PROCEEDINGS

MATHMOD VIENNA 09

Abstract Volume

I.Troch, F.Breitenecker, Eds.

6th Vienna Conference on
Mathematical Modelling
February 11-13, 2009
Vienna University of Technology

ARGESIM Report no. 34 **ASIM Mitteilung AM 123**

ISBN print 978-3-901608-34-6 ISBN ebook 978-3-901608-08-7 DOI 10.11128/arep.34


MATHMOD
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ARGESIM – Publishing House, Vienna, 2009
ISBN 978-3-901608-34-6

ARGESIM Reports

Published by **ARGESIM** and **ASIM**, German Simulation Society,
Div. of GI – German Society for Informatics / Informatics and Life Sciences

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ARGESIM Report no. 34

Titel: Proceedings MATHMOD 09 Vienna – Abstract Volume

Editors: Inge Troch, Felix Breitenecker
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ISBN 978-3-901608-34-6

Full text conference contributions to MATHMOD 09 are published in
Proceedings MATHMOD 09 Vienna – Full Papers CD Volume, ISBN 978-3-901608-35-3

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

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Preface

At MATHMOD Vienna scientists and engineers using or developing models or interested in the development or application of various modelling tools are offered an opportunity to present ideas, methods and results and discuss their experiences or problems with experts of various areas of specialisation.

The scope of the *MATHMOD Conference Series* covers theoretic and applied aspects of various types of mathematical modelling. Comparison of modelling approaches, model simplification, modelling uncertainties, and port-based modelling are discussed. Moreover, besides applications of modelling in traditional areas such as engineering and natural sciences also new ones are of growing importance. Further, the topics to be discussed during the conference reflect also the fact that mathematical modelling is now used more and more in industries. Moreover, numerical aspects are now often already part of the modelling process and, automation of modelling and the use of IT are of growing importance. All these facts can be recognized on one hand in the many special sessions, which were organized by experts in the specific area. But, on the other hand, also the various sessions, where submitted papers will be presented and discussed, show the broad variety of the MATHMOD conference.

Moreover, it is to be observed that traditional classifications such as theory, applications, numerics, computer science, simulation etc. becomes more and more obsolete. Scientific work often presents new results in several areas.

A look on the special sessions illustrates this quite well and underlines the fact that working teams are now often already international:

Modelling the Swarm
Thomas Schmickl (Univ. Graz, Austria), Heiko Hamann (Univ. Karlsruhe, Germany)

Numerical Methods in Quantum Simulations
Othmar Koch (Vienna, Austria)

Modeling and Simulation in Systems Biology
Wolfgang Wiechert (Univ. Siegen, Germany),
Aljoscha Wahl (Delft Univ. of Technology, The Netherlands)

Advances in Model Order Reduction
Boris Lohmann (TU München, Germany),
Peter C.Müller (Univ Wuppertal, Germany), Tatjana Strykel (TU Berlin, Germany)

Tools for Modelling of Reaction Systems
Rudibert King (TU Berlin, , Germany)

Modelling of Fuel Cells and Chemical Engineering Applications
Kurt Chudej (Univ. Bayreuth, Germany), Michael Mangold (Max-Planck-Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany)

Mathematical Modelling and Control of Chemical and Bio-chemical Processes
Philippe Bogaerts (Univ. Libre de Bruxelles, Belgium),
Jan Van Impe (Katholieke Univ Leuven, Belgium)

Numerics of Ordinary Differential Equations with Uncertainties
Michael Günther (Univ Wuppertal, Germany),
Utz Wever (Siemens AG, Corporate Technology, Germany),
Peter Rentrop (TU München, Germany)

Mathematical Models and their Correspondence to the Physical Reality
Peter Dabnichki (Univ. of London ,England)

Computational Micromagnetics
Markus Melenk, Dirk Praetorius, Dieter Suess (all: TU Vienna, Austria)

Nonlinear Oscillations
Alois Steind, Horst Ecker (both: TU Vienna, Austria)

Selected Examples in Biomechanical Modelling and Simulation
Arnold Baca (Univ. Vienna, Austria)

Modeling of Decentralized Service Systems in Automation Technologies
Ulrich Epple, Henning Mersch (both: RWTH Aachen, Germany)

Object-oriented Modelling and Simulation
Gianni Ferretti, Francesco Casella (both: Politecnico di Milano, Italy)

Control of Dynamical Systems
Felix L. Chernousko (Russian Acad. Sciences, Moscow, Russian Federation)
Georgy Kostin (IPM RAS, Moscow, Russian Federation)

Discrete and Hybrid Simulation: Methodologies, Techniques and Applications
Gasper Music (Univ. Ljubljana, Slovenia)

Modelling, Simulation and System Dynamics through E-Learning
Maja Atanasijević-Kunc (Univ. Ljubljana, Slovenia)

Computational Modeling and Simulation in Multi-Modal Transportation
Dietmar P. F. Moeller (Univ. Hamburg, Germany)

Carbon Capture and Storage
Bernt Lie (Telemark Univ. College, Norway)

Meeting With IT Advances in Modeling and Simulation Tool Developments
Kaj Juslin (VTT, Finland)

Modelling and Simulation of Biological Water Treatment
Esko Juuso (Univ. Oulu, Finland)

Modelling, Analysis and Control of Distributed Parameter Systems
Markus Schöberl, Kurt Schlacher (both: Univ. Linz, Austria)

Circulating Fluidized Beds
Erik Dahlquist (Sweden)

Also the invited lectures reflect to some extend this wide spectrum of important topics of current interest ranging from applications in engineering, biology to methodological and theoretic aspects of various types and also that scientific work now usually belongs to more than one area of classification:

Networked Control Systems
Frank Allgoewer (Univ. Stuttgart, Germany)

Modeling and Control in Heavy Plate Mills
Andreas Kugi (TU Vienna, Austria)

Hybrid Modelling - Control and Optimisation
Alberto Bemporad (Univ. Siena, Italy)

Design of Nonlinear CMOS Circuits in the Nano-GHz Era and its Mathematical Challenges
Wolfgang Mathis (Univ. Hannover, Germany)

Modeling and Finite-element Simulation of Heating Effects in Semiconductor Devices
Ansgar Juengel (TU Vienna, Austria)

System-theoretic Methods for Model Reduction of Large-scale Systems: Simulation, Control, and Inverse Problems
Peter Benner (TU Chemnitz, Germany)

Model Order Reduction for Object-oriented Models: a Control Systems Perspective
Gianni Ferretti, Francesco Casella, Dr. Filippo Donida (Politecnico di Milano, Italy)

Adaptive Extremum Seeking Control : A Survey
Denis Dochain (CESAME, UCL, Louvain-la-Neuve, Belgium)

Modelling in Systems Biology, Neurology, and Pharmacy
Ales Belic (Univ. of Ljubljana, Slovenia)

Furthermore, two plenary contributions deal with mathematics and fine arts:

Algorithms, Mathematics and Art
Vlatko Ceric, Univ. Zagreb, Croatia

Laura and Petrarca - True Emotions vs. Modelled Emotions
Felix Breitenecker (TU Vienna, Austria)

A novelty in MATHMOD 2009 is the contribution type *Short Papers*. Short Papers are intended for presentation of recent developments and work in progress in all areas of modelling and simulation. Short Papers are published in the Conference Proceedings with a 1-page abstract and with a 4-page full text paper. Short papers are presented with a poster in the Poster Session (no oral presentation).

MATHMOD 2009 Proceedings consist of two volumes. *Proceedings MATHMOD 2009 Vienna – Abstract Volume* contains (ISBN 978-3-901608-34-6) one-page abstracts of all invited plenary talks, of contributed papers to regular sessions and to special session, of short papers, and of student posters. *Proceedings MATHMOD 2009 Vienna – Full Papers CD Volume* (ISBN 978-3-901608-35-3) consists of the full text versions of invited papers, of regular papers, of regular papers in special sessions, and of short papers.

Both volumes of these Proceedings start with the manuscripts of the plenary lectures. Then follow contributed papers (*Regular Papers*) which were either contributed upon invitation of a session organizer or, which were selected for presentation after a reviewing process which was based on extended abstracts. All these contributions were collected and arranged in sessions according to their main thematic point. Such a grouping is by no means easy because many contributions address several different aspects in a balanced manner.

Therefore, the arrangement chosen for this volume follows rather closely the one of the conference where also time limitations had to be observed:

- Control Systems
- Discrete Systems and Manufacturing
- Robotics – Applications, Tools
- Traffic and Transportation Systems, Guidance
- Environmental Systems and Processes
- Numerical Methods and Algorithms
- Modelling in Physics and Natural Sciences
- Process Engineering
- Electrical/Electronic Engineering and Communication
- Modelling Methods, Theory and Tools
- Biology, Physiology, Medicine
- Fuzzy Systems – Modelling and Applications
- Mechatronics – Applications, Modelling, Tools
- Stochastic Modelling
- Modelling in Economics and Finance
- Agent-based and Alternative Modelling Techniques

Next, abstracts of the *Short Papers* follow, which have been peer reviewed in the same way as the *Regular Papers*. The *Abstract Volume* contains as its last part the abstracts of the *Student Posters*, which were undergoing also a review procedure. Posters of *Student Poster* contributions and of *Short Paper* contributions were on display during the whole conference and discussed in a special *Poster Session*.

As editors we wish to express our sincere thanks to all who have assisted us by making the idea of this symposium known within the scientific community or by acting as sponsor or cosponsor. We want to thank especially the members of the International Program Committee who assisted us in the reviewing process – some of them did indeed a tremendous work by reviewing some 30 extended abstracts in rather short time. Further, we want to thank all colleagues who have done an excellent job by putting together special sessions devoted to one main topic. Last but not least we like to thank the ARGESIM team for their support in the preparation of these Proceedings.

Vienna, January 2009 Inge Troch and Felix Breitenecker

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Plenary Lectures

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODEL ORDER REDUCTION FOR OBJECT-ORIENTED MODELS A CONTROL SYSTEMS PERSPECTIVE

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Equation-based, object-oriented modelling techniques, languages, and tools emerged during the '90s, and are now well established in the modelling and simulation field, in particular to support the design of modern integrated systems, which require multi-physics modelling capabilities. Object-oriented models are usually non-linear, and mostly used for simulation purposes. There is a strong interest in object-oriented modelling for control system analys and design, but so far the use of such models to support control-related activites has been mostly limited to the verification of the control system performance in closed loop by simulation, rather than giving direct support to controller design [1]. For this specific purpose, the equations that correspond to object-oriented models built by aggregation of reusable components are usually too complex, and not formulated in a way that can be directly employed in the controller design.

In the field of electronic circuit analysis and design, a research interest has recently emerged in Model Order Reduction (MOR) techniques for nonlinear circuits. The main motivation behind this interest is to support hardware design activities. On one hand, as pointed out by [2] and [3], the design of modern mixed-signal (analog and digital) integrated circuits represent a challenge for modelling and simulation software, due to the ever-increasing complexity of the circuits allowed by the progress of integrated circuit manufacturing technology. In order to master the complexity, it is necessary to provide good macro-models of basic functional units, which are then used at a higher level for the design of the integrated system. These macro-models are usually developed manually by skilled designers, but this activity is very labour-intensive, and might lead to neglect parasitic and secondary phenomena which have a significant impact on the overall system performance, expecially as the features of the integrated circuits get smaller and smaller. This motivates the development of techniques to extract these macro-models automatically from finer-detail models of the hardware. On the other hand, as noted by [4], MOR techniques can help to highlight the influence of key design parameters of the hardware on the dynamic performance of the system, e.g., the frequency and damping of poles in the transfer function of the linearized model, thus providing valuable information for the optimization of the system design.

Similar issues also arise in the field of control system design, even though with some significant differences. The aim of this paper is then to review some of these recently developed MOR techniques, putting them in a control system perspective, and motivating the need for further research and extensions in order to make them more effective for control applications.

At first, it is shown how object-oriented models could be used for direct support of control system design, with emphasis on the specific requirements of control-oriented models. Then, several recently developed MOR techniques are reviewed, and finally open issues and future research work which is needed to make these techniques more effective for control system design support are pointed out.

[1] Casella F., Donida F., and Lovera M. "Beyond simulation: Computer aided control system design using equation-based object oriented modelling for the next decade," in *Proceedings 2nd International Workshop on Equation-Based Object-Oriented Languages and Tools*, Paphos, Cyprus, Jul 8 2008. Available: {http://www.ep.liu.se/ecp/029/005/}

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[3] Schwarz P., Bastian J., Clauss C., Haase J., Köhler A., Otte G., and Schneider P.: *A Tool-Box Approach to Computer-Aided Generation of Reduced-Order Models*. In: Proc. EUROSIM 2007, September 9–13, 2007, Ljubljana, Slovenia.

[4] Sommer R., Halfmann T., and Broz J.: *Automated Behavioral Modeling and Analytical Model-Order Reduction by Application of Symbolic Circuit Analysis for Multi-Physical Systems*. Simulation Modelling Practice and Theory, 16, (2008), 1024–1039.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

COMMUNICATION NETWORKS IN CONTROL: NEW DIMENSIONS OF COMPLEXITY

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Rainer Blind, Ulrich Münz, Peter Wieland
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University of Stuttgart, Germany

Abstract. During the history of control, the system complexity steadily increased. First simple first order systems were studied. Then higher order linear systems and finally nonlinear and uncertain systems have been investigated and by now a good level of understanding has been achieved.

Since in practice many application relevant systems are composed of several subsystems, the analysis and design of interconnected systems and Multi-Agent Systems (MAS) became increasingly important, but introduced a new dimension of complexity: the topological complexity. First, simple and regular topologies between the subsystems where considered. Nowadays, the investigation of large and time-varying topologies between the subsystems is state-of-the-art.

Traditionally, the communication links between the subsystems are assumed to be perfect. However, real communication links, e.g. via Ethernet or WLAN, are not perfect. In particular in packet-switched networks, the information exchange suffers from packet loss and delay. The influence of these non-ideal links on control systems is currently investigated thoroughly in the area of Networked Control Systems (NCS), where the plant and controller are connected via an imperfect network. Hence, the incorporation of appropriate link models adds a third dimension of complexity to control theory: the link complexity.

In this talk, we give an overview on recent trends how to deal with both the topological complexity and the link complexity in control theory. Thereby, we mainly focus on two topics: high-order linear and nonlinear Multi-Agent consensus problems with and without communication delays as well as Networked Control Systems with packet-switched networks.

DESIGN OF NONLINEAR CMOS CIRCUITS IN THE NANO-GHZ ERA AND ITS MATHEMATICAL CHALLENGES

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Abstract. During the last 25 years silicon CMOS became the main technology in microelectronics and following the IRTS roadmap for industrial applications CMOS will be the dominant technology in the next 15 to 20 years. One reason for the success of CMOS is related to the possibility that almost all circuit concepts survived the downscaling process from the μm to the sub-μm scale. In the meantime state-of-the-art technologies are below 100 nm scale and enter the *nm* regime. Therefore we have to reconstruct all parts of the modelling process for the CMOS devices. Also the functionality of today's microelectronic circuits used for technologies above 100 nm must be analyzed in order to be sure that the desired circuit properties can be preserved also in the *nm* regime. Accurate modelling of *nm* semiconductor devices and its consequences for the properties of *nm* circuits become a challenging problem and close related to that interesting mathematical problems arise.

However nano-scaling in CMOS technology not only a subject of difficulties. Obviously a main advantage of each downscaled CMOS technology is that the devices density and therefore the complexity of circuits increases. However in high-speed digital CMOS circuits (e.g. memory circuits) downscaling is connected with the disturbance of the ideal circuit functionality and their performance decreases. Additional problems arise if more advanced semiconductor device concepts are considered. The problems of modelling high-speed circuits are discussed elsewhere (see [1], [2]) and for alternative concepts beyond CMOS see [3]. Although a similar tendency can be observed in nano-scaled analogue CMOS circuits the frequency behavior of RF CMOS devices will be improved because of the decreasing parasitic dynamic effects. If nano-scaled MOS devices are used in RF microelectronics we have the above mentioned advantages and disadvantages and therefore a trade-off is needed for a specific technology with its corresponding characteristic length. Furthermore the particular limits with respect to the circuit functionality of a certain technology are of special interest. Heterojunction bipolar transistors (HBTs) are superior to frequencies of 100 to 200 GHz [**?**] but deep sub-100nm CMOS technology seems to be useful for RF circuits for a few GHz since we can combine them with digital circuits. This approach is called system-on-chip (SOC)concept. Therefore we have to consider modelling of nano-scaled CMOS transistors including RF modelling aspects such that we have Giga challenges in combination to the nano challenges.

In order to study the properties and the behavior of such nano RF circuits we need semiconductor device models which based on quantum mechanically coherent and incoherent charge transport. For studying RF circuits advanced MOS compact models are needed for circuit simulation. Most recently new MOS models of this kind are developed using a surface potential formulation; see chapters 2 and 3 in [4]. In contrast to the threshold or charge sheet formulations this formulation can be generalized in such a manner that quantum effects can be incorporated. Additionally in contrast to most intrinsic quasi-static quantum mechanically device models non-quasi-static effects have to included; see [5]. Although advanced MOS compact models incorporate some quantum effect more elaborated models have to be developed for fully coherent transport; see [6] and our chapter 8 in [4]. In this paper we discuss different modelling approaches and their results with respect to the design of nano-scaled RF circuits as well as the corresponding mathematical challenges.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

LAURA AND PETRARCA - TRUE EMOTIONS VS. MODELLED EMOTIONS

Felix Breitenecker[1]
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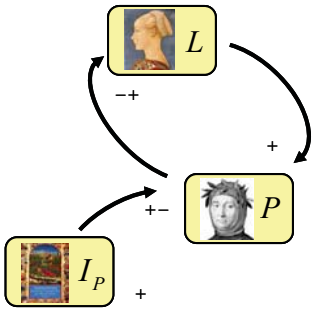
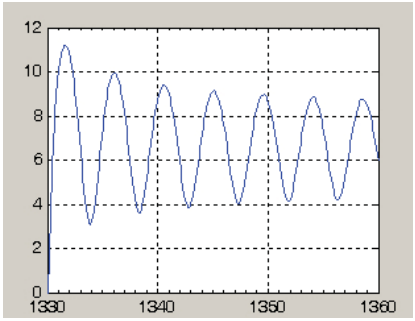
Laura, a very beautiful but also mysterious lady, inspired the famous poet Francesco Petrarca for poems, which express ecstatic love as well as deep despair. F. J. Jones – a scientist for literary - recognised in these changes between love and despair in the years 1328 to 1350 an oscillating behaviour, which he called Petrarch's emotional cycle. It is evident, that this cycle is based on the emotional relations between Laura and Petrarch and on Petrarch's inspiration. How to model this emotional behaviour, this love dynamics mathematically?

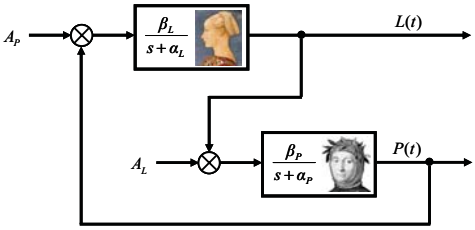
This contribution introduces and reviews modelling approaches for emotional dynamics and inspiration by means of a fully mathematical approach using ODEs, by System Dynamics, and by transfer function modelling.

The mathematician S .Rinaldi investigated as first this cycle and established a mathematical model based on ordinary differential equation of predator-prey type: two coupled ODEs with nonlinear reaction functions, reflecting Laura's and Petrarch's emotion for each other, drive an inspiration variable, which coincides with Petrarch's emotional cycle. These ODEs were starting point for the investigations in two directions: mapping the mathematical model to a suitable modelling concept, and trying to extend the model for love dynamics in modern times.



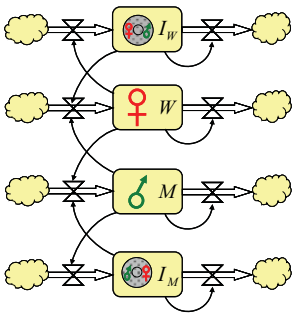
The modelling concept of System Dynamics fits very well to model the qualitative behaviour. In principle, emotions and inspiration emerge from a source, and are fading into a sink. But the controlling parameters for increase and decrease of emotion create a broad variety of emotional behaviour and of degree of inspiration, because of the nonlinearities. These nonlinearities must be 'fitted' by appropriate auxiliaries.





Emotions and inspiration are fading over time – behaving like a transfer function approaching a steady state. This observation suggests a modelling approach by transfer functions. Emotions and inspiration are modelled by first order lags driven by the other's emotion and by inspiration as inputs. But the linear behaviour does not reflect reality, so that gains and time constants must chosen state-dependent using appropriate nonlinear relations.

Both approaches make the basic modelling easy, but for nonlinear influences again the nonlinear reaction functions must be used. In any case, the model parameters can be identified, so that Petrarch's emotional cycle described by F. J. Jones can be retraced by the model. But simulation experiments also allow interesting 'what-if' – analysis in history: what, if Petrarch would have been more attractive ? - what, if Laura would have left her husband and would have married Petrarch ?



In times of gender equality woman as well as men may play an active part in a love affair. Consequently also women express their love by poems or other media, and they confess their love to public. For Laura and Petrarch this would mean, that also Laura writes poems, that Petrarch's appeal is influenced by Laura's poetic inspiration, and that Petrarch shows more sensibility in his reaction to Laura. In modelling terms, a second inspiration state is used – and the model becomes symmetric. By this, the *Laura-Petrarch* model develops to a *Woman-Man* – model, expressed by ODEs, stock-flow diagram or transfer functions.

Experiments with an implementation of these models (Maple and MATLAB) and selected simulations provide interesting case studies for different kind of love dynamics - attraction, rejection and neglect, - stable equilibriums and chaotic cycles.

MODELLING IN SYSTEMS BIOLOGY, NEUROLOGY, AND PHARMACY

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Area description. In the last decade some significant changes occurred in biomedical area with introduction of systemic view to the area. In neurology, the paradigm that contribution of systems that consist of simple elements can be more than just a sum of contributions of the elements was already well accepted, while other areas of bio-medicine were more or less accepting the reductionism paradigm where systems were studied through the analysis of its isolated sub-systems. Genome project showed that it is not possible to explain the diversity of life only with combinations of genes. The discovery strongly affected the way of thinking in the community which resulted in a new science called systems biology. Systems biology is, in contrast to reductionism, interested in characteristics that emerge from interactions of large groups of simple sub-systems that form a whole system. The ideas were adopted also in pharmacy, where the rate of success in discovery of new drugs is relatively poor in compare with the improved measuring methods. To explore the characteristics of the system that originate from the cooperation of sub-systems, modelling of biological systems has become a necessary procedure. The origins of the idea that biological systems can be viewed as special sort of machines can already be found in Leonardo Da Vinci's anatomical studies, however, it took a few additional centuries for the idea to evolve to systems biology. Mathematical modelling as one of the principal tools of theoretical physics and control engineering is becoming essential tool for solving complex problems in life-sciences as well. Feedback mechanisms play important role in all biological systems thus it is important to understand the dynamical nature of the feedback mechanisms. Two different approaches to the systems analysis seem to be in a constant struggle, statics and dynamics. Many great results have been achieved by using statical approaches, however, it becomes more and more clear also in life-sciences that statical analysis of dynamical systems can be sometimes misleading. There is also a big gap between the life-sciences and engineering in the understanding of the term "understanding the mechanisms". While life-sciences mostly define the process through symptoms, engineering struggles to create a working prototype of the system. Only when the prototype is operational in the desired manner, the mechanisms have been correctly understood. Thus modelling and simulation, as integral tool of the systemic approach paradigm, is important addition to the standard analysis procedures for studying biological systems.

Conclusions. In the area of life-sciences any procedure that requires mathematics is usually understood as bioinformatics, however, there are substatntial differences between the approaches. While bioinformatics looks for patterns in large databases with some inclusion of expert-knowledge, modelling and simulation tries to recreate observed systems in mathematical form, with maximum possible inclusion of expert-knowledge and validates the model against the database. Considering the complexity of the observed systems, development lead to several modelling techniques that are in between the data-driven and knowledge driven approaches. In reality, bio-systems are too complex to be analysed with only a single approach; measurements are problematic and structural knowledge of bio-systems is incomplete.

With increasing importance of systems biology to all areas of bio-sciences the models are becoming more and more complex that leads towards several problems. First, the problem of identifiability of such complex models cannot be neglected. Since the models are mostly of non-linear type (enzyme reactions) the optimisation methods must be used to identify the model parameter values, thus introducing the well known problems of optimisation in high-dimensional spaces to the area. Next, a serious problem with simulation methods of complex, non-linear, high-order dynamical systems cannot be neglected. The problem has two consequences, questionable precision of results and very long simulation times (or necessary use of supercomputers). The experimenting with and understanding of the behaviour of such complex models is of central interest, when trying to understand the modelled system. However, if model becomes too complex to understand, it also becomes obsolete. Simplification of such models is thus becoming a necessity. Simplification can be viewed as selective scale of different parts of the model. While it is not possible to neglect the holistic nature of the model, details that are not studied in detail can be simplified, however, not omitted.

There is also a significant problem with modelling goals. In order to use modelling and simulation efficiently, modelling goals must be set at the beginning, since modeller must decide which part of the system should be modelled in detail and which parts can be simplified. The idea is however somewhat strange to bio-scientists, since their model organisms are completely formed per se prior to experiments, while mathematical model must first be designed through sensitive design cycles, before it can be used for experiments. Since the system is extremely complex, not all the details should be included in the model in detail. In this sense, standardised descriptions of models, such as SBML (Systems Biology Markup Language) might result in false understanding of modelling and simulation and lead to the goals of the type: "life, universe, and everything".

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

EXTREMUM SEEKING CONTROL AND ITS APPLICATION TO PROCESS AND REACTION SYSTEMS : A SURVEY

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Most adaptive control schemes documented in the literature [4]-[6],[9] are developed for regulation to known set-points or tracking known reference trajectories. In some applications, however, the control objective could be to optimize an objective function which can be a function of unknown parameters, or to select the desired states to keep a performance function at its extremum value. Self-optimizing control and extremum seeking control are two methods to handle these kinds of optimization problems. The goal of self-optimizing control is to find a set of controller variables which, when kept at constant set-points, indirectly lead to near-optimal operation with acceptable loss [2][10][11]. The task of extremum seeking is to find the operating set-points that maximize or minimize an objective function.

In the past few years, Krstic et al. [7][8] have presented several schemes for extremum-seeking control of nonlinear systems. First the system is perturbed using an external excitation signal in order to numerically compute the gradient [1][8].Their framework allows the use of black-box objective functions with the restriction that the objective value to be minimized is measured on line. Although this technique has been proven useful for some applications [13], the lack of guaranteed transient performance of the black-box schemes remains a significant drawback in its application. Alternatively an adapted model of the system is used for analytical evaluation of the gradient [3]. The extremum seeking framework proposed by Guay and Zhang [3] assumes that the objective function is explicitly known as a function of the system states and uncertain parameters from the system dynamic equations. Parametric uncertainties make the on-line reconstruction of the true cost impossible such that only an estimated value based on parameter estimates is available. The control objective is to simultaneously identify and regulate the system to the lowest cost operating point, which depends on the uncertain parameters. The main advantage of this approach is that one can guarantee some degree of transient performance while achieving the optimization objectives when a reasonable functional approximation of the objective function is available.

This survey is organized as follows. We shall first concentrate on the Þrst class of methods, i.e. perturbation-based extremum-seeking control methods, then to the second one, i.e. model-based extremum-seeking control. In both cases, theoretical results are provided and the performance are illustrated in numerical simulations.

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ALGORITHMS, MATHEMATICS AND ART

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Algorithms, mathematics and art are interrelated in an art form called algorithmic art. Algorithmic art is visual art generated by algorithms that completely describe creation of images. This kind of art is strongly related with contemporary computer technology, and especially computer programming, as well as with mathematics used in algorithms for image generation.

We first discuss two aspects of algorithmic art: the fact that it is based on rational approach of constructing algorithms and that it involves a strong constraint that image has to be created by an algorithm.

Importance of mathematics for artists is emphasized by Swiss artist, architect and graphical designer Max Bill in his well-known text on the mathematical approach in contemporary art [1]. He wrote that he is convinced that "it is possible to evolve a new form of art in which the artist's work could be founded to quite a substantial degree on a mathematical line of approach to its content". We describe mathematical influences to art during history, and especially in Renaissance and during the 20th century. It is well known that for example two famous Renaissance artists, Leonardo da Vinci and Albrecht Dürer were studying and using knowledge on perspective, human body proportions, optics and science of colours in creation of their works. The best known 20th century artist that was influenced by mathematics was by no means Dutch graphic artist M. C. Escher who attempted to visually express various mathematical concepts like infinity, recursion and self-similarity and studied the use of regular periodic divisions of a plane, convergence to a limit and various transformations of shapes. Among interesting mathematically based artistic objects are sculptures based on mathematical objects, as well as different type of perspectives painted on the sphere [2]. We present here Helaman Ferguson, mathematically oriented sculptor who is using mathematics as a design language for his sculptures, as well as Dick Termes, one of the leading artists working with perspectives painted on a sphere.

Development of computer technology and particularly graphic cards and software in the second part of the 20th century made an enormous influence on the ability of visualizing mathematics and using these visualizations in design and art. Here we present main idea of fractals and cellular automata as well as their visualization.

Then we are describing algorithmic art as art based on generation of visual artworks using algorithms, and its main principles. Algorithmic artists as a rule don't use special graphical software but rather general program languages that enable drawing basic graphical elements like line, circle or rectangle. Such approach requires more work but offers much more flexibility and freedom in expression. After the image is generated no further intervention with image processing tools like Photoshop is done. Interventions for changing image are done merely by changing the algorithm. We present some of the best known algorithmic artists: Vera Molnar, Jean-Pierre Hébert, Roman Verostko, Manfred Mohr and Charles Csuri and their background and approach to algorithmic art.

Algorithmic art itself, a discipline that unites mathematics, computing and art, has a rather specific character since the author has to possess rational abilities required to compose the algorithm and write the corresponding computer code correctly from both the syntactic and semantic point of view, but he also needs intuitive and aesthetic abilities required to select visually promising alternatives. The author of algorithmic artworks constantly evaluates visual outputs obtained during experimentation with the program and on the basis of these evaluations makes changes to the program until satisfactory visual results are obtained. Although experimentation is also present and important in a traditional art, algorithmic art is using its full potential.

Besides we discuss algorithmic art as a form of visual art notation and compare it with musical notation.

Finally we discuss some algorithmic art methods and techniques in order to provide better understanding about generation of algorithmic art. We present examples of three methods developed by the author of this text: constructivist approach, mathematical modelling approach and digital manipulation of photographs (or any kind of images).

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

SYSTEM-THEORETIC METHODS FOR MODEL REDUCTION OF LARGE-SCALE SYSTEMS: SIMULATION, CONTROL, AND INVERSE PROBLEMS

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Introduction. Model (order) reduction, MOR for short, is an ubiquitous tool in the analysis and simulation of dynamical systems, control design, circuit simulation, structural dynamics, CFD, etc. In order to state the problem treated in our contribution, we consider linear, time-invariant (LTI) systems of the form

$$\dot{x}(t) = Ax(t) + Bu(t)\,, \qquad y(t) = Cx(t) + Du(t)\,, \tag{1}$$

where $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{p\times n}$, $D \in \mathbb{R}^{p\times m}$, and $x^0 \in \mathbb{R}^n$ is the initial state of the system. Here, n is the order (or state-space dimension) of the system and $x(t) \in \mathbb{R}^n$, $y(t) \in \mathbb{R}^p$, $u(t) \in \mathbb{R}^m$ are the state, output and input of the system, respectively.

The model reduction problem considered here consists of finding a reduced-order LTI system,

$$\dot{\hat{x}}(t) = \hat{A}\hat{x}(t) + \hat{B}u(t)\,, \qquad \hat{y}(t) = \hat{C}\hat{x}(t) + \hat{D}u(t) \tag{2}$$

of order r, $r \ll n$, with the same number of inputs m, the same number of outputs p, so that for the same input function $u \in L_2(0,\infty;\mathbb{R}^m)$, we have $\|y-\hat{y}\| \le \mathrm{tol}\cdot\|u\|$ for a given error tolerance tol and appropriate norms.

Balanced Truncation and Related MOR Methods. In systems and control, MOR methods based on balanced truncation (BT) and its relatives have been widely used. The basic concept is to balance two positive definite matrices $P,Q \in \mathbb{R}^{n\times n}$ via a so-called contragredient transformation, i.e., they are simultaneously diagonalized. This is achieved using a nonsingular matrix $T \in \mathbb{R}^{n\times n}$ chosen such that

$$TPT^T = T^{-T}QT^{-1} = \mathrm{diag}(\sigma_1,\ldots,\sigma_n)\,,$$

where $\sigma_1 \ge \ldots \ge \sigma_n$. (Generalizations to positive semidefinite matrices exist, leading to only partially balanced $TPT^T, T^{-T}QT^{-1}$.) Using T as state-space transformation $x \mapsto Tx$ yields a new realization $(TAT^{-1}, TB, CT^{-1}, D)$ of (1). The reduced-order model is then obtained by truncating this realization w.r.t. r, i.e., by taking the leading principal $r\times r$, $r\times m$, etc. submatrices as realization of the reduced-order model. Efficient implementations never form T explicitly, but compute the reduced-order model directly employing only the necessary submatrices of T and T^{-1}. In BT, P,Q are chosen as the controllability and observability Gramians of (1), satisfying the dual Lyapunov equations

$$AP + PA^T + BB^T = 0\,, \qquad A^TQ + QA + C^TC = 0\,.$$

Related methods use the stabilizing solutions of certain algebraic Riccati equations (LQG and positive real BT), or balance P as above versus the stabilizing solution of yet another algebraic Riccati equation (balanced stochastic truncation), see [1, 3] for overviews and more variants of balancing-related methods.

In other application areas, balancing-related MOR methods have been less successful as it is common belief that their computational complexity is too high to apply them to large-scale problems involving sparse matrices due to the large computational cost attributed to solving the large-scale matrix (Lyapunov, Riccati) equations. We will review the recent development of efficient algorithms for solving matrix equations [2] that make balancing-related model reduction methods competitive to other MOR approaches - these new implementations fall into the same complexity class as the omnipresent Krylov subspace methods. As balancing-related methods offer the advantage of computable error bounds that allow for an adaptive choice of the order of the reduced model and moreover, they can be shown to preserve certain system properties like stability, passivity, dissipativity, etc., these new BT implementations become attractive in various application areas. These include

- nanoelectronics/VLSI design, where MOR is inevitable for circuit *simulation*,
- (optimal) *control* of physical processes described by PDEs,
- *inverse problems* related to the identification of input signals, e.g., for tracking control.

We will discuss some particular aspects arising in these areas when applying BT-related MOR techniques. The performance of several BT-related approaches will be demonstrated using examples from a variety of application areas.

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MODELING AND SIMULATION OF ELECTRON TRANSPORT AND HEATING IN SEMICONDUCTOR DEVICES AND CIRCUITS

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Self-heating is becoming of paramount importance in modern ultra-integrated circuits and power devices since it influences strongly the circuit behavior or even lowers its performance. The standard approach for the modeling of integrated circuits is to replace the semiconductor devices by equivalent circuits consisting of basic elements and including (thermal) fitting parameters. Due to the decreasing feature size and increasing operating frequency, however, a very large number of basic elements and a careful adjustment of the large number of fitting parameters is needed in order to achieve the required accuracy. Therefore, it is preferable to model thermally relevant semiconductor devices by transport equations and to develop a coupled model for the particle temperatures, the lattice temperature in the device, and the temperatures of the circuit elements. The goal of this presentation is to review the derivation of the energy-transport equations and the modeling of electric circuits and thermal networks and to present some numerical examples illustrating the self-heating behavior.

Self-heating is described by the following models. First, the energy-transport equations allow for the computation of the particle temperatures. Collisions of the charge carriers with the crystal lattice (modeled by a relaxation-time ansatz) leads to an increasing lattice temperature which is described by a heat equation derived from thermodynamic principles. Second, the circuit is modeled by electric network equations resulting from the so-called modified nodal analysis. Third, a thermal network model describes the heat evolution in the (lumped and distributed) circuit elements. These three subsystems are coupled by thermo-electric, electric circuit-device, and thermal network-device interfaces.

We describe the modeling of these subsystems in detail (joint work with M. Brunk, Trondheim). In particular, the derivation of the energy-transport equations from the semiconductor Boltzmann equation is sketched. Moreover, the heating effects are illustrated by several numerical examples.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELING AND CONTROL OF HYBRID DYNAMICAL SYSTEMS: THE HYBRID TOOLBOX FOR MATLAB

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Hybrid systems describe the dynamical interaction between continuous and discrete signals in one common framework. This paper focuses on discrete-time models of hybrid systems that are suitable for setting up and solving model predictive control (MPC) problems through mixed-integer and multi-parametric optimization: discrete hybrid automata (DHA), piecewise affine systems (PWA), and mixed logical dynamical (MLD) systems. After introducing the modeling framework for DHA, PWA and MLD systems and of MPC for linear and hybrid systems, the paper present the Hybrid Toolbox, a MATLAB/Simulink tool for modeling, simulating, and verifying hybrid dynamical systems, for designing and simulating model predictive controllers for hybrid systems subject to constraints, and for generating linear and hybrid MPC control laws in piecewise affine form that can be directly embedded as C-code in real-time applications.

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Control Systems

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELLING OF AIR PRESSURE DYNAMICS FOR CLEAN ROOM FACILITIES

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Introduction. In the pharmaceutical industry clean room pressure is important in terms of product quality, because overpressure guarantees that only preconditioned air enters the facilities. Strict specifications prescribe overpressure and differential pressure between different clean room classes. Therefore, the pressure has to be actively controlled. When doors between different control zones are closed, pressure surges occur and the pressure may exceed specified limits.

There already exist multi-zone air flow models, which model the air flow and contaminant distribution in buildings [2]. They are quite extensive and for simulation require solving an overall mass balance for the whole building. Most existing models focus on air conditioning and ventilation technologies, where air flows through doors are not implemented and energetic considerations are most important [1], [3].

The motivation for the work presented here is to create a modular and easy to parameterize model in Simulink, which covers the dynamics of the system and the cause of the phenomenon “pressure surge”.

Component modelling. The mathematical modelling follows state of the art procedures using linear 1^{st}-order differential equations for the pressure of each room based on non-stationary mass balances and the ideal gas law, where temperature T and density ρ are considered to be constant and the room volume is a dominant model parameter. In order to apply the model to a realistic room topology detailed experimental identification of actuation devices was performed in laboratory, pointing out the hysteresis and the nonlinear static characteristic of the actuator. The pressure sensor is a ring balance and is modelled as a PT1 element. Measurement bias in the room pressure signal is considered. Ventilation facilities and pipe networks are idealized and air flows through doors and leakages are implemented. Additionally, measurements at the clean room facilities were used for parameter identification, optimization, and model validation.

Results. The phenomenon “pressure surge” turns out to be the consequence of integral controller action and measurement bias, which was proven by both the model prediction and measurements.

The room module itself turns out to be a quasi static model. The slope of step responses of the real plant corresponds to the limited rate of the actuator, which indicates, that the room pressure reacts synchronously to the position of the actuator. The fast dynamics of the systems were proven by high-bandwidth pressure sensors, an additional reference measurement with poor stationary accuracy, but low cost effort. The slowest dynamic element in the system is the ring balance with its PT1 behaviour.

Conclusion. Experimental validation at the structure of one ventilation system of the real plant shows excellent results. The low order, modular simulation model is easy to parameterize and gives the possibility of flexible adaptation to a given topological map of rooms. Therefore, device manuals or readily available measurement data are sufficient to provide the parameters and the nonlinear static characteristic of the actuator.

Moreover, the model is a basis for testing and evaluating different control concepts in terms of robust pressure control.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

ZONAL MODEL OF CLIMATIC CONDITIONS IN A LECTURE ROOM

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Due to the rising standards demanding energy-efficient heating and cooling systems, t improvements of the existing systems are required. Moreover, the indoor air quality standards require a low level of pollutants in the room [1]. This means that the air in the room should have an appropriate chemical composition. In addition to the aspects of heat and pollutants in the indoor air, we may also consider measuring the level of relative humidity. This aspect is important from the viewpoint of comfort and health. The most common problems caused by inappropriate relative humidity level are the presence of bacteria, fungi and respiratory infections.

The purpose of this study is to develop a model of climatic conditions in a lecture room. Various types of mathematical models can be applied to the description of climatic conditions in order to obtain the desired model accuracy. The main aspects of modelling climatic conditions inside the buildings can be classified into three main approaches: nodal, zonal and CFD (*Computer Fluid Dymanics*) modelling. The nodal type of modelling describes the climatic conditions in each room with a single set of equations, where the uniform distribution of air and heat is assumed. The CFD approach divides space into a fine grid of cells where the air flow between the cells is described by the Naiver-Stokes's set of equations. A link between the nodal and CFD modelling is zonal modelling. A zonal model may be described as a CFD model with a rather coarse grid with a nodal type description of sub zones. Each sub zone is described by a set of equations specifying the mass and heat flow [3]. It will be shown in this paper that by using a zonal modelling with a low number of zones a good approximation of the realistic situation may be achieved.

The purpose of this modelling was to develop a model that might be used as an evaluation tool for testing the quality of regulating indoor air parameters. Besides, we wanted to create a model that might be used for prediction pe of regulation; moreover, our desire was also to develop a model that could explain the climatic relations from the physical points of view. This knowledge can then be used to further improve the regulation.

The model was developed in order to evaluate the regulation of three parameters which indicate the indoor air quality, i.e. the temperature, CO_2 concentration and relative humidity. Due to the correlation between the measured parameters, we included in the model all the necessary physical interactions in order to maintain nonlinearity of the system and coupling between parameters.

The room that was subject to modelling is provided with a HVAC (*Heating, Ventilation, and Air-conditioning*) system, by which the room is heated and cooled by controlling the input temperature of the air at the ventilation inlet. This means that there are two main situations: the one in which the room conditions are governed by the main air jet and the other with numerous air plumes. These two conditions have a significant impact on heat and mass transfer estimation. Since the expected ventilation air speed varies from zero to its maximum value, the building envelope model includes the model for natural and forced convection for estimation of the heat transfer from the envelope to air [2].

The impact of a human person on indoor air quality is included in the model from three aspects: The first and foremost aspect is heat being transferred from the human person to its surroundings; the second and third aspects are metabolism products of being emitted into the air, such as CO_2 and water vapour. The zonal modelling offers the possibility of localizing the presence of persons within the room. This is important for a precise calculation of the observed parameters that then compared to the measurements

The main principles of modelling employed will be explained in this paper and results will be compared to a real case where the number of people varies with time and internal and external conditions change during the experiment.

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SIMULATOR FOR TESTING MEASUREMENT, ESTIMATION AND CONTROL METHODS IN 2D PROCESSES

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Introduction. Industrial web processes, such as paper making and plastic film extrusion, use scanning gauges to measure properties of the web while it is produced. Measurements are made by sensors that are mounted in a frame, which allows the sensor to scan back and forth across the web. As the web is moving the sensor draws a zig-zag measurement path on the web. The variations of the paper web are classified into three categories, cross directional (CD), machine directional (MD) and residual variation. CD and MD variation have separate control systems: thus the measurement signal has to be separated into CD and MD variation estimates. Residual variation is normally not estimated and cannot be controlled. Despite the development of new measuring systems [1], the single scanning sensor continues to be the predominant measurement system in the paper making and plastic films industry.

Estimation and separation of the CD and MD components have been intensively studied for some three decades. There have been many attempts to solve the estimation problems by using different kind of methods, for example [2-3]. There exist also new camera-based commercial measuring systems that measure 2D variation down to submillimeter spatial resolution. The problem with such systems is that the cameras do not measure directly any of the relevant quality variables and therefore images from the system must be combined with scanning measurement.

CD control systems usually have an array of identical actuators located across the web. MD variation is usually controlled with the feeding pump.

Simulator. We present a Matlab-based simulator for 2D quality variations of the paper web such that the effects of incoming – user defined or based on process data – variations and actions of CD and MD controls are combined. Arbitrary scan paths, estimation methods of 2-D variation, methods of separation to CD and MD components, and CD and MD control methods can be studied. Furthermore, the inaccuracy of process models in the control can be analyzed. As results the simulator provides the simulated quality variation, estimated quality variation and their variances, the estimate separated into CD and MD variations, and the CD and MD control actions and the effect of the controls. Furthermore, the measurement and prediction error signals can be studied. Hence the overall control system performance and the robustness, of the estimation and control algorithms can be assessed.

Figure shows an example of simulated web variation and its estimate

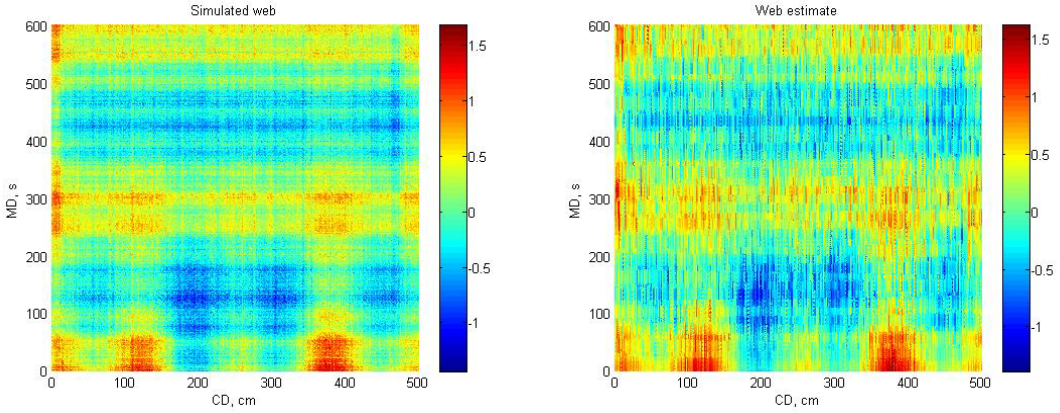

Figure 1 Simulated web and estimated web

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

APPROXIMATING DISTRIBUTIONAL BEHAVIOUR, SYSTEMS THEORY AND CONTROL

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Abstract. In many engineering and generally speaking more physical dynamic differential systems, the problem of transferring the initial state of the system to a desired in (almost) zero-time time is very significant. For instance, in biology, it is well known the famous Leslie population growth model. Thus, in this particular application the kicking of the initial state in (almost) zero time is being appeared whenever an environmental conservational organization (for instance WWF) reveals new populations in their habitats. In practice, this can be succeeded by using a linear combination of Dirac δ-function and its derivatives. Additionally, some good reasons for this choice are discussed in this paper. Obviously, such an input is very hard to imagine physically. However, we can think of it approximately as a combination of small pulses of very high magnitude and infinitely small duration. In this brief paper, an overview of the approximating distributional behaviour of descriptor differential systems is presented. Based on several new research results, a concrete mathematical framework is provided for our approximation procedure. Some important elements of system and control theory are also available. Finally, a numerical example is appeared.

ENGINE MODELING AND CONTROL SYSTEM DESIGN CONSIDERING TWIST OF A CRANKSHAFT

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Summary. The exhaust emission regulations and improving safety of cars become strict year by year, and better fuel efficiency and more comfortable driving response are also desired strongly. The present engine works are based on the crankshaft angle, i.e. the timing of the spark angle and fuel injection depend on the crankshaft angle. However, the twist of the crankshaft cannot be neglected in the measurement of the crankshaft angle and it influences the engine control. In this paper, the influence of the twist of the crankshaft is studied by using a model of an engine and its simulators. The engine model is derived by the Projection Method. [3].

Introduction. The engine torque control is important for a lot of reasons, e.g. automobile emissions, safety, fuel efficiency, comfortable driving response and so on. And, in the recent year, high speed and high performance semiconductors that are able to execute more complex control method are cheaper and cheaper. On these backgrounds, in order to improve the engine torque control drastically, it is imperative to control and to estimate engines based on the nonlinear model of the engine. The current engine is controlled by the crankshaft angle, i.e. the spark timing depends on the crankshaft angle. In the current engine, in generally, the crankshaft angle is measured from a sensor mounted in the front of the engine. However, the twist of the crankshaft cannot be neglected in the measurement of the crankshaft angle and it affects the engine control. This problem is pointed out by McKelvey [1] and Kallenberge [2]. The gap of the combustion timing between the front side and the rear side is occurred because the twist is generated in the crankshaft of an in-line multi-cylinder engine and it causes undesirable variation of the torques. In this case, irregularity of rotational speeds causes vibrations. This problem can be solved to measure the crankshaft angle of every piston. But it is difficult to attach sensors on the every piston, because of the space of sensors, costs of the engine and so on. So the crankshaft angle is measured on either the first-cylinder or the end cylinder, and it is important to estimate the engine torques by it. In our recent research, the piston crank mechanism has been expressed by a nonlinear model[**?**]. In this study, considering the twist of the crankshaft, the engine model is enhanced more realistic, and is applied to the high precision engine torque estimation.

In this paper, at first, a nonlinar model of the engine considering the twist of the crankshaft is proposed using the Projection Method [3]. Then the way to estimate the engine torque is also proposed. The proposed method is verified by numerical simulations.

Future works. As a future work, using the advantage of the model, i.e. accuracy andnonlinearity, we will tackle to design a observer that estimates torques and inmeasureable angles. As another future work, the proposed nonlinear model and the torque estimation method will be verified experimentally using the engine for the radio control car(Figure 1).

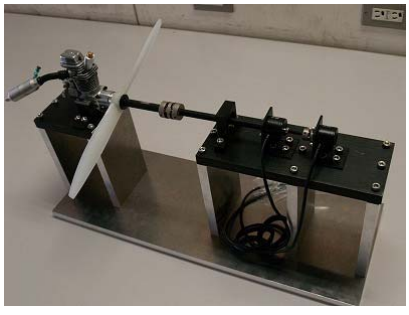

Figure 1: real machine of engine

Figure 2: four-stroke engine

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

ROBUST CONTROL APPROACH FOR INPUT-OUTPUT LINEARIZABLE NONLINEAR SYSTEMS WITH MODELING ERRORS BASED ON HIGH-GAIN PI-OBSERVER

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In this contribution, a robust control design approach is proposed for input-output linearizable nonlinear MIMO systems with modeling errors. The presented approach solves the robustness problem and the requirements of all the states information in the classical nonlinear control method (the input-output linearization method) and provides the estimation of the disturbances/modeling errors at the same time. A detailed application of the approach on mechanical systems shows the applicability and the potential of the developed idea.

If modeling errors, disturbances or other unknown effects acting on the nonlinear system are considered as external unknown inputs to the system, denoted by $Nn(x,t)$, an 'exact' system model can be set up by

$$\dot{x} = f(x)+g(x)u+Nn(x,t)\,, \tag{1}$$
$$y = h(x)\,, \tag{2}$$

where the assumed as known matrix N locates the external unknown inputs $n(x,t)$. The dimension of the unknown inputs vector $n(x,t)$ is assumed as p, with $0 < p \leq n$, while m denotes the dimension of the outputs y. With the classical input-output linearization method, the model (1) can be transformed into the following form

$$\begin{bmatrix} y_1^{(r_1)} \\ \vdots \\ y_m^{(r_m)} \end{bmatrix} = \begin{bmatrix} v_1 \\ \vdots \\ v_m \end{bmatrix} + \tilde{N}(x)n(x(t),t)\,, \text{ with } \tilde{N}(x) = \begin{bmatrix} L_{N_{col_1}} L_f^{r_1-1} h_1(x) & \cdots & L_{N_{col_p}} L_f^{r_1-1} h_1(x) \\ \vdots & \ddots & \vdots \\ L_{N_{col_1}} L_f^{r_m-1} h_m(x) & \cdots & L_{N_{col_p}} L_f^{r_m-1} h_m(x) \end{bmatrix}, \tag{3}$$

which can be written in a unique state space form

$$\dot{x} = Ax+bu+\bar{N}\bar{n}\,, \tag{4}$$
$$y = cx\,, \tag{5}$$

with $\bar{N} = \begin{bmatrix} 0 & \cdots & 0 & 1 \end{bmatrix}^T_{r_i \times 1}$ and the state vector $x = \begin{bmatrix} y_i & \dot{y}_i & \cdots & y_i^{(r_i)} \end{bmatrix}^T$, $i = 1,\cdots,m$ for different outputs. The system is obviously fully controllable and fully observable. PI-Observers can be constructed for the m motions separately

$$\begin{bmatrix} \dot{\hat{x}} \\ \dot{\hat{\bar{n}}} \end{bmatrix} = \begin{bmatrix} A & \bar{N} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \hat{x} \\ \hat{\bar{n}} \end{bmatrix} + \begin{bmatrix} b \\ 0 \end{bmatrix} u + \begin{bmatrix} L_1 \\ L_2 \end{bmatrix} (y-\hat{y})\,,$$
$$\hat{y} = \begin{bmatrix} c & 0 \end{bmatrix} \begin{bmatrix} \hat{x} \\ \hat{\bar{n}} \end{bmatrix}. \tag{6}$$

With properly chosen observer gain matrices L_1 and L_2, which fulfill given conditions [1, 2], the transformed states and the transformed disturbances $\bar{n} = \sum_{j=1}^{p} L_{N_{col_j}} L_f^{(r_i-1)} h_i(x) n_j(x,t)$ can be estimated.

As a robust control, the state feedback control $u = K\hat{x} - \bar{N}\hat{\bar{n}}$ can be taken to stabilize the transformed system dynamics, because the estimations $\hat{x}$ and $\hat{\bar{n}}$ are available from the PI-Observer and the transformed system is fully controllable. At the same time from the m PI-Observers m external inputs/disturbances $\bar{n}$ can be estimated in the transformed coordination and the disturbances in the original coordinates can be calculated by back transformation. Of course all the states and outputs in the original coordinates should be available to realize the input-output linearization as usual and this can be easily realized for mechanical systems based on the PI-Observer.
The whole control loop will be stable, while the transformed system dynamics is stabilized and the remaining zero dynamics of the input-output linearization is assumed stable.
An example is taken to illustrate the proposed approach. The results show clearly the effects and advantages of the proposed robust control method with the help of PI-Observer technique.

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INTELLIGENT CONTROL USING ONLINE STABILITY-BASED KNOWLEDGE REPRESENTATION

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In this paper, a new concept for intelligent control of stability in technical systems is proposed with the modified Situation-Operator-Model-based cognitive architecture of autonomous system [1].

An example of stabilizing a pendulum with unknown impulse disturbances is utilized to illustrate the concept. Suppose the pendulum's structure information, such as the weight, length and so on, is unknown, and only the two actual states are measurable. The control task is to implement a control to keep the pendulum within its stable region (the neighborhood near the lower position) when the pendulum is disturbed by an unknown impulse disturbance.

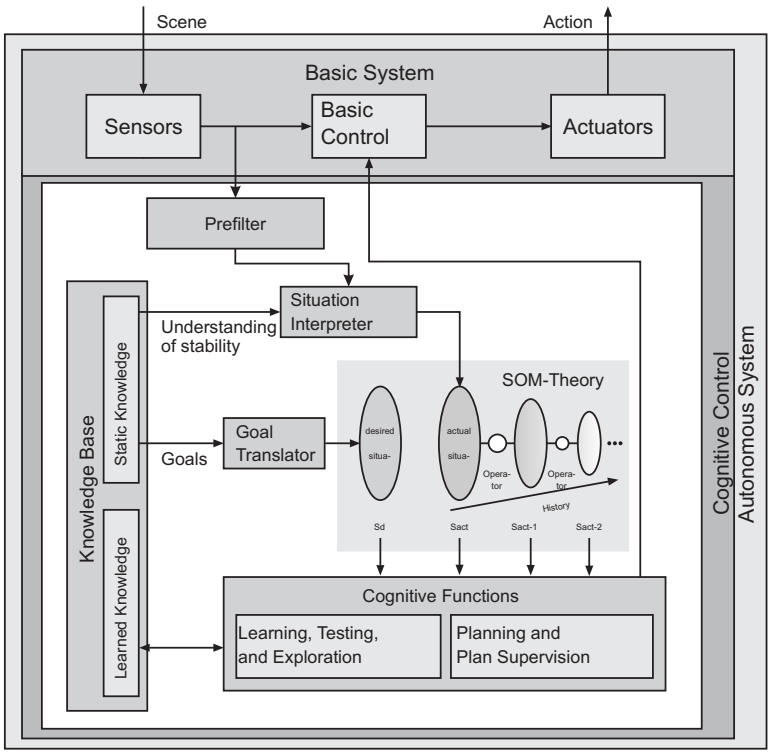

Figure 1: From pre-filtered situation to interpreted situation

The schematic structure of control is shown in Fig.1: The pre-filter takes the measurements of the states, compresses the information contained in phase portraits into the SOM description [2] which is transferred to the situation interpreter. Given in advance the static knowledge base about how to understand the stability, the situation interpreter can detect stability features of the system as a new characteristic in the situation, and give out a stability judgement. The cognition functions compare this judgement and the desired situation, generate a suitable feedback control to the basic system, by which a loop is formulated. The history of experienced control with respect to specific disturbances is stored in the learned knowledge base for the improvement of the control performance.

The novelty of this method is that controller does not have to know the detailed structure of the system plant, nor its physical behavior, because all the information needed in the stability control are gained by studying the phase portrait during the interaction process between the system and the environment, with the help of the static knowledge. Further more, the performance of the control can be improved according to the experiences of the controller which are gained by the cognitive functions and stored in the learned knowledge base.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

STABILIZATION OF NONLINEAR SYSTEMS WITH INPUT SATURATION USING SOS-PROGRAMMING

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The stabilization of an equilibrium point of a nonlinear system with input saturation including an estimation of the region of attraction is an important problem in control theory. Especially the input saturation has a significant influence on the region of attraction. Hence, it is necessary to consider the input saturation within the control design procedure.

The stability theory of Lyapunov is a tool to prove the stability of an equilibrium point and to estimate the region of attraction (for details see [2]). Using this theory, a suitable Lyapunov function must be constructed which is positive definite on the region of attraction and additionally the time derivative has to be negative definite. This theory can also be used for the purpose of controller design, i.e. a control law is constructed such that a Lyapunov function candidate becomes a Lyapunov function for the closed loop system. This Lyapunov function proves the stability of the equilibrium point and can be used to estimate the region of attraction of the equilibrium point of the closed loop system.

Although, the Lyapunov theory is the instrument to give the answer to the stability question, there is no easy way of constructing an appropriate Lyapunov function. In the last decade, beginning with the work of Parrilo [3], a numerical approach to find a Lyapunov function for systems with polynomial nonlinearities was presented in different publications, e.g. [1], using the so called SOS-programming (SOS - sum of square). It is shown in [3] that every SOS-program can be transfered in a semidefinite program which can be solved efficiently by a numerical software package. Furthermore, the region of attraction of the considered equilibrium point can be estimated using SOS-programming. As already mentioned the basic problem finding a suitable Lyapunov function is to test nonlinear functions for positive definiteness on a certain region in state space. The advantage of the SOS-programming technique is to solve this problem for polynomial functions with a restriction. Actually the polynomial is checked if a sum of square representation exists which is naturally positive semidefinite (for details see e.g. [3]). Furthermore, the SOS-programming technique can construct Lyapunov functions of degree larger than 2 systematically which may result in better estimates of the region of attraction when compared to quadratic Lyapunov functions.

Jarvis-Wloszek used the SOS-programming method in his dissertation [1] to compute a polynomial control law together with a polynomial Lyapunov function with the intention to stabilize the equilibrium point and maximize the estimation of the region of attraction of the equilibrium point of the closed loop system. In this paper the SOS approach of Jarvis-Wloszek is extended to polynomial systems with input saturation. The basic idea of this method is to construct a Lyapunov function and maximize a region in which all conditions for stability are fulfilled. To this end, the degrees of freedom of the control law are used to stabilize the system and to gain a maximum for the estimation of the region of attraction by the construction of an appropriate Lyapunov function. This yields an optimization problem with constraints which can be formulated as polynomial function which have to be checked for a SOS-representation. By considering the input saturation two additional conditions, one for the upper and one for the lower saturation, are derived which can easily be included in the SOS-program. It is easy to show that state constraints can also be handled by an similar procedure and yield an additional condition for every limited state.

Another modification compared to [1] is the application of rational control laws which consist of polynomial nominators and denominators. Furthermore, the denominator is chosen such that it is strictly positive in the whole state space in order to avoid singularities in the input signal. The integration of a rational control law in the constraints of the optimization problem yield after small rearrangements polynomial constraints which can be solved with the SOS-programming technique.

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INTEGRATED MODELLING, SIMULATION AND OPERATION OF HIGH FLEXIBLE DISCRETE EVENT CONTROLS

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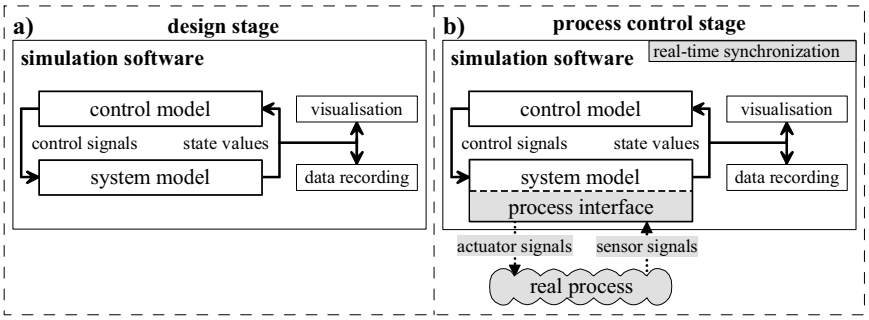
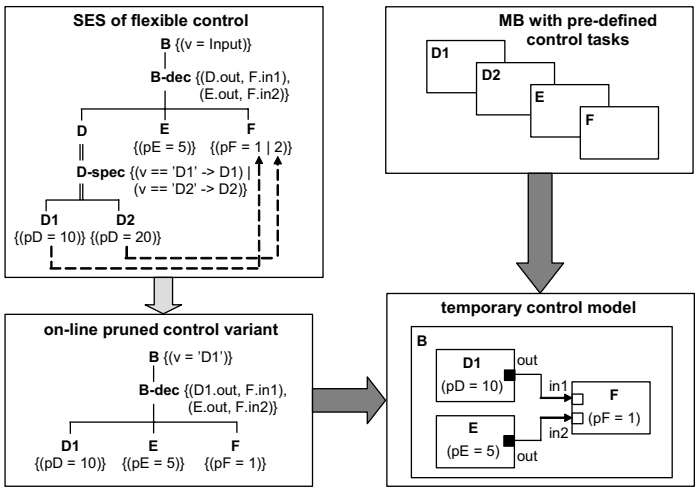
Modelling and simulation of discrete event dynamic systems is a well established method in engineering science, particularly in control engineering. In contrast to control engineering of continuous systems there is a gap between design stage and operation stage up to now. In the design stage modelling and simulation are used for system performance analysis and to develop optimum control strategies. In the subsequent process control development the control strategies are re-implemented in specific process control software, which functionality is often quite limited [1]. This research proposes a holistic approach extending a simulation model for process control after the same simulation model has been used in design stage. Necessary requirements such as the overall structuring of simulation models, its extension with a process interface, a task-based specification of the control model and new possibilities for discrete event process control, like e.g. model-based state observation, are discussed.



Extending a simulation model developed in the design phase (a) to a model-based process control system (b)

The system and the control model can be composed by sub-models in a modular, hierarchical manner. However, when in a high flexible control [2] the control model structure and its parameters have to be adapted depending on the actual system state, it is difficult or even impossible to specify the control in a closed modular, hierarchical model. Therefore, we employ the System Entity Structure and Model Base framework (SES/MB) according to Zeigler et al. [3] for the specification and operation of modular and high flexible controls. In contrast to [3] a new algorithm for stepwise generation of the control model from a SES under real-time conditions is introduced and demonstrated by a high flexible robot control application. Finally, a prototyping environment with an industrial robot cell for test and validation of the introduced research is described.



Employing SES/MB framework for specification and generation of high flexible controls

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELLING AND EVALUATION OF DESYNCHRONIZATION STRATEGIES FOR CONTROLLABLE COOLING DEVICES

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Introduction. Due to the time-varying availability of energy from renewable resources like sunlight or wind and their increasing use, the development of new load balancing mechanisms becomes a major task of grid operators. The storage of large quantities of electrical energy is very difficult. So "spinning reserve" generators, which are inefficient and expensive, are used to ensure stability of the grid frequency. An approach to reduce the use of such generators can be found in demand side management, where load balancing occurs on customer side by the use of intelligent devices. Such devices may be completely autonomous through monitoring the AC frequency and reacting to frequency changes by adapting their power consumption to reduce the stress in the grid. On the other hand, devices may react to dynamic price information from the utility in order to minimize operational costs. In this approach the devices can partly be influenced by the grid operators. A third approach moves the ability to control devices completely to the grid operator by using control signals. These signals can be used to directly modify the devices' behaviours in order to reduce stress in the grid.
Here, we follow the third approach. We analyze the collective behaviour of a great number of devices after processing a control signal and investigate some of the emerging problems. Stadler et al. [2] adressed the use of refrigerators in private households as controllable thermal storage. The authors explored different control signals for a simulation model of a great number of cooling devices. They concluded, that control signals to these devices can be used for short time reserves. However, the signals lead to a synchronization of the simulated devices, which in turn was followed by a periodic oscillation of the overall load of the population.

Approach. Based on the simulation model by Stadler et al. [2] and the findings from Hinrichs in the Master's thesis [1], we discuss and compare in this paper two strategies to desynchronise a population of cooling devices in order to damp an oscillation resulting from a control signal to the device. For this objective, we extend the simulation model by two algorithms to restore a particular distribution of fridge states after the impacts of a control signal.
The first algorithm performs a state recovery in order to produce a distribution of device states after the reactions to a control signal which is the same as immediately before the signal. For this task, a device controller has to store state information when a control signal arrives. After the reaction to the signal, the controller has to calculate and execute a behaviour which leads to a state similar to the stored information as soon as possible.
The second algorithm tries to achieve a state distribution which is not the same but similar to the situation before a control signal. For this objective, a device controller will have to randomize the device's behaviour after the reactions to a control signal.

Results. Both developed algorithms lead to a complete desynchronisation of the devices, but differ in their implementation and operation complexity. We show that using a simplified, linear model of a cooling device for the algorithms allows the controller logic to be kept simple. On the other hand, the linear calculations produce errors in the prediction of the device's behaviour which must be specially handled.

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A NEW METHOD TO IMPROVE PERFORMANCE OF CONTROLLERS DESIGNED BY LQR METHOD

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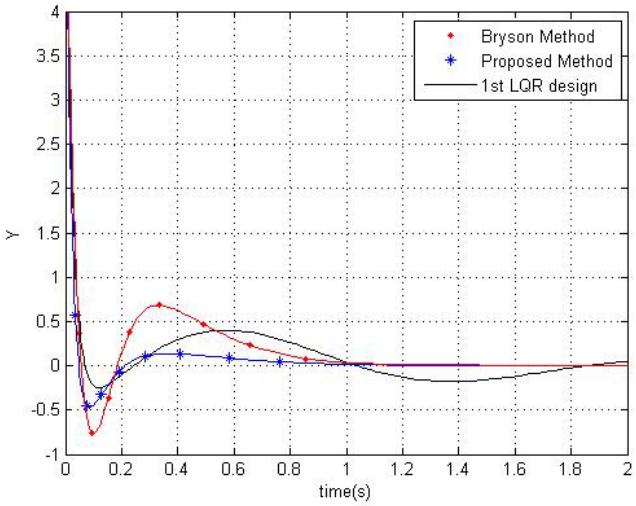
LQR is a powerful method for control of multi inputs multi outputs (MIMO), linear systems. Using LQR theory, it is known that for a controllable linear time invariant system, a set of optimal feedback gains may be found which minimizes a quadratic index and makes the closed loop system stable. The main difficulty in working with LQR method is to choose proper values for **Q** and **R**, the weighting matrices of state vector and inputs, to achieve acceptable performance for closed loop system. Commonly a trial-and-error is used to construct the matrices **Q** and **R**. This method is very simple to use, but very difficult to produce good control performance. Also it takes a long time to choose the best value for **Q** and **R**. Bryson [1] developed a method to solve this problem using a simple iteration algorithm to optimize the elements of matrices **Q** and **R**. Robandi et al. [2] proposed a method based on genetic algorithm to produce optimal values for matrices **Q** and **R** to improve the settling time of the system. The computational cost of these methods is high and they do not guarantee a solution to the problem.

In this paper a method is proposed to improve matrix **Q** such that the dominant poles are pushed beyond a specific value, which can guarantee desired performance. To introduce the method we first present a formulation for finding appropriate matrix **Q** which may be used in a LQR design process to put the closed loop pole of a first order linear time invariant system, LTI, at a desired location. Then a similar formulation is given for second order system with two complex conjugate poles. It is also shown that for two similar LTI systems related trough a similarity transformation, T, two weighting functions Q and Q' which are transformed with the same transformation matrix would result in similar closed loop systems. Taking advantage of these developments, a method is presented which can improve the choice of Q in a step by step procedure to push the poles beyond a specified value.

A numerical example in which it is intended to decrease settling time of a sixth order system to less than one is solved, which shows validity of the proposed method. The same problem is also solved with the method proposed by Bryson and Ho [1]. The results prove the proposed method to work better and faster as compared to previously available methods. Figure shows time history of the output for the solved example.



Time response of the closed loop systems designed by LQR method

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

OPTIMAL SENSOR PLACEMENT IN FLEXIBLE STRUCTURES: ENERGY VS. INFORMATION BASED CRITERIA

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The static and dynamic behavior of a physical system is described by system variables, which allow for a description of the system state at any given time. However, the system states are usually not directly available and appropriate variables have to be measured by physical sensors to guarantee observability of all system states. While classical observability criteria only give qualitative information on observability (yes or no), more advanced methods yield quantitative results in terms of robustness with respect to numerical issues and modeling errors or sensor noise. Thus, both the careful choice of the sensing principle as well as optimal placement of the sensors are important system design tasks.

This paper is concerned with the optimal placement of sensors (OSP) on flexible dynamical structures, a frequently discussed research topic during the last ten years [1]. The goal is to establish a criterion which specifies where to place displacement, force, inertial acceleration, or other sensors, such that either the energy or the information is maximized in the sensor outputs. Typical applications cover modeling, identification, fault detection, and especially active control of large flexible structures such as bridges, rail wagons, or space structures. Thus, various methods and criteria for OSP have been developed, whereas the remainder of this paper focuses on the comparison of two of them.

The first method is information based and analyzes the information content in the sensor measurements via the output mode shape matrix, which describes the propagation of the modes into the outputs [2]. An iterative elimination algorithm, denoted as EFI (for "Effective Independence") has been developed that repeatedly deletes those lines of the initial full output shape matrix which contribute the smallest amount of information. The criterion used in the EFI method quantifies the information content in the considered set of sensors, measured by either the trace or the determinant of an underlying Fischer information matrix, which is defined as the inverse of the output estimation covariance matrix. An appropriate defined selection vector enables an iterative ordering and selection of the sensors by their amount of information. This process is repeated until the number of remaining sensors equals to the preset value.

The second approach for optimal sensor placement considered in this paper is based on maximizing the amount of the energy of the signal that can be received by the sensors [3]. The signal energy is evaluated for two different cases of system inputs: transient and persistent excitation. Utilizing a special choice of modal state coordinates (where all structural modes are decoupled), both excitations lead to the same Lyapunov equation with the observability gramian as a quantitative measure for the observability of the structure. For structures with small damping and well-spaced natural frequencies, the observability gramian is diagonally dominant and the diagonal elements can be calculated in a closed form. This feature of the gramian is finally well-suited for a performance index definition for each possible sensor location out of a set of location candidates.

A comparison of the information based approach with the energy based approach shows the basic coincidence of them. Up to a scalar factor, the vector expressing the information content and the vector containing the total energy are equal, which is also verified on a simple example. Furthermore, it is shown that an appropriate definition of a performance index is useful with respect to the observability of higher frequency modes, since considering only the signal information content or total energy, respectively, can lead to sensor positions unable to observe certain higher order modes.

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Discrete Systems and Manufacturing

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MULTI-AGENT ADAPTIVE MECHANISM LEADING TO OPTIMAL REAL-TIME LOAD SHARING

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General Context. To reduce manpower or other resource costs is an everlasting managerial challenge in any production and service network. Such contraction of the operating costs obviously relies on an optimized workload sharing between the available operators. Hence, to process the full incoming load by using the minimum number of engaged operators, while still respecting given due dates, is clearly the basic optimization objective. The operator random failures as well as the non-stationary fluctuating incoming workload force the optimal load sharing policy (LSP) to be based on a real-time monitoring of the system state (*i.e.* queue contents, instantaneous traffic, etc). While this information updating process, on which our adaptive optimal LSP will be based, is often fulfiled by a central dispatcher, our present contribution shows how fully decentralized mechanisms, of multi-agent type, are also perfectly suitable to achieve the same objective. Whereas our research topic shares similarities with well-known congestion control problems arising in the Internet, it definitely differs from them by the fact that, in the present case, the agent character is carried by the circulating items themselves rather than by the servers. More specifically, our LSP relies on "smart tasks" which produce, via ad-hoc stigmergic interactions, the emergent optimal job dispatching. Beside its manifest relevance for applications, our class of models is analytically tractable, a rather uncommon feature when dealing with multi-agent dynamics and complex adaptive systems.

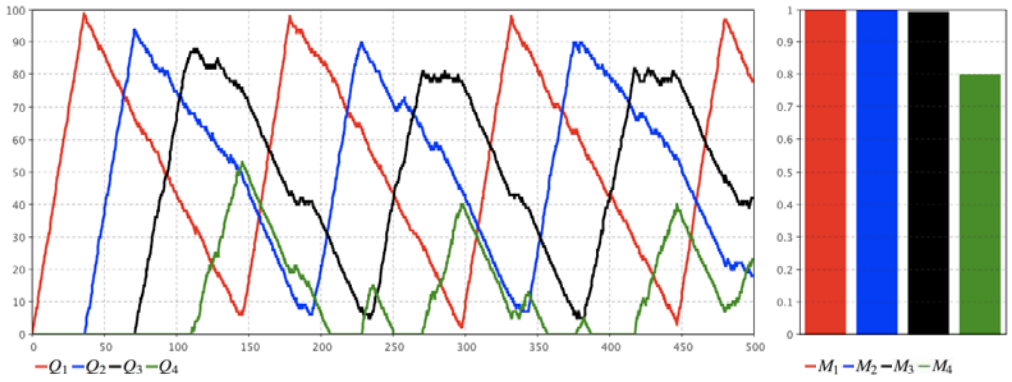
Basic Modelling Framework. We consider a production center with N parallel servers fed by an incoming non-stationary random flow of tasks. The objective is to realize an optimal load sharing defined by:

($\mathscr{O}$): *i)* "Process the global incoming workload by permanently engaging the minimum number of servers" or similarly, using queueing system terminology, "maximize the busy period of the engaged servers".

ii) "Keep the average waiting time below a given level".

Each "smart task" is endowed with an individual capability to monitor its sojourn time in the system and can thus warn the following tasks, using an ad-hoc informational feedback mechanism, of possible server congestions. The tasks use these warnings when they autonomously compute their individual routing strategy through the network.

Emergence of Self-Organized Optimal Load Sharing Dynamics. By the construction of the above multi-agent dynamics, our LSP permanently ensures *i)* the engagement of the minimum number of servers and *ii)* queue stability. Specifically, we observe that the queue contents exhibit stable temporal oscillations whose maximum and minimum values can be explicitly calculated. Tuned by control parameters, these maximum possible queue contents can be used to calibrate the waiting room sizes and hence, due to Little's law, to limit the task waiting times. Moreover, we show that the queue contents of the engaged servers never vanish, thus ensuring maximum busy period and hence optimal load sharing. As clearly illustrated in the figure below, the system dynamics reveals itself to be very robust and objective $\mathscr{O}$ is always reached despite the strong fluctuations affecting the system behaviour. This robust and quasi-deterministic temporal evolution, which is a direct consequence of the law of large numbers, arises independently of the interarrival and service time distributions. Our optimal LSP leads to highly reactive response (*i.e.* the length of the transient adaptive phase is almost negligible), which is in particular perfectly suitable for non-stationary incoming workload.



Left: Temporal evolution of the queue contents Q_α, $\alpha \in \{1,2,3,4\}$, for task interarrival times uniformly distributed in $[0.16; 0.36]$ and service times uniformly distributed in $[0.5; 1.5]$. *Right*: Corresponding server utilization.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODEL-BASED SAFETY MONITORING OF PRODUCT FLOW PATHS*

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Introduction A basic and essential operation performed by processing plants is the movement of material, i.e. products, between plant elements. We denote the routes that products take while flowing through a plant as *product flow paths* [1]. The operation of plants with flexible structures requires adequate working states of plant elements like valves in order to restrict the flow of material to a desired path, as well as to ensure the safety of the flow operation by avoiding undesired and potentially hazardous situations. Process control systems usually fulfil the task of ensuring and monitoring the correct and safe transport of material. However, the development of these plant-specific solutions is based on informal knowledge and is time-consuming and error-prone, and must be repeated as soon as the plant itself changes. This motivates the development of automated approaches that may partly or completely replace this engineering work, ensuring its correctness at the same time. With this goal, we have developed a formal and abstract plant model which defines a simplified plant representation that considers the possibility of flow through its components, and is generic enough to represent practically any type of plant and plant device. We present a formalisation of the safety of a product flow path at a given plant state based on our abstract plant model. This formulation may be used as a guideline for automating the construction of systems which perform safety monitoring of product flow paths. An outline for the design of such a system following a decentralisation scheme is also presented.

Abstract plant model A plant is formally represented based on sets of elements and product connectors. A mapping associates connectors to elements, and a binary relation represents the interconnection of element connectors as is found in the physical plant. The plant is hereby modelled by a special kind of graph: the elements of the plant are represented by graph nodes, and rather than connecting the nodes directly, the edges of the graph link so-called connectors, which are in turn embedded in the element nodes.

Flow allowance model We follow a *plant-oriented* and *passive* approach for representing product flow. The possibility of flow through the plant is denoted as *flow allowance*, which represents a *necessary* condition for actual product flow. Therefore, the absence of flow allowance guarantees the absence of product flow in the plant, and we use this reasoning when defining the structure and safety of product flow paths. Our model describes the allowance of flow of material into and out of every plant element, as well as *among* neighbouring plant elements by means of a *flow allowance relation*.

Flow path model A flow path is defined as a sequence of neighbouring plant elements which follows the flow allowance relation, and which may be used by a product to flow from an initial element to a final element. Flow paths are free from any repeated elements, which causes flow paths to be free of cycles, guarantees that flow paths have a finite length, simplifies the representation of flow path data and the algorithms which work with flow paths, rules out any form of simultaneous bidirectional flow and captures the essence of product flow operations.

Product flow path safety Based on our flow allowance model, we formulate a definition of safety of a product flow path at a given plant state with the intention of identifying general scenarios which correspond to undesired and potentially hazardous situations that may arise during the usage of a product flow path. We identify two subclasses of plant elements: *sources* and *sinks*. The basic principle behind the definition of product flow path safety is the avoidance of leaks and unintended mixtures. A leak occurs when the flow of a product diverges from the intended path and reaches a sink. An unintended mixture occurs when another material is able to flow from a source and mix with the product flowing through a flow path. The conditions for the occurrence of these situations may be determined in a step-wise manner. The successive application of a flow step safety function to each flow step in a flow path is achieved by means of a recursive function which defines the safety of a flow path inductively over the structure of the path. In this manner, a simple and unambiguous way of determining the safety of a product flow path based on our abstract plant model is obtained.

Decentralised safety monitoring of product flow paths The decentralisation of process control systems is advantageous for many reasons. A system for product flow path safety monitoring which operates in a decentralised fashion may be developed using the model-based definition of product flow path safety presented in this paper. We give a general description of the composition and operation of such a system.

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*This research has been partially funded by the DFG Research Training Group 1298 "Algorithmic synthesis of reactive and discrete-continuous systems" (AlgoSyn).

DISCRETE-MODELLING OF PROCESS COMPONENTS INTERACTIONS USING THE DESIGN STRUCTURE MATRIX

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Abstract. The product development community faces new challenges due to a drastic increase in the scale and complexity of engineered systems. Modelling these systems is becoming increasingly important as it allows a better process/product understanding for analysing changes while avoiding several iteration loops. Therefore, knowledge about involved feedbacks and their effects is of particular importance, as they help in better understanding the dynamical behavior of the considered processes.

One of the most famous modelling approaches for live systems was established by Jay W. Forrester and is known as *System Dynamics* [1]. It is a structured approach for modelling complex systems with applications in urban commuter and social systems and industrial dynamics. Various theoretical and practical developments made *System Dynamics* to a powerful modelling and simulation tool. However, it still suffers from some disadvantages: e.g. problems in getting appropriate *Causal Loop Diagrams* or *Level-Rate-Diagramms* [3] and problems in modelling purely discrete-time dynamical systems [2].

In this article a new modelling approach is introduced based on extending a recent decomposition principle called DSM (*Design Structure Matrix*) to a discrete-time dynamical system in order to bypass some disadvantages related to *System Dynamics*. The system is modelled as detailed as necessary by aligning the used interaction knowledge to an introduced weighting coefficient. Proportional, functional and qualitative knowledge of the coherences is considered and linguistic process knowledge is thereby included via *Fuzzy-Logic*. Hence, the developed strategy allows to handle nonlinear relations as well as uncertainties. First applications are shown on two simplified examples, together with analyses of process fixed points and attracting regions using well-known mathematical methods.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

AIRSIDE AND LANDSIDE MODELLING FOR DETERMINING AIRPORT CAPACITY

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Introduction. Air traffic is carried out in selected air zones that are controlled by Air Traffic Services. One of the main problems they encounter is the traffic congestion. The biggest congestion is observed in the Terminal Area (TMA). To provide safety of controlled aircrafts one must know so called airport capacity, i.e. number of airplanes that can stay in Terminal Area in given meteorological conditions, traffic organization, etc.

Airport capacity. At present, worldwide, there are no accepted methods of determining the airport and TMA capacity. Establishing a method for determining capacity would have a significant impact on the development of methods for controlling air traffic worldwide. In this paper, the airport capacity is precisely defined basing on so-called practical capacity. Then a method of calculating the capacity is proposed. It was assumed that the airport consists of two areas: airside - related to the aircraft service and landside - related to the passengers' service. Both sides influence on each other. Late passengers delay aircraft's takeoff, late landings delay passengers' end-of-the-journey time.

Model. For systems, which take as an evaluation criterion the amount of time lost for servicing a large number of objects, the correct method of modelling is treating them as systems of mass service. These models, on one hand, may properly express transport phenomena related to the movement of transport units. However, on the other hand, they characterize by possibilities of effective computer realization, already verified in practice. In the theory of mass services, it is the lost time (delay) to be analyzed as a fundamental value. It changes, in relation to the kind of a performed operation (for example, airport approach or taxing, passenger's check-in) and place, where the service is performed (TMA area, taxing areas). It may be observed that the whole service consists of several successive stages, where each of them is an independent system of mass service. On each of the entrances we may face a different probability distribution of the application's sequence. Moreover, from each of the entrances an aircraft may go to any of the exits, and yet the time of crossing in any of the cases may have a different probability distribution.

Method. It has been proposed to carry out a study over a terminal area seen as a network, multi-phase queuing system, in which the output streams from one sub-system are the input streams for the next sub-system (the next phase of service). If in the case of an analytic model we have to deal with a kind of very complex queuing model, for which determining stationary characteristics is at present impossible, in the case of a simulating model the numerical experiments show easiness of obtaining the results. The proposed method of solution of the problem of airport capacity consists of the following stages:
1. Determination of model of studied space.
2. Recording the model with the use of special language of description.
3. Execution of series of simulating experiments
4. Analysis of received statistical sample and determining the capacity.

Simulation and results. In order to carry out simulation experiments, statistical data was collected, both in airside and in landside. For instance in landside collected data describe: intensity of passengers' requests, passenger's traffic within terminals, duration of service in given points etc. Simulation experiments were conducted, which consisted in testing of a real check-in systems', so as to point out the system's bottlenecks. Later on, some other experiments were realized, which were to evaluate the impact of the flight schedule, the configuration of passenger's check-in procedure, on the system's capacity. As the result of executing the series of simulating experiments a random sample of realisation of two-dimensional random variable (X,D) is obtained. Pairs X,D define: intensity of air traffic, size of average delay. On the basis of these data a table is created, which corresponds to the distribution of probability of relative average delay for all accessible values x_0 (intensity of air traffic). For this table the values of function G_x are calculated, which is the probability of that the average delay is larger or equal to a pre-set maximum value D_{max}. This function is a base for airport capacity determination.
Examples of results for a real situation's simulation and a planned reconfiguration of modeled system are presented in the paper.

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BEHAVIORAL ANALYSIS OF FLEXIBLE MANUFACTURING SYSTEMS WITH MULTIPLE CLASSES AND FINITE CAPACITIES [1]

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Introduction. Flexible Manufacturing Systems(FMS) are complex manufacturing systems where multifunctional computerized machines are united together with a material handling systems. Their costly investment requirement necessitate the study of system performance under operating conditions.

FMS systems are usually modeled as multi-chain closed queueing networks with a central server configuration. Multi-chain queueing networks consist of different classes of customers which vary in their routes, service requirements, costs, waiting spaces etc.

Behaviors of Multi-class networks with finite buffers We consider closed queueing networks with multiple customers. Further, we assume that the stations may have limited waiting spaces and a customer can be blocked after service. With a FCFS queueing discipline, these networks may have the following surprising behaviors:

Benefiting from Finite Capacity

An interesting, observation in closed finite queueing networks with multiple customer classes is that increasing the buffer size of a workstation may not necessarily lead to better performance of the system. So far, as conjectured and generally believed, the throughput of a finite capacity network is less than or equal to the same network without blocking. That may be the case in a single class network, however, the customers in multiple class networks can benefit from finite capacities and may have higher throughput than their infinite node capacity counterparts.

In this context, we propose the following result for a multiple class closed queueing network with FCFS queueing discipline:

Theorem 1. *A multi-class closed queueing network with infinite node capacities does not provide an upper bound for the throughput of the customer classes as the same network with finite node capacities.*

Detriments of Finite Capacity

Another behavior which contrasts with the previous property is the negative effect of finite buffers on chains. Due to the interactions of customers arising from use of finite capacities, the performance of a class can be affected significantly, although, there is no blocking station on its route. This is intuitively understandable, especially in a network with single servers, FCFS scheduling and BAS. Once a customer is blocked by its downstream station, it continues to occupy the upstream station. During this time, the server cannot provide service to other customers although it is idle. The blocked customer functions as a barrier forcing the customers in the queue to wait longer.

Conclusion and Future Research In this research, we have investigated the behavior of multi-class finite closed queueing networks and showed that they can benefit from existence of finite buffers. On the other hand, we also have illustrated that finite capacities may significantly reduce the performance of the system if not carefully positioned.

As demonstrated in numerical experiments, the relative percentage difference of finite networks compared to non-blocking ones can be very high. Estimating the performance of the finite buffer queueing from non-blocking network is not suitable, and hence, finite networks require a particular treatment.

There are several important applications of such networks: packet-switching communication networks with different types of packets and priorities, job-shop manufacturing systems and multi programmed computers systems, to name a few.

The findings here open new areas of study in closed queueing networks. One possible area is that of studying the achievable performance bounds of customer chains. Since, the classes may exceed their non-blocking network counterparts in performance they do not provide an upper threshold anymore. Specific calculations and distinct algorithms should be derived for finite buffer systems in order to predict their performance.

Another area is optimization. While optimizing the system performance or/and determining the number of customers in each chain, the influence of the finite buffers may contribute to the objective function. Hence, the finite buffer factor should be included in decision process.

[1]This research has been supported by the The Scientific and Technological Research Council of Turkey(TUBITAK) under the programme National Young Researchers Career Development (Career Programme) by grant number 106M367.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Robotics – Applications, Tools

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELING AND OPTIMAL OPERATION OF ROBOTIC MANIPULATORS WITH DISCRETE CONTROLS

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Introduction. The use of hydraulic or pneumatic actuators in industrial robots allows to generate high specific forces in a compact design. A further simplification of the manipulator design becomes possible by the restriction to only discrete control levels. This is the case, if e.g. magnetic valves are installed. It is no longer necessary to generate continuous pressure profiles with high accuracy, only exact switching times have to be realized. The aim of this article is to set up a mathematical model for such an industrial robot and carefully investigate the effects of discrete controls compared with the continuous case.

System modeling. The example manipulator is modeled as a set of n rigid links connected in a chain by revolute joints; joint angle θ_i corresponds to joint i. The equations of motion of the manipulator in the joint space are derived by a modified version of the recursive Newton-Euler algorithm. For optimal control applications, efficient access to accurate derivative information is important. Derivatives of the rigid body system are obtained by differentiating the Newton-Euler recursion with respect to $\theta_j, \dot{\theta}_j$. For every joint j, the differentiation process again results in outward and inward recursions. Only discrete levels of torque are allowed for control. Transitions between different control levels are not idealized by step functions, but described more realistically by continuous transition profiles. During transition time, no control commands are accepted by the respective control. This leads to a control problem with reduced dimension of the control vector during switching times. In addition, multiple state constraints have to be fulfilled.

Optimal control problem. A Maximum Principle based approach is used to calculate optimal trajectories with high accuracy. The original optimal control problem with discrete controls is embedded into a continuous problem of higher dimension. By this, optimality conditions are not only evaluated at discrete times, but the system dynamics and sensitivity properties on the full solution interval are coupled to the switching points of the system. The extended problem of optimal control is transformed into a multi-point boundary value problem. By recursive modeling techniques, the formulation of the boundary value problem including nonlinear state and control constraints is automated to a great extent [2]. An advanced multiple shooting method [1] provides significantly improved stability of the numerical solution process.

The sequence of different torque vectors along the optimal trajectory and thus the structure of the problem is derived from a modification of Bellman's idea of dynamic programming, using the solution of the infinite-dimensional case with continuous controls as a reference for the finite-dimensional case with discrete controls.

Example. Time-optimal point-to-point trajectories subject to state and control constraints are calculated for a three-link example robot. With discrete controls properly determined, a similar performance of the robotic manipulator is achieved as with continuous controls. However, the solution structure is more complicated than in the continuous case, especially if state constraints are active.

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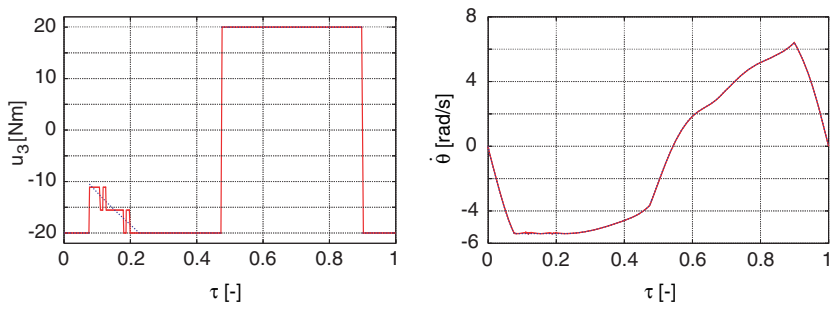

Figure 1: Finite-dimensional problem: State constrained solution, four discrete control levels are active (thick line). Motor torque u_3 and link velocity $\dot{\theta}_3$ vs. time for the example problem. The solution of the infinite-dimensional case is given for comparison purposes (dashed line).

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MATLAB BASED ROBOT CONTROL DESIGN ENVIRONMENT FOR RESEARCH AND EDUCATION

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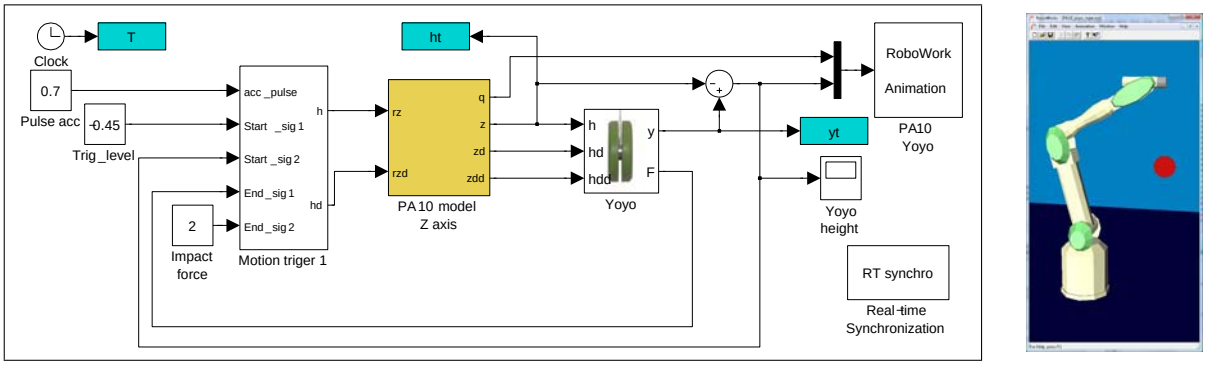
Introduction. Research in the field of robotics is tightly connected to simulation tools for many reasons. On one side, simulation supports the development of new advanced control algorithms and on the other side it is always not feasible to built a whole robot system to test some algorithms or it is not safe to perform tests on a real system (at least in the first design stages). In the paper we present an integrated environment for the design and testing of advanced robot control schemes, including visual tracking, force feedback on a single robot or in multi-robot applications. Our simulation framework is not intended as an alternative to different available software tools for robotics systems. The aim is to support the control design in such a way that the user can focus on the control issues and not on the simulation details.

The main capabilities supported by our simulation environment are: the simulation of the kinematics and dynamics of manipulators, the integration of different sensor systems, scenarios for complex robot tasks, the visualization of robots and their environment and the integration of real robots in the simulation loop. The main advantage of our system is the simplicity, which allows easy integration of different robots, sensors and other devices. Although the kernel of our environment is MATLAB/Simulink, some of these can be easier simulated by using other tools. Hence, other simulation tools can be used for the simulation of particular parts of the system and then these subsystems are integrated in the simulation environment into the complete system. To integrate such a diversity of components in unique framework we have decided use the ethernet communication and the UDP protocol.

The scope of our research is lately oriented more in the development of control systems for humanoid and service robots. This advanced robot systems are characterized by the variety of complex sensory system like vision and force sensors. It is important to have available accurate sensor models. As these systems require high computational power and can run on more than one computer, we have developed special protocol classes for integration of different sensors, actuators and other subsystems into the simulation environment.

When dealing with complex tasks for these robots, the desired motion depends on the system/environment states. To provide all the flexibility needed we have developed a special Matlab Robot Language (MatRoL) and a corresponding MATLAB/Simulink interpreter block. MatRoL is BASIC like programming language extended with special commands for the robot control and supports all MATLAB interpreter commands. In this way we have the advantage of a simple robot task definition and access to comprehensive MATLAB computation capabilities.

To show the efficiency and usability of our control design environment we outline some typical experimental examples using our robots. We explain some typical control design procedures from the “pure” simulation to the testing of algorithms on real robots. The simulation examples illustrate another important feature of our system, i.e. easy final testing of developed control algorithms. Namely, for final testing of the control algorithms the models in the simulation scheme are just replaced by interface blocks for real system and the user does not need to consider implementation details.



Yoyo simulation: Top level block scheme in Simulink and animation of the PA10 robot and yo-yo in RoboWorks

The presented control design environment has proved to be a very useful and effective tool for fast and safe development and testing of advanced control schemes and task planning algorithms, including force control and visual feedback. The software can be very easily extended and adapted to different requirements and applied to any types of robotic manipulators. Last but not least it is an efficient tool for educational purposes. Thus, it should be of interest to the researchers involved in the development of advanced robot systems, and for teaching laboratories.

MODELLING, SIMULATION AND CONTROL OF A REDUNDANT PARALLEL ROBOT USING INVARIANT MANIFOLDS

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Introduction. This contribution presents a systematic approach of modelling, simulation and control of a parallel robotic manipulator. In contrast to classical industrial robots that are well understood and consist of only one open serial kinematic chain such parallel robots with several closed kinematic chains are considerably harder to describe. In many cases even the number of the mechanical degrees of freedom and therefore a suitable set of generalized coordinates is difficult to find or unknown. Often auxiliary dependent coordinates are introduced to simplify the process of modelling. These coordinates have to be either eliminated which requires the analysis of the possibly ambiguous inverse kinematics or additional differential kinematic equations have to be introduced for system analysis and numerical simulation.

Contribution. In this paper a different approach will be followed that gets along without the described elimination. Regarding the framework of structured analysis of dynamical systems, it is often useful and convenient to divide the overall system into smaller parts. This way of modelling is quite intuitive and less complex, even though the aggregation of those subsystems requires some additional compatibility conditions. Considering the standard state space approach, these conditions appear as algebraic equations defining relations between single state variables. Such differential-algebraic systems are also known as descriptor systems.

As an example the parallel manipulator shown in figure 1 is first divided into its three arms which can easily be modelled as serial chains using any method for multi-body systems, such as Langrange's equations or Kane's method. In addition, the assembly of the whole system requires the definition of four additional holonomic constraints. The overall dynamics can be transformed into a nonlinear state space representation in descriptor form which is defined on the manifold $\mathscr{M}$. Based on the approach in [1] for linear descriptor systems, the problem is interpreted as a coupling or constraint control problem. This is achieved by defining a number of additional input and output variables which just equals the number of algebraic equations. Now, an appropriate state feedback controller $\mathbf{u}_e = \alpha(\mathbf{x}_1) + \beta(\mathbf{x}_1)\mathbf{v}$ can be constructed, which meets certain requirements. First of all it renders the submanifold $\mathscr{N} \subset \mathscr{M}$ of consistent/allowed states an invariant manifold, e.g. $\mathbf{a}(x) + \mathbf{b}(x)\alpha(x) \in T_x\mathscr{N}\ \forall x \in \mathscr{N}$ and $\mathbf{c}(x) = \mathbf{0}\ \forall x \in \mathscr{N}$. This basic idea can be found in [2] for nonlinear input affine systems. Introducing some modifications it is furthermore possible to make the invariant manifold $\mathscr{N}$ an attracting submanifold, such that all inconsistent initial conditions tend asymptotically towards $\mathscr{N}$. This is especially important for simulation purposes. The remaining degrees of freedom in the controller design procedure can now be used to make the system behave in a desired way on the submanifold $\mathscr{N}$ of allowed states. This can either be used in order to design a controller in the classical sense to solve some trajectory following problems or to simulate the robotic system without any exterior control. The latter control object is achieved by introducing some structural constraints into the feedback law. This feedback just recovers the finite dynamics of the original differential-algebraic system on $\mathscr{N}$ and is therefore a suitable tool for the numerical stable simulation of the parallel robotic manipulator by means of standard simulation tools.

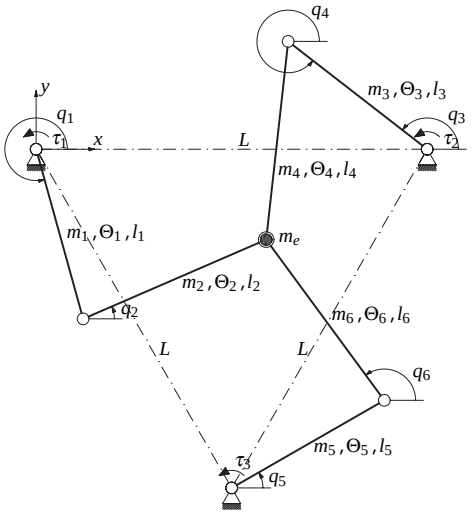

Figure 1: Planar redundant parallel robot

Numerical results are shown for the two cases of system simulation and an exact feedback linearisation on $\mathscr{N}$ that allows trajectory tracking and prestressing of the whole structure in order to increase accuracy.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

APPLICATION OF NON-DIMENSIONAL MODELS IN DYNAMIC STRUCTURAL ANALYSIS OF CRANES UNDER MOVING CONCENTRATED LOAD

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Introduction. This paper deals with the analysis of dynamic behaviour of the large ship-to-shore (STS) container cranes under moving concentrated load (modelled as moving mass including the effects of mass inertia, centrifugal and Coriolis force) – crane trolley carrying the container. The application of moving load problem in cranes dynamics has obtained special attention on the engineering researchers in the last years, but unfortunately little literature on the subject is available, e.g. [1]. The container crane boom (waterside outreach), due to its large dimensions, structural flexibility and self-weight, is identified to be the most important structural element for dynamic analysis, having in mind the cantilevered nature of STS container cranes. The stiffness of the structure affects the magnitude of the deflection and the vibration frequency. By increasing the stiffness of the crane structure, the deflection will decrease and the vibration frequency will increase. In practice it is very difficult and expensive to do an experimental research on a real mega STS container crane, or on a scale-model. For that reason the investigations on mathematical models and numerical experiments are necessary, especially during the design stage of such large structures. This paper discusses the problem of dynamic interaction between the structure and the moving trolley. The idealized equivalent reduced mathematical model of the boom structure is obtained in [2].

Non-dimensional model. In addition to the analysis presented in [2] this paper present the analysis of the non-dimensional mathematical model for the prediction of the boom dynamics of operating large STS container crane. The non-dimensional mathematical model implemented in this paper presents a conceptual substitution of the real system of mega STS container crane and provides general understanding of the dynamic behaviour of container crane boom under the action of moving trolley. So, the obtained results can be applied for analyzing dynamic behaviour of a series of similar constructions of STS container cranes, as well as other related constructions such as are slewing tower cranes, unloading bridges, gantry cranes, etc. The non-dimensional differential equations of motion are solved numerically by using the Runge-Kutta-Fehlberg method.

Parameter sensitivity analysis. The deterministic computer simulation of the non-dimensional mathematical model of the STS container crane boom, as a kind of the numerical experiment, simulates the trolley motion alongside the STS container boom from shore-to-ship. For obtaining the qualitative estimation of the structural parameters and the dependencies of the non-dimensional boom deflection under the moving mass on the dimensionless structural parameters, such as are stiffnesses, masses and geometric configuration, the parameter sensitivity analysis method is used. Parameter sensitivity analysis techniques also provide useful methods for the validation of the problem as suggested in [3]. Also, the parameter sensitivity analysis is used to validate the simulation model in relation to the model obtained by FEM. The variation of some dynamic parameters is done in the real diapason (not in the theoretical one) for modern constructions of large STS cranes. Hence, the investigation done in this paper is particularly important from the aspect of an engineer's viewpoint. Also, the external validation of the model and obtained results is done by the experts and experienced professional engineers (expert scrutiny) dealing with problems of large container cranes.

Conclusions. The main conclusions obtained by parameter sensitivity analysis are:

- The variation of the values of structural parameters (stiffness, geometry and mass) in the real diapason has the significant impact on the dynamic values of deflections. This conclusion can be used for making a new and more rational approach in the design of mega STS container cranes.
- Before adopting the final design solution of the STS container crane it is necessary to analyze in detail the values for stiffnesses and geometry of stays, as well as the location of the point of attachment of inner stay to the boom.
- The results obtained in this work may be used as a basic point for setting new and improved control algorithms by considering the structural flexibility of the boom.

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ROBBIT: AN OPEN SOURCE SIMULATOR FOR EDUCATION IN ROBOTICS

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Teaching of control and robotics to computer science students can take great advantage in using practical demonstrations, both in laboratory or via numerical simulations. In recent years, both the decrease of the hardware costs and the diffusion of the *open source* philosophy made accessible to most of the universities the set-up of an educational laboratory for robotics applications. Together with the teaching of basic mathematics, physic and dynamic systems theories, in order to fully appreciate a robotic class a fundamental role is played by the practical aspects of design, implementing and tuning a controller. A well designed software tool, moreover, may be of crucial importance also in allowing the studens to better understand the importance of the modeling and identification steps of the design procedure. The use of software tools may be also used to teach basic feedback control to high-level students.

In this paper a new project, named ROBBIT, is presented. ROBBIT enables the users to write their own controllers, modify the environment and, in future release, use the sensors. It is not designed to provide a real world simulation and it is kept simple, modular and extensible. In case, the user can easily add obstacles, sensors or define a new robot.

Several educational experiences are possible through the use of ROBBIT, the user can design and implement a customized control algorithm or acquire insights into the control design by, e.g., modifying the control gains of existing controllers. An unicycle-like kinematics has been implemented, car-like and Dubin kinematics will follow. Moreover, the software is written for the general case of multiple robots acting on the same environment, thus allowing also its use for more advanced concepts such as coordinated control. At an higher control level it is possible to simulate navigation or exploration algorithms for single or multiple mobile robots. Advanced control strategies, such as, behavioral or cognitive control, fuzzy logic, network control or genetic algorithms may be implemented as well.

The project's home page is provided in [2], while the SVN server in [1]. ROBBIT is released under the GNU General Public License (GPL).

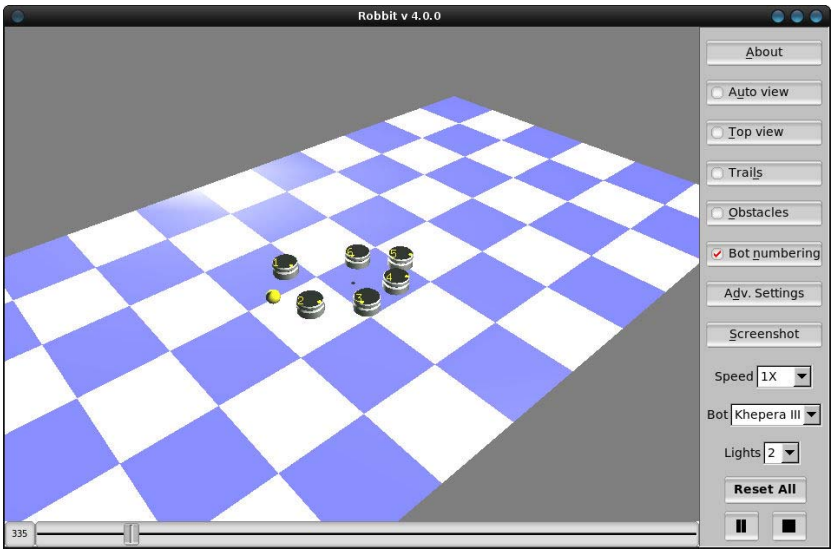

Figure 1: Snapshot of the main ROBBIT's windows simulating 6 mobile robots with a tennis ball as obstacle.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELING AND ANALYSIS OF A BICYCLE ON THE THREE-DIMENSIONAL SPACE USING THE PROJECTION METHOD

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Abstract

Our final goal of this study is to develop a bicycle riding support system. To develop the such system, because difficulties to ride bicycle are caused by its non linearity, it is important to consist of a strict nonlinear model of a bicycle. In this paper using the Projection Method and making out some appropriate constraint conditions, a way to derive a nonlinear bicycle model on the three-dimansional space is proposed. Some numerical simultions show the validity of the model.

Introduction. The automobile is one of the most familiar vehicle. But, in the recent years, the automobile has a lot of problems such as the greenhouse gases caused by automobiles, the cost of fuel up and so on. In this situation, riding a bicycle attracts attentions again as a no-emission vehicle. The bicycle also has many advantages such as keeping and increasing rider's health, relief of traffic congestion and energy efficiency. However, since the bicycle is an unstable system, a certain amount of skill is needed to perform stable riding. Especially, when the speed is low, its instability is increased. Therefore, riding support systems are needed for elderly people who can't treadle by an appropriate force at statring time, so the speed of the bicycle is low. Riding support systems are also needed for beginners for the same reason like as the elderly people. Many study on two-wheeled vehicles such as bicycles and electric motorbikes have been done[**?**][**?**]. Saguchi[1] has realized stable running on straight-line and curve motions using a model which is considered the skid of the wheels. Satou[2] has realized stabilizing a bicycle to control a handle and center of gravity(COG) by an attached cart-mass system. In these conventional studies, since only stabilizing at the upright position is considered, linear models that are linearized near the operating point is used. Especially, there is no literature using a model that is considered strict nonlinearity of the bicycle on the three-dimensional space, so it is difficult to consider stabilizing a bicycle when its speed is low. Therefore, our final goal of this study is to develop a stable bicycle riding support system using a strict nonlinear model of a bicycle.

In this paper, to consist of a strict nonlinear bicycle model, the Projection Method[3] is used. Each part of a wheel, a handle and a frame are modeled as subsystems, and these are connected by appropriate constraint forces that are not easy to derive. Validity of the model is shown using numerical simulations.

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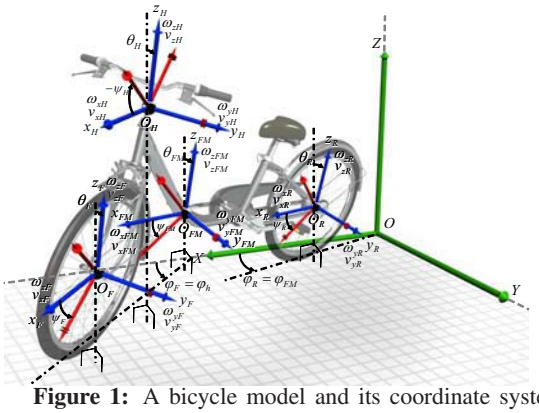

Figure 1: A bicycle model and its coordinate systems and parameters.(a)

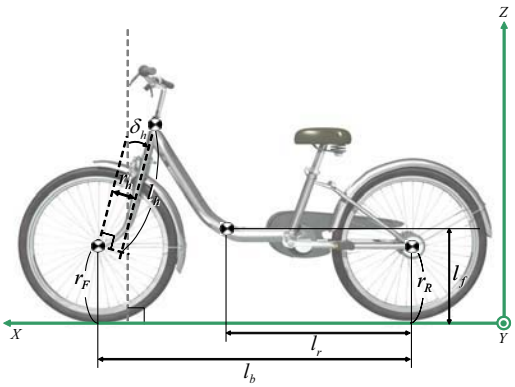

Figure 2: A bicycle model and its coordinate systems and parameters.(b)

MODELS OF COMPUTATION FOR REACTIVE CONTROL OF AUTONOMOUS MOBILE ROBOTS

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Abstract. The motivation of this paper is to develop computation models for tasks performed by autonomous mobile robots. Such models can help to analyze the functioning of the associated control algorithms and to study their stability properties [1]. Reactive control has been successfully applied to autonomous mobile robots and has enabled robotic vehicles to perform various tasks, such as parallel parking or motion with desirable speed in uncertain environments [2-4]. Reactive systems receive inputs, react to them by computing outputs and wait for the next inputs to arrive. Reactive systems correspond to finite state machines which in turn can be represented with the use of Petri nets [5]. The evolution of reactive control systems can be described using different models of computation which have as distinguishing feature the abstraction level of time. Thus, three computation models are defined: the untimed model, the synchronous model and the timed model [5].

First, the *untimed model* of computation is considered. This adopts the simplest timing approach, in which processes are modeled as state machines which are connected to each other via signals. Signals transport data values which do not carry any time information but preserve their order of emission. Values that are emitted first are assumed to be received first by the receiving process. Second the *synchronous model* of computation is considered. This can be based on partition of time either into time slots or into clock cycles [6]. The *perfectly synchronous* model assumes that no time advances during the evaluation of a process. Consequently, the results of a computation on input values are already available in the same cycle. The *clocked-synchronous* model assumes that every simulation step of a process takes one cycle. Hence the reaction of a process to an input becomes effective in the next cycle. Third, the *timed model* of computation is examined which assigns a time stamp to each value communicated between processes. This allows to model time-related issues in great detail, but it complicates the model and the task of analysis and simulation. It will be shown that the clocked-synchronous model of computation is more appropriate for describing the controller for the parallel parking task.

The structure of the paper is as follows: In Section 2 the use of finite state machines and Petri Nets in the modeling of computation processes is analyzed. In Section 3 the basic elements of the various models of computation (MoC) are presented and the untimed model of computation is explained. In Section 4 the synchronous model of computation is introduced. In Section 5 the timed model of computation is presented. In Section 6 the modeling of a parallel parking controller by a finite state machine is analyzed and the associated untimed, synchronous and timed models of computation are studied. Finally, in Section 7 concluding remarks are stated.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELING EXERCISING ON WRIST EXERCISER

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Introduction. Powerball® is commercial name of a gyroscopic device that is marketed as a wrist exercisers. The device has rotor with two unactuated DOFs and can be actuated with suitable motion of additional human or robot wrist axis. After initial rotor's spin, applying the properly torque about wrist axis lead to spin-up of the rotor. Finding this torque intuitively is easy job for most peoples, but not so easy for technical consideration for example in robotics.

The articles main contributions are dynamic models with considered friction effects. Working principles of this device in all three modes: free rotor and both modes of rotor rolling in the hous-ing are described. The work introduces reduction to 1 DOF excitation, considering preliminary re-search results, which enables laboratory control experiment. Estimation of friction parameters is also discussed. Both, the simulation with animation and experimental results are presented.

Content. In the case of rolling the model enables to compute excitation wrist torque components: first for coupling compensation , and second for the acceleration.

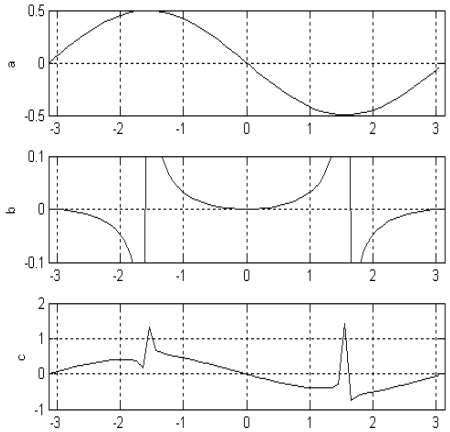

Figure. Accelerating in one rolling mode: a) torque for conditional rolling, b) torque component for acceleration, and c) resulting torque M_1.

Torque components and the resulting excitation are documented on Figure. With acceleration torque it is easy to identify the nature of Powerball® coupling. For the one DOF excitation, singular positions, and the constant acceleration the effort becomes infinite.

Developed model serves also for calculating the cinematic variables:

$$\begin{aligned} \ddot{q}_2 &= \frac{1}{J}\left(T_{2S} - h_2(q,\dot{q}) - T_{2d}\right) \\ \ddot{q}_3 &= \frac{1}{J_3}\left(T_{3S} - h_3(q,\dot{q}) - J_3\cos(q_2)\ddot{q}_1 - T_{3d}\right) \end{aligned}, \tag{1}$$

where is $\ddot{q}_1$, $\dot{q}_1$ and q_1 cinematic chain of wrist excitation for the Powerball® experiment shown in the paper.

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A LEARNING ALGORITHM FOR TIME-OPTIMAL OPEN LOOP CONTROL OF MANIPULATORS ALONG SPECIFIED PATH

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Time optimal solution has always been an interesting subject among researches working on path planning and control of manipulators. The minimum time problem of tracking specified path by a serial manipulator was extensively studied by many researchers. Bobrow et al. [1] proposed a method for time optimal motion of serial manipulators based on phase plane analysis. Considering that the solution is bang-bang, the method reduces the problem into calculating the maximum and minimum acceleration along the trajectory in each step, and to find the switching points. The problem of minimum time motion along specified path for cooperative multi manipulators (CMMS) was also studied by several researchers. Moon and Ahmad [1] employed a similar algorithm as Bobrow et al [2]. to find the time-optimal trajectory for a cooperative robot. They showed that to find the maximum and minimum values of acceleration at each point, one should solve a linear programming problem. Hasan Ghasemi and Sadigh [3] proposed a direct method for computation of critical points for parallel manipulators and presented an algorithm to construct the switching curve.

In spite of all above mentioned advancements in this area during last two decades, which made it possible to compute the maximum and minimum acceleration on line, switching points needs off line computation. This fact, which is due to computation of critical points, and backward integration for first and last switching points, prevents this method to be used as a control algorithm. So far, the method can only be used for time optimal path planning.

This paper takes advantage of the previous theoretical developments in this area and presents a learning algorithm to find switching points and near-minimum time solution online. As a result of that this method can be used as a feed forward time-optimal control law. The method can be used both for serial and parallel manipulators. Basic idea behind the method is to move the manipulator on the specified path on consequent segments of maximum acceleration, constant velocity, and maximum deceleration and to learn the manipulator to reduce and adjust the constant velocity period in each step of learning process. As the constant velocity period gets smaller and smaller, the solution converges the time optimal and two switches on the start and final time of constant velocity period converge the exact switch. Adjustment of second switch also pushes the final error to zero.

The validity of the method is checked by solving time optimal problem for two cases of a double three link planar parallel manipulator, along a straight line and then along a circular line. The results for straight line are shown in table. As can be viewed from the results, in six steps of training, the final error is less than 0.44% and the travelling time is 0.28% more than the exact minimum time. These results are very promising both in accurate tracking and in fast learning process.

step	s_{a1}^i	s_{a2}^i	ds_a^i	$\dot{s}_a^i$	ε^i	s_{b1}^i	s_{b2}^i	ds_b^i	$\dot{s}_b^i$	t^i
1	0.1058	0.3998	0.2940	5.8781	0.0050	0.5406	0.9900	0.4494	5.7351	0.2278
5	0.1168	0.3763	0.2595	6.1843	0.0050	0.7406	0.8028	0.0622	6.6891	0.2019
10	0.1328	0.4107	0.2779	6.6381	0.0050	0.7656	0.7977	0.0321	6.9572	0.196
15	0.1398	0.1767	0.0369	6.8417	0.0050	0.7856	0.7860	0.0004	7.0930	0.2013
20	0.1403	0.1792	0.0389	6.8515	0.0050	0.7856	0.7860	0.0004	7.0930	0.2011
25	0.1408	0.1817	0.0409	6.9005	0.0050	0.7856	0.7860	0.0004	7.0930	0.2009
30	0.1413	0.1842	0.0429	6.9005	0.0050	0.7856	0.7860	0.0004	7.0930	0.2007

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

INVESTIGATION OF MASS CENTER UNCERTAINTY FOR SAFE GRASPING BY A TWO FINGER HAND

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As the robotic systems improve and become more autonomous, grasping becomes more important and more attention is paid to that by researchers. Holding and manipulating delicate objects such as a glass of water, introduces the concept of safe grasping. When a robot manipulates a delicate object, it must grasp it in a stable way to prevent slipping by applying the minimum necessary grasping force to avoid object breaking or deformation. Last decade, considerable research work has been done in the area of object manipulation using tactile sensors. Two classes of problems seem to predominate in this area of research: (i) detection of object slippage (ii) real time force control of a gripper fragile object.

Some researcher worked on designing different type of tactile sensors [1]. They present appropriate models for slippage detection based on frequency response of measured contact forces. As opposed to the issue of slippage detection, the subject of force control for safe grasping shows less progress. Most of controllers used to achieve stable grasp need good knowledge of relative motion, i.e. relative velocity and relative acceleration between gripper and the object. This type of controllers face two kinds of difficulties the first is due to errors resulted from numerical derivatives needed for calculation of relative motion. The second difficulty arises from the fact that this type of controllers has no sense of excessive normal forces which might be exerted on the object by gripper, so it is not capable of reducing the normal force to its minimum necessary value. Sadigh and Ahmadi [2] proposed a control scheme based on sensing normal and friction forces, instead of relative motion. They also presented an estimation algorithm for friction coefficient.

Uncertainties in mass and mass distribution are two important uncertainties which might be encountered during grasping of unknown objects. The robustness of controller proposed in [2] in presence of mass uncertainties are investigated in that paper. In contrast to mass uncertainty, mass distribution uncertainty is difficult to investigate. For, uncertainty in mass center may cause the object to rotate with respect to gripper, so the mathematical model must account for different possible contact points and a distribution of contact and friction forces. To this end, a mathematical model is developed which assumes that contact forces are applied along a contact line between gripper and object. The method is applied to control a two-finger hand which is grasping an object with mass uncertainties. However, The results show that the controller is robust in presence of mass uncertainties. The results also reveal that two-finger hand is not a good choice for safe grasping of objects with uncertainties in center of mass, and suggests use of a third finger or multi-segment fingers to reduce applied forces.

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Circulating Fluidized Beds

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

ON MODELLING THE MIXING IN A DIGESTER FOR BIOGAS PRODUCTION

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Introduction. The technology for biogas production is not optimized and thus not fully cost-effective. To be fully commercially competitive with other types of fuels, efficiency improvements of the process is needed. One important part for possible improvement of the performance is to increase the reaction rate by optimizing the mixing and gas distribution in the digester. The fermentation process relies on a good and even mixing for distribution of microorganisms and nutrition, inoculation of fresh feed, homogenizing of the material and for the removal of end products of the metabolism [1]. In the Växtkraft biogas plant, in Västerås, Sweden, organic waste from households and restaurants is mixed and fermented with crops from graze land in a 4000 m^3 digester. Not much is known about the quality of mixing inside the digester and since it is complicated to study the mixing while it is in operation, this investigation is based on an advanced CFD study. In this study the unconfined release of biogas from the bottom is simulated to give a better understanding of the digester and the process as a whole. Some work has already been done in this area but for other types of gas driven mixing that can give useful insights in the problems that this type of mixing still exhibits [2].

Simulation. The geometry of the digester is axisymmetric with a height of 19.5 m and a radius of 8.5 m. The gas injection is simplified to two inlet rings at the bottom so that a high quality mesh could be produced. As part of the liquid recirculation system a liquid outlet is placed on the bottom next to the centerline axis and the liquid is then reintroduced with an inlet through the side wall close to the bottom. A gas outlet is also placed above the liquid free surface. The numerical calculation was made using the volume of fluid (VOF) model which allows us to predict all the flow local and global quantities including a detailed description of the liquid free surface deformation.

Results. To study the mixing dynamics of the Växtkraft biogas plant five different rates of gas (air) recirculation were simulated with a gas velocity of 0.6, 0.48, 0.36, 0.24 and 0.12 m/s. The lowest gas flow rate is the closest one to the actual set up at the biogas plant and this gas flow rate is also simulated in combination with the liquid circulation to see what effect it has on the overall mixing. Gas flow rate and liquid recirculation impact are studied and commented.

Simulation	Gas flow rate	% of max flow rate	liquid circulation	Mean Liquid velocity	Mean Liquid Turbulent kinetic Energy
1	0.6	100	off	0,22	0,064
2	0.48	80	off	0,18	0,056
3	0.36	60	off	0,16	0,036
4	0.24	40	off	0,13	0,029
5	0.12	20	off	0,10	0,015
6	0.12	20	on	0,09	0,014

Table. Setup and results of the simulations using different gas flow rates and an evaluation of the liquid circulation.

Conclusions. Our simulation results suggest that the positioning of the liquid outlet is not optimal for the gas-lift mixing configuration and that energy savings and better mixing can be accomplished by finding a new position for the outlet. The zones with lower circulation are not significantly influenced by fine tuning the gas flow because the volume of the digester is so large compared to the narrow rising bubbly liquid stream. It seams that a complete review of the digester design is necessary to be able to improve seriously the process and probably reduce the energy consumption. Experimental work to validate these results is crucial for further investigations of the digester at the Växtkraft biogas plant.

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FLUIDIZED BED COMBUSTION AND GASIFICATION MODELING AND UTILIZATION OF THE MODELS FOR DIAGNOSTICS, CONTROL AND DECISION SUPPORT

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Abstract: In both gasification and combustion in fluidized beds it is important to keep control over the actual process, to avoid sintering or blow out of bed material in the actual bed, or in the down comer G-valve. It is also important to keep control over the sensors. If the sensors are faulty, you may make the wrong control actions that may cause severe problems or just poor performance generally, where you will be on the boarder of what is acceptable with respect to economy and environmental emissions.

Malardalen University has been working together with power plants like Malarenergy in Vasteras and Eskilstuna Energy and Environment in Eskilstuna and vendors like ABB to develop models for both CFB and BFB for combustion, as well as gasification. Malarenergy has a CFB for biomass combustion, 170 MW, and Eskilstuna Energy and Environment a BFB for biomass combustion, 95 MW. ABB developed a Black liquor gasification process using CFB. All these processes have many common functions and thus we have tried to model them using a program Modelica, and then use this program for process performance monitoring, diagnostics and model based control.

The mathematical models include the energy and mass balances for all relevant components. The dynamics is introduced primarily as change of temperature and chemical composition in a number of inventories. For the actual main fluid bed we have one, a second for the G-valve fluid bed and a third one for the steam system.

On line data then is collected from all the sensors in the fluidized bed and the surrounding systems. These are introduced as initial conditions to the model, which then makes a simulation to a balanced solution is reached, using the simultaneous solver of the Modelica model. The balanced values are compared to the original measured values and the difference between these is then plotted as a function of time for each variable.

By this we can see how difference of temperature measurements, gas composition, pressures and flows may be jumping up and down around an average values, or start to deviate upwards or downwards. When the deviation is above a certain level a message is sent to the operators, that something may be wrong. This information together with other data is fed to a Bayesian Net, giving probabilities for different type of faults. In this way we get a diagnostics and decision support system that can be used also for maintenance on demand. Tendencies for sintering in the fluidized bed, risk for irreversible fouling and other important process functions as well as sensor condition are included.

Key words: Simulation, modeling, boiler, digester, MPC, control, diagnostic

MODELING OF PROCESS STATES BY USING ARTIFICIAL NEURAL NETWORKS IN A FLUIDIZED BED ENERGY PLANT

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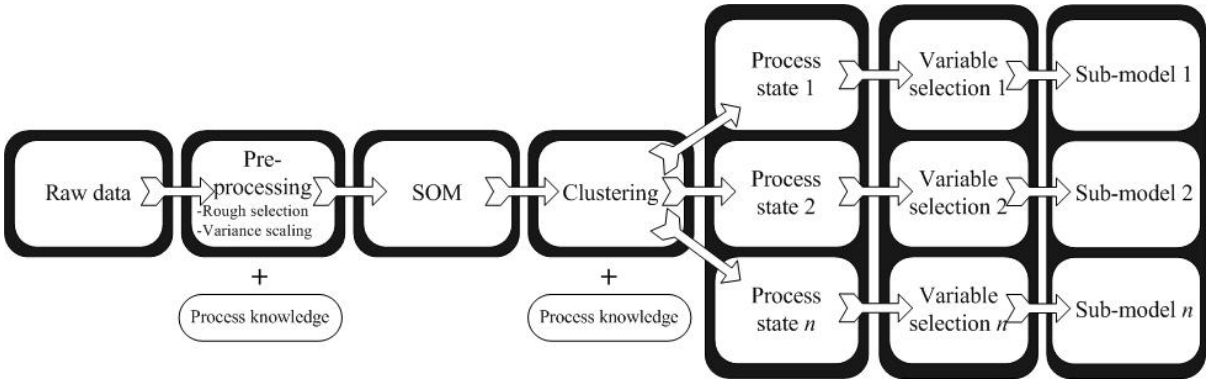
Introduction. The efficiency of energy plants is becoming a more important issue because of tightening environmental regulations and increasing fuel costs. One of the main future issues is to minimize the process emissions, including harmful emission components such as nitrogen oxides (NO_x). Despite the growing environmental issues, the production must be capable of reacting fast to changes in the boiler load and to variations in the fuel quality, which necessitates a faster and more accurate operational control of the process. Due to this, such advanced and intelligent systems for process monitoring and optimization are needed that can respond to these new dynamic demands.

Process and data. Fluidized bed combustion is a common energy production technology designed mainly for the combustion of solid fuels such as coal. The main parts of a typical circulating fluidized bed (CFB) boiler include a combustion chamber, a separator and a return leg for the recirculation of the bed particles. The combustion occurs in a zone that is fluidized by the primary combustion air brought in from the bottom of the chamber. The size of the data matrix used in this study is 10 000 x 42 (10 000 rows, 42 variables in columns).

Methods. The formation of NO_x in a circulating fluidized bed (CFB) boiler was modeled by using a sub-model -based artificial neural network (ANN) approach, whose stages are represented in the figure below. After appropriate pre-processing, the process data are processed by using a self-organizing map (SOM) [1] and k-means [2] clustering to create subsets representing the separate process states in the boiler. Expert process knowledge can be combined with the cluster information to identify these states. The process states can include for example start-ups, shutdowns, and idle times in addition to the normal process flow. After the determination of process states, a variable selection procedure based on multilayer perceptrons (MLP) [3] is performed to create sub-models and to determine whether different variables are affecting the NO_x formation in the defined process states. Eventually this data analysis procedure produces process state -specific sub-models that can be used to simulate the NO_x content of the flue gas.



The method in a nutshell

Conclusions. The results show that this kind of approach can be a fruitful way to get new information from combustion processes. The created sub-models proved to be 2–3 % more accurate than the generic process model including all the process data. This suggests that dividing the overall process model into separate process state -specific models clearly improves the model goodness. Additionally, the ability of the method to reveal nonlinear and multivariate interactions brings additional value to the models. For these reasons, the presented data analysis method offers a fruitful option to identify the different process states and their corresponding sub-models.

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FLUIDIZED BED COMBUSTION AND GASIFICATION MODELING AND UTILIZATION OF THE MODELS FOR DIAGNOSTICS, CONTROL AND DECISION SUPPORT

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Abstract: In both gasification and combustion in fluidized beds it is important to keep control over the actual process, to avoid sintering or blow out of bed material in the actual bed, or in the down comer G-valve. It is also important to keep control over the sensors. If the sensors are faulty, you may make the wrong control actions that may cause severe problems or just poor performance generally, where you will be on the boarder of what is acceptable with respect to economy and environmental emissions.

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By this we can see how difference of temperature measurements, gas composition, pressures and flows may be jumping up and down around an average values, or start to deviate upwards or downwards. When the deviation is above a certain level a message is sent to the operators, that something may be wrong. This information together with other data is fed to a Bayesian Net, giving probabilities for different type of faults. In this way we get a diagnostics and decision support system that can be used also for maintenance on demand. Tendencies for sintering in the fluidized bed, risk for irreversible fouling and other important process functions as well as sensor condition are included.

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Control of Dynamical Systems

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

COMBINED CONTROL FOR COMPUTATIONALLY EFFICIENT ACTIVE NOISE REDUCTION IN AVIATION HEADSETS

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Abstract

In commercial aviation ANR-headsets (Active Noise Reduction), the simple and computationally efficient non-adaptive feedback control approach is commonly used. However, this strategy causes a limited active attenuation performance. Especially in case of aircraft noise with narrowband dominant frequencies, it is favorable to attenuate these dominants more effectively. The reduction of the dominant frequency results in an enhanced hearing protection as well as in improved speech intelligibility of the communication signal.

In this paper, a computationally efficient control approach, which permits the reduction of low frequency noise with a single dominant frequency, is presented. In the framework of the proposed control strategy, the combination of a non-adaptive feedback controller and an adaptive narrowband feedforward controller is suggested. While the non-adaptive feedback controller permits the reduction of the broadband low frequency noise, the dominant frequency is further reduced by the adaptive narrowband feedforward controller. The performance of the proposed control strategy is discussed and concluding remarks are given.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

PERIODICAL OSCILLATIONS OF CONTROL SYSTEMS. ANALYTICAL AND NUMERICAL APPROACH.

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The method of harmonic linearization, Lyapunov quantities, numerical methods, and the applied bifurcation theory together discover new opportunities for analysis of periodic oscillations of control systems. In the present work these opportunities are demonstrated. Here the quadratic system is reduced to the Lienard equation and by the latter the two-dimensional domain of parameters, corresponding the existence of four limit cycles: three "small" and one "large", was evaluated. This criterion together with numerical estimates of oscillations amplitude give an estimate of occurrence of chaotic oscillations in the Henon system. In the work it is also considered the Feigenbaum effect for nonunimodal maps which describe discrete phase-locked loops.

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TIME-OPTIMAL SWING-UP AND DAMPING FEEDBACK CONTROLS OF A NONLINEAR PENDULUM

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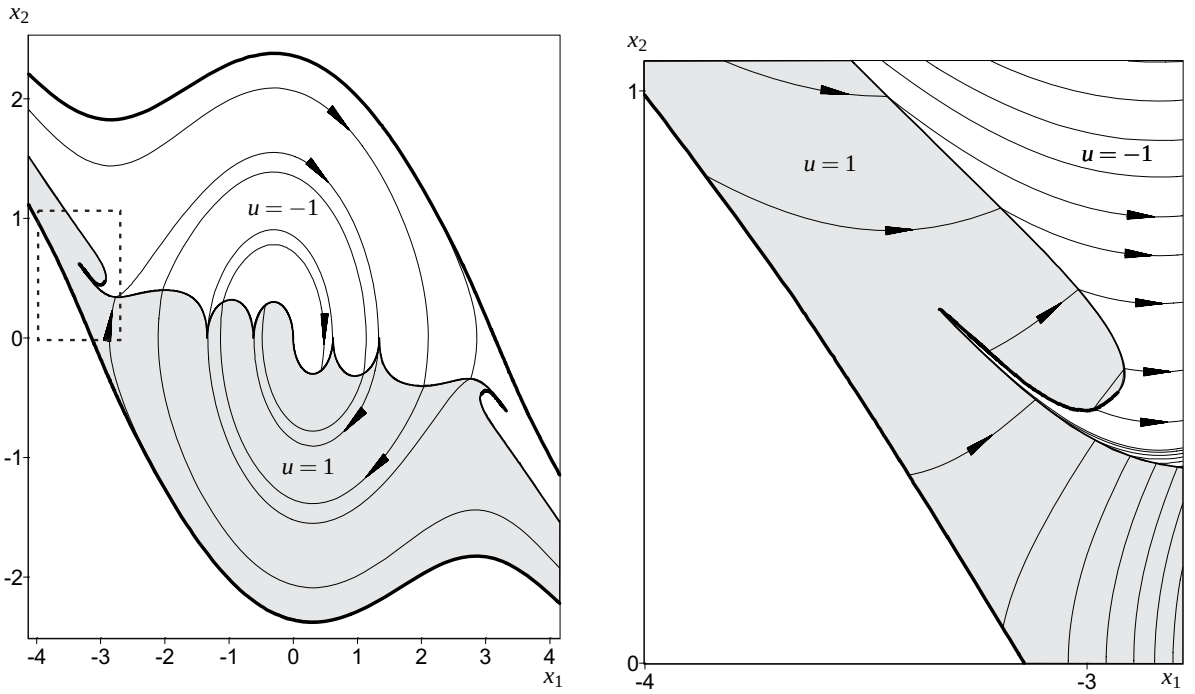
A pendulum is a well-know example of a nonlinear mechanical system that is often regarded as a benchmark for control algorithms. In a number of papers, various feedback controls have been proposed that bring the pendulum to the upper unstable or lower stable equilibrium position. These controls are called swing-up and damping controls, respectively. Time-optimal controls have been also considered, but the solutions obtained were not complete.

In this paper, the time-optimal feedback controls both for the swing-up and damping control problems are obtained. The solution is based on the maximum principle and involves analytical investigations and extensive numerical computation for a wide range of parameters. As a result, the switching and dispersal curves are obtained that bound the domains in the phase plane corresponding to different values of the optimal bang-bang control.

Optimal trajectories can intersect the switching curves but not the dispersal curves. The latter curves have the following property: two different optimal trajectories start from each point of the dispersal curve.

The switching and dispersal curves are obtained for various values of the maximal admissible control torque. These curves completely determine the feedback optimal control.

Fine details of the structure of these curves as well as of the field of optimal trajectories are analyzed. The structure depends essentially on the magnitude of the control torque. In particular, numerical results show how the breaks of the switching curves (in the case of the damping control) are formed at the transition from high torques where these curves are smooth to low torques corresponding to the switching curves with breaks.



The switching curve with breaks (in the case of the damping control).

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

STATE ESTIMATION IN CONTROL PROBLEMS UNDER UNCERTAINTY AND NONLINEARITY

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The paper is devoted to state estimation problems [1, 2, 3, 4] for nonlinear uncertain dynamic systems with system states being compact sets. The topics of this paper come from the control theory for systems with unknown but bounded uncertainties related to the case of set-membership description of uncertainty. The motivations for these studies derive from applied areas ranged from engineering problems in physics to economics as well as to ecological modelling. The paper presents recent results in the theory of tubes of solutions (trajectory tubes) to differential control systems with uncertain parameters or functions.

The paper deals with the problems of control and state estimation for a dynamical control system

$$\dot{x}(t) = A(t)x(t) + f(x(t)) + G(t)u(t)\,,\ x \in R^n\,,\ t_0 \le t \le T\,, \tag{1}$$

with unknown but bounded initial condition

$$x(t_0) = x_0\,,\ x_0 \in X_0\,,\ X_0 \subset R^n\,, \tag{2}$$

and with control constraints

$$u(\cdot) \in U = \{u(\cdot) : u(t) \in U_0\,,\ t \in [t_0\,,T]\}\,,\ U_0 \subset R^m\,. \tag{3}$$

Here matrices $A(t)$ and $G(t)$ (of dimensions $n \times n$ and $n \times m$, respectively) are assumed to be continuous on $[t_0\,,T]$, X_0 and U_0 are compact and convex sets in related finite-dimensional spaces. The nonlinear n-vector function $f(x)$ in (1) is assumed to be of quadratic type

$$f(x) = (f_1(x)\,,\ldots,f_n(x))\,,\ f_i(x) = x'B_ix\,,\ i = 1\,,\ldots,n\,, \tag{4}$$

where B_i is a constant $n \times n$ - matrix ($i = 1\,,\ldots,n$).

Let absolutely continuous function $x(t) = x(t\,,u(\cdot)\,,t_0\,,x_0)$ be a solution to (1) with initial state x_0 satisfying (2) and with control function $u(t)$ satisfying (3). The differential system (1)–(3) is studied here in the framework of the theory of uncertain dynamical systems (differential inclusions) through the techniques of trajectory tubes [4]

$$X(\cdot) = \bigcup\{\, x(\cdot) = x(\cdot\,,u(\cdot)\,,t_0\,,x_0) \mid x_0 \in X_0\,,\ u(\cdot) \in U\ \} \tag{5}$$

combining all solutions $x(\cdot\,,u(\cdot)\,,t_0\,,x_0)$ to (1)- (3).

The main problem consists here in describing and estimating the trajectory tube $X(\cdot)$ of the nonlinear system (1)-(3). The point of special interest is to find the t – cross-section $X(t)$ of this map which is actually the attainability domain (reachable set) of the system (1)–(3) at the instant t. It should be noted however that the exact description of reachable sets of control systems is a difficult problem even in the case of linear dynamics and ideas of construction outer and inner set-valued estimates of reachable sets were proposed and developed in [1, 2] for linear control systems.

In this paper the modified state estimation approaches which use the special structure of nonlinearity of studied control system (1)–(4) and advantages of ellipsoidal calculus [1, 2] are presented. We develop here new ellipsoidal techniques related to construction of external and internal estimates of reachable sets and trajectory tubes of the nonlinear system. Some estimation algorithms basing on combination of discrete-time versions of evolution funnel equations and ellipsoidal calculus [1, 2] are given. Examples and numerical results related to procedures of set-valued approximations of trajectory tubes and reachable sets are also presented [3]. The applications of the problems studied in this paper are in guaranteed state estimation for nonlinear systems with unknown but bounded errors and in nonlinear control theory.

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OPTIMAL CONTROL FOR GAS-LIFT WELL

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Summary. Natural oil flowing conditions finishes when energy of oil reservoir is insufficient to a lifting of oil to the ground surface. Since this moment it is required submissions of additional energy from a surface of the ground for a lifting of a liquid. Thus it is spoken about the mechanized methods of oil exploration, one of which is gas-lift.
The gas-lift is one of the most mechanized methods of oil well operations and high profitability. For gas-lift operation of wells at an optimal conditions in practice are guided by well flow rate (production) curves from the injected gas flow rate and the working agent specific flow rate from the injected gas flow rate. Thus it is considered to be an optimal mode the one which is characterized by the minimal value of the specific gas flow rate *(R)* or coordinate of a point *"A"* where the tangent through the beginnings of coordinate system adjoins to curve *Q=f (V)*. The point *"A"* corresponds to the maximal efficiency of gas injection work in a well of gas, though thus flow rate *(Q)* is not maximal. In practice it is accepted to maintain wells in conditions, which belong to piece *AB* on curve *Q (V)*.
The process of optimal control of the gas-lift well is examined and has been solved in this work.

Introduction. The authors are based on the models of gas lift process that they have got with due regard for real processes in pump-compressor tubes and the reservoir (i.e. changes of physical parameters and reological features of reservoir-collector and filtering fluids of the reservoir pressure) and also the influence of the neighboring wells. The last means that the problem consists of two interrelated processes – the process of gas movement, gas oil mixture in pump-compressor tubes and filtering (flowing) processes in the reservoir (its permeability and porosity depend on importance of reservoir pressure). And flow of oil and gas to bottom-hole zone depends on it.

Gas injection and movement of gas-liquid mixture in lifting tubes may be described by the next system of equations [1].

$$-\frac{\partial P}{\partial x}=\frac{1}{F}\frac{\partial Q}{\partial t}+\frac{2a}{F}Q, \tag{1}$$

$$-\frac{\partial P}{\partial t}=\frac{c^2}{F}\frac{\partial Q}{\partial x}, \tag{2}$$

where $Q=F\rho w$, F - area of horizontal section of pump-compressor tubes and is permanent on the axis x, P- is a pressure, t, x- time and coordination, ρ ,Q – density and volume flow rate of gas, oil and gas-liquid mixture depending on the coordinate; $2a=\frac{g}{w_c}+\frac{\lambda_c w_c}{2D}$. Movement of oil in this case is depicted in the next equations.

$$\frac{1}{r}\frac{\partial}{\partial r}\left\{r\left[\frac{p\beta\gamma_г f_г(1-\rho_н)}{Z(p)p_{am}\mu_г(p)}+\frac{S(p)f_н(\rho_н)}{a(p)\mu_н(p)}\right]k(p)\frac{\partial p}{\partial r}\right\}=-\frac{\partial}{\partial t}\left\{\left[\frac{p\beta\gamma_г(1-\rho_н)}{Z(p)p_{am}}+\frac{S(p)}{a(p)}\rho_н\right]m(p)\right\} \tag{3}$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left\{r\left[\frac{f_н(\rho_н)}{a(p)\mu_н(p)}\right]k(p)\frac{\partial p}{\partial r}\right\}=-\frac{\partial}{\partial t}\left\{\left[\frac{\rho_н}{a(p)}\right]m(p)\right\}, \tag{4}$$

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

THE CONTROL OF LINEAR SYSTEMS UNDER FEEDBACK DELAYS[1]

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The problems of measurement feedback control are at the heart of control theory [2, 6, 3, 1]. These problems were mostly treated in a stochastic setting. In this paper we consider problems of feedback control under delayed measurement output feedback and set-membership noise. The delays considered here may be due to errors in communication channels as well as to the processing time in the observers and controllers.

The suggested solutions are based on a combination of Hamiltonian techniques with methods of set-valued analysis. They rely on ellipsoidal approximations of information and solvability sets which describe the solution strategies [4]. These approaches allow to solve problems of realistically high dimensions. Their practical implementation may be based on the Ellipsoidal Toolbox [5].

We first consider the situation with feedback noise but no delay. This problem is dealt with by reduction to one in the metric space of information sets. The key point is that the problem further reduces to a standard one in finite-dimensional space.

After that we consider bounded noise in the delayed output measurement. A control strategy for the related problem of control is indicated. (Everything is exact.)

We finally present the results of numerical modelling for oscillating systems (of dimension up to 20). We show the realized control inputs, and how the quality of solution depends on delay time.

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MODELING AND NONLINEAR CONTROL OF MAGNETIC LEVITATION SYSTEMS WITH HYSTERESIS

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Abstract. Magnetic levitation systems are nonlinear and hysteretic systems which have many application area such as high speed trains, frictionless bearing and vibration isolation system. Control problem of these systems is very important since magnetic levitation systems are nonlinear and open-loop unstable. In the literature, most of controllers have been designed for linearized model around an operating point. In this case, deviating from operating point can cause deterioration of system behavior. Therefore, it is necessary to design nonlinear controller for a large domain of stability. Besides, the losing of energy due to hysteretic feature of the system, such as the heating of electromagnet or the change of inductance should be considered. Feedback linearization is commonly used method to developed nonlinear controller for magnetic levitation systems, see [1, 2]. However, these works ignored hysteresis effects in magnetic levitation systems. So far, very little work has been published that controls magnetic levitation system with effecting of hysteresis feature. For example, magnetic levitation system has been modeled with Preisach model of hysteresis and the inverse of hysteresis has been applied to the system for its compensation in [3]. Moreover, magnetic levitation system has been modeled with input backlash, and the smooth adaptive inverse of backlash has been applied to controller design with backstepping approach in [4].

In this work, a magnetic levitation system is modeled with its hysteresis characteristic and a nonlinear controller is developed by using feedback linearization method. Hysteresis nonlinearity of the system is modeled with Duhem model which is very efficient to model electromagnetic hysteresis, see [5, 6]. An equivalent linear system is obtained by nonlinear controller, and the linear system is stabilized with pole placement.

In magnetic levitation system, a ferromagnetic object is suspended in space by a magnetic force which is produced by an electromagnet. Mathematical model of magnetic levitation system is given with

$$u(t) = \frac{R}{N}H(t) + \frac{L}{N}\frac{dH(t)}{dt}, \text{ and } \frac{d^2y(t)}{dt^2} = \frac{K}{m}\frac{B^2}{y^2} - g,\ B = \Phi(H),$$

where u is the controlled voltage applied to the electromagnet, y is output of the system which is distance value between the ball and the electromagnet, Φ is hysteresis nonlinearity between magnetic field H and magnetic induction B, and R,L,N,K and m are constants. Using $x_1 = H$, $x_2 = y$ and $x_3 = \dot{y}$ the system can be represented by

$$\dot{x} = f(x) + g(x)u,\ y = h(x),$$

where $x = (x_1, x_2, x_3)^T$. For feedback linearization, f,g and h functions have to be smooth. But, the function f is nonsmooth at some points where Duhem hysteresis is non-differentiable at $\dot{H} = 0$, see [6]. Using Lipschitz continuity of Duhem hysteresis, we give following definition as

$$\frac{d\Phi(x_1)}{dx_1} = \begin{cases} \frac{d\Phi(x_1)}{dx_1}, & for\ \frac{dx_1}{dt} \neq 0, \\ \lambda, & for\ \frac{dx_1}{dt} = 0, \end{cases}$$

where λ is Lipschitz constant. Thus, a nonlinear controller is developed with feedback linearization method. The obtained linearized model is stabilized with pole placement. Consequently, simulation results show that the system with hysteresis nonlinearity tracks the desired reference input either sinusoidal or fixed.

Acknowledgment. This work has been supported by TUBITAK with Project No: 105T446.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELING AND VARIATIONAL ANALYSIS OF CONTROL PROBLEMS FOR ELASTIC BODY MOTIONS

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Introduction. Elastic properties of structure elements can essentially affect the dynamical behavior of the whole system. Some parts of mechanical structures with distributed parameters are modeled as elastic bodies with given stiffness and inertia characteristics. Modeling problems for controlled motions of an elastic body is considered. A variational principle, in which displacement and stress fields are varied, is proposed based on the method of integrodifferential relations and the linear theory of elasticity [1]–[7]. A regular numerical algorithm of constrained minimization for the initial-boundary value problem is worked out. The algorithm allows us to estimate explicitly the local and integral quality of numerical solutions obtained.

Content. We consider an elastic body occupying a bounded domain with an external piecewise smooth boundary. Taking into account the assumption of the linear theory of elasticity about smallness of elastic deformations and relative velocities the controlled motions of the body can be described by a system of partial differential equations. In the presented work the statement of the dynamic linear elasticity problem is discussed. The method of integrodifferential relations and a new variational formulation of the initial boundary problem in displacements and stresses are presented. The stationary conditions equivalent to the constitutive relations are obtained. A numerical algorithm used finite approximations of unknown functions (displacements and stresses) is developed [2] and the effective integral and local bilateral estimates of solution quality are obtained relying on the extremal properties of the finite dimensional variational problem. An example is devoted to numerical modeling, optimization, and analysis of controlled motions of a 3D elastic beam.

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LIMITING PERFORMANCE ANALYSIS OF SHOCK ISOLATION FOR A NON-RIGID OBJECT

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Limiting performance analysis is performed for shock isolation of an object that is modeled by two rigid bodies connected by a viscoelastic element with a linear characteristic. The object is attached to a movable base by means of a shock isolator. A shock isolator is a medium or a structure that generates a control force between the base and the object. The base and the object are assumed to move along the same straight line. The base is subjected to an external shock disturbance characterized by the time history of the acceleration of the base. A control law for the shock isolator is chosen so as to minimize the maximum magnitude of the displacement of the object relative to the base, provided that the magnitude of the force of interaction between the object's components does not exceed a prescribed value. An algorithm for solving this problem is given. It is shown that the optimal control has impulse components. Examples of calculation of the minimum peak magnitude of the object's relative displacements are given for some typical shock disturbances. Applications of two-component models similar to that considered in the paper to describe the mechanical reaction of the human body to shock compressive loads of the spine [1, 2] or the thorax [3] have been reported. Therefore, the problem under consideration can serve as a benchmark problem of optimal control of a shock isolation system for injury prevention. Solution of such problems is highly topical for the design of effective safety systems in vehicles.

The limiting performance analysis is a technique for evaluating the absolute minimum of a performance index that characterizes the level of protection of objects from shock loads. The absolute minimum corresponds to a theoretically perfect shock isolator. The limiting performance analysis involves the solution of an optimal control problem but does not take into account the design configuration and hardware implementation of a specific shock isolator. For details, see [4, 5].

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Traffic and Transportation Systems, Guidance

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELING AND SIMULATION - A LANE KEEPING ASSIST STUDY

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Vehicle routes that are marked by long and monotonous driving situations lead to decreasing attention of the driver. Nearly 14 % of all sole accidents with injured persons go back to driving situations where the vehicle leaves the lane. Driver assistance systems and especially the lane keeping assist task can help in reducing these accidents by a correcting steering intervention. This correcting steering intervention is executed for example by an electric motor that is mounted at the steering column of the vehicle. The electric motor executes an overlay torque that can be introduced to the driver as a trapezoid overlay torque or as a continuous operating lane guidance controller.

In this contribution the mathematical modeling for the lane keeping assist task is derived. The modeling contains the vehicle, the steering system and the situation model for the driver interaction. The external rack force couples the vehicle model and the steering model. In a simulation study two control approaches for the lane keeping assist task are compared and specific driving manoeuvres on specific road tracks show the working method of each approach.

For the lane keeping assist task the vehicle and the steering system are modeled. The vehicle is modeled as a bicycle model, known from e.g. [1,2], which is sufficient for a lane keeping assist task (see figure 1). The steering system of the car is modeled in this paper by an electro-hydraulic power assist rack and pinion steering gear. The first lane keeping assist approach computes the electric motor torque in a lookup table in dependence on the lateral position error [3]. The second approach makes use of a lane guidance controller similar to the one in [2].

In the simulation study the trapezoid overlay torque approach shows that the vehicle is pushed back to the road centre line adequately if the lane boundary is reached. The lane guidance controller approach is capable to deal without a lateral position error deadband and to deal with higher bend radii.

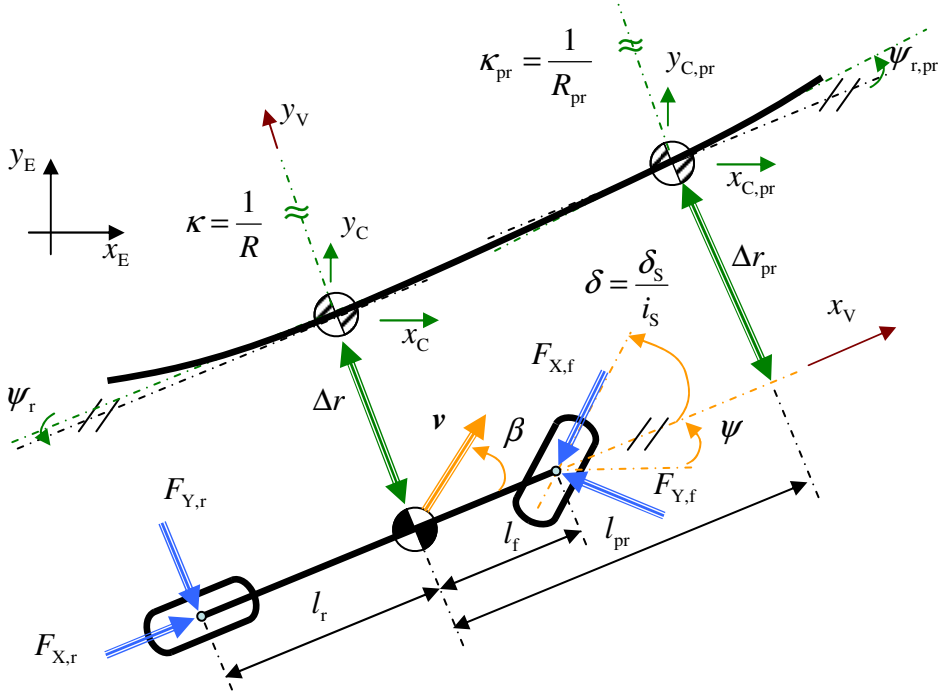

Figure 1. Modeling the vehicle dynamics and the vehicle motion relative to the reference road trajectory.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELLING AND SIMULATION OF INTERACTION IN DRIVER/VEHICLE DYNAMICS

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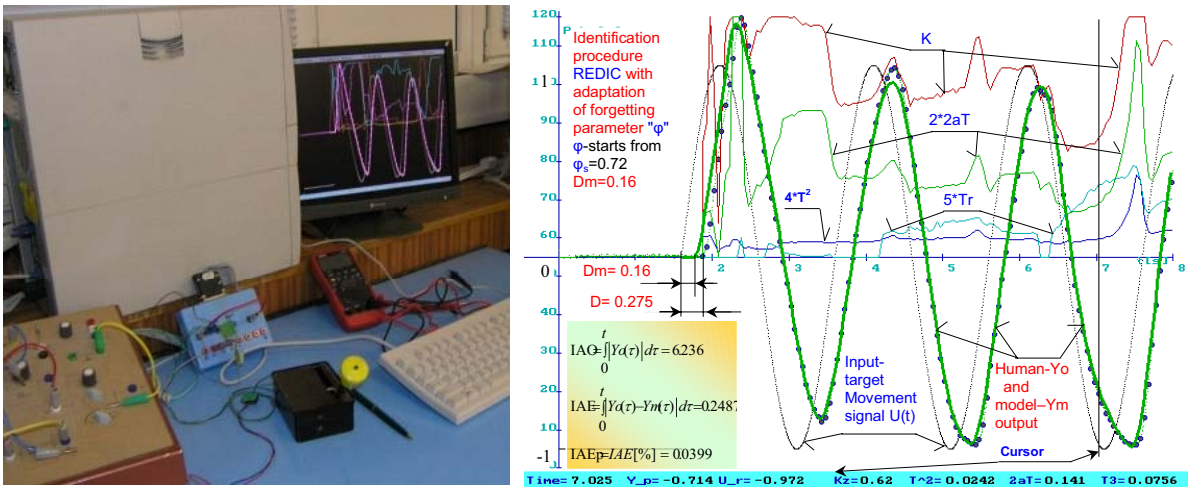
Future requirements of vehicle control dynamics especially cars, requires to consider ability of driver systematically. This research is needed in recent information and automation technologies, which have the potential to change vehicle control towards a new quality that shall be called "decision making in human/vehicle system". This paper describes conceptual model for driver's behaviour, control levels in the intelligent control system driver/vehicle/traffic situation and conceptual simulator model for generation and measuring of dynamics in this system. To study this, mathematical (cybernetic) and simulation models which represent (in the first research steps) dynamics between driver's eye-hand/legs will be needed. In the paper there is detailed description of experiments for obtaining operator's/driver's responses (eye/hand, eye/leg channels) and also identification procedures for obtaining parameters in their models. Particular results of simulation experiments, which have been made with linear models (constant and changeable parameters), are finally given at the end of the paper. Simulation experiments made until now show that key parameter which described operator dynamics behaviour acts as their "dead time," or "delay". It was supposed as constant in simulation experiment but in real driver behaviour it varies in large scale and fundamentally represents driver dynamics. Also experiment with changeable dead time in the channel eye-leg was made, but research of more accurate drivers models needs to continue. On the next figure left, is photo from laboratory environment for measurement of the driver responses. On the figure right is comparison of model - driver performance by model with varying parameters, when driver follows sinusoidal target movement.



Laboratory environment for measurement of the driver responses and simulation experiments with varying parameters.

Models with varying parameters are able to characterise operator's behaviour better but the wide range of the model parameter changes is a sort of disadvantage. For better study of driver/vehicle interaction especially in the unavoidable (emergency) situations it is needed taking into consideration not only drivers "dead time" but also all drivers' time constants. This is reason to solve problems with measurement and identification of variable delays and time constant in driver dynamics.

In further research it is needed to focus on identification methods applicable for varying dead time and on realisation of context and structure oriented level of behaviour in human/vehicle interaction. Using parallel computation methods for continuous identification of varying parameters and varying dead time, it will be possible to carry out also on-line identification of operator behaviour. One example of this method is documented in this paper. Exact, certain and clear models for eye-hand, eye-leg channels are basic predisposition for building qualitative models of operators' decision making in particular situation, planning of future activities and impact of instant actions on development of future situations.

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INTRODUCING SOFTWARE COMPONENTS TO ROAD TRAFFIC MODELING AND SIMULATION

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Introduction to Road Traffic Modeling. Modeling and simulation of road traffic has gained in popularity in recent years. This is not surprising, because it constitutes the only tool available so far for predicting behavior of a traffic system. Using traffic models, it is possible, for example, to evaluate the impact of the traffic restrictions related to a road work (whether construction or maintenance) and to determine which combinations of road works can be performed simultaneously without causing unnecessary congestion, or to compare the performance of several different road design alternatives. In connection with the recent onset of intelligent traffic management and information systems, traffic models can also be used to test these systems during their development in a real-like environment.

Basically, there are two different approaches to road traffic modeling. The first one, called macroscopic, is based on physical theories of fluid dynamics and describes the traffic by differential or difference equations using physical quantities such as traffic flow and traffic density. Macroscopic models are not suitable for simulating every problem and their results often lack precision once the simulated traffic system gets congested. The second approach, called microscopic, describes the behavior of the individual traffic participants (cars, trucks, streetcars, and so on) by a combination of difference equations and decision trees, using quantities such as acceleration and speed. The capabilities of microscopic models are almost unlimited, but their computational complexity (both in terms of time and space) can be enormous.

Software Components. Software components are extensions to objects or modules in an effort to achieve a higher level of reusability. They differ from objects or modules by so-called contractually specified interfaces, that is, by explicit definition of any functionality they provide as well as any functionality they require from other components. Most often, Meyer's Design by Contract is used. These contractually specified interfaces have an interesting implication: any two components implementing the same contract can be substituted one for the other. In other words, replacing one of them with the other does not require any changes in the rest of the software. Components thus make the functionality of the software much more flexible and adaptable to changes.

Components in Road Traffic Models and Their Advantages. Every traffic system can be decomposed into two different aspects: its topology (the layout of road segments and intersections) and its behavior (the way in which the state of the system is changed). These two aspect can be modeled each by a separate set of components. Structural components constituting the road topology and behavioral components constituting the behavior can then make use of the above-mentioned component substitutability. This way, is is possible to test and compare different road design alternatives or to easily adjust the road traffic model to the simulated conditions (such as a different traffic law). Especially the changes in behavior is otherwise difficult to achieve in most of the existing road traffic modeling and simulation tools.

However, even two components that do not implement the same contract can be substituted one for the other if that there is an adapter able to overcome the differences between their contracts. An adapter in this sense is actually an intermediate component that implements both contracts and provides a logic to translate from one to the other. Adapters can be used to implement hybrid road traffic models, that is, models capable of switching between the microscopic and the macroscopic level of details. This way, it is possible to simulate the area of interest using a microscopic model, while the rest of the traffic system can be simulated using a macroscopic model in order to reduce the computational intensity of the overall simulation. But, even if the areas out of interest are simulated using a macroscopic model, the overall computational intensity may still be too high for a single computer. In such situations, a distributed computing environment may be necessary to get the simulation results in a reasonable time. But this also means that the simulation model needs to be adapted for a distributed environment (in particular, divided into several parts). This time, component-based approach in connection with remoting adapters may help. The model can be divided between any two structural components, where an remoting adapter can be placed in order to make the remote communication completely transparent.

Summary. Using component-based approach, it is possible to develop a single multi-adjustable road traffic model suitable for simulating an almost unlimited spectrum of problems.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Agent-based and Alternative Modelling Techniques

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

INTERPERSONAL TRUST MODEL

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Introduction. Trust is a unique phenomenon and its acceptance is wide; from honesty, truthfulness, confident expectation or hope, something managed for the benefit of another, confidence of ability or intention to pay for goods or services in the future, till business credit. We will understand trust as a given credit, hope, confidence in ability or intention of some subject to perform to benefit of other subject at some future time.

Trust plays an important role in the relationships among subjects in the communities. These subjects need not be only humans. Trust among the machines, servers, and network nodes gains more and more on importance. Trust models, and interpersonal trust models particularly, e.g. [1], [2], [3], [4] are usually focused on merely one of the factors which trust determine. Each of these factors (reputation, recommendations, and initial trust) can be modelled as an individual component. Our model tries to integrate more of trust affecting factors, i.e. initial trust, reputation, recommendations, realized contacts, and trusting disposition for trust determination.

Trust Representation. Generally, trust can be quantified by a value from the interval $\langle a, b\rangle$, where a, b ($a<b$) are integer or real numbers. Value a represents complete distrust and value b is blind trust. Other verbal trust levels are possible to be represented by values from this interval. Without loss of generality, we will use real values from the interval $\langle 0, 1\rangle$. Next, we specify an interpersonal trust representation, i.e. trust between two subjects. Consider a group of n subjects represented as the set $X = \{x_1, x_2, \ldots, x_n\}$. The measure of interpersonal trust between the subject x_i and x_j is introduced as follows:

$$t_{ij} = t(x_i, x_j),\ t_{ij} \in \langle 0,1\rangle,\ \ i,j = 1, \ldots, n,\ \ i \neq j.$$

Further we suppose that both values t_{ij} and t_{ji} exist, thus providing the reciprocal trust.

We consider the following factors in our model: reciprocal trust, initial trust, subject reputation, number of subject recommendations, number of reciprocal contacts and trusting disposition. The tendency of reciprocal trust is reflected by geometric mean. Initial trust to subject is got on the start. The reputation of the subject comes after individual experience and by some information dissemination about subject in its neighbourhood and influences trust formation considerable. Trust depends also on the frequency of mutual contacts of subjects. Next, trust is formed by information about another subject that other subjects have passed on. This information is called recommendation. Trusting disposition representing a degree of non rational behaviour of a subject is modelled by random factor.

Experiments. The interpersonal trust model behaviour was examined by a number of parameter studies. Initial trust matrix and reputation matrix that implement initial trust and reputation of the subjects were randomly generated. Number of contacts among selected subjects and number of recommendations of selected subjects were stepwise increased and trust forming was pursued. Experiments studying influence of reputation size and initial trust size were performed. Number of contacts and number of recommendations were stepwise increased to illustrate trust forming. Trusting disposition was generated randomly for each subject and each step. Then the study of all parameter weights finished the experiments. The results of these experiments were presented graphically, too.

The experiments proved that the trust formation is reasonably sensitive to the parameters in proposed formula. Hence, they can be tuned to reflect the trust formation under various conditions.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODEL-BASED ANALYSIS OF AGENTS' INCENTIVES IN A DISTRIBUTED AIR TRAFFIC MANAGEMENT PROCESS

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Air Traffic Management (ATM) can be understood as a distributed multi-stakeholder system with a large number of economically and organizationally independent actors. Within the system a wide range of subprocesses are currently being redesigned towards more interactive and cooperative planning processes, often including elements of negotiation between different agents [4, 1, 6]. The redesign follows the aim of reaching better coordination and usage of limited resources and thus a higher global system efficiency. However, if potential new interaction protocols and planning mechanisms are not designed properly, the self-interested behavior of individual agents can also run counter the realization of the global system objective [3]. A suitable modeling of new protocols and their careful formal analysis is a key element for validating that the design objective can actually be reached [7].

The contribution presents a model-based approach to analyze agents' behavioral incentives in a distributed air traffic management process. The approach is demonstrated on the specific example of a new planning process for arrival management [8, 5] which was implemented as a Coloured Petri Net (CPN) model [2]. Aim of the new arrival management process is to provide an optimized scheduling of arrival traffic, based on state information and time estimates for Earliest Times of Arrival (ETA) submitted by the various arriving aircraft. In order to reach that goal, a planning system AMAN (Arrival Manager) computes a set of potential candidate sequences (possible schedules), which are evaluated using different rating functions. The objective of the model-based analysis introduced in this work, is to provide a formal argument, if agent's incentives and interest emerging from a certain design variant of the AMAN will or will not be compatible with the behavioral expectations towards the agents as formulated by the system designer.

The Coloured Petri Net model supports the formal analysis of the mechanism by calculating state spaces with the reactions of the planning system to all possible combinations of behavior of the aircraft. In this work, the model is used to investigate an operational traffic scenario where aircraft have to adapt their submitted time estimates ETAs for a common merging point as a reaction to a change in wind. The behavioral expectation of the system designer would be that all aircraft submit their corrected estimates to the planning system as soon as possible. However, the analysis shows that this behavior is not always profitable for the aircraft. Particularly aircraft which are slowed down might generally profit from delaying the update of the ETA. The desired instant update can be shown to be irrational in terms of MaxMax, MaxMin, and MaxAverage strategies. The result will be examined on a more varied set of scenarios in the future and potential cures to this incompatibility will be further discussed.

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AGENT REASONING BASED ON TRUST AND REPUTATION

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Trust is very important aspect in our everyday interaction with people, groups and institutions in our society. We should have a trust in the surrounding environment, people and institutions as well. We are often rated and judged on the basis of our trustworthiness and this defines a different manner of the interactions in our social life. We behave more openly towards subjects on account of the strong confidence and trustworthy subjects can access different types of information which can be confidential. In the case of abuse of the information, the trust of the subject rapidly decrease and it is usually very hard to restore it again.

In branch of intelligent systems especially in multi-agent systems we can adopt some trust and reputation principles which we know from every day interactions. The terms trust and reputation is also know from information technology security domain, namely from reputation systems.

Recent researches shows that system based on trust and reputation have great potentiality, for example in the e-commerce and autonomous distributed computer systems. This can be seen for example on the leading auction server *eBay*, where the selection of seller (from the buyer point of view) is based also on his or her reputation. All participants in the system are treated on the bases of his or her reputation. Trustworthiness of a seller so as of a buyer is represented by some value, which is update by the *eBay* system and depends on cumulating positive and non-positive ratings from other sellers or buyers. This reputation system, from our point of view, can be considered as relatively simple and closely aimed system.

In more sophisticated systems, we must deal with trust as strictly *subjective* and *context specific* metric, because it is assessed from the unique perspective of the element which has to trust somebody or somewhat and our interest is limited only to those actions (context) of a trustee that have relevance to the trust value. In our proposal, we need to take into account many specific problems which come with *trust based reasoning*.

This paper describes preliminary proposal core for *agent reasoning framework* based on trust and reputation principles. We proposed how a trustworthy value will *create*/*receive*, *store* and *represent* and *use* to agent decision. Our framework does not create next multi-agent architecture. We are trying to build new layout based on known and well formalized bases (such as BDI). This layout allow to agents to use trustworthy value to be more effectively in decision making and interacting with other agents.

We describe theoretical background of trust and reputation in different disciplines of the real word. Trust in our model is internal rating of each agent towards other agents in the system. Terms such as *reputation* and *recommendation* was also explicitly defined to provide core of formal proposal of our reasoning framework. We show that reputation is clearly a context-dependent quantity. Two cases of contexts in the system will be identified and in this paper and we use multiple contexts environment, which is most suitable for distributive multi agent systems and reflect the real world principles. We also describe phases of an agent trust evaluation process from reputation or agent belief base (knowledge - facts). In this evaluation process we will combine reputation history with recommendations. Process of inference reputation from facts, respectively inferencing facts from reputation will be also provided.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Computational Modeling and Simulation in Multi-Modal Transportation

A SIMULATION MODEL FOR DETERMINING CONTAINER THROUGHPUT AT AN EXPANDING SEAPORT

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Introduction. Over ninety percent of cargo currently transported worldwide is shipped as containerized cargo. As supply chains become more global and the use of containerized cargo increases, the ports throughout the U.S. are improving operations and undergoing major expansions. The Alabama State Port Authority is currently enhancing container and intermodal operations at the Alabama State Docks in Mobile, Alabama. The focus of this research was to determine the container throughput given a predefined set of operation parameters. The design goal for the container terminal is 325,000 containers annually.

Model. The simulation model was written in ProcessModel and has five submodels: ship unloading and loading of containers, train unloading and loading of containers, truck unloading and loading of containers, movement of containers from dock to container yard and movement of containers from container yard to dock. These submodels run independently of one another, each with a different entity type. Data are passed between the submodels by a number of global variables. A number of attributes are assigned to the entities. These variables and attributes control entity movement, branching and activity operations.

Conclusions. The goal of 325,000 containers annually is feasible with the proposed design parameters. dRun12 exceeded the goal and Run7 came close to the goal. To achieve this design goal the time between arrivals of ships must drop from three days for Run1 to one day and the time between arrivals of trains must drop from three days for Run1 to twelve hours. Increasing the entity arrivals had no impact on the entities time in the terminal. For Run12 ships averaged thirty-three hours in the terminal, trains averaged nine hours and trucks twenty-four minutes. Again these times were well within the desired turn around times. Values added times were twenty-two hours for ships, five hours for trains and thirteen minutes for trucks. The differences in the times in the terminal and the value added times are the times waiting for containers, resources or activities. The model is very sensitive to the interaction of arrivals of ships and trains. For example, a decrease in the time between arrivals of ships may not necessary increase throughput if there are not adequate trains available to remove the containers from the terminal. The same holds for a decrease in the time between arrivals of trains. Decreasing the time between arrivals of ships or trains may actually increase the time the entities are at the terminal. For example, a decrease in the time between arrivals of ships will result in a demand for more containers that are available to load on the ships. If there is not an adequate supply of containers arriving from trains, the ships will have to wait. As a result, the time the ship is in the terminal increases drastically. This point is reinforced in the selection of Runs2, 7 and 12 with overall low times in the system and large container handling. In these three runs a decrease in the time between arrivals of ships was also accompanied by a corresponding decrease in the time between arrivals of trains. The utilization of resources was relative low. However, these low utilizations are misleading. For example when two ships are in port all berths are fully utilized as well as the cranes unloading the ships. Likewise, the carts moving containers from the docks to the container yard are probably fully utilized. In many instances the terminal resources utilizations drop to zero when ships leave the terminal. ProcessModel was adequate to addressing the stated research objective. The ProcessModel was developed in less than forty hours that included collecting the necessary input data. The ProcessModel label feature that allowed the displaying of container content through the terminal proved to be an excellent tool for not only V&V but also to observe the running of the model and the movement and buildup of containers.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

NAVIGATION OF BIG SHIPS IN PORTS AND WATERWAYS

– A CHALLENGE FOR NUMERICAL MODELLING –

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Introduction. 30 years have passed since the maritime world copied the idea of simulation from the aircraft industry to train navigators but it is only in the last few years that the power of this tool for serving port and waterway planning has been fully understood. However there are some shortcomings to be compensated for in order to enhance simulation of complex human – machine –environment systems in shipping. programs established in engineering are the product of a marriage between science and mathematics. Ship traffic infrastructure, i.e. ports and waterways, cannot become adequately adapted to the ever increasing ship sizes, thus maneuvering has become a true challenge. However, the potential hazards from ships colliding with other ships or infrastructures, or from grounding, do not allow for any kind of gambling. Port and waterway access policy by maritime administrations needs to be based on reliable assumptions of opportunities and risks. This is also in the interest of the shipping companies who accept neither excessive risks for their ships nor delays in the ships' extremely tight schedules. Whereas expanding existing ports requires lots of effort, new ports can more easily become adapted to current and future ship sizes. However the luxury of too spacious ports is extremely expensive and investors there-fore just want tailor-made ports fulfilling minimum requirements. Thus those minimum requirements must be determined.

Maneuvering of ships can be simulated by

- Scaled models, remote controlled, towed or manned
- Numerical fast time simulation
- Numerical real-time simulation.

Only real-time simulation allows for the complete human-machine-environment system. Manned scaled models are useful to elucidate hydro-dynamic effects but because the time constants are very different from real operations these models are not adequate to develop sophisticated maneuvering strategies. State of the art ship simulators provide a realistic, controlled environment, the ship's bridge, displaying computer-generated information on off the shelf equipment. Also the visible environment is computer-generated and projected to large screens surrounding the ship's bridge. Such simulators are used for investigation and training, however their suitability depends on the ability of the mathematical model to mirror ship motion characteristics. Usually this is achieved by parameterised model-ling of reality. To allow real-time behaviour even under highly dynamic conditions, not all forces are calculated numerically, just the influence of governing scalar parameters. Each degree of freedom of ship motion is covered by a differential equation where coefficients provide the particularities of an individual ship. Surge, sway and heave describe the motions along the three main axes (x, y, z) and roll, pitch and yaw the rotation around these axes. The degrees of freedom required for simulation depend on the complexity of simulation. For simple simulation tasks surge and sway as linear motions and yaw as rotation is sufficient. This approach works fine for deep water conditions at quasi-stationary speeds. It also allows some conclusions for port design or maneuvering strategies at unsteady speeds and within a restricted environment like a waterway or a port. There the ship's behavior is dependent on

- under keel clearance
- distance to banks
- presence of other ships to become overtaken or encountered
- propeller thrust
- rudder
- other propulsion or steering devices like podded (azimuth) drives or bow and stern thrusters
- dynamics of engine
- current pattern
- wind forces

to only list the most prominent ones.

The most advanced ship simulators provide plug-ins to replace an inherent mathematical model or sub-set by a more sophisticated one computed by an external processing unit.

The smaller margins of safety in maneuvering mean that simulation must mirror reality to allow its application as a reliable tool for port design. Current conditions for big ships in tight ports no longer allow for significant uncertainties.

SCENARIO PLANNING AND ANALYSIS ON MULTIMODAL TRANSPORTATION IN METROPOLITAN HAMBURG SIMULATING A TERRORIST ATTACK ON RIVER ELBE TUNNELS

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Introduction. This paper presents a scenario planning and analysis embedding a simulation case study of an assumed terrorist attack on river Elbe tunnel to calculate the impact of the resulting bottlenecks on multimodal transportation in metropolitan Hamburg. A scenario analysis can be performed to predict possible future events of a given entity considering alternative possible outcomes, assuming changing scenarios but inherently consistent framework conditions, for improved decision-making, that require as prerequisite a scenario planning, a method based on simulation games for decision making. This games combine known facts about the future, with plausible alternative trends that are key driving forces. The scenario analysis used in this paper is an improved decision making allowing consideration of outcomes and their implications on transportation chains through river Elbe tunnel tubes in metropolitan Hamburg. Hence the major facts of the tunnels concerning the transportation chain must be known. But scenario analysis in general is no substitute for a complete and factual exposure of survey error in the respective studies under test. In commonly prediction, the data given are used to model the problem under test, with a reasoned specification and technique and the analyst in charge with the respective analysis feels in duty bound, within a certain percentage of statistical error, to state the likelihood of previous specified coefficients being within a certain numerical bound. To scale down this expectations it should be noted that this exactitude need not come at the expense of very disaggregated statements of hypotheses of a real scenario analysis., i.e. it has to be considered causal inference, as well as the evaluation of the counterfactuals. Based on what is perceived would be the outcome of each and the basis to plan the next step, which finally require testing to perceive a good scenario. For this reason the scenario planning is necessary to understand as best as possible likely future trends to make strategic decisions based on an analysis of the consequences of the most likely scenario. Such contemplation at least result in the following topics that have to be taken into account. As result of this topics a traffic network model was developed, based on modifying VITS (Virtual Intermodal Transportation System), that support multi-modal traffic and provides reasonable tradeoff between macroscopic computational efficiency and microscopic/agent-oriented accuracy, but require data nearly impossible to obtain. The traffic network consist of nodes and links. For the road mode vehicles can be modelled individually, attributes including current location, speed, and destination. Vehicles stochastically appear at any node (inter-arrival time exponentially distributed) and traverse fixed routes, i.e. sequence of road links, reaching destination. Based on that previous mentioned methods a bottleneck-analysis can be used to predict the impact of shortages in metropolitan Hamburg, as part of an terrorist attack. In general a bottleneck analysis is a process related approach used to identify shortages. In relation to transportation chains it is concerned with analysis of resource planes, depth of optimization of multimodal transportation, consideration of timeliness and concurrency while using resources, analysis of transactions in the network, etc. Thus the main advantage of a bottleneck-analysis is the possibility of shortage identification and, if possible, rectification on the very spot to achieve optimized transportation chains. In general, the results obtained from a bottleneck analysis distinct between best -, worst -, und real case results, based on their respective approach. Assuming that a bottleneck-analysis in transportation deals with the calculation of the adequate availability of resources, the three different cases are:

Best Case Analysis: resources for multimodal transportation chain are available and no shortage will appear. This result in a high priced solution, basically the resources available can't be used in an optimal way, because there are more resource available than necessary.

Worst Case Analysis: resources for multimodal transportation chain are not available in the required amount or at the worst only one component is available but several of which are needed. Henceforth, shortages will appear. Result is a cheap priced solution, basically resources available are not adequate.

Real Case Analysis: real available resources for multimodal transportation chain have been taken into account. Basically the solution achievable is in between beast case and worst case because the results obtained by the real case analysis are sub-optimal.

As a result the paper will evaluate the impact onto the multimodal transportation chains and show possible solutions based on the scenario analysis on how to overcome the bottlenecks.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

ON SELF-ORGANIZING TRANSPORT NETWORKS – AN OUTLINE

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Transport networks. This paper presents an outline of a PhD project currently in progress. The target is the optimization of *transport networks*, defined as a graph topology where entities are forwarded from node to node following different routes. The progress of such entities is limited by capacity restrictions of both nodes and edges (links). Examples include networks seemingly as different as urban traffic (vehicles proceeding from one intersection to the next), conveyor-based manufacturing systems (items processed successively by different workstations) and telecommunication networks (e.g. IP packets being forwarded from router to router).

Decentralized optimization. Transport networks can be interpreted as complex adaptive systems [3]; attempts to adaptively optimize (i.e. minimization of waiting or travel times despite traffic conditions continuously changing) such a network centrally typically imply exponential computational complexity and depend on the availability of a central server and the communication to this authority. This motivates applying a decentralized approach: In the absence of a central controller, each node (router, traffic light) uses local rules to independently decide about the order in which entities (IP packets, vehicles) are processed. Existing work indicates that in *self-organizing* [1, 6] networks, a performance better or at least not significantly worse than in centrally controlled systems where solutions determined from global knowledge are enforced may emerge [2]. However, decentralized transport networks require less communication and their behaviour is adaptive, scalable and robust. A measurement for the "disorder" of a transport network is proposed, which is sharing typical properties of entropy in Thermodynamics [7] and Information theory. The problem of engineering self-organizing systems is discussed: Self-organizing systems can neither be developed top-down (unless suitable local rules are already known) nor bottom-up (undesired emergentes may occur), which facilitates pattern-based approaches in-between micro- and macro-level.

Model logic. A simulation model to empirically evaluate the performance of a transport network is presented next. This model is queue-based and well-suited for discrete event simulation. The underlying idea is to keep track of the earliest possible arrival at the next node for every entity; depending on queue lengths and whether or not passing slower entities is permitted, actual arrival may by significantly later than the earliest possible arrival.

Local rules. Microscopic rule components [5] from which efficient network performance on a macroscopic level may emerge primarily rely on selfish behaviour, like (using terminology from urban traffic here) minimizing average local delays subject to a minimum "green" length per direction and to an upper bound to the "red" waiting duration for any link [4]. At the same time, it is desirable to maximize the absolute flow or flow per traffic blocked, e.g. protected left-turning in right-hand traffic is more expensive in terms of traffic blocked than right-turning. Adaptivity includes dynamically adjusting phase and lane allocation (compare Figure 1). Selfish local rules have to be balanced against cooperative behaviour, e.g. facilitating *green waves* by retaining platoons of approaching vehicles (even if side road traffic has to wait longer) unless the subsequent links are congested.

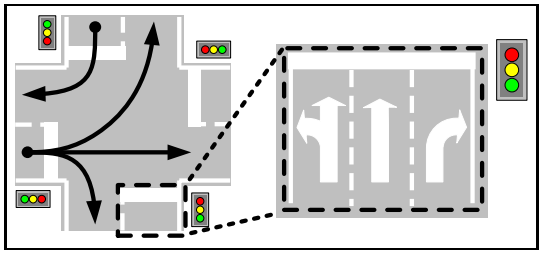

Figure 1: Possible configuration of phases (left) and lanes (right) at an instant.

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A COMPREHENSIVE FAST TIME SIMULATION TOOL FOR MODELLING AND EVALUATING APRON GROUND TRAFFIC AT AIRPORTS

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Initial situation. Fast time simulation has become an important methodology for supporting airport planning and optimisation of operational concepts. Using a computer model of the airport, selected processes are simulated based on the chronological proceeding of the flights at the airport. In the past several tools have been developed in order to cover the different parts of an airport with the main focus on the passenger flow through terminals and the aircraft movements on the runway and apron. Permanent expansion of the airports within recent years led to a great demand for a capable simulation tool that supports in optimisation of infrastructure and solving problems with the growing ground handling traffic on airports.

Based on the requests from the aviation industry and looking back on a long term experience in simulation development, *Airport Research Center GmbH*, together with different partners, have developed CAST – Comprehensive Airport Simulation Technology. In addition to the passenger terminal module and an aircraft traffic module in cooperation with *Fraport AG* and *Fraunhofer IML* a vehicle and ground handling simulation module has been developed.

CAST Vehicle. CAST Vehicle is a new generation of simulation tool that allows for the first time to link logistical processes with vehicle based traffic. It provides special functions for modelling and evaluating the complete airside ground handling processes and traffic on airports.

CAST Vehicle enables the rapid evaluation of layout concepts and operational strategies. Besides the application on the strategic level the software can be used on a tactical and operational level in order to provide essential information for an improved airport management and support the control of the system as well. The super ordinate aim is to constantly reduce the cost of infrastructure and operations, guarantee safe operations, and reduce negative environmental impact.

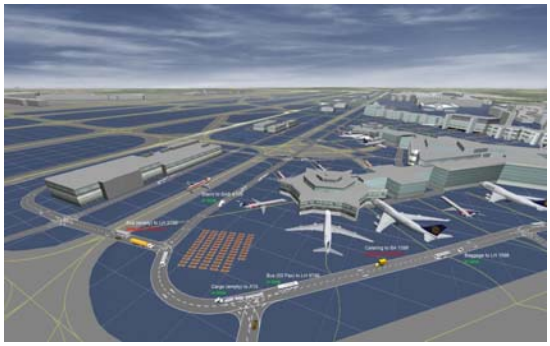

Figure: 3D view of CAST Vehicle

Figure: 2D colour coding of infrastructure capacity utilisation

Functionalities. Baseline for the vehicle simulation is a 3D model of the airside infrastructure including aircraft stands, apron areas, vehicle roads, depot and parking areas, aircraft taxiways and their intersections with vehicle roads as well as push back areas. Furthermore, representations of components providing data and control systems as an airport database and the disposition centres are included. CAST Vehicle generates a schedule-based dynamic traffic that takes into account flight load information (e.g. passenger baggage and cargo), as well as individual ground handler responsibilities and their dispatching strategies.

A detailed routing module provides automated and realistic routing. Vehicles find their routes considering e.g. blockings by taxiing aircraft and the actual traffic situation on potential route segments. The software provides an accurate model of microscopic driving behaviour: vehicles accelerate, turn, change lanes and overtake according to their kinematic and dynamic properties and give way at road junctions while obeying the respective traffic rules.

Different performance indicators can be logged for extensive analysis and – via simulation-synchronic animation and in-run analysis functionalities such as graphs or colour coding – can already be assessed during the simulation run.

Conference presentation. An overview on the main components and functionalities of CAST Vehicle is given from the user's point of view. The required integration of different sub-functions and algorithms are pointed out.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

OPTIMIZING THE GROUND HANDLING AT AIRPORTS: A STUDY CONCERNING A BUS DISPATCHMENT ALGORITHM

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Abstract. Hamburg Airport is currently being equipped with a new traffic control system. With the help of such a system the actual position of air and ground vehicles can be located and thus the system enables an updated and exact geographical position of all vehicles. This functionality not only increases safety aspects at the airport but also serves as a basis for further optimization. For example, a route planning for ground vehicles based on their current geographical position, the current traffic situation on the apron, and the current task list for the fleed is possible.
For the example of the passenger bus dispatching unit an optimizing algorithm is worked out that has

- to be able to integrate frequent changes in the timetable for arrivals and departures under real time conditions
- to offer an interface that consolidates the needs of an automatic dispatching with the must of interactive interventions by the dispatcher
- to consider the geographical situation to calculate realistic driving times
- to consider the restricted hardware equipment that makes an overall optimized day schedule impossible

In this situation, the paper describes a solution, that introduces different states for the buses (as resources) and the diving tasks (as tasks in general) and permanently controls the criterion “shortest service time” with respect on the current position of the buses and the distances between the locations on the apron for a set of the n next tasks to be served.

The paper is structured as follows:

- Introduction to the application area “airport logistics” and to the objectives for optimization
- Specification of the data areas such as resource list, daily schedule for arrivals and departures, traffic graph for the routing, and the estimated traveling times.
- Afterwards, the dispatching problem itself will be specified: For resources and for tasks a state-transition model is introduced, that allows a formal treatment of the dispatching process.
- For the optimization algorithm itself, a set of tasks is introduced that holds the currently optimized jobs and that is automatically updated if external changes in the flight schedule or in the job sequence in general occur. Special attention is paid to the interactions of the human dispatcher who influences the set of currently optimized tasks by selecting the set of tasks currently treated by the optimization and even by manual assignments of resources.
- A separate section will describe the optimization algorithm in a pseudo-code version.
- The interface is described by a detailed explanation of a typical screenshot.
- In the final discussion, the experiences with the solution are referred with special emphasis on the conflict between completely automatic dispatching and the acceptance by the people working at the airport.

AN M&S-BASED TRANSPORTATION ENGINEERING PROGRAM

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Introduction. Many programs established in engineering are the product of a marriage between science and mathematics. For example, the Electrical Engineering program emerged from a combination of physics and math when people found more practical ways of applying them that didn't require a detailed solution every time. The same was true for Computer Engineering which emerged from the application of math and Electrical Engineering.

Transportation Engineering is currently an area of specialization in Civil Engineering and has a good chance to be recognized as an independent field due to its need. This field concentrates in the issues involved with the design, planning, and safe operation of highways, waterways, and airways as well as the issues involved with handling traffic under normal and emergency conditions, such as the bottlenecks created during the rerouting/detouring and/or mass evacuations during emergencies. The range of applications for this field vary from bike path designs to airport runway designs to transit modes of operation from pedestrians to rail to air.

Determining the accuracy, financial viability, and utility of a new transportation project depends increasingly on computational modeling and simulation. M&S, being an inexpensive and safe method for designing for unavailable physical circumstances, is used to provide details for design issues by verifying and validating the models of the design and analyzing the results obtained from the model. No design is complete unless its accuracy has been verified by simulation.

M&S may be considered as a field in applied math using engineering and computer science concepts for development and testing of the models. Due to the vast opportunity for application areas of M&S in both science and engineering, establishment of an M&S program is needed in both areas. This program is heavily dependent on math, software engineering, and the student's field of specialization. Since M&S applications can be in any field, the program should emphasize the utilization of the concepts in the student's area of specialization.

Recognizing the importance of M&S, the 2006 NSF Blue Ribbon Panel reported that continued advancement in the M&S field is critical for resolving a multitude of scientific and technological problems facing the United States. In addition, the White House American Competitive Initiative report identified M&S as a key enabling technology of the 21st century. With pressure to cut costs while increasing technological development, researchers are turning more and more to M&S in order to increase the development and understanding of the systems and their interactions.

Due to many potential applications of M&S in transportation, much attention has been focused recently on what should be a proper M&S educational program in transportation engineering and what qualifications the graduates of this program should posses for a career in M&S. This has motivated the educators to focus on developing a model curriculum for Bachelor of Science (B.S.) and/or Master of Science (M.S.) degrees in M&S-based Transportation Engineering to assist engineering schools in establishing a new program in this field.

However, defining a curriculum for a degree program in computational modeling and simulation in Transportation Engineering is difficult. This is because 1) M&S is usually regarded as a fragmented subject with components in a range of disciplines but with a wide range of applications, and 2) Transportation Engineering is an area of specialization in Civil Engineering. The following is a first draft of the proposed elements for a program in M&S-based Transportation Engineering.

The first version of a model curriculum for an undergraduate degree in M&S-based Transportation Engineering is proposed. We hope this proposal can be used as a basis for wide-ranging discussions that will lead to a published version sponsored by interested professional bodies such as ASCE, SCS, and SIM SUMMIT.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

TIME AND ENERGY EFFICIENT TRANSPORT

A PROPOSAL FOR A TRANSPORT SYSTEM ASSESSMENT

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Introduction. Different transportation systems compete with each other in a multilayered contest around market shares in the constantly growing transportation market of the 21st century. To optimize the transportation systems and chains it is necessary to characterize the transportation efficiency of a transport vehicle like aircrafts, trains or automobiles by the relevant parameters along the entire energy and mission track from door to door. Based on this analysis transportation efficiency can be characterized by

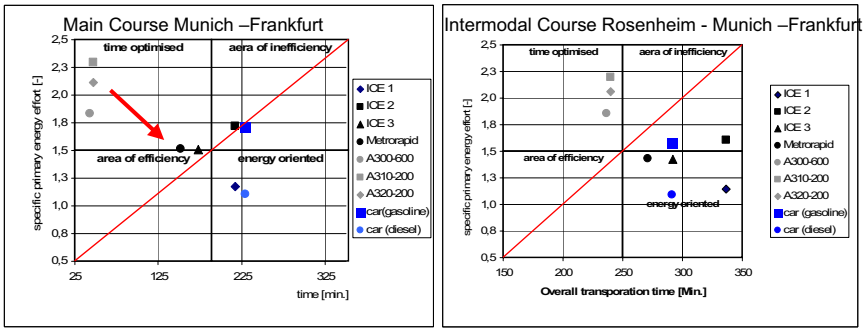
- the energy needed to perform a dedicated transportation task from door to door
- the time needed for the overall transport mission
- the operating cost associated with the transportation task
- the emissions and noise a transport system creates

An integrated approach is used in the following based on a 5 phases model and a graphical efficiency criterion to develop a method to correlate the energy demand with the transport time and the transport performance in intermodal transport tasks

Content. Generally, this *Proceedings Abstract* is a summary of your contribution. The body of the *Proceedings Abstract* should start with a short description of the problem and the state-of-the art in treating/solving it. Mainly, you should describe the fundamental idea and the approach and implementation of your presented work, highlighting, what is new in your approach or method. From this description one should see in which respect your paper will be of interest to colleagues interested in one or the other aspect of modelling.

Analysing the various transportation processes of passenger and cargo transport from door to door one can identify a common structure represented by five main phases. All phases are characterized mainly by the time needed to perform it and the energy to be used, where the transition phase is of major importance because no transport performance is received but a lot of time is needed.

Modelling the technical characteristics of the most competitive transport vehicles and calculating the primary energy demand along an intermodal chain from door to door one can see, that e.g. the aircraft has a high energy demand to compensate the time consumption of the departure, transition and destination phases, while other transports show significant less overall energy demand associated with a limited increase in time, when the inter modal chain is considered, right picture below.



Example of transportation efficiency assessment on the main course Munich – Frankfurt

The investigation has shown, that the five phases model is useful to identify time related bottlenecks without modeling to much details. In addition the assessment criterion is applicable to compare different transport systems in intermodal transport chains. In the next step more dynamic models will be developed to investigate the sensitivity of the criterion and it will be extend to cost and environmental assessment capability.

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Modeling and Simulation in Systems Biology

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

CALCULATING THE *K*-SHORTEST ELEMENTARY FLUX MODES IN METABOLIC NETWORKS

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Abstract. In the post-genomic era elementary flux modes represent a key concept to analyze metabolic networks from a pathway-oriented perspective. In spite of considerable work in this field, the computation of the full set of elementary flux modes in large-sized metabolic networks still constitutes a challenging issue. In this paper we illustrate that the full set of elementary flux modes can be enumerated via integer linear programming. Technically, our approach produces elementary flux modes in increasing order of number of reactions by sequentially solving an optimization problem. Though our procedure is not particularly efficient in computing the full set of elementary flux modes for large-sized metabolic networks, it is very flexible. It can be applied to calculate the elementary flux modes satisfying a given criteria without having to calculate all the solutions first, in contrast to what is typically done by current methods. This greatly speeds up computation by focusing only on that part of the solution space that is of interest. Since computation time increases as the length increases, it is promising to start with the shortest, second shortest, etc., (overall called *K*-shortest) elementary modes. Detection of these is indeed of interest for several biological applications. Experimentally, it is difficult to insert and express a large number of heterologous genes and shorter pathways can carry higher fluxes. To illustrate the scope of our approach, we analyse a subset of elementary flux modes that produce L-lysine in *Escherichia coli*. Our analysis shows that our mathematical approach can be an effective tool to explore the capabilities of metabolic networks at the genome scale.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

DETECTING METABOLIC CONVERSIONS IN GENOME-SCALE METABOLIC NETWORKS ON THE BASIS OF ELEMENTARY FLUX PATTERNS IN SUBNETWORKS

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Elementary modes (EMs, [2]) represent a powerful means in the analysis of metabolic networks and their characteristic properties. However, EM analysis cannot be applied to genome-scale systems since their number is growing exponentially with network size [1]. Thus, EMs can only be computed in networks usually not corresponding to the entire known system and hence they might not reflect the true metabolic capabilities of the entire system. Here we present a novel concept, elementary flux patterns, which allows to circumvent these problems. Within a large or genome-scale metabolic network elementary flux patterns are defined as sets of reactions that represent the basic routes of any steady-state flux of the genome scale network through a particular subsystem. Equipped with this method we analyze the EMs obtained for two networks within the central metabolism of *Escherichia coli* that have been studied previously [2, 3]. We integrate these networks as subnetworks into a publicly available genome scale metabolic model of *E. coli*. Thus, we find that 6 of the 16 elementary modes of the first system cannot be present in any steady-state flux of the genome-scale system. For the second system, all EMs are part of global steady-state fluxes. Furthermore we analyze the elementary flux patterns of the subnetworks and find several alternative routes on which intermediates of the subnetworks can be produced from species in the growth media. We conclude that the concept of elementary flux patterns offers two major advantages. First, elementary flux patterns more faithfully reflect the possible steady-state fluxes through a subsystem of a large metabolic network by taking into account the entire system. Second, they enable the application of tools from EM analysis to genome-scale metabolic networks.

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Determination of Flux Directions by Thermodynamic Network Analysis: Computing Informative Metabolite Pools

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Network thermodynamics [4] focus on the energetic analysis of complex metabolic networks. The method connects metabolite concentrations, free Gibbs energies (under standard conditions), and flux directions by the thermodynamic laws. Applications are given by consistency checking of mixed concentration/flux data, computing possible flux direction patterns [1, 3], or narrowing the concentration space of the unmeasured pools in a biochemical network [2]. To deal with uncertainty, metabolite concentrations and Gibbs energies are treated as intervals of values which can be determined (measurement error) or very wide (no concentration measurement).

Here, a new application of network thermodynamics is presented, that determines those metabolite pools that have to be measured in order to determine as many flux directions as possible. The following questions are addressed:

- Which pools in a given network need to be measured for determining a specific flux direction?
- Which direction information is given by a set of measurable pools?
- Which information is contained in one or more measurable pools on directing all reversible reactions?
- Are there reactions whose direction cannot be determined at all?
- How important is the measurement of energetic currency metabolites ATP, NAD, NADP etc.?

The general concept that is used to predict a net flux direction for a specific set of measurable pools includes the following operations: First, Monte Carlo samples are generated in the thermodynamically feasible concentration space of all metabolites in the network. Then, the high-dimensional space of the samples is projected to the subspace of some few chosen pools. Next, it is checked how far a given subspace sample uniquely determines the direction of a reversible reaction. This is computed by checking the affiliation of the data set to the feasible concentration subspace concerned to the forward and the backward directed flux. Finally, the probability of unique flux direction determination from the subspace data set is taken as a measure of information.

An example is given by analyzing the network model of the central carbon metabolism of *C.glutamicum*. This network contains 23 measurable pools and 18 reactions, that are known to be unidirectional. In the tested case, the flux direction prediction shows trivial and nontrivial results. Clearly, the flux direction of reactions whose substrate and product pools are measured can directly be derived. Nontrivial cases are not obvious from the measured pool pattern. Interestingly, for some cases the pools aren't even attached to the affecting reaction. Because cofactors are involved in many reversible reactions their measurement is expected to be very important. This assumption is confirmed for many but not all cofactors in the given network of *C.glutamicum*s central metabolism.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A SOFTWARE FRAMEWORK FOR MODELING AND SIMULATION OF DYNAMIC METABOLIC AND ISOTOPIC SYSTEMS

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Ongoing development of technical and analytical procedures for measuring metabolic intermediates with and without tracer information (e.g. ^{13}C) [4] led to the requirement to formulate different model approaches describing the measurement data. Thereby a classification can be made between the model's assumption on metabolic and isotopic (non-)stationarity.

While ^{13}C-MFA has become a powerful tool in elucidating the fluxome in different organisms of bacteria and plants [3, 5] under metabolic stationary conditions, this approach is not capable of describing in vivo metabolic regulation and control. Therefore it has only minor predictive power. To reveal underlying kinetic mechanisms of metabolic regulation, pulse experiments have been established to generate dynamic data of metabolic intermediates. For the description of this data, dynamic metabolic networks are formulated that are based on kinetic models describing enzyme catalysis and regulatory metabolic interactions [1]. Validation of such models is a challenging task since usually a huge amount of parameters have to be identified with a limited number of measurements. In order to improve parameter identification, an extension of the dynamic model approach using ^{13}C labeling has been suggested [6].

Accordingly, for the underlying modeling approaches a diversity of *in silico* tools have been developed. The full exploitation of this potential to address metabolic processes is hampered by mainly three principal issues. First, not all currently realizable experiments are covered by these tools. Secondly, an easy switching between existing tools allowing for a flexible description of different experimental states is not possible. The third item addresses the universality of underlying modeling concepts which usually have a restricted focus.

We propose a general modeling concept which allows modeling and simulation of all combinations of metabolically and isotopically variants in their stationary and dynamic states and which is embedded in an unique software platform. The basic idea is to build up dynamic metabolic networks relying on mass balances for intermediate labeling pools, i.e. systems of ordinary differential equations (ODE) describing dynamically changing cumomer (cumulative isotopomer) concentrations as state variables. Starting from biochemical network descriptions (including stoichiometry, C-atom transitions, initial conditions) using the software 13CFlux, consistent algebraic equation systems (AE) of mass balances for all cumomer pools are generated. These AE's are then transformed into Modelica specific code consisting of ODEsystems for all cumomers. Due to the general model structure all types of experimental states mentioned above can be simulated using one model with different scenarios settings.

A workflow is presented that allows the automatized generation of models of any size and complexity specially tailored for the experiment of choice. The Modelica models are directly compiled into highly efficient executable simulation code. Model simulations, parameter fittings as well as comprehensive statistical evaluations are performed in the Matlab environment. As an essential ingredient of model based inference, sensitivity analysis for model variables and parameters is performed using an automatic differentiation method developed for Modelica source code (ADModelica, [2]).

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REACTION ENGINEERING APPROACH APPLIED TO THE PRODUCTION OF ANTIBIOTICS BY *Saccharothrix algeriensis*

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Almost a quarter of the deaths in the world results of infectious diseases more and more caused by bacteria having developed a resistance to antibiotics. This phenomenon stresses the importance of constantly renewing the pool of bio-active molecules. In this context, a new bacterial specie *Saccharothrix algeriensis* NRRL B-24137 has been isolated in 1992 from the Sahara desert (Algeria). This filamentous bacterium belonging to the actinomycetes family is able to produce dithiolopyrrolones, molecules which present antibacterial, antifungal, and anticancer activities. A previous work [2] highlighted the influence of the culture medium on the dithiolopyrrolones production. Its capacity to produce antibiotics upon request by precursor-directed biosynthesis facts that the study of *Saccharothrix algeriensis* presents a fundamental undeniable interest, in addition to an obvious useful interest. As this bacterium has been recently discovered and characterised, no deep knowledge on its metabolism is available. Several studies have been undertaken in parallel to better understand the dithiolopyrrolones production pathway by *Saccharothrix algeriensis*. For the study presented here, a macroscopic approach has been chosen to investigate the bacterium metabolism. No data coming from "omics" are used but the "reaction engineering" approach adopted to analyse the metabolism from a qualitative and quantitative point of view enables to get more knowledge about the mechanism of dithiolopyrrolones production. The advantage of this approach is that, while remaining at the extra cellular scale, with experimental information relatively easy to obtain, it allows getting information on the metabolism of the cell. Stoichio-kinetic models consist of the decomposition of bacterial growth in some reactions of invariant stoichiometry with time. It is based on the bilinear structure of the component mass balances in a batch reactor. In that case, for *nr* occuring reactions and *nc* measured components on *ns* samples, the data matrix *D*, consisting of *ns* rows containing the result of cumulative molar amount of each of the *nc* measured species can be written as the product of two matrixes *R* and *S* respectively the matrix of the reaction extend (ns,nr) and the matrix of stoichiometry coefficients of the *nr* reactions (nr,nc). Different authors have proposed to determine R and S by factor analysis in two steps [1]. Fillon et al. [3] showed the sensitivity of this method to measurement errors and suggested to first reconciliate raw data on elemental balance. By reducing the noise intensity using data reconciliation based on elemental balances, errors become negligible compared to reaction extends and in that case, the discrimination of reactions is possible and reliable. The factor analysis is interesting when the number of active reaction is unknown. When a qualitative analysis of the raw data enables to be aware of the active reactions, we suggest a direct determination of *R* and *S* by solving the constrained optimization problem based on reconciliated data ($\hat{D}_{exp}$):

$$\underset{R,S}{Min} \sum_i \frac{\sqrt{\sum_j (\hat{D}_{exp}(i,j) - D_{calc}(i,j))^2}}{Max(|\hat{D}_{exp}(i,j)|)} \text{ and } \begin{cases} D_{calc} = RS \\ \text{R is coherent with the elemental balances} \\ s_{i,j} > 0 \text{ for i = 1, ns and j = 1, nr} \\ s_{i+1,j} - s_{i,j} > 0 \text{ for i = 1, ns-1 and j = 1, nr} \end{cases} \quad (1)$$

This approach was successfully applied to the analysis of the growth of *Saccharothrix algeriensis*. A four reaction scheme has been suggested as a macroscopic view of the growth of this bacterium and the associated production of thiolutine. It was shown that *Saccharothrix algeriensis* was able to grow on both free amino acids and glucose as carbon source. The amino acids of weak molar weight are consumed preferentially to glucose. They seem to be directly integrated to the proteinic synthesis and enriched the medium with ammonia. This ammonia is then assimilated during the growth on glucose. It has been established that the thiolutine production was the result of a secondary metabolism, decoupled from growth. In our experimental conditions it seems to be initiated as soon as a nitrogen source depletion occurs. These results open an interesting way to deepen the knowledge on the behaviour of this bacterium of a rare kind. They give tracks for an exploration of the metabolism to an intracellular level and pose the bases for the production of dithiolopyrrolone at an industrial scale.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODEL INVALIDATION AND SYSTEM IDENTIFICATION OF BIOCHEMICAL REACTION NETWORKS

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Introduction. An important modeling issue in systems biology is system identification, comprising both estimation of model parameters and model structure analysis. System identification can be very difficult, due to uncertainties of the involved reaction mechanisms leading to concurring structural hypotheses. Moreover, kinetic parameters can not be determined experimentally and may therefore be completely unknown. To obtain a model that captures the essential behavior of the process under study, it is important to discriminate between the structural possibilities and to estimate model parameters.

Current approaches to discriminate between model alternatives and to estimate model parameters are often inappropriate for biochemical reaction networks. This is because often only noisy measurements and sparse experimental data are available, and since they do not take the special structure of biochemical reaction networks into account.

Content. In this work a set-based approach for model invalidation, parameter and state estimation, is presented. The key idea is to reformulate the invalidation task as a feasibility problem, while taking into account the measurements and parameter bounds as constraints. In general, this is a hard non-convex optimization problem, where non-convexity results from the nonlinearities of the model equations. As shown, due to the polynomial structure of many biochemical reaction systems, it is possible to *relax* the non-convex feasibility problem into a convex semidefinite program (SDP) ([1]). Such SDPs can then be solved efficiently, e.g. via interior point methods. As the relaxation process is conservative, infeasibility of the original feasibility problem can be certified via the corresponding SDP.

This approach allows to obtain conclusive results on model invalidity based on the certification of *non-existence* of a feasible parametrization even if only imprecise or sparse measurements are available. Competing model alternatives can thus be discriminated by proving inconsistency with the available data for (some of) the wrong alternatives.

To provide estimates of parameter and state sets being consistent with the measurements, subregions in the surrounding are certified as infeasible and discarded. Herefore, the initial parameter or state space is partitioned and the partitions are checked for infeasibility. In order to reduce the overall computational cost, we provide a bisection algorithm, so as to check groups of partitions simultaneously.

Summary. Our framework allows us to consider the arising difficulties posed by biochemical reaction networks by taking the polynomial structure of the dynamics and model outputs into account. We have studied the problems of model invalidation, parameter and state estimation of discrete-time polynomial systems.

The proposed method allows to discriminate between different model hypotheses, and allows to discard large parameter regions, thus complementing existing identification methods. We also applied this method to estimate the model states from the measurements.

We have shown with an example, considering two alternative enzyme-substrate reaction mechanisms, that with this method it is possible to prove invalidity of one of the two mechanisms. Extending this example, we also demonstrated the applicability of the approach to estimate the model parameters. In summary, our approach is a reliable and computationally manageable method for dynamical model invalidation, and parameter and state estimation.

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A Model Based Analysis of Multiple Steady States in Continuous Cell Cultures

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Metabolic regulation is of fundamental importance for understanding the dynamic behavior of biological systems. While it allows the microbial cells to survive under changing environmental conditions, it can be also the source of intricate nonlinear behavior in biotechnological production processes. As a consequence of the interconnections between metabolism, signal transduction and gene expression, complex nonlinear behavior in the form of steady state multiplicity and bistability may appear in continuous cultures. Depending on the initial conditions, different asymptotic states can be attained with completely different amount of biomass and/or internal metabolite concentrations. Hence suitable start-up strategies may be required to achieve an optimal production rate with high cell density [2]. Suitable mathematical models can contribute to a better understanding and may guide the way to suitable process conditions and operating strategies.

In the present paper, a model based analysis of steady state multiplicity in continuous cell cultures is presented for two different types of models. The first type of model is based on the cybernetic approach, which was proposed by Ramkrishna and co-workers and has been under continuous improvement (see [7] and references there). Cybernetic models are models of moderate complexity, which take into account metabolic regulation by using some cybernetic variables which control enzyme synthesis and activity in order to maximize the growth rate. More recently, cybernetic models were used for the nonlinear analysis of bioreactors in [5, 4, 3] and [6]. In particular it was shown, that the experimental findings in [2] could be predicted theoretically with a cybernetic model [4].

The second model is a detailed mathematical model which was developed by Kremling and co workers and later extended in series of papers (see Bettenbrock et al. (2006) [1] and references therein). The final version of the detailed model used in the present contribution describes the growth of *E. coli* on a mixture of up to six carbon sources and takes into account the regulation (activity as well as gene expression) of the uptake reactions. In particular, the complete signal transduction pathway, starting from the sensory system, the carbohydrate phosphotransferase systems (PTS) to the activation of the global transcription factor Crp is included.

Advanced computational tools employing simulation and parameter continuation methods are used to determine the multiplicity regions in the space of adjustable operating parameters of the corresponding models. Further insight into the solution structures of the cybernetic model is gained from an analytical approach. In particular, it is shown that the cybernetic model always predicts multiplicity if the fraction of the preferred substrate in the feed is sufficiently low, no matter which particular substrate or micro-organism is considered. It is further shown for growth of *E. coli* on mixed substrates of glucose-6-phosphate and glucose, that the overall behavior predicted by the cybernetic model is agreeing qualitatively quite well with the detailed model. Quantitative differences are also discussed and conclusions are drawn for future work.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

CONSTRUCTIONS OF KINETIC MODELS FOR METABOLIC REACTION NETWORKS: LESSONS LEARNED IN ANALYZING THE SHORT TERM PERTURBATION DATA

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Construction of dynamic models of large scale metabolic networks is one of the central issues of engineering of living cells. However, construction of such models are often hampered by a number of challenges e.g. data availability, compartmentalization and parameter identification coupled to design of in vivo perturbations. As a solution to the latter, short-term (<200 s) perturbation experiments are proposed and are proven to be a useful experimental method to obtain insights on the in vivo kinetic properties of metabolic pathways. This approach consists of perturbing a well-characterized culture state by external stimuli and subsequently monitoring the response of the intra- and extracellular metabolites over a short period of time. During this time, it may be assumed that enzyme concentrations do not change, allowing the observed responses to be attributed to kinetic interactions at the metabolome level alone. In this respect, construction of kinetic models is a central issue in analyzing and interpreting such data.

The aim of this work is to construct a kinetic model using the available experimental data obtained via short term perturbation experiments, where the steady state of a glucose limited anaerobic chemostat culture of Saccharomyces cerevisiae was perturbed and the dynamic response of extracellular/glycolytic intracellular metabolites were monitored [1]. In constructing the model, we first determined the steady state flux distribution using the data prior to the glucose pulse and the known stoichiometry. For the rate expressions, we used approximative linlog kinetics, which allows the enzyme-metabolite kinetic interactions to be represented by an elasticity matrix. We performed a priori model reduction based on time-scale analysis and parameter identifiability analysis allowing the information content of the experimental data to be assessed, as described in [2]. The final values of the elasticities are estimated by fitting the model to the available short term kinetic response data [3].

The final model consists of 16 metabolites and 14 reactions. With 25 parameters, the model adequately describes the short term response of the cells to the glucose perturbation, pointing to the fact that the assumed kinetic interactions in the model are sufficient to account for the observed response.

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MODELING AND ANALYSIS OF THE DIFFERENTIATION PROGRAM OF A MODEL ADULT HUMAN STEM CELL

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Abstract. Understanding the molecular basis of stem cell differentiation programs is one of the grand unmet challenges facing modern cell-biology. In this study, we integrated computational and experimental network analysis tools to unravel the response of HL-60 human myeloblastic leukemia cells to Retinoic Acid (RA). HL-60 is an uncommitted precursor cell-line that is responsive to RA signals. Thus, HL-60 is an archetype model to study the molecular architecture of human differentiation programs. Our initial studies have focused on the role of the BLR1 receptor in the transduction of RA signals. BLR1, a G-protein coupled receptor expressed following RA exposure, is required for RA-induced cell-cycle arrest and differentiation and leads to atypical persistent MAPK signaling. A dynamic mathematical model of the molecular programs governing RA induced cell-cycle arrest and differentiation was formulated and tested against BLR1 wild-type (wt), knock-out and knock-in HL-60 cell-lines with and without RA. The current HL-60 model architecture described the dynamics of 729 proteins and protein complexes interconnected by 1356 interactions. An ensemble strategy was used to compensate for uncertain model parameters. Consistent with previous experimental studies, the initial HL-60 model showed up-regulation of BLR1 expression following RA exposure along with sustained MAPK activation. The initial simulation studies led to several testable structural linkages between BLR1 expression and MAPK activation. When taken together, our modeling efforts have established a prototype organization the differentiation program in HL-60. BLR1 acts as part of a feed-forward control element which drives its own expression and that of other components required for differentiation. More broadly, we have demonstrated that modeling of molecular programs can help prioritize experimental directions and expand current biological knowledge despite model uncertainty.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

Proceedings
MATHMOD 2009 Vienna
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Mathematical Models and Their Correspondence to the Physical Reality

CALIBRATION OF FLEXIBLE STRUCTURES FROM MULTIPLE MEASUREMENTS

(REDUNDANT MEASUREMENTS BETTER THAN COMPLEX MODELS)

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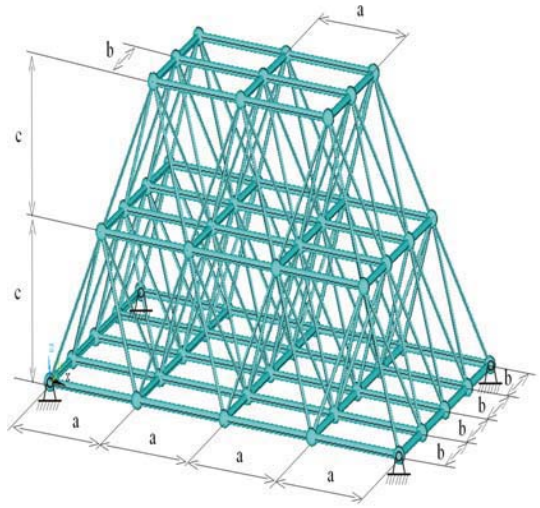
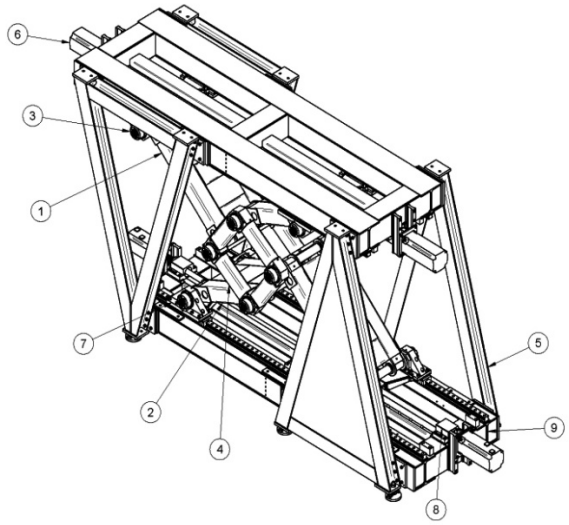
Introduction. The paper deals with calibration and identification of mechanical properties of mechanical structures of truss type. It includes both the structures of civil engineering constructions and the parallel kinematical structures of robots, machine tools and measuring machines.

Concept. The common concept is that the mechanical structure is equipped with network of multiple sensors and based on the measurements the properties (models) of the investigated structure are reconstructed. The important problem is the selection of ratio between the number of reconstructed parameters and the number of measurements and/or the complexity of applied models.



Spatial frame structure



Parallel kinematic machine Sliding Star

Frame structures. One problem [1] deals with the identification of structural stiffness model of a spatial frame structure (Fig. left) using network of multiple sensors measuring the deformations of particular nodes (joints) for several loading cases. The necessary network of measurements can be significantly reduced. The structure treated as truss is more difficult to be identified than the frame structure. On the other hand the eliminated measurements in the inside nodes worsen the problem conditionality. The frame structure can be generalized to the complete identification of continuum model.

PKM structures. Another problem [2] deals with the determination of the TCP position of machine tool accurately during the operation of the machine tool in case of parallel kinematic machines (PKM) (Fig. right) that is treated as compliant mechanism. Two approaches for the determination of TCP position of deformable PKM can be distinguished. The first one is based on the model of compliant mechanism of PKM. The second one replaces this complex model by redundant measurement. The first approach uses relatively complex model of compliant mechanism and is based on the belief that simulation can truly predict the reality. The second approach uses just the geometrical model where the flexibility is described by the variability of mechanism dimensions. This approach is based on extensive redundant measurement.

Conclusion. The common conclusion from both cases is that the usage of complex models should be replaced by redundant measurements for simpler models. The method of redundant measurement seems more robust and promising for industrial usage.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

THE UNSTEADY KUTTA CONDITION

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A potential flow based Boundary Element Method was developed to estimate the hydrodynamic forces on flapping wing [1,2]. A new formulation of the unsteady Kutta condition, postulating a finite pressure difference at the trailing edge of the oscillating wing, was implemented in the numerical procedure: its theoretical and physical foundations are here discussed.

The trailing-edge condition, necessary to obtain a unique solution, is derived from the unsteady Bernoulli equation, that is, the conservation of momentum equation for incompressible fluid and irrotational flow. It implies that the second derivative of every involved function, such as the fluid velocity and pressure, exists and is continuous (C^2 space). This is not the case everywhere in the considered domain as the airfoil is a C^0 profile with one singularity at the trailing edge.

There is not any experimental evidence supporting the notion that the pressure difference at the trailing edge ought to be equal to zero for unsteady motion, as it is usually assumed in the literature [1,2]. In essence a logical first step in the formulation of a comprehensive unsteady Kutta condition could be the relaxation of the postulated zero pressure difference at the trailing edge. This would allow considering the variation in direction and magnitude of the velocities in the vicinity of the trailing edge, that is, the formation and shedding of trailing-edge vortices.

More generally, such an assumption implies that the energy supplied for the wing motion would generate trailing-edge vortices. Their overall effect, which depends on the motion initial parameters, would be a jet of fluid that propels the wing. As the kinetic energy is transferred from the jet back to the wing, the vortices would disappear. The postulated pressure difference at the trailing edge is then fundamental for such a model as it can justify the velocity difference that generates the thrust-producing jet.

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UNSTEADY FLUID MECHANICS EFFECTS IN WATER BASED LOCOMOTION

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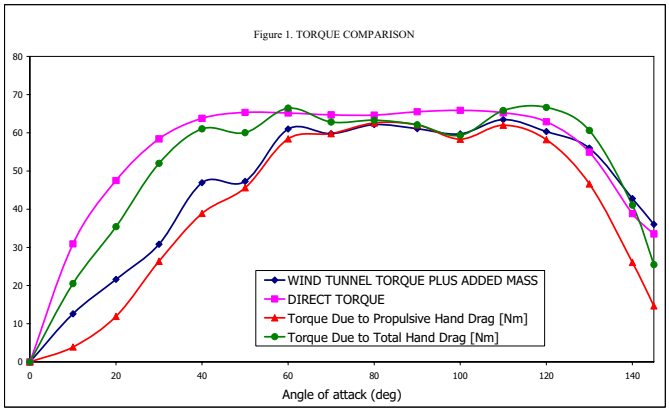
Introduction. Water based locomotion as well as the flights of birds have been studied with a different intensity over the last 70 years. Most of the emphasis has been on development of analytical methods for estimation of the forces. However, such models have limited success as the resulting mathematical equations are too complex and analytical approximations are only appropriate for Stokes flow. The emergence of powerful Computational Fluid Dynamics (CFD) commercial packages shifted the attention towards the development of powerful computational methods that leads sometimes to compromise of physical models and mathematical rigour [1]. For example some of the most used computational methods such as Large Eddy Simulation (LES) and Direct Numerical Simulations are not proven mathematically but are very widely used in industry. The author aimed to establish the physical soundness of the use of simpler but rigorous mathematical to model and assess the relative importance of different unsteady flow factors in modelling human arm propulsion during a front crawl stroke.

Method. The present work aimed to estimate the hydrodynamic forces during front stroke in swimming by considering different unsteady effects such as the added mass effect, flow turbulence and free-surface effect on the propulsion. The model was implemented into stages to establish the relative importance of the different effects. Initially only a quasi-static model of the drag and lift was implemented and this model showed large discrepancy with experimental data obtained from an instrumented robotic arm [2, 3]. The next stage was to model the added mass effect which is specific for accelerating bodies in water or denser fluids in general. The added mass effect was modelled with the use of Boundary Element Method. Despite using the La while the free surface effect was modelled by CFD software (Fluent®) by using the Volume of Fluid (VOF) technique. From these data the Drag, Lift Forces and Torque were calculated assuming quasi static conditions and compared with those obtained with the same software and model but in absence of free surface. Both laminar and turbulent flows were considered and compared. The results show clearly that the importance of the added mass far supersedes the free surface effect.



Discussion. The proposed approach in essence quasi-static showed very food agreement with the experimental data which was somewhat surprising as an accuracy of 3% average d 5% maximum error was a lot better result than expected. Complex and less physically meaningful models as the free surface simulation and turbulent flow added relatively little improvement of about 1% but their physical meaning is dubious as input parameters cannot be measured. The success of the quasi-steady approach is probably due to the relatively low frequency of human swimmers and for aquatic species this is not adequate as the dynamic thrust generation is the major propulsion contributor. This dynamic approach as presented in [4,] allows to better understand where exactly are the main mechanisms for water propulsion of aquatic species. Understanding of these principles is important if we are to produce successful biomimetic designs. In order to do this sound physics models are essential. Understanding of the added mass effect is an important step in this direction.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

Proceedings
MATHMOD 2009 Vienna
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Nonlinear Oscillations

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

DELAY TUNED PHASE-LOCKING IN A PAIR OF COUPLED LIMIT CYCLE OSCILLATORS

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Coupled limit cycle oscillators have been studied in the context of many different disciplines including but not limited to physics (Strogatz and Mirollo, 1988; Kuramoto, 1984), chemistry (Bar-Eli, 1985) and biology (Kawato and Suzuki, 1980). In particular, dynamical behavior of a pair of coupled limit cycle oscillators has been studied quite extensively for coupled van der Pol oscillators, both for the case of strong and weak coupling (Storti and Rand, 1982; Chakraborty and Rand, 1988), with (Wirkus and Rand, 2002) and without time delay (Rand and Holmes, 1980).

Our study is motivated by the dynamics of the central pattern generator of primitive vertebrate like lamprey. The mathematical model considered in this paper is a proposed scaled version for traveling wave generation mechanism in lamprey spinal cord assuming uniform immediate neighbor coupling. Hence, the time delay originates either due to signal transmission (communication delay) or due to segmental processing (inevitable for a robotic implementation with distributed computing). In particular, we study the dynamics of two delay-coupled limit cycle oscillators. The mathematical model considered here involves time delay in the state as well as in the derivative of the state, both of which constitute the coupling.

The equations for the pair of coupled oscillators have the form:

$$\ddot{x}_1 + (x_1^2 + \frac{\dot{x}_1^2}{\omega^2} - A_1^2)\dot{x}_1 + \omega^2 x_1 = \alpha x_2(t-\tau) + \beta \dot{x}_2(t-\tau)\,,$$
$$\ddot{x}_2 + (x_2^2 + \frac{\dot{x}_2^2}{\omega^2} - A_2^2)\dot{x}_2 + \omega^2 x_2 = \alpha x_1(t-\tau) + \beta \dot{x}_1(t-\tau)\,,$$

where α and β are the coupling strengths, A_1 and A_2 are the amplitudes of each uncoupled oscillator, ω is the common angular frequency, and τ denotes the time delay in coupling. First, the equilibria of the actual system are found and linear stability analysis is performed. Next, we analyze the system for the case of weak coupling by the averaging method. It is shown that the weakly coupled oscillators can achieve phase-locked solutions only at the expense of delay tuning. All such "delay-driven equilibria" were computed and their stability were characterized (using linear stability and center manifold analysis).

Numerical simulations of the original as well as the averaged system matches the analytical predictions. Further, the numerics reveal some more qualitative behavior of the system dynamics including the destruction of the four dimensional tori with the variation of parameters.

One important result revealed was the dynamics of the phase locking as the time delay was varied. It was shown that only two cases may result stable equilibria, one of them for the case of in-phase locking and the other one for out-of-phase locking. The global dynamics exhibits dependence on the intersegmental coupling strength.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

Wave Propagation in Periodically Excited Fluid Transmission Lines with a Nonlinear Compressibility Law

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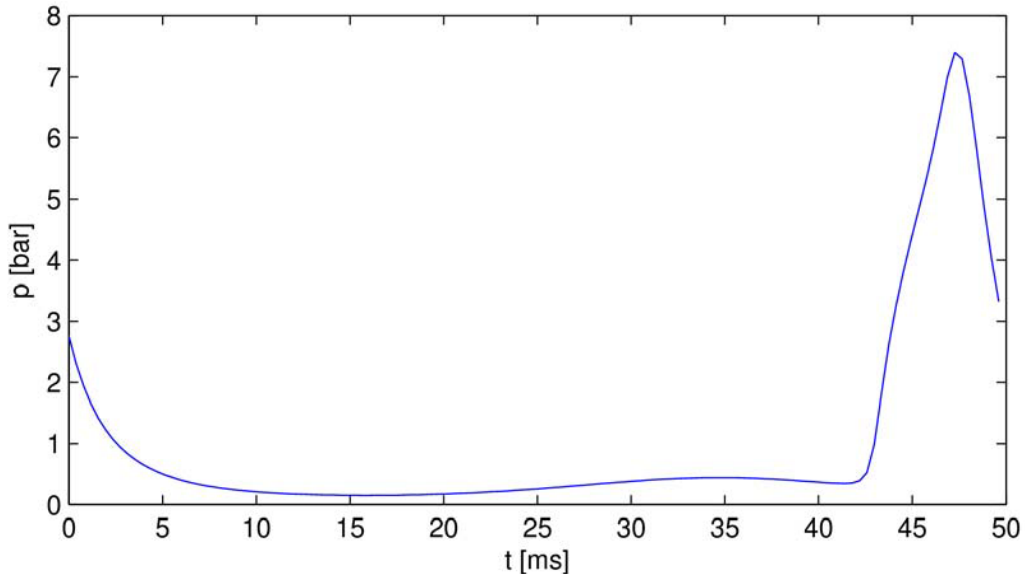
Abstract. Pipelines filled with a weakly compressible fluid such as mineral oil or water play an important role in many fields of technology such as internal combustion engines or hydraulic drives. A number of interesting problems such as the prediction of pressure ripples for piston pumps or the simulation of fuel injections systems at a single operating point share the property of periodic boundary conditions. The phenomenon of wave propagation in transmission lines is well understood in the case of a weakly compressible fluid with a linear material law. For this type of problem, the periodic case can be treated with high computational efficiency by using transcendental transfer functions in the frequency domain. This paper aims at the computation of pressure and flow waves arising in liquid transmission lines with periodic pressure and/or flow boundary conditions and a nonlinear law of liquid compressibility. The nonlinearity is due to the presence of small gas bubbles in the liquid. This condition frequently occurs in the low pressure part of fluid power systems where dissolved air is released. An isothermal behaviour of the gas bubbles is assumed in this paper for computational simplicity. The validity of this assumption or more likely the need for a refined model with a detailed description of the gas behaviour will be the focus of experiments in the near future.

The proposed method. The equations for the wave propagation in a fluid filled transmission line are solved for a special material law which describes the behaviour of a mixture of a liquid and a gas. The liquid is weakly compressible with a constant bulk modulus of compressibility and the gas is assumed to be evenly distributed throughout the liquid in the form of small bubbles with an isothermal state change without any dynamics in the material law. Especially the process of air release and back-solution is not modelled. The combined behaviour of the liquid and gas fractions has been cast into a material law giving the mean mass density of the liquid and gas mixture as a function of the hydrostatic pressure. This algebraic equation is substituted into the equations derived form first principles, i. e. the conservation equations for mass and momentum in axial direction. The viscous friction is modelled using a transfer function known as the frequency-dependent friction model for transient, laminar pipe flow. After a discretization in space using a Galerkin approach on a staggered grid and a discretization in time by a simple point-collocation scheme with centered differences for the time derivatives, a large equation system is solved for the periodic answer to the sinusoidal flow-rate excitation. The result given in the figure below clearly shows the strong nonlinear effects in the system. While the system without gas bubbles has an almost constant speed of sound at least for moderate pressure variations, the solution of the nonlinear system is far from an harmonic response. A broad region of very low pressure is due to the influence of the highly compressible gas fraction which provides for a very large compliance of the fluid column within the transmission line at low pressure values. However, the incoming wave hitting the flow-rate boundary condition generates a high pressure peak due to the progressive stiffness behaviour. All in all, the proposed approach is capable of reproducing some phenomena observed in low pressure lines of fluid power systems. The experimental verification – probably together with some amendments to the model – will be published by the author in the near future.

Figure: Periodic response of a transmission line with a nonlinear fluid compressibility to a sinusoidal excitation.



COMPUTATION OF STABILITY BOUNDARIES OF OSCILLATIONS STARTING FROM EQUILIBRIA

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Periodic oscillations are ubiquitous in models in the physical and life sciences. One question that arises is how such oscillations depend on one or two model parameters and the size of the parameter domain. This can be studied by numerical bifurcation analysis using a software package such as MATCONT [2]. Typically, one then encounters stability boundaries of these oscillations in a parameter plane. When there is a transition from stable equilibria to oscillations, such stability boundaries usually emerge from codimension two bifurcation points as codimension one bifurcation curves. We present a new method to start the computation of the related bifurcation curves directly from these equilibria [1]. These are generalized, fold- and double Hopf points. A more intuitive approach is discussed in a classical example. We indicate why this intuitive approach can be time consuming and how this is circumvented with the new method. The algorithm is implemented in MATCONT which we use to study a system of coupled excitatory and inhibitory cells.

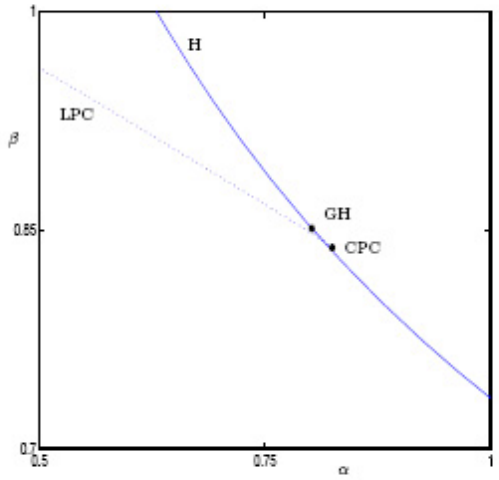

Figure 1: Bifurcation diagram of the Watt-Governor system in (α, β)- space [3]. The equilibrium is stable below the Hopf curve (H), while the stable oscillations exist in the parameter region above the boundary delimited by the Hopf curve and the saddle-node of cycles curve (LPC). There are two codimension two bifurcations: GH Generalized Hopf, CPC Cusp of limit cycles. The LPC curve is very close to the Hopf curve near the GH point before turning at the cusp. Therefore it is not easy here to start the computation of periodic orbits from the Hopf curve and to find a point on the LPC curve by continuation of the periodic orbits. The new method computes the LPC curve directly.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Modelling the Swarm

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

THE EFFECTIVENESS OF THE "COMMON STOMACH" IN THE REGULATION OF BEHAVIOR OF THE SWARM.

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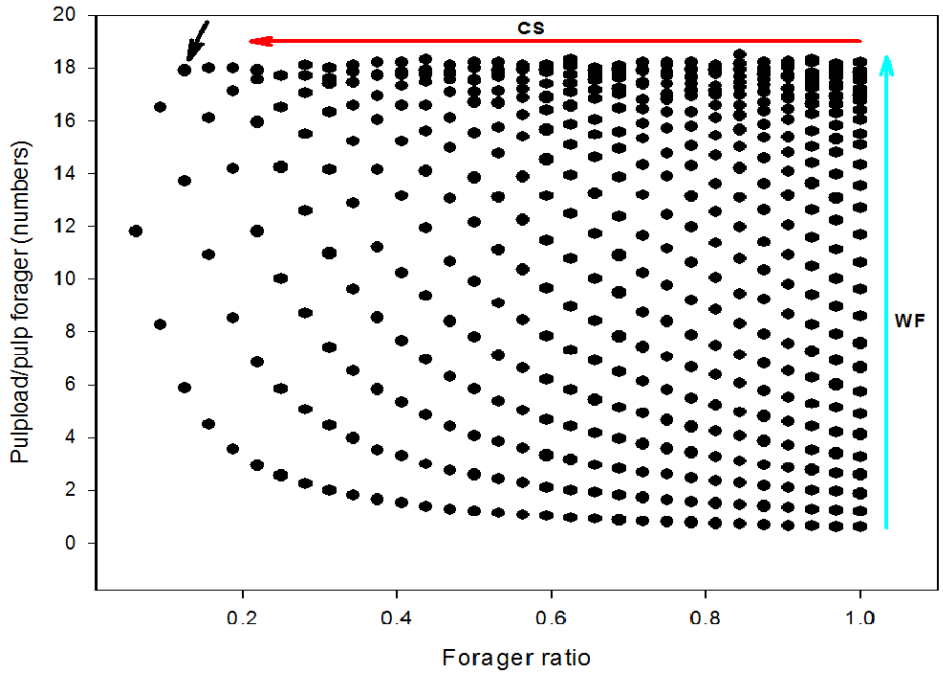
Wasp nests are the center of social life and inter-individual interactions for wasp societies, therefore building and maintaining these nests are crucial for the colony. This requires building materials, pulp and water foragers, builders and also an organization of workforce for effective construction. Inspired by the construction behavior of social wasps, [1] an agent-based model is presented. Our goal is not to model the exact behavior of wasp societies, but rather to investigate in a more abstract way some of the features of the common stomach. The central hypothesis of this study is that the societies developed a social crop or common stomach which stores water and provides a mechanism for worker connectivity, which in turn regulates building.



Effectiveness of the pulp forager (pulp load/pulp forager: pulp delivered by a single pulp forager between 100 and 200 time steps) as the function of the forager ratio ((WF+PF)/swarm size) in the swarm. Dots with the same forager ratio represents different WF and PF mix while the total number of foragers stays the same. Blue arrow shows how the number of water foragers increases in the mix. Red arrow shows how the number of common stomach wasps increases in the mix. Black arrow shows the first highly productive colony with 1 pulp forager 3 water foragers and 28 common stomach wasps. Average values of 25 simulations, colony size 32 wasps.

We demonstrate how colony efficiency changes as a function of colony size and the constitution of the labor distribution, as well as how indirect interactions increase efficiency. Our findings imply that the effective and low risk use of a worker force via worker connectivity (common stomach) is reliant upon larger colony sizes. Our studies showed that the usage of common stomach wasps decreases the number of foragers and maximizes the effectiveness of the pulp forager. Using the common stomach as a regulator and buffer also keeps most wasps on the nest where they can provide additional work while they hold water, such as patrolling, defense, and so on. The use of the common stomach seems to be an efficient mechanism of self-organization in the behavior of the swarm. The benefit of organizing colony level performance through worker connectivity may function as an important evolutionary pressure for increasing colony size for insect societies [1].

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

AN INDIVIDUAL-BASED MODEL OF COLLECTIVE ATTENTION

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With the ongoing growth of mass media and communication technologies, people are every day confronted with an increasing amount of information of any kind. Pieces of information can be broadcasted through television, urban advertisements or Internet, or exchanged directly between people through emails, phone calls or personal communications. As a side effect, the amount of information an individual is facing in its everyday life exceeds by far its processing abilities and attention capacities. Therefore, people have to *select* which elements of their environment are relevant and which will be ignored or roughly checked out.
Interestingly, when selecting items they will pay attention to, individuals are strongly influenced by other people's choice. First, because people like to share the same topics of interest as their friends, second, because popular novels are more relayed in the media, which increases their level of attraction and, finally, because people are naturally curious about what others are attending to.
The study of collective attention is, therefore, a main issue in the understanding of various herding phenomena, such as the spread of ideas or the outbreak of commercial trends resulting in best sellers or blockbusters.

In this article, we develop an individual-based model of collective attention to better understand the internal dynamics of such a system. We suggest that each agent of our model owns a limited amount of attention that can be shared over many items. We also define an environment made of N items, each item being characterized by its age and popularity. The age of each item naturally increases in time, while the popularity is the amount of attention the item received from the agents. Given this framework, we rely on early empirical observations to define a set of rules defining the agents' behavior:

1. Agents are attracted by what other agents already attend to.
2. Agents give a certain amount B of their attention to these items, where B is proportional to the novelty of the considered items.
3. Agents continuously recover a small amount of attention they previously gave to each items.

The above model has been tested in various simulation setups. In a situation where 100 agents are facing a flow of many items per time step, the model predicts a burst of attention around novel items that deceases and vanishes some times later, as it has actually been observed. Moreover, the distribution of the maximum level of popularity each item has reached at the end of the simulation shows that most items are barely considered by the agents while a few of them reach a high level of popularity.
Finally, the exploration of the model predicts an interesting form of competition between the events: an item appearing when many others are present will be less considered, since all the population is already attending to something else. This competition may be compared to situations where several commercial products (e.g. movies or books) are released at almost the same time.

FUNCTIONAL EFFICIENCY OF BIOLOGICAL TRANSPORT NETWORKS: WHY THE BEHAVIOUR OF NETWORK USERS MATTERS

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Recent studies on transport networks in social insects have mostly focused on the structural properties of these networks. Based on topological measurements and comparisons with theoretical networks, these studies have estimated the efficiency and the robustness of various insect transport networks, especially in termites and ants. The structure of a network however does not necessarily reflect the way it is exploited by its users. Social factors for instance, as attraction toward or repulsion from conspecifics, may favour the use of certain parts of a network, whatever its underlying topology. As a consequence, topological measurements do not always give a reliable picture of the functional efficiency of a given network.

In this contribution, we illustrate this statement through the example of foraging trail networks in ants. These trail networks form in general one or several dendritic trees originating from the nest of the colony. In several ant species, field and experimental studies have shown that these trees display a particular structure: the mean angle between trail bifurcations as they branch out from the nest is 50°-60° (*Atta sexdens*, *A. capiguara*, *A. laevigata* and *Messor Barbarus*: Acosta et al. 1993; *Monomorium pharaonis*: Jackson et al. 2004; *Formica aquilona* and *Linepithema humile*: data not published). Therefore an ant exiting the nest and moving toward food sources located at the periphery of the network generally faces symmetrical bifurcations, i.e. the two trails that follow a bifurcation deviate by approximately 30° from the original direction of the ant. An ant coming back to its nest on the other hand faces asymmetrical bifurcations: at a bifurcation, the trail leading to the nest that follows the bifurcation deviates less (~30°) from the ant original direction than the other trail (~120°) that lead away from the nest.

At first, we experimentally investigated the individual behaviour of the Argentine ant *L. humile* while crossing symmetrical and asymmetrical network bifurcations in gallery networks. We showed that this ant behaved differently according to the direction it approached a network bifurcation. In the absence of any other orientation cue, fed (coming from the source) and unfed (coming from the nest) ants crossing a bifurcation from its symmetrical side equally selected both branching trails. On the contrary, 2/3 of the ants reaching the asymmetrical side of a bifurcation chose the branch that deviates by a 30° angle, while the remaining 1/3 chose the branch that deviates by a 120°.

As a second step, we studied with computer simulations the consequences of this individual behaviour at asymmetrical bifurcations on the foraging efficiency of the colony. We simulated colonies of 500 ants foraging within a dendritic trail network, which bifurcations mimicked those found in natural trail networks. While foraging within their networks, Argentine ants lay down a pheromone trail that is followed by other ants, which in turn lay down additional pheromone deposits that attract even more ants. This self-enhancing mechanism may eventually lead to the selection of the shortest route that connects the nest of the colony to a food source (Goss et al. 1989).

Our simulation results clearly showed that the performance of the colony to find the shortest path linking the nest to a food source was better when virtual ants expressed the preference for the branch that deviates by 30° at asymmetrical bifurcation. If this preference is removed from the simulations, the ants dispersed more evenly inside the network and were less capable to select a path toward the food source. Moreover after only fifteen minutes the foraging e ciency, measured as the proportion of returning ants carrying food, was three times higher when ants expressed the preference.

We conclude that biased individual behaviours coupled with social factors can have a major impact on the pattern of exploitation of transport networks in ants. Understanding the coupling between their behaviours and the structure of their networks is essential to accurately evaluate the efficiency of their nest galleries or their foraging trails.

In a more general context, our results emphasize the role of the individuals that operate within a transport network. Therefore, their interactions with the structure of the network in one hand, and with other network users in the other hand, should not be investigated separately.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A MACROSCOPIC PROBABILISTIC MODEL OF ADAPTIVE FORAGING IN SWARM ROBOTICS SYSTEMS

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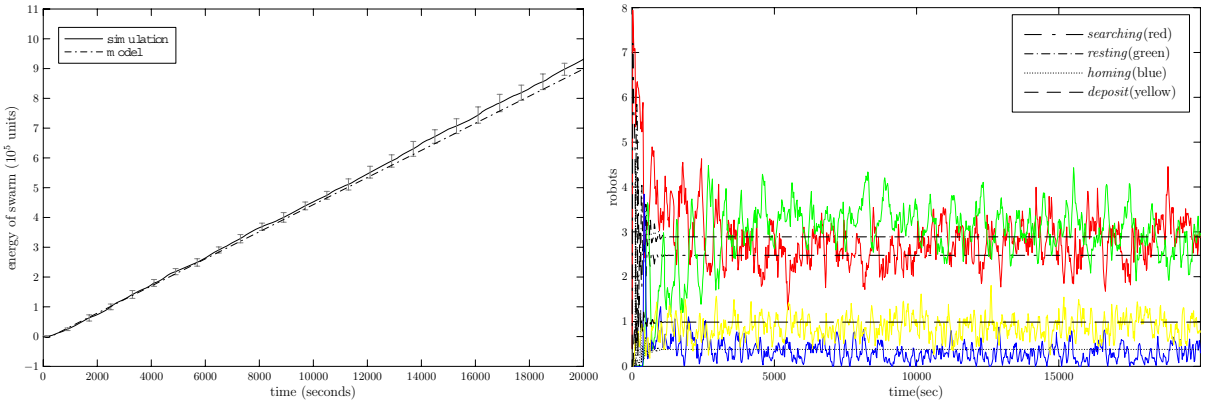
In this paper, we extend a macroscopic probabilistic model of a swarm of foraging robots from the homogeneous to the heterogeneous case. In the swarm, each robot is capable of adjusting its searching time threshold and resting time threshold following the rules described in our previous paper [1]. In order to model the difference between robots, private resting time and searching time thresholds are introduced. The robots resting at home are divided into two subsets according to which states they are transferred from, either state *Deposit* or state *Homing*. For each subset of robots, private resting time and searching time thresholds are used to calculate the effect of social and internal cues. The transition between state *Resting* and state *Searching* is then decided by the corresponding private resting time threshold. Corresponding to private resting time thresholds, a public resting time threshold is used to track the contribution of the social cues, internal cues and environmental cues for the whole swarm, which is a global property owned by all robots. Although the public resting time threshold doesn't affect the behaviours for the individual robots directly, it affects the private resting time threshold and vice versa. Similarly, a public searching time threshold is introduced to track the contributions of the adaptation cues. The behaviours for the robots searching for food in the arena are constrained with the corresponding private searching time threshold, which is 'inherited' from the public searching time threshold but will affect it as well. With these considerations, a number of equations are then developed to work out the relationship between these private time thresholds and public time thresholds based on previously developed difference equations in [2]. The resting time and searching time thresholds are dealt with separately because each of them has its own valid scope. The extended macroscopic probabilistic model has been tested using the simulation tools Player/Stage. A set of intuitively chosen adjustment factors which are presented in our previous paper are used to validate the macroscopic model. Figure 1 (a) illustrates the instantaneous energy of the swarm from both the simulation and macroscopic probabilistic model with the food growth rate set to 0.05. The error bars represent the standard deviations of data recorded from 10 experimental runs. This shows clearly that the data from simulation fits very well to the curves obtained from the macroscopic model. Figure 1 (b) then plots the instantaneous number of robots in selected states from the simulation and the model. We see that the number of robots in each state predicted by the macroscopic model reflects the corresponding average number of robots from the simulation. Given the accuracy of the model, we can use any appropriate searching techniques to find an approximate optimal solution for the previously developed adaptation algorithm. Although the model is specific to adaptive foraging, We believe the methodology can be extended to other systems in which the heterogeneity of the system is coupled with its time parameters.



(a) **(b)**

Figure 1: (a) The instantaneous energy of the swarm (8 robots). (b) The average number of robots in selected states, where the horizontal dashed lines are from the model while the coloured curves from simulation.

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FINDING OPTIMAL COLLECTIVE STRATEGIES USING INDIVIDUAL-BASED SIMULATIONS: COLONY ORGANIZATION IN SOCIAL INSECTS

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Abstract. Social insects like ants and bees live in cooperative colonies containing up to millions of individuals. These colonies are sometimes termed "superorganisms", and have evolved tightly integrated and sophisticated collective behaviors. Different species, however, often differ in the type and mechanisms of communication and collective organization employed. I show here how individual-based models can be used to identify the non-intuitive benefits of different mechanisms of collective organization. This allows us to understand under what ecological conditions particular types of communication or division of labor may have evolved, and thus can also explain variation among species. I will present the results of two modeling efforts, one concerned with different communication systems, the second focusing on different mechanisms of task allocation within the nest. In studying self-organized collective behavior, individual-based models are ideal. To implement such models, I use SeSam (www.simsesam.de) and the SWARM library in Objective C (swarm.org). Because my models are spatially explicit and contain behavioral or information-heterogeneity among agents, they often contain a (relatively) large number of parameters, whose numerical values may have an impact on the predictions produced by the model. This necessitates the use of similar techniques as empirical research, namely a strict hypothesis-testing approach and extensive sensitivity analyses [1-3]. I found that in the case of bee foraging, recruitment is most beneficial if there are few, low quality resources, but that patchiness per se, and colony size, have no impact on benefits of recruitment [1]. This shows that recruitment evolved in honey bees and not bumble bees likely because of differences in their ecology, not their colony size. In division of labor, I show that the ratio of workers to work available has an impact on the optimal task allocation system. Further studies in this direction may help to understand the evolution of diverse task allocation mechanisms in social insects.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

INDIVIDUAL BASED MODELLING OF TEMPERATURE INDUCED AGGREGATION BEHAVIOUR

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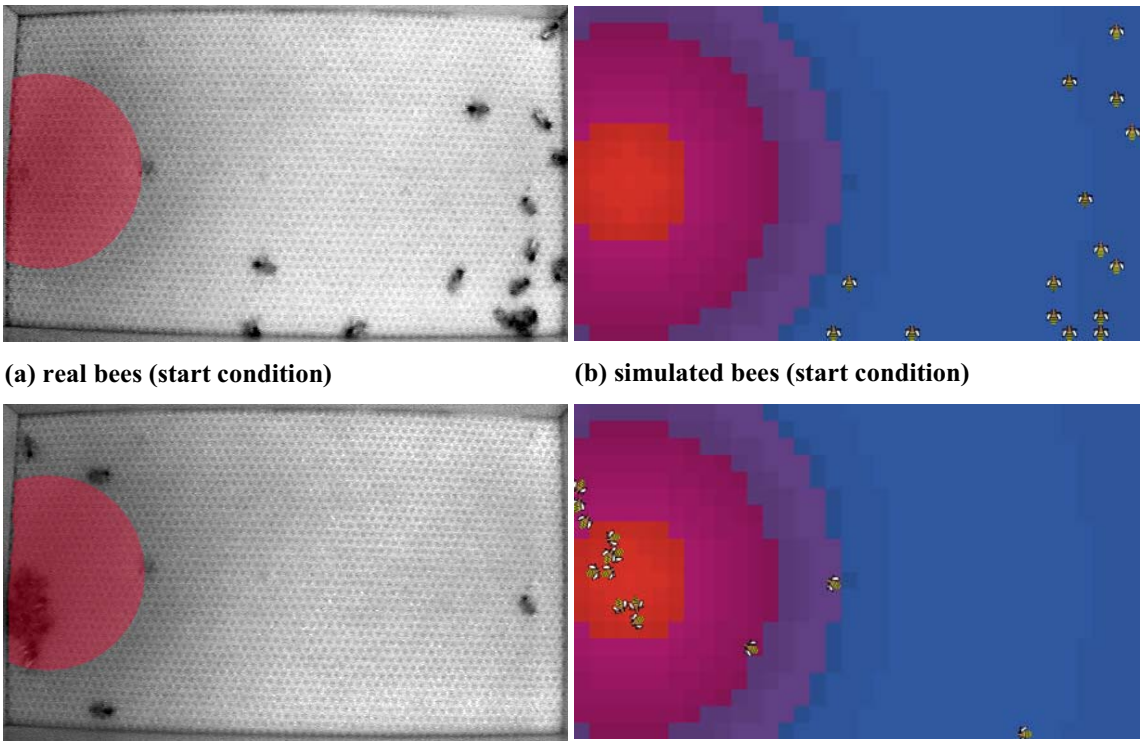
There are several species of animals from different phyla that are known to exhibit diverse forms of social behaviour. Certain insect species like honeybees implement an interesting form of emergent social behaviour, based on a simple set of rules for individual behaviour rather than on complex cognitive interactions between individuals or with a leader. A good example for the bees' swarm behaviour is temperature induced aggregation. Young bees show a clear preference for temperatures around 36° C [1]. If a group of bees is allowed to move freely on a ground exhibiting a two dimensional temperature gradient, their likeliness to come to rest in an area of preferred temperature is positively correlated to the number of interacting individuals up to a certain level. We suggested four different hypotheses to explain the basic mechanisms of this behaviour. In order to test them, we developed an individual based (bottom-up) NetLogo [2] model which allows us to simulate a group of bees moving in a temperature gradient. By varying the influence of each of the four hypothetical mechanisms and comparing the result of the respective simulation to the results of real life experiments, we receive valuable clues to determine the likeliness of each hypothesis.

The model proved successful in replicating many aspects in the bees' behaviour. As an example, the figure below demonstrates the model's ability to reproduce certain aspects of the real bees' behaviour. It shows a comparison of the results of a real experiment with bees in an arena exhibiting a temperature gradient on its ground and a simulation with a similar setup.



(a) real bees (start condition) **(b) simulated bees (start condition)**

(c) real bees (end condition) **(d) simulated bees (end condition)**

(a) and (b) show the starting setup of a real experiment and a comparable simulation run, (c) and (d) show the clustering resulting after 10 minutes. In both cases, a steep temperature gradient was used (real experiment 26 - 36° C, simulation 22 - 36° C). The area of optimum temperature in the real arena is marked by a circle.

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[2] NetLogo website: ccl.northwestern.edu/netlogo/

Robustness of Two Interacting Robot Swarms Using the BEECLUST Algorithm

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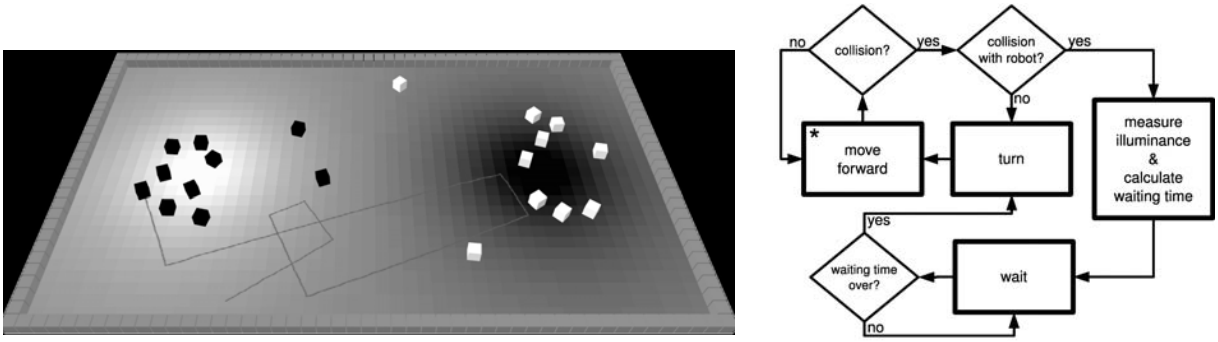
Compared to single robot systems, robot swarms have the advantage to work quite robust, because the removal or malfunction of single individuals affects the behaviour of the whole swarm only slightly. Robot swarms are also able to act "swarm intelligent" which permits a group of individuals to make decisions to reach a common goal in a decentralised manner [1].

In the work of [2] it has been shown that a swarm of Jasmine III robots using the BEECLUST algorithm, which is inspired by honeybee behaviour, is able to find locations of maximum illuminance using a few simple rules. Based on this work we investigated how the robustness of the BEECLUST algorithm is affected by the swarms population and how it is influenced by a second group of robots in the same arena performing a different task at the same time.

For our experiments we used SMARS (Small Robot Simulator). In this simulation environment we were able to simulate two different castes of Jasmine III robots which were implemented with the physical properties of the real robots. One caste waits longer at places of high illuminance ("light finders") after robot-to-robot collisions, the other one at places of low illuminance ("shadow finders") after such collisions. We added two different kinds of optima, a light-spot with 1000 lux for the "light finders" and a shadow-spot with 0 lux for the "shadow finders". To test the robustness of a robot swarm against disturbances caused by another swarm performing another task we added groups of variable numbers of "shadow finders" and observed how they affect the aggregation behaviour of the "light finders".



Left: Screenshot of the simulation environment SMARS. The bright area is the optimum for the "light finders" with 1000 lux and the dark area is the optimum for the "shadow finders" with 0 lux. The ambient illuminance is 500 lux. Robots are represented by boxes: black boxes represent"light finders", white boxes represent "shadow finders". The line shows a trajectory of a randomly chosen robot for demonstration purposes. Right: Finite state machine of the BEECLUST controller. Boxes represent the different behavioural states of a robot. * indicates the starting point. Diamonds represent control structures (if-else decisions).

We found that small populations of "light finders" aggregate faster and more efficient by an increasing number of "shadow finders", thus we observed a sort of cooperation emerging within our heterogeneous robot swarm. Medium populated swarms only take small disadvantages by increasing numbers of "shadow finders" and large "light finder" populations take strong disadvantages in speed but are not affected in their aggregation efficiency.

With the work at hand we show that the BEECLUST algorithm is not only capable of working robust in a homogeneous robot swarm, but it is also suitable in heterogeneous robot groups with differing controller strategies, even without discrimination of caste affiliation of other robots.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

PATTERN FORMATION AS A TRANSIENT PHENOMENON IN THE NONLINEAR DYNAMICS OF A MULTI-AGENT SYSTEM

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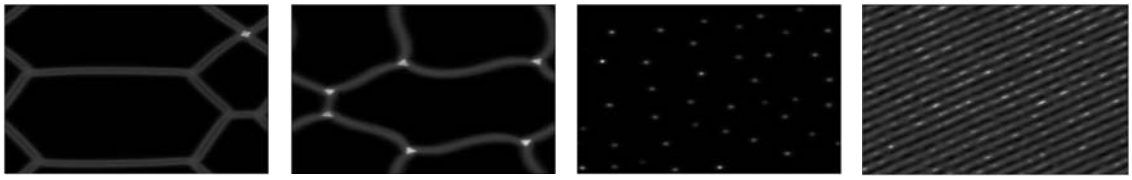
This paper presents a microscopic model (agent positions, directions, and interactions are explicitly modeled) of mobile agents (or self-propelled particles) that is inspired by and similar to the "complex transport networks" reported by [1]. In the system reported here, however, the agents' positions are modeled continuously. This multi-agent system (or artificial swarm) shows a wide variety of self-organized pattern formations. The self-organization is based on the nonlinearity of the agents' turns (discrete jumps in the agents' directions) and the indirect interactions of the agents via a potential field that determines their motion (high values are attractive) and which is changed by themselves (agents increase the value of the potential field at their positions). At least most of the irregular and complex patterns are transient. Fig. 1 shows some typical examples of the patterns found in the potential field and obtained by varying the rotation angles (value of the discrete jumps in the direction). These plots demonstrate the variety of patterns that are generated by the investigated system. The patterns found during the transient are more complex than those the system converges to. Still, I believe this transient behavior is relevant because most complex self-organized phenomena seem to be based on transient behavior. I empirically investigate the transient times in dependence of the system's size and give examples.



(a) 45^o (b) 80^o (c) 165^o (d) 255^o

(e) 300^o (f) 330^o (g) 350^o (h) 355^o

Figure 1: Patterns for a varied parameter (rotation angle).

It is well known that transient times scale exponentially with the dimensionality in many high dimensional systems. I estimate a lower bound of the average transient time depending on the system's size. This is done by measuring the time until a simple pattern (without bifurcations) is reached. The result (not shown) indicates an exponential increase of the average transient time with increasing system size as expected.

The behavior of the system is more complex for bigger sizes and bigger agent numbers. In the full paper we give diagrams for two examples of bigger systems based on a parameter a representing the activity in the potential field (percentage of potential field areas with high values). In some cases the behavior is dynamic most of the time. New patterns emerge and break down again. Even very low values of a are reached corresponding to patterns of very low complexity. However, these states are not stable and more complex patterns emerge again. Also time intervals of little dynamics are found. Whether this irregular behavior is transient stays unanswered. In contrast, in other cases the system (most likely) converges to a stable pattern after a long transient.

I conclude that the transient is the most relevant phase in at least some self-organized dynamical systems. Thus, it is a concern of these natural systems or of the designer of artificial systems to extend the transient.
An investigation of the influence of noise to this system is pending. In first experiments, no qualitative changes for reasonable intensities of noise were found concerning the formation of patterns and the influence to transient lengths. This will be the focus of future work.

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Modelling, Analysis and Control of Distributed Parameter Systems

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

HAMILTONIAN FIELD THEORY AND MECHANICS

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The Hamiltonian formalism is well known describing phenomena which can be modeled by ordinary differential equations. The main ingredients of the theory are a representation of the equations in an evolutionary first order form and under some regularity assumptions the Legendre transform yields a connection with the well known Lagrangian description. There exist several approaches that extend this Hamiltonian description to systems that are described by partial differential equations, where the general question arises if the formulation as an evolutionary description should be maintained. A description in evolutionary form requires to single out an evolution parameter, for example the time, and this leads to the introduction of the variational derivative with respect to the Hamiltonian. This approach is well known in the literature [2]. Another possibility to describe field theory is an approach going back to *De Donder*, which is based on the conservation of the symmetry with respect to all the independent variables, i.e., the time and the space. This leads to the introduction of so called multimomenta and of course the Legendre transform differs from the case of the evolutionary approach. There exists an extensive literature describing the polysymplectic or the multisymplectic formulation, see for example [1, 2].

An interesting question is to analyze conserved quantities. This will be treated based on a Lagrangian description, which leads to well known results. These results are crucial in the Hamiltonian formulation since the desire to have a Hamiltonian description, where the Hamiltonian is a conserved quantity is desireable for control theoretic purposes.

This paper aims to give a geometric description for both approaches. We consider the polysymplectic one, and the evolutionary one, in a geometric fashion, describing the differences in the bundle construction and to show how this two approaches differ in the case of first order field theory in mechanics. As an example we will treat continuum mechanics in great detail, see [3], where we assume that a stored energy function exists. We will analyze the Lagrangian picture as well as the Hamiltonian one, where we point out the differences of the polysymplectic and the evolutionary point of view especially with respect to regularity of the corresponding Legendre morphism. Beside an analysis of higher order problems, further directions of research will include preeminently a detailed discussion of the boundary conditions.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A FORMAL METHOD FOR IMPROVING THE TRANSIENT BEHAVIOR OF A NONLINEAR FLEXIBLE LINK

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Most control systems employ two distinct kinds of control actions: a *feed-back action*, to improve the stability properties of the system and increase its robustness with respect to parameters variations and/or disturbances, and a *feed-forward action*, usually needed to achieve a rapid response and improve tracking performances with respect to a time-varying reference signal. Designing a feed-forward controller requires, generally speaking, to invert (at least partially) the dynamics of the system to be controlled in order to obtain a output-input relationship which is then put in cascade with the open loop system itself.

This paper focuses on designing a feed-forward controller for flexible beams. In robotics, this problem has been usually addressed by solving the Lagrange's inverse equation of motion in time domain. In this case, the flexible beam is a finite dimensional system of proper order, obtained under the hypothesis that the position of a point of the link is described by a virtual rigid body motion *plus* a deflection, modeled by an Euler-Bernoulli beam model with "some" zero boundary conditions compatible with the rigid coordinates (e.g. clamp-free, pin-free or pin-pin), [1, 2, 4].

The same problem has been also addressed in the context of flatness-based control, mainly with reference to the Euler-Bernoulli beam model, [3, 7]. On the other hand, the procedure illustrated in this paper is applied to the nonlinear flexible elastic beam model introduced in [6] with time-varying boundary conditions on the position/orientation of the extremities of the link and/or on the applied forces/torques. Upon linearization around the unstressed configuration, this nonlinear model simplifies into the well-known Timoshenko beam model for which a formal expression of the dynamics, i.e. of the solution of the PDE with time-varying boundary conditions, can be computed. This solution is expressed as an infinite series whose convergence properties, differently from [3, 7], are not addressed here and are currently under investigation. Some analogies in the approach can be found in [5] where a similar feed-forward control strategy for the Korteweg-De Vries equation is proposed within the flatness framework. Then, the synthesis of the feed-forward control law (i.e. the time-domain inversion of the equation of motion) is an application of well-known results for linear dynamical systems.

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GEOMETRIC REDUCTION OF DISTRIBUTED PARAMETER SYSTEMS USING PSEUDO-SPECTRAL METHODS

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Abstract.

A reduction method which preserves geometric structure and energetic properties of non linear distributed parameter systems is presented. It is stated as a general pseudo-spectral method using approximation spaces generated by polynomials bases. It applies to Hamiltonian formulations of distributed parameter systems which may be derived for hyperbolic systems (wave equation, beam model, shallow water model) as well as for parabolic ones (heat or diffusion equations, reaction-diffusion models). It is defined in order to preserve the geometric symplectic interconnection structure (Stokes-Dirac structure) of the infinite dimensional model by performing exact differentiation and by a suitable choice of port-variables. This leads to a reduced port-controlled Hamiltonian finite-dimensional system of ordinary differential equations. Moreover the stored and dissipated power in the reduced model are approximations of the distributed ones. The method thus allows the direct use of thermodynamics phenomenological constitutive equations for the design of passivity-based or energy shaping control techniques.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

GEOMETRY OF COUPLED INFINITE-DIMENSIONAL SYSTEMS

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Modeling is an essential or even the most important step for the analysis and design of dynamic systems. Hence, it may turn out that certain components of physical systems cannot be described by finite-dimensional systems due to their inadequateness to incorporate some physical effects like transportation delays, spatially-distributed parameters, hysteresis nonlinearities, and the like; this often leads to infinite-dimensional systems, which are frequently termed distributed-parameter systems. In particular, the present work considers coupled lumped- and distributed-parameter systems, whose evolution along continuous-time is allowed to be governed by coupled ordinary and/or partial differential equations in general.

In many publications, see, e.g., [1, 2, 3, 4] and references therein, differential geometric methods have already emerged as a (standard and) useful tool for the geometric analysis of finite- and infinite-dimensional systems. Hence, the approaches inherently rely on a proper geometric description of the considered dynamic systems. With regard to the class of coupled infinite-dimensional systems there are often important related aspects neglected resp. can not be captured appropriately, like (distributed and lumped) system inputs, system outputs, boundary and coupling conditions, etc. Complementarily, the main issue of this contribution is to emphasize that by some adequate adaptions and extensions of those methods as well as the introduction of appropriate geometric structures a proper geometric description of the considered systems is obtained. Thereby, the dynamic systems are associated with some suitable geometric objects reflecting their dynamics in such a manner that the description is provided in a coordinate-free manner. In this context the systems equations are supposed to describe (locally) a family of regular fibred submanifolds of some appropriately-constructed manifolds.

In addition, the first order Lagrange formalism (with first-order Lagrangian density) is considered for coupled infinite-dimensional systems, especially, including boundary and coupling conditions. It is illustrated that the proposed geometric structures fit well into this theory resp. for the derived systems. Several examples are arranged to illustrate the proposed theory.

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STABILITY ANALYSIS OF PIEZOELASTIC STRUCTURES FOR ROBUST VIBRATION CONTROL

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Abstract. Compensating for harmonic vibrations induced by rotating machinery and other periodic disturbances is a common problem in the industry and robust controller solutions accompanied by self sensing actuation for lightweight mechanical constructions, are essential to the breakthrough of active technologies in industrial applications. In fact, self sensing actuation of functional materials enables collocation of actuator and sensor. In the case of piezoelectric actuators, self sensing requires a robust separation of the time derivative of the actuation voltage from the measured electric current in order to obtain a signal which is proportional to the strain rate integrated over the piezoelectric patch area. Due to the unfavorable ratio of these two signals, the design of an observer for the electric current due to the direct piezoelectric effect seems most appropriate. The design of observers relies on accurate modelling of the underlying piezoelastic structure which in our case is chosen to be a rectangular plate equipped with two piezoelectric actuators and two opposite edges either clamped or free, see figure 1. When de-

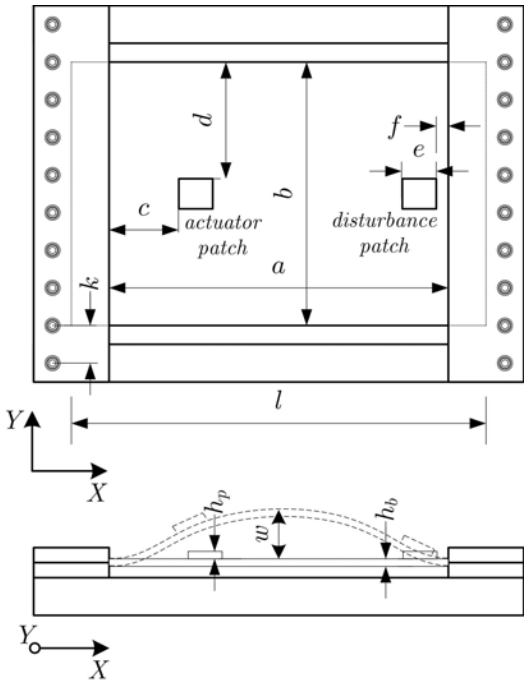

Figure 1: Geometric configuration of the piezoelastic structure under investigation.

signing a controller for the purpose of suppressing harmonic vibrations, i.e. we require the regulated output to tend to zero as time goes to infinity, the special mathematical structure of the model tremendously facilitates controller synthesis and resolves stability issues of the infinite-dimensional model in a straightforward manner by applying results on positive real transfer functions in conjunction with the small gain theorem. This result has been reported on a previous occasion, see [1]. In many cases, however, the disturbance frequency is unknown. In this case, the proposed controller can be extended by a nonlinear ordinary differential equation for the unknown frequency where the proof of stability of the infinite-dimensional closed loop involves the Hamilton Jacobi inequality together with the small gain theorem. The resulting update law for frequency estimation is only driven by the observed direct current and the regulator states.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

ACTIVE CONTROL FOR THE RE-ENTRY OPERATION OF FLEXIBLE RISERS

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This paper presents an active control dedicated to a re-entry problem found in the offshore oil industry. The re-entry operation consists in connecting the bottom of a very long pipeline to the wellhead, by dynamically modifying the pipeline top position, which is linked to a floating device (vessel or platform). These long pipelines are usually called risers, because they are used to rise the drilling mud or the hydrocarbons from the wellhead to the platform. Nowadays the re-entry operation is done manually. The use of an active control intends to reduce the operation time, and to make it possible even under bad weather conditions. The considered offshore structure can be analyzed as a cable submerged in a flow. A convenient model is given by the Bernoulli's historical cable equation, completed with a damping factor, that linearly depends on the structure speed. The damping factor is developed in series around zero, to get an approximate solution. The corresponding model turns out to be differentially flat[1], a property directly used in the control design, providing an extension to previous works of Petit and Rouchon [2], Thull et al [3], and Sabri [4]. This paper presents an overview of the results of [5]. Furthermore it contains material concerning a new tracking system, that uses the system inversion to define the feedback control.

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A HYPERELASTIC REISSNER-TYPE MODEL FOR NON-LINEAR SHEAR DEFORMABLE BEAMS

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Abstract. The present paper is concerned with the non-linear modelling of plane deformations of beams that are bent and stretched by external forces and moments. Our task is to present a continuum mechanics based extension of the celebrated large displacement finite deformation structural mechanics theory for plane shear deformable beams, which was laid down by Eric Reissner in [1].

The principal result derived by Reissner in [1] was a system of non-linear strain displacement relations being consistent with exact one-dimensional equilibrium equations for forces and moments via an appropriate structural mechanics version of the principle of virtual work. Reissner first derived the local structural mechanics relations of beam equilibrium by directly studying the equilibrium of a deformed beam element of differential length. In the plane case, this involves normal force, shear force and bending moment as generalized static entities. Reissner then assumed constitutive relations at the structural mechanics level to exist in the form of functional dependencies between these static entities and a set of generalized strains, namely a bending strain, an axial force strain and a shear force strain. In order to find out the correct kinematic meaning of the latter generalized strains, Reissner in an a-priori manner postulated a virtual work expression that connects the generalized static entities and the generalized strains in a particularly simple manner. He then required that this virtual work relation must lead to the local structural mechanics relations for beam equilibrium that he had derived before, from which he in turn found the required kinematical meaning of the generalized strains.

A main advantage of Reissner's structural theory [1] is that it is variationally consistent, due to his special construction of the generalized strains based on the principle of virtual work. Reissner himself however indicated a conceptual problem associated with this formulation, namely that the constitutive relations between the generalized static entities and the generalized strains must be evaluated from appropriate physical experiments to be performed for the beam under consideration as a whole. This severe drawback can be attributed to the fact that the notions of stress and strain, which are basic for continuum mechanics, were not used by Reissner in the above sketched structural mechanics derivations, such that the usual constitutive modelling at the stress-strain level could not be used in connection with Reissner's theory so far in a rational manner.

In order to overcome this problem, we present a continuum mechanics based converse to Reissner's structural mechanics modelling. We show that substituting the kinematical assumptions of Reissner's shear-deformable beam theory directly into the continuum mechanics version of the principal of virtual work is equivalent to the virtual work relation postulated by Reissner in [1] between the static structural entities and the generalized strains. This derivation then automatically attaches a continuum mechanics meaning to the generalized static entities and the generalized strains introduced in [1] by relating them, e.g., to the work-conjugate notions of second Piola-Kirchoff stress and Green strain. In the present contribution, we particularly derive relations between generalized static entities and generalized strains valid for a simple hyperelastic constitutive relation proposed by Simo and Hughes [2]. This model allows writing the constitutive relations in a series representation, the first terms of which do coincide with representations well-known from the linear theory of beams. In principle, however, the presented methodology should enable to introduce any suitable continuum mechanics based constitutive modelling at the stress-strain level, be it elastic or inelastic, into the structural theory laid down by Reissner in [1]. The present work represents an extension of a previous paper by the authors devoted to the case of beams rigid in shear, so-called Bernoulli-Euler beams, [3]. The relations derived in the latter paper turn out to be compatible with the present results, when shear deformation is neglected.

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Acknowledgement. Support of the present work in the framework of the Comet-K2 Austrian Center of Competence in Mechatronics (ACCM) is gratefully acknowledged.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

NUMERICAL STUDY OF FLATNESS BASED MOTION PLANNING FOR A HORIZONTALLY MOVING BEAM WITH A POINT MASS

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Introduction. In today's pick and place machines – like rack feeders for logistic facilities – residual vibrations are limiting the throughput of the machines. There are two ways to cope with residual vibrations. First way, simply drive slower with the cost of a larger transition time. As a second one, attach the top of the beam to another actuator. With this, the stiffness of the structure is increased by modified boundary conditions and the amplitudes of residual vibrations are reduced at the cost of a reduced energetic efficiency, because of more accelerated mass. Flexibilities of a machine's structure have to be taken into account if high precision and high speed positioning at a minimum of energetic and economical costs are desired. Thus, the system's efficiency can be increased by consideration of its flexibilities in the control design instead of using a stiffer and, therefore, heavier structure. In this work, systems are considered which can be mechanically well modelled as sketched in Figure 1.

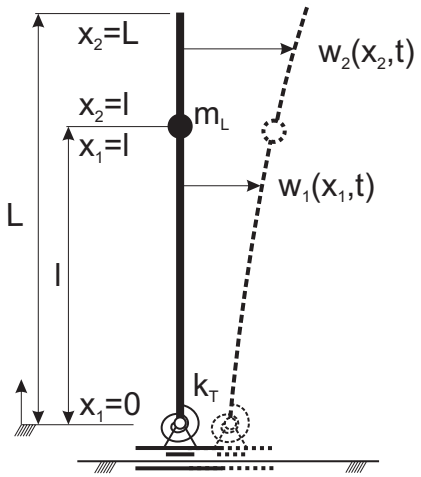

Figure 1: Linear actuator with attached elastic structure. Elasticities of the slide bar are modeled by a rotational stiffness k_T. The structure between the actuator and the payload m_L — for instance a tool like a gripper — as also the structure beyond the mass m_L are taken into account as two Euler-Bernoulli beams.

Flatness Based Feed Forward Control Law. For linearly actuated robots, like placement machines or rack feeders, an explicitly parametrized feed forward control law is presented. With this mathematical exact planning strategy, positioning of elastic structures with a constant mass distribution can be performed, by avoiding residual vibrations. In [1] a feed forward control law addressing this problem based on the theory of [2, 3] can be found, neglecting the dynamics of the beam above the payload. In this work an enhanced feed forward control law is presented, which takes the dynamics of the part of the beam situated above the payload into account. This improves the results especially for very long structures.

Numerical Study of Robustness. The efficiency and aspects of robustness of this approach are investigated numerically, using a finite element and a finite difference model. For this reason a huge number of numerical simulations has been performed, investigating the effects of parameter variations in respect to the occurring residual vibrations.

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CONTROL OF FLEXIBLE VIBRATIONS IN A TWO-LINK ROBOT BY PIEZOELECTRIC ACTUATION

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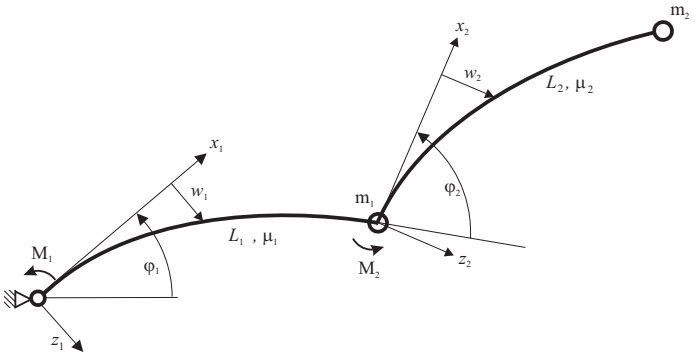
Introduction. This paper concerns the control of flexible vibrations in a two-link robot by piezoelectric actuation. The robot consists of two elastic arms with concentrated tip masses. The robot is moving in a horizontal plane, such that gravity loads are not taken into account. Flexible vibrations are caused by distributed and concentrated inertial forces. The scope of this work is to find an appropriate distribution of piezoelectric patch actuators and suitable control algorithms in order to minimize the elastic vibrations.



Flexible two-link robot

Shape control. In the first step, it is assumed that the geometrical properties and masses of the robot are known, and that any distribution of piezoelectric patches can be realized. The so-called shape control problem needs to be solved, i.e. to find the distribution of piezoelectric actuation in order to completely compensate the flexible vibrations. Using a floating frame of reference formulation [1] the equations of motion for the two-link robot are derived. The distribution of piezoelectric actuation in order to completely compensate the inertial forces follows from the equations of motion [2]. The spatial distribution of the actuating piezoelectric moment is given by the distributed and concentrated masses, the time-dependency is prescribed by the rigid-body angles, velocities and accelerations of the robot arms. It turns out that for each arm, at least three spatially distributed actuating moments with different time responses are needed in order to completely compensate the inertial forces.

Approximation by patch actuators. By use of piezoelectric patches, it is not possible to exactly realize the derived distribution of the actuating piezoelectric moments. Additionally, in practical applications the number of piezoelectric patches is limited. By means of numerical computations with beam elements [3], which have been extended to include the piezoelectric actuation, the response of the system is analysed for a limited number of patches. Having this methodology in hand, an efficient configuration of the patches can be evaluated for practical applications.

Closed loop control algorithms. In the second step, it is assumed that mass-distribution and geometrical properties of the robot are not exactly known and that the realisation of the actuating moment by piezoelectric patches is an approximation of the exact solution. Thus, it is not possible, to completely compensate the flexible vibrations with the help of the above shape control solution, which can be considered as feed-forward control strategy. In order to minimize the remaining vibrations, an additional closed loop control algorithm is employed. A PD-controller is added to the piezoelectric actuated patches. The proportional (P) part of the controller keeps the curvature of the beam near the value given by the optimal distribution of the patches. The differential (D) part of the controller aims to damp the vibrations of the beam. By assuming that the third time-derivative of the joint angle cannot be measured accurately, the differential part only damps out low frequency vibrations of the robot arms. A numerical example of a highly flexible robot with three patches per arm is studied which shows significantly reduced vibrations and turns out to be robust with respect to variation of system parameters.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

Proceedings
MATHMOD 2009 Vienna
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Modelling and Simulation of Biological Water Treatment

INTELLIGENT ANALYSERS AND DYNAMIC SIMULATION IN A BIOLOGICAL WATER TREATMENT PROCESS

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Introduction. This paper presents an overview of different modelling and simulation methods used in biological water treatment in pulp and paper industry. The treatment in an activated sludge plant is a complex biological process, where several physical, chemical, and microbiological mechanisms simultaneously affect purification results. Limits of the emissions are defined by authorities. A lot of process measurements are available, but measurement sets do not include sufficient information on special features of the influent nor on microbial composition of the sludge. Populations of microorganisms are highly important, e.g. sludge bulking cause especially poor treatment efficiency results when biosludge escapes from secondary clarification. Activated Sludge Models (ASM) have been in active use in many fronts from industry to the science and many practical projects. However, most applications are directed to municipal wastewater. AS models need to be simplified for pulp and paper applications since all the parameters cannot be identified from the sparse measurement data.

Methods. Basic dynamic simulation is based on LE models, which have been earlier used in chemical water treatment. The models consist of two parts: interactions are handled with linear equations, and nonlinearities are taken into account by membership definitions. Activated Sludge Models provide a basis for phenomenological modelling and can be linked to process expertise. Hybrid models based on a cascade approach are needed in biological wastewater treatment to cover different operating conditions. The overall model consists of three interacting models: load, biomass and treatment. The treatment model has three submodels corresponding to three types biomass. Smooth transitions between these models are handled with fuzzy set systems. Uncertainty handling needs to be included, since the measurement material is rather sparse, especially for on features of the influent and microbial composition.

Operating conditions can be detected by clusters obtained from measurements. Variable selection is important in these approaches. Performance of different dynamic submodels can be used as indications supporting specific operating conditions. Trend analysis of process measurements provides valuable information also about slow changes. This paper introduces new trend and deviation indices, which use the same nonlinear scaling approach as the LE models. For any variable j, a trend index $I_j^T(k)$ is calculated from the difference of the short and long term average of the scaled values X_j. Interpolation is needed since the measurements are sparse and the time between measurements varies. Outliers are removed before interpolation. The index value is in the range $[-2,2]$ representing the strength of both decrease and increase of the variable x_j. The derivative of the index $I_j^T(k)$ is used for analysing triangular episodic representations. Severity of the situation can be evaluated by a deviation index, which its highest absolute values, when the difference to the set point is very large and is getting still larger with a fast increasing speed.

Results and discussion. Variables selection is based on process knowledge. Influent quality depends on suspended solids (SS), chemical oxygen demand (COD), biological oxygen demand (BOD) and concentrations of nitrogen and phosphorus. In pulp and paper industry, additional nitrogen and/or phosphorus dosing is needed to keep the biomass in good condition. Changes in biomass population may cause sludge bulking which is seen as deterioration of sludge settling properties, described with sludge volume index (SVI) or diluted sludge volume index (DSVI). For example, if there is lack of oxygen or nutrients compared to biomass population, filamentous sludge leads into poor settling properties. Operating conditions are detected with trend and deviation indices. These indices provide a basis for hybrid modelling by indicating suitable time periods for specialised submodels. The weights of the submodels are calculated from the indices.

Conclusions. Hybrid models based on a cascade approach are needed in biological wastewater treatment to cover different operating conditions. Changes in operating conditions can be detected with new trend and deviation indices. Indices can be used both in selecting modelling areas and in combining the submodels of the water treatment.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

OXYGEN UPTAKE RATE MEASUREMENTS AS A TOOL FOR DETERMINISTIC MODELLING OF PULP AND PAPER WASTEWATER TREATMENT PLANTS

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Introduction. Deterministic modelling of biological wastewater treatment plants took a great leap forward in 1987 when the first IAWPRC model, Activated Sludge Model no 1 (ASM1), was released [1]. Since then new models have evolved from ASM1, the models have been implemented in commercial modelling software, bench marking of the different models has been made and especially universities have started to utilise the tools in research. In contrast, the practical use of modelling was and is still limited. The main reason is assumed to be that the basic requirements in terms of measurements of wastewater and sludge characterisation is too time and economy demanding.

The present paper is an attempt to present a modelling strategy for wastewater treatment plants within the pulp and paper industry based on simple measurements of oxygen uptake rate (OUR) combined with existing standard measurement programs from the treatment plants. The measurements have been used to estimate the maximum oxygen uptake rate of the sludge of the plant. Together with routine measurement from the influent and effluent uptake rate measurements have also been used to estimate the fractions of the incoming chemical oxygen demand (COD) to the plant. The model calibration procedure is also presented.

Results and discussion. OUR measurements were made using sludge and wastewater sampled from an activated sludge plant treating pulp and paper mill wastewater. Heterotrophic yield coefficient that is required to calculate the biodegradable COD fractions, and fractions of readily biodegradable and slowly biodegradable COD were estimated using the OUR measurements. Soluble inert COD was estimated from the amount of COD that is constant in the secondary clarifier effluent. Almost all COD (95%) in the mill effluent is soluble. Therefore estimating particulate inert COD is not of great significance in this case. Results of the fractionation are presented in the table below. Heterotrophic yield coefficient was estimated to be $Y_H = 0.75$. The maximum respiration rate of the sludge was found to be 27.8 mg O_2 / gVSS · h. Estimated biodegradable fractions seem reasonable as they make most of the COD that is not soluble inert.

	Fraction of COD
Readily biodegradable	30.6%
Slowly biodegradable	11.8%
Soluble inert	45%

Results of the COD fractionation

Building the plant and adding all physical properties is straightforward in commercial simulation programs. The wastewater characterisation can be added based on the principles above. Model constants can be changed in order to reach the same maximum specific oxygen respiration found in the experiments. Typically the maximum growth rate of heterotrophic bacteria is the only model constant that is needed to adjust in order to get a reasonable calibration. Further a fine tuning of the model can be based on comparison of modelled results with measured data, and making final changes to influent characteristics and parameters based on this comparison. The calibrated model may next be used for a number of purposes such as trouble shooting or for evaluation of different control strategies and optimised process operation. For plants treating wastewater from pulp and paper mills different nutrient control strategies could be a good choice for utilisation of the calibrated deterministic model.

Conclusions. Practical use of deterministic models of the activated sludge process needs to be based on calibration of the important model parameters specific for the actual type of the plant and the intended use. Also the incoming wastewater has to be characterised with respect to the significant fractions of substances. A model of a biological wastewater treatment plant treating wastewater from a pulp and paper mill only needs information about the oxygen uptake rate of the sludge and the fractions of the COD in the wastewater with respect to degradability. A simple Activated Sludge Model calibration procedure based on oxygen uptake rate measurements is presented. Both model parameter optimisation and COD fractionation is made utilizing only OUR, soluble and total COD, and suspended solids measurements. The described calibration procedure has been tested and found to be feasible with samples from Stora Enso Fine Paper Nymölla pulp and paper mill, and will be used in a more comprehensive measurement campaign with Stora Enso Fine Paper Oulu pulp mill.

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PREDICTING COD CONCENTRATION OF ACTIVATED SLUDGE PLANT EFFLUENT USING NEURAL NETWORKS AND GENETIC ALGORITHMS

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Introduction. Biological wastewater treatment in an activated sludge process is the most common way of treating pulp and paper mill effluents in Finland. Even though the treatment of forest industry wastewaters has improved a lot, incidental discharges are still an issue and have become a significant proportion of the total amount of discharges, because the microbial population in biological wastewater treatment is sensitive to unusual discharges from the mill and changes in operating conditions. Modelling the activated sludge process and using the model for predicting discharges is a possible method for achieving better control of the process. Modelling the activated sludge process is a difficult task, and there is a need for better methods of predicting discharges.

Both deterministic and data driven black-box modelling have been used with the activated sludge process. For example in [2] multilayer perceptron artificial neural network was trained with four years of process data, and was used for predicting pulp and paper mill wastewater treatment plant effluent COD concentration. One problem with the data driven approach is the tremendous variation in the process behaviour, making it difficult to train one black-box model to take into account the time varying behaviour of the activated sludge process over a time period of even one year. Time varying behaviour of the process was studied in [1] using self-organising maps and K-means clustering, and the method was found to be capable of clustering the process data according to the different operating regions of the process.

Applied algorithm. The approach in the study reported in this paper is to use routinely measured data from the UPM-Kymmene corporation pulp mill databases for black-box modelling of the activated sludge process. One year of process data was used for the purposes of this study. COD concentration in the effluent of an activated sludge plant treating pulp and paper mill wastewater was predicted two days ahead using the measured data as model inputs. Due to the time varying behaviour of the process, the process data was first clustered using self-organising maps and K-means in order to separate data from different operating regions of the process into their own clusters. Submodels were trained with the data of each cluster. Multilayer perceptron artificial neural networks were chosen as the model structure for the submodels due to their ability to describe nonlinear processes. In the available process data there are over hundred variables measured from the influent water, the process itself and the effluent water. It is very difficult to justify the choice of input variables for each submodel if the choice is made manually. Therefore automatic variable selection using genetic algorithms was implemented.

Results and discussion. The process data was clustered into six clusters with SOM and K-means in order to separate data from different operating regions of the process using three important variables describing operating region of the process as the inputs to the SOM: sludge load, DSVI and aeration basin temperature. From the results of the clustering it can be seen, that there is a clear distinction between different operating regions of the process in the clusters.

From the results for the prediction of the effluent COD presented in the paper it can be seen, that the predicted values follow the measured values quite closely. The exact values are not always predicted perfectly, but the submodels trained and validated with the clustered data are able to predict the direction of change.

Conclusions. Reducing incidental discharges from activated sludge plants treating pulp and paper mill wastewater is important in order to reduce the total amount of discharges to the environment. Modelling the activated sludge process and using the model to improve process control is a possible method for reducing discharges. The results presented in this paper show that using SOM and K-means for finding different operating regions of the process and training MLP submodels for the operating regions with input variable selection by genetic algorithms is an efficient way to predict COD concentration in the activated sludge plant effluent.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

SOM-BASED SUBTRACTION ANALYSIS TO PROCESS DATA OF AN ACTIVATED SLUDGE TREATMENT PLANT

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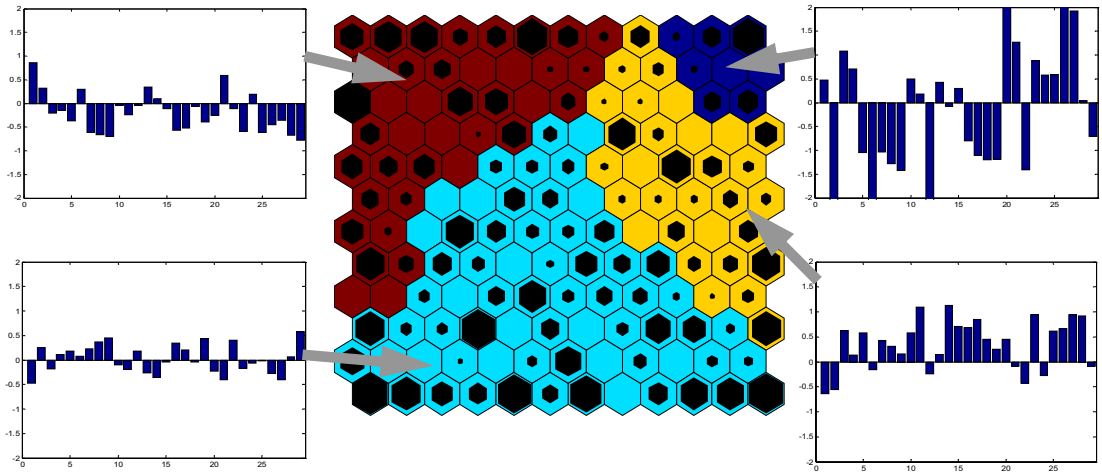
Abstract. This paper presents an overview of an analysis method based on Self-Organizing Maps (SOM) which was applied to an activated sludge treatment process of the paper and pulp mill. The aim of the study was to determine whether the neural network modelling method could be a useful and time-saving way to analyze this kind of process data and to investigate process states. The used analysis procedure went as follows. At first, the process data is modelled using the SOM algorithm. Next, the reference vectors of the map were classified by K-means algorithm into four clusters, which represented different states of the process. At the final stage, the center vectors of the clusters were used for subtraction analysis to indicate differences between different process states. The results show that the method presented is an efficient way to analyze activated sludge process states and it could lead to better process control.

Process and data. The raw data (on-line data and laboratory measurements) was extracted from the databases of the UPM-Kymmene Wisaforest pulp mill. The wastewater of pulp mill is handled in an activated sludge wastewater treatment plant. This unit treats an average of 86 000 m^3/day of waste water in a typical activated sludge process consisting of: (1) pre-sedimentation and equilibration, (2) aeration and (3) secondary clarifying. The selection of variables that were used in the analysis was made by a process expert. The complete data set contained values of 29 variables for 4 years with one day resolution.

Methods. After appropriate data pre-processing, the process data are processed by using a Self-Organizing Map (SOM) [1] and K-means [2]. The center vector of the clusters, solved by K-means algorithm, can be used for identifying differences of clusters by subtraction analysis. In subtraction analysis center vector of the clusters subtracted from each other and it revealed differences in process factors between clusters.



SOM using the data of activated sludge treatment process showing the number of the hits on the size of the depicted neuron. The background colours show the four main clusters of the map. The bar graphs represent the reference vectors related to four clusters.

Conclusions. Because of the growing need for optimizing industrial processes due to, for example, environmental regulations of process, developing new methods for process analysis is very important. The results presented in this paper show that the applied SOM-based neural network method is an efficient and fruitful way to model data acquired from the activated sludge treatment process. By means of this data-driven modelling method, some new findings were discovered concerning the dependencies between the process parameters.

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MODEL BASED ON-LINE SYSTEM IN ACTIVATED SLUDGE PROCESS TREATING PULP AND PAPER WASTEWATERS

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Introduction. Activated sludge is mainly composed of micro-organisms, which grow continuously and rapidly adapt to changes of conditions and wastewater to be treated. The management of activated sludge in dynamic conditions in space limited process requires knowledge and expertise.

Suspended solids separation in clarifier often is the limiting factor. Effluent quality of treated water depends on effluent suspended solids amount because solids carry other commonly used quality criterions like BOD, COD, P and N. Activated sludge process treating nutrient poor wastewaters are controlled with following: return sludge flow, excess sludge flow, air flow, dosage of phosphorous and nitrogen. The control of temperature and pH can be done easier with high-low limits or fixed set points.

Procedure. The procedure of model based on-line system is based on three levels: 1 selection of process status target, 2 set point estimation of devices and 3 control loops of devices. Details of the properties of system levels are shown in table.

Table. Operational properties of the procedure based on three levels

	1 selection of process status target	**2 set point estimation of devices**	**3 control loops of devices**
Operational principle	Steady state mass balance models	Expert system	Automatic control loops
Operation frequency	Once a month	Once a day	Continuously
Operator	AS-process expert	AS-process operator	AS-process control system

In level 1 loading figures, process dimensions and process circumstances are the input of steady state model of activated sludge process. The formation of biomass is based on models of growth, degradation and accumulation. Activated sludge distribution and behaviour is modelled in both basic unit processes: aeration tank and secondary settling tank. Results as function of sludge age are: sludge amounts in aeration and clarification, effluent BOD, COD, N, P and suspended solids, excess sludge as well as required oxygen, phosphorus and nitrogen.

Results are used to select limits and target values in level 2. Following three factors should be considered in selection: safe operation, high effluent quality and low costs. Factors form a triangle, where each factor is in the corner of triangle. If one of the factors is emphasized then the others are understated.

In level 2 part of the data from activated sludge process status is based on indirect measurements. Results of laboratory analysis are sparse. Process status is calculated from the last possible measured data. Part of the status variables are exponentially filtered during calculation. Result variables are compared with set of limits and target values. Comparison produces new set point values, which are then used in low level control loops on level 3.

Practical experiences. During the last ten years the above-mentioned procedure is used on some activated sludge plants in Finland. Procedure is run either in normal workstation individually with data transfer or fully integrated on the mills data and control systems. Experiences have been promising, when the personnel of the wastewater treatment plant are motivated and the measured data is accurate enough. Motivation to use the procedure is not sufficient in cases, when effluent quality of treated water completes the requirements of the authorities with lower effort.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

NET-EFFICIENCY SURVILANCE IN A NON-LINEAR PAPERMAKING PROCESS METHODOLOGY FOR WATER CIRCULATION AND PURIFYING SYSTEMS

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Introduction. Most of the papermaking processes intensively looking for a better solution to improve their net-efficiency score at its wet-end and overall profit in the end product on reel. Papermakers have been trying to bring new technologies in control systems and mechanical arrangements including process chemicals to avoid sucking up in between; and have been successful too in certain extent; but to do more! Paper engineers are looking principally on their "home-made-solutions." They consult on very popular issues; with machine builders or academic sources; to ensure their thinking are on the right TRACK or not. However, when a new thing appears in the market; they try to avoid it, due to "so-called proto-users." This conspiracy is a long-lasting immune for centuries; and would remain generation to generation; at the mill site. We execute sophisticated technologies in predicting, changing and controlling money-minds! Globalization and one-community framework in papermaking; become an additional headache to the paper machine building companies because of the competition that cannot perform, as in the past century; one large group of corporations owns, many mills including their centralized decision model on investments. The audacities of hope in many cases with obtainable tool systems; are significantly inefficient to meet the requirements of usual paper mill. This is due to basic functions; such as version management, configuration selection, concurrent and distributed developments, etc.; in making possible to store, retrieve, and compare versions and variants of a document; to create and select associated versions or branches of different documents; controlling simultaneous access by several users; providing mechanisms for building software without unnecessary rebuilding, release managements, workspace controls, change management and seamless integration with other tools in the system. Therefore, it is practiced that the papermaking is a multi-scientific approach, there is no generational change; but challenge ensembles enormously.

Methodology. In this presentation, I would offer a methodology that might lend a hand in understanding the well-known savvy; the control of water input, water cleaning; and its circulation phenomenon. Fundamental issues are; how to control the non-linear behavior before the headbox inlet flow systems? And how to mirror the water – chemicals and fiber supra-molecular intimacies; complimentary effects and manage to redirect them; into self-regulating channels; not to the pit; but take them away; into separate means; Clean them "on-line" and put them back to process; save energy, labor, and input chemicals! Nonlinear activities are welcomed in this doctrine; due to the process paradigm and comforts in that fashion, which is coupled with mechanical processing; diluted with chemistry, signal processing and control engineering areas.

Results and discussion. A segment; where one could focus though the needs for effective engineering skills to adapt. In running or inserting such a system as explained above; is rather cute when all the disciplines of art of papermaking go hand-in-hand flawlessly then there would not be any problems that would create grade changes, cleanings in between the grades and multi-grade paper productions. Some other results on the outage of different fading statistics and also considering the multiwall path loss in the process are significant. Different technologies, comprising Bluetooth, Zigbee, and Ultra Wide Band among others, are compared with on hand today's automation engineering; is almost on crossroads. Those are related to routing, localization and time synchronization, etc.; several protocols and algorithms used in the mills are reported and described, and some of them are evaluated through the use of suitable frameworks. Signal processing affects several aspect of paper machine design under a cross-layer view; so to say, the silent technology needs more time to modernize by itself or through the generational change. Similarly, the use of routing protocols for wireless voice and data; traditional networks are not suitable for wireless sensor networks in the paper producing mill environment. Wireless sensor networks in fact are characterized by many specific aspects that differentiate them from the traditional communication networks. First of all, nodes are based on batter supply and a typical applications environment does not allow to simply changing batteries – especially in running high speed paper machines. Secondly, often nodes are deployed in an ad hoc way rather than with careful pre-planning; they must then organize themselves to create a communication network. The sensor networks are generally composed by a high number of nodes; furthermore, node with many neighbors and it can also vary during time. The traffic in the network is generated by sensing events.

Conclusions. This approach would; let one to improve the net-efficiency, fundability of the paper or board machine; less or no breaks and chemicals; cheaper investment prospective and all-in-all better profit at the reel than before.

Proceedings
MATHMOD 2009 Vienna
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Selected Examples in Biomechanical Modelling and Simulation

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

DETERMINATION OF INDIVIDUAL NEUROMUSCULAR PROPERTIES AND APPLICATIONS IN SPORTS SCIENCE

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Introduction. An essential factor in modelling human movements is to find the values of the subjects' neuromuscular properties individually and in vivo. Most applications of models found in literature use mean values for the persons' properties, possibly scaled to the body dimensions, as input parameters for the model equations. Sometimes, even movement dependent quantities or combinations of properties and conditions of the movement are used (e.g., explosive strength). We use a method for determining movement independent neuromuscular properties of knee extensors and elbow extensors. Furthermore, we relate these properties to fiber composition and efficiency of the muscle, and we give examples of applications in the planning and controlling of training.

Method. Isometric and dynamic knee extensions pushing a sliding sledge on an inclined leg press are performed. We measure the position, as well as the velocity and force of the pushed sledge. Applying a mathematical model of the movement we identify all parameters of the model equation that cannot be measured directly using a modified Levenberg-Marquardt algorithm [2]. Among the identified parameters are the neuromuscular properties describing the activation rate by an activation parameter A [1/s] and the parameters f_{iso} [N] (isometric force in the muscle), p_{max} [W] (maximum possible power of the muscle), and v_{max} [m/s] (maximum possible contraction velocity) of a Hill-type extensor model muscle. The muscle properties can equivalently be expressed by Hill's parameters a, b, and c. Using an analoguous method we also determine the neuromuscular properties of the elbow extensors. [1]

Let n be the number of parameters in the model equations, $k<n$ the number of parameters describing the movement conditions (such as the mass of pushed object, inclination of plane,…) and $m<n$ the number of the person's properties (such as activation rate, mass, muscle properties,…), $n = k + m$. Let parameter values of conditions be fixed. Then for every possible set of values of properties we can define a performance of the movement, e.g., the maximum velocity of the sledge. Therefore, we can construct a mapping between the set of properties and a one-dimensional performance space. The graph of this mapping is a surface showing the relation between the properties and the performance.

Applications. Relation between the neuromuscular properties and other individual properties can be found such as the ACE genotype (related to a combination of neuromuscular properties), the fiber distribution (related to Hill's parameter b normalized to the muscle length) and efficiency (related to the curvature of the force-velocity relation in the muscle) [2],[3].

The inter- and intra-individual differences in the neuromuscular properties can be quantified. Especially, there are large differences between different subjects, confirming the statement that parameters of the model equations have to be determined individually.

The influence of a change in movement condition on the performance can be calculated. Change in conditions such as mass of a pushed load leads for example to different power output of the muscles. The amount of the differences depend on the value of all other parameters and therefore can only be predicted individually by evaluating the model. Measurements only lead to statistical results.

The above defined mapping between properties and performance space gives information about the connection between the person's properties and his/her performance and shows where the largest gain in performance increase can be achieved.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

NET-BASED PHASE-ANALYSIS IN MOTION PROCESSES

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Although data can be taken from motions automatically it is still a problem to get useful information from them. In contrast, the huge amount of automatically recorded data can hide that information. Standard analysis and search algorithms are not helpful as long as the 'striking' property is not known a priori – e.g. if the unknown reason for a non-optimal motion is looked for.

Approaches and experience from the last ten years have shown that artificial neural networks of type SOM (Self Organizing Map) can be extremely successful in the task of making data transparent and transferring them to useful information.

To meet the different requirements of data pre-processing, net training, and data analysis our working group has developed the DyCoN-approach (Dynamically Controlled Network), which offers a number of helpful concepts and components.

Three typical examples are introduced in case studies, dealing with motion processes from different disciplines and demonstrating the way how networks like DyCoN together with phase diagrams support the analysis of motion processes.

APPLYING A PRINCIPAL COMPONENT ANALYSIS TO MOVEMENT COORDINATION IN SPORT

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Because sports movements are very complex biomechanical analyses contain many kinematical or dynamical parameters and characteristic curves. PCA is a technique for simplifying a dataset by reducing multidimensional datasets to lower dimensions for analysis. By means of the PCA it is researched how the variance of a data vector is composed of the variances of the single components. Especially, we interpret the number of the components or also named components with relative high eigenvalues as the number of degrees of freedom. The purpose of this paper is the presentation of several studies which used the PCA to solve some problems in the movement science in sport.

The aim of the first study was the characterization of the walking and running movement as well as the transition by means of a systems parameter and analysing its changes under the condition of varying velocity. It can be discovered that the first component is distinguished by the greatest eigenvalue. Additional drawing of phase plots show similarities and differences between walking and running. The determination of the systems parameter [1] offers the estimation of the variability of the movement coordination. The variability of walking is particularly high immediately before transition to running.

The purpose of the second study was the estimation of the number of PCA-components and their eigenvalues relating to the rehabilitation process for patients with a knee joint endoprosthesis. It could be found the dominance of the first component and the growth of its eigenvalue during the rehabilitation.

In the third study the running coordination after prior cycling exercise in triathlon was analysed. By means of the PCA significant differences between a normal run and the run after the cycling period could not be found.

The PCA was used in the fourth study to compare the different gaits in horseback riding. This investigation was interesting in view of the fact that horseback riding concerning the three interactive systems of horse, saddle and rider is a very complex movement which is difficult to characterise by single biomechanical parameters or characteristic curves. It was assumed that the movement coordination of trot can be described as sufficiently accurate with only one systems parameter.

In summary we found out that the PCA presents a useful method to characterise the movement coordination in its entirety.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

STRESS AND STRAIN IN BIOLOGICAL TISSUES – MATHEMATICAL DEFINITION AND PHYSICAL CONCEPTS

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Problem background. The role of mechanical deformations in cell response is known as mechanotransduction. However, it is still not clear as how exactly do cells react to external loads. One of the important issues is that the transfer of continuum mechanics concepts to microbiological level has not been entirely successful. There are several reasons for this but one is the lack of analytical methods for analysis of cells due to the dominance of digital equipment that in effect imposes discrete image representation. Dabnichki {1,3] and Dabnichki and Zhivkov [2] is that is that is designed to integrate different stages of cell analysis – from image processing to global analysis of cell dynamics combined with an interface to continuum mechanics based computational analysis. However, the main focus of the current work is to establish a method of identifying the non-deformed cell status or more precisely a method for identifying a group of equivalent reference state that could be used to analyse cell response to loading. It is argued that at micro-level the classic continuum mechanics definition of stain and stress is not applicable as cell shape is affected by the functionality. Hence the homeostatic state is not necessarily the equivalent of stress free state but a reference state.

Method. The method developed is based on the hypothesis that cells could be geometrically reconstructed by using an ellipsoid as an initial shape

$$E_0: \quad A_1x_1^2 + A_2x_2^2 + A_3x_3^2 + A_4x_1x_2 + A_5x_1x_3 + A_6x_2x_3 + A_7x_1 + A_8x_2 + A_9x_3 + A_{10} = 0 \qquad (1)$$

From 1 every deformed shape could be obtained by "adding and removing" mass from the ellipsoid to obtain the "deformed shape" of the ellipsoid. This transformation is performed by using specifically designed functions with a compact carrier that allow to obtain a family of pseudo-ellipsoids as seen in fig.1 below.

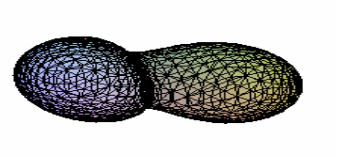

Fig.1 Reconstructed deformed cell shape

The cell shape above was obtained by a custom algorithm where

$$E_1: \quad E_0 + A_{11}e^{(x-x_0)^2+(y-y_0)^2+(z-z_0)^2} = 0 \qquad (2)$$

$$E_{i+1}: \quad E_i + A_{10+i}e^{(x-x_0)^2+(y-y_0)^2+(z-z_0)^2} = 0 \qquad (3)$$

The above procedure is based on pre-set value for the quadratic error. It is self evident that the method allows analytical reconstruction and hence proper classification of families of pseudo-ellipsoid in different state of "deformation". All the important geometric invariants could be obtained directly.

Discussion and conclusion. The developed method was tested on specially designed experiments where mechanically instrumented cells were artificially deformed and their state digitised. The method successfully reconstructed the deformed cells beyond biologically admissible level. The proposed technique allow to identify a family of equivalent shapes and hence establish a reference state which is not a mathematical but biological problem. The achieved accuracy is less than 2% of the greatest radius. Unfortunately to date the method could not be properly tested on microscopic images as they are processed and approximated by ellipsoids as reported in earlier works [1,3].

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MATHMOD 2009 Vienna
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Carbon Capture and Storage

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

DYNAMIC MODEL FOR REMOVAL OF CARBON DIOXIDE FROM A POST COMBUSTION PROCESS WITH MONOETHANOLAMINE

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Abstract
Capture and storage of carbon dioxide from post combustion gases produced by burning fossil fuels are an important operation in the global aim of reduction of CO_2 emissions. Up to 60% of CO_2 emissions are from fossil fuel point sources, mostly from coal, oil and natural gas fired power stations [1].
A dynamic rate based model for simulating a CO_2 capture system from post combustion gases is developed. The model consists of an absorber, a de-absorber, a re-boiler, a condenser, two heat exchangers and two pumps. More attention is given to the distribution models of the reactive absorber and the reactive de-absorber as they are considered to be the main components. The reactive absorber/de-absorber is discretized into a number of slices, while the mass transfer between the phases are modeled using the classical two-film theory approach in each stage. Multicomponent mass and heat transfer, and reaction kinetics are considered for the development of the model. A major effort is dedicated to defining the interface concentrations, diffusion fluxes, fluid properties and equilibrium constants.
Monoethanolamine solvent system is considered for modeling along with the Montz B 200 metal structured packing [2] for the absorption and de-absorption towers.
The model is implemented in Matlab, and the effect of the number of slices on the computation time, geometry of the absorber and de-absorber, and accuracy of the model are analyzed. The equilibrium constants used for defining the reaction kinetics are validated with speciation diagrams. Certain perturbations are made to observe the model efficiency in various conditions. The model equations are solved using the method of lines (MOL).

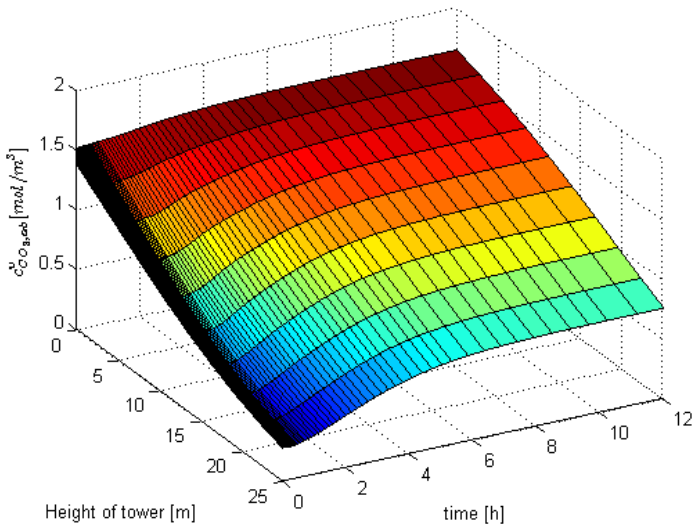

Figure 1. Concentration profile of CO_2 in the gas phase of the absorption tower

Simulations gave reasonable results and confirmed the tendencies of the concentrations and temperatures. The concentration profile of CO2 in the gas phase of the absorption tower is given in Figure 1. The results of the simulations helped to conclude that it is possible to model both the absorption and de-absorption towers using the rate based model which saved some model development time.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

CO_2 CAPTURE BY THE ABSORPTION PROCESS IN THE MEMBRANE CONTACTORS

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Abstract. Post combustion CO_2 capture is corresponding to the most widely applicable option in terms of industrial sectors and is compatible to a retrofit strategy. In addition to the conventional chemical absorption process, membrane gas absorption is considered as one of the promising alternatives to conventional techniques for the CO_2 separation from the flue gas of fossil fuels combustion. As a hybrid approach of chemical absorption and membrane separation, it may offer a number of important features, e.g., economical viability due to its larger interfacial area, no flooding at high flow rates, no foaming and channeling, linear scale-up with predictable performance. This paper is to describe and present the state-of-the-art of the R&D efforts on membrane contactors focused on the microporous hallow fiber structure. The operating principles, liquid absorbents selection, influence of membrane wetting phenomenon, membrane materials and module types have been intensively reviewed. Model parameters including economic performance has been evaluated with comparison of other technologies. Technical obstacles of applying membrane contactors in CO_2 capture process have also been discussed. The knowledge and application gaps have been examined and identified, thus providing a recommendation for the future studies.

Keywords: CO_2 capture and storage; carbon dioxide; hollow fiber membrane; membrane contactors; numerical modeling

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MATHMOD 2009 Vienna
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Meeting with IT Advances in Modeling and Simulation Tool Developments

CO_2 REMOVAL BY ABSORPTION, CHALLENGES IN MODELLING

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Abstract. CO_2 can be removed from exhaust gases by several methods. The traditional large scale method is by absorption in a mixture of an amine and water. MEA (monoethanol amine) is the most actual amine for CO_2 removal at atmospheric conditions. The absorbed CO_2 is regenerated in a desorption column, and the solvent is recirculated to the absorption column.

The models for solving specific tasks of the CO_2 absorption process differ in accuracy, complexity and robustness. The main purpose of this paper is to pinpoint areas where further modelling can lead to important improvements. One main challenge is how to combine different models in existing tools.

The tasks of modelling this process can be divided in detailed description of

- absorption and reaction kinetics
- gas/liquid equilibrium
- gas and liquid flows
- pressure drop
- energy consumption
- mechanical equipment dimensioning
- economical optimization

Process simulation tools containing models for most of these tasks are commercially available. A process model made with the program Aspen HYSYS is used as an example. Another example using the program Aspen Plus is given by Kucka et al., [2]. Other process models have been made with e.g. Fortran code and Matlab. One example is the model from Al-Baghli et al., [1]. Calculation convergence of the models is important, especially the column convergence is critical.

There is still a challenge to search for improved gas/liquid equilibrium models. There is need for improved accuracy, and the models should be easy to converge and to use in combination with kinetic models.

For some simplified conditions, e.g. by using MEA under traditional conditions, calculation of stage efficiencies can give a satisfactory description of the absorption process. Under more complicated conditions, especially when using mixtures of amines, a more rigorous description of the interactions between mass transfer and reaction kinetics is necessary. There is a challenge to find out under which conditions a simplified method is satisfactory.

CFD (Computational Fluid Mechanics) is an efficient tool for calculating flow conditions, pressure drop and temperature profiles, especially for one fluid phase. An overview is given by Valluri et al., [3]. It is a challenge to make use of CFD for gas/liquid processes. An unsolved problem is the description of the gas/liquid interface area, and especially combined with absorption.

A major challenge is the combination of models. In the case of process simulation programs, Cape-Open is an example of a standard interface for introducing a new model into an existing program package. An improvement in one specific model must be available to other tools to be utilized.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

EXPERIENCES AND CHALLENGES IN DEVELOPMENT OF SUSTAINABLE MODELLING AND SIMULATION TOOLS

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Abstract.

Modelling and simulation software tools should be sustainable even if it is not definitely required for temporary research projects with a publication as outcome. Especially, when using modelling in simulation as an integrated tool supporting both engineering and operation of industrial processes - the models should sustain for the whole life cycle of the target process - from initial design to decommission, at least 60 years.

The solution relates, first, to apply such formal specifications of the physical model that easily can be carried as simple text files between generations of computer and operation system platforms. Second, reliable simulation engines are needed that are programmed in high level language enabling for transportation to the new platforms and. Third, standardised procedures for re-verification of the computational functionality are required. Fourth, easy connectivity to concurrently developing engineering databases and graphics interfaces is needed, as well. Digital catalogues are already available over Internet for various kinds of construction materials and production plant components. The ISO 15926 interoperability standard provides a basis for interconnecting systems [1].

New challenges are set for the simulation engines, on the other hand on increased computational speed, much faster than real-time, but also on more detailed description of the processes and on replication of more complicated physical phenomena. The advance of multi core processors, even on laptop computers, calls for reconsideration of the mathematical methods used so far in order to make use of the inherent computing power. Companion model graphs are supposed to have a significant mission in automated computer model generation from semantic plant specifications, as well as in even distributing to computation load on available cores [2]..

However, to grab the possibilities now soon available, the source codes need to be revised. The program data organisation needs to be re-developed to minimise required cash operations to main memory. The computing algorithms need to be re-developed to promote on chip operations and minimize communication between computer nodes. OpenMP standard provides means for instructing the compiler on what parts of the code that can be run in parallel [3]. At the same time the mathematical solver algorithms need to be developed to support multi scale modelling of heterogeneous processes requiring that separate parts of the integrated model are simulated with different time-steps [9]. It seems that Niclas Wirths law: "Software gets slower faster than hardware gets faster", will come true even with regard to scientific computing subject that the software architectures and mathematical methods not are strongly adapted to the hardware developments. Multicore processors are already installed in our laptop computers [4]. It is time to review our serial computation algorithms, perhaps in European research context.

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SIMULATION-BASED PLANNING AND OPTIMISATION IN SUPPLY CHAINS: APPLICATION IN ECLIPS PROJECT

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Introduction. For the last decade, supply chain planning has become a critical factor in the success and profitability of an enterprise, especially given a global competition and rapidly changing markets. Traditionally, researchers and practitioners have primarily investigated so called single echelon approach, where a stage or facility in the supply chain is managed. Recently, increasing attention has been placed on the performance, design, and analysis of the supply chain as a whole. A multi-echelon environment considers multiple processes (e.g. purchasing, production and transportation) and multiple stock points (buffer or storage). Cyclic and non-cyclic planning policies can be used within a multi-echelon approach. The main idea of a cyclic schedule is to use fixed order intervals at each echelon while synchronizing these cycles in a supply chain. In practice, cyclic policies are more preferable, as they easier to control and reduce administrative costs. However, when a customer demand is variable and uncertain, e.g. at the product introduction or end-of-life phases, flexibility in spacing of planning periods can result in lower costs for the non-cyclic policy. The ECLIPS Project is addressing both academic and business state-of-the-art in supply chain planning and management. Simulation is used intensively in the project. It supports supply chain management processes (e.g., optimization, decision making), providing conditions for minimization of inventories and provides a platform for testing algorithms and tools, being developed within the project. The project scope in the paper focuses on development of simulation-based methodology and tools for optimising multi-echelon cyclic schedules, and analysing planning policies over the product life cycle to prove efficiency of a cyclic schedule or to switch from a cyclic policy to non-cyclic one.

Simulation-based multi-echelon cyclic planning and optimisation. The multi-echelon cyclic planning problem is formulated as a simulation-based optimisation problem that is aimed to determine optimal parameters of cyclic schedules at different supply chain echelons in conditions of demand variability and uncertainty. A supply chain simulation model is built as process oriented model with a one-directional flow of goods. The supply chain generic network is constructed from basic sub-networks, such as linear, convergent and divergent. The replenishment and delivery logic for each sub-network is defined. The simulation environment for cyclic planning and optimisation provides automatic generation of the network simulation model described in the Excel format by using the Promodel ActiveX technology, definition of an initial point for simulation optimization using analytical calculus, and performing simulation optimization. The environment includes database; procedural component by using analytical calculus to generate products cyclic schedules; process component where the network is built up and simulated, cyclic schedules are modelled, inventory levels are controlled, and the network performance measures are estimated; and optimisation component. Optimisation of a multi-echelon cyclic schedule refers to a multi-objective combinatorial optimisation problem. To solve the problem, simulation optimisation algorithm is developed based on the cooperative search of the multi-objective genetic algorithm (GA) that is well suited to solve combinatorial problems and RSM-based linear search to improve GA solutions.

Simulation-based comparative analysis of cyclic and non-cyclic planning policies. Simulation-based scheme for comparative analysis of supply chain planning alternatives over the product life cycle allows evaluating the difference between total costs of cyclic and non-cyclic planning policies, analysing an additional cost of a cyclic schedule (ACCS), determining the most efficient policy for switching from one policy to another one. Cycles and order-up-to levels are used as parameters of a cyclic planning policy, while a non-cyclic policy is defined by reorder points and order quantities per each chain echelon. These parameters are defined using either analytical calculus or simulation optimisation techniques. Supply chain simulator model behaviour of alternative planning policies, and their performance measures, i.e. total costs mean values and ACCS values, are received from simulation experiments. Cost comparison is based on estimation of the difference between policies total costs mean values by using the Paired-t confidence interval method. It is aimed to discover if two mean values are significantly different. If the Paired-t confidence interval excludes zero with a probability $1-\alpha$, then two mean values are considered as significantly different with α significance level. In this case, the cyclic policy will outperform the non-cyclic policy or vice versa. Otherwise, the final decision is made based on the ACCS analysis. The software for comparative analysis of cyclic and non-cyclic planning policies is developed using Promodel, Ms Excel and VBA integration possibilities. As a test bed, the chemical manufacturing supply chain is simulated. The results presented demonstrate efficiency of the proposed methodology and tools.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

APPLICATIONS OF SIMULATION MODELS FOR DIAGNOSTICS AND MODEL BASED CONTROL IN PULP AND PAPER AND POWER PLANT APPLICATIONS.

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ABSTRACT: Dynamic process models have been produced for bubbling bed combustors, circulating fluidized beds and pulp digesters. The models were made in Modellica and thereafter transferred as objects into Mathlab/Simulink, with OPC link to the process computer system via the data-base. In the application at a pulp mill the model also has been combined with a NIR measurement on ingoing wood chips, to determine the reactivity of the wood as a function of residence time, chemical additions and temperature. Later on the NIR will be used as feed forward for both model based control and for diagnostic purposes with respect to channeling and hang-ups. In the power plant applications models have been used for dynamic data reconciliation for a CFB boiler and for MPC-control using NIR for moisture measurements of ingoing bio-fuel to a BFB-boiler. The applications will be presented at the conference.

Keywords: Modelling, Applications, Pulp, Power plant

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Environmental Systems and Processes

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MATHEMATICAL MODELLING OF FOREST FIRE FRONT EVOLUTION: WAVE APPROACH

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Introduction. Forest fires belong to destructive natural phenomena which cause every year large damages, threaten people's lives and block significant human resources. However, they have not been sufficiently well described yet due to still inadequate knowledge about the complex processes determining behaviour of the phenomenon and a huge amount of data suffering from serious difficulties with the data extraction and gathering. Advances in computers and information technologies stimulate the development of advanced program systems for the fire management, prevention and planning purposes. Mathematical modelling of the forest fire spread in time plays a key role in such systems. In particular, fire behaviour predicting systems are capable to simulate the evolution of forest fire front in time and are able to describe not only the spatial and temporal fire behaviour but also to quantify and often even display fire characteristics for fire effects evaluation. Such simulation systems can be used even for operational purposes. The computer fire simulation can help to increase the effectiveness of fire management response for concrete active or hypothetical fires and to better understand the circumstances causing human incidents during past tragic fires [3].

Modelling of forest fire front evolution. In the literature several types of fire spread models are distinguished. *Semi-empirical models* which represent a certain substantial simplification of modelled combustion process allow to develop effective operational tools for forest fire simulation under real conditions (e.g. Behave and Farsite). On the other hand, *physical models* represent a physically much more detailed approach to the fire spread modelling but they lead to differential equation systems which often require sophisticated and time-consuming numerical calculations and advanced high-performance computing environments. That is why the simulation of more extensive real forest fires applicable for operational purposes, which could be realized on currently available computer equipment, is still generally restricted for semi-empirical and empirical models. This paper summarizes some recent results on the analysis of application of Huygens' principle of wave propagation on the problem of description of global steady-state forest fire spread in time based on the assumption of locally elliptical fire spread. Each point on a starting fire front at a given time t can be considered as an ignition point of a small local fire which causes burning out of the area of elliptical shape at time $t+dt$. Assuming that each such an ellipse is defined by burning conditions at its generating ignition point, the resulting fire front at time $t+dt$ can be defined by the envelope of all the ellipses (Huygens' principle applied for the forest fire spread). The use of Huygens' principle for the fire front evolution was formulated analytically by G. D. Richards who derived a non-linear system of differential equations of the first order describing the fire front growth in time [2]. To express points lying on envelope of the set of ellipses, a linear transformation was applied transforming ellipses into circles to utilize specific geometrical properties of points lying on common tangent line of two circles. The envelope of the set of circles was then calculated by spatial limiting process. Then applying time limiting process and the inverse linear transformation, the resulting system of differential equations describing the fire evolution in time was derived. Despite certain restrictions, this equations system is of a great significance for the forest fire modelling and simulation. We demonstrate a new approach to the model derivation based on the knowledge of envelope theory of sets of curves to derive explicit formulae for the envelope of ellipses which form the resulting fire front [1]. This procedure avoids the necessity of the linear transformation used by Richards. Following the same assumptions as Richards, the equivalence between both presented approaches is shown. However, the new procedure requires to derive a new relation between the functions representing variability of burning conditions and their spatial derivatives which allows us to formulate some of substantial model assumptions in original way. The use of classical envelope theory of curves sets from differential geometry enables to obtain better insight into the complexity of the problem of mathematical modelling of forest fire front evolution in time using Huygens' wave principle. Such analysis allow us to better understand assumptions and limitations of the model. The knowledge of mathematical fire spread model is significant not only for better understanding the model itself, but also for its effective implementation, and its correct use under variable topographic, meteorological and fuel conditions, and for proper interpretation of simulation results in real conditions. The readers engaged in the use of systems and models developed for forest fire modelling and simulation can benefit from this deeper analysis.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

OPTIMIZATION OF A H_2O/CO_2 CONDENSER FOR CAPTURE OF CO_2 USING ROBUST SIMULATION SOFTWARE

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Abstract: There is rising anxiety that the increasing emission of carbon dioxide (CO_2) to the atmosphere will result in climate change with undefined consequences. This has lead to development of technologies for reduction of CO_2 emissions from power stations, involving capture and sequestering of generated CO_2. New knowledge, based on both advanced combustion and gasification technologies hold promise for economically achieving CO_2 reductions through improved efficiencies. Based on judgement of the three main methods that are used for the capture of CO_2 from gas-fired power plants the author has studied Oxy-fuel cycles with internal combustion of gas using pure oxygen including the chemical looping combustion cycle.
This article provides technical research methods of capturing CO2, which involves separating the CO_2 from the other constituents in the flue gas using a condenser. The CO_2/steam separation and condenser unit is an essential part of all oxy-fuel cycles and the CO_2 handling tools does in fact represents a considerable contribute to the total cost for such power plants. Improvements regarding cost efficiency and compactness of the CO_2/steam condenser systems is hence of vital importance if the oxy-fuel power plant concepts are going to be developed as realistic commercial alternatives. The CO_2/steam separation process does also influence the thermal efficiency and hence the operational cost of the cycle through the effect of pressure loss and through the effect of purity of re-circulated water and CO_2. The methods discussed in this paper are the CO_2/steam separation process in an oxygen fuel combustion system. The main goal is to develop a thorough understanding of the separation process at varying thermal conditions and with varying fluid compositions. A CFD tool has been used for simulation of the proposed condenser to separate H_2O and capture CO_2. It has been carried out as an optimization study that also may lead to reduced capital costs and increase the thermal efficiency of the power plants. Accurate knowledge about the thermo physical and fluid dynamic properties of CO_2/H_2O mixtures is required in order to carry out reliable process simulations and hence to optimise the condenser and the process cycles. Some experimental thermodynamic data like compressibility, dew point, density and enthalpy for CO_2/H_2O mixtures are available in previous works by the two latter authors. Fluid flow, heat transfer rate and pressure drop characteristics are studied as function of CO_2/H_2O mixture composition. Resulting velocity profile, gas/liquid ratio, degree of turbulence, two phase flow regime for H_2O/CO_2 mixtures are also presented.

MODEL-DRIVEN ENGINEERING FOR TRANSPARENT ENVIRONMENTAL MODELING AND SIMULATION

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Models are an important means to gather, store and communicate the (assumed) knowledge about a system. One well known issue in modeling and simulation (M&S) is to provide model reusability and transparency across different application contexts. It is particularly challenging to consider both, technical aspects and the process of how a model and the knowledge associated with it has been obtained, including, for example, the experimental setup [1, 2]. Thus, is vitally important that both, the model and the process of how a model has been created, modified and used, are transparent.

Transparency means that model descriptions are comprehensible and that all artifacts associated with the modeling and simulation (M&S) process are consistent. Existing M&S-frameworks may provide transparency to some degree, e.g. with the provision of domain-specific modeling languages (DSLs), but modelers are usually bound to their chosen framework [3]. Moreover, many M&S-technologies are designed for particular class of models and respective modeling formalisms, particularly domain-specific technologies, e.g. for environmental M&S. This is an issue when models are reused within different application contexts with different functional or non-functional requirements. Usually, the reuse of models requires the re-implementation or transformation of models in another implementation technology with other functional and non-functional properties and different modeling languages [4, 5]. Important contextual information is likely to be lost this way.

Technologies and concepts from Software Engineering, in particular meta-model-based model-driven engineering (MDE), offer means to meet the challenge of transparency and reuse in M&S. With meta-modeling there are many possible ways of achieving reusability. Meta-model-based MDE can also be used to couple different DSLs and their respective models, if the DSLs' meta-models conform to the same meta-meta-model.

We apply the concept of MDE with meta-modeling to environmental modeling and simulation in order to support transparent M&S. The main contribution is the transfer of concepts from software engineering to the M&S domain. We provide the concept and architecture for a model-based development of an integrated modeling system including meta-model-based DSL and experiment management. We applied this approach to environmental modeling with cellular automata, with a respective modeling language and experiment management system (EMS). The DSL provides the means to specify a model independently from implementation technology. The EMS ensures consistency of M&S-artifacts.

The use of model-driven engineering facilitates the separation of model descriptions and implementation technology. With our prototype (ECA-EMS) we showed that ECA models can be transformed to the target technologies jDisco and Geotools. These technologies are exemplary for a number of similar technologies, providing common simulation modeling and GIS functionality. Meta-meta-modeling facilitates the integration of several DSL for technology independent modeling. However, it must be clear that the possible models defined by all DSLs are limited by the functionality of the possible target technologies. Tools that are needed for M&S are already available or can be implemented in an efficient way. This is facilitated by meta-modeling and automatic tool generation (e.g. editor, generator). The Eclipse Rich Client Platform is a suitable platform for integrating our tools under one uniform GUI and additionally, it provides standard interfaces for user specific extensions.

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A QUANTITATIVE ASSESSMENT & MATHEMATICAL MODEL OF EMBEDDED ENERGY AND TOTAL CO2 EMISSIONS FOR FUTURE PROJECTIONS

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Introduction. In the present study the GHG emissions from energy final consumption, not only energy in the producing sector, but also indirect energy embedded in other inputs for the sector are considered and the embedded energy emits GHG during conversions of energy in the whole energy chains are included.
The Input–Output Analysis (IOA) is used to calculate energy intensities and GHG emission factors of various final consumptions in the economy. IOA is applied to full-energy-chains analysis in the estimation of GHG emissions from energy activities in all producing chains, of final consumptions of economic sectors. The flows of energies through various sectors are traced back through infinite transactions within the economy, and GHG emissions embedded in the flows are initially quantified.
Methodology. The energy-related GHG emission including emissions from burning of fossil fuel, fugitive emissions, and emissions from industrial process are considered. The revised 1996 IPCC guidelines (IPCC) are applied to sectoral derivation of carbon dioxide (CO2). Emissions from the Indian economy have been estimated based on the sectoral energy consumption and Input–Output (I–O) tables. This study considers fossil fuels that are used as feedstock in some production processes, but there are no GHG emissions. Embedded emission in imported secondary energy is also taken into account. The statistical data is thereby generated on Total energy consumption and related carbon dioxide emissions. These data is organized to form matrices of energy consumption and Carbon Dioxide emissions. As far energy inputs to Indian economy is concerned, the system can be considered to be formed of five energy intensive sectors. Out of them the four sectors Agriculture, Residential, Industrial and Transport are consumers of fossil fuels like Coal, Oil and Natural Gas, where as the fifth sector the power sector is considered in terms of hydro, thermal and nuclear. The energy consumed in each sector for all the inputs has been obtained and arranged in form of a matrix Esi. The Emission factors of each of the fossil fuel are worked out on the basis of the IPCC guide lines to form the matrix Ef. Direct and indirect emissions are derived by the physical amount of each type of fossil fuel that is directly combusted within the sector. Than the indirect energy flows are truncated to modify the energy consumption. Finally total emissions generated from all production sectors are derived.
Data preparation. Indian energy consumption tables in four sectors published by the Energy Directory [TERI – TEDDY] are obtained. The recent disaggregated data is used for construction of the matrix E i.e. Energy consumption. The e-c table is tailor-made for a structural matrix. Each element is the sum of the 'wholesale fuel consumption margin' plus the 'retailed fuel consumption margin', the 'transportation' and the 'import'. Indian energy consumption tables, available in four sectors, are published by many authorities. In order to assign each sector and represent average energy consumption I–O approach is applied for the analysis. The TEDDY also provides recent disaggregated data for construction of the matrix Esi for the period 1980 to 2007.
Conclusions and Discussions. The IOA method applied to the energy sector in the present study reveals the implications of the indirect as well as the direct energy related GHG emissions in the Indian economy. The energy intensities and total GHG emissions in final consumptions found in this study could be further applied for comparative assessment in other energy projects in India. Though the energy related GHG have to be derived from the amount of energy consumption, there is no proportionality between 'energy intensity' and 'greenhouse gases intensity'. There are two explanations: firstly, disparity of GHG emissions from combustion of different fuels, and secondly, GHGs could be emitted in some other activities rather than combustion of fuels. Delineation of most sectors into sub process orders and activities reveals that we could not neglect indirect effects beyond the direct combustion in the conversion stage of any commodities' production. The assessment of GHG emissions from the selected case studies reveals that input requirements in the operating stage directly affect direct and indirect emissions and energy intensities. As the global warming is an important issue, long-term policy making on a lower GHG emitting project should be done in terms of full-energy-chains analysis.

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PARAMATER SENSITIVITY OF AN EUTROPHICATION MODEL

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Abstract. Modern environmental management decisions are based on mathematical models of ecosystems or ecological processes. To get suitable simulation results for management purposes the process of setting up of parameter values and initial conditions is of high importance. Management options for eutrophication control will be obtained by scenario analyses with changing parameter values (Straškraba and Gnauck 1985). The goal of sensitivity analysis is to determine how sensitive is the model to changes of parameter values, which is the basis for model validation and parameter estimation. Investigations of parameter changes are carried out for an eutrophication model of a lowland river basin. Estimating sensitivity to external parameters , those connected with driving variables or site constants, a picture is getting how would a given freshwater ecosystem behave under different conditions. One particular problem is the sensitivity to sampling intervals or kinds of approximation of driving variables. For internal parameters, those characterising state variables, the goal is too determine the importance of parameters for the approximation of the model to reality. Attention has to be devoted mainly to those parameters, to which the model is most sensitive. Eutrophication is referred to algal growth and intensive increase of dissolved nutrients within the water body. These man-made impacts influence matter fluxes and biological activity of a freshwater ecosystem. Therefore, those parameters connected with algal growth are of special interest for eutrophication management. The importance of parameters are visualised by ranking with Hasse diagram technique.

Investigations of parameter sensitivity are essential tasks of the modelling procedure. Especially for complex systems like freshwater ecosystems these investigations are necessary to mark the parameter range of validity for environmental management decisions. The output of the eutrophication simulator investigated is most sensitive for parameters characterising phytoplankton growth and dynamics. A second level of sensitivity is given by parameters describing nutrient cycles within the water body. In opposite of that, the influence of zooplankton to phytoplankton was found very stiff.

Keywords. modelling, parameter optimisation, parameter sensitivity, euthrophication

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MATHEMATICAL MODELING OF LARGE FOREST FIRES INITIATION

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Great interest of the problem concerned is explained by the influence of large forest fires on the ground level layer of the atmosphere, which causes medium temperature drop due to the area smoke screen and leads to the damage or delay of agricultural plant ripening and different ecological disasters. Considering that, natural investigations of these problems are merely impossible, methods of mathematical modeling are urgent. The paper suggested in the context of the general mathematical model of forest fires [1] gives a new mathematical setting and method of numerical solution of a problem of a large forest fire initiation. Mathematical model of forest fire was based on an analysis of known experimental data and using concept and methods from reactive media mechanics. The forest and combustion products are considered as a homogeneous two temperatures, reacting, non - deformed medium. Temperatures of condensed and gaseous phases are separated out. The first includes a dry organic substance, moisture (water in the liquid-drop state), condensed pyrolysis and combustion products (coke, ash) and mineral part of forest fuels. In the gaseous phase we separate out only the components necessary to describe reactions of combustion (oxygen, combustible products of pyrolysis of forest fuels and the rest inert components). The solid phase constituting forest fuels has no intrinsic velocity, and its volumetric fractions, as compared to the gaseous phase, can be neglected in appropriate equations because a volume unit of wood. It is considered that 1) the flow has a developed turbulent nature, molecular transfer being neglected, 2) gaseous phase density doesn't depend on the pressure because of the low velocities of the flow in comparison with the velocity of the sound, 3) forest canopy is supposed to be non-deformed porous medium. The research is done by means of mathematical modeling of physical processes. It is based on numerical solution of Reynolds equations for chemical components and equations of energy conservation for gaseous and condensed (for canopy) phases [2]. To describe the transfer of energy by radiation we use a diffusion approximation. To obtain discrete analogies a method of control volume of S.V.Patankar is used. Calculation method and program have been check. The boundary-value problem is solved numerically using the method of splitting according to physical processes. In the first stage, the hydrodynamic pattern of flow and distribution of scalar functions are calculated. The system of ordinary differential equations of chemical kinetics obtained as a result of splitting is then integrated. A discrete analog for equations is obtained by means of the control volume method. The accuracy of the program is checked by the method of inserted analytical solutions. Analytical expressions for the unknown functions are substituted in the system of differential equations and the closure of the equations are calculated. This is then treated as the source in each equation. Next, with the aid of the algorithm described above, the values of the functions are inferred with an accuracy of not less than 1%. The effects of the dimensions of the control volumes on the solution are studied by diminishing them. The time interval is selected automatically. As a result of mathematical modeling the fields of temperatures, mass concentrations of components of gaseous phase, volume fractions of components of solid phase, as well as vectorial fields of velocity at different instants of time. It allows to investigate dynamics of forest fire initiation under influence of various external conditions: a) meteorology conditions (air temperature, wind velocity etc.), b) type (various kinds of forest combustible materials) and their state(load, moisture etc.). In this paper attention is given to questions of description of the initial stage in the development of a mass forest fires initiated by high altitude radiant energy source (for example Tunguska celestial body fall and etc.). Ignition outlines which fit well with the results of survey in the location of Tunguska celestial body fall were obtained. Contours derived for collision catastrophes look like a circle arc in the neighbourhood of epicenter of the explosion and take the form of the ellipse extended in the flight trajectory projection direction of Tunguska celestial body. As distinct from collision catastrophes, ignition contours take the form of a circumference as illustrated as the result of numerical experiments for the ignition of a homogeneous vegetation layer by radiation from the air nuclear explosion. The results obtained agree with the laws of physics and experimental data [1,2]).

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Numerical Methods and Algorithms

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

ON A CHARACTERIZATION OF PHYSICAL SYSTEMS BY SPACES OF NUMERICAL EVENTS

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Let S denote the set of all states of a physical system $\mathbf{S}$. The probabilities $p(s)$ of the occurrence of an event obtained by observing $\mathbf{S}$ for different states $s \in S$ determines a function from S to $[0,1]$ called a numerical event (or multidimensional probability).

Let P be a set of functions from S to $[0,1]$. Then P is ordered in a natural way by the partial order of functions, i. e. $p \leq q$ if $p(s) \leq q(s)$ for all $s \in S$. It is apparent to assume that P has the following properties:

(1) $0 \in P$. (2) $p \in P$ implies $p' := 1 - p \in P$. (3) If $p + q \leq 1$ for $p, q \in P$ then $p + q \in P$.

0 and 1 denote the corresponding constant functions. If $p + q \leq 1$ then p and q are called orthogonal. Three elements $p, q, r \in P$ which are pairwise orthogonal are called an orthogonal triple (p, q, r).

If, in addition to (1) – (3), P fulfils that

(4) $p + q + r \leq 1$ for every orthogonal triple (p, q, r)

then P is called an algebra of S-probabilities.

Examples of algebras of S-probabilities:

(a) $\{0, x, 1-x, 1\}$ is an algebra of $[0,1]$-probabilities.

(b) Let H be a Hilbert space, S denote the set of all one-dimensional subspaces of H and for every $s \in S$, let a_s be a fixed unit vector in s. If we denote the set of all projectors of H by $P(H)$ and write $(.,.)$ for the inner product in H then $\{s \to (Qa_s, a_s) \mid Q \in P(H)\}$ is an algebra of S-probabilities, which, in general, is not a Boolean algebra.

Algebras of S-probabilities serve for generalizations of classical event fields in case of quantum mechanical systems. A classical physical system can then be characterized by the fact that the corresponding algebra of S-probabilities is a Boolean algebra.

In this paper we first identify algebras of S-probabilities among sets of numerical events and specify conditions for these sets to be Boolean algebras. From the obtained results we then derive possibilities to determine by means of appropriate measurements whether one deals with a quantum mechanical system or a classical one, as well for small sets of states as for infinitely many.

Example for a small set of states:

If every $p \in P$ can only assume the values 0 and 1 then P is an algebra of S-probabilities if and only if $P = \{I_X \mid X \in M\}$ where M is a set of subsets of S satisfying

$\emptyset \in M$; $A \in M$ implies $S \setminus A \in M$; $A, B \in M$ and $A \cap B = \emptyset$ together imply $A \cup B \in M$.

If, moreover, $A \cup B \in M$ for all $A, B \in M$ then $(P, \leq')$ is a Boolean algebra. (I_X denotes the indicator function corresponding to X.) Now, if S is finite, say $S = \{s_1, \ldots, s_n\}$ then $p \in P$ can be represented by an n-tuple $(p(s_1), \ldots, p(s_n))$ of 0 and 1, and it is easy to check the conditions (i) – (iii), at least if n is not too large. Having already verified that P is an algebra of S-probabilities one has evidence to deal with a classical physical system if the join of any two n-tuples $(p(s_1), \ldots, p(s_n)) \in P$ belongs to P.

In case of infinitely many states we apply a theorem which we derive by endowing P with a further operation that can be interpreted by logical operations. The well-known experiment contradicting classical logical results by observing "spin up" and "spin down" of an electron in a magnetic field will fit into this concept.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

BOUNDARY CONDITIONS IN LINEAR 3D-AEROACOUSTIC NUMERICAL SIMULATION

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Introduction. The focus of this contribution lies in the modelling, analysis and simulation of realistic boundary conditions. We are especially concentrating on wave number dependent boundaries including reflection, transmission and absorption of acoustic waves [2]. The underlying numerical research deals with the Spectral Method for benchmark problems, [4]. The realistic treatment of boundary conditions within accurate aeroacoustic simulations is of interest for [1], [3] et alii.

Content. To introduce the spectral approach, which includes a global differentiation technique, we study the homogeneous Helmholtz equation. After developing the theory for equispaced and clustered grids in 1D, convergence relationships and the treatment in higher dimensions as well as the inclusion of arbitrary homogeneous boundary conditions are discussed. Finally numerical results for selected 1D and 3D examples in the time domain and in the frequency domain for the related Wave equation and the Helmholtz equation are shown.

With our simulations we could verify, that analytic solutions end up in spectral accuracy. Additionally it is almost unpretentious to include arbitrary combinations of homogeneous boundary conditions. The simulation examples in the time domain hold very low dispersion and dissipation errors without conspicuous spurious oscillations in long-term integrations. Regrettably it is not possible to expand this method to complex geometries. The global approach, in combination with the tensor product grids for higher dimensional problems, only allows simple benchmark geometries like cuboids, spheres and cylinders. Another difficulty is, that it becomes very fast too expensive to calculate problems with more dimensions and growing degrees of freedom.

Because of these results we want to use the Spectral Method to compare its accurate solutions with solutions of Spectral Finite Element Methods, which can cope with complex geometries, in simple benchmark geometries in the future.

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TAYLORIAN INITIAL PROBLEM

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Introduction. In recent years, intensive research in the field of numerical solutions of systems of ordinary and partial differential equations has been done at the Brno University of Technology, Faculty of Information Technology. The basic numerical method employed is the so-called Modern Taylor Series Method (MTSM). It has been described, studied, and numerous aspects have been investigated such as processing in parallel systems. Also a simulation system TKSL has been developed which is based on the Taylor series method. For some results see [2].

The MTSM is based on a transformation of the initial problem into another initial problem with polynomials on the right-hand sides. This is a precondition for a Taylor series method to be successfully applied to the task of finding a numerical solution. The solution of the transformed initial problem then includes the solution of the original system.

This approach has been implemented in a simulation language TKSL (an implementation of the Modern Taylor Series Method on a personal computer) [1].

Automatic integration method order setting The best-known and most accurate method of calculating a new value of a numerical solution of a differential equation is to construct the Taylor series in the form

$$y_{n+1} = y_n + h * f(t_n, y_n) + \frac{h^2}{2!} * f^{[1]}(t_n, y_n) + \cdots + \frac{h^p}{p!} * f^{[p-1]}(t_n, y_n) \tag{1}$$

where h is the integration step.

The main idea behind the Modern Taylor Series Method is an automatic integration method order setting, i.e. using as many Taylor series terms for computing as needed to achieve the required accuracy.

The Modern Taylor Series Method used in the computations increases the method order ORD automatically, i.e. the values of the terms

$$\frac{h^p}{p!} * f^{[p-1]}(t_n, y_n)$$

are computed for increasing integer values of p until adding the next term does not improve the accuracy of the solution.

As an application of the automatic integration method order setting the solution of the well known *Van-Der-Pol's equation*. Another application of the automatic integration method order setting is focused on a particular problems with the integration of *stiff systems*.

Definite integrals and integral equations, due to the number of applications, are very important mathematical tools. Their solution using the Modern Taylor Series Method is also the subject of this paper. For all functions that have Taylor series the calculation of their integrals can be conducted indirectly via their derivatives. Thus, the problem of solving a definite one-dimensional integral taken as a function of the upper boundary can be transformed to solving a system of differential equations.

Conclusions The principal objective of the paper is to provide an idea of a mathematical background for the practical research in the field of numerical solutions of systems of differential equations that has been conducted at the Brno University of Technology for some time. This particularly concerns the problem of transforming a system of differential equations into a new system with polynomials on the right-hand sides.

Another problem that the paper deals with has also arisen in practical research. It is the problem of a suitable stopping rule, that is a rule that decides that no other step needs to be undertaken since the set accuracy requirements are satisfied. Various methods can be devised, more or less ingenious, but the basic question remains, namely, at a given point in calculation, how many subsequent steps must actually be "inspected" to get a satisfactory conviction that the sum of increments provided by the rest of the infinite series will not exceed the required accuracy. In particular, when solving some relatively simple problems using the basic version of the Taylor series method algorithm, situations occurred where the calculation could not be stopped using a straightforward stopping rule since all the contributions equalled zero for several consecutive terms. Knowing the exact solutions to these particular problems it was clear that, in extremely unfavourable circumstances, the calculation might end with considerable errors. This can be helped by using an improved version of the basic Taylor series method algorithm.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

EFFICIENT DIRECT SEARCH ALGORITHMS FOR SOLVING A LARGE-SCALE STOCHASTIC DYNAMIC PROGRAM

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Introduction. Many general-purpose decomposition techniques and heuristics have been introduced to minimize the computational cost of solving large models. However, many models tend to remain utterly large and costly prompting the application-oriented practitioner to exploit the structure of the specific problem at hand and devise decomposition techniques and solution algorithms that render efficient solutions. In this paper, a large stochastic dynamic program is formulated to address the problem of managing a water reservoir under several operational constraints and subject to stochastic effects. By inspecting the structure of the problem, and under suitable assumptions on the interdependence among the stochastic variables, and given the finite range within which the variables lie, an efficient solution algorithm was developed. The procedure considers the discretization of some of the key variables and searching for values of the decision variables that would maximize the objective set forth in the model. Furthermore, to avoid the need to specify functional forms for the stochastic variables, a simulation routine was embedded in the model's solution procedure, as well as a validation tool of the model's performance through the direct calculation of the system reliabilities and comparing them to the model solution's output.

Related Literature To solve large stochastic problems, several techniques have been proposed in the literature. These include heuristics, decomposition techniques, and in the case of stochastic programs, the use of stochastic dynamic programming (SDP). For a detailed review of stochastic optimization, heuristics and decomposition techniques, the reader is referred to Fouskakis and Draper (2002), Silver (2005) and Dominguez-Ballesteros et al. (2002), respectively. In the SDP case, modelers often run into the so-called *curse of dimensionality* whereby the problem becomes exponentially large as more stages and evaluations are required. To alleviate this problem, researchers have proposed various aggregation, decomposition, and hybrid simulation-decomposition techniques. In this paper, an integrated simulation-optimization approach is used in conjunction with decomposition techniques that exploit the problem structure to generate very efficient solution algorithms. Under lenient assumptions on the dependence between random variables, the solution cost is significantly reduced

Problem Statement. To illustrate the approach, we develop a stochastic dynamic programming model for the reservoir problem involving multiple periods representing 12 months of operation, see Saadouli and Edirisinghe (2005) for a detailed description. The main source of randomness in the reservoir is the monthly water inflow to the reservoir. The downstream demand for irrigation water is prescribed *a priori* and thus it is not random. During any month, the randomness of inflow will be modeled by a sample of discrete outcomes, generated randomly subject to the history of inflows up until that month. In the sequel, we will describe how such samples are generated to develop a *scenario tree* of potential future inflow patterns. The degree of violation of a constraint is considered explicitly and is controlled. The state of the system is completely defined by the state space $(\mathscr{H}_{t-1}, S_{t-1})$. The history of inflows $\mathscr{H}_{t-1}$ provides the information on what scenario of inflows has realized up until period t. The model is to select the release R_t that would minimize the expected penalty cost, less energy benefits, relative to the inflows.

Solution Procedure. Solving the dynamic program requires the solution of a nonlinear program at each node $\mathscr{H}_{t-1}$, for a specified S_{t-1}. This is an orenous task as the number of such nodes increases exponentially with the addition of periods and/or outcomes. Furthermore, the latter computation needs to be performed for every possible S_{t-1}, as determined by a suitable grid of values for S_{t-1}. Efficient solution algorithms of the DP under the assumption that the monthly inflows are independent and then under the assumption that the monthly inflows are only dependent on the cumulative inflows are developed and tested. The simulation analysis shows a high level of the various reliabilities controlled by the model.

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NUMERICAL EXPLORATION OF KALDORIAN INTERREGIONAL MACRODYNAMICS: ENHANCED STABILITY AND PREDOMINANCE OF PERIOD DOUBLING UNDER FLEXIBLE EXCHANGE RATES

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Aspects of international macroeconomics and regional economics are studied recently by methods of nonlinear economic dynamics (see, e.g. [1], and [2]). In this paper we employ such methods to study the economic interdependency between two regions.

We present a discrete two-regional Kaldorian macrodynamic model with flexible exchange rates. The structures of the two regional economies are assumed similar. The model is five-dimensional with three basic parameters, the common speed of adjustment of the goods markets (α) and the degrees of economic interaction between the regions through trade (δ) and capital movement (β).

We then proceed to explore our two-regional macrodynamic model numerically focusing on the stability of equilibrium under variations of the model parameters and on the asymptotic behavior of the system outside the stability region, and consider in particular the possibility of occurrence of business cycles. We use a grid search method in two-dimensional parameter subspaces, and coefficient criteria for the flip and Hopf bifurcation curves, to determine the stability of equilibrium region and its boundary curves in several parameter ranges (as in Figure).

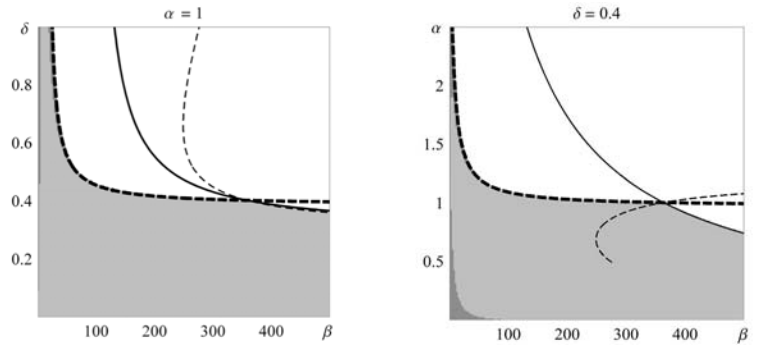

Figure: Region of stability of equilibrium in (β, δ) plane for $\alpha = 1$ and in (β, α) plane for $\delta = 0.4$

By considering the geometry of the locus (thin dashed curve in Figure) of the points of intersection of the flip bifurcation curve (bold dashed) and the Hopf bifurcation curve (continuous) we deduce the trade threshold for the occurrence of cycles in the form of restrictions described by inequalities that must be satisfied by the parameters δ, α and β.

We find that the present model is characterized by enhanced stability of equilibrium, while its predominant asymptotic dynamical behavior when equilibrium is unstable is period doubling. This evolves to chaotic behavior by going through an intermediate phase of period–2 cycles. Business cycles are scarce and short-lived in parameter space, occurring at large values of the degree of capital movement β. A characteristic difference from the fixed exchange rates system considered previously is that in our present system of flexible exchange rates for cycles to occur sufficient amount of trade is required *together* with high levels of capital movement. Examples of bifurcation and Lyapunov exponent diagrams illustrating period doubling or cycles, and of cycles in two-dimensional projections, are given.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A FLEXIBLE TIME INTEGRATION METHOD FOR THE 1D HEAT CONDUCTION PROBLEM

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In process control, there is a need for mathematical models which are both computationally inexpensive as well as reliable in terms of accuracy and convergence. Motivated by these needs, a method to compute the *temperature field* in a *one-dimensional domain* of a solid with *nonlinear material parameters* and *radiation boundary conditions* is proposed [1]. The approach originates from an application in the steel industry, where slabs or rolled products are to be heat-treated or reheated according to specific temperature trajectories [3]. However, the method is transferable to other diffusion-convection systems described by parabolic initial-boundary value problems.

A nonlinear, time-invariant *transformation of the temperature values* allows to isolate the nonlinear material characteristics into a *single* parameter of the heat conduction equation [1]. By means of this transformation, the temperature is replaced as a system state by a quantity proportional to the specific enthalpy. For the time being, *Neumann boundary conditions* are considered, and the *Galerkin method* is employed for spatial discretization of the problem. The remaining nonlinear material parameter is extracted from the weak formulation, and it is shown that the Galerkin approach with just *three* polynomial trial functions suffices to achieve acceptable accuracy.

An analytical solution of the obtained explicit ordinary differential equation was not found. Utilizing a standard numerical time integration scheme would be possible, yet the entailed computational load is undesirable in view of the intended practical application. Therefore, an *approximate time integration method* is proposed, where the system inputs are constrained to *piecewise linear, discontinuous signals* to obtain a discrete-time system. Because of the shape of the input signal, the approach may be classified as a *first-order-hold type method*, and it allows to account for batch processes or discontinuous process steps.

Only after the discretization of the problem, the Neumann boundary conditions are substituted by *radiation boundary conditions*. Hence, the ambient temperatures serve as control inputs, and an exact satisfaction of the boundary conditions is only achieved at the sampling points. The radiative heat exchange is computed by means of the *Stefan-Boltzmann law* [2], which contains a fourth-power nonlinearity. However, the model finally constitutes a *nonlinear, implicit difference equation*, which can be reliably solved by the Newton-Raphson method or by fixed-point iteration. The implicit structure of the difference equation is advantageous for the numerical stability of the integration method. The chosen *sampling period* may be *large* as well as *highly variable*.

The feasibility and accuracy of the proposed method are demonstrated by means of an example problem of heat treatment of a steel slab. Numerical results are compared to the *finite difference method* using various grid sizes. The advantages and the flexibility of the proposed approach are based on robustness against variations of the sampling time, reliable convergence behavior, small model dimensions, and low computational costs. Therefore, the model is suitable for (real-time) applications, like trajectory planning, optimization, or control tasks, where constraints on computing time are often tight.

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THE PROPOSAL OF THE ALTERNATELY EVOLVING GENETIC ALGORITHM AND ITS APPLICATION

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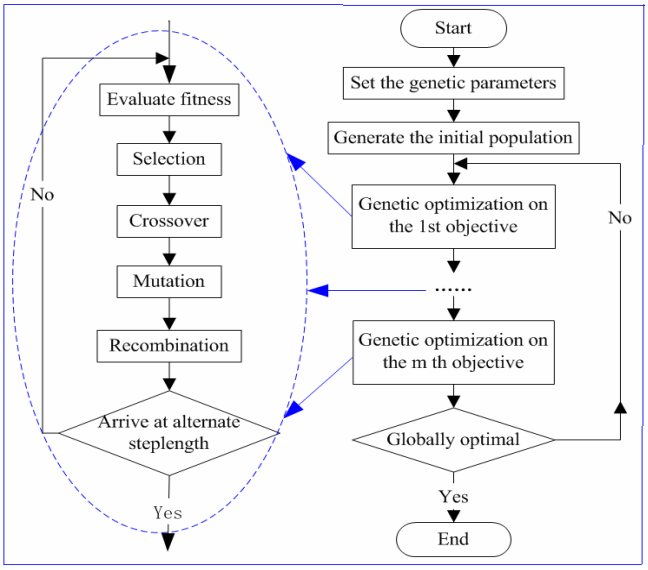
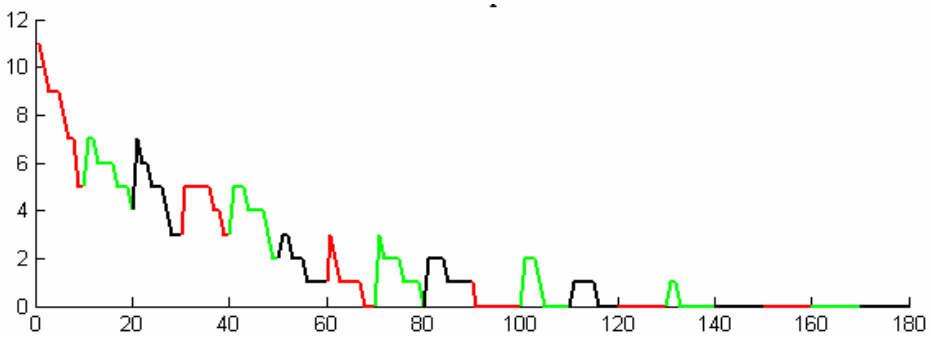
The proposal of the alternately evolving genetic algorithm. Genetic algorithm (GA) is a random searching algorithm, and has been widely applied to many fields. When dealing with multi-objective combinatorial optimization problems, the usual genetic algorithm usually employs a comprehensive weighed objective to replace multiple objectives through constructing an evaluation function, and then uses unified genetic operators to optimize the weighted objective in a unified coding scheme. This method may be ineffective in some cases for the objectives may conflict with one another in the evolutionary process. By way of contrast, this paper puts forward an alternately evolving genetic algorithm from the opposite direction, which adopts alternate strategy to optimize multiple objectives one by one circularly. The flow char of alternately evolving GA is shown below:



Experiment. In order to verify the feasibility and high efficiency of the alternately evolving GA, take Sudoku as an example. The most common Sudoku puzzle consists of 9×9 grid and 3×3 blocks for a total of 81 cells. And the objective is to make each row, column and block have no repeated digits. So the Sudoku puzzle is a combinatorial optimization problem of three objectives. The solving result is shown as follows:



The change of each objective's punishment. The graph's abscissa refers to evolving generations, and the ordinate refers to row, column or block objective's punishment. The curve's fluctuation in the graph is the very result of alternate evolution, in which the red, the green and the black curve represents the row, the column and the block objective's evolution respectively.

As can be seen from the graph, although every evolution's alternation always makes punishment fluctuate, the general trend of the three kinds of punishment is convergent. And when the three kinds of alternate steplength are all set to 15, the three kinds of punishment all converge to 0 at about 150 generations. The sensitivity of each objective's evolutionary depth is also analyzed in the paper.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Advances in Model Order Reduction

PRECONDITIONING TECHNIQUES IN LINEAR MODEL ORDER REDUCTION

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Model order reduction is a field of research that receives increased interest in recent years. A closer look at the techniques being used reveals that there are essentially a number of classes. In [1], these classes are identified, and a state-of-the-art overview is provided. Besides the well known balanced truncation methods originating from systems and control theory, there is also the popular class of Krylov subspace based techniques. Methods from the latter class are closely related to iterative solution methods for linear systems such as ICCG, biCGstab and CGS. Using Krylov subspaces a basis is built up in such a way that the dominant (and most important) part of the solution is found within an acceptable and preferably low number of iterations.

Within the field of numerical linear algebra, it is well known that the number of iterations within iterative solutions is very much dependent on the conditioning of the coefficient matrix. This explains the need for preconditioning techniques, which provide ways to improve the conditioning by multiplying the system by scaling matrices. In fact, one could argue that preconditioning is equivalent to applying a direct solution method (such as Gaussian elimination or Choleski decomposition) in an incomplete or partial sense. Popular choices are the incomplete Choleski decomposition for symmetric systems, and incomplete LU decompositions with thresholding (ILUT) for more general systems.

Since Krylov subspace based linear MOR is very much related to iterative solution methods for linear systems, it seems natural to also employ some kind of preconditioning. In this way, one would hope to reduce the number of basis vectors in the Krylov subspace, and hence obtain a more reduced model. So far, this concept seems not to have been pursued seriously. The main reason is that the transfer function often depends on the product of two matrices, which makes it more difficult to employ preconditioning. This is comparable to the situation encountered in generalized eigenvalue problems.

In order to assess the applicability of preconditioning within the area of model order reduction, we started our investigations with static electronic circuits, more specifically with large resistor networks. For this type of problem, the transfer function contains only a single matrix, thereby opening up a host of possible preconditioning strategies. Ordering techniques are an important ingredient, and we use the recently developed BBD algorithm for this purpose in combination with graph theoretical methods. The results are impressive, as is demonstrated in Table 1. For the more general case involving also capacitors and resistors, new research has started recently, and we will present first results of preconditioning such systems.

Table 1: Results for the resistor network reduction

	Network I		Network II		Network III		Network IV	
	Original	ROM	Original	ROM	Original	ROM	Original	ROM
#terminals	3260		1978		15299		8000	
#int nodes	99k	8k	101k	1888	1M	180k	46k	6k
#resistors	161k	56k	164k	39k	1.5M	376k	67k	26k
#other elements	1874		1188		8250		29k	
#other unknowns	0		0		0		11k	
CPU time reduction	130 s		140 s		1250 s		75 s	
CPU time simulation	67 hrs	6 hrs	20 hrs	2 hrs	–	120h	–	392s
Speed up	10x		12x		∞		∞	

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

EFFICIENT BALANCING BASED MOR FOR SECOND ORDER SYSTEMS ARISING IN CONTROL OF MACHINE TOOLS

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Behavioral simulation of machine tools is using discrete structural models. These models result from a finite element analysis being applied to their mechanical structure. Therefore they are in general sparse but very large since many details have to be resolved. This accounts for unacceptable computational and resource demands in simulation and especially control of these models. To reduce these demands and to be able to compute solutions and controls in acceptable, i.e. applicable, time frames model order reduction is applied. Classically modal truncation is used for this task. The reduced order models (ROMs) generated are normally relatively large and often need manual modification by addition of certain technically motivated modes. That means they are at least partially heuristic and cannot be generated fully automatic. Engineers are therefore searching for alternate reduction methods.

Here we will concentrate on the application of balancing based model order reduction techniques. A central topic is to provide a reduced order model for the construction and parameterization of a practicable controller for the application. Our main focus will be on presenting a way to efficiently compute the ROM exploiting the sparsity and second order structure of the FEM semi-discretization, rather than presenting a new reduction technique.

BALANCING OF DISSIPATIVE HAMILTONIAN SYSTEMS

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Model reduction is a major issue for control, optimization and simulation of large-scale systems. We present a method for model reduction of perturbed linear Hamiltonian systems. The Hamiltonian approach involves also second-order equations that appear in a variety of physical contexts, e.g., in molecular dynamics or structural mechanics. Common spatial decomposition methods such as Proper Orthogonal Decomposition, Principal Component Analysis or the Karhunen-Loève expansion aim at identifying a subspace of "high-energy" modes onto which the dynamics is projected (Galerkin projection). These modes, however, may not be relevant for the dynamics. Moreover these methods tacitly assume that all degrees of freedom can actually be observed or measured. Unlike the aforementioned approaches *Balanced Truncation* accounts for incomplete observability. It consists in finding a coordinate (i.e., balancing) transformation such that modes which are least sensitive to the external perturbation (controllability) also give the least output (observability) and therefore can be neglected. Accordingly, a dimension-reduced model is obtained by restricting the dynamics to the subspace of the best controllable and observable modes (truncation). A great advantage of the method is that it gives computable *a priori* error bounds; a drawback is that it typically fails to preserve the problem's physical structure (e.g., being Hamiltonian) and that its second-order variants suffers from lack of stability [1].

Here we adopt a Hamiltonian framework that allows for a generalization of Balanced Truncation to second-order problems [2]. The control variable function may be either deterministic or random where systems of the latter class are known by the name of second-order (also: underdamped) Langevin equations [3]. Confining a Hamiltonian system to a given subspace is well understood in terms of (holonomic) constraints and, although the balancing transformation mixes positions and momenta, the truncation step can be formulated as a holonomic constraints. The negligible modes in the system are associated with certain small *Hankel singular values*, and it turns out that, borrowing arguments from singular perturbation theory, sending them to zero forces the dynamics to the best controllable and observable subspace. The resulting low-dimensional system is a again a stable and passive Hamiltonian system with collocated inputs and outputs.

It is interesting to note that the singular perturbation argument applies to both the deterministic and the noisy case although the types of convergence are very different. In particular the stochastic dynamics does not converge point-wise to the controllable and observable subspace as the small singular values go to zero but rather in the mean square sense. Nonetheless the coefficients of the reduced stochastic systems are exactly the same as that of the deterministic control system. The deterministic problem has been addressed in [2] and we shall focus mainly on the stochastic case here, discussing convergence and issues of structure-preservation.

For the stochastic system the balancing transformation can be computed from simulation data without solving Lyapunov equations, and the similarity between the deterministic and the stochastic case suggests to exploit this property as well for the deterministic system if the dimension of state space is too high to solve the corresponding Lyapunov equations. We explain how to compute balancing transformations from sampled data in general and give numerical examples that illustrate the method in either case.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODEL ORDER REDUCTION FOR SEMI-EXPLICIT SYSTEMS OF DIFFERENTIAL ALGEBRAIC EQUATIONS

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Increasing complexity of mathematical models demands techniques of model order reduction (MOR) that enable an efficient numerical simulation. MOR methods are well developed for linear systems of ordinary differential equations (ODEs), whereas the nonlinear case represents still an open field of research, see [1]. We investigate MOR for semi-explicit systems of differential algebraic equations (DAEs). Systems of DAEs result in the mathematical modeling of a wide variety of problems like electric circuit design, for example. We consider a semi-explicit system of DAEs

$$\begin{aligned} y'(t) &= f(y(t),z(t)), & y:\mathbb{R}\to\mathbb{R}^k \\ 0 &= g(y(t),z(t)), & z:\mathbb{R}\to\mathbb{R}^l \end{aligned} \tag{1}$$

with differential and perturbation index 1 or 2. For the construction of numerical methods, the direct and indirect approach can be used. The direct approach applies an ε-*embedding* of the DAEs (1), i.e.,

$$\begin{aligned} y'(t) &= f(y(t),z(t)) \\ \varepsilon z'(t) &= g(y(t),z(t)) \end{aligned} \quad \Leftrightarrow \quad \begin{aligned} y'(t) &= f(y(t),z(t)) \\ z'(t) &= \tfrac{1}{\varepsilon} g(y(t),z(t)). \end{aligned} \tag{2}$$

Techniques for ODEs can be employed for the singularly perturbed system (2). The limit $\varepsilon \to 0$ yields an approach for solving the DAEs (1). The applicability of the resulting method still has to be investigated.

Alternatively, the indirect approach is based on the *state space form* of the DAEs (1) with index 1, i.e.,

$$y'(t) = f(y(t),\Phi(y(t))) \tag{3}$$

with $z(t) = \Phi(y(t))$. To evaluate the function Φ, the nonlinear system

$$g(y(t),\Phi(y(t))) = 0 \tag{4}$$

is solved for given value $y(t)$. Consequently, the system (3) represents ODEs for the differential variables y and ODE methods can be applied. The part (4) includes constraints. More details concerning techniques based on the ε-embedding and the state space form can be found in [3].

In this work, we focus on the direct approach for semi-explicit systems of DAEs (1). For reducing the singularly perturbed system (2), two different scenarios to handle the artificial parameter ε exist. In the first scenario, we fix a small value ε and then use a standard technique for reduction of ODEs. Finally, we obtain a reduced ODE (with a small ε inside). In the second scenario, we consider the parameter ε as an independent variable (value not predetermined). We can use a parametric MOR for reducing the ODE system (2). The applied parametric MOR is based on [2] in this case. The limit $\varepsilon \to 0$ provides us a reduced system for approximating the original DAEs (1). The existence of the approximation in this limit and its quality still has to be analyzed. The input-output behavior of each system can be described by a transfer function in frequency domain. We investigate the discrepancy between the transfer function of the original DAEs (1) and the regularized system (2). We present simulation results of both scenarios corresponding to linear test examples, which model electric circuits.

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MACHINE TOOL SIMULATION BASED ON REDUCED ORDER FE MODELS

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Introduction. Numerical simulations of the behavior of machine tools are usually based on a finite element (FE) model of their mechanical structure. In order to capture all necessary details FE models are usually very large and sparse. Hence the computation of the simulation takes an unacceptable long time and requires much memory space. To calculate the results in reasonable time typically modal reduction is used to obtain a model of lower order. This method is based on the eigenvalue decomposition and has the disadvantage of a huge amount of computation time and space when the dimension of the model is large. Benner and Saak are reporting on efficient balancing based MOR in another contribution. Here the model order reduction with Krylov subspace based methods is considered.

Abstract. The simulation of a machine tool is based on two parts: the model of the control loop and the model of the mechanical structure of the machine tool. To describe the behavior of the mechanical structure a system of partial differential equations is used. After linearization and discretization by means of finite elements or finite differences one obtains a system of ordinary differential equations of second order:

$$M\ddot{x}(t) + D\dot{x}(t) + Kx(t) = Bu(t)\,, \quad y(t) = C_v^T\dot{x}(t) + C_p^T x(t) \tag{1}$$

where $M, D, K \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times p}$, $C_v^T, C_p^T \in \mathbb{R}^{m\times n}$, $x(t) \in \mathbb{R}^n$, $u(t) \in \mathbb{R}^p$, $y(t) \in \mathbb{R}^{m\times p}$. The system matrices are usually sparse, of high order and non-symmetric.
Now one is interested in a reduced system with dimension $k \ll n$:

$$\hat{M}\ddot{\hat{x}}(t) + \hat{D}\dot{\hat{x}}(t) + \hat{K}\hat{x}(t) = \hat{B}u(t)\,, \quad \hat{y}(t) = \hat{C}_v^T\dot{\hat{x}}(t) + \hat{C}_p^T\hat{x}(t)\,,$$

where $\hat{M}, \hat{D}, \hat{K} \in \mathbb{R}^{k\times k}$, $\hat{B} \in \mathbb{R}^{k\times p}$, $\hat{C}_v^T, \hat{C}_p^T \in \mathbb{R}^{m\times k}$, $\hat{x}(t) \in \mathbb{R}^k$, $u(t) \in \mathbb{R}^p$, $\hat{y}(t) \in \mathbb{R}^{m\times p}$, which is expected to capture essential dynamical properties of the original system.
Alternatively before the reduction process any second order system (1) can be transformed into a first order system:

$$E\dot{z}(t) = Az(t) + Gu(t)\,, \quad y(t) = C^T z(t) \tag{2}$$

where $E, A \in \mathbb{R}^{2n\times 2n}$, $G \in \mathbb{R}^{2n\times p}$, $C^T \in \mathbb{R}^{m\times 2n}$, $z(t) \in \mathbb{R}^{2n}$, $u(t) \in \mathbb{R}^p$ and $y(t) \in \mathbb{R}^{m\times p}$.
After reduction one obtains the reduced first order system:

$$\hat{E}\dot{\hat{z}}(t) = \hat{A}\hat{z}(t) + \hat{G}u(t)\,, \quad \hat{y}(t) = \hat{C}^T\hat{z}(t)\,, \tag{3}$$

where $\hat{E}, \hat{A} \in \mathbb{R}^{k\times k}$, $\hat{G} \in \mathbb{R}^{k\times p}$, $\hat{C}^T \in \mathbb{R}^{m\times k}$, $\hat{z}(t) \in \mathbb{R}^k$, $u(t) \in \mathbb{R}^p$, $\hat{y}(t) \in \mathbb{R}^{m\times p}$.
In engineering the modal reduction [2] is most common. In the last years new methods to reduce large and sparse dynamical systems were presented [1]. Here we concentrate on Krylov subspace methods, e.g. the Lanczos method applied to $E^{-1}A$ with starting vectors G and C generates matrices $V \in \mathbb{R}^{2n\times k}$ and $W \in \mathbb{R}^{2n\times k}$ with $W^TV = I_k$ such that (3) is constructed by applying the Petrov-Galerkin projection $\Pi = VW^T$ to (2):

$$\hat{E} = W^TEV, \quad \hat{A} = W^TAV, \quad \hat{G} = W^TG, \quad \text{and} \quad \hat{C}^T = C^TV.$$

The so generated reduced order model matches at least the first $\lfloor k/p + k/m \rfloor$ moments of the original system (that is at least the first $\lfloor k/p + k/m \rfloor$ terms of the Laurent series expansion of the transfer function around zero are equal). By applying rational Krylov methods, reduced order methods are obtained that match moments at different points in the complex plane. Doing so yield better approximations of the original system in a wider range of frequencies.
We implemented a method to reduce first and second order systems based on the Interpolation-Rational-Krylov-Algorithm (IRKA) [3]. We applied several Krylov methods based on moment-matching (PVA, PVL) and multi-point rational interpolation (MRI) to generate matrices V and W.
The approximation abilities of the reduced systems were evaluated by embedding them into the simulation control loop and comparing the results with the results obtained with the original system. Numerical results demonstrating the advantage and disadvantage of the different approaches for the simulation of a machine tool will be presented.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

HANKEL-NORM-BASED LUMPING OF INTERCONNECTED LINEAR SYSTEMS

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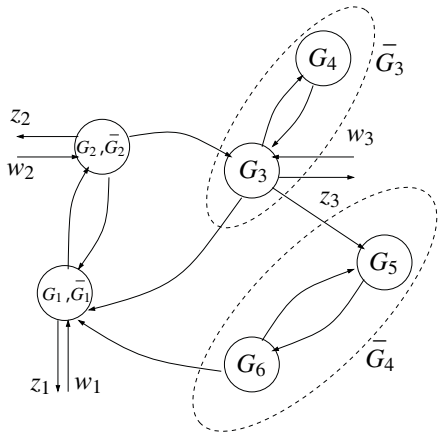
In this paper, we consider the problem of how and when to lump subsystems together in large linear interconnected systems with external inputs and outputs. The motivation for this work is that we often want to reduce the model order of large interconnected systems, see for example [3, 1, 2]. But before the reduction, we should identify what interconnection structures that are worth preserving. Let us illustrate the problem with an example. Consider an interconnection of linear dynamical systems, such as the one depicted below.



This system consists of six subsystems, $G_1, \ldots, G_6$, and it is being excited by the external signals w_1, w_2, w_3, and the signals z_1, z_2, z_3 are measurements on the system. We want to come up with a rationale for when to lump some of these subsystems together, in order to simplify its representation. Lumps are indicated with bar notation, $\bar{G}_k$, in the figure. The interconnection structure generally becomes less complicated for a lumped system, and it can be easier to understand and analyze the overall system behavior. Also, if we want to apply structure-preserving model reduction on the interconnected system, see for example [3, 1, 2], then the fewer structure constraints there are, generally the more the model order can be reduced.

Denote the transfer function from w to z in an interconnected system by the linear fractional transform $\mathscr{F}_l(N, G)$, where N models the interconnection topology and G is a block-diagonal transfer function with subsystem transfer functions G_k on its diagonal. We can now define a *constrained Hankel-norm* by

$$\|\mathscr{F}_l(N, G)\|_{H,k} := \sup_{w \in L_2(-\infty, 0] \neq 0; x_{-k}(0)=0} \frac{\|\mathscr{F}_l(N, G)w\|_{2,[0,\infty)}}{\|w\|_{2,(-\infty,0]}},$$

where x_k is the state of G_k. Hence, the entire interconnected system is at rest at $t = -\infty$, and is then maximally excited during $(-\infty, 0]$ using w such that all the states x_{-k} (all states except x_k) are zero at $t = 0$. Then the interconnected system is released from this state with zero input, and we measure the energy in the output. If the subsystem G_k is highly controllable and observable independently of all other subsystems in the interconnected system, then the number $\|\mathscr{F}_l(N, G)\|_{H,k}$ is large. In this paper, we show how the constrained Hankel-norm can be computed, and define the so-called *lumping index* γ_k by

$$\gamma_k := 1/\|\mathscr{F}_l(N, G)\|_{H,k}.$$

A subsystem with a large index γ_k is not a very visible and controllable subsystem by itself. We propose that one computes the lumping indices for all subsystems G_k, and compare them to each other. If there are large differences in the magnitudes of the lumping indices, then we propose that subsystems with large indices are lumped together. After a successful lumping, the lumps $\bar{G}_k$, are roughly equally controllable and observable subsystems, and thus of similar importance in the interconnected system.

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COUPLING SMOOTHED PARTICLE HYDRODYNAMICS AND REDUCED ORDER HEAT TRANSFER FOR EFFICIENT CASTING SIMULATION

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Introduction. Microcasting is a metal forming process based on lost-wax lost-mould investment casting, allowing for very complicated parts even with undercuts. Its simulation for microscale components requires modelling of both the melt fluid dynamics as well as the heat exchange with the macroscopic mould. The results allow to detect early solidification (which may hamper complete filling) and determine cooling curves for, e.g., the computation of the micro structure. This multiscale challenge can be solved by modeling the mould by a finite element method and applying model order reduction (MOR) to the resulting system of ordinary differential equations (ODEs). For the simulation of the free surface flow of the melt, smoothed particle hydrodynamics (SPH) is used which is a Lagrangian discretisation of the Navier-Stokes equations, thus providing automatic convection of internal degrees of freedom (DOFs). In this work, we couple these methods in an integrated implementation.

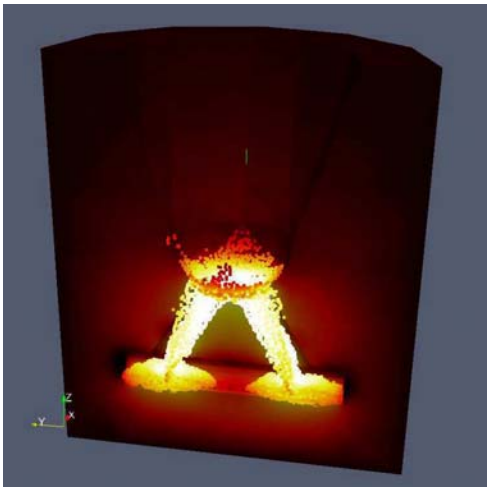

Figure 1: Melt's heat being transfered into the surrounding cast. Brighter color indicates higher temperature

Smoothed particle hydrodynamics. SPH [1, 2] interpolates a quantity f using a set of particles with DOF f_i, mass m_i, and a kernel $W(r)$ with width r_c. Let ρ_i be the mass density, r_i the particle's position and $r_{ij} = r_i - r_j$, then $\langle f_j \rangle = \sum_i \frac{m_i}{\rho_i} f_i W(r_{ij})$. For Fourier's law of heat conduction, we use the following discretisation:

$$\langle \nabla \cdot (\kappa \nabla T(f)) \rangle \approx \sum_j m_j (\kappa_j + \kappa_i)(T(f_j) - T(f_i)) \nabla W(r_{ij}) r_{ij} / (\rho_j \rho_i r_{ij}^2),$$

where f is the enthalpy, T the temperature, and κ the heat conductivity.

Model order reduction. The mould is modelled using finite elements, so that local refinement can be employed close to the micro-structure. The resulting system is large and redundant. Given the resulting ODE system $\mathbf{E}\dot{\boldsymbol{x}} = \mathbf{A}\boldsymbol{x} + \mathbf{B}\boldsymbol{u}$, where $\boldsymbol{u}$ are the input terminals, the Arnoldi method finds a subspace $\mathbf{V}$ for a Padé-type approximation of the system, where the first q moments of the Taylor expansion in complex frequency of the transfer functions match [3]. The number of equations is often reduced by a factor of more than 1000, while only insignificant deviations in the system response are observed.

Coupling. The SPH system and the reduced order model of the ODE system are coupled by a special kind of particle beyound the mould's wall. The wall particles interact with the fluid by providing temperature values T calculated from the state vector of the reduced system and by collecting transfered heat for the inputs $\boldsymbol{u}$ to the thermal system.

Results. The model has been applied to a non-trivial test geometry. The solution of the FEM system, resulting in $O(10^6)$ floating point operations per timestep, is reduced to $O(10^4)$ floating point operations per timestep, which is substantially less than the $O(10^6)$ floating point operations required for the SPH timestep integration.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODEL ORDER REDUCTION OF ELECTROMAGNETIC DEVICES WITH A MIXED CURRENT-VOLTAGE EXCITATION

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Modeling methods that are based on the finite spatial discretization approaches (e.g. finite elements, finite volume, finite difference, etc.) have become very popular in a wide range of modeling fields. This is due to their generic nature, and to their applicability to a large number of engineering problems. However, a well-known disadvantage of those modeling methods is the high dimensionality of the generated models, which generally makes the computational cost of solving their underlying system of equations very expensive. This in turn restricts their use, specially in the fields where several components models have to be coupled and solved simultaneously, as the cost of such a simulation may rapidly go beyond the available computational resources.

Model order reduction techniques present a solution for this problem, by offering the possibility of generating accurate reduced-order models that are able to approximate the behavior of the original large-scale models, while being much faster in the required simulation time [1]. Hence, by generating reduced models of the different components of a system, the simulation of the whole system can be performed very efficiently.

When modeling linear electromagnetic devices with electrical excitation coils, the input-output behavior of the device's model changes significantly when switching the applied excitation signal from voltage to current or vice versa [3]. This change in the behavior represents a challenging issue for applying the Krylov-based model order reduction techniques [2], as two different reduced-order models in two different state-spaces have to be generated in order to approximate the behavior of the original current and voltage-driven models, respectively. This dissimilarity in the state-spaces of the generated models imposes the need of performing a coordinate transformation whenever the excitation signal type is switched from current to voltage or vice versa during the simulation.

In this work, the input Krylov subspaces of both the voltage and current-driven models are proved to be equivalent. This equivalence allows halving the computational costs of reducing the order of both original models, by projecting them onto the same input Krylov subspace. Moreover, it significantly simplifies the procedure needed for switching the excitation signal during the device simulation using the reduced-order models. As an example, the presented results are applied to reduce the BEM-FEM models of an electrical transformer.

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MODEL ORDER REDUCTION FOR MULTIPLE GEOMETRIC PARAMETERS

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Summary In this contribution we consider finite element (FE) approximations to linear time-invariant systems which are parameterized by multiple parameters. The system responses of such FE models can be analyzed very efficiently by projection-based multi-parameter model order reduction (MOR) methods; for a pioneering work, see [1]. The considered methods can be characterized as single- or multi-point [2] methods or combinations thereof. Single-point methods are very attractive in the FE context, because they require one matrix factorization only. However, since the direct computation of the projection-basis is ill-conditioned, early implementations were limited to low polynomial order. Nowadays, numerically robust algorithms for multilinear [3] and multivariate polynomial parameterization [4] are readily available.

When geometry parameters are present, the application of such methodologies is hampered by the following two difficulties: first, tracking the impact of geometry parameters from the solid model through the meshing process to the resulting FE matrices and right-hand sides turns out to be a very intricate task. For complicated real-world problems, explicit knowledge of the parameter-dependence of the resulting FE model may just not be available. Second, a closer analysis reveals that, even under the assumption of smooth changes in mesh geometry, the global FE matrices are parameterized by multivariate rational functions. Hence MOR methods for polynomial parameter-dependence do not apply. To bypass these difficulties, we propose an approximate approach, whose main steps are as follows:

1. Mesh parameterization. Given an initial mesh $\mathscr{M}_0$ in the expansion point, construct a parameterized mesh $\mathscr{M}(\mathbf{s})$ which is topologically equivalent to $\mathscr{M}_0$. Furthermore, the node coordinates of $\mathscr{M}(\mathbf{s})$ have to be smooth functions of the parameters.
2. Interpolation. Evaluate the FE system at unisolvent points in parameter space and interpolate its parameter-dependence by multivariate polynomials. Note that explicit representations of the underlying functional dependencies are not required.
3. MOR. Since the interpolated FE system features polynomial parameter-dependence, the MOR method of [4] becomes applicable.

Numerical Example As a practical example, we analyze the bandpass filter of Fig. 1, which consists of three metallic posts within an empty waveguide. We consider four model parameters: the diameters of the posts, d_1 and d_2, their distance l_{12}, and the operating frequency f. Using the proposed MOR approach, a single matrix factorization is sufficient to generate a whole family of 20 dB bandpass filters; see Fig. 2. ROM errors are typically in the order of 10^{-4} to 10^{-3}, and evaluation time is 324 times faster than for the full model.

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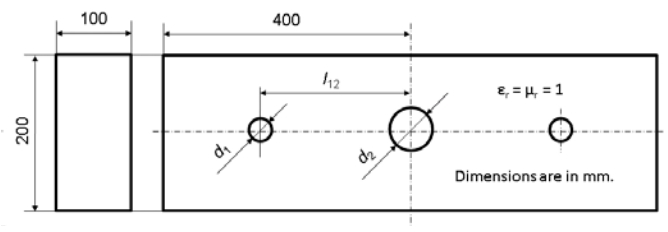

Figure 1: Structure of bandpass filter.

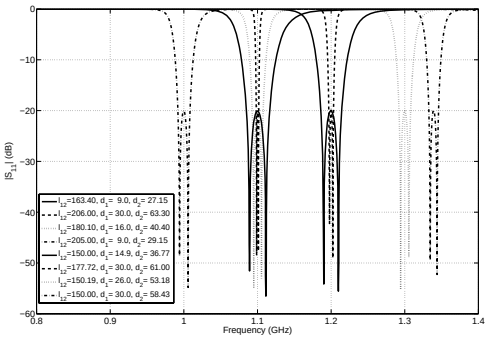

Figure 2: Magnitude of S_{11} versus frequency for selected filter configurations, based on a 5^{th} order ROM.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

EFFICIENT REDUCED MODELS FOR PARAMETRIZED DYNAMICAL SYSTEMS BY OFFLINE/ONLINE DECOMPOSITION

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Reduced basis (RB) methods are effective methods for model reduction of parametrized partial differential equations (P^{2}DEs). During the last years various types of stationary and time-dependent, linear and nonlinear P^{2}DEs have been treated. An overview with many recent references is given by [5]. In the field of dynamical systems' order reduction, these methods are largely unknown, but the interest in reduction of parametrized systems is increasing [2, 4, 3]. In the current presentation, we show that some characteristic components of RB-methods, in particular the offline/online decomposition and the a posteriori error estimation, can be transfered to model reduction of parametrized dynamical systems. We assume the following parametrized linear dynamical system for a state variable $x(t) \in \mathbb{R}^n$, input $u(t) \in \mathbb{R}^m$ and output variable $y(t) \in \mathbb{R}^p$ for $t \in [0,\infty)$

$$\frac{d}{dt}x(t) = \mathbf{A}(t,\mu)x(t) + \mathbf{B}(t,\mu)u(t)\,, \qquad y(t) = \mathbf{C}(t,\mu)x(t) + \mathbf{D}(t,\mu)u(t)\,. \tag{1}$$

The system matrices $\mathbf{A}(t,\mu) \in \mathbb{R}^{n\times n}, \mathbf{B}(t,\mu) \in \mathbb{R}^{n\times m}, \mathbf{C}(t,\mu) \in \mathbb{R}^{p\times n}, \mathbf{D}(t,\mu) \in \mathbb{R}^{p\times m}$ depend on a parameter $\mu \in \mathscr{P} \subset \mathbb{R}^d$ from a bounded parameter domain $\mathscr{P}$. The parameter μ is assumed to be fixed during a single simulation of the dynamical system. But a system is wanted, that allows multiple simulations with different parameters μ. Given a projection matrix $\mathbf{V} \in \mathbb{R}^{n\times k}$ with reduced order $k << n$ and $\mathbf{W} \in \mathbb{R}^{n\times k}$ biorthogonal, i.e. $\mathbf{W}^T\mathbf{V} = \mathbf{I}_{k\times k}$, the reduced system is, cf. [1]

$$\frac{d}{dt}\hat{x}(t) = \hat{\mathbf{A}}(t,\mu)\hat{x}(t) + \hat{\mathbf{B}}(t,\mu)u(t)\,, \qquad y(t) = \hat{\mathbf{C}}(t,\mu)\hat{x}(t) + \hat{\mathbf{D}}(t,\mu)u(t)\,. \tag{2}$$

For efficient computation, we assume a separable parameter dependence, e.g. $\mathbf{A}(t,\mu) = \sum_{q=1}^{Q_A} \sigma_A^q(t,\mu)\mathbf{A}^q$. with scalar parameter- and time-dependent coefficient function σ_A^q and parameter- and time-independent matrices $\mathbf{A}^q$ and small number of components Q_A. By this parameter dependence, an offline/online decomposition can be realized. In the offline phase, the parameter-independent quantities of the reduction scheme are computed. This phase is run once and may be arbitrary time consuming, as it will pay off in view of sufficiently many online simulations with varying μ. First, the the biorthogonal projection matrices $\mathbf{V}$ and $\mathbf{W}$ may be generated by any algorithm. Then parameter independent reduced components are computed, such as $\hat{\mathbf{A}}^q$. In the online phase, the parameter μ is known and the reduced simulation matrices, e.g. $\hat{\mathbf{A}}(t,\mu) = \sum_{q=1}^{Q_A} \sigma_A^q(t,\mu)\hat{\mathbf{A}}^q$, can be assembled and the reduced simulation can be run in complexity independent of n.

A further attractive aspect of RB-methods is rigorous error analysis. In particular a-posteriori error estimates can be obtained based on suitable definitions of the error $e(t,\mu)$ and residual $R(t,\mu)$. As an example, we obtain the following a posteriori error estimator under suitable additional assumptions

$$\|y(t,\mu) - \hat{y}(t,\mu)\| \le \Delta_y(t,\mu) := C\left(\|e(0,\mu)\| + \int_0^t \|R(\tau,\mu)\|\,d\tau\right)\,. \tag{3}$$

This simple result is practically relevant, as a full offline/online decomposition of the error bound is possible, hence enabling fast and rigorous error estimation during the reduced simulation. The error bound does not put strong assumptions on the basis apart from biorthogonality of $\mathbf{V}$ and $\mathbf{W}$. Hence in particular, these a-posteriori error bounds are as well valid for Krylov-subspace bases $\mathbf{V}$, bases obtained from balanced truncation, POD, etc.

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Object-oriented Modelling and Simulation

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

GROWING AN EQUATION-BASED OBJECT-ORIENTED MODELING LANGUAGE

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Equation-based object-oriented (EOO) modeling languages are typically rather complex. Such languages can unfortunately not be designed correctly once and for all, not least because all requirements and use cases are not known initially, and may never be known completely. Hence, there is a need to plan for modeling languages to grow [2] in a sound manner. This paper discusses and analyzes how EOO languages in general can be designed for growth, and in particular how this relates to the evolution of the Modelica [1] language. A language can grow in many different ways and directions. However, in the end, it is all about changing the language's syntax and/or semantics. The relationship between syntax and semantics regarding language growth is illustrated in Figure 1.

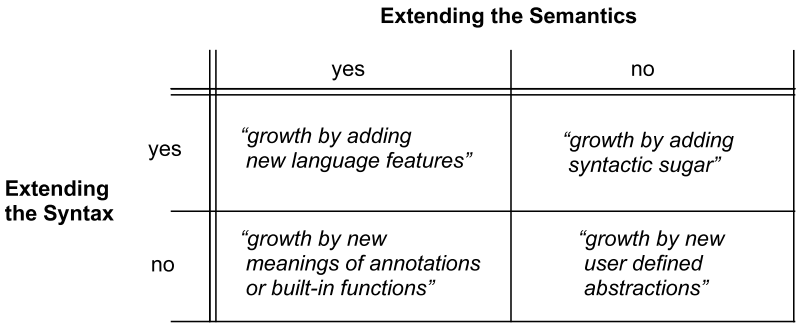

Figure 1: Categorization of different ways of growth.

Which is the right way to grow? The right way to grow a modeling or programming language is not always the easiest way. The easy way is not always easy for everyone. We will in this paper discuss and analyze the benefits and drawbacks of the various ways of growth from different stakeholders' perspectives:

- *Language Designers*. Person(s) inventing and designing the actual language.
- *End Users*. The users who use the language for modeling and analysis. In the Modelica case, these are usually engineers who create the model mainly using a graphical component-based user interface.
- *Library Users*. Engineers and scientists who develop reusable model libraries. Libraries are created by editing textual Modelica code. The free Modelica standard library is one example.
- *Tool Vendors*. Computer scientists and computer engineers who develop the compiler and tools for viewing, editing, compiling, and executing models.

Finally, the importance of different ways of growth are concluded and summerized as follows:

- *Growth by adding new language features*. Always changing both the syntax and the semantics is the most drastic kind of change of a language and should be minimized or avoided, especially for mature and widely used languages. The stakeholders that are most negatively affected of such changes are language designers and tool vendors, while library users might be the ones that push most for such extensions.
- *Growth by adding syntactic sugar*. Extending only the syntax by using syntactic sugar and at the same time keeping a core semantics is one of the preferable approaches to language growth. It gives both a precise language definition for the tool vendors as well as an understandable language for the user.
- *Growth by new meanings of annotations or built-in functions.* Growth by only changing the semantics and not the syntax might first seem to be a very attractive approach, especially for language designers since few changes are needed in the specification. However, it can also be dangerous, e.g., in cases where many tool dependent annotations might make different tools incompatible.
- *Growth by new user defined abstractions.* Finally, growth by user defined abstractions, i.e., neither the syntax nor the semantics are changed, is the preferable approach in the long term. However, it is far from obvious how to achieve this, especially in such a young language research area as EOO languages.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

JMODELICA—AN OPEN SOURCE PLATFORM FOR OPTIMIZATION OF MODELICA MODELS

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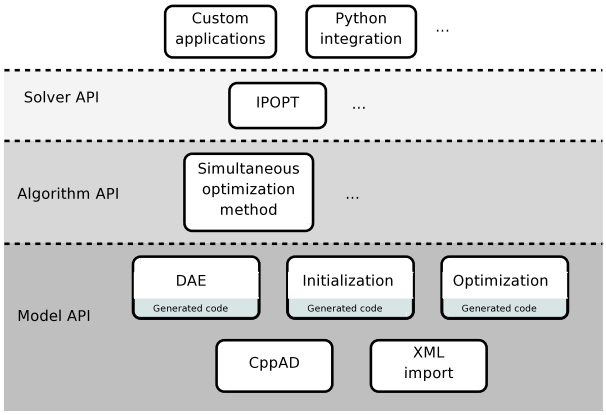
Optimization is becoming a standard methodology in many engineering disciplines in order to improve products and processes. The need for optimization is driven by factors such as increased costs for raw materials and stricter environmental regulations as well as a general need to meet increased competition. As model-based design processes are being used increasingly in industry, the prerequisites for optimization are often fulfilled. However, current tools and languages used to model dynamic systems are not always well suited for integration with state of the art numerical optimization algorithms. As a result, optimization is not used as frequently as it could, or less efficient, but easier to use, algorithms are employed.



Architecture of the model and optimization interfaces.

This paper reports a new Modelica-based open source project entitled JModelica, targeted towards dynamic optimization. The objective of the project is to bridge the gap between the need for high-level description languages and the details of numerical optimization algorithms. JModelica is also intended as an extensible platform where algorithm developers, particularly in the academic community, may integrate new and innovative methods. In doing so, researchers gain access to a wealth of industrially relevant optimization problems based on existing Modelica models, while at the same time facilitating industrial use of state of the art algorithms. The JModelica project rests upon three pillars, namely a language extension of Modelica for optimization entitled Optimica, software tools, and application. In this paper, these three topics will be high-lighted. The JModelica platform is intended to be released as open source software during 2009.

The JModelica platform consists of a collection of software modules, including two compiler front-ends for Modelica and Optimica respectively, a code generation back-end for C, a run-time library in C, a simultaneous optimization algorithm, and a library for integration with Python. Together, these pieces of software form a complete tool chain for formulating and solving dynamic optimization problems based on Modelica models. The foundation of the JModelica platform in its current form was presented in [1]. As part of this PhD project, a prototype compiler was developed, which is currently being further developed into the JModelica open source platform. The project is scheduled for public release during 2009.

The C code generated by the Optimica compiler is intended to be integrated with numerical algorithms. To meet this end, an Application Program Interface (API) consisting of a set of C functions is provided. The architecture of the JModelica API is depicted in the figure. As can be seen, the software is structured into three main parts, namely the Model API, the Algorithm API, and the Solver API. The Model API has three parts, namely the DAE interface which gives access to the DAE system, the initialization interface which represents the equations that must be solved in order to consistently initialized the DAE, and finally the optimization interface which provides access to e.g., the cost function and the constraints. The division of the Model API is motivated by the fact that not all parts of the interface may be provided in all cases. The Model API functions encapsulates the generated code, and also provides means to access the XML meta data files that are generated along with the C code. On top of the Model API a simultaneous optimization algorithm has been implemented as well as an interface to the optimization code IPOPT.

The JModelica platform and Optimica has been used in projects both in industry and in academia. In the present paper, a project reported in [2], considering optimal control of a car is highlighted.

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ENCAPSULATION IN OBJECT-ORIENTED MODELING FOR MECHANICAL SYSTEMS SIMULATION – COMPARISON OF MODELICA AND BEAST

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In this paper we compare two object-oriented modeling approaches, one is Modelica used for systems engineering as well as modeling of multi-body systems and the other one is BEAST which is a specialized multi-body systems tool with good support for contact modeling. The current Modelica approach requires strict interfaces with encapsulation of internal components, whereas BEAST allows connections to internal components which are visible in a 3D view, which is often natural from the 3D mechanical systems point of view. For 3D mechanical systems, Modelica might be too strict, whereas BEAST might be too forgiving. Two different solutions are presented and discussed (in the form of possible Modelica extensions) to combine the advantages of both approaches.

The comparison led to the following main observations

- Modeling of contacts between mechanical parts requires accessible interfaces. Contacts in multibody systems are possible between any two bodies in the model that do not have any intervening object or boundary that prevents physical contact. For example, if the surface of a body is exposed to the outside world it can in principle be connected to any outside body, whereas a body which is hidden within a physical container (e.g. a box or a sphere) cannot be connected to outside bodies. If the simple solution of making all interfaces globally accessible is used, additional (geometrical) checking will be needed to prevent unphysical impossible contacts.
- Composition hierarchies can be created in several ways. One method of creating object hierarchies is object-oriented composition where the part objects are declared as belonging to a containing object. More flexible hierarchy composition can be achieved at runtime, e.g., adding or removing child objects on demand using flexible data structures such as linked lists to represent the containment relation.
- The modeling process is often very domain dependent. A general target domain of the simulation tool also requires a general modeling process. For example, general multi-physics modeling requires a high level of flexibility, i.e., class and interface design, while pure mechanical modeling can utilize predefined classes of objects.
- Graphical user interfaces are often domain dependent. For example, regarding 3D mechanical system modeling a user interface with support for three dimensional visual representations of the complete system is desirable.

The main difference, however, is data encapsulation in conjunction with contact modeling. Modelica requires strict interfaces with encapsulation of internal components, whereas BEAST allows connections to internal components which are visible in a 3D view, i.e., all bodies or their surfaces, which are exposed to the outside environment, must be accessible. Contacts in BEAST therefore have access to any child component at any lower level in the model hierarchy. Model designers (BEAST users) create the contacts that are of interest for a particular system analysis and are responsible to avoid the creation of contacts between bodies whose surfaces are not physically accessible. For instance, contacts between two physically contacting gear-wheels in a gearbox model can be neglected (or replaced by simpler joints) if they are not of interest for the current system analysis. This is typically done to improve simulation performance. On the other hand, contacts between two gears that are physically not in contact could be created by mistake in BEAST. Modelica on the other hand uses a more strict approach in deep connection modeling. Connections through multiple sub-levels in the model hierarchy require the connector to be propagated through all sub-levels.

Finally, different solutions have been briefly presented and discussed (in the form of possible Modelica extensions) to combine the advantages of both approaches, these are:

Global connectors that are propagated through all parent levels. This is a special connector type that is accessible through all higher levels of the model hierarchy.

Connector references that can be used to reference a connector on any hierarchical sub-level.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

EFFICIENT SIMULATION OF HYBRID CONTROL SYSTEMS IN MODELICA/DYMOLA

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Abstract

Hybrid control systems generally involve both continuous and discrete dynamic behavior. In the context of digital control systems (Figure 1), the discrete sub-system representing the digital controller and sampling devices governs the continuous sub-system representing the plant under control by specifying discrete event switching logic. On the other hand, the continuous sub-system operates according to newly assigned states.

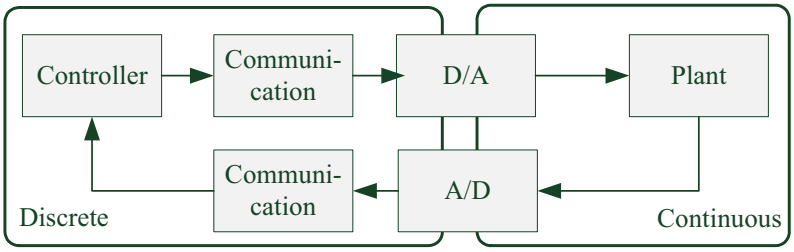

Figure 1. Hybrid control system

Simulation is commonly utilized for comprehensive analysis of hybrid systems. Though systems with mixed discrete/continuous behaviors can be handled by proper hybrid simulation tools, the efficiency of simulation is often not satisfactory. The performance of simulation is affected by a number of factors from the models themselves and the simulation settings including the frequency of events, the number of state variables, the chosen integration algorithm, the length of the output interval, and so on. In an ordinary modeling and simulation approach, the hybrid system is considered as a whole thus every local event has global effects. I.e. An event triggered by any element of the system causes the numerical solver to detect the event and recalculate all state variables. This works well if the discrete event logic couples tightly with continuous behavior evolution. A tight coupling means that the discrete event sub-system governs the whole system and all its events necessarily trigger the switch of equation system or stop/restart of the numerical solver. However, in case of a loose coupling, i.e. not all the events from the discrete event sub-system are relevant to the continuous sub-system, this approach is excessively expensive.

This paper gives a general approach to achieve more efficient simulations of hybrid systems with loose coupling, especially for stiff systems such as the Networked Control/Automation Systems (NCS/NAS) in which different system components have strongly distinguished temporal characteristics. The method is based on classification of events and separation of event domains. It cuts off the unnecessary coupling between events and variables and separates the integrated simulation into two synchronized simulation instances (Figure 2). This approach provides efficient simulation while holding the accuracy of simulation results. Advantages of this approach are demonstrated using the simulation tool Modelica/Dymola.

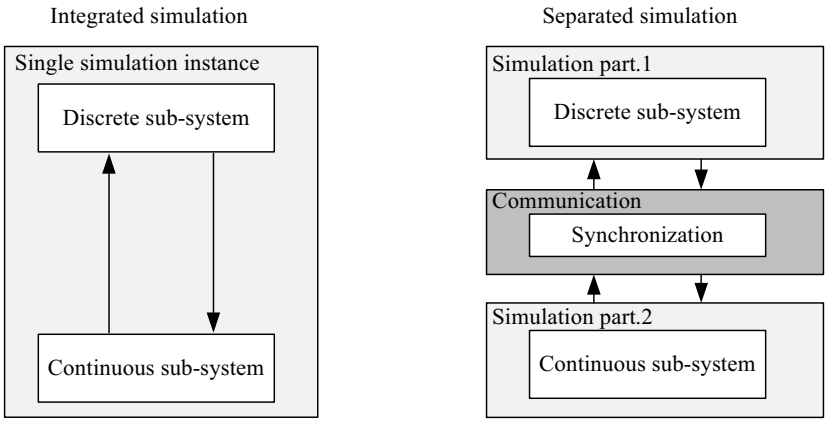

Figure 2. Integrated simulation vs. separated simulation

The Modelica libraries presented in this paper are available at www.eit.uni-kl.de/frey.

MODELICA LIBRARY FOR LOGIC CONTROL SYSTEMS WRITTEN IN THE FBD LANGUAGE

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Abstract This paper presents an object-oriented model library, written in the Modelica language, for the simulation of logic control systems written in the FBD (Functional Block Diagram) language. The library is part of a larger research project, the aim of which is to allow the joint simulation of plants - modelled as systems of nonlinear, differential and algebraic equations - and of the relative control systems, written as per the IEC61131-3 industry standard. The presented FBD library contains interchangeable models of different complexity, so that the user can specify a control system either as a continuous-time or an event-based model.

Introduction and motivation For the purpose of control commissioning, or process/control co-design, an accurate representation of both the process and the control system is of paramount importance.

In synthesis, one would like to choose the level of detail for the representation of the control system in a transparent manner, i.e., specifying that system adhering to some standard, and then simply selecting which type of representation (continuous-time model or algorithm) to use.

Nowadays, more and more control systems are implemented adhering to the IEC61131-3 standard, that defines five programming languages (Ladder Diagram or LD, Sequential Functional Chart or SFC, Functional Block Diagram or FBD, Structured Text or ST, Instruction List or LD) basically oriented to *logic* control, although most systems adhering to the standard also offer *modulating* control functions. In the last years, the IEC61131-3 standard has become very popular for example - but not only - in the arena of PLC (Programmable Logic Controller) programming, therefore spreading out in a vast number of contexts and applications.

In parallel, the object-oriented modelling (OOM) paradigm has been encountering in the last years a steadily growing success. With reference to the scope of this study, the main advantages of OOM are the following.

Modelling IEC 61131-3 controls The IEC 61131-3 standard defines five programming languages: three are textual, two graphic. The modelling approach used here can be exemplified by starting from the implemented language, namely the FBD. The key point in the discussion is that a controlled plant can be modelled, in total adherence to the way IEC-compliant controllers are realised, by greatly simplifying the problem of managing events.

A simulation example This section reports a simulation example. to show the usefulness of the possibility of simulating the same regulator as continuous-time and as event-based model. The example refers to some PI/PID control loops, and deals with set point step and ramp responses where the antiwindup mechanism of the regulator comes into play. The process to be controlled is described by the transfer function

$$P(s) = \frac{1}{1 + 2s + s^2/0.016} \tag{1}$$

and the PID regulator

$$R(s) = 10\left(1 + \frac{1}{30s} + \frac{3s}{1 + 0.3s}\right) \tag{2}$$

is applied to it, in the continuous-time version and as an event-based model with a sampling time of 0.01 s. The results of the simulations are then analysed.

Conclusions The library adheres to the FBD specifications as defined in the IEC61131.3 standard, and contains not only strictly logic blocks, but also the main types of industrial controllers, particularly of the PID type. The adoption of an industrial standard facilitates information sharing and greatly reduces ambiguities.

With the presented library, that the user can specify a control system as a continuous-time or an event-based model, for maximum flexibility in fulfilling the simulation needs.

Some simulations were presented to illustrate the usefulness of the library, which will be extended in the future, with respect to both FBD and other IEC-compliant languages.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

AUTOMATIC GENERATION OF LFTS FROM OBJECT-ORIENTED NON-LINEAR MODELS WITH UNCERTAIN PARAMETERS

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The process of developing control-oriented mathematical models of physical systems is a complex task, which in general implies a careful combination of prior knowledge about the physics of the system under study with information coming from experimental data (leading to the so-called problem of grey-box modelling, see, e.g., [1]), in view of the application of the model to control systems analysis and design. As recently discussed in [4], the critical issue in the development of an effective approach to control-oriented grey-box modelling lies in the integration of existing methods and tools for physical systems modelling and simulation with methods and tools for parameter estimation. Furthermore, throughout the modelling exercise, one should always keep in mind that the eventual application of the model is control system analysis and design, so the mathematical structure of the model has to be compatible with currently available methods and tools for such problems.

In this paper an approach is proposed to bridge the gap between physical and control/estimation-oriented system modelling, by automatically deriving standard model structures used in system identification and control starting from object-oriented (OO) models of nonlinear plants. As far as OO modelling is concerned, the Modelica modelling language has been considered, as it allows to describe the plant dynamics in a very general and user-friendly way. On the other hand, the Linear Fractional Transformation (LFT) model structure has been considered as the natural target as a goal for identification and control applications (see, e.g., [3]).

The LFT representation of the plant dynamics is shown in Fig. 1: the LTI block represents a static linear, time-invariant mapping between the inputs and the outputs, the I_n/s block contains a bank of integrators, the Δ block contains the uncertain parameters of the model, and the Θ block represents a nonlinear mapping between the inputs and the outputs. This model structure allows to describe linear and nonlinear dynamics with uncertain parameters, and is the starting point for many control design and system identification problems.

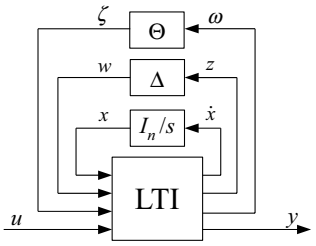

Figure 1: Block diagram of the considered LFT representation.

Deriving such models from first-principles physical models is a non-trivial, error-prone and tedious process, if carried out manually, so there is clearly a strong need of user-friendly tools to perform this task automatically. A first step in this direction is taken by control-oriented tools such as the LFR Toolbox [5], which is based on MATLAB's Symbolic Toolbox. This tool provides several functionalities, but can only handle causal models, where the interaction between the different sub-models is expressed in terms of input/output interaction. A further step is to obtain an LFT representation starting from a system model written with the Modelica language, which allows to describe the plant dynamics in a much more general way.

The paper presents the latest results obtained in the development of an algorithm to obtain an LFT representation, starting from a system model written with the Modelica language. The paper extends the preliminary results presented in [2], which were limited to linear models, to generic nonlinear models with uncertain parameters.

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KNOWLEDGE-BASED SIMULATION MODEL GENERATION FOR CONTROL LAW DESIGN APPLIED TO A QUADROTOR UAV

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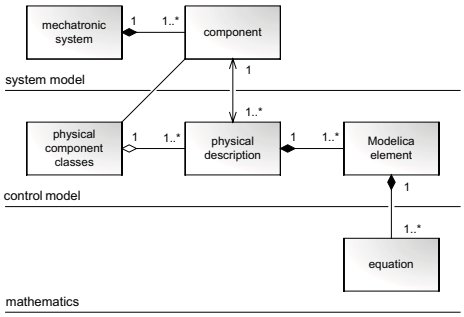
Introduction. With the advances in computing capabilities, the role of the embedded control system in the mechatronic system design is becoming more and more prominent. The 'traditional' sequential design approach, in which mechanical, electrical, electronics and software components are designed and optimized sequentially, is therefore becoming inefficient. The increasingly important role of control software is prominent in the aerospace field, where both aircraft and spacecraft operations benefit from the application of software. Apart from passenger and military jets, which use software with millions of lines of code, software has enabled the use of unmanned aerial vehicles (UAVs) for a wide range of purposes.

Control model generation. To support the development of control software and to cope with the multidisciplinary nature of mechatronic systems, an automatic control software generation framework has been proposed previously [1]. Part of the supported development process consists of creating models used for control algorithm and control software design and verification, often referred to as plant or simulation models. The aim is to apply the developed methods enabling further control law design for a quadrotor UAV.

In the framework the multi-disciplinary system architecture is build-up from mechatronic system components. However, in control design the system is often represented as a set of (linear) transfer functions, either in the time or in the frequency domain. In contrast to the use of transfer functions, with the 'physical modelling' paradigm supported by Modelica a component-based model corresponding to physical elements, using parameters directly related the real world, can be obtained. As control design often requires linear models, the generated model can be linearized where necessary.



Relationships between components at different viewpoints, adapted from [2].

Knowledge base. Although a direct, one-to-one mapping from system component to control model component is relatively straightforward, this kind of mapping ignores the possible interaction occurring in or between elements of different domains. Reference [3] denotes these additional interaction as 'unpredictable interaction', resulting in behaviour which occurs within a domain or by interactions between domains.

To be able to find these interactions, a knowledge-based approach is proposed. As a first step for setting up the knowledge base supporting the model generation process, a language ontology for Modelica models has been created. Based on the language specification, the concepts and relations in the ontology are restricted such that only 'structurally' correct models can be created with it. Based on the ontology, a database containing Modelica libraries is created, initially providing an insight in the relation between, and the properties of classes.

Results. The fidelity of the quadrotor UAV model primarily depends on the level of detail in which the rotors are modelled. Taking into account local flow fields however requires more design parameters and aerodynamic analysis results. The paper shows one-to-one component mapping does not suffice, e.g. in case of a DC-motor component used as actuator and as part of the structural subsystem, thus requiring modelling components representing these two domains.

Conclusions and future work. As part of a framework supporting the development of control software for mechatronic systems, first steps for a knowledge-based approach for generating simulation models has been presented. The need for, and advantages of such an approach is illustrated by considering the development of non-linear simulation models of a quadrotor UAV.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

Simulation of Faults in Electric Drive Systems with Modelica®

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Abstract For simulating electric drive systems the `freeFOClib` [3] is being developed. This Modelica® library can be seen as an extension to the *Modelica Standard Library* (MSL). The library can be used to build a field-oriented control system for existing machine models from the *Modelica Standard Library*, investigate the impact of electric faults (e.g., battery faults, inverter faults, machine faults) on a electric drive system, and run simulations to estimate the fuel consumption of hybrid electric vehicles.

Introduction The simulation of systems is a very useful method to investigate scenarios and procedures which will give prior unknown experimentation results. Thus we can test if a certain experiment will damage the test equipment or even worse might prove to have dangerous impacts on test-engineers.

Especially fault scenarios are the ideal application field for simulation runs up front. We like to know hat happens if certain devices fail and perhaps derive security measures which will protect our applications if a certain fault occurs.

In automotive applications there are a huge number of electric motors involved. Some of them bigger some smaller. Some with a more severe impact on the safety of the car and especially its passengers. Taking into account that electric motors are now also used for traction (hybrid or pure electric vehicles), braking (brake-by-wire), and steering (steer-by-wire) a lot of (expensive) tests have to be carried out.

As noted before, simulation can help here but the models must represent signals from different physical domains (e.g., electrical, mechanical, thermodynamical). The modelling language Modelica was especially developed to simplify the simulation in different physical domains within one simulation model (see Fig. 1). The multidomain capability allows us to build simulation models of hybrid electric vehicles easier than with other simulation tools. Furthermore it allows us to concentrate on the physics of a model rather than building models which represent mathematical equations which in turn then represent the actual physical behaviour [1, 2].

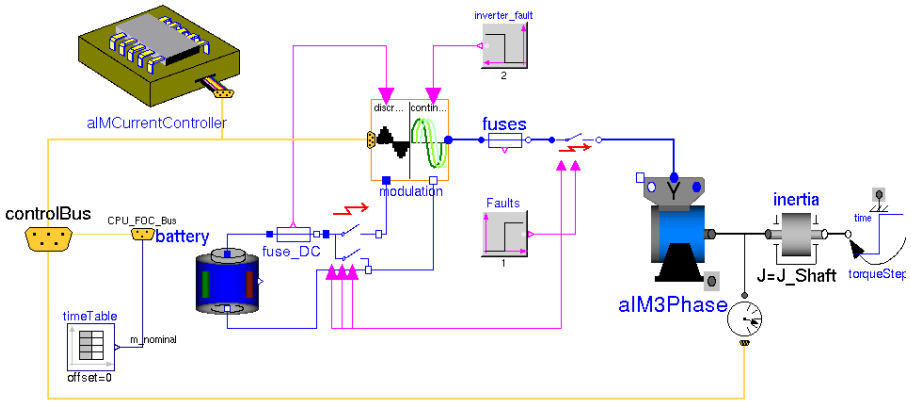

Figure 1: Example model of an electric drive system.

This paper will introduce some of the physical equations to model electrical induction machines using a equivalent circuit diagram. We show how these equations can be transformed into Modelica syntax. A short overview of the to be published library `freeFOClib` is given and some example fault simulations are shown.

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INTEREST OF MODEL-DRIVEN STUDIES OF FOULING PHENOMENA IN STEAM GENERATORS OF NUCLEAR POWER PLANTS

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Abstract. Pressurized water reactor steam generators (PWR SGs) are large components whose main function is to cool the fission reactor by extracting the thermal power conveyed by the primary coolant, and thus to produce steam for the turbine-generator. Fouling phenomena may occur in the SG when iron oxide particles carried in the secondary feedwater get unavoidably deposited inside the SG structure, and specifically in two main regions: on the 3,600 U-tube outer walls, and on the quadrifoil sections of the plates that support the U-tubes. They may reduce its cooling efficiency and impact its dynamic behaviour, thus leading to possible safety issues.

Methods based on local inspections of the SG have been designed and are already in use. They produce estimators of the local fouling rate, during the yearly outage of the plant for refuelling and maintenance.

A new method to assess a global estimator of the fouling rate is presented. This method is based on a 1D physical model of the SG that reproduces the complex dynamics of the two-phase flow phenomena inside the SG. The model was developed in the Modelica language.

This model is used to compute response curves of the SG characteristics to a particular transient that challenges the dynamics of the SG, when affected by fouling. The estimator is obtained by comparing the computed response curves to real response curves measured on-site.

The method is still under validation. However, first results show that it is able to give global estimators that are consistent with local ones.

This new method is expected to improve the monitoring of possible SG sludge fouling phenomena by producing fouling rate estimators with better accuracy, with a quarterly periodicity while the plant is in operation.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODEL-DRIVEN OPTIMIZATION OF BIOMASS CHP PLANT DESIGN

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Keywords : *Power Plant, CHP Models, Biomass Model, Steady State Modelling, Inverse Problems*

Abstract. Steady state 0D/1D models are useful to check, validate and improve through simulation the energy performances of existing heat and/or power plants. They are also used to find the best design that meets required economical criteria.
A library of fully static 0D thermal-hydraulics component models was built. It contains the models of a grid furnace, gas combustion chamber, electrical boiler, steam boiler, multifunctional heater, waterwall gas/water steam exchangers, tubular air heater, steam turbine, condenser, aero-condenser, pump, drum, valves, pipes, gas turbine, compressor, kettle boiler, mixer and splitter etc...
This library now enables us to build models of any CHP plant. A 0D multi configurations steady state model of a combined heat and power biomass plant was built, the plant satisfies the steam demand during all the year and produces electricity with its remaining energy.
Model was built by connecting the component models in a technological way, so that its topology reflects the process flow diagram of the plant.
A generic model was developed for design optimisation of CHP biomass plants. This model includes all typical configurations, thus enabling its use through a user-friendly Excel interface. With this interface, comparisons between various architectures according to given criteria and constraints are easy, thus helping the user to define the best design.
The model was then able to compute precisely the distribution of the steam/water mass flow rates, pressure and temperature across the network, the exchangers thermal power, and the performance parameters of all the equipments. It converges very quickly, provided that the iteration variables are properly fed in by the user (approx. 5% of the total number of variables).

MODELING OF HEAT PUMPS WITH AN OBJECT-ORIENTED MODEL LIBRARY FOR THERMODYNAMIC SYSTEMS

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The object-oriented structure of a new Modelica library for modeling of thermodynamic systems is described. The design strictly aims on flat inheritance structures and good readability of the resulting code. The basic model concepts of important component models are discussed. Modeling concepts for fin-and-tube heat exchangers, the most complex model in the library, are described in detail.

The library is used to simulate a CO_2 heat pump system for low energy buildings. The typical requirements of low energy buildings are low heating power at a relatively high temperature level in order to provide not only heating but also potable hot-water. Because of the transcritical process CO_2 heat pumps have the potential to achieve higher energetic effectivness than heat pumps using other refrigerants when delivering heat at high temperatures. The simulation results are validated by measurement data. The additional information gained by simulation is used to identify improvement potential of the system. Simulation results of an improved cycle are used to estimate the possible performance gain by improving the evaporator's refrigerant-side heat transfer. An *COP* increase of 3.4% results when doubling the refrigerant-side heat transfer coefficient from 5000 to 10000 W/(m^{2}K).

There have been many research activities about simulation of thermodynamic systems during the last decades. A variety of different programming and modeling languages are used. Richter [1] gives an overview of the state of the art in this topic. The latest activities concentrate on component model libraries written in Modelica. The mathematical description of thermodynamic systems leads in general to non-linear equations, which are numerically difficult to solve. Different scopes of research require different levels of detail. Therefore it is useful to replace non-linear equations case-dependent by linear ones or even constants. Object-oriented modeling languages provide convenient concepts to include this switching of levels of detail in one model. A drawback is that this often leads to very complex and hard to read model libraries. A short overwiew of state-of-the-art thermo-fluid flow modeling in Modelica is given below.

A common approach in object-oriented modeling of thermodynamic systems is to split fluid property models and component models - mostly even two separated libraries are used. The fluid property library *Modelica.Media* that is part of the Modelica Standard Library uses Modelica packages to model the fluid properties of various different fluids such as ideal gas, mixtures, or two-phase fluids which all inherit from one base class [2]. This library tries to combine all possible fluid models into a single framework to allow for an easy fluid property model exchange in component models. The resulting object-oriented structure is rather complex. *Modelica_Fluid*, developed by the Modelica Association, is a free component library for 1-dimensional thermo-fluid flow modeling [2]. It uses *Modelica.Media*.

The *AirConditioning* library is currently the most widely used library to simulate air-conditioning systems in Modelica. It is developed by the Swedish company Modelon AB and presented by Tummescheit et al. [3]. The structure of the *AirConditioning* library is also rather complex.

The main difference of the presented library compared to other state-of-the-art libraries is that it is not tried to combine all different fluid property models (e.g. ideal gas, two-phase fluids) into one common framework. Fluid property models are distinguished into different types. Component models are explicitly written for one fluid type (e.g. refrigerants, gases). The object-oriented structure is based on a few rules. The most important ones are: Inheritance should only be used if the relation between two classes can be described as an is-a-relation, multiple inheritance should be avoided whenever possible, and the inheritance structure should be as flat as possible. These rules and the fluid types concept lead to a sustainable library which allows new users to get familiar with the modeling concepts quickly and to write his own extended models.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

SIMULATION OF THE MEAN-VALUE INTERNAL COMBUSTION ENGINE IN MODELICA

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Abstract. The Modeling and simulation play an important role in automotive engineering applications. Several well-known system based simulators (based on causal modeling) such as Matlab/Simulink and standard Scilab/Scicos allow Engineers to investigate and design control strategies for complex systems. There are also component based simulators (based on acausal modeling) such as AMESim give good insight for the design with the physical components. In this paper, we evaluate at IFP the potential of Modelica as an object-oriented programming language in modeling the vehicle engine. The model of the engine components is validated using real data logged from a spark-ignited two cylinders engine as well as models developed with other simulators. After modeling the engine, the Modelica model will be simulated in Dymola (V6.1) and Scicos simulators to perform a comparison between these two Modelica simulators.

PEM FUEL CELL DYNAMIC SIMULATION USING *FuelCell*LIB

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Our society is suffering from fossil fuel shortage. Fossil fuels also contribute to a number of environmental problems during their extraction, transportation, and use. As an alternative for the devices consuming fossil fuels, fuel cells are one of the most promising means of producing energy in portable systems.

The mathematical modelling of PEMFC (proton exchange membrane fuel cells) is a challenging topic, due to the complexity and variety of phenomena involved in the operation of these devices, including fluid-dynamic of gases and liquids in complex media, electrochemical reactions, heat transfer, and ion conduction in electrolytes. Different approaches to the modelling and simulation of PEMFC are based on the use of different software tools:

- Computational fluid dynamics (CFD) software, such as FLUENT, CFX and STAR-CD, has been used for 2D and 3D steady-state modelling of PEMFC.
- Numerical code written in a programming language, such as C, Fortran, etc.
- The Matlab/Simulink simulation environment has been used by other authors and commercial tools (e.g., Emmeskay and FEMLAB).
- Object-oriented modelling languages (e.g., Modelica and gPROMS) have been used to develop libraries of components intended for PEMFC modelling. The Modelica library implemented by Steinmann and Treffinger [1] allows composing 0D steady-state PEMFC models. A 0D dynamic model of PEMFC written in Modelica and intended for real-time simulation was proposed in [2].

Another Modelica library for PEMFC modelling is *FuelCell*Lib [3, 4]. In contrast with the two aforementioned libraries, *FuelCell*Lib facilitates 1D dynamic modelling of PEMFC. *FuelCell*Lib models are based on physical-chemical principles. The balances of the species (i.e., water, oxygen, protons and electrons) are enunciated in each physical layer of the fuel cell. The finite volume method has been applied to discretize the PDE in the spatial coordinate perpendicular to the layers. The modelled physical-chemical phenomena include:

- Membrane: transport of water in liquid and steam phase, and protonic conduction.
- Catalytic layer of the cathode: transport of water in liquid and steam phase, transport of oxygen in steam phase, protonic and electronic conduction, and electro-catalytic reaction.
- Diffusion layer of the cathode: transport of water in liquid and steam phase, transport of oxygen in steam phase and electronic conduction.

*FuelCell*Lib models allow reproducing relevant PEMFC phenomena, including the cathode flooding, the membrane drying, the electro-osmotic drag, the diffusion of liquid and gases through the porous media, the coexistence of steam and liquid water, the electrochemical reactions in the cathode, and the double-layer capacitance. The library provides a set of alternative models describing certain phenomena [3, 4], allowing the user to select the adequate hypotheses for the particular application. *FuelCell*Lib models are isothermal: the temperature dependence of the phenomena is modelled, but the temperature of each layer is constant during the simulation run.

The first version of *FuelCell*Lib was released in 2005. The second version of the library, which can be freely downloaded from [5], is presented in this manuscript. The modelled phenomena, modelling hypotheses and structure of the library are discussed. In addition, the effect of selected parameters on the voltage response after current interruption, the cell polarization curve, the flow of liquid water in the membrane, the dynamic of the cathode flooding process, and the steady-state spatial distribution of water load and oxygen is analyzed using *FuelCell*Lib. As a conclusion, *FuelCell*Lib allows enhancing the understanding of the physical-chemical phenomena involved in the PEMFC operation and therefore it is a useful tool for optimizing the PEMFC performance.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELING PHYSICAL SYSTEMS AS PHYSICAL NETWORKS WITH THE SIMSCAPE LANGUAGE

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Engineers are relying more and more on simulation to accelerate development processes. Combining computer simulation with Model-Based Design techniques enables engineers to not only complete tasks in a shorter period of time, it makes it possible to find design errors before building hardware, making the errors easier and less expensive to fix. As the systems they develop require integrating control systems with physical systems spanning multiple physical domains (mechanical, electrical, etc.), a useful model of the physical system (plant) is critical for developing an optimized system.

Traditional methods (C, FORTRAN, etc.) and signal-based or input-output (causal) methods in graphical software tools (Simulink, etc.) were useful for control engineers because they were written in a language they could easily understand and integrate with their control system models. However, these models can be difficult to reuse, leading to redundant work. A technique which has been applied to electrical systems for quite some time is now being used on multidomain physical systems. The physical network approach, often referred to as acausal modeling, enables engineers to create reusable models of physical components that can span multiple physical domains.

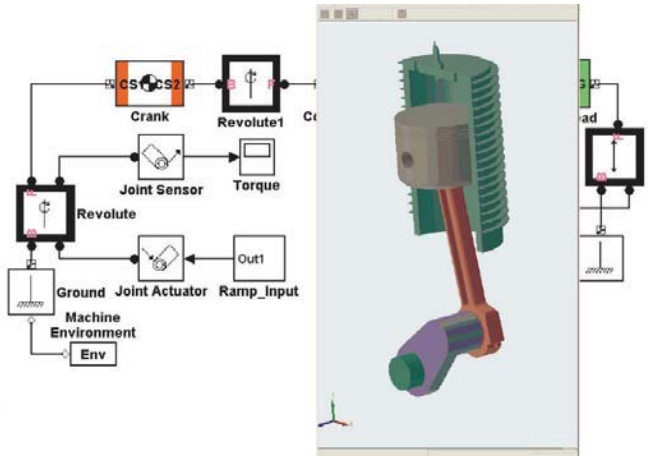

Figure 1: Component-based acausal modelling

Simulation tools that support this method (Simscape, etc.) then build up the equations for the system and solve the differential algebraic equations directly, resulting in accurate simulations of the entire system. This paper focuses on the physical network technique for modeling physical systems and its use in Simscape within the Simulink environment. The figures give a short glance on Simscape language and modelling structures using Simscape

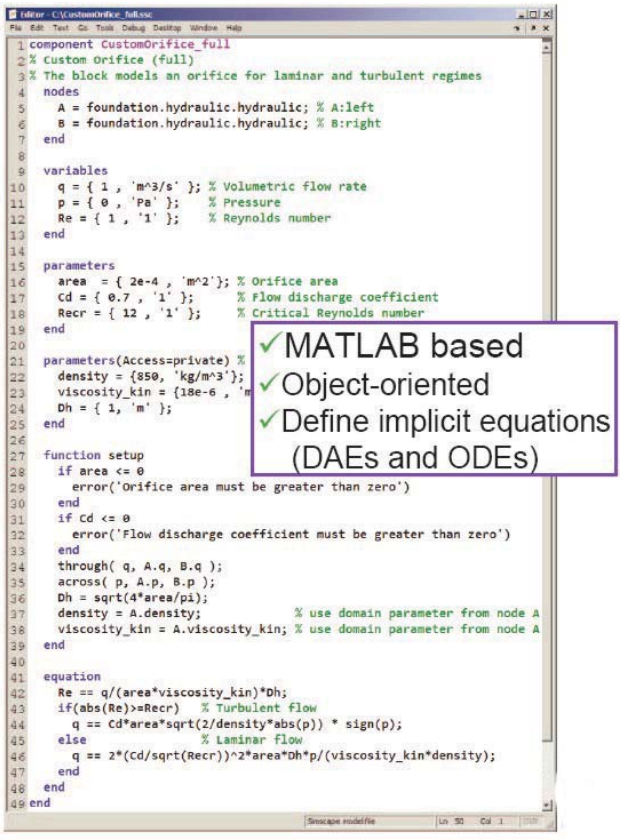

Figure 2: Textual DAE model of a component in Simscape Language

MODELLING STRUCTURAL DYNAMIC SYSTEMS: STANDARD MODELICA VS MOSILAB STATECHART

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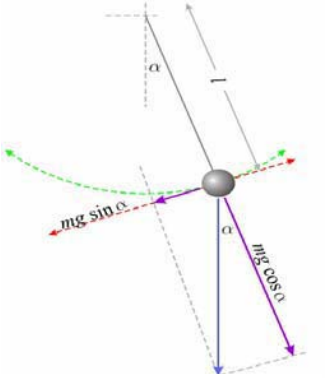
Introduction. Object-Oriented modelling is a fast-growing area of modelling and simulation that provides a structured, computer-supported way of doing mathematical and equation-based modelling. Modelica is today the most promising modelling and simulation language in that it effectively unifies and generalizes previous object oriented modelling languages and provides a fundament for the basic concepts [1].
The Modelica modelling language offers easy to use multi domain physical modelling approaches as well as acausal equation based modelling and simulation. Classical hybrid systems can be implemented using *if-then-else* or *when* equations, these are conditional equations. This construction can be used in the so called equation section or outside in an algorithm section, which is used for sequentially sorted source code.

Mosilab (***Mo****delling and* ***Si****mulation* ***Lab****oratory*), developed by Fraunhofer-Gesellschaft in a cooperation of six Fraunhofer-Institutes (FIRST, IIS/EAS, ISE, IBP, IWU and IPK) in the research project GENSIM, is a Modelica based multi domain modelling and simulation environment. Besides the classical way of modelling, as defined in the Modelica standard, Mosilab offers an extension in graphical and textual way for representing structural dynamic systems by using the language extension Mosila [2].

Content. The main focus of the presented work lies on the comparison of standard Modelica implementations of structural dynamic systems and the additional possibilities offered by Mosilab. Using two examples from classical physics, the constrained pendulum and the free pendulum on a string, and one from electronics we show the influence and power of state event modelling using the graphical environment in Mosilab in combination with the textual description to implement hybrid structures. The graphical hybrid structure layer in Mosilab is UML (Unified Modelling Language) based, and thereby intuitive handling is possible.

Starting with the constrained pendulum and the discussion how to model the state event (tangential velocity versus angle velocity) different approaches and types of state changes are modelled and simulated [3]. The results of the time point of state detection and the computation time are calculated and compared for different integration methods. The standard solution method hereby is Dassl code developed by L. Petzold.



Force diagram of the implemented pendulum

The second example deals with the problem of different state space dimensions during runtime and how to handle such kind of system. As example the free pendulum on a string is chosen.
The system acts in two states: in state one the string is tight and therefore the pendulum is rotating; in state two the string is sagging and the mass on the end of the string is free falling until the string is tight again.

Summary. Using these examples different methods for model implementation in the advanced simulation environment Mosilab are shown in detail and compared with standard Modelica implementations. The implementation of an UML based state machine makes it useable for problems in which the state space dimension does not stay the same over the whole simulation time and thereby a very powerful extension for advanced modelling and simulation.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

ACAUSAL PHYSICAL MULTIDOMAIN MODELLING IN MAPLESIM: MODEL STRUCTURES, MODEL TRANSLATION AND MODELICA - COMPATIBILITY

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This contribution demonstrates how MapleSim, a new modelling module in Maple, addresses the limitations of current signal-oriented simulation technology. MapleSim does this by:

- Allowing engineers to use both acausal and causal modelling paradigms in the same model, so plant models and control systems can be prototyped in a manner that suits each task best
- Using symbolic technology to remove the complexities that would cause other tools to fail during numerical simulation, and to create computationally efficient models
- Offering multibody technology that produces highly efficient descriptions of even the most complex 2-D and 3-D multibody systems
- Supporting design documentation and engineering analysis through integration with Maple
- Allowing natural multi-domain modelling that enables the interaction between many physical domains to be simulated

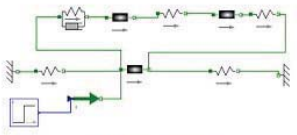
The development of MapleSim was, in part, motivated by a growing market demand for tools that can successfully model the increasingly complex systems that engineers need to simulate. Mainly, Maplesim understands itself as answer of Maple to the Modelica development

Hybrid Physical and Signal-Flow Modeling. MapleSim allows both modelling at the physical component and signal-flow level within the same model. This enables both the plant model and the control system to be prototyped with the modelling approach that suits each task best.

Multibody Dynamics. MapleSim uses graph-theoretic methods to generate the equations of motion for multibody systems. One feature of this approach is that it allows for the systematic separation of terminal equations (which describe how individual components interact) from topological equations (which describe how components are connected). This is significant because by managing topological equations intelligently, MapleSim's multibody engine can directly control the state variables for a given system. Since the nature and number of the equations of motion are a direct result of the chosen state variables, controlling the state variables gives the multibody engine unprecedented control over equation complexity during the equation formulation process. This delivers computationally efficient sets of symbolic equations that are simplified further by Maple, and delivers faster simulations than approaches restricted to only using absolute coordinates as state variables. Benchmarks have shown much higher execution speeds than the most popular existing multibody tools.

Multi-Domain Modeling. Many physical modelling tools (such as those based on SPICE) are dedicated to a single domain. This is highly restrictive because engineers often need to model the subtle effects that one domain has on another. For example, given the appropriate set of operating conditions, there is a high correlation between the variation of the voltage across a motor and the vibration of an attached mechanical arm. That critical relationship would be far more difficult to discover (and to correct, if needed) if the electrical motor and the mechanical system were simulated in separate systems. MapleSim is naturally multi-domain, and contains components from rotational and translational mechanics; analog, digital, and multiphase electric circuits; multibody mechanics; and thermodynamics. It also has standard continuous and discrete functionality.

Symbolic Simplification and Computational Efficiency. After automatically generating the system equations, MapleSim simplifies them with symbolic techniques that include index reduction, differential elimination, separation of independent systems, and elimination of redundant systems. Symbolic simplification has two primary benefits. By symbolically resolving algebraic loops and through reducing the complexity of DAEs, symbolic simplification makes many (previously intractable) problems numerically solvable. The simplified equations are provided to the numerical solvers in a computationally efficient form. This reduces the total simulation time, in some cases, by many orders of magnitude.



MapleSim model

Modelica Compatibility. MapleSim works with generic component libraries, but allows also direct use of Modelica models, and Modelica libraries.

EXTENDING BUILDINGS' THERMAL-DYNAMICS MODEL IN MODELICA WITH EXTERNAL ILLUMINATION MODEL

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Introduction An intelligent dynamic building's envelope is a promising concept for future low-energy building design. For assuring pleasant living conditions multiple quantities have to be controlled and due to complexity and diversity of systems (living and working rooms), the corresponding control can become very complicated. A good reusable model can play crucial role in the successful control design procedure.

Our previous work was based on experimentations with a real test chamber. To assist the control development of the illumination and thermal status and to improve knowledge about the system (test chamber), we started with modeling in *Matlab/Simulink*. This model was found to be inappropriate due to disadvantages of the non-object-oriented modeling tool when the extension to experimentations on a real-world buildings are required. So we decided to reimplement it in a more powerful modeling tool *Dymola* which offers modeling in object-oriented modeling language *Modelica*. Thermal dynamics of the building in our model is described with differential-algebraic equations using energy balance principle. With object-oriented approach an intuitive, reusable and easily expandable modeling of buildings' thermal dynamics is enabled. Similarly flexible and easily maintainable model was desired also for illumination. For this purpose we adapted *Radiance lighting simulation and rendering tool* [2] and incorporated it in *Modelica* model of thermal dynamics.

Illumination model in *Radiance* *Radiance lighting simulation tool* is a powerful rendering package using backward ray-tracing and is primarily intended for visualization and lighting analysis [2]. The tool reads scene-description sources and then generates image of a specific view or trace a single ray from a particular stand-point in a selected direction. During the simulation run of the building's thermal response and illumination also the scene changes. In order to diminish the overhead of reading scene-description sources anew in each simulation step, the *Radiance* tracing utility was changed to re-read only parts of the scene that changes during the simulation run. So, *Modelica* model needs to send two types of information to *Radiance* submodel: the change of scene (e.g, new sun position, change in position of the shading, etc.) and position and orientation of the spot of interest. The *Radiance* subsystem sends back to the *Modelica* the information about illumination value of the spot. The interface to Modelica is thus simple, it consists of only four functions: initialization and finalization routine, function to inform about the changes in the scene and function to actually perform calculation of the selected spot's illumination.

Modelica Interface Models in *Modelica* can interact with other models through the use of external functions [1] written in other programming language. *Dymola* in the version used supports only *C* language. For each external function a Modelica interface must be declared, that is four declarations in our case. All the declarations were organized inside a partial class. This class can be expanded easily and in the extended class, which is a specific model of the room, the information exchanged with *Radiance* subsystem through API function calls is dispached to other *Modelica*'s submodels over appropriate *Modelica*'s connectors, so the illumination model can be smoothly integrated in *Modelica*'s model as a submodel.

Illumination model of the test chamber The usage of described *Modelica* interface to *Radiance* is illustrated on the example of our experimental test chamber.

Conclusion *Modelica* has a well defined interface for the use of external functions and we were able to implement clear interface to *Radiance* lighting simulation tool in the sense of easy integration to existing model of building's thermal dynamics. No nasty hacks were needed and easy reusability and extensibility, as one of the main advantages of the object-oriented modeling, were not lost or diminished.

However, the described smooth incorporation of external model in the *Modelica* model is only possible if the external model has no dynamics, i.e., it has no internal continuous states, otherwise there is currently no neat solution.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

CLASSIFICATION AND EVALUATION OF FEATURES IN ADVANCED SIMULATORS

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Introduction. This contribution elaborates, classifies and compares features of modern simulation systems. First a short overview on the CSSL standard is given, with discussion of standard and extended features for CSSL simulators. Then main emphasis is put on the developments in the last decade: object-oriented approaches, acausal modelling, physical modelling, structural dynamic systems and impacts from computer engineering (e.g. statecharts). Based on solutions of the ARGESIM Benchmarks, finally classification and comparison of features in modern simulators is given.

Extended Features. CSSL simulation languages range from simple ODE state space description to graphical DAE systems. In this context *Extended Features* are elaborated, which classify improvements of the classical standard (except Sorting, being a basic feature for CSSL): MS – Model Sorting, TEH - Time Event Handling, DAE - DAE Solver, ED -Event Description, SEH - State Event Handling, and IR - Index Reduction.

Structural Features. While the *Extended Features* address the CSSL-standard, *Structural features* should classify advanced and modern properties of simulations systems, more or less far beyond CSSL. They characterise e.g. features for physical modelling, for structural dynamic systems, and others. Features investigated are:

- Acausal physical modelling textual (PM-T) or graphical (PM-G)
- Modelica standard (MOD)
- simulation-driven visualisation (VIS)
- Structural dynamic systems features (SD)
- PDE support (PDE
- parallelisation (PAR)
- State chart modelling- textual (SC-T) or graphical (SC-G)
- frequency domain analysis (FA)
- extended environment (ENV)

Evaluation and Comparison. Based on a very time-consuming evaluation of some simulation systems, mainly in context with solutions for the ARGESIM Benchmarks, a comparison on these features was elaborated. As measure for availability, 'yes' and 'no' is used (feature available or feature not available), a more detailed analysis gives an additional classification with '(yes)' and '(no)': a 'yes' in parenthesis '(yes)' means, that the feature is (too) complex to use, so not really available; and a 'no' in parenthesis '(no)' means, that the feature is yet not available, but there is some other way around, so the feature is not really not available. In the following the investigated simulators and simulation systems, and a snapshot of the evaluation list are given.

- MATLAB
- ACSL
- Dymola
- Open Modelica
- Simulation X
- Scilab
- Scicos
- Scilab/Scicos
- Maple
- Mosilab
- AnyLogic
- MathModelica
- Simulink
- MATLAB / Simulink
- Maplesim
- MathModelica / Mathematica
- Simulink / Stateflow
- Simulink/ Simscape
- Simulink/ Simscape/Stateflow
- MATLAB/ Simulink/ Simscape/Stateflow

	MS - Model Sorting	ED -Event Description	SEH -State Event Handling	DAE - DAE Solver	IR - Index Reduction	PM-T - Physical Modelling -Text	PM-G - Physical Modelling -Graphics	VIS – 'Onlie' - Visualisation	MOD – Modelica Modelling	SC-T – State Chart – Modelling - Text	SC-G – State Chart Modelling - Graphics	SD – Structural Dynamic Systems	FA – Frequency Analysis	ENV – Extended Environment
MATLAB	no	no	(yes)	(yes)	no	no	no	(yes)	no	no	no	yes	yes	yes
Simulink/ Simscape/Stateflow	yes	yes	yes	yes	(yes)	yes	yes	(yes)	(no)	(yes)	yes	no	yes	(yes)
ACSL	yes	yes	yes	yes	no	no	(no)	(yes)	no	no	no	no	yes	yes
Dymola	yes	yes	yes	yes	yes	yes	yes	yes	yes	(yes)	(yes)	no	(no)	(yes)
MathModelica	yes	yes	yes	yes	yes	yes	yes	(yes)	yes	(no)	(yes)	no	(no)	(no)
……..	…	…	…	…	…	…	…	…	…	…	…	…	…	…
Mosilab	yes	yes	yes	yes	(no)	yes	yes	(no)	(yes)	yes	yes	yes	no	(yes)
Open Modelica	yes	yes	yes	yes	yes	yes	(no)	(no)	yes	(no)	(yes)	no	no	no
AnyLogic	yes	yes	(yes)	(yes)	no	no	no	yes	no	yes	yes	yes	no	no
Scilab/ Scicos	yes	yes	yes	yes	(yes)	yes	yes	(yes)	(yes)	yes	(yes)	yes	yes	yes
MapleSim	yes	(yes)	(yes)	yes	yes	yes	yes	yes	yes	no	no	(yes)	(yes)	yes

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Modelling of Fuel Cells and Chemical Engineering Applications

METABOLIC MODELLING FOR THE CONTROL OF INTRACELLULAR PROCESSES IN PLANT CELLS CULTURES

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Introduction. Plant secondary metabolism has been used for decades as a way of producing high value molecules such as dyes, pigments, antibacterial agents and anti-cancer drugs. The production of these molecules in a controlled environment is extremely important, especially if the product is used therapeutically.

Achieving controlled conditions in bioprocesses is not a problem for basic variables such as pH, temperature and dissolved oxygen. However in plant cultures, the control of extracellular states is not sufficient to ensure a proper operation, as the cells can accumulate significant intracellular nutrients reserves, which in turn affect productivity. Thus, adequate feeding of medium is a critical problem in plant cells cultures. To that end, a precise quantification of the system dynamics is required, as contradictory effects are reported when modulating plant cells cultures medium.

Metabolic model. A dynamic metabolic model developed in previous work [1-2] was used to obtain a feeding profile for a plant perfusion bioreactor culture. This model can describe the major nutritional dynamics (extracellular and intracellular) of plant and hairy roots cultures. The cell line used in this study is the California poppy (*Eschscholtzia californica*) with the key products being a variety of alkaloids compounds.

Perfusion culture. The feeding of nutrients can be achieved in chemostat, fed-batch or perfusion culture. A chemostat requires continuous growth, which is not suitable for secondary metabolites production. A fed-batch operation dilutes the biomass during the production (non-growth) phase. Thus, the perfusion culture seems to be the most appropriate design, given the constraints imposed by the slow growth and non-growth associated production. A lab-scale 3L perfusion bioreactor for plant cells was previously developed in our group and was used here to implement a culture strategy based on these premises. Further details on the culture system can be found in [3].

Results and discussion. The feeding profile was calculated to allow stabilization of key intracellular state variable (glucose concentration), which showed to be critical in improving cell productivity. The simulation results indicated that it is possible to manipulate the nutrients feeding rates in order to circumvent the intracellular 'open-loop' dynamics that might reduce the productivity in batch cultures.

These experimental results confirmed the soundness of the proposed perfusion bioprocess strategy, as GLC concentration showed very little variation between days 2 and 11 of culture with a concentration of 0.28±0.07 $mmol \cdot gDW^{-1}$. The increase in productivity that was observed from simulation is also observed experimentally, except where phenomena like product degradation and/or cell death might be significant. The agreement between model simulation and experimental results shows that the model has sufficient predictive capacity to be used for bioprocess design.

Model simulation at the intracellular level to improve the production of biomolecules could also be pushed further. Optimization techniques could be used with different objectives (yield, production rate, product concentration, harvest time etc.) depending on the specific cellular system. This is already performed with standard methods like Metabolic Flux Analysis, but not in closed-loop, and most of these approaches are limited to steady-state operation, which is not always achievable, depending on the cell culture method.

Our work suggests that not only dynamic modelling, but also closed-loop control of intracellular processes will be key for further improvements on bioprocesses. The case study presented here for plant cells shows that this approach should definitely be considered.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

METABOLIC MODELLING OF WINE-MAKING : A STATE OF THE ART

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So far the macroscopic behaviour of the alcoholic fermentation has been widely studied, resulting in particular in dynamical mass balance models that provide a mathematical formalism of the main process phenomena (sugar and nitrogen consumption, ethanol production, biomass synthesis).

This work focuses on the organoleptic properties transferred to the wine during the fermentation under the action of yeast (*Saccharomyces cerevisiæ*). Flavour markers, as higher alcohols, esters, and sulfur compounds result from complex biochemical reactions and their modelling requires a good knowledge of the yeast metabolism. It is important to note that these compounds represent less than 5% of the yeast production and correspond to (very) low concentrations, and that their measurements involve specific and expensive measuring devices.

In this context **M**etabolic **F**lux **A**nalysis is a useful tool that can provide an accurate description of these compounds biosynthesises since the intracellular behaviour is taken into account. A metabolic network linking metabolites is assumed to represent the system behaviour under steady state conditions [5], and the fluxes through the pathways of the bioreaction network are estimated from measurements of substrate uptake and product formation rates (via stoichiometric balances).

The possible flux pathways connecting the concerned metabolites are traced and this cartography of the cell allows to determine which substrate is necessary to obtain one product (via the application of convex algebra concepts to define elementary flux modes, [4]). Macro-reaction schemes can be deduced and corresponding differential equations can be derived to obtain a dynamical model of the process [3].

Stoichiometric models have been developed for *Saccharomyces cerevisiæ* in wine-making conditions (e.g. [1]). These metabolic networks are limited to the main products synthesis as ethanol, glycerol, and some amino acids. Moreover the biomass synthesis is simplified.

In some recent studies (e.g. [6]) MFA has been performed to better understand the intracellular behaviour during the fermentation (when nitrogen is depleted, for example). Models are sometimes studied to determine elementary flux modes (EFMs) governing the cell macro-reactions in order to identify which enzyme subsets are important at different growth conditions or to optimize product yield.

A dynamic model is rarely derived from these considerations. Nevertheless, in some works [2], kinetic expressions and metabolic network are coupled to predict the fermentation evolution.

Flavour markers are never included into the resulting metabolic network because MFA thus needs measurements of extra- and intra-cellular species related to these specific compounds.

Further development in this research will involve the development of a metabolic network oriented to the synthesis of flavour-active compounds. MFA and EFMs will hopefully provide enough information to derive a reliable dynamical model.

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METABOLIC FLUX INTERVAL ANALYSIS OF CHO CELLS

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Introduction. A detailed metabolic network of $CHO-320$ is built based on available information gathered from the literature [1, 2]. The fundamental assumption of quasi-steady state is applied to exponentially growing CHO cell cultures, and together with the measurements of the time evolution of a number of extracellular metabolites, the classical methodology of Metabolic Flux Analysis can be applied to a well constrained metabolic network [4]. However, the available measurement information is usually not sufficient and the system of equations is underdetermined. Nevertheless, the set of solutions can be studied and admissible ranges for the flux distribution can be defined using tools of positive linear algebra, particularly the algorithm METATOOL [3].

Flux Interval Analysis. In general, the resulting linear system of mass balance equations representing the metabolism of mammalian cells is underdetermined. Therefore, the solution of the system is not unique but a set of admissible flux distributions ca be determined. This space of solutions provides the limiting values of the flux interval for each metabolic flux, i.e., among all possible values of v_i, there are an upper and a lower value which define the bounds v_i^{max} and v_i^{min}, respectively. This way, despite the exact flux distribution remains unknown, it is possible to define an interval of values for each flux and thus, have a preliminary insight of the metabolic state of the cells.

Network Structure. Based on a set of available measurements of extracellular components, alternative network configurations, corresponding to different net directions of several reversible pathways, are systematically investigated. Among the 16 candidate configurations, only 2 appear feasible, as they correspond to an admissible solution space. However, only one of them is likely to occur, depending on the level of concentration of ammonia.

Measurements Sensitivity. The influence of the availability of the measurements of the uptake or production rates of the 20 amino acids is assessed. As a result, the amino acids can be classified in two groups, one with limited influence and the other with critical influence. Considering the first group, it is possible to evaluate reasonable flux distributions, even in the situation where up to 5 measurements are missing.

Hypothetical Additional Measurements. It is of interest to consider the situation where the measurements of all 20 amino acids are available (as well as standard measurements of glucose, lactate and ammonia) and to evaluate the benefits of additional measurements such as urea uptake rate, CER, antibody production rate ($INF-\gamma$), choline and ethanolamine uptake rates. The more informative measurements appear to be CER, urea and choline uptake rates, which allow the flux intervals to be significantly reduced. Interestingly, the resulting flux ranges can be quite narrow, thus providing a very useful insight in the cell metabolism, even in the situation where some extracellular component measurements are missing and the underlying system of mass balance equations is underdetermined.

Acknowledgments This work presents research results of the Belgian Network DYSCO (Dynamical Systems, Control, and Optimization), funded by the Interuniversity Attraction Poles Programme, initiated by the Belgian State, Science Policy Office.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

INDIVIDUAL-BASED MODELLING AND SIMULATION OF MICROBIAL PROCESSES: YEAST FERMENTATION AND MULTI-SPECIES COMPOSTING

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Controlled microbial activity is the core of many industrial processes that require efficient, cheap and clean bio-chemical transformations of input products. Two examples are yeast fermentation and composting processes carried out by multi-species microbial ecosystems. In alcoholic fermentation glucose is transformed into ethanol. Composting is the aerobic decomposition of organic matter into a specific final product used as fertilizer in agriculture. Different kinds of microbes are mainly involved in this process: bacteria, actynomycetes and fungi.

Both of the above-mentioned processes have been widely studied and modelled in order to better understand, predict and control the evolution of industrial systems from a given initial state. Most of the existing models are population based continuous approaches (top-down). They describe the population dynamics and the changes in the concentration of relevant extracellular compounds using differential equations. This modelling approach of fermentation and composting processes provides a wide pool of useful and interesting results [5, 6], but is limited by the inherent complexity of the systems under study.

An alternative approach is Individual-based Modelling (bottom-up). INDISIM is a discrete and spatially explicit Individual-based Model (IbM) [2]. First, it sets the rules that govern each microbe and its interaction with its local environment and neighbouring cells. The physical space is divided into spatial cells, and the environmental processes are also locally defined. Then, it performs simulations including a large number of microbes. Finally, the behaviour of the whole system emerges as a result of these simulations. INDISIM was initially developed to study bacterial cultures, and it has shown to be versatile and useful to deal with other kind of microorganisms [1]. INDISIM-YEAST [3] and INDISIM-COMP [4] are two examples of this. They have been successfully applied to the study of yeast fermentation and composting processes respectively.

Continuous models and IbMs are not excluding but complementary methodologies: both have strengths and weaknesses that can be profited and counterweight. In this work, we present some examples of INDISIM specific contributions to the modelling of fermentation and composting processes with special attention to the challenges faced by continuous models in dealing with (i) microbial activity, (ii) environmental conditions and processes and (iii) external manipulations. INDISIM provides a tool that covers heterogeneity in the population, stochasticity in the cellular processes and inhomogeneity or/and anisotropy in the environment. It also consists in a basic core that remains appropriate to study microbial systems operating under different external protocols.

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TWO EXAMPLES OF TESTING GLOBAL IDENTIFIABILITY WITH THE DAISY SOFTWARE

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Abstract

DAISY (Differential Algebra for Identifiability of SYstems) is a recently developed computer algebra software tool which can can be used to automatically check global identifiability of (linear and) nonlinear dynamic models described by differential equations involving polynomial or rational functions. Global identifiability is a fundamental prerequisite for model identification which is important not only for biological or medical systems but also for many physical and engineering systems derived from first principles. Obviously, once a priori identifiability is assessed, the accuracy of the estimates will eventually depend on other different factors, as for example, noise, the paucity of the available data and/or the complexity of the model with respect to the available data.

The software does not require understanding of the underlying mathematical principles and can be used by researchers in applied fields with a minimum of mathematical background.

We demonstrate the DAISY software by checking the a priori global identifiability of two benchmark nonlinear models taken from the literature. The analysis of these two examples includes comparison with other methods and demonstrates how identifiability analysis is simplified by this tool. It includes discussion of some specific aspects related for example to the role of observability and knowledge of initial conditions in testing identifiability. The main focus of this paper is not on the description of the mathematical background of the algorithm, which has been presented elsewhere, but on illustrating its use and on some of its more interesting features.

DAISY is available on the web site http://www.dei.unipd.it/∼pia/.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

LINEAR REGRESSION TECHNIQUES FOR STATE-SPACE MODELS WITH APPLICATION TO BIOMEDICAL/BIOCHEMICAL EXAMPLE

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Introduction. In literature, various parameter estimation methods have been proposed. Often, non-linear least squares methods are used to iteratively estimate parameters in models that are so-called non-linear in the parameters. However, unlike the ordinary least squares methods, the non-linear least squares methods do not guarantee a global minimum, especially in non-convex optimization problems [1]. Alternatively, for some problems it is possible to generate a linear-in-the-parameters model to approximate the system by applying a logarithmic transformation or via reparametrization. However, it is not always possible to apply these methods directly to a more complex model. It is also well-known that applying the classical linear regression technique on a general discrete-time LTI system poses a significant shortcoming, which is the loss of physical knowledge of the system. Usually, the estimation of unknown parameters is obtained solely by the use of an input-output data relationship, as represented by the discrete-time transfer function, and thus black-box parameters result. The main objective of this paper is to estimate parameters in an LTI state-space model structure while retaining the physical knowledge.

Approach. Essentially, this novel approach to estimate parameters in an LTI state-space model structure is based on a so-called pqR-decomposition of the numerator and denominator polynomials of the system's transfer function (see [2] for a first introduction of the idea). As an illustrative example, a continuous-time biomedical/biochemical process with two compartments in parallel and with first-order reaction is used (see [3], p.80). First, the process is approximated by a discrete-time state-space model. Next, after deriving the corresponding discrete-time transfer function, the rational transfer function is decomposed into pqR form and then reparametrized to obtain a set of linear regressive equations. Subsequently, the unknown linear regression parameters, which are a polynomial function of the original physical parameters, are uniquely estimated from real data of the biomedical/biochemical process using the ordinary least-squares method.

Conclusion. The linear regression estimation via pqR-decomposition takes into account the physical structure of the model. The pqR-decomposition generates a direct realization of the physical model with physical interpretation. This approach is favourable when there is a need to preserve physical interpretations in the parameters and regressors. Furthermore, by taking into account the original model structure, a smaller number of parameters than in the case of direct transfer function estimation may result. Typically, estimation of a corresponding transfer function related to an n-compartment model leads to $2n+1$ parameters. On top of that, we can easily check identifiability by only looking at the regression weighting matrices M and N of the pqR-decomposition.

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A photobioreactor model in nitrogen limited conditions

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Microalgae use light as energy source to fix carbon dioxide (CO_2). These microorganisms have recently received a specific attention in the framework of renewable energy. Their high actual photosynthetic yield compared to terrestrial plants (whose growth is limited by CO_2 availability) lead to large potential algal biomass productions of several tens of tons per hectare and per year. After a nitrogen limitation, this biomass can reach a very high lipid content (up to 80% of dry weight under some stress conditions. These possibilities have led some authors to consider that microalgae could be one of the main biofuel producers in the future [5, 2].

These advantages put microalgae in a good position for renewable energy production at large scale [2]. This means that in the coming years there might be large scale industrial plants to produce microalgae. In the specific case of biodiesel production, nitrogen limitation is known to increase the lipid content of phytoplankton. But, by changing the pigment composition and concentration [4, 7], it also strongly affects the radiative transfer properties in the culture medium [7]. The objective of our modelling approach is to propose a new model that can predict the behaviour of a photobioreactor in conditions of nitrogen limitation.

The basis of our development is the Droop model ([3]) which has been deeply investigated ([8]) and proved to accurately reproduce situations of nitrogen limitations ([6, 1]). A link between particulate nitrogen and chlorophyll will then be introduced, so that a simplified light distribution within the reactor can be proposed. We relate the nitrogen status to the chlorophyll content, for a given photoadaptation light. In a second step, we compute the light distribution thanks to a Beer-Lambert model. It results in a model where biology (growth in nitrogen limited conditions) and physics (radiative transfer) are deeply coupled. The model is validated with experimental data of *Isochrysis galbana*.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

CARDINAL TEMPERATURES ESTIMATION VIA OPTIMAL DYNAMIC EXPERIMENT DESIGN FOR PARAMETER ESTIMATION: VALIDATION ON *Z. bailii*

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Introduction. In predictive microbiology, models are developed that can describe the influence of environmental conditions on microbial evolution in food products. Model parameters are often determined based on static experiments. Dynamic experiments are, however, a better alternative as they lower the experimental load and allow evaluation of model validity under time-varying conditions. Optimal experiment design for parameter estimation (OED/PE) forms an excellent basis for the selection of informational experiments, aiming at unique and accurate parameter estimation. This procedure was already successfully adopted for the estimation of the parameters of the Cardinal Temperature Model with Inflection (CTMI) [2] for *E. coli* K12 MG1655 [3]. This nonlinear kinetic model describes the effect of temperature on the microbial growth rate and encloses four parameters, i.e., T_{min}, T_{opt}, T_{max} (the minimum, optimum and maximum growth temperature, respectively) and μ_{opt} (the specific growth rate at T_{opt}). The design problem was reduced to a series of two-by-two optimization problems. Given the four CTMI parameters, six combinations of two parameters are obtained, for each of which a D-optimal experiment was designed. Realistic CTMI parameters were obtained and implementation of OED/PE returned a high statistical quality on the kinetic model parameters. However, a major drawback of the use of OED/PE for CTMI identification was uncovered. A reliable T_{max} estimate is only obtained when temperatures very close to the true T_{max} are included. Therefore, a realistic initial estimate of T_{max} is required.

In the presented work, the OED/PE strategy, as developed for the *E. coli* case study, is validated for *Zygosaccharomyces bailii*, a common spoilage yeast mostly found in food products with low pH values and high sugar concentrations, like apple juice and ketchup.

Results. Realistic initial parameter estimates, i.e, nominal values, are derived from a small series of static experiments and literature. Attention is paid to the selection of a realistic nominal T_{max}. D-optimal experiments are calculated for all six combinations of two CTMI parameters and implemented in a computer controlled bioreactor. In general, the trends in the growth curves are accurately described by the selected models. Compared to the nominal values and values published in [1], the T_{min}, T_{opt} and T_{max} estimates are reliable. Associated standard deviations are very small. The largest estimation error is associated with the T_{min} estimate. The nominal T_{min} value is chosen too high such that the optimal experiments lack information in the most informative region. Additionally, accurate estimation of T_{min} is hardened by the lower sensitivity of the CTMI model with respect to T_{min}, and the slow growth rates at low temperatures. Estimation of T_{min} can most likely be improved in a second OED/PE design round with revised nominal values and an adapted lower temperature boundary.

The advantage of OED/PE is proven by comparing the CTMI parameters to parameters estimated from a series of non-optimized dynamic experiments. More accurate and realistic CTMI parameters are derived from the OED/PE experiments. The overall validity of the OED/PE parameter estimates is confirmed by the accurate prediction of the six non-optimized experiments.

Conclusion. In general, the main conclusion drawn from the *E. coli* case study can be confirmed: by selecting the informative temperature regions, the application of OED/PE enables reliable and accurate CTMI parameter estimation from a limited set of dynamic experiments.

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MODELLING CONTINUOUS CULTURES OF MICROALGAE COLIMITED WITH NITROGEN AND PHOSPHORUS

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The culture of microalgae is more and more developed at the industrial scale. In many applications, a substrate limitation is necessary to induce the production of a specific metabolite. To achieve a better yield, the idea of inducing a stress by two nutrients simultaneously has been investigated. It motivated a better modelling of microalgae colimited by two nutrients.

We present a new model that represents growth of microalgae colimited both by nitrogen and phosphorus. We show that the key point in modeling this complex biological system is the expression for the absorption rate. Phosphorus uptake must be a decreasing function of the phosphorus internal quota. The situation for the nitrogen uptake is different and we show that it must be an increasing function of the phosphorus quota to be able to represent experimental observations. Finally we end up with a model that explains the *a priori* paradoxical opposite response of nitrogen and phosphorus to dilution rate. The proposed model is compared with data of *Selenastrum minutum* and is validated both qualitatively and quantitatively.

Our Droop-based model suggests that the interaction between N and P should be considered at the acquisition rather than at the assembly level. Indeed we feel that the Droop function between growth rate and quota remains unaffected by the N-P interaction while the N-quota construction is tightly tied to the P-status of the cell. The combination of the uptake-limiting effect of P through energy availability needed by NO_3 porters and the concept of uptake-inhibition by the internal quota allowed the model to reproduce the experimental data of the few studies dealing with the two nutrients and particularly under extreme N:P input ratios. We therefore suggest that regarding the colimitation concept, N and P would better be considered as dependent nutrients rather than operationally independent ones.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

SIMULATION AND OPTIMIZATION OF ALCOHOLIC FERMENTATION IN WINEMAKING

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Alcoholic fermentation is an important step of wine making process. Nowadays, it is generally empirically and traditionally conducted. Automatic techniques using on line monitoring of fermentation, modelling and process optimisation would be a valuable new instrument for winemakers. In fact, the fermentation duration and the total energy required for temperature regulation could be predicted and optimised, not only in one tank but also in the whole winery.

We proposed a dynamic model of alcoholic fermentation based on the main yeast physiological mechanisms [1]. In this model, the speed at which ethanol is produced is related to the effects of the main factors involved: (i) temperature, which can vary within a predefined range and (ii) assimilable nitrogen additions, which has a major impact on the yeast activity). The resulting model consists of ordinary differential equations including numerous parameters that need to be identified and important interactions between explanatory variables. These parameters were identified by uncoupling the effects of variables during specific experiments. The model predicted accurately the fermentation kinetics of >80% of a large number of experiments performed with 20 wine yeast strains, 69 musts and different fermentation conditions [2].

We then elaborated a thermal model to calculate the amount of energy produced by the fermentation and consequently the evolution of temperature inside the tank and/or the power consumption for temperature regulation. This model is based on the transient equation for power conservation: $P_{accumulation}(t)=P_{fermentation}(t) - P_{wall}(t) - P_{evaporation}(t) - Q_c(t)$, with $P_{fermentation}$ the power generated by the fermentation, $P_{accumulation}$ the power accumulated by the must, P_{wall} the power exchanged by convection through the tank wall, $P_{evaporation}$ the power lost through evaporation and Q_c the power required to cool the tank.

Thanks to the wide domain of validity of the models, a simulator was developed to help winemakers to optimize tank management [3]. It not only predicts the end of the fermentation and changes in the rate of fermentation, but also includes an optimization module based on fuzzy logic. Optimized temperature profiles and nitrogen addition strategies are proposed to decrease the duration of fermentation and energy requirements at winery scale, according to user specifications. The calculation of a precise, optimal solution for a large number of tanks is very time-consuming and may not be compatible with an interactive interface. Taking this into account, we developed a heuristic approach combining precomputed solutions and a fuzzy logic approach.

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NON-LINEAR DISTRIBUTED PARAMETER OBSERVER APPLIED TO A DENITRIFICATION REACTOR

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Abstract. In this paper, the state observation of a denitrification reactor modelled by a parabolic PDE system is developed. The strategy is to design a distributed parameter Luenberger observer by a late lumping approach such as to keep the distributed nature of the system as long as possible in the construction of the state observer. The numerical implementation of the observer is based on the method of lines and the approximation of the spatial derivatives using a finite element discretization. It however results in a high order ODE system, which is then reduced to a lower order system involving only some dominant modes. Such dominant modes are obtained by modal decomposition.

Keywords: *Parabolic PDE, distributed parameter observer, method of lines, finite element method, modal analysis.*

1 Introduction

Biofiltration has proven to be a promising reaction system for wastewater [3] or drinking water treatment [4], but also in aquaculture or for control of air pollution. Such a device is compact, fairly simple to build and operate, and has shown good efficiency for biological treatment associated to low energy consumption. On the other hand, closed-loop control or supervision is quite limited due to the lack of on-line efficient and low cost instrumentation. Dealing with this problem then requires to implement state observation strategies.

Moreover, such biofiltration units are characterized by spatial distribution of micro-organisms which are fixed on a solid support [5]. Such distributed parameter systems (DPS) are represented by partial differential equations (PDE) to describe their distributed nature [2]. The state observation problem is formulated as an estimation of the complete spatial profiles of the state variables [7]. Key problems related to the state observation of such PDE systems are:

- the location of measurement sensors [6] and associated observability considerations [1],
- the choice of an observation strategy, e.g. a Kalman filter, a Luenberger observer, an asymptotic observer, etc [7].
- the choice of an early or late lumping approach [7].

The main idea of this work is to design a distributed parameter Luenberger observer following the approach devised in [7] for a denitrification reactor represented by a parabolic PDE system and then, by using the method of lines, observer PDE equations are solved. Following a method of lines strategy, the observer PDEs are solved using the finite element method (FEM). In this way, a semi-discrete ordinary differential equation (ODE) system is obtained. Since the ODE system is usually of high dimension, a modal analysis is done such as being able to use only a selection of the dominant modes to integrate the solution.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

BALANCING PREDICTION QUALITY AND FAULT DETECTION PERFORMANCE IN BATCH PROCESS MONITORING

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Introduction. In the chemical and biochemical process industry, batch processes are commonly used for the production of products with a high added value (e.g., medicines, enzymes, high-performance polymers). To achieve a constant product quality, a close online monitoring of these batch processes is necessary. Hereto, multivariate statistical methods have been extended to batch processes in the context of *Statistical Process Control* (SPC).

Most research effort in this area has been directed towards fault detection and identification using *Principal Component Analysis* (PCA) and derived techniques. However, these PCA-based techniques are unable to provide estimates of batch-end quality parameters because the underlying empirical model only focuses on the measurement (input) space of the process, and disregard the quality (output) space. *Multiway Partial Least Squares* models (MPLS) are capable of making batch-end quality predictions when required. While batch-end quality prediction and fault detection have been combined in a single MPLS model [2], a suboptimal method for obtaining the online estimates was used . More recently, PLS-type models have been employed for online fault detection and final quality estimation of a batch fermentation [3], but the estimates are provided only at specific times during the operation and are not available online. Therefore, a true online combined batch-end quality prediction and fault detection scheme based on an MPLS model is presented in this paper.

Methodology. The performance of four different MPLS model types is investigated with regards to true online batch-end quality prediction and fault detection. A relevant case study of a simulated fed-batch penicillin fermentation process forms the basis of comparison [1]. The first investigated MPLS model type takes all available measurements from a complete batch run as input variables. The input variables for the second MPLS model type are a reduced (optimized) set of input variables, in which only those measurement variables with a significant influence on the batch-end quality are retained. This optimal input variable set is obtained through *bottom-up branch-and-bound leave-one-out crossvalidation*. The third MPLS model type is of the phase-wise genre, and is composed of one submodel for each phase of the fermentation process under study. Likewise, the fourth model type model is phase-wise, but employs an optimized input variable set.

Results & Conclusions. Based on extensive simulation results, it is concluded that those model types displaying good batch-end quality prediction typically exhibit a poorer fault detection performance, and vice versa. By combining a phase-wise MPLS model with unoptimized input variables for fault detection with either an optimized phase-wise or full MPLS model for batch-end quality prediction in a multi-model methodology, however, superior results can be achieved. The performance of the multi-model is better than the sum of its parts, as the impact of a process fault on the final product quality can be determined, something not possible with the traditional single-model fault detection methods. Hence, implementing this multi-model scheme will result in only those specific batches where the disturbance impacts the batch-end quality significantly being corrected and/or terminated. In turn, this will lead to a more efficient use of the available raw materials and energy, and reduce the downtime between subsequent batch runs, resulting in a more cost-efficient, cleaner, and safer process.

Acknowledgements. Work supported in part by Projects OT/03/30 and EF/05/006 (Center-of-Excellence Optimization in Engineering) of the Research Council of the Katholieke Universiteit Leuven, Leverage Project IOFH-BKP/06/002 (SCORES4CHEM) of the Industrial Research Council of the Katholieke Universiteit Leuven, and the Belgian Program on Interuniversity Poles of Attraction, initiated by the Belgian Federal Science Policy Office. The scientific responsibility is assumed by its authors. The authors would like to thank J. De Wilde of CYTEC (Drogenbos, Belgium) for the industrial polymerization data set provided for this study.

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OBSERVERS FOR THE ESTIMATION OF FUNCTIONAL GROUPS OF THE ANAEROBIC DIGESTION

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Introduction. In the field of wastewater treatment processes engineering, anaerobic digestion is now a "model for modelers". By this expression, we mean that anaerobic digestion has become an important process to be studied in particular because it is a possible alternative to recover green energy from waste. However, it is an unstable process (and thus it must be controlled) and a number of biological pathways are still poorly understood. The actual models – that are functional models – do not take into account the biodiversity dynamics. In other words, each "biomass" is a virtual functional biomass grouping sometimes not less than hundred of different species. Before introducing as many species as there may exist in reality into models, we need to better understand the microbial ecology of anaerobic digestion. In particular, it is important to establish links between the functions of the ecosystem and its biodiversity. More precisely, it is crucial to assign to each species a particular function. This "assignation problem" is related to the question of "who does what?" in a complex ecosystem (here, "complex means that we consider ecosystems involving several interacting species, each of them possibly realizing different functions).

Content. Molecular fingerprint techniques offer a way of monitoring microbial ecosystems by providing new pictures of microbial ecosystems. In a recent work, it has been shown, under appropriate conditions, that the relative abundances of species could be monitored with these techniques, [1].

Assuming a functional model and the relative abundances of most abundant species are available (typically a mass-balance type model describing both biomass and substrates/products dynamics and the concentrations of most abundant species), one "direct" solution is to test all possible combinations of measured species relative abundances that are then considered as inputs of the model. However, this solution necessitates testing an unfeasible number of possibilities under a dynamical context. Instead, we propose an "indirect" approach based on specific tools of automatic control theory to solve this problem in two steps, cf. [2].

In a first step, functional biomass trajectories which best explain the substrate/products dynamics are generated in using optimal control or observers-based theories while, in a second step, the combination of individual species concentrations which best approximate these functional biomass trajectories are searched for using optimization techniques (in this case, the optimization problem is static and feasible), cf. [3].

In this paper, the approach is proposed for the large class of biosystems involving P coupled bioreactions catalyzed by P microbial functional consortia in which the substrates and products are monitored which may typically be the case of anaerobic digestion.

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STABILITY LOSS DELAY IN THE CHEMOSTAT WITH A SLOWLY VARYING WASHOUT RATE

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In this paper, we propose to study a model with two competitors competing for a single nutrient in a chemostat with a slowly varying washout rate. We show that the model exhibits the delayed loss of stability phenomenon when the washout rate crosses the bifurcation value at which the growth curves of the two competitors intersect.

Constant washout Rate. Consider the chemostat model with two competitors on a single resource, of concentration $s(\cdot)$:

$$\frac{ds}{d\tau} = D(s_{in} - s) - \mu_1(s)x_1 - \mu_2(s)x_2 \qquad \frac{dx_i}{d\tau} = (\mu_i(s) - D)x_i, \quad (i = 1,2)$$

The concentrations of the two different micro-organisms in the system are denoted $x_1(\cdot)$ and $x_2(\cdot)$. The concentration of the input nutrient, denoted by s_{in}, is kept constant. The growth functions $\mu_i(\cdot)$ are assumed to be strictly monotonic and such that $\mu_i(0) = 0$. The term D is called the *washout rate*. Considering values of D less than $\min(\mu_1(s_{in}), \mu_2(s_{in}))$, we denote by λ_i the break-even concentrations $\mu_i^{-1}(D)$. When D is kept constant, it is well known from the Competitive Exclusion Principle (CEP) that generically at most one competitor survives asymptotically [3]. More precisely, when $\lambda_1 < \lambda_2$ (resp. $\lambda_1 > \lambda_2$), the CEP claims that $(s(\tau), x_1(\tau), x_2(\tau))$ converges asymptotically to $(\lambda_1, s_{in} - \lambda_1, 0)$ (resp. $(\lambda_2, 0, s_{in} - \lambda_2)$) when τ tends to infinity.

Varying washout Rate. We assume that growth curves μ_1 and μ_2 intersect in exactly one point $s^* > 0$, where $\mu_1(s^*) = \mu_2(s^*) = D^* < s_{in}$. We assume that $\mu_2(s) < \mu_1(s)$ for $0 < s < s^*$ and $\mu_2(s) > \mu_1(s)$. Furthermore, we consider a slow time varying washout rate $D = D(\varepsilon\tau)$, that is $\varepsilon > 0$ is small, that alternatively favors competitor 1 and competitor 2, see Figure 1.

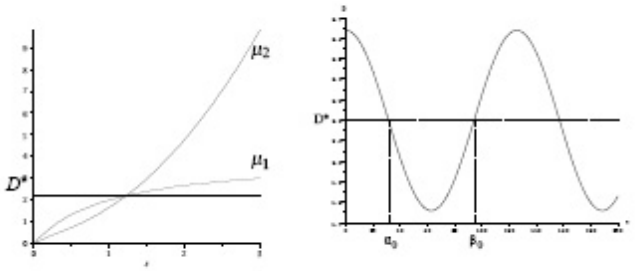

Figure 1: On the left, the growth functions $\mu_i(\cdot)$. On the left, the whashout $D(\cdot)$ with respect to time τ.

In real-life bioprocesses, such as waste-water treatments, inputs are often time-varying. Usually the time scale of theses variations is faster or about the same than the biological one. This is a motivation for studying the chemostat with time-varying inputs (s_{in} or D) favoring alternatively one of the competitors, as it has already been made in the literature [3]. Then, an asymptotic coexistence has been proved to occur, under particular conditions on the variations of the inputs. Designing periodic inputs is a way to maintain more than one competitor above some thresholds at any time.

On the opposite, in natural ecosystems, such as in mountain lakes for instance, one may expect that the variations of the environment are much slower than the biological time scale. This is the purpose of the present work. We focus here on the transient behavior of the dynamics, and show that when D crosses the bifurcation value D^* i.e. gets more favorable to the other species, one may have to wait a large time before observing the density of this later species becoming dominant. This phenomenon is known in slow-fast dynamics as a stability loss delay [1, 2]. Here, we provide also an approximation of this delay.

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DYNAMIC OPTIMIZATION OF CHEMICAL AND BIO-CHEMICAL PROCESSES USING AN EFFICIENT GLOBAL OPTIMIZATION METAHEURISTIC

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Dynamic optimization of chemical and biotechnological processes has received major attention in recent years. Dynamic optimization allows the computation of the optimal operating policies to maximize a predefined performance index such as productivity or other economical indexes. Most bioprocesses present a nonlinear dynamic nature and constraints in both the state and the control variables, which calls for the use of robust dynamic optimization techniques in order to successfully obtain their optimal operating policies. From the existing numerical methods for the solution of dynamic optimization problems, the control vector parameterization (CVP) approach [2] seems to be the most convenient method for dealing with large scale ODE systems [3], such as those resulting from distributed systems.

The CVP approach proceeds dividing the time horizon into a number of ρ time intervals. The control variables are then approximated within each interval by means of basic functions, usually low order polynomials, with fixed or variable length along the time. This parameterization transforms the original (infinite dimensional) dynamic optimization problem into a non-linear programming problem where the systems dynamics (differential equality constraints) must be integrated for each evaluation of the performance index. NLPs arising from the application of direct approaches (such as CVP) are frequently multimodal. Therefore, gradient based local optimization techniques may converge to local optima. Global optimization methods are robust alternatives to local methods. Recent advances in global deterministic methods for dynamic optimization have been achieved in recent years [4] but they still need some requirements regarding the functions differentiability and the path constraints type to be handled. Besides, the computational effort is still a barrier for the application of these methods. Stochastic and hybrid global optimization methods have been successfully applied to dynamic optimization problems [5].

In recent years, a special class of stochastic global optimization methods called metaheuristics has appeared as efficient optimization techniques. Some examples of the use of metaheuristics for dynamic optimization problems can be found in the recent literature (e.g., see [1] and references therein). Scatter Search (SS) is a population-based metaheuristic based on the formulations by Glover [6]. Unlike genetic algorithms and/or evolutionary methods, SS does not use randomization for choosing population members to be combined. Instead, it creates sets of population solutions and combines them systematically. Another difference is that the number of population members is relatively small. SS incorporates a memory term to avoid doing combinations among population members previously combined, which makes the search more efficient.

Here we present a SS-based algorithm for the global dynamic optimization of chemical engineering processes using the control vector parameterization (CVP) approach. It is designed to overcome typical difficulties of nonlinear dynamic systems optimization such as noise, flat areas, non-smoothness and/or discontinuities. It balances intensification and diversification by coupling a local search procedure with a global search. It has been applied to three multimodal dynamic optimization problems from the bioprocess engineering area: ethanol production in a fed-batch reactor, penicillin production in a fed-batch fermenter for and the drying operation of a bioproduct. Its results, compared with those obtained by other state-of-the-art global optimization algorithms, prove its efficiency and robustness, showing also a very good scalability.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Process Engineering

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

DETERMINATION OF INITIAL AMOUNT OF MATERIAL OF INTERMEDIATE STORAGES BY DIFFERENCE EQUATIONS IN DISCRETE STOCHASTIC MODELS

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Intermediate storages play important role in process engineering systems. Using them one can fit each other the subsystems with different operational characteristics. The processing system investigated consists of batch and batch subsystems which are connected by a reservoir. Two natural questions arise: how large the intermediate storage should be in order to avoid overflow, and how much initial amount is needed in order to avoid running out of material. In this paper we deal with the problem of determination of the appropriate initial amount of material. Most of the works dealing with these questions suppose stochastic operation conditions. If conditions concerning the operations assume random variables with continuous distribution functions concerning both the time values between consecutive fillings and the amount of the filled material, the functions describing reliability satisfy integro-differential equations. But in some cases the material arrives at the storage in discrete time points and the amount of material can also be given by random variables with discrete distributions. Such model will be investigated in this paper.

The model that will be investigated in our presentation is the following. The filling process ($N(t)$) is a general renewal process, hence the time intervals between the consecutive fillings (t_k) are supposed to be independent identically distributed random variables. We suppose that they have discrete distributions with integer values and with notation $P(t_k = j) = f(j)$, j=0,1,2,3…The amounts of the filled material are also random (Y_k), they are assumed to be discrete random variables, as well, with notation $P(Y_k = i) = g(i)$ i=0,1,2,3…The withdraw of material from the intermediate storage happens in batches in integer time points and the amounts of the withdraw are unit. In order to avoid running out of material the following inequality has to be held:

$0 \le z_0 + \sum_{k=1}^{N(t)} Y_k - t \quad t \ge 0$ where z_0 denotes the initial amount of material.

If we introduce the probability

$$x(n) = P(n + \sum_{k=1}^{N(m)} Y_k - m < 0 \quad for \quad some \quad m \in N \ ),$$

which is probability of running out of material, using the theory of renewal theory we could prove that $x(n)$ satisfy the following difference equation:

$$x(n) = \sum_{j=0}^{\infty} \sum_{i=0}^{n-1} x(n-j+i) f(j) g(i) + \sum_{j=n}^{\infty} f(j) \quad n = 0,1,2,....$$

We analyse this equation and we prove the existence and the uniqueness of the solution under certain conditions, we investigate the rate of the convergence of the solution. We solve the difference equation in special cases and we use the solutions to determine the initial amount of material appropriate to a given reliability level.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELLING OF HEAT TRANSFER PROCESSES WITH COMPARTMENT/POPULATION BALANCE MODEL

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Fluidized bed heat exchangers are characterized by favourable gas-solids-wall contacting, and, because of the high solids hold-up and intensive motion of particles, particle-particle and particle-surface collisions play significant role in controlling the thermal characteristics of beds. For modelling and simulation of collisional heat transfer processes, a population balance model has been developed [1]. The aim of the paper is to present an extension of the population balance model for describing also the spatial distributions of the gas and particle temperatures in gas-solid fluidized bed heat exchangers.

In the model, collisional particle-particle and particle-wall heat transfers are formulated as discontinuous heat exchange processes characterized by collision frequencies and random variables with probability density functions determined on interval [0,1]. The spatial distribution and transport of gas, particles and the heated fluid are described by a compartmental model, while the gas-particle, gas-wall and wall-fluid heat transfers are described as continuous processes with linear driving forces. The heat conduction in the wall is also described by a discrete model corresponding to the bed compartments.

If $n_k(T_p,t)$ denotes the population density function for the k^{th} cell, k=1,2…K, in the compartment model by means of which $n_k(T_p,t)\mathrm{d}T_p$ provides the number of particles from interval $(T_p,T_p+\mathrm{d}T_p)$ in a unit volume of the cell at time t, $T_{g;k}(t)$ denotes the gas temperature in the k^{th} cell and $T_w(t)$ stands for the temperature of the wall, then the set of population balance equations for particles takes the form:

$$\frac{\partial n_k(T_p,t)}{\partial t}-\frac{\partial\left[K_p\left(T_{g;k}(t)-T_p\right)n_k(T_p,t)\right]}{\partial T_p}=\frac{(1+S_kR)q}{V_k}n_{k-1}(T_p,t)+\frac{Rq}{V_k}n_{k+1}(T_p,t)-$$
$$-\frac{(1+Z_kR)q}{V_k}n_k(T_p,t)-k_{2k}n_k(T_p,t)+k_{2k}\int_0^1 n_k\left(\frac{T_p-p_wzT_w}{1-p_wz},t\right)b_2(z)\frac{1}{1-p_wz}dz+ \qquad (1)$$
$$-k_{1k}n_k(T_p,t)+\frac{k_{1k}}{M_{0,k}}\int_{T_{p\min}}^{T_{p\max}}\int_0^1 n_k\left(\frac{2(T_p-S)}{z}+S,t\right)n_k(S,t)b_1(z)\frac{2}{z}dzdS,\quad k=1,2...K,\ t>0$$

where $n_0(T_p,t)=n_{in}(T_p,t)$, $n_{K+1}(T_p,t)\equiv 0$, and the auxiliary symbols, introduced for the sake of shortness, are: $S_1=0$, $S_K=1$, $Z_1=Z_K=1$, $S_l=1$, $Z_l=2$, and $l=2,...,K-1$. Further, q is the volumetric flow rate, V_k is the volume of the k^{th} cell, V_k=V/K, V is the volume of the bed, and R denotes the back-flow coefficient. The factors $p_2=(m_pc_p)/(m_pc_p+m_wc_w)$ and $p_1=(m_wc_w)/(m_pc_p+m_wc_w)$ characterize the ratios of particle-wall heat capacities where m and c denote, respectively, the mass and specific heat, while the indices p and w denote particle and wall. The second term on the left hand side of Eq.(1) describes the gas-particle heat transfer with coefficient K_p, while on the right hand side: the first three terms represent the transport of particles between the cells, the next two terms describe the collisional wall-particles heat transfer with collision frequencies k_{2k}, and the last two terms describe the collisional particle-particle heat transfer with collision frequencies k_{1k}. The model of the system is formed by the population balance equations (1) for the particulate phase coupled with the heat balance equations for the fluidizing gas, the wall of the bed, and for the heated fluid.

The model was validated by fitting the model parameters to measured data of a fluidized bed heat exchanger [2,3], and properties of the model were investigated by numerical experiments using the second order moment equations reduction. The model describes the temperature distribution of the particle population, and allows separating the effects of the fluidizing gas-immersed surface and particle-immersed surface heat transfers. The second order moment equations reduction, generated from the population balance equation has proved to be an efficient tool for studying the behaviour of heat exchanger.

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MODELLING OF A VISCOSE-FIBRE DRYING PROCESS

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Introduction. Convective Through-Air Drying is a highly efficient state-of-the-art drying technology in the paper and textile industry. This technology features an intense contact between drying air and the good to be dried. Therefore, high rates of the simultaneous heat and mass transfer can be obtained.

The goal of this investigation was to construct a mathematical model of an industrial drying process for viscose staple fibres which is suitable for a Model Predictive Controller (MPC). In this thermal process a belt of fibrous web is moved on the surface of so called rotating drum sieves while heated air is sucked through the web by means of a ventilator. After passing the web at each drum the drying air is heated up again by heat exchangers which are fed with vapour or hot water. This type of dryer can consist of numerous drums up to a number of 20 and even more. In this case the loose fibre flakes enter the predryer (8 sieve drums) forming the fibrous web followed by the main dryer (16 sieve drums) and two remoistening drums, which provide a higher homogeneity of the desired moisture at the end of the process.

There exist a lot of publications about Through-Air Drying. Most of them refer to paper drying and modelling of this process e.g. [1] and [2]. Ghazanfari [3] introduced a drying model for flax fibres using Fick's second law but with no special application. To summarize, there is no literature about modelling drying processes for viscose fibres with distributed drum sieves which leads to a system with distributed parameters

Modelling. The structure of the desired model is modular and scalable. This means that a model of a single drum sieve dryer is established in which it is possible to adapt parameters like geometrical values and process or plant parameters. By joining several of these modules it is possible to model the whole drying process. The main equations of the model are balance equations of mass and energy which generally leads to partial differential equations (system with distributed parameters). In order to obtain a system with lumped parameters the model is being discretised. This ensures that the equations turn into common differential equations which can be solved numerically, on the other hand that for calculations always mean parameter and input values are used, and therefore, also the results are mean values for the discrete place. In the actual model one module corresponds to a unique discrete place. This implies that each state of every module has to be passed with correct time delay (dead time) to the next module.

To be able to describe the airflow through the web qualitatively and to calculate important dimensionless characteristic numbers (Reynolds, Nusselt, Sherwood) a model of the airflow is necessary. The fibres are described as bulk material with a certain porosity and specific surface. It is assumed that the drying air passes the fibre web in flow channels or pores with an average diameter, which can be described as a pipe flow.

Viscose fibres are hygroscopic, so generally three different parts of drying kinetics are distinguished. In the first stage of drying, superficial water that evaporates from the surface of the fibres is assumed to be present. The second stage of drying starts when superficial humidity is removed from the good and the water surface draws back into the capillaries of the fibres. Hygroscopic materials like the viscose fibres have a third stage of drying kinetics, where equilibrium of humidity is established between the good and the surrounding air. In this case, the PEK-model (Parallel Exponential Kinetics) is applied.

Results. The primary goal was to simulate the longitudinal progression of fibre water content through the dryer, knowing the main influence factors on the process like incoming humidity of fibres and drying air as well as the drying temperature distribution along the dryer. Simulation results of transient behaviour of the drying process and a sensitivity analysis of the drying air temperature level in the predryer and the main dryer are shown. Stationary validation at different operating points (different fibres, different temperature levels) of the process model generally gives a good accordance between the model simulation results and measured data. Due to the fact that measurements of the remoistening drums show an impossible high fibre moisture, simulation results have motivated that closer investigations in the plant are being performed.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

SPATIOTEMPORAL DYNAMICS AND SIMULATION OF THE THERMAL FUSING PROCESS IN ELECTROPHOTOGRAPHIC PRINTING

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Introduction. In this contribution a model for the spatiotemporal dynamics of the thermal fusing process in electro photographic printing is derived. The model is a dynamical system consisting of two hyperbolic partial differential equations (PDEs) for the temperature and moisture content of the paper web. In the following the Method of Characteristics and the geometrical interpretation of a first order PDE is employed as a vital tool to simulate different control strategies with high accuracy and determine the state of the paper web during launching of the printing machine and transient steps in the process.

Content. Xerographic images are composed of numerous toner particles deposited on well defined locations on paper by control of adhesive forces. When the toner is first transferred from the photo conductor to paper, it adheres to the paper fibers because of electrostatic and dispersion forces. In this condition the image is easily rubbed off by the slightest contact with another surface, so the image must be fixed permanently to the paper substrate. In the process at hand the toner is fused to the paper and the energy required for this thermal activated process is transfered to the surface by radiation. Due to events taking place further upstream, the fusing process cannot be operated continuous, in fact the way of processing is semi-batch: A certain amount of paper is carried through the domain at a constant pace, before the process stops. During the break, already fused paper elements are drawn back into the machine. At the end of the break, the paper web is accelerated in the direction of processing and finally the velocity returns to a constant pace and the process operates at steady state until the next break is required.

A process model will be derived from first principles, here the conservation of energy and the conservation of mass. Particular attention is given to the different mechanisms of heat transfer and mass transfer dominating the process, especially the evaporation of water, which is found in the capillaries of the paper web, and the radiant intensity of the emitting surfaces, which depends on the spatial variable [1]. The resulting model consists of two hyperbolic partial differential equations (PDEs). From the control engineers point of view, the process is a distributed parameter system with the action of the manipulated variables not taking effect on the boundary conditions, but being distributed in the domain. Furthermore the coefficient of the spatial differential operator, namely the process velocity, depends on time. This fact poses difficulties for the design of a controller as well as for simulation of the process: The deviation from the steady state process velocity is of an extend, s. t. a linearization can not longer be justified. The second part of the paper is focused on simulation of the thermal fusing process and a method for simulation of the nonlinear transport equations is presented, which is capable of dealing with time varying coefficients in the main part of the PDEs.

Dynamical systems described by hyperbolic PDEs have some characteristic properties which are desired to be preserved in simulation of the process. First, their impulse response settles in a finite time. Secondly the eigenvalues of the spatial modes of the spatial differential operator cluster at minus infinity, which essentially means that each mode contributes an equal amount of energy to the impulse response [2]: Reducing the order of the system by neglecting fast modes is impossible. This is the reason why simulation methods like Discretization on Finite Elements, Finite Differences or Finite Volumes do not predict the evolution of the system satisfactorily: Lumping of the parameters leads to a finite dimensional system whose impulse response settles in infinite time and whose poles are distinguishable from each other. Thus the lumped parameter system has slow and fast parts that may be neglected. More difficulties associated with spatial discretization arise when transient steps in the process are supposed to be simulated: Then the process velocity varies in sign. To overcome the difficulties arising with discretization and preserve the characteristic dynamics of the system, the Method of Characteristics and the geometrical interpretation of a first order PDE is applied to simulate the plant output and the distribution of the state variables in the domain [3]. It will be shown, that this method preserves the characteristic dynamics of the system and does require less numerical effort than classical lumping techniques. To illustrate the effectiveness of the simulation method, the current control configuration of the plant is simulated and as a part of the conclusions, based on the prediction of the model, possible improvements are discussed.

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SIMPLE MODELS FOR PROCESS CONTROL

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A second–order–plus–dead–time model is derived from the data used for the characterization of a self–regulating process with a view to its PID control. This modeling approach provides guidelines for the design of the controller and tuning relations are proposed which provide flexibility in the choice of the control system responses and guarantee of stability and robustness. These features are illustrated by simulation results.

The first-order plus dead-time (FOPDT) model which can be constructed from this three parameter characterization is not a realistic model neither for simulation nor even for controller design if the normalized dead time is small (below 0.5). In any control loop indeed, there are more than one single time constant, there may be additional time constants in the process itself and there are others in the various components of the control loop, especially in the actuator. Consequently, in the time domain the step response of the controlled system exhibits a smooth start-up whereas that of the FOPDT model shows an abrupt take-off. In the frequency domain the gain diagram of the FOPDT model has a slope of $-20\ dB/decade$ at frequencies beyond the inverse of the apparent time constant whereas the additional time constants hidden in the control loop result into a steeper descent of the gain diagram at high frequencies. These discrepancies between the true transfer function of the controlled system and its FOPDT model are minor for processes where the apparent dead time is relatively long ($\tau > 2/3$), they may be significant in other cases. Then, a second-order plus dead time (SOPDT) model would be more appropriate for designing a controller. Such a model can be obtained by various identification methods ; in the sixties already van der Grinten had proposed formulas determining the model parameters from the process reaction curve and graphical methods. Here it is proposed to construct a SOPDT model with only three independent parameters closely related to that of the usual FOPDT model ; the values of these parameters can be determined from the same two moments used for determining the parameters of the FOPDT model, or directly from the latter or from any transfer function representing the process to be controlled.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

FLUE GAS CONDENSER MODELLING FOR IMPROVING THE CO2 CAPTURING EFFICIENCY

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Among the main greenhouse gases that contribute in the global temperature rising, the main anthropogenic greenhouse gas is CO_2. CO_2 is produced mainly from fossil fuel combustion in the industrial process and plants. Thus carbon dioxide capturing and sequestration is of critical importance to reduce the release of CO_2 to atmosphere. One of the most recent proposed methods for CO_2 capturing from flue gas is Oxyfuel process. Oxyfuel system uses oxygen instead of air for combustion of the primary fuel. This results in production of a flue gas that contains mainly high CO_2 concentration (greater than 80% by volume) and water vapour. The water vapour is then removed by cooling in a flue gas condenser. To gain the high efficiency in water vapour removal from flue gas and preparing a pure CO_2 stream, there is a great demand for precise design of condenser. Most of the former studies in the CO_2 capturing field have pointed to the condensing method itself without any further discussion on technical aspects of condenser which is not a usual condenser.

In the current paper, the available numerical multiphase flow approaches are investigated and governing mathematical equations for this flow regime are defined precisely. Then a numerical approach is implemented to simulate the two-phase flow behaviour in a simple condenser. It has been found that the Mixture and Eulerian two-phase flow models are both appropriate choices for simulation of condensation phenomena when a non-condensable gas like CO_2 exists in the flue gas stream.

The “mixture” method is implemented to capture the multiphase flow and flow behaviour inside the condenser. This model is combined with the turbulent flow and energy equations via additional source terms in these equations. The calculated flow field shows flow mainly influenced by the cooling tube configuration and spray tube location. The distribution of the velocity and CO_2 fraction can be seen. Furthermore the model shows that CFD has ability to predict the condensation from flue gases. Anyhow the should be verified against some experimental data. Currently such data are not easily available as the oxy fuel process is under the research phase.

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Discrete and Hybrid Simulation: Methodologies, Techniques and Applications

MODELING AND SIMULATION OF MANUFACTURING SYSTEMS BASED ON MACHINE-JOB INCIDENCE MATRIX

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Using today's classification of systems, manufacturing systems (MSs) can be treated as hybrid systems that contain a mixture of various dynamic behaviors—continuous and discrete control loops, Boolean variables related to process states, and discrete events, all embraced by a usually hierarchical decision-making overhead. This means that an MS structure contains both hard and soft technology, first focused on the product fabrication, assembly and distribution, while later the focus is on the support and coordination of manufacturing operations.

The MS's hard technology is split into several levels – from the factory level via the operating center, workcell and robotic station levels to a particular manufacturing process level. The accompanying soft technology is also split into several levels – from the highest strategy level, via lower planning, supervisory, and manipulating levels to the basic manufacturing task level.

Today, simulation models provide a very inexpensive and convenient way for complete factory design. Instead of building real systems, a designer first builds new factory layouts and defines resource configurations in the virtual environment and refines them without actual production of physical prototypes. Allowing clear understanding of all potential problems caused by the factory layout and/or dispatching strategy, modeling and dynamic simulation of manufacturing processes has traced a completely new route to analysis and design of MSs [1]. Simulation of robotized manufacturing systems has become much easier and more effective with specialized programs for virtual-factory modeling and simulation. Many virtual-factory simulators have origin in the academia [2]. Each of these tools has a mathematical core in a form of an algorithm used to describe dynamic behavior of MS elements. In this paper we exploit so called machine-job incidence matrix (MJI) for purpose of deriving such an algorithm.

Construction of MJI matrix, presented in the paper, is based on two well known matrices: resource requirements matrix, also know as machine-part incidence matrix (MPI), and Steward sequencing matrix, also referred as design structure matrix (DSM). An extension of MJI to design of MS recursive simulation model is given, followed by illustrative example. The recursive mathematical model of free choice multiple reentrant flowlines (FMRF) is presented in detail [3]. We consider FMRF systems with multiple flowlines, where resources can hold an arbitrary number of parts simultaneously (k-limited systems). The recursive model forms the basis of the developed system simulator, which is presented at the end of the paper. We conclude the paper with final remarks and an outline for future work. Although manufacturing systems have been used for validation of the proposed modeling technique, the method can be applied on other discrete event systems as well.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

COLOURED PETRI NETS: TIMED STATE SPACE EXPLORATION EXAMPLES AND SOME SIMULATION SHORTAGES

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Introduction. The paper deals with the problem of timed state space generation and exploration in the frame of simulation-optimization approach for discrete-event systems. Coloured Petri net [1] representation of a system is considered and corresponding techniques of timed state space generation and timed simulation are addressed.

Coloured Petri nets (CPNs) include a time concept that makes it possible to apply CPNs for simulation-based performance analysis, and also for model representation within the simulation-optimization approach. Within this approach, an optimization algorithm is used to arrange the simulation of a sequence of system configurations so that an optimal or near optimal system configuration could eventually be obtained [3].

In order to be able to reach the optimum, it is important to be able to generate any possible trace of the system behaviour. It can be observed that in most of the discrete-event simulation tools this is not always the case. They are generally able to represent only a subset of timed state space of a simulated system.

Timed state space exploration. For simplicity, a timed state space exploration of Place/Transition Timed Petri nets (TPNs) is considered. This allows more focused presentation on time aspects while the mechanism of time inclusion are kept as close as possible to the one of CPNs.

While the concept of time is not explicitly given in the original definition of Petri nets in [2] a general concept is applied, which assigns delays to individual arcs, either inputs (enabling duration) or outputs (holding duration) of a transition. This paper builds on some ideas presented in [2] although in a substantially simplified way. When modelling several performance optimization problems, e.g. scheduling problems, it is sufficient to use holding durations. This principle is also used in the timed version of CPNs. While CPNs allow the assignment of delays both to transition and to output arcs, we further simplify this by allowing time delay inscriptions to transitions only. This is sufficient for the type of examples investigated here, and can be generalized if necessary.

Classes of timed state spaces. In the definition of the firing rule of a TPN the exact moment of firing can be defined in a number of different ways. Depending on this one can distinguish among several classes of timed state spaces [2]. Most general is the *timed state space TSS* where a firing of an enabled transition is not tied to any specific firing time. To better define the firing time it may be required that a transition fires at the earliest possible time at a given marking. This way the *earliest time state space* is defined. Other transitions that can fire from the same marking at a later time are also taken into account when generating *ESS*. This possibility is eliminated by the reduced earliest time state space *RSS*, which only allows the inclusion of transitions in conflict that can fire at the same time. Most of the timed state space generating algorithms found in various software tools actually generate *RSS*. An example is CPN Tools software [1].

Simulation can be regarded as an exploration of a single path in the timed state space of the model. Most of the available simulation packages for TPNs or CPNs are also based on RSS generation principle. Of course only one transition is chosen to fire at every simulation step.

Examples. It is shown that the established simulation techniques do not perform adequately in some application relevant examples since in general, only a subset of a timed state space of a simulated system is represented. Clearly, this rules out some of the possible paths in the timed state space. When using simulation for performance optimization, this may cause the obtained solutions being not optimal.

Two examples are provided to illustrate the effect of timed state space reduction. Both *ESS* and *RSS* are generated for each example. The later is generated by standard CPN Tools software. While the optimal solution is preserved within the reduced state space in one example, in the second example this is not the case and the optimum is missed. This indicates that the underlying simulation technique has to be carefully designed in order to be suitable for the simulation-optimization approach.

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APPLYING HYBRID TOKENS TO THE ESTIMATION OF THE THERAPEUTIC OUTCOME OF PSYCHIATRIC TREATMENTS

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Introduction. In the field of health care simulation studies have different objectives: Existing structures and processes of health care systems are to be optimized [1] and treatment costs are to be predicted [2]. Furthermore, prognoses are made about the workload of the health care provider depending on the expected number of patients and their different medical conditions.
One example question is the estimation of the influence of a particular form of therapy on the therapeutic outcome. In Germany somatic treatment follows strict clinical pathways determining the form of therapy that has to be administered. In mental health care clinical pathways are highly controversial and have not been officially established. The chosen therapy is within the sole discretion of the psychiatrist or psychotherapist. However, surveys indicate that different treatments of the same disease can lead to different therapeutic outcomes [3]. In our simulation study *outcome* is defined as either the successful completion or the discontinuation of the treatment. In case of a discontinuation the probability of the mental disturbances occurring again is higher than in the case of a successful completion. This has a direct influence on the number of future patients of the mental health care providers and thus on the system's input and output parameters. If the therapeutic outcome is to be evaluated, a detailed model of the patients is might be necessary.
Psychiatric Treatment. In our example we would like to examine the treatment of in-patients with addictive disorders in a psychiatric hospital. After admission to the hospital, diagnoses are proposed including a leading diagnosis and, if necessary, one or more secondary diagnoses covering comorbidity. According to these diagnoses and the condition of the patient different combinations of treatments are possible. In a psychiatric hospital these usually include the prescription of drugs such as antidepressant or mood stabilisers and setting up a psychotherapeutic treatment. Possible treatments for addictive disorders are among others psychoanalysis, cognitive behavioural therapy or interpersonal therapy [3] in individual and group sessions. The compliance of the patient, that is the motivation for taking part in the treatment, is crucial for the success of a therapy. Each patient shows a different compliance to different kinds of treatments, based on parameters such as the patient's mood. As these parameters are changing continuously during the treatment we need a simulation technique allowing continuous attributes of entities in a discrete-event-driven system. For that reason we would like to apply the introduced concept of hybrid tokens in stochastic Petri nets to model the course of a treatment in a mental health care facility. This will enable the estimation of the therapeutic outcome.
Simulation Model. We use hybrid tokens [4] for modelling the treated in-patients with both discretely and continuously changing attributes. For that purpose, a sufficient mathematical description of the in-patients' mental parameters and their development over time has to be derived. In order to do that, a comprehensive statistical analysis has to be performed. The provision system and the resulting Petri net are comparatively simple. Instead, a high number of tokens that has to be created and the computation of their attributes during the simulation run are the challenges that we are facing. In our previous work the computation of these attributes in constant intervals lead to a large error of the method. For that reason, we now want to use the described problem from mental health care and the collected data for reviewing and improving our modelling approach and the assumptions made.
Results. After building the simulation model of the therapy processes we were able to run experiments by varying characteristics and treatments of the patients and observe the system's output, for example the rate of discontinuations if administering additional treatments for reducing somatic symptoms. But due to the limited sample size, some of the results can only provide a vague indication on the underlying interrelationships. Nevertheless, we believe that the implemented model provides a decision support for physicians and therapists. It enables the estimation of the therapeutic outcome and thus the choice of the most promising treatment according to the patient's mental disturbances.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

PARALLEL ASPECTS OF MODELLING VERSUS IMPLEMENTATION IN HYBRID SIMULATION APPROACHES

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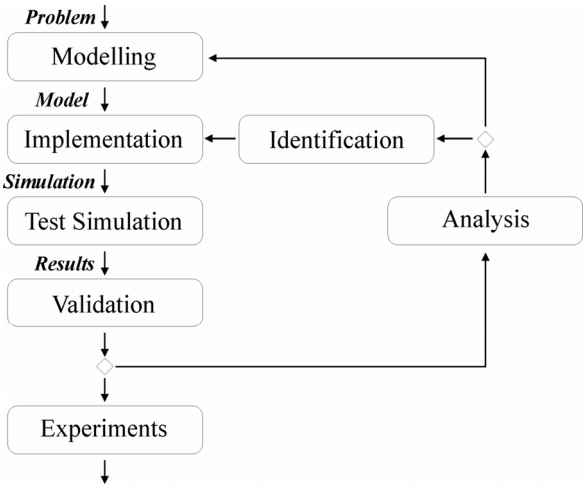
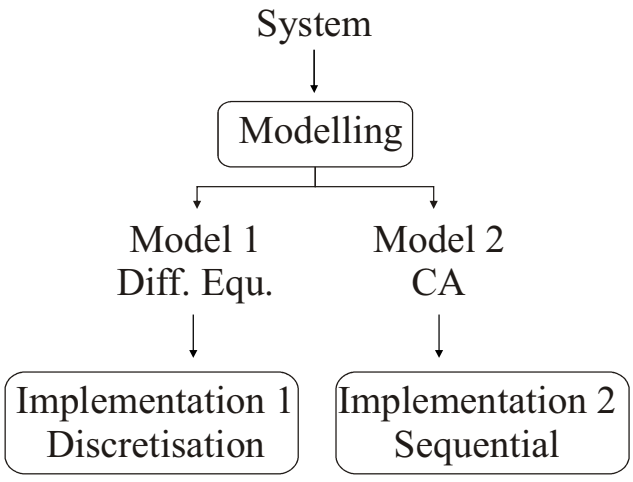
Introduction. Parallelisation as a key word is widely used when processes have to be speeded up. Typically a problem has to be divided in different sub problems *("divide and conquer")* and will be faster solved by simultaneous computing of similar calculations. In our case the key word *"Parallel Aspects"* is used in a different way. It describes a principal conclusion concerning the permutability of modelling and implementation in general and especially the consequences of this permutation for hybrid models, in which different modelling approaches representing a real system are used.

Permutability. While developing and generating a model for simulation reasons in principle different stages are passed through. In a classical way the problem will be described. After the analysis of the problem we have modelling, implementation, parameter identification and simulation. A key question is where is the end of the modelling section and where does the implementation section start. For example the aspect of discretisation of equations can be considered in the same way as the modelling assumptions in the section above. Both define the structures and in this way the behaviour of the model representing a real system strongly. This will be shown presenting different models for epidemic spread.



In the same way the choice of adequate parameter sets will affect not only numerical stability but will also be influenced by the eradication of the steps described above. In our case a cellular Automata and a system of differential equations have to be identified with different parameter sets for simulating equivalent simulations.

Hybrid Simulations. This aspects have to be focused on, especially in the case of hybrid simulations and models. In this case two or more different models of the same real system will be computed simultaneous. Different cases have to be considered as mentioned above: Identification can be obtained with the same parameter sets is the simple case. More complicate is the situation when the permutation of the processes mentioned above leads to models that have to be identified with different parameter sets to compute the same simulation scenario. These situation will conclude in problems validating and verifying the model and the simulation. On the other hand new possibilities structural mapping of real systems can be achieved.



Modelling of actual structure vs. target structure
Similar to classical controllers where the actual value is adapted to comply with the set point, the same situation can be assumed for whole structures of complex real systems. So we can assume a current system or structure not representing a Set Point Structure. Within one simulation scenario we have to switch between these different representations of one system. In general this seems to be a well described problem of hybrid simulation (switching between different model spaces) but in this special case we have the problem of optimization of the model structure itself heading to the set point structure. This problem will be described on the basis of a health economy model.

MODELING HYBRID SYSTEMS IN MVSTUDIUM

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Abstract
A new version of graphical environment MvStudium 6.0 for modeling and simulation of complex dynamical systems enables to design hierarchical event-driven systems using blocks with oriented (Inputs and Outputs) and non-oriented (Contacts and Flows) connections (oriented and non-oriented blocks), whose internal activity may be described by Behavior-charts (B-chart is a state machine with continuous do-activities and without orthogonal states).

1. MvStudium 6.0

MvStudium 6.0 [1-5] **MvStudium 6.0** – is a graphical environment with universal equation- and UML–based object-oriented modeling language, which graphical form based on B-charts and hierarchical functional diagrams. The environment supports technology of designing hierarchical models using oriented and non-oriented blocks, that behavior is may be described by hierarchical B-Charts. The environment consists of Model Editor and Virtual Test-bench.
Model Editor has four user's interfaces that sequentially become more complex for different types of models: 1) an isolated classical dynamical system, 2) an isolated hybrid system, 3) a hierarchical model with components from multiple domains, 4) a model with predefined plan of computer experiment. User can build model using his own original blocks or imported blocks from other projects or libraries. A solved system of differential-algebraic equations for each current model mode is formed and analyzed on compilation stage for models with oriented blocks, and it formed on runtime for models with non-oriented blocks. Designed by user model is checked and compiled. A model may run under Virtual Test-bench, may be a standalone executable program, or may be realized as hidden or un-visual model in the form of DLL for using as a component of more complex model or for parameter optimization with the help of Virtual Test-bench toolbox.
Virtual Test-bench is used for debugging, simulation and computer experiments with visual model.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

FEEDFORWARD CONTROL OF A CLASS OF HYBRID SYSTEMS USING AN INVERSE MODEL

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Introduction. The basic idea of this paper is to present the feedforward part of a control algorithm suitable for controlling MISO systems, which can be modelled by a hybrid fuzzy model. The presented feedforward control algorithm is based on an inverse of a hybrid fuzzy model.

The control scheme. The control scheme we are discussing in the paper splits the control algorithm in two parts: the feedforward part and the feedback part. In the paper, we deal with the feedforward part of the control algorithm.

Modelling of a hybrid fuzzy model. We focus on using the hybrid fuzzy model formulation. The details concerning modelling and identification can be found in [1].

Feedforward control using an inverse model. The basic idea of the control approach is to derive a hybrid fuzzy model of the MISO system we are to control and use the inverse model as a sort of feedforward controller. Of course, it is also very important to take into account the eventual constraints of the system.

We assume that the hybrid fuzzy model of the system is known in advance. Furthermore, we assume the system has a single output and the model should be fuzzyfied with regard to the output. In addition, we assume the system has a single continuous input. The operating mode is defined by the discrete inputs.

The control law presents the core of the control algorithm: the appropriate input signal is calculated from the inverse model so that the desired output signal is obtained. Note that due to causality reasons, the actual output will be delayed by one time-step with regard to the reference signal. The operating mode (and hence the discrete input signal) is selected on a higher level: by calculating the continuous input for each operating mode individually, we can select the most suitable continuous input and in this manner determine the most suitable operating mode.

In most industrial applications the inputs are inherently constrained. Therefore, the control algorithm has to take these constraints into account. The idea is to use the hybrid fuzzy model of the system to calculate the range of the predicted output in the next time-step for each operating mode individually. In case the reference signal is in the range of the hybrid fuzzy model, the reference trajectory is feasible and the inputs can be calculated as described above. However, in case the reference signal is out of range of the hybrid fuzzy model, the prescribed reference is not feasible considering the input domain. Therefore, the reference signal has to be adjusted by moving it into the range of the hybrid fuzzy model. The inputs are now calculated from the adjusted reference signal.

Control of a batch reactor. We introduce a batch-reactor process. The modelling of the batch reactor is tackled and the results of the simulation experiments using the proposed control algorithm are presented. The experiments involve controlling the temperature of a batch reactor by using two on/off input valves and a continuous mixing valve.

Conclusion and future work. The main advantage of the proposed approach is that the feedforward part of the control algorithm can bring the system close[1] to the desired adjusted feasible trajectory. Therefore, in order to obtain a suitable control performance, a simple design of the feedback part of the control algorithm should be sufficient. For instance, one could use a model predictive controller employing a model, which is linearized at the operating point of the system. Since the feedback part of the algorithm takes into account the output signals of the system, the combined control algorithm could easily compensate for the inaccurate modelling, noise and eventual disturbances on the real system. What is more, such algorithm presents a low computational burden; both the feedforward and feedback part are computationally simple, particularly comparing to the standard model predictive control algorithms. These usually require a considerable computational effort, which often thwarts their implementation on real industrial systems.

The future work will therefore focus on developing and including the feedback part in the control algorithm and verifying its usefulness it on the studied batch reactor example.

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A HYBRID MODEL FOR SIMULATING ROOM MANAGEMENT INCLUDING VACATION TIMES

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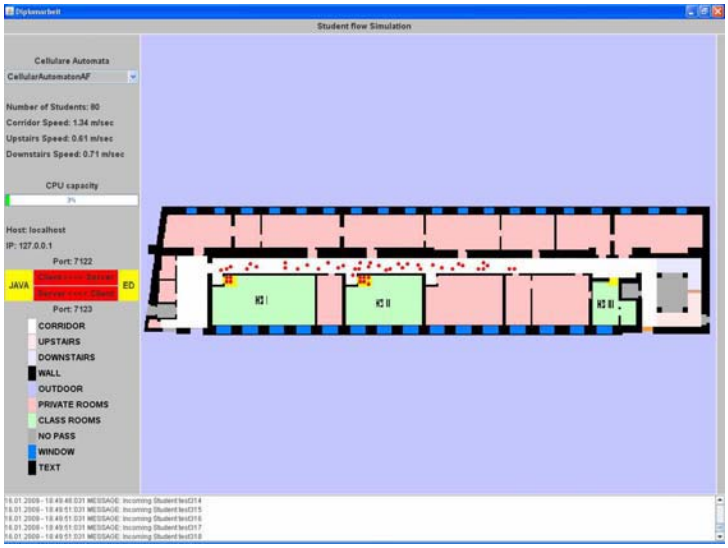
Introduction. Aim of this project as a part of the simulation system <more space> is to simulate the movement of students between lecture rooms, attending their regular curriculum to implement dynamic vacation times. Major outcome is the calculated time which they need to move from a starting point (for example an auditorium) to another location (arrival point). The program is realized in the object-oriented programming language "JAVA" and connected to "Taylor ED". Modeling approaches are *"Cellular Automata" (CA) and discrete simulation* because the literature of this approach is widely spread, and after analysis of the project, the cost-benefit calculation for this modeling was the best. One advantage especially shows that the CA can manage the dynamic behavior of the students finer and more efficient. This justifies the cost of planning and implementation of the corresponding interfaces.

The goal of the project *<more-space>* is to develop software that shall support the planning phase of "University2015" - a project of the Vienna University of Technology (TU Vienna) to renovate all university buildings and to improve the existing infrastructure and the inherent processes - by determining and evaluating the (spatial) resources required and introducing a model for the room management that can simulate the usage of resources to optimize the planning of the rooms and the future "real-life" usage. The dynamic model implemented in *"Taylor ED"* is the main model and simulation system including the data model, process descriptions and dynamic behaviour as using of resources depending on different system or environmental dependencies.

The model. Main elements of the hybrid model are "Students", these entities are moving through the existing structure of CA and the "Building structure". The students are forwarded from the simulation from ED, and processed as long as they do not reach their goal and then send back to ED. In order to make a smooth cooperation and for automatization the capture of data, the following approaches have been chosen. The building structure and related data are saved as an image file in Portable Network Graphics (. PNG) format and a text file (. txt). The image file includes the ground plan of the section who should be read and represents the structure of the Cellular Automata. Lecture halls, stairs, private rooms, etc. are coded in different colors. The exact color coding with the RGB values is saved in the text file. The maximum speed of students moving through the CA is recalculated at every step, it depends on the actual ground (its distinction between corridor, up stairs and down stairs) After studying the literature, the size of a cell is assumed with 0.125 x 0.125m (64 cells per square meter) and each student occupies 4 x 4 cells or 0.5 x 0.5 m. (This value is different for students in class rooms).



GUI in JAVA with CA of the currently simulated level

Interfaces. The Cellular Automatas for different levels are connected at certain points, the gates or stairs. Superior structure of the cellular automata is a weighted undirected graph. *Nodes* are stairs, rooms and gates, *Edge*s are the routes between the nodes with the distance as weight. In order to search for the shortest route across several CAs the Dijkstra algorithm is used. The connection between Java and ED is realized by TCP/IP.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MORE SPACE – A HYBRID DYNAMIC APPROACH FOR MODELLING LECTURE ROOM MANAGEMENT

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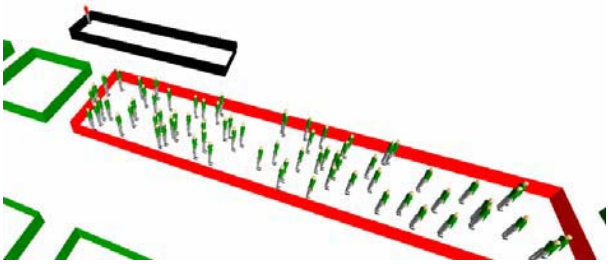
Problem Definition. In the course of the project "Univercity2015" Vienna University of Technology (TU Vienna) is undergoing a major reconstruction process. The projects two main ambitions are to firstly renovate all university buildings and improve the existing infrastructure, and secondly to pool ever two departments at each of the four existing inner-city locations. This of course leads to a vast amount of construction work and relocations due to which — among others — many of lecture rooms are blocked (for at least some time).

The goal of the project <more-space> is twofold. On one hand the developed software shall support the planing phase of "University2015" by determining and evaluating the (spatial) resources required. On the other hand it is to play a significant role during the (re-)construction phase as it will be used to generate an optimum scheme for the blocking of lecture rooms in order to guarantee sufficient rooms with sufficient seats for all scheduled lectures.

Simulation in Facility Management. Despite being a well-known tool in several fields of resource management Discrete Event Simulation (DEVS) is fairly new to the whole Facility Management (FM) branch. Thus for applying DEVS in FM one needs to find an entity– (resources) or entity-flow concept equivalent to the existing one: entities (e.g. work pieces) are searching for a way through the process to their respective resources (e.g. industrial robots) while events are defining and controlling this way.



Screenshot of pseudo-3D model

Model Setup. For setting up our model of the (lecture) room utilization at the TU Vienna an approach was chosen which is breaking down the group of persons up to the respective individuals (i.e. all students). Thus in the present model students (entities) with a common mission — their respective curriculum (control logic) — are finding their way through lecture rooms (resources). The model is being generated using Enterprise Dynamics (ED) and a special module developed by the research group *"Mathematical Modelling and Simulation"* from TU Vienna.

This module is capable of automated database-driven model generation which becomes necessary for the reproduction of an ever changing structure — which is the case for the university's room structure during the construction period. It would be extremely inefficient to manually model a new room structure as it changes every few days or weeks. Of course such an approach also requires the appropriate databases that feed the model with necessary information.

For the calculation of travel times the model is connected to cellular automata (CA) in which the buildings, (lecture) rooms, hallways and stairways of the TU-buildings and streets and crossings of the TU area are mapped. The entities are being transferred from the ED model into the CA in which they travel from their respective sources to their given destinations. As they reach the preset destinations they are handed over again to the ED model and placed into the appropriate (lecture) room.

Findings. In the course of the project <more-space> several scenarios have been set up and simulated with some quite interesting results. One of the outstanding ones being the reduction of erroneous entries — those requests for booking a room of appropriate size that cannot be fulfilled — by more than 75% only because of room management changes. Further the model runs showed significant fluctuation of studentnumbers during the semester leading to the reccomendation of spatially flexible lecture rooms. It was shown that with such a room-structure the changing demand can be encountered much more satisfactory.

MODELLING OF END-STAGE RENAL DISEASE ECONOMICS

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Influence of globalization can be observed practically everywhere, also in an everyday life of each individual, where long working time, unhealthy nutrition habits, stress and lack of recreation have significant influence to health condition all over the world. Such unhealthy lifestyle in combination with population ageing and, partly at least, also because of more intensive and systemized medical examinations in developed countries, revealed that the number of patients with chronic diseases like type-2 diabetes, hypertension and hypercholesterolemia has reached epidemiological proportions. For example, the International Diabetes Foundation (IDF) has reported that 194 million people suffered from D2 in 2003. In 2007, it was estimated that 7.3% of adults aged 20–79 in 172 countries, covering 90% of the world's population, have diabetes. The highest prevalence of diabetes is in North America (9.2%), followed by Europe (8.4%). Based on information from the IDF it can be expected that the number of patients with D2 will double by 2030. Regarding some predictions the number of D2-patiens will reach even 500 million in the next 20 years. The consequence of such situation is a non-negligible economic burden for treatment, which is important not only for governments, hospitals and medical insurance companies, but also for individuals, especially when taking into account also the significant influence of these diseases, and risk factors like obesity and smoking, on serious health complications among which it is important to mention the strokes, peripheral arterial-vascular disease, coronary heart disease, congestive heart failure and end-stage renal disease.

The aim of this modelling and simulation study is to develop a mathematical model with which it would be possible to identify the main dynamic properties of the observed diseases and risk factors, to estimate the number of patients in terms of their age, to identify any possible overlapping of the observed groups of patients, to estimate the healing effects and treatment costs, to predict the social burden of treatment, to estimate and evaluate possible savings, and to enable model extensions, with which a study of an ageing population's influence on the distribution of diseases as well as the economic burden would be possible.

Such types of modelling results are not directly available in the literature. They often cover some of the mentioned aspects, and are frequently connected with a specific region or country. In this paper the results are evaluated for Slovenia, and then an extrapolation is suggested, which can be applied to the countries with a similar demographic and social situation. We can expect that the circumstances are similar in practically all the EU countries.

To cover all the mentioned goals, and taking into account also the available data, the modelling structure was developed as is presented in Fig. 1. That means that the work was realized in three main phases. In the first phase mentioned risk factors and chronic diseases were described taking into account also all possible combinations of observed patients. In the next phase the influence to serious health complications is studied. In the paper the influence to end-stage renal disease is presented. In the third phase the information of population distribution was applied and accomplished by price-treatment evaluation.

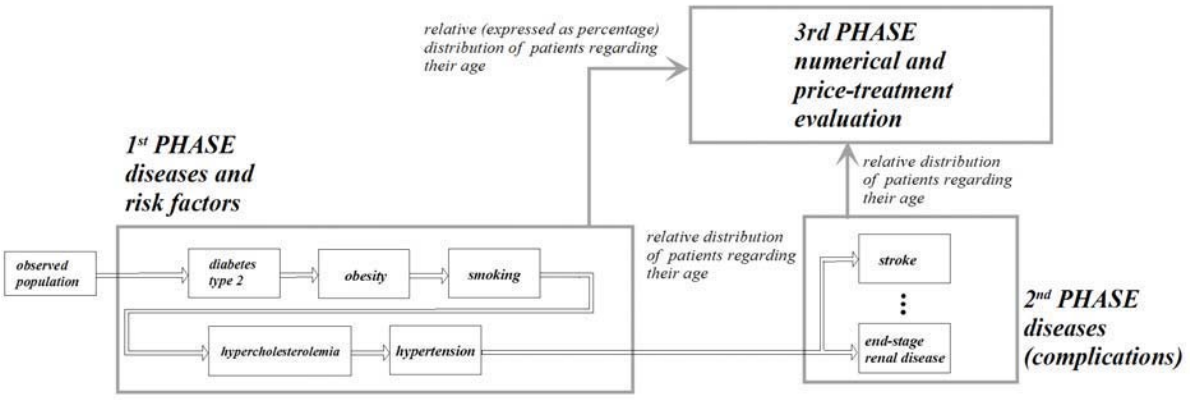

Figure 1. Modelling structure.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

LEARNING OVER SETS WITH HYBRID RECURRENT NEURAL NETWORKS: AN EMPIRICAL CATEGORIZATION OF AGGREGATION FUNCTIONS

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Numerous applications benefit from parts-based representations resulting in sets of feature vectors. To apply standard machine learning methods, these sets of varying cardinality need to be aggregated into a single fixed-length vector. Taking classification as an example, we define the classification task over sets $X_i := \{x_{i,1}, x_{i,2}, \dots, x_{i,n_i}\}$ of feature vectors $x_{i,j} \in \mathbb{R}^m$

$$f \circ g: \mathbb{R}^{m \cdot n_i} \mapsto \{-1,1\}$$
$$X_i \mapsto c_i := (f \circ g)(X_i)$$

as the composition of the aggregation function $g: \mathbb{R}^{m \cdot n_i} \mapsto \mathbb{R}^k, X_i \mapsto a_i$ computing the fixed length k-aggregate a_i and the classification function $f: \mathbb{R}^k \mapsto \{-1,1\}, a_i \mapsto c_i$. Since, per-se, no order is imposed on the set elements, the aggregation function has to be order invariant.

Related Work. Some work has been done on classification of structures containing an unknown number of elements [1], where the authors propose to use *generalized recursive neurons* to represent the structure of a graph. The problem is similar to ours in that the number of input elements can vary, however their approach uses the structure present in the input to deduce the order in which to present the elements to the network. Recently kernel functions have been proposed operating on sets of features [2]. These approaches either assume that direct correspondences exist between the elements of sets or require sets of equal cardinality.

Approach. We propose using Recurrent Neural Networks (RNN) to perform both aggregation and classification of the features of potential faults. The n input vectors x_1, x_2, …, x_n will be processed by the network as if they were a time sequence. The classification result will be available at the output after n "time steps". However, since this sequence of vectors has no inherent ordering special methods for achieving invariance of the RNN have to be applied. Order invariance of RNNs is realized by reshuffling of the data during training: The sequence of the feature vectors in the set is randomly permuted after each training epoch of the network. The neural network should thus learn to be order-invariant.

Evaluation. We have evaluated three common RNN architectures, Elman, Williams&Zipser and Long Short Term Memory (LSTM) [3] networks, on approximating eight aggregation functions g of varying complexity. Data sets have been produced by applying aggregation functions to sets of scalar entries $x_{i,j} \in \mathbb{R}$. The goal is to establish baseline results showing whether existing RNNs can be applied to learn order invariant aggregation functions. The accuracy of the approximation is assessed by the Pearson correlation coefficient R of the network's output with the target value on test data not presented during training.

The results indicate that the aggregation functions can be categorized according to whether they entail (a) *selection* of a subset of elements and/or (b) *non-linear* operations on the elements. We have found that RNNs can very well learn to approximate aggregation functions requiring either (a) or (b) and those requiring only linear sub functions with R greater than 85%. However, if both selection and non-linear operations are required, the accuracy achieved is less than 60%.

Definition	Selection	Non-linear
$a := \sum_j x_j$	no	no
$a := \sqrt{\sum_j {x_j}^2}$	no	yes
$a := \frac{1}{n_i}\sqrt{\sum_j {x_j}^2}$	no	yes
$a := x_u + x_v$ $x_u \geq x_v \geq x_j, j \in \{1, \dots, n\} \backslash \{u, v\}$	yes	no
$a := \max_j x_j$	yes	no
$a := \lvert x_u \rvert + \lvert x_v \rvert$ $\lvert x_u \rvert \geq \lvert x_v \rvert \geq \lvert x_j \rvert, j \in \{1, \dots, n\} \backslash \{u, v\}$	yes	yes
$a := \max_j \lvert x_j \rvert$	yes	yes
$a := \min_{j,k,j \neq k} \lvert x_j - x_k \rvert$	yes	yes

Definition and categorization (see Text) of the aggregation functions underlying the 8 data sets under evaluation.

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PULSE WAVE ANALYSIS BASED ON INTELLIGENT, MULTICHANNEL SENSORS FOR PERIPHERAL BIOSIGNALS

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Introduction. The risk to suffer from various cardiovascular diseases increases dramatically in the last years. These diseases are jointly responsible for around 50 % of fatalities in the developed countries. Current statistics show that mortality motivated by cardiovascular complications like cardiac infarction, stroke or renal dysfunction is much higher than mortality caused by cancer. In order to characterize the cardiovascular risk several parameters are used. High blood pressure and Hypercholesterolemia are the most popular ones. But epidemiological data show that only 40 % of the diseases can be described with these two risk factors.

In the current treatment guidelines of the European Society of Cardiology and the European Society of Hypertension the view is held that hypertension is not an isolated disease but rather a combination of cardiovascular syndromes. A mix of several risk factors enhances the occurrence of cardiovascular diseases. Thus, there is a need for additional relevant and independent risk indicators. Aortic or central pulse wave velocity has turned out to be significant. Unfortunately pulse wave velocity within the Aorta can only be measured invasively.

Motivation. The aim of this work is the development of a sensor whereby non-invasive, peripheral biosignals can be acquired as a tool for the calculation of the central aortic pulse wave velocity. Furthermore, the influence on the measurement site is negligible, because no external pressure is necessary to obtain the signals. Current commercial solutions concentrate on the measurement of the peripheral pulse wave velocity. It is basically measurable with available sensor systems and can be used for certain applications (e.g. non-invasive continuous blood pressure measurement). However, this approach has two problems for determining the cardiovascular risk:

a) The peripheral measured pulse wave velocity is not a significant cardiovascular risk indicator.
b) Unsatisfactory signal quality by limited scope of available sensors.

Aims. The mean pulse wave velocity is defined as distance over time. Starting point of the measurement is the ascending Aorta, as the cardiac activity is the origin of the pulse wave signal. Thus the R-peak of the derived electrocardiogram, which estimates the moment of the blood ejection from the heart into the Aorta, can be used as reference point for time measurements. The ejected pulse wave travels through the vascular system. The peripheral onset point of the pulse wave, which is acquired at the A. carotis, A. femoralis or A. radialis, defines the elapsed transit time. Based on these peripheral signals a digital signal processor computes the pulse transit times and pulse wave velocities.

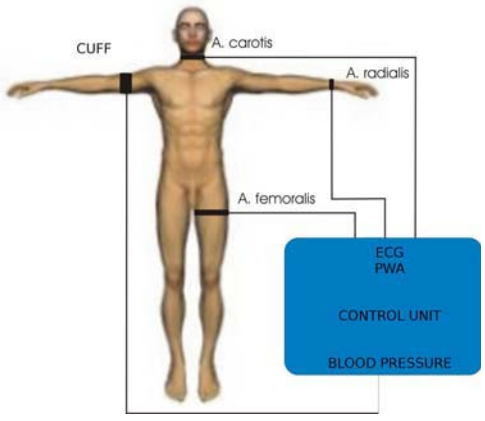

Figure 1: Schematic view of the measurement system

The development of intelligent, active sensors for synchronous, non-invasive measurement of haemodynamic parameters in the blood circulation based on two or more peripheral signals and their joint evaluation in diagnosis and therapy, is a unique possibility in ambulatory treatment to estimate the arterial status and individual cardiovascular risk. The described method is so simple that the functional status of the arteries can be estimated without special efforts by each doctor at each ambulatory patient. Thus, the developed tool can be a major contribution to the prevention of cardiac death.

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Biology, Physiology, Medicine

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

INFLUENCE OF DETECTOR BANDWIDTH AND DETECTOR SIZE TO THE RESOLUTION OF PHOTOACOUSTIC TOMOGRAPHY

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Introduction. High spatial resolution is one of the major aims in photoacoustic tomography. Two main factors limiting the resolution of photoacoustic tomography are the detector size and the finite bandwidth of the ultrasound detection system. We present a quantitative analysis of those effects for "approximate point detectors" and for "approximate line detectors".

Photoacoustic tomography. Photoacoustic tomography (PAT) is based on the excitation of high bandwidth acoustic waves by illuminating a probe with pulsed electromagnetic energy, see [2, Section 1.5] for a detailed mathematical description. It has proven great potential for important medical applications including cancer diagnostics and imaging of vasculature. If the probe is acoustically homogeneous, then the excited acoustic pressure $p : \mathbb{R}^3 \times [0,\infty) \to \mathbb{R}$ satisfies

$$\begin{aligned} \left(\partial_t^2 - \Delta\right) p(\mathbf{x},t) &= 0 , & (\mathbf{x},t) &\in \mathbb{R}^3 \times (0,\infty) , \\ p(\mathbf{x},0) = f(\mathbf{x}) \,, \partial_t p(\mathbf{x},0) &= 0 , & \mathbf{x} &\in \mathbb{R}^3 , \end{aligned}$$

where Δ denotes the Laplacian and ∂_t the derivative with respect to t. We assume throughout that $f \in C_c^\infty(B_R)$, where $B_R \subset \mathbb{R}^3$ is a ball with radius R. The goal of PAT is to reconstruct the initial pressure f (representing the probe) from measurements of $p(\mathbf{x},t)$ taken outside of B_R.

Approximate Point detectors. The classical approach in PAT is to assume that point data

$$(\mathbf{P}_{\text{point}} f)(\mathbf{z},t) := p(\mathbf{z},t) , \qquad (\mathbf{z},t) \in \partial B_R \times (0,\infty) ,$$

are given. In practical applications, the detection system has a finite bandwidth, and standard ultrasound transducers are used to approximate point data. Hence,

$$(\mathbf{P}_{\phi,w} f)(\mathbf{z},t) = \left[\phi *_t \int_{\partial B_R} w\left(|\mathbf{z}-\mathbf{z}'|\right) p(\mathbf{z}',\cdot)\, dS(\mathbf{z}') \right](t) , \qquad (\mathbf{z},t) \in \partial B_R \times (0,\infty) .$$

are the actually available data. Here $w(r)$ is the sensitivity of the detector surface and $\phi(t)$ the impulse response function of the ultrasound detection system. Insufficient knowledge of w and ϕ, as well as the severe ill-posedness of deblurring problems make it impossible to stably invert $\mathbf{P}_{\phi,w}$. It is therefore common to apply the exact inverse of $\mathbf{P}_{\text{point}}$ to $\mathbf{P}_{\phi,w} f$, which results in a blurred reconstruction.

Approximate line detectors. In [1] we proposed PAT with line integrals

$$(\mathbf{Q}_{\text{line}} f)(\mathbf{z},t) := \int_{L_\mathbf{z}} p(\mathbf{x},t) dL(\mathbf{x}) , \qquad (\mathbf{z},t) \in \partial B_R \times (0,\infty) ,$$

where $L_\mathbf{z}$ is the unique line passing through $\mathbf{z}$, being tangential to ∂B_R, and orthogonal to $\mathbf{e}_3$. In practical applications a line detector is approximated by laser beam in an interferometric setup. Hence

$$(\mathbf{Q}_{\phi,w} f)(\mathbf{z},t) = \left[\phi *_t \int_{\mathbb{R}^3} w\big(\operatorname{dist}(L_\mathbf{z},\mathbf{x})\big) p(\mathbf{x},t) d\mathbf{x} \right] , \qquad (\mathbf{z},t) \in \partial B_R \times (0,\infty)$$

are the actually available data.

Again, application of exact inversion formulas for $\mathbf{Q}_{\text{line}}$ leads to blurred reconstructions. However, the laser beam can be made very thin, suggesting that the one dimension approximation with approximate line detectors gives less blurred images than the zero dimension approximation with approximate point detectors. Our aim is to make such statements precise, by calculating analytical blurring kernels and to investigate the resolution for both kind of detectors.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELLING FREE OXYGEN EFFECTS IN ANAEROBIC DIGESTION

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Introduction. Anaerobic digesters (AD) are susceptible to considerable amounts of free oxygen loads. One may expect those aerobic invasions to deteriorate the performance of the digestion systems. But experience shows that in most of the cases the digesters are capable of maintaining high activity despite of the unavoidable aerobic loads. And few researchers reported observing even improving performances under mild aerobic conditions in AD [2], [3]. However, according to the authors' knowledge, no attempt has been made before to explain the dynamics of free oxygen in an anaerobic digester with a comprehensive mathematical modelling approach. This study is intended to establish a sound model basis for analyzing digester aerobic-anaerobic interactions based on the presently known biochemical pathways.

Oxygen Effects -Theoretical and Experimental Basis. Facultative anaerobic acidogenic organisms can consume oxygen rapidly when available, to oxidize readily available carbon sources into carbon dioxide, making energy available for cell synthesis. Meanwhile, the activity of obligatory anaerobic acetogenic and methanogenic organisms is inhibited due to the presence of free oxygen. By conducting an experimental series on oxygen effects in AD, Johansen and Bakke [2] discovered that in fact oxygen enhanced the hydrolysis stage of anaerobic digestion. They further revealed that additional oxygen lead to consumption of available soluble carbon by oxidizing it into carbon dioxide, greatly reducing the methane potential of the system. Thus it is expected that facultative anaerobic acidogenic organisms can improve the hydrolysis process by using oxygen and at the same time can induce detrimental effects on biogas methane yield by oxidizing soluble carbon resource.

Model development. The free oxygen included anaerobic digestion model ADM 1-Ox (oxygen) is developed based on the generally accepted anaerobic digestion model ADM 1 structure [1], developed by the International Water Association (IWA). The amended model ADM 1-Ox has 25 components and 22 biochemical processes, including 3 additional aerobic uptake processes. Saturation type Monod kinetics is used for aerobic uptake processes and a non competitive inhibition function is used for introducing oxygen inhibition of obligatory anaerobic organisms. Biomass dependent first order hydrolysis kinetics is used so that the oxygen induced increase in biomass growth would be reflected in increased hydrolysis.

Simulations. The developed model ADM 1-Ox was programmed and simulated using the AQUASIM 2.1 software package. The initial simulation results are satisfactory in the sense that simulations are similar to the behaviour observed and expected in anaerobic digesters where no or some free oxygen is introduced. Comparison of simulation results with and without oxygen interactions gives insight into the possible free oxygen effects in an anaerobic digester.

When comparing the cases of zero oxygen, 1 mg/L oxygen and 7 mg/L (nearly saturated) oxygen in the influent, no significant difference is observed for most of the simulated parameters (including biomass concentrations, gas flow, methane concentration). When the simulation for 1 mg /L influent oxygen concentration is repeated, but after removing three aerobic uptake processes defined under ADM 1- Ox model, a number of detrimental effects are noticed including high oxygen inhibition, reduced growth rates, less methane yield and accumulation of intermediates.

Conclusions. ADM 1-Ox model is developed in order to simulate the known effects of free oxygen in anaerobic digestion. Simulations are in accordance with common observations. Low oxygen loading conditions, such as typical oxygenated influent feed streams have no significant negative effects in anaerobic digesters, primarily due to the rapid oxygen consuming ability of facultative acidogenic organisms. Further model expansions and improvements are suggested in order to predict the overall effects of oxygen in more precise detail. The initial simulations are used planning relevant experimental studies to validate/improve the model and gain a better understanding of digester aerobic-anaerobic interactions.

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MODELLING A HORMONE-BASED ROBOT CONTROLLER

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Abstract. For all living organisms, the ability to regulate internal homeostasis is a crucial feature. This ability to control variables around a set point is found frequently in the physiological networks of single cells and of higher organisms. Also nutrient allocation and task selection in social insect colonies can be interpreted as homeostatic processes of a super-organism. And finally, also behaviour can represent such a control scheme. We show, how a simple model of hormone-regulation, inspired by simple biological organisms, can be used as a novel method to control the behaviour of autonomous robots. We demonstrate in our article the formulation of such an 'artificial homeostatic hormone system' (AHHS) by a set of linked difference equations and we explain how the homeostatic control of behaviour is achieved by homeostatic control of the internal 'hormonic' state of the robot. The basic idea of our controller is that the inner space of the robot is virtually compartmentalized in a way that the model of compartments reflects the robot's morphological structure. Each compartment can hold different concentrations of hormones which are produced at a constant base rate and which decay at a constant rate. In addition to that, sensor inputs can intensify the secretion of virtual hormones in the compartments they belong to and, in turn, hormones can affect (activate/deactivate) the behaviour of actuators in a compartment. The dynamics of the hormone concentrations in the compartments are described by a set of linked difference equations, as the robots perform their programs in discrete time steps.

The test task that we used to check the quality of our AHHS controllers was a very simple one, which is often a core functionality in controller programs that are used in autonomous robots: obstacle avoidance. We demonstrate two implementations of such an AHHS controller that perform this task in differing levels of quality. Both controllers use the concept of homeostatic control of internal variables (hormones) and they extend this concept to include also the outside world of the robots into the controling feedback loops: As they try to regulate internal hormone levels, they are forced to keep a homeostatic control of sensor values in a way that the desired goal 'obstacle avoidance' is achieved. Thus the created behaviour is also a manifestation of the acts of homeostatic control. The two described controllers were evaluated by using a stock-and-flow model, which allowed sensitivity analysis and stability tests. In addition to that, we have tested both controllers also in a multi-agent simulation tool, which allowed us to predict the robots' behaviours in various habitats and group sizes. The examples shown in this article represent a first step in our research towards autonomous aggregation and coordination of robots to higher-level, modular robotic organisms, that consist of several joined autonomous robotic units. In the end we plan to achieve such aggregation patterns also by using AHHS controllers, as they are described here.

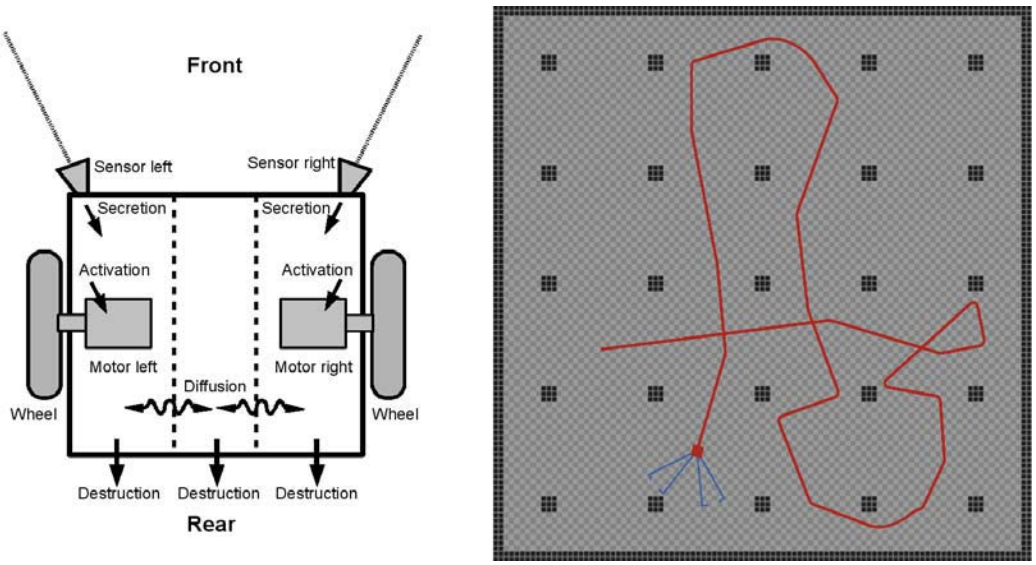

Figure 1: Left: Spatial model of a simple AHHS, showing the compartmentalization, sensors, actuators, decy, and diffusion of a hormone. B: Simulation of the controller in a multi-agent simulation of an aoutonomous robot.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

FINDING THE RIGHT PLACE: CONTRIBUTION OF SPACING TO THE ATTRACTIVENESS OF MALES IN AN INSECT AGGREGATION

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Abstract. In many acoustically communicating insect species males attempt to attract females by calling songs. In natural populations, males differ in their source levels and louder signalling males are known to attract a higher proportion of mating partners compared to softer signalling males in two-choice situations. Another, but related reason for an increased attractiveness of louder than average males is thought to be a larger broadcast area, in which their signals are detectable by receivers. Theory suggests that softer signalling males should stay far from louder ones, in order to increase the area in which their signals are perceived louder than that of opponents. Therefore, male density often found in aggregations facilitates competition for available broadcast area and suggests broadcast area as an important male resource.

In the current simulation study the influence of the spatial arrangement of signallers in such aggregations was investigated concerning a correlation of source level and the accrued broadcast area. In addition, the attractiveness of signallers differing in their source levels was investigated by simulation of female phonotaxis, which is based on a passive attraction to the louder of competing sound sources. This was investigated in three different spacing scenarios: Random spacing, in which signallers exhibit random inter-agent distances. A spacing in which the nearest neighbour is perceived at a sound level of 65 dB and an 'optimised spacing', which is the result of an evolutionary optimisation algorithm aiming to maximise the perceived sound level in an aggregation. All three spacing scenarios were performed at four different male densities mimicking different degrees of inter-male competition. In a variant of this simulation, males signalled from elevated positions, which is known to result in a reduction of excessive attenuation, but on the other hand increases competition for broadcast area in a dense aggregation due to an increased signal radius.

As a result of this study, a significant positive correlation of the source level of individual males and the number of attracted females was restricted to 'optimised aggregations'. In contrast, such a correlation was absent in 'random aggregations' and in '65 dB aggregations' of senders signalling on ground. Simulating *Mygalopsis marki* bushcricket aggregations, in which males signal from elevated positions and inter-male distance fulfils 65 dB spacing criteria, resulted in an average inter-male distance similar to what was found in a real population of this species. In such aggregations, a significant correlation between the source levels of males and the percentage of accrued broadcast area was found. Nevertheless, louder males in simulated *M. marki* aggregations did no succeed in attracting a higher number of females, although such a correlation was found in 'optimised aggregations' of the same senders. This result strongly suggests that despite the regularity of sender spacing, which can be found in *M. marki* aggregations, louder than average signalling males do not attract a higher percentage of females that are passively attracted to the louder of competing sound sources. This result is a direct consequence of an increased zone in which signals belonging to different senders are perceived at a similar loudness.

Finally, female encounter rate of sender aggregations simulated after *M. marki* males was investigated concerning its robustness against perceived sound level fluctuations, minimally discernable sound level differences and turning errors occurring during phonotaxis. Only the magnitude of the minimally discernable sound level difference, which is required for a receiver in order to head towards the louder of competing sound sources, was found to exert an influence on the correlation of source levels and female encounter rates. Interestingly, this correlation was increased at higher sound level differences, suggesting that louder males may benefit from a situation in which a receiver needs to perceive signals at higher intensities in order to locate the source of a sound signal. Such a situation is easy imaginable in a chorus situation with many heterospecific signallers contributing to a high background noise level.

MODEL AND GLOBAL SENSITIVITY ANALYSIS OF *E. COLI* CENTRAL METABOLISM

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In this work mathematical model of central metabolism of *E. coli* upon glucose impulse was analized. The mathematical model is based on the experimental data by Degenring *et al.* [1]. Model of *E. coli* central metabolism includes 24 biochemical reactions and 132 kinetical parameters which are initially estimated by the nonlinear Least Squares Method and improved by several global optimization algorithms [2]. The parameter fitting proces results in relative small erors, but because of the very high dimension of the parameter space there are significant uncertainties in parameters values. For purpose of identification the most sensitive parameters and reactions included in *E. coli* central carbon metabolism (glycolysis and pentose phosphate pathway) the FAST algorithm (Fourier Amplitude Sensitivity Test) was applied [3]. Application of FAST algorithm provides sensitivities to large and simultaneous change of the complete set of the model parameters. Complete set of 132 parameters is transformed to one dimensional space of a single parameter. Results of the output functions (fluxes) are decomposed in Fourier series based on which sensitivity indices are evaluated.
Results of FAST analysis, expressed as percentages of the total variance due to the parameter variations, evaluated for the first 5 seconds of the response to the impulse are: for PTS flux (60 % phosphofructokinase and 22 % PTS mechanism), for nucleotide biosynthesis flux (nucleotide biosynthesis mechanism 39 %, mureine synthesis 30 %, 6-P-gluconate dehydrogenase 6 %, transketolase-transaldolase 4 %) and for pyruvate to biomass flux (pyruvate to biomass rate 24 %, PTS mechanism 16 %, phosphofructokinase 14 %, aldolase 12 %, and pyruvate dehydrogenase 9 %). On average, the contribution of the rest of the metabolic rates is between 15-30 %.

To analyze the glucose consumption in the metabolic network 1 C-mol balance for the input and output fluxes are evaluated. There are two positive in-fluxes, PTS and the reaction of PEP production from OAA. These two fluxes are considered as the inputs to the central metabolism. The input-output 1 C-mol fluxes for the central metabolism reveal that based on 100 % of glucose intake 50 % is directed toward polysaccharide synthesis and 30 % is the flux of oxaloacetate for replenishment of phosphoenolpyruvate (PEP) needed for PTS activity. The flux toward biomass synthesis from pyruvate accounts for 11.7 % of the glucose carbon intake. The results lead to better understanding of the central metabolism regulation and for biotechnology process improvement by application of a rational planning in genetic engineering.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A MODEL FOR A MILDLY-SEVERELY STAGED DISEASE

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Mathematical epidemiology studies the infectious disease propagation among populations. The basic assumption consists in partitioning the whole population into a few classes, of which susceptible and infected individuals are compulsorily present in the model. Other classes could account for instance for latent individuals, i.e. those infected but in which the disease is still not able to spread to others, removed individuals, i.e. those who have been recognized as infectious and therefore quarantined, and so forth.

For many diseases that were considered fatal long time ago, but for which suitable cures were developed, a recrudescence is observed in these days, due to the fact that the infectious agents develop strains that are resistant to the administered drugs, when the latter perhaps are not assumed regularly or with the prescribed protocol. The goal of this paper is the study of the transmission of a disease which shows a weak, curable form, and a strong, possibly lethal stage. From the either one of the two stages individuals can move to the other one, this being the result of success or failure in the cures.

Our results show that if the net birth rate of the population is negative, the system collapses and the population is wiped out. However if the net birth rate is positive, there occur two possible equilibria: the origin now becomes unstable and an interior endemic equilibrium now arises. We have shown numerically that it bifurcates to originate stable limit cycles around it, for suitable choices of the parameter values.

Predictions of carbon fixation during a bloom of *Emiliania huxleyi* as a function of the regulating inorganic species

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Large scale precipitation of calcium carbonate in the oceans by coccolithophorids is a phenomenon that plays an important role in carbon sequestration. However, there is a controversy on the effect of an increase in atmospheric CO2 concentration on both calcification and photosynthesis of coccolithophorids. Indeed recent experiments, performed in conditions of nitrogen limitation, revealed that the associated fluxes may be slowed down, while other authors claim the reverse response. We have designed models to account for various scenarii of calcification and photosynthesis regulation in chemostat cultures of Emiliania huxleyi, based on different hypotheses of regulation mechanism. These models, which are kept at a general and generic level, consider that either carbon dioxide, bicarbonate, carbonate or pH is the regulating factor. These models are calibrated to predict the same carbon fluxes in nowadays pCO2, but they turn out to respond differently to an increase of CO2 concentration. Thus, we simulated a bloom of Emiliania huxleyi using the 4 considered regulation scenarii. For high biomass concentration, the coccolithophorids can significantly affect the inorganic carbon and the pH in their environment, thus leading to a feedback in their growth rate which is, depending on the model, positive or negative. It results that the prediction of the carbon fixed during the bloom varies by a factor 2, depending on the assumed regulating mechanism hypothesized for growth and calcification.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

INTERMINGLING OF DISEASE-AFFECTED POPULATIONS

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Population models date back to the Malthus model of the early nineteenth century. Verhulst corrected it a few decades later to avoid its only two possible outcomes, either exponential growth or decay. His logistic correction allows the population to tend to a constant value representing the carrying capacity of the environment for this population. The early twentieth century saw the predator-prey works of Volterra prompted by the data on fishing in the Adriatic sea collected by the biologist D'Ancona. The now called Lotka-Volterra model contains an interior equilibrium point which exhibits neutral stability. It has been later modified to avoid this drawback and to make it more realistic, by including quadratic and other nonlinear models, accounting for logistic growth or feeding saturation. These models have also been generalized to food webs, with a top predator feeding on some other populations, this possibly going down to several levels.

Mathematical epidemiology was founded by Kermac and McKendric who studied an SIRS (Susceptible-Infected-Removed-Susceptible) system. A disease spreads by contact in a population of fixed size. The major aim consists in searchig for strategies to control the disease, possibly by devising suitable vaccination policies. The population is divided into classes of susceptibles, infected and removed, i.e. quarantined, individuals. The mathematical analysis sheds light on the epidemics spread, remarking that the problem is given by the infectives, which are not identified until they show the disease symptoms, but in the while they have been able to infect other individuals. The most important success of this discipline has been the decision of the WHO in 1980, by which smallpox has been declared worldwide eradicated, and consequently compulsory smallpox vaccination has been discontinued. This decision has been made on the basis of a suitably validated mathematical epidemics model. Specifically, it is the basic reproduction number that tells whether a disease will ultimately propagate or not. A variety of other models in this field of study are also possible.

Ecoepidemiology is a rather new subject of study, in that it considers interacting populations in which an epidemic is spreading. It therefore merges characterists belonging to both types of models described above. In most of the work so far undertaken by several researchers, various types of interactions between the populations have been considered. The disease has always been taken to spread only in one population, either the prey or the predators, or one of the two competing or symbiotic species described by the underlying demographic model. Only fairly recently epidemics in both populations have been considered.

We consider a rather complicated ecosystem in which two populations thrive, and both are disease-affected. The epidemics can pass from one species to the other one by contact. We analytically and numerically investigate the feasibility and stability conditions of the equilibria of the system. We also study possible interesting behaviors of special cases of the proposed model. Some relevant findings are outlined below.

In the proposed ecoepidemic model the disease cannot be eradicated while at the same time preserving both populations, thus the two sound populations cannot thrive together, while this currently happens in the corresponding purely demographic models.

The predators' presence in the model destabilizes the prey endemic equilibrium population, although it is not a priori easy to determine the outcome of a possible predator introduction into the environment. The system will tend to one of its equilibria, where the disease for the prey may not or may be present, but perhaps in such case even affect them more.

The introduction of the disease in the prey may save the sound predators from extinction; in fact predators may go to extinction in the ecoepidemic model should the prey be disease-free.

In the ecoepidemic model considered here the disease cannot disappear just from the predators. It can vanish from the prey leaving only the sound prey as the sole subpopulation thriving in the system. Otherwise, the disease remains endemic in the ecosystem.

NOVEL CONCEPT OF MODELLING EMBRYOLOGY FOR STRUCTURING AN ARTIFICIAL NEURAL NETWORK

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The morphological structure of an Artificial Neural Network (ANN) is very important for its functionality. In our work we present a novel method to organise the nodes and links of an artificial neural network in a biological motivated manner [2] using a new model of virtual embryology. Using this technique, we plan to optimise the structure od ANNs in a biologically inspired manner by Artificial Evolution. Our concept of virtual embryogenesis is mimicking processes observable in biology during the developmental phase of most multicellular lifeforms, like *Drosophila m.* or other species. A virtual embryo consists of individual cells in our system. These cells can develop to nodes in the final ANN. The embryo is implemented as a multi-agent model, in which each single cell is represented as an agent. These cells interact with each other via virtual physics and via virtual chemistry.

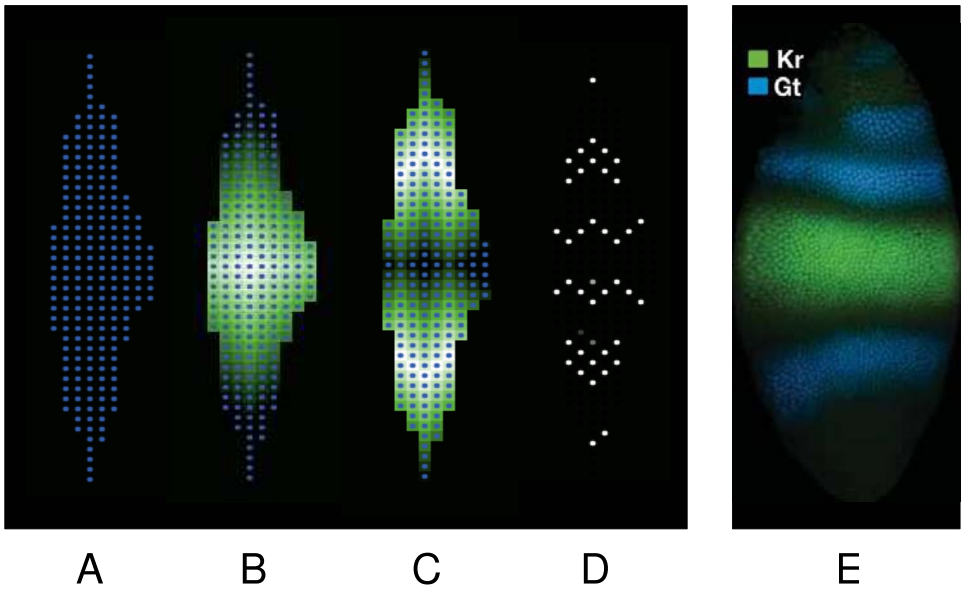

Figure 1: Comparison of virtual and real-world embryogenesis: A: Virtual embryo, consisting of cells (dots); B: Morphogene gradient in embryo; C: Gradient of another morphogene, inducing cell differentiation. D: Embryo consisting of differentiated cells (white dots) and non-differentiated cells (invisible). E: natural examples of gene expression: Activity domains of gap genes in *Drosophila m.* (from [1]; 'Kr' and 'Gt' indicate areas of active gap genes.)

Using our system of virtual embryogenesis, we can show the development of an embryo governed by a simple handcoded genome for the purpose of structuring an artificial neural net (see figure 8). The shape of the embryo, as well as the internal specialisation of cells is controlled by a system of feedbacks, which arise from the process of embryogenesis, from the genome, from the spatial distribution of the cells within the embryo and from the diffusion properties of the morphogenes. The specialisation of cells within the embryo allows the development of different tissues, neural cells or structure cells, which have no neural function but morphological function. The resulting patterns are comparable with patterns found in nature during embryological development. In figure 1 we compare the self-organised segmentation processes in our virtual embryogenesis (figure 1 A-D) with images from natural embryogenesis in *Drosophila m.* (figure 1 E).

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

SIMULATION OF EXUDATION BY ROOT HAIRS

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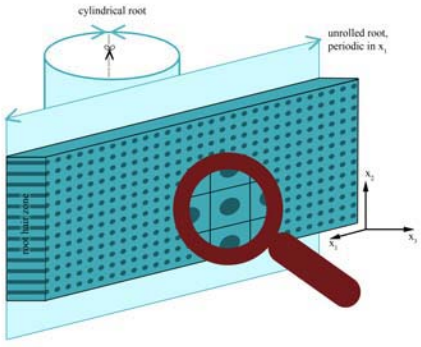
Summary Modelling and simulation is an important tool in describing and analysing plant and soil interactions. In this work we investigate the release of organic compounds (exudation) from roots with root hairs. Exudation by root hairs is thought to increase the bioavailability of nutrients. Therefore they represent a major factor for plant uptake of nutrients which have low mobility in soil, such as phosphorus. In this paper we use the method of homogenisation to analyse the effect of root hair geometry on exudation in the root hair zone. The resulting effective homogenised equations for the root hair zone are used to develop a new exudation model. We solve the model with Comsol Multiphysics and investigate exudation patterns in a hydroponic culture.

Introduction We introduce an effective equation for exudate transport in the root hair zone of roots which contains the relevant information about the root hair geometry. In a first step, we consider a root with root hairs in hydroponic culture, thereby avoiding diffusion limitation due to soil properties. Our aim is to analyse the development of exudate patterns around a root with root hairs for different morphological and physiological root properties.

A root with root hairs represents a complex 3-dimensional structure and therefore direct simulation is computationally challenging. For such problems, the method of homogenisation [**?**] represents a tool to transform the spatial heterogeneities into a tractable homogeneous description. Effective equations of the model valid on macroscale, i.e. root scale, can thus be derived which still contain the relevant information about the microscale geometry. Instead of calculating the movement of solutes around each root hair we consider a composite material whose properties change rapidly compared to the macroscopic length scale L, which is in the order of the root length (cm). On the microscale we consider individual root hairs surrounded by water. The characteristic microscopic length scale of these geometrical heterogeneities l is given by the distance between the root hairs (in the order of μm). If the ratio between the characteristic microscopic and macroscopic scales is small *i.e.,* $\varepsilon = \frac{l}{L} << 1$, it is possible to find effective macroscopic properties.

The Model We consider one single root with a root hair zone in a nutrient solution. Root hairs excrete exudate which moves by diffusion and convection. In the model the geometry is simplified in the following way: The cylindrical root is unrolled yielding a rectangular domain with periodic boundary conditions on two sides, which contains a smaller rectangular domain representing the root hair zone, see figure. This is justified as long as the distance between the root hairs ε is small and the ratio between root hair length and root radius is not larger than order one. In this case the distance between the tips of the root hairs is of order ε. The resulting domain contains cylindrical root hairs orthogonal to the root, which have small radii and are close to each other.



Geometry of a root with a root hair zone

Acknowledgements This work was supported by the Vienna Science and Technology Fund (WWTF, Grant No.: MA07-008) and the Austrian Science Fund (FWF, Grand No.: T341-N13). Andrea Schnepf is a Hertha-Firnberg Research Fellow. Tiina Roose is a Royal Society University Research Fellow.

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A NOVEL MAGNETICALLY METHOD PLANNING TO FETUS HEART RATE MONITORING WITHOUT SIDE EFFECTS

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Abstract. At present, the most common way of diagnosing fetal heart ailments is through an ultrasound examination. While ultrasound can reveal the shape of the heart and provide some information about the working of the heart and blood flow, it is unable to provide the type of electrophysiological information directly related to cardiac activity that is furnished by an electrocardiogram or magnetocardiogram. Attempts have been made to obtain electrocardiograms from the fetal heart using electrodes placed on the mother's abdomen or using the surface touch of solenoids and receiver devices. However, the electrical fields emitted by the fetal heart are so minute that it is difficult to separate them from the electrical signals generated by the mother's heart.

Based of individual researcher reports, there are indeed some potential dangers to the fetus in administring ultrasound tests. They are: "Postnatal thermal effects, fetal thermal effects, postnatal mechanical effects, fetal mechanical effects, and bioeffects considerations for ultrasound contrast agents. Ultrasound energy produces a mechanical pressure wave through soft tissue. This pressure wave may cause microscopic bubbles in living tissues, and distortion of the cell membrane, influencing ion fluxes and intracellular activity. When ultrasound enters the body, it causes molecular friction and heats the tissues slightly. This effect is very minor as normal tissue perfusion dissipates heat. With high intensity, it can also cause small pockets of gas in body fluids or tissues to expand and contract/collapse in a phenomenon called cavitation (this is not known to occur at diagnostic power levels used by modern diagnostic ultrasound units). The long-term effects of tissue heating and cavitation are not known.

According to mentioned side effects, it needs to design a new device to fetus heart rate measuring without dangerous. It has proved that human organs make poor magnetic fields. In the fetal magnetocardiography method the magnetic activity of the fetal heart is measured. Fetal magnetocardiography (F-MCG) is a non-invase technique in which the magnetic field caused by electrical activity within the fetal heart is measured.

Consequently, using robust sensors, equipped apparatuses, power full software and algorithm fetus heart rate should be simulated and compared with test results to validate of defined heart model. This research will present a new and beneficial method to monitor of fetus heart rate without any side effects. As the mentioned above, due to ultrasonic wave's problem this method can be used in fetus heart rate monitoring. Non stress test and other showed methods can not compete with this healthy method.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

TEMPERATURE DISTRIBUTION DURING HIFU TREATMENT AND EFFECT OF LARGE BLOOD VESSEL

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Introduction. Ultrasound hyperthermia is used to treat tumors in human tissue by heat and uses heat in an attempt to destroy cancer cells by localized heating of tumors. Ultrasound hyperthermia is used for liver cancer, with increasing use in other organs such as kidney, lung, bone, and adrenal gland [1].

Ultrasound is mostly utilized for those tumor patients who are not candidates for surgical resection due to complications such as awkward size and location of the tumor. The heat due to ultrasound hyperthermia causes tissue necrosis at predictable temperatures in relatively predictable volumes. The goal of hyperthermia treatment is to define the power deposition pattern such that while the tumor is adversely affected, there would be only minimal impingement on the normal tissue. HIFU (High Intensity Focused Ultrasound) is a non-invasive method for hyperthermia. This technique creates short and local elevations of temperature at the focus. HIFU is a non-invasive treatment modality for a variety of cancers, including breast, prostate, kidney, liver, bone, uterus, and pancreatic cancers. The main goal of HIFU is to maintain a temperature between 50 and 100 °C for a few seconds (typically less than 10 s), in order to cause tissue necrosis. Typically, focal peak intensity between 1000 and 10,000 W/cm2 is used with pulse duration between 1 and 10 s and a frequency of 1 to 5 MHz [2]. HIFU has the advantage of no-invasiveness, better penetration, better selectiveness and ease of power control, over other physical methods such as lasers, microwaves, or radio frequency (RF) fields.

Computer models have been used to determine tissue temperatures during ultrasound hyperthermia. In this work, we consider a liver tissue with a tumor at its center. The liver is a highly perfused and the largest organ in human body and is located in the right upper quadrant of the abdomen. Presence of a large blood vessel next to the tumor is often seen in liver tumors. We calculated temperature distribution in the presence a large blood vessel. When ultrasound is focused on tumor adjacent to large vessels, the blood flow would drag thermal energy away from the tissue. These vessels can change the shape of the zone of necrosis. We used the Pennes bioheat equation for modeling heat transfer. A finite element method (FEM) was used to obtain the temperature distribution for a heat transfer equation. The Comsol Multiphysics software package is used for the FEM implementation. This software performs thermal field analysis and provides all the elements needed to build the model.

A 3-D model for simulation of tumor tissue utilized a cylinder with 4-mm diameter and 10-mm height located in the center of the cylindrically modeled liver tissue. The study proved that temperature distribution in HIFU treatment is independent of the vessel locations in short durations and large distances. Furthermore, simulation results demonstrated that as the vessel diameter was reduced, the temperature of the tumor was increased and lastly with the use of HIFU, the temperature at the centre of tumor increased.

Most computational models of ultrasound hyperthermia used Pennes equation. Frequently simulations consider effect of large vessels by either assigning constant temperature at the surface of the vessel or applying a constant convective heat transfer coefficient (h). We preformed simulations to clarify the essence of flow distribution in vessels. Our study implied that the flow in the vessel is laminar and the thermal boundary layer is fully-developed, thereby resulting in a constant h throughout the procedure. However, since the heated region during the procedure varies in time and the vessel heated length is small, the thermal boundary layer is not fully-developed.

Heat transfer between tissue and blood vessel has been investigated by a number of various models. However, it seems that previous studies have hardly considered a 3D HIFU treatment which includes the effect of large blood vessel presence in the vicinity of tumors for liver tumor.

By increasing distance from the blood vessel to tumor, temperature slightly increased. In our models, the diameter of the large blood vessel is 10mm, which is the typical size of the portal vein. Presence of a large blood vessel next to the tumor is often seen in liver tumors. When ultrasound is focused on tumor adjacent to large vessels, the blood flow would drag thermal energy away from the tissue.

Keywords: HIFU, Bioheat equation, temperature distribution, large blood vessel, FEM, liver tissue

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Electrical/Electronic Engineering and Communication

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

vICERP – THE VIRTUAL INSTITUTE OF CENTRAL RECEIVER POWER PLANTS: MODELING AND SIMULATION OF AN OPEN VOLUMETRIC AIR RECEIVER POWER PLANT

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The virtual Institute of Central Receiver Power Plants (vICERP) founded in the beginning of 2008 is a research network consisting of five research centers under the coordination of the Helmholtz Association. vICERP works in the field of *solar thermal energy* using *central receiver systems* (CRS) with emphasis on the *open volumetric air receiver technology*. This technology is at this time being realized in the research and demonstration plant in Jülich, Germany. The focus of the work is on modeling and simulation of the dynamic system behavior as well as the development of an optimized control and operation strategy.

In order to analyze the behavior during changes in load and operation points, an object-oriented model library using *Dymola/Modelica* is being developed. Models for the central components such as the receiver, the heliostat field, the thermal storage system and the power block are included in the library as well as additional components like pipes, compressors, and valves. The library is based on the open source *Modelica* library *Modelica_Fluid* [1].

The optical part of the heliostat field is modeled using the ray tracing software called *STRAL* [2]. It is coupled with *Dymola* in a master-slave arrangement setting *Dymola* as the master. This way, a very detailed heliostat field model can be integrated with the option of aim point optimization. Validation of the models will be done with experimental data from the solar tower power plant in Jülich.

Feedback control system models are developed using *Matlab/Simulink*. After application of a basic automation concept based on classical PID controllers, it is intended to use a *model-based predictive controller* (MPC) for certain control tasks in the system. The MPC uses an internal, simplified dynamic plant model to calculate the prospective output of the plant. By converting a simplified *Modelica* model to a compilable language such as C/C++, state-of-the-art algorithms for non-linear optimization and optimal control can be used, including, but not limited to (possibly stochastic) weather forecasts and complex objective functions taking into account risks and electricity demand.

For the simulation, the two environments *Dymola* and *Simulink* are interfaced to each other using a co-simulation tool called *TISC* [3]. In that way, the models can be designed and simulated in the best-suited environments and then coupled during the simulation. In addition, other tools can easily be integrated in the simulation. The control trajectories will be validated with experimental data from plant in Jülich.

In the paper presented, the general system setup of a central receiver system using *Dymola* and *Simulink* as well as the co-simulation with *TISC* is shown. The modeling of two central components, namely the open volumetric air receiver and the thermal storage, using the object-oriented modeling language *Modelica* are discussed. In addition, the tool coupling of *Dymola* and *STRAL* is described. Some first simulation results of the solar components are shown.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

STOCHASTIC MODELLING OF POWER SYSTEM NETWORK DEPENDABILITY

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Introduction. In performing the design of a power system a reliability analysis of the power system should be done. There are three approaches for dependability prediction of fault-tolerant systems [2]: combinatorial models, simulation technique (Monte-Carlo), Markov and Semi-Markov models. Markov models are capable of handling phased missions, state dependent failure rates, common mode failures, physical interconnection dependencies, time dependent transitions, maintenance policies. To describe the Markov chain (MC) for a complex system is a very difficult task. In this case a Stochastic Petri Net (SPN) equivalent to MC, is usually used in modelling power system failure-repair behavior [3].

Content. This paper uses the power system dependability model based on Generalized Stochastic Petri Nets (GSPN) but having a simplified structure, named Logical Explicit Stochastic Petri nets (LESPN) developed by the authors [1]. The model is used for fault analysis of power systems networks. The structural simplified LESPN model is obtained by extracting from inside the GSPN model the logical subnets and including predicate/transitions nets facilities. A computerized tool, Stochastic Petri Nets Evaluation (SPNE), predicting dependability metrics of complex repairable power system, was developed. Primitive architectural modules are built and used to construct a modular architecture [1]. The paper exemplifies the LESPN model for simple systems and extends the results for complex power delivery systems.

Radial power delivery network (RDR) has a separate electrical transport line for each electric load supply. Electrical equipments in power delivery network are usually bus bars, cables, electrical transport lines, electrical sources, switches. Ring power delivery network (RDI) supplies all the electrical loads from two electrical sources using the cables i serial connection. This could be done in two distinct networks alternatives RDI_A and RDI_B. Loop power delivery network (RDB) is a combination of radial and ring power delivery types, but the network has many electrical transport lines C, in order to increase the network reliability.

LESPN high level colored Petri Net model for RDI_B network has different colours for electric generators, electrical transport lines supplying bus bar, cables. LESPN model has three architectural modules. All the architectural modules use transitions modelling fault events and also repair. The system functional dependencies are modelled by the arcs connecting the architectural modules. The predicates/transition sets dictate how many and what kind of tokens are moving in each one of the transition execution type. Performance logical conditions are presented in the LESPN associated table. For availability metrics evaluation, the SPNE tool gives: general dependability indices as system success probability P_S, system failure probability P_F; power system dependability specific indices as, System Average Success Time $M[\alpha(T_p)]$, System Average Failure Time $M[\beta(T_p)]$, System Average Failure Interruptions Number $M[\nu(T_p]$, System Average Interruption Frequency Index SAIFI, Customer Average Interruption Frequency Index CAIFI, Customer Average Interruption Duration Index CAIDI, Momentary Average Interruption Frequency Index MAIFI.

The comparative study of the analyzed power delivery networks gives the following results:
- RDR power delivery network model has only 9 states but the dependability metrics P_S and $M[\alpha(T_P)]$, in the planned operational time $T_{p,}$ are the lowest of the investigated networks. This conducts to the highest Average Failure Interruptions Number $M[\nu(T_p]$.
- both RDI_A and RDI_B power delivery networks have almost the same dependability metrics. System success probability P_S and, System Average Success Time $M[\alpha(T_p)]$ are smaller for RDI_B case because of the series bus bars failure/repair events modelling. Also the model complexity in RDI_B case is bigger than in RDI_A case, but dependability metrics P_S, $M[\alpha(T_p)]$ are not much more reduced, because failure rate of the bus bars is generally low. RDI network is more available than RDR network.
- RDB is the most available power delivery network of all studied cases. Also RDB has the most complex MC of all, having NT=225 states, obtained using LESPN model. Number of success states is very high NS=118, so success probability P_S and, System Average Success Time $M[\alpha(T_p)]$ are important.

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Multiport Communication Model of The Low-voltage Power Line Network

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This paper presents a modeling methodology of LV PLC channel based on a multiport analysis and telegraphers' equations in the matrix form. Representing power-line cables in the form of multiconductor system, LV PLC channel communication characteristics are determined in the radio-frequency range and are derived for different coupling schemes of communication equipment with the respect to the power line.

Power lines are primarily used for the transmission of electric power. During the last fifty years different models of utilization of power lines for the transfer of information have been implemented. However, during the analogue era, communications via power lines, also known as power-line carrier (PLC), was mainly used by power utilities for their internal purposes.
Proper design of digital communication systems requires the specification of the following communications channel characteristics: amplitude characteristics, group delay and input impedance. PLC communication utilizes a frequency spectrum in the MHz range regardless of the underlying power network. Since the power grids are optimized for the transfer of electric power and not for the flow of information, there is an increased need for modeling of PLC, especially for LV PLC, in order to adequately estimate the degradation introduced in the communications channel.

It is difficult to model LV power-line network due to the branched topology, lack of power-line data and impedance fluctuations in the network. Initial modeling approaches were based on the frequency-characteristics measurements and derivation of empirical formulas. These models, known as multipath propagation models, use actual measurements for determination of coefficients in the transfer function. Alternative modeling approach is to describe signal propagation via LV power cable utilizing telegraphers' equations with impedance matrix Z and admittance matrix Y. Matrices Z and Y are determined by the dimension and shape of the cable cross-section. Telegraphers' equations are coupled equations since they correspond to a multiconductor power line. Using decoupling procedure, solution of the differential equations is obtained for the incident and reflected voltages at the line terminals.

In this paper, analysis starts with the matrix telegraphers' equations and matrices **Z** and **Y**. Analysis of the signal propagation is conducted through the modal analysis since such approach decouples signals propagating through different conductors. Proposed methodology uses modal analysis based on the eigenvalue decomposition and multiport description of a power line. This approach is then applied to 50 m long LV cable with a standard cross-section. Results of numerical simulations are presented in the paper. The advantage of the model that we proposed in this paper is deterministic which requires cable impedance and admittance matrices. The derived procedure is applicable for determination of the transfer function for an arbitrary coupling of communication equipment with a LV power line.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

GAS INFRASTRUCTURE INVESTMENT: TWO SECTOR DYNAMIC OPTIMIZATION MODEL

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The topic about gas markets becomes a hot one. Because of costly investment in pipelines and LNG facilities, gas has a clear pattern of regional prices. That is why this market is much less competitive than one for oil. When the distance between producer and consumer is relatively small, investment in pipeline gives cheaper final price. Another technology (LNG) is liquidating gas, using relatively cheap trans-ocean transportation and de-liquefaction it at the port of final consumer. The paper presents dynamic optimization model about optimal investment path in two capitals related to gas-exporting industry.

Since gas prices are regional, they differ across space. The open problem is about the interplay between the prices of pipeline gas and LNG. There is some evidence about externality effect, related to positive influence of growing pipeline network on the demand for gas. There exist several countries that are net exporters of gas and which have technical possibilities to develop both pipeline and LNG infrastructures: Russia, Iran, Venezuela, Algeria, Nigeria. The paper considers several formalizations of the problem of an optimal investment of a monopolist into spatial infrastructure, with application to gas delivery using pipelines and LNG. There exists a (local) monopoly in pipeline gas supply and perfect competition in LNG supply.

It is assumed that gas exporting firm can behave as a monopolist is local region but takes the world price of liquid gas as given. Every time period t the firm possesses capital stocks $K_L(t)$, $K_P(t)$ and invests I_L, I_P in infrastructure. It also can decide about exporting price of pipeline gas, p_p taking into account capacity constraint. In the simplest set up (model 2), we consider the linear demand function for pipeline gas with a positive externality effect from capital invested: $Q_P=aK_p - p_P$. The exporting firm solves the optimization problem related to the maximization of the integral from discounted inter-temporal profit function π (t), which is calculated as the revenue in time t minus variable cost and investment from both activities, pipeline gas and LNG. The capital stock dynamics is determined by the difference between investment and depreciation. Investment cost is assumed to be a quadratic function of investment intensity. The variable cost for both technologies depends positively on capital stocks, however with different coefficients. Since LNG sector is assumed to be competitive, it always makes sense to produce at full capacity: $Q_L=K_L$. The price of pipeline gas within a period is chosen to maximize profit within period given existing capacity. After the substitution of this optimal price there emerges the problem with two states (capital stocks) and two controls for the Hamiltonian. Differentiations with respect to controls give two linear relationships between controls and co-states: $\lambda = 1+2\beta I_L$, $\mu = 1+2\gamma I_p$. Thus, controls can be excluded, and we stay with the system of four first order differential equations for states and co-states. Under our initial assumptions, they can decomposed into two pairs of non-interacting equations, and 4-dimentional phase space separates into two 2-dimensional sub-spaces: (K_L, λ) and (K_p, μ). In the first subspace (that describes LNG sector) the isocline $dK_L/dt=0$ is upward sloping, while another isocline $d\lambda/dt=0$ is downward sloping, crossing the axis λ at the point $\lambda^*=(p_L-c_0)/(r+\delta_L)$. For $p_L-c_0 > r+\delta_L$, there exists a unique internal equilibrium point. In the second subspace (describing pipeline sector) both isoclines, $dK_p/dt=0$ and $d\mu/dt=0$, have positive slopes, and all depends on the relative values of slopes. For some parameter values, there is a unique equilibrium in the positive quadrant. Under some set of parameter values, both LNG and pipeline sectors grow to some optimal size. Under other sets of parameters, only one sector is being developed, and we observe corner solution.

Since model results are sensitive to our assumptions, we have also studied alternative models. In the specification of model 1 (when both choke price and demand slope depend linearly on capital stock) the nonlinear interaction between capitals can lead to emergence of two internal steady states. However, under certain parameter values there is unique saddle point.

The shape of externality also plays the role. If it is weaker, the system becomes more complex, but we still can have convergence to unique steady state in some cases. In model 3 it is assumed that pipeline gas and LNG may have identical price, $p_L=p_p=p$. This assumption reflects the effect of globalization, leading to evaporation of local monopoly powers and convergence of gas prices in different regions. The topology of dynamical system becomes more complex in this case, as 4 differential equations no longer separate into two non-interacting pairs.

A NOVEL INVESTIGATION ON COLD ROLLING CONTROL SYSTEM TO OPTIMIZE OF CONTROL DESIGN

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Abstract. The main aim of cold rolling is reduction of strips to the desired final thickness. As the cold rolled strip is being manufactured from hot rolled strip, the uniformity of width, thickness, hardness, etc. are all now intended for improvement. To reach to this target, need to abound control system to reach the higher quality of slabs. It should satisfy the several factors, as regards geometrical, mechanical, chemical and surface properties.

Process control has taken advantage of new measurement equipments, new control actuators and algorithms. Automation and automatic process control can advance the quality further than what is achievable by manual control. This is an important desideration in rolling industry that rolling of slabs needs advanced and optimized process control to increase the productivity and reduction of the variations in the final properties.

A typical cold rolling stand performs one step in a chain of processes in the cold rolling mill, which can include pickling, rolling, annealing, temper rolling and downstream processes. All these processes contribute to the final properties of the strips. When the main process or the main objective is well controlled, it is important to continue with the other processes. In continuous annealing furnaces, the temperature controls the mechanical properties, but temperature differences and bending around rollers change the flatness. Temper rolling needs the same flatness control as other cold rolling processes. Cooling and lubrication can affect several properties of the strips.

Precise general control of the strip in a cold steel rolling mill will be discussed in this article.

Typically, the rolling process is modelled with numerical techniques. But these are not appropriate for a controller design, because they are too difficult. Thus, a linear mathematical model for the rolling process is presented here, which describes the interaction of the required influencing parameters. The attempt leads to numerically professional algorithms, which are essential to run in a real-time situation. With the help of these linear descriptions, the vital elements for the control are investigated. Modern rolling mills are equipped with a servo-hydraulic gap adjustment system, eccentricity control of the rolls, thickness, speed, force and tension controls.

A model to optimize of the control design process and increasing of accuracy is presented. In this way using the process transfer function in system at different control mode like to thickness, flatness, shape and etc designed a PID and PI optimized controller with using of the best optimization method, final properties increased. The measurements are used to verify the model approach and to detect the most significant sources of disturbances.

A new linearised numerical model for the rolling process which is suitable for closed loop control has been developed. The model is based on the calculation of the operating point using an available numerical method, followed by determining the partial derivatives at the operating point with respect to all input parameters. Finally, the partial derivatives are combined using superposition to describe the behaviour of the complete system. In this manner, the changes in the output parameters can be determined for small changes in the input parameters. This calculation is numerically efficient and suitable for use in closed loop control.

Moreover, we describe the roll eccentricity problem and the possibilities to perform compensation. Due to the great variety of solutions, a classification of the methods will be sketched. The basic properties of these classes are discussed. Then, a special solution is presented, which has proved its worth already in a practical application. The investigation of its properties is proposed to be typical for the whole class, to which the method belongs.

Finally measurement data which can be used to verify the new model will be performed. The model has been incorporated as a simulation system developed by the authors who enable the simulation of a multi-pass single stand rolling process. To get practical information about the rolling process, a data logging system was developed and installed in Sura AB for data collection.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

NUMERICAL STUDY OF CELLS MOLECULAR UPTAKE DUE TO ELECTROPORATION BY USING DIFFERENT SHAPES OF HIGH VOLTAGE ELECTRIC PULSES

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High voltage electric pulses have been reported to enhance molecular uptake of cells significantly due to formation of transient aqueous pores in the cell membrane. This technique (named electroporation) nowadays is widely used in delivery of a large variety of molecules such as drugs and DNA in biotechnology and medicine. It was experimentally demonstrated in several studies that the efficiency of electroporation is under the control of electric pulse parameters such as pulse amplitude, duration, and shape. However, the theoretical basis for these experimental results and dependences is theoretically not fully explained.

In order to predict the outcome of experiments and optimize the efficiency of electroporation before each treatment, we developed a model and compared simulation results with experimental results. In our present study, we thus investigated the effect of pulse shape on efficiency of electroporation using modelling and simulation. Our model was based on chemical-kinetics scheme with two types of pores [1] which has been confirmed recently. We used developed equations with field dependent rate coefficients in order to obtain distribution of pores on the membrane. In addition, the conductivity of pores was defined based on trapezium barrier model for the image forces which is also field dependent. The pulse switching-on results in increasing induced transmembrane voltage and affects the pores distribution. Moreover, with increasing the field strength, conductivity of the pores and membrane increase, which results in decreasing of induced transmembrane voltage and this, in turn, affects the distribution of pores. Thus in our model we used self-consistent set of equations to consider all these changes simultaneously and the distribution of pores on the cell membrane was obtained spatially and temporally.

Previously described model was supplemented with a molecular transport model for a single cell to acquire the molecular uptake of cells. Based on experimental observations, we suggested two different mechanisms for uptake: the interactive diffusion through the pores (due to transient contacts of the molecules and the lipids of the membrane) which lasts for seconds after the pulse and long lasting endocytotic-like process in the electrically perturbed area of the membrane [2]. The total uptake was computed with integration of transported molecules through the cell membrane over the time and the cell surface. To investigate the efficiency of electroporation with different pulse parameters, molecular uptake of the cells was calculated.

We used this model to compare the time and position dependence of induced transmembrane voltage, plasma membrane conductivity and permeability, and molecules uptake of the cell for different pulse shapes. The investigated pulse shapes in this study were unipolar rectangular pulses with different rise and fall time, triangular, sinusoidal and bipolar rectangular pulses and also sinusoidal modulated unipolar pulses with different percentages of modulation. The results show that among the pulses, considered rectangular bipolar and triangular pulses are the most and the least effective pulses, respectively. Moreover, the results indicated that the higher the percent of unipolar pulses modulation with sine shape pulses of 50 kHz, the lower uptake enhancement of the cells. Moreover the rise and fall times of unipolar rectangular pulses are not significantly effective in the uptake increase of the cells. Our simulation results are consistent with experimental observations [3].

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Modelling Methods, Theory and Tools

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

AUTOMATED DETECTION OF HUMAN ERRORS BASED ON MULTIPLE PARTIAL STATE SPACES

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Introduction. The development of assistant systems, supporting human operators during supervisory tasks is a field with increasing significance and a wide range of applications. Typical examples are safety critical Human-Machine-Systems like the control and supervision of the operation of nuclear power plants or airplanes. In these scenarios the human operator's flexibility is in practice often used as a fallback level to handle unexpected dangerous situations. However, the human interaction behavior is also not free of various kinds of errors [1]. Here, assistant systems analyzing the Human-Machine-Interaction (HMI) could help the human in critical situations.

Simulation and analysis of human behavior. In [2, 3] an approach for automated detection of human errors in human interaction with complex dynamical systems is presented by formal representation [3] and related automatic detection [2]. As a basis of the approach, the interaction between a human operator and a technical system is formalized using a Situation-Operator-Modeling (SOM) approach [3]. The implementation of a SOM-based model of interactions is realized using Coloured Petri Nets (CPNs). From the CPN model in [2] a full state space can be generated, which contains all possible situations of the system. The considered human errors are described by formal query functions in a generic manner and are detected by analyzing the state space.

The approach was already realized and tested successfully for different human errors by a simulation environment named HMI Analysis Architecture. Here, the interaction between a human operator and a (real or simulated) process is modeled using the SOM approach. This model is implemented with high-level Petri Nets. From the Petri Nets describing the interaction of the real world a state space is generated. An analysis model uses the state space as well as the actions of the real world (modeled as operators) as inputs to evaluate the behavior of the human. As an example, the interaction between a human operator (gamer) and a computer (arcade game) was chosen. The arcade game enables the design of custom scenarios and is easy to replace by other simulated or real technical processes. The modeling and analysis of the interaction is realized by the software CPN Tools providing modeling and simulation of CPNs as well as formal analysis based on an automatically generated state space.

Analysis of multiple partial state spaces (MPSS). Using the approach demonstrated in [2], the online detection of human errors is possible for systems with small complexity. With growing complexity of the considered system, the computational effort for the generation of complete state spaces increases exponentially. Also, the execution of state-space-based queries needs increasingly more time and quickly becomes prohibitive. To solve this problem, a modified analysis approach based on the generation of multiple partial state spaces is proposed here.

Instead of attempting to generate one full state space a priori with all possible system states starting from the initial system state (before actually starting a simulation), multiple partial state spaces of limited size are computed a posteriori starting from observed intermediate states which actually occurred during simulations. Compared to the approach presented in [2] the handling of more complex systems and more extensive simulations now becomes possible.

Regarding the definition and detection of human errors based on incomplete state spaces (when not all reachable situations and situation trajectories are known) the modeling and the analysis also have to be modified. The goal directed behavior can no longer be evaluated with respect to a set of known final goal situations as it was possible in the case of a complete state space. To compensate for that, the definition of sub goal situations becomes necessary. Furthermore, the analysis of several state spaces may be required to calculate all necessary information for the error detection.

As an example for the MPSS-based detection of human errors, the formalization and detection of the human error 'rigidity' [1] based on a full state space as well as the differences resulting from the extension with partial state spaces is decribed. Within an experimental example, the detection of 'rigidity' is implemented and tested for the arcade game application.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

BLOCK BASED PHYSICAL MODELS DERIVED FROM BOUNDARY VALUE PROBLEMS

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Introduction. Practical simulation programs for complex systems usually consist of a library of component blocks and of a software environment for the construction of system models from these components. This software environment may be a simulation language or a graphical user interface for the arrangement and connection of various components. The construction of component blocks requires considerable expertise in science, engineering, and mathematics. This knowledge is "canned" in a component block and is at the service of the user who can rely on the correct implementation whithout knowing about its inner life. Thus the task of simulation of complex systems is separated between two groups of experts, here called the *block designers* who build all the component blocks in the library and the *model builders* who select and connect the appropriate components to form a complex system.

This approach has been successfully applied mostly for component blocks with clearly defined inputs and outputs and for systems described by "pipe models" of different kinds. The situation is different when the single components are described by differential equations for potential and flow variables. Since there are no predefined inputs and outputs, the connections between different components are defined in terms of port variables for e.g. voltage and current or pressure and flow. For distributed parameter systems described by partial differential equations defined on a finite domain, the connection to other system components is given by boundary conditions.

Here arises a fundamental problem for the construction of flexible simulation environments: Mathematical rigor requires that the description of a distributed parameter system is given by a properly posed problem, i.e. that the boundary conditions are specified. However in a simulation environment the block designer has to implement a numerical model for unspecified boundary conditions. These are given later by the model builder through connection to other blocks.

Previous Work. Possible solutions to this problem have been discussed lately in specific applications fields like acoustic simulation and virtual musical instruments. More formal approaches from the perspective of control theory are port-Hamiltonian systems [1] and the behavioral approach [2]. The interconnection of transmission lines and electrical circuits has also been a topic of classical circuit theory, where descriptions by impedances, admittances, etc. for voltage and flow representations or by scattering matrices for wave variable representations have been introduced. The wave variable representation has been carried to the discrete-time domain by the wave digital principle.

Content. It seems that the relations between these different theoretical approaches and other practical solutions for special cases have not yet been fully explored. This contribution presents a small step in this direction by linking the general idea of the behavioral approach to some well-known tools from circuit theory and digital signal processing. The presentation starts with the connection between the behavior of a distributed parameter system and possible input output assignments induced by the boundary conditions. Then the relations to the well known two-port parameters from circuit theory are shown. A major topic are the implications between block design and model building, i.e. the design of a component block for later use in a larger model. It is shown that a block for a distributed parameter system can be designed according to standard boundary conditions and that the boundary conditions can be modified subsequently without opening up the component block. This method is extended to include not only effort and flow variables but also wave variables. It is explained how component blocks designed for effort and flow variables can be connected to those designed with wave variables. Finally a multiport description is obtained from the formulation of a distributed parameter system as a boundary value problem.

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MODELLING SYSTEMS WITH ORDINARY DIFFERENTIAL EQUATIONS: DERIVATIVE ORDER REDUCTION OF INPUT SIGNALS

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Many systems that process input signals can be described by ordinary differential equations (ODE). Common test input signals are impulse or step functions, which are very often used to study electrical devices. Problems may occur, if the right hand side or source term of an ODE contains a derivative of a non-differentiable input signal. However, this can often be cured analytically for many good-natured source terms by using Fourier or Laplace transform methods, but not generally when solving an ODE numerically. Here we show that the application of ODE dependent forward and backward transformations can be useful to improve numerical ODE solvers.

Assume that the n-dimensional ODE of interest can be written as

$$\dot{\mathbf{x}} = A\mathbf{x} + B_0\mathbf{s} + B_1\dot{\mathbf{s}} + B_2\ddot{\mathbf{s}} \tag{1}$$

where A and B_i are constant $n \times n$-matrices and where $\mathbf{s} = \mathbf{s}(\mathrm{t})$ is the input signal. Using the transformation

$$\mathbf{y} = \mathbf{x} - B_1\mathbf{s} - B_2\dot{\mathbf{s}} \tag{2}$$

we have consequently to solve the ODE given by

$$\dot{\mathbf{y}} = A\mathbf{y} + (B_0 + AB_1)\,\mathbf{s} + AB_2\dot{\mathbf{s}} \tag{3}$$

Note that the second oder derivative of the input signal has been eliminated or, more exactly, the orders of the derivatives of $\mathbf{s}$ have been reduced. This approach will be generalized for time dependent matrices and for ODE that can be written as

$$\dot{\mathbf{x}} = \mathbf{f}(t,\mathbf{x},\mathbf{s}) + \mathbf{g}(t,\mathbf{s},\dot{\mathbf{s}},\ddot{\mathbf{s}},\ldots) \tag{4}$$

For this ODE the transformation approach

$$\mathbf{y} = \mathbf{x} - \mathbf{h}(t,\mathbf{s},\dot{\mathbf{s}},\ddot{\mathbf{s}},\ldots) \tag{5}$$

leads to

$$\dot{\mathbf{h}}(t,\mathbf{s},\dot{\mathbf{s}},\ddot{\mathbf{s}},\ldots) = \mathbf{g}(t,\mathbf{s},\dot{\mathbf{s}},\ddot{\mathbf{s}},\ldots) \tag{6}$$

Thus $\mathbf{g}$ should be integrable. Further conditions for $\mathbf{g}$ will be given. And it will be shown that the repeated application of the introduced transformation approach can be used to eliminate all derivatives of the input signal present in ODE's source term. However, the costs of this approach are the transformation of ODE's structure and the required backtransformation of its solution to obtain the solution of the original ODE. The potential advantage of the method will be demonstrated by examples.

The ODE dependent transformation approach can be used to eliminate or to reduce the order of derivatives of input signals present in the source term of the ODE model of the system to be analysed. The notion behind this transformation approach is the fact that many ODE structures are intrinsically exploited to a transformation-based order reduction of input signal derivatives present in ODE's source terms. However, more important is the fact that some additional mathematical operations can be useful to improve the performance and, certainly, the range of applications of numerical ODE solvers.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

STOCHASTIC PARTICLE APPROXIMATION TO THE GLOBAL MEASURE VALUED SOLUTIONS OF THE KELLER–SEGEL MODEL IN 2D

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This paper is concerned with the mathematical modelling of chemotaxis, a biological phenomenon in which living organisms (typically cells) direct their movements according to certain chemicals in their environment. In particular, we construct a discrete scheme for approximation of the global measure valued solutions to the parabolic-elliptic Keller-Segel model of chemotaxis [2] in the 2D full space case,

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \nabla S - \nabla \rho) &= 0 \,, \\ -\Delta S &= \rho \,, \end{aligned}$$

for $t > 0$ and $x \in \mathbb{R}^2$, subject to the initial condition $\rho(x,t=0) = \rho_I(x)$. Here, $\rho = \rho(t,x)$ denotes the number density of cells, and $S = S(t,x)$ the concentration of the chemoattractant. When the Poisson equation for S is understood in the sense of the Newtonian potential solution,

$$S[\rho](x) = -\frac{1}{2\pi} \int_{\mathbb{R}^2} \log(|x-y|)\rho(y)\,\mathrm{d}y \,,$$

we obtain the classical result

$$\frac{\mathrm{d}}{\mathrm{d}t} \int |x|^2 \rho(x)\,\mathrm{d}x = \frac{M}{2\pi}(8\pi - M) \,, \qquad \text{with } M := \int_{\mathbb{R}^2} \rho_I(x)\,\mathrm{d}x \,,$$

indicating the well known dichotomy in the qualitative behavior of the system with the critical mass 8π. Biologically, the possible concentration of the cell density in the supercritical case $M > 8\pi$ represents aggregation of cells, and the description of the dynamics of these aggregates is of natural interest. One such description has been derived in [1], based on a regularization of the Newtonian potential. The cell density ρ becomes a time dependent nonnegative Radon measure; making the ansatz $\rho = \bar{\rho} + \sum_{n=1}^N M_n(t)\delta(x - x_n(t))$, where $\bar{\rho}$ is smooth and t varies in a time interval where the atomic support of ρ consists of N smooth paths $x_n(t)$ carrying smooth weights $M_n(t) \geq 8\pi$, the following system of equations is obtained:

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \nabla S[\bar{\rho}] - \nabla \bar{\rho}) - \frac{1}{2\pi} \nabla \bar{\rho} \cdot \sum_{n=1}^N M_n(t) \frac{x - x_n}{|x - x_n|^2} = 0 \,, \tag{1}$$

$$\dot{M}_n = M_n \bar{\rho}(x = x_n) \,, \tag{2}$$

$$\dot{x}_n = \nabla S[\bar{\rho}](x = x_n) - \frac{1}{2\pi} \sum_{n \neq m = 1}^N M_m \frac{x_n - x_m}{|x_n - x_m|^2} \,. \tag{3}$$

A local-in-time rigorous existence result is known only [3]; in general, one has to expect blow-up events in the smooth part $\bar{\rho}$ and/or collisions of point aggregates in finite time. At such instants, a restart is required with either an additional point aggregate after a blow-up event or with a smaller number of point aggregates after a collision.

In our paper, we construct a discrete approximation of (1)–(3) based on a system of stochastic interacting particles. After a discretisation in time, this leads to a stochastic numerical method for computation of approximate solutions. The main novelty of our method against existing numerical schemes is that it detects both the (possible) blow-up instants in $\bar{\rho}$ as well as collisions of point aggregates and captures the solution even after these events. Moreover, a formal application of the Ito formula shows that our method reproduces the 8π-dichotomy of the qualitative behavior of the system. On the other hand, the numerical cost of our scheme compared to "traditional" methods (finite differences, volumes or elements) is relatively high.

We describe our method in detail and present some numerical examples. Moreover, we make a first step toward the convergence analysis of our scheme by proving the convergence of the stochastic particle approximation for the Keller-Segel model with a regularized interaction potential. The proof is based on a BBGKY-like approach for the corresponding particle distribution function.

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HIDDEN NON-MARKOVIAN MODELS: FORMALIZATION AND SOLUTION APPROACHES

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Introduction The modeling of real systems usually involves direct study and measurement of the systems' behavior. However, some system can only be observed through their interaction with the environment. An example of such a system is a machine which produces either working or defective parts, the portion depending on the production mode, which is not transparent to the observer. An analysis of the sequence of produced parts could enable a production manager to find out if the machine is working within the manufacturer's specification and when to schedule the next maintenance. Using existing modeling paradigms, it is not easily possible to use these signal sequences to draw direct conclusions about the exact system behavior that produced them. Hidden Markov Models (HMM) can analyze hidden systems, but are limited in their modeling power. On the other hand, discrete stochastic models (DSM) have a large modeling power, but they have to be completely observable. Combining these two paradigms will enable the analysis of more realistic hidden models with the tools of HMM, specifically it will enable to link recorded system output to possible system behavior.

Formalization of Hidden non-Markovian Models The definition of HnMM uses the state space of the model with transitions of arbitrary type between the states. A Hidden non-Markovian Model is described as a 6-tuple $(S, C, V, A(t), B, \pi)$ = *(states,state changes,output symbols, state transition process, symbol output process, initial system state)*. The extension to DSM requires every symbol and every transition to be associated with the time stamp. The trace becomes a sequence of pairs $(symbol, timestamp)$ and the path a sequence of pairs $(transition, timestamp)$. Several special cases can be considered when designing an HnMM, each leading to a different formal description or modified solution algorithms. The first option is whether all model transitions emit symbols or only some produce observable output. The second choice is whether an state change can be realized by only one or by several transitions. The third choice is whether transitions can keep their activation time when a state change happens, or whether all non-Markovian transitions are reset when a state change happens.

Adapting Solution Algorithms for HnMM For the calculation of the state changes probabilities, several possibilities to compute these based on the instantaneous rate function are discussed. We will adapt the algorithm definitions taken from [1] to HnMM. The Forward and Backward algorithms determine the probability of a given output sequence for a given model. The Viterbi algorithm determines the most likely generating path of a given output sequence for a given model. The Forward, Backward and Viterbi algorithms were successfully adapted for the simple HnMM configuration. How to handle models containing transitions that do not emit symbols is not yet clear. The Baum-Welch algorithm solves the training task of a model using an observed output sequence. The adaption to HnMM is not easily possible. The training of a model also involves the training of the state change rates, and it is not clear, how the IRFs can be changed in an meaningful way to reflect that. For HnMM that are not Markov regenerative concurrently activated non-Markovian transitions are not reset, their activation times need to be remembered as transition ages. This approach eventually results in the solution algorithms already described in [2]. Considering all of these restrictions, the adaption of the algorithms was only partially successful. However, the main contribution of the paper consists in the formalization of HnMM themselves.

Conclusion We hope that HnMM will combine the advantages of DSM and HMM. The new paradigm will enable the following: output sequences of real systems can be used to deduce possible system behavior that produced them. One can determine the probability of an output sequence. In general, the extension to more general hidden models utilizes the capabilities of HMM for more realistic system representations. The training method is currently not applicable to HnMM and the evaluation and decoding tasks can only be solved if the model is of Markov regenerative type. However, other solution approaches using Proxel-bases simulation have already been described in previous papers. HnMM make it possible to solve problems not solvable with existing paradigms. The formalization of HnMM is a necessary step to the further examination and development. One drawback is that currently the existing and the adapted solution algorithms are computationally expensive. Increasing the efficiency of the algorithms is a task of future research. Another task is the comparison of the modified original HMM algorithms and the solution algorithms based on Proxels and phase-type distributions. We hope that in the future HnMM will present a practically applicable tool for analysts in various fields.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

ENERGY-BASED MODEL REDUCTION OF LINEAR SYSTEMS

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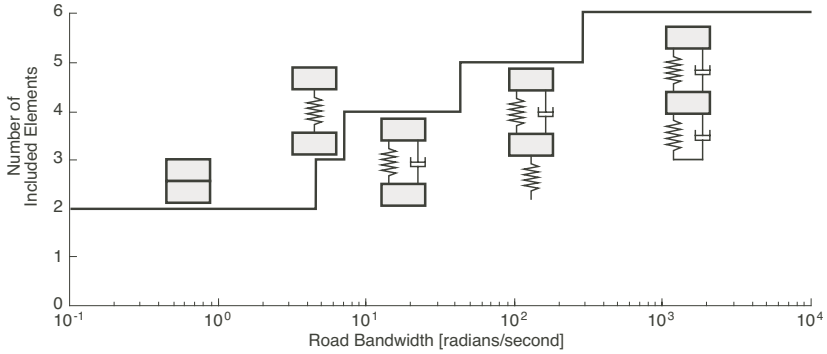
Summary: A previously developed concept, an energy-based modeling metric called activity, [1], is applied to linear systems to compare model complexity as a function of frequency. It is shown that when considering the sinusoidal steady state response, the derivation of analytical expressions for the activity as a function of the input frequency is possible. Furthermore, the activity due to a general system excitation (e.g., input with a given frequency content or bandwidth) can be computed based on the "steady state" activity and the Fourier expansion of the excitation. It is also shown that the activity varies with the frequency content of the excitation. Thus, a previously published algorithm, MORA, which is based on the activity metric, can generate a series of models. This series of models are shown to be ordered such that as the model complexity increases the model is accurate over a wider frequency range. These results are compared to those obtained using a previously published Model Order Deduction Algorithm (MODA). It is shown that MORA generates models of similar complexity to those generated by MODA for a given frequency range. Finally, in contrast to MODA, MORA is shown to account equally for the contributions of all the energy elements to the total system response. The results of this paper provide more insight into the nature of the reduced ordered models produced by MORA, and therefore, demonstrate that MORA is an even more useful tool than previously realized for the production of proper models of nonlinear systems. Furthermore, it appears to have some advantages over MODA for the creation of proper linear system models.

Activity Analysis of Linear Systems: The activity metric and MORA, as previously developed by the authors, are applicable to nonlinear systems. By restricting the use of MORA to linear systems, analytical expressions for the activity can be obtained. The analysis is simplified even more if, in addition to the linearity assumption, the system is assumed to have a single sinusoidal input, and only the steady state response is examined. These assumptions are motivated from Fourier analysis where an arbitrary function can by decomposed into a series of harmonics. Using this decomposition, the analysis is first carried out for a single input sinusoidal excitation under steady state conditions. Then, the effects of each harmonic are superposed, using the superposition principle, to get the aggregate response of the system caused by a general input. Furthermore, the superposition principle can also be used in the case where the system has more than one input. Therefore, the applicability of such approach to linear systems, with a generic input with frequency content within a given frequency range, is maintained even with the previous assumptions.

Results: A quarter car model is selected as the linear system to which we apply MORA and compare the results to those obtained from MODA applied to the same system. This model is chosen because it has been extensively used in the automotive literature and the frequency dependent properties of the system are well understood. At low bandwidth excitation only the rigid body model with the two masses are included in the reduced model. As the bandwidth increases the suspension stiffness must also be included. Just before the first natural frequency the suspension damping is also added to the reduced model as its activity increases above the specified elimination threshold. The tire stiffness is the next element included in the model before the second natural frequency. Eventually, at a bandwidth beyond the second natural frequency, MORA does not eliminate any energy elements. This is intuitive, because a rich input excites all system dynamics, and therefore, a model that includes all the dynamics of the system (full model) is needed to accurately predict the system behavior.



Quarter car reduced models

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PORT-HAMILTONIAN FORMULATION OF PHYSICAL SYSTEMS CONTAINING MEMRISTORS

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Motivation. In the early seventies, Chua [1] postulated the existence of a new basic electrical circuit element, called the memristor, defined by a nonlinear relationship between charge and flux-linkage. The memristor, a contraction of memory and resistance that refers to a resistor with memory, completes the family of the well-known existing fundamental circuit elements: the resistor, inductor, and capacitor. Although a variety of physical devices, including thermistors, discharge tubes, Josephson junctions, and even ionic systems like the Hodgkin-Huxley model of a neuron, were shown to exhibit memristive effects, a physical passive two-terminal memristive prototype could not be constructed until very recently scientists of Hewlett-Packard (HP) Laboratories announced its realization in Nature [2]. Strukov et al. show that memristance naturally arises in nanoscale systems when electronic and atomic transport are coupled under an external bias voltage.

Apart from HP's prototype memristor and its promising developments in the context of nonvolatile computer memory, the memristor concept has not yet played a significant role in modeling problems. This can most likely be explained by the fact that so far the majority of practical devices are reasonably well modeled by some (though often artificial) combination of standard modeling building blocks, like resistive, inductive, and capacitive elements, and their nonlinear and multiport versions. However, as nanoscale electronic devices become more and more important and complex, it might be beneficial, and on the longer term even necessary, to enlarge our repertoire of modeling building blocks that establishes a closer connection between the mathematics and the observed physics.

Contribution. In this paper, the port-Hamiltonian modeling framework [3] is extended to a class of physical systems containing memristive elements. First, the concept of memristance is generalized to the same generic level as the port-Hamiltonian framework. Secondly, the underlying Dirac structure is augmented with a memristive port. Since both an integration and a differentiation is involved in this process, a memristor, like a resistor, appears to be causally neutral. This leaves two possible choices to configure the memristive port. The inclusion of memristive elements in the port-Hamiltonian framework turns out to be almost as straightforward as the inclusion of resistive elements. However, although a memristor is a resistive element, it is also a dynamic element since the associated Ohmian laws are rather expressed in terms of differential equations. This means that the state space manifold, as naturally defined by the storage elements, is augmented by the states associated to the memristive elements. Hence the order of complexity is, in general, defined by the number of storage elements plus the number of memristors in the system. Some simple examples are provided to illustrate the theory.

One of the strong aspects of the port-Hamiltonian formalism is that a power-preserving interconnection between port-Hamiltonian systems results in another port-Hamiltonian system. Based on this principle, complex, multidomain systems can be modeled by interconnecting port-Hamiltonian descriptions of its subsystems. Moreover, several control design methodologies are available that can be directly applied to such port-Hamiltonian descriptions of complex nonlinear systems. It is precisely in this context that a memristive port-Hamiltonian description can be of added value.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MINIMAL PARAMETERIZATIONS IN DIAGNOSIS–ORIENTED MULTIVARIABLE IDENTIFICATION

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Introduction. A dynamical system is a mathematical entity that can be described by means of several families of models like state–space ones, transfer functions, polynomial models etc. Inside most families it is possible to consider equivalence relations that define partitions into equivalence classes so that every specific system can be described by any of the infinite models belonging to the associated class. The selection of specific models inside a class to solve analysis or synthesis problems is an established praxis in System Theory because it can lead to a reduction of the complexity of the involved procedures and/or to a better numerical robustness. In many applications any model inside an equivalence class can be used without drawbacks; only some of the models inside a specific class are however parameterized by the minimal number of scalars necessary to describe the associated system and, in all models with a non minimal parameterization, a variation in one parameter could be compensated by variations in other parameters without exiting from the class i.e. without introducing any variation in the behaviour of the associated system. This aspect is important when the models are identified from operating records and used for fault diagnosis by adopting fault detecting criteria based on the parameter values. In these applications it is important to make reference to models described by the minimal number of parameters in order that their variations can be interpreted only as variations of the underlying system [1].

Minimal parameterizations for dynamical systems. Denote a set with X and an equivalence relation defined on X with E. Then denote with S a second set and with $f : X \to S$ a function. If x' and x'' are two elements of X, and f is such that $x' \, E \, x''$ implies $f(x') = f(x'')$ then f is called an *invariant* for E. Moreover if $f(x') = f(x'')$ implies $x' \, E \, x''$ then f is called a *complete invariant* for E. A set of invariants $f_1, \ldots, f_n$, $f_i : X \to S_i$ for E is called a *complete set of invariants* for E if the function $f = (f_1, \ldots, f_n) : X \to S_1 \times \ldots \times S_n$ defined by $x \to (f_1(x), \ldots, f_n(x))$ is a complete invariant for E. A set of invariants for E, $f_1, \ldots, f_n$, $f_i : X \to S_i$ is called *independent* if the associated invariant $f = (f_1, \ldots, f_n) : X \to S_1 \times \ldots \times S_n$ is surjective. A set of invariants $f_1, \ldots, f_n$, $f_i : X \to S_i$ for E is called a *complete set of invariants* for E if the function $f = (f_1, \ldots, f_n) : X \to S_1 \times \ldots \times S_n$ defined by $x \to (f_1(x), \ldots, f_n(x))$ is a complete invariant for E [3].

Consider now the set S_o of polynomial input–output models $Q(z)\,y(t) = P(z)\,u(t)$ for multivariable systems where $Q(z)$ and $P(z)$ are polynomial matrices in the unitary advance operator z and $u(t)$, $y(t)$ denote the system input and output. Consider also the equivalence relation E defined by the premultiplication of $Q(z)$ and $P(z)$ by a square nonsingular unimodular matrix $M(z)$. Then the minimal number of parameters that can be used to describe the pair $(Q(z), P(z))$ coincides with the image of $(Q(z), P(z))$ in a complete set of independent invariants for E [2]

Parameter dispersion in identification. A Monte Carlo simulation of 100 runs has been performed for an order 4 ARX model with one input and two outputs whose minimal parameterization consisted in 11 scalars and has been repeated by using equivalent models described by 12 and 13 parameters. The cost function that has been considered to describe the dispersion of the identified parameters is given by the ratio between the standard deviation and the mean value of their estimates.

minimally parameterized model	0.38	0.15	0.075	0.58	–	–	0.19	2.56	0.070
model with one extra parameter	0.39	0.16	0.075	0.91	141.28	–	0.27	2.51	0.069
model with two extra parameters	0.40	0.18	0.077	0.91	93.08	98.52	0.27	3.49	0.069

Table 1: Ratio between the standard deviation and the mean value of the estimated parameters (first subsystem)

Table 1 reports the value assumed by the cost function for the parameters of the first subsystem (the considered model consists in two interconnected subsystems). It can be observed that the dispersion of the estimates for a minimally parameterized system is modest (maximal value of the cost function equal to 2.56). In the second simulation, where the model contains only one extra parameter, the cost function jumps to a maximal value of 141.28 while in the third simulation (two extra parameters) we observe two peaks with values of 98.52 and 93.08. In all cases the use of non minimal parameterizations has had very adverse effects on the dispersion of the estimates.

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EVALUATION OF LYAPUNOV EXPONENT IN GENERALIZED LINEAR DYNAMICAL MODELS OF QUEUEING NETWORKS

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The evolution of actual systems encountered in economics, management, engineering, and other areas can frequently be represented through stochastic dynamic models of the form

$$\boldsymbol{x}(k) = A(k)\boldsymbol{x}(k-1),$$

where $A(k)$ is a random state transition matrix, $\boldsymbol{x}(k)$ is a state vector, and matrix-vector multiplication is thought of as defined in terms of a semiring with the operations of taking maximum and addition [2, 3].

In many cases, the analysis of a system involves evaluation of asymptotic growth rate of the system state vector $\boldsymbol{x}(k)$, which is normally referred to as Lyapunov exponent. In the semiring with the operations of maximum and addition, the mean growth rate is defined in terms of the semiring as

$$\lambda = \lim_{k\to\infty} \|\boldsymbol{x}(k)\|^{1/k}.$$

Note that for queueing networks, the value of λ can be considered as the mean service cycle time in a system, while its inverse can be thought of as system throughput.

Existence conditions for the above limit can normally be established based on the ergodic theorem in [7]. Specifically, examples of the conditions can be found in [1, 2]). Note however, that these conditions frequently require that the system state transition matrix is of particular form or type (matrix with finite entries, irreducible matrix).

For stochastic systems with random state transition matrices, evaluation of λ normally appears to be a difficult problem. Existing results (see e.g., [2, 6]) include the exact solution to the problem for second-order systems determined by matrices with entries that are independent and have either normal or exponential probability distributions. It is shown in [4, 5] how the value of λ can be found for systems with particular matrices of arbitrary size, including triangular matrices, similarity matrices, and matrices of rank 1.

In the current paper we consider the problem of evaluation of Lyapunov exponent, which arises in the analysis of a wide class of queueing networks. We consider a general model of stochastic dynamical system governed by the vector equation with the random matrices $A(k)$ which are assumed to be independent and identically distributed for all $k = 1,2,\ldots$New general conditions for the limit that determines the Lyapunov exponent λ to exist are given which involve the spectral radius of the mean state transition matrix.

We present results of evaluating λ for systems with matrices of particular types, including diagonal and triangular matrices, similarity matrices, and matrices of rank 1. A new approach to evaluation of λ is then proposed based on a decomposition of $A(k)$. The approach allows one to reduce the problem with the original matrix $A(k)$ to that with a matrix of particular type and known solution.

Furthermore, we discuss application of the above results to the analysis of a general class of queueing systems. Some particular systems including open and closed tandem queues with finite and infinite buffers, a fork-join network, and a system with round-robin routing are examined. For these queueing systems, we show how to obtain the mean service cycle time through evaluation of Lyapunov exponent in their associated dynamical systems. Related results are given in the form of some functions of the mean values of random variables that determine the service time in the system.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

SPACE-ADAPTIVE REDUCED BASIS SIMULATION FOR TIME-DEPENDENT PROBLEMS

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We address the task of model reduction for *parametrized* evolution equations. These are problems which are characterized by a parameter vector $\mu \in \mathscr{P}$ from some set of possible parameters $\mathscr{P} \subset \mathbb{R}^p$, and the evolution problem is to determine $u(t,\mu) \in L^2(\Omega)$ on an open bounded domain $\Omega \subset \mathbb{R}^d$ and finite time interval $t \in [0,T], T > 0$ such that $\partial_t u(\mu) + \mathscr{L}(t,\mu)(u(t,\mu)) = 0$ and suitable initial and boundary conditions are satisfied. Here $\mathscr{L}(t,\mu)$ is the parameter dependent spatial differential operator. Discretization with finite element or finite volume schemes and first order time discretization, yields discrete solutions $u_H^k(\mu) \in \mathscr{W}_H, k = 0,\ldots,K$ in the H-dimensional discrete space $\mathscr{W}_H \subset L^2(\Omega)$ approximating $u(t^k,\mu)$ at the time instants $0 = t^0 < t^1 < \ldots < t^K = T$. Detailed simulations are frequently expensive to compute due to the space resolution and not suitable for use in multi-query settings, i.e. multiple simulation requests with varying parameters μ.

Reduced Basis Methods are increasingly popular methods to solve such parametrized problems, aiming at a problem-dependent simulation scheme, that approximates the detailed solutions $u_H^k(\mu)$ by efficiently computed reduced solutions $u_N^k \in \mathscr{W}_N$. Here $\mathscr{W}_N \subset L^2(\Omega)$ is an N-dimensional *reduced basis space* with suitable *reduced basis* $\Phi_N = \{\varphi_i\}_{i=1}^N$ which is generated in a problem specific way based on *snapshots* of detailed solutions for suitably chosen time instants k_i and parameters $\mu_i \in \mathscr{P}$, i.e. $\Phi_N \subset \text{span}\{u_H^{k_i}(\mu_i)\}$. A reduced basis Φ_N is hierarchical in the sense, that for $1 \leq N' \leq N$ the bases $\Phi_{N'} := \{\varphi_i\}_{i=1}^{N'} \subset \Phi_N$ span N'-dimensional reduced spaces $\mathscr{W}_{N'} := \text{span}(\Phi_{N'})$ which are nested by $\mathscr{W}_1 \subset \mathscr{W}_2 \subset \ldots \subset \mathscr{W}_{N-1} \subset \mathscr{W}_N$. An important focus of RB-methods is a posteriori error estimation of the model error $\left\|u_N^k(\mu) - u_H^k(\mu)\right\| \leq \Delta^k(\mu)$ in suitable norms $\|\cdot\|$. The estimators $\Delta^k(\mu)$ can be rapidly computed during the reduced simulation and are rigorous and sharp upper bounds of the true error. The currently existing RB-methods for time-dependent problems, e.g. [1, 2], use identical dimensionality $N^k := N$ for all timesteps k. This may be suboptimal, as different solution structures may require different dimensionalities N^k at different times. Given a certain desired error threshold $\varepsilon > 0$, a too large N will result in an unnecessarily good simulation result with unnecesarily large simulation time. On the contrary, a too small N may result in an intolerable error estimator value and require refined simulation. Hence it may be favourable in time-dependent simulations, to choose the model depth N^k during the reduced simulation.

In the current presentation, we extend the RB-scheme of [2], in order to adaptively choose N^k. For the N-adaptive approach, a heuristic rule for adjusting N^k must be defined. A simple strategy is to aim at a certain target for the a posteriori error estimator, e.g. linear development in time, and define suitable increases and decreases in model dimension depending on the deviation of the current estimator from the target curve. We provide experimental insights based on two advection-diffusion problems. Qualitative results of the corresponding N-adaptive RB simulation are depicted in Fig. 1. The trial and error process of choosing a correct value of N can obviously be prevented with N-adaptivity. The error estimator is steered in such a way, that it approximately reaches the desired prescribed tolerance level at end time. We show, that the N-adaptive approach may be particularly useful for examples with time-variant data functions, implicit discretization components and solution structure variety in time.

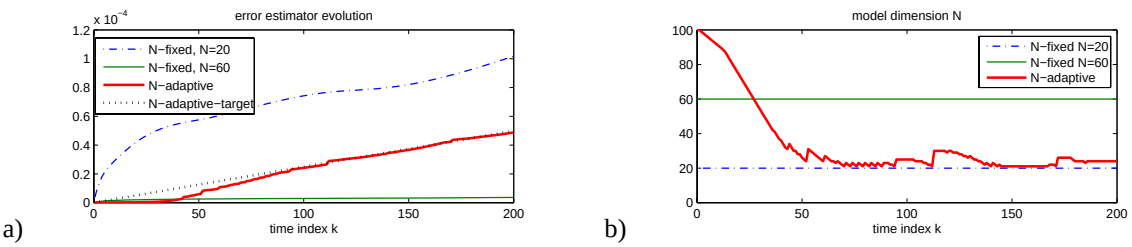

Figure 1: N-fixed and N-adaptive RB Simulation results over time. a) Error estimator development, b) model order N.

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SOME PARAXIAL APPROXIMATIONS OF VLASOV-MAXWELL EQUATIONS

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Introduction. Quite complete mathematical models to solve charged particle problems are based on the time-dependent Vlasov-Maxwell system of equations, sometimes under the relativistic assumption. Indeed, the Maxwell equations are related to electric charged particles, the motion of which being a source for generating an electromagnetic field. Conversely, for a population of charged particles with a mass m and a charge q, the main force field is the electromagnetic Lorentz force

$$\mathbf{F} = q\,(\mathscr{E}(\mathbf{x},t) + \mathbf{v}(t) \times \mathscr{B}(\mathbf{x},t))\,, \tag{1}$$

that describes how the electromagnetic field $\mathscr{E}(\mathbf{x},t)$ and $\mathscr{B}(\mathbf{x},t)$ acts on a particle with a velocity $\mathbf{v}(t)$. In the Vlasov model, one considers a population of charged particles, submitted to a given force field $\mathbf{F}(\mathbf{x},\mathbf{v},t)$ given by (1). Each particle is characterized by its position $\mathbf{x}$ and its velocity $\mathbf{v}$ in the so-called phase space $(\mathbf{x},\mathbf{v})$. Then the distribution function $f(\mathbf{x},\mathbf{v},t)$ is solution to the following transport equation, named the Vlasov equation

$$\frac{d}{dt} f(\mathbf{x}(t),\mathbf{v}(t),t) = \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \frac{q}{m}(\mathscr{E}(\mathbf{x},t) + \mathbf{v} \times \mathscr{B}(\mathbf{x},t)) \cdot \nabla_{\mathbf{v}} f = 0\,. \tag{2}$$

In this paper, our aim is to take into account the particularities of the physical problems to derive some approximate models leading to faster and cheaper computations.

Approximate Models From a numerical point of view, the Vlasov-Maxwell system is a very complete model but it also leads to very expensive computations, in particular in a three-dimensional domain. Evenhougth this is necessary in several cases (see [1], [2]), one easy understands the need of deriving simpler (but accurate) models, by exploiting given physical assumptions. Let us give an example: the relativistic paraxial model, that exploits the paraxial property, i.e the property that the particles of the beam remain close to an optical axis.

Consider a particle beam that is highly relativistic i.e., satisfies $\gamma >> 1$. Since the velocity is close to light velocity c for any particle in the beam, it is convenient to rewrite the Vlasov-Maxwell equations in the beam frame, i.e. in a frame which moves along the z-axis with the velocity c. According to [3], it is worthwhile to distinguish the transverse quantities from the longitudinal ones. Now, to derive a paraxial model, the first step is to introduce a scaling of the equations. Assuming that the dimensions of the beam are small compared to the longitudinal length of the device, and that the longitudinal particle velocities v_z are close to the light velocity c, whereas the transverse particle velocities $\mathbf{v}_\perp$ are small compared to c, we can introduce a small parameter η and rewrite the Vlasov-Maxwell system of equations in the beam frame using dimensionless variables It remains now to develop asymptotic expansions of all the quantities $(f,\rho,\mathscr{J},\mathscr{E},\mathscr{B},...)$ in powers of the small parameter η, and to retain the first four terms (in that case) of this asymptotic expansion to obtain a new mathematical model. An important theoretical result was to prove that such a model is accurate up to fourth order. As expected, this leads to far cheaper computations than the full Vlasov-Maxwell model.

Another approximate model can similarly be derived. By retaining only the zero-order terms of the relativistic paraxial model, one can prove that one thus obtains a Poisson-like model, also written in the beam frame. This remark motivates numerical comparisons between these two approximate models. Writting the axisymmetric Poisson equation in the beam frame (r,ζ), we obtain

$$\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r}\frac{\partial \phi}{\partial r} + \frac{\partial^2 \phi}{\partial \zeta^2} = \frac{1}{\varepsilon_0}\rho\,, \qquad \mathscr{E} = (\frac{\partial \phi}{\partial r}, \frac{\partial \phi}{\partial \zeta})\,. \tag{3}$$

Then, one can derive numerical schemes for Vlasov-Poisson equation by straightforward finite differences approximation. In the full paper, numerical results will be detailed and discussed.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELING AND SIMULATION USING THE COMPOSITIONAL INTERCHANGE FORMAT FOR HYBRID SYSTEMS

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One of the major challenges towards a broad industrial acceptance of hybrid systems techniques and tools is the large number of modeling formalisms and the resulting manual effort for the tool-based solution of many complex design or analysis tasks. A promising approach to achieve inter-operability between hybrid systems tools is to develop translations of their formalisms via a general and sufficiently rich interchange format. This paper gives an intuitive introduction to such a formalism, the *Compositional Interchange Format* (CIF) [1], that was recently developed within the European Network of Excellence HYCON.

The CIF has been developed with two major purposes in mind - to provide a generic modeling formalism with formal semantics (and appropriate tools) for a wide range of general hybrid systems, and to establish interoperability of a wide range of tools by means of model transformations. In this way, the implementation of many bilateral translators between specific formalisms can be avoided. The latter idea is employed in the new European research project MULTIFORM (http://www.ict-multiform.eu) whose main objective is the integration and the support for interoperability of tools and methods based on different modeling formalisms in order to make a significant step towards integrated coherent tool support for the design of large complex controlled systems from the first concept to the implementation and further on over their entire life cycle. Within MULTIFORM, algorithms and tools for the translation to/from the CIF will be defined for a large variety of modeling languages, including CHI, GPROMS, MATLAB/SIMULINK, MODELICA, MUSCOD-II, PHAVER, and UPPAAL. Using these (and future) translations, we expect that the CIF will help to significantly increase the applicability of hybrid systems techniques in industrial practice.

A CIF model can be specified in two different formats: 1) the *abstract* format that formally defines the syntax and semantics of a CIF model in terms of an interchange automaton in a mathematically sound way and thus enables correctness proofs of translations to/from other formalisms, and 2) the *concrete* format that provides a user-friendly syntax that adds the concepts of hierarchy and reusability, improves the readability of CIF models, and thus facilitates the manual modeling process. The semantics of the concrete format is defined by means of a mapping to the abstract format.

The CIF language contains, among others, modeling primitives for the specification of:

- Different classes of variables (discrete, continuous, and algebraic).
- Continuous dynamics that are specified as fully implicit DAEs.
- Steady-state initialization.
- Different kinds of urgency (urgency allows/restricts the passing of time up to a certain point), including many urgency concepts found in literature.
- Interaction between parallel processes using different mechanisms.
- Structural information, such as classification of variables as input, output, and/or internal and external.
- Process re-use (automaton definition/instantiation) and hierarchy.

In this paper, the CIF tool set is introduced that enables visualization and simulation of CIF models. The tool set is implemented in PYTHON. The CIF simulator supports both, numerical simulation (using DASSL) and symbolic simulation (using MAPLE), and the CIF visualizer is based on the open visualization toolkit GRAPHVIZ.

In addition, the capabilities of the simulator as well as the large expressiveness and the ease of use of the concrete CIF format are illustrated with a complex case study, the hybrid model of a supermarket refrigeration system under logic control [2]. This system exhibits nonlinear DAE dynamics as well as significant discrete dynamics and serves as a challenging case study for hybrid control techniques in several European research projects.

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CPL CLUSTERING BASED ON LINEAR DEPENDENCIES

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A method of discovering a variety of linear dependencies in data sets is presented in the paper as a tool for data mining (exploratory analysis) [1]. The proposed method is based on the minimization of a special type of convex and piecewise linear (*CPL*) criterion functions defined on a given data set C [2]. The basis exchange algorithms, which are similar to linear programming, allow one to find the minimum of these *CPL* function efficiently, even in the case of large multidimensional data sets [3]. The division of the set C into a family of linearly dependent clusters C_k allows to form a family of local regression type models. In result, each subset C_k can be characterized C_k by its own linear model.

The *K-plans* algorithm which is similar to the *K-means* algorithm can be used for the purpose of the dividing the set C into a family of linearly dependent clusters C_k. The central points m_k are identified for each subset C_k during the *K-means* procedure [4]. On the other hand, the minimization of the *CPL* criterion function during the *K-plans* procedure allows to identify the central hyperplane $H(w_k,\theta_k)$ for each subset C_k. The central hyperplane $H(w_k,\theta_k)$ defines the local dependency characteristic for a given subset C_k.

The proposed approach can be used for solving a variety of problems of data mining. One of them is discovering linearly dependent patterns in data sets and analysing them in this manner. Feature selection or separable data aggregation can be also carried out in this way.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

EXP-FUNCTION METHOD FOR KHOKHLOV-ZABOLOTSKAYA-KUZNETSOV (KZK) EQUATION

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Introduction. The Exp-function method is used to obtain exact solution for some nonlinear evolution equations arising in mathematical physics using symbolic computation. The KZK (Khokhlov-Zaholotskaya-Kuznetsov) equation is chosen to illustrate the effectiveness and convenience of the method.

Many new approaches have been proposed to introduce analytical solutions to nonlinear evolution equations. Many new approaches with advantages on the one hand and disadvantages on the other hand have been suggested to solve various nonlinear equations, such as the variational iteration method, the homotopy perturbation method, the tanh-method, the sinh-method, the homogeneous balance method, the F-expansion method, the extended Fan's sub-equation method [1].

The Exp-function method introduced by J.H. He has been developed to find solitary solutions, compact-like solutions and periodic solutions for nonlinear evolution equations in mathematical physics [2]. In this study, we focus on KZK equation. There are some numerical methods for solving KZK equation that nearly all of them are based on finite difference method [3]. To date, no explicit analytical solutions exist for the KZK equation.

When an acoustic source of finite size radiates into free space, the effects of diffraction must be considered. The KZK nonlinear parabolic wave equation is known to describe accurately the propagation of a finite amplitude sound beam by including, to the lowest order, the combined effects of diffraction, absorption, and nonlinearity; in addition, it models the propagation of plane wave finite amplitude sound beam.

In the derivation of the KZK equation, the sound waves are assumed to form a directive beam that permits a parabolic approximation to be made in the terms which account for diffraction. The parabolic approximation introduces errors at field points that are far away from the acoustical axis, and at near field (e.g. locations close to the source). However, these restrictions are relatively weak in practice, and the main regions of interest in a directive beam are accurately modelled by the KZK equation.

The behaviour of Burgers equation solution represents shock waves in propagation of mechanical waves; the KZK equation is somehow more general than Burgers equation and in fact it is a perturbation of Burgers equation and hence the diffraction effect is modelled in it. In previous studies some solutions are prepared for Burgers equation, but no analytical solution is proposed for KZK. Therefore, we discuss solutions of KZK equation with definite boundary conditions by Exp-function in this letter.

Keywords: Exp-function, nonlinear acoustic, KZK equation, boundary conditions, diffraction, absorption

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Proceedings
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Mechatronics – Applications, Modelling, Tools

AN AUTOMATIC MODELLING APPROACH TO MOBILE ROBOTS

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Introduction. Both mechanical and mathematical models of a robot, whatever is its configuration or application, are the most significant steps on a robot design to fulfil. The mechanical model is normally used to present the visualization of the robot, to define the direction of the movements as well to provide the mechanical plans for the components construction. The mathematical model composed by kinematics and dynamics equations is the base to simulation, to determine trajectories, angles and necessary torques for certain movements.
This paper presents a straightforward procedure to model and simulate mobile robots. Starting from the design of each robot part or component and adding all its mechanical characteristics and material properties it is possible to obtain the CAD assembly model. Since the CAD assembly is ready a XML file can be generated. The XML file (physical model) contains all relevant parameters necessary to create the Simulink blocks, such as mass, inertia matrix, coordinates of center of mass, etc of each link. At this time, this physical model can be imported into a SimMechanics model in Simulink environment. The Simulink model obtained can be used to determine the necessary torques to produce a given movement. With the torques values the actuators can thus be chosen. A four legged tree climbing robot example is used to illustrate the procedure. Obviously the same approach could be used to model any robotic manipulators.

Kamanbaré Platform. Legged robots were demonstrated to be the ideal option for many applications where the working environment is difficult to access or even dangerous or risky for human beings, such as exposure to hazardous substances or environments and risk conditions. Productivity increase and quality issues are also extremely relevant and are considered [1].
Besides the varied applications and areas, there still remains a little explored area: environmental research. As in any other area, different applications or problems can be addressed or solved with the help of a robotic platform.
Purporting the main goal to climb trees for environmental research applications, to be applied in tasks such as presented above, a bio-inspired robotic platform named Kamanbaré was proposed [2]. The project's main application is climbing trees for non-invasive search purposes, reaching points (at high altitudes) that may offer risk to humans. However, together with the larger mobility offered by legged robots, a more complex modelling emerges depending on the robot structure and configuration. This complexity depends on if the robot has identical or different legs, a rigid or flexible body, number of legs and the corresponding DOF (degrees of freedom) for each one.
In this way, the modelling task can be arduous, take a lot of time and the most relevant factor to be considered is that this assignment is critical since it is susceptible to insert errors to the final model.

Simulink Models. A method that can be used in order to minimize possible errors is an automatic robot modelling using CAD software translation together with MatLab SimMechanics. Simulink and SimMechanics software use a block diagram approach to model control systems around mechanical devices and simulate their dynamics. With CAD translation, it is possible to combine the power of CAD and SimMechanics software. The translator transforms geometric CAD assemblies into Simulink blocks using a so called CAD-to-SimMechanics translator.
The translation process is based on two major steps: i.) to export the CAD assembly into a physical modeling XML format file and ii.) to import the generated XML file into a SimMechanics model in Simulink environment.
The XML files contains all relevant parameters necessary to create the Simulink blocks, such as mass, inertia matrix, coordinates of center of mass, etc of each link.
The CAD model of the Kamanbaré robotic platform was designed using Solidworks CAD software. Thus a Kamanbaré model was generated using the SolidWorks-to-SimMechanics translator.
The resultant models obtained for the Kamanbaré platform is presented in this work.

Simulation Results. For the simulation process a simplest mode of movement generation, or gait, was initially implemented, i.e., the robot follows a straight path at the highest speed allowed by the surface.
The proposed realistic and practical SimMechanics model is further employed to simulate the designed controller which is implemented using Simulink, in this case just a gait generator.
The mode of movement (gait) generation contains information corresponding to the body movement and the foot trajectories, as well as the joint angles of the legs. Using these inputs and running simulations in an inverse dynamics option in Simulink, all the necessary joint torques to produce a simple desired movement for each joint of all legs were obtained and presented.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

OPTIMIZATION BASED MEAN VALUE MODEL OF TURBOCHARGED DIESEL ENGINES

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Abstract

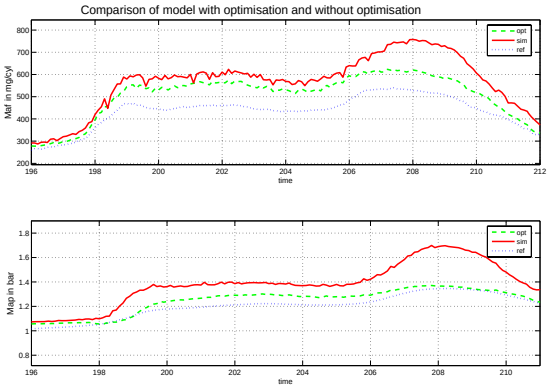
While engine control is still widely based on heuristic approaches and maps, there is a wide consensus that model based control is an indispensable component to meet the coming challenges and exploit at best the increasing number of degrees of freedom offered by modern and coming engines.

Unfortunately, model based control requires models, whose determination is not a trivial task and usually the most demanding step in the control system development. Indeed, a good physical insight in engine dynamics and combustion properties allows deriving the main physical relationships between different components of the system, but the resulting models tend not to be sufficiently precise to enforce an optimal or almost optimal behavior of the engine as many "small" extremely hard to model effects - like friction nonlinearities, thermal properties etc. are critical for the precise behavior prediction. This is the main practical reason for the classical approach consisting in measuring almost all operating conditions and tuning the feedforward – basically the inverse inverse – to enforce optimal operation.

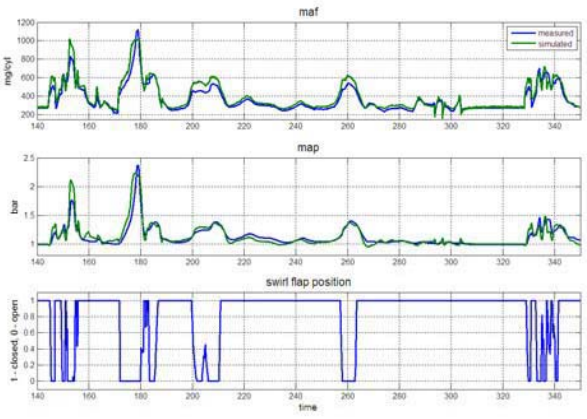
Identification would be a suitable alternative, but unfortunately identification can be used efficiently only for few model classes, especially for linear ones, who do not easily capture the system behavior to the desired precision.

Against this background this paper proposes a mixed approach. The model structure is determined by physical understanding, the complexity of each block corresponding to its relevance for dynamical measurements and not to the physical complexity. The use of producer information is kept as limited as possible, and the parameters of each component are determined from standard overall measurements and optimization routines and not by component specific measurements, in such a way that a tracking of parameter changes during normal operation and wear could be possible along the same way. An important consequence of this is that the parameters eventually include also the non-modeled nonlinearities and special effects responsible to a large extent for the model precision.

The device under test for the mean value engine model (MVE-Model) was a BMW M47TÜ-OL Diesel engine with an external exhaust gas recirculation and variable geometry turbine turbocharger.



Effect of the I/O parameter optimization



Overall model performance during swirl valve operation

COUPLED MODELS OF COMBINED DRY FRICTION BASED ON PADE EXPANSIONS

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Introduction. There are a large number of studies devoted to dry friction. At the most of these publications authors are using the Coulomb model of dry friction supposed that the friction force at the point of contact is direct opposite the relative velocities of sliding and it is not depend on the module of velocity. However, there are many experimental facts about the violation of this law at case when the rubbed bodies are participated simultaneously in the translational, whirling and rolling motions.

Coupled models of the sliding, whirling and rolling friction for circle areas of contact. In correspondence with [1], the main influence of the rolling on the force state in the area of contact consists in the asymmetry of the diagram of the distribution of the normal contact stresses. At the proposed models, this asymmetry is described by the linear function with one dimensionless coefficient $k_r, |k_r| \le 1$ that defined by the direction and value of the rolling velocity Ω_r: $\tilde{\sigma} = \sigma(1 + k_r (x\Omega_y - y\Omega_x)/(R\Omega_r)), \Omega_y = \Omega_r \cos\beta, \Omega_x = \Omega_r \sin\beta$, where σ - symmetric distribution of normal contact stresses at absence of rolling in the rectangular coordinate system $\{xOy\}$, axis x of which is directed alone the velocity of sliding v, R - radius of contact circle. Integration of the differentials of the net force and torque on the spot of contact, at the supposition that Coulomb's friction law is valid in the local form for the differential of the tangential forces of friction on any area element inside the contact domain, yields the exact integral model of the combined dry friction. This model shows that asymmetry at distribution of the normal contact stresses at the case of circle areas of contact cause the appearance of the component of the friction force directed on normal to the trajectory of motion and, consequently, the net vector of friction forces is not opposite directed to the vector of sliding velocity. In addition, this asymmetry leads to shift of the gravity center of contact circle respectively the geometric centre in the direction of whirling and to appearance of torque of rolling parallelly directed to the plane of sliding [2]. However, integral model is inconvenient for application to the problems of dynamics because it requires calculating multiple integrals in the right-hand sides of the equations of motion. In order to avoid this difficulty, it is possible to replace the exact integral expressions by the corresponding Pade expansions. The simplest is the fractional linear approximations (model of the first order) [2]:

$$F_{\parallel} = \frac{F_0 v + k_r F_r u \Omega_x/\Omega_r}{v + au} \equiv \frac{F_0 v + k_r F_r u \sin\beta}{v + au}, F_{\perp} = \frac{k_r F u}{u + bu} \frac{\Omega_y}{\Omega_r} = \frac{k_r F_r u \cos\beta}{u + bv}, F_0 = F_{\parallel}\big|_{u=0}, F_r = F_{\parallel}\big|_{v=0}, M_0 = M_C\big|_{v=0}, M_{ur} = M_C\big|_{u=0}$$

$$M_C = \frac{M_0 u + k_r M_{ur} v \Omega_x/\Omega_r}{u + mv} \equiv \frac{M_0 u + k_r M_{ur} v \sin\beta}{u + mv}, \frac{1}{m} = \frac{v}{M_0} \frac{\partial M_C}{\partial u}\bigg|_{u=0}, \frac{1}{a} = \frac{u}{F_0} \frac{\partial F_{\parallel}}{\partial v}\bigg|_{v=0}, \frac{1}{b} = \frac{v}{k_r F_r} \frac{\partial F_{\perp}}{\partial u}\bigg|_{u=0}$$

where $F_{\parallel}$ and $F_{\perp}$ are the modules of the net vector components which are directed, correspondingly, on the tangent and normal to the trajectory of motion, M_C - the torque of whirling, $u \equiv \omega R$ - velocity of whirling.

The model of the first order is sufficient for the dynamics investigation, but for more precise qualitative analysis the model of the second order is required. This model not only good approximates the exact integral models but conserves all their properties such as behavior of these functions and their first derivatives at zero and infinity.

$$F_{\parallel} = \frac{F_0 (v^2 + auv)}{v^2 + auv + u^2} + \frac{k_r F_r u^2}{u^2 + v^2} \frac{\Omega_x}{\Omega_r} \equiv \frac{F_0 (v^2 + auv)}{v^2 + auv + u^2} + \frac{k_r F_r u^2 \sin\beta}{u^2 + v^2}, \; F_{\perp} = \frac{k_r F_r (u^2 + buv)}{v^2 + buv + u^2} \frac{\Omega_y}{\Omega_r} \equiv \frac{k_r F_r (u^2 + buv) \cos\beta}{v^2 + buv + u^2}$$

$$M_C = \frac{M_0 (u^2 + muv)}{v^2 + muv + u^2} + \frac{k_r M_{ur} v^2}{u^2 + v^2} \frac{\Omega_x}{\Omega_r} = \frac{M_0 (u^2 + muv)}{u^2 + muv + v^2} + \frac{k_r M_{ur} v^2 \sin\beta}{u^2 + v^2}, a = \frac{u}{F_0} \frac{\partial F_{\parallel}}{\partial v}\bigg|_{v=0}, m = \frac{v}{M_0} \frac{\partial M_C}{\partial u}\bigg|_{u=0}, b = \frac{v}{k_r F_r} \frac{\partial F_{\perp}}{\partial u}\bigg|_{u=0}$$

Models of the first and second order can be considered as reological models, because there is no required in solving of real problems to calculate the double integrals, defined the coefficients of Pade approximations. These coefficients can be defined from the experiments. The main advantage of coupled models of combined dry friction based on Pade expansions is obviating a necessity to solve the problem of the theory of elasticity and exactly define the boundaries of area of contact.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

BOND GRAPH SIZING OF MECHATRONIC SYSTEMS: COUPLING OF INVERSE MODELLING WITH DYNAMIC OPTIMIZATION

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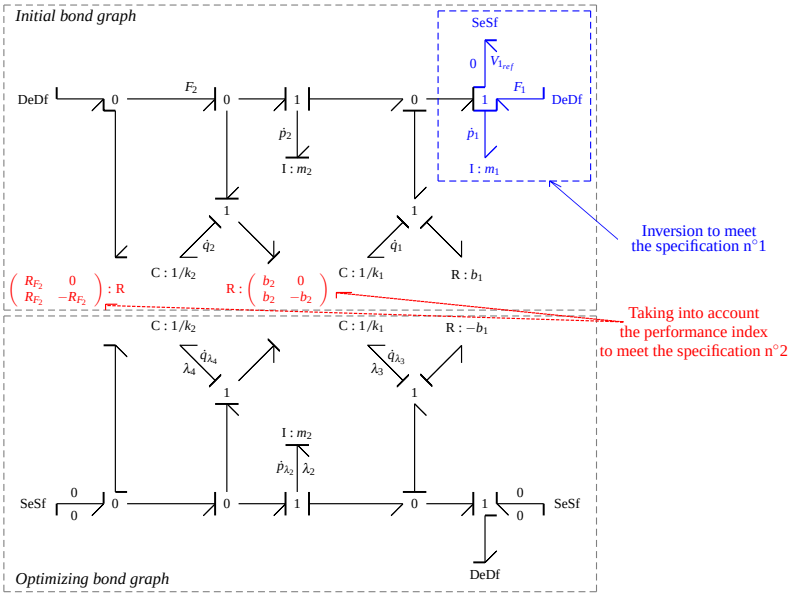
Introduction. For the last 15 years, a methodology has been developed for sizing mechatronic systems. Based on the use of inverse models described by bond graph, it has in particular the advantage of drastically decreasing the number of calculus iterations, compared to the trial and error procedure of the classical direct approach. The aim of this article is to extend this sizing methodology to the case where only a part of the specifications can be translated in terms of functions of time (and so where only a part of the model can be inverted) and where the other part can be formulated as an optimal control problem.

Bond graph formulation of dynamic optimization. In order to handle design constraints formulated as an optimization problem, recent articles developed an optimization procedure which leads to graphically construct what it is called an *optimizing* bond graph, and to couple it with the *initial bond graph* model of the system under study. The resulting *augmented bond graph* then mirrors a system of equations, identical to the *optimality conditions* given by the Pontryagin Maximum Principle. The first advantage of this optimization procedure lies in the fact that the *optimality conditions* are obtained in a systematical and graphical manner contrary to the Pontryagin Maximum Principle which requires analytical developments.



Augmented bond graph model coupling both inversion and optimization.

Coupling of inverse modelling with dynamic optimization. Up to now this optimization procedure was considered only for direct models. To initiate the coupling between inverse modelling and dynamic optimization, this article focuses on the example of two masses in series, joined by springs and dampers in parallel. Then it is supposed that the sizing problem is to find the two inputs so that: the speed of the first mass follows a given trajectory (specification n°1) and the dissipative energy due to the second damper is minimized (specification n°2). To meet specification n°1, the bond graph model of the example is partially inverted. Then specification n°2 is met by adapting the optimization procedure to the remaining dynamic part of the inverse model thus obtained. As a consequence, not only the *optimality conditions* resulting from the corresponding *augmented bond graph* are identical to those obtained by analytical developments but some numerical results are also given to prove the feasibility of such an approach.

Conclusion. Coupling the sizing methodology to the optimization procedure has the advantages of the two approaches by limiting their drawbacks. In fact the optimization procedure enables the handling of design constraints not expressed as functions of time, while the inversion gives a stronger constraint in term of trajectory tracking. It then enables to size mechatronic systems with specifications of a heterogeneous kind. The full version of the article compares the two possible manners of treating such a coupling (inverting then optimizing or optimizing then inverting). It also shows how this can be useful for writing the specifications.

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OBJECT-ORIENTED MODELING OF ELECTROMECHANICAL SYSTEMS WITH SWITCH CIRCUITS BY USING TRANSMISSION ELEMENTS

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Modern drive systems, e.g. the hydromechanical or electromechanical, are generally composed of components from different physical domains. Using the signal-oriented approach to model such systems usually results in a huge amount of effort to derive the explicit form of the equations. Beyond this drawback, models of the signal-oriented approach are lack of hierarchical structures, and hardly reusable. The object-oriented modeling of physical systems, first introduced by Elmqvist [2], can be used to overcome such difficulties. In recent years, this paradigm in the form of the *Modelica* language has gained more and more significance in the industrial application. But its acausal declarative nature makes the simulation performance particularly dependent on the stable and powerful *Modelica* language compiler and its preprocess optimization, which are, at least right now, not as easy to be accessible as a C++ one for the developers of simulation programs.

The object-oriented modeling via transmission elements may offer the same features of most importance that the physical modeling paradigm should offer. However, it provides a method to generalize the equations of complex physical systems in a numerical, consecutive manner. This approach was primarily used for modeling the kinematics and dynamics of multi-body systems by Kecskeméthy, see e.g. [3]. In this paper, it is applied to model electrical and electric systems, and implemented in the simulation software named *D&C Engine*. The application example is a permanent-magnet-synchronous-motor drive system [4].

The switching power converters are frequently applied in the modern electric drive systems. They are used to control the electrical motors. Simulation of such converters is problematic for several reasons. They are operated by the frequent switching up to several Megahertz. In contrast, some of the time constants, at least for the mechanical parts, are more orders of magnitude larger than the switching period. This property makes the equation system potentially stiff. On the other hand, each switching event, in an ideal sense, is a discontinuity. Typical power converter simulations can run for hundreds or thousands switching cycles, which may lead to problems for the simulation software that does not have the explicit mechanism for handling these discontinuities. Problems are for example long simulation time, lack of convergence, and convergence to an erroneous solution. Here the implicit integration with an event-handling algorithm [1] is applied to deal with the discontinuities and the potentially stiff equation systems.

In many simulation tools, the switch is non-ideally modeled by a variable resistor, in which the resistance is assumed to be a small value at switch-on and a large value at switch-off. This could introduce the artificial stiffness to equation systems and may lead to inaccurate results. In most cases of simulating complex electric drive systems, the dynamics of circuits during switching is of little interest. Hence, the switch operation can be regarded as instantaneous, and the switch itself can be treated as ideal and controlled by discrete states, such as the variables of the enumeration type ON and OFF. The ideal switch model in the object-oriented fashion, however, involves the change of the modeling causality and leads to variable structure systems in simulation. The complete power converter applied in the drive system is developed as a whole object of transmission elements. Thus, it is, on the level of the individual ideal diode, still structure variable system, but not on the level of the complete power converter.

The performancewise advantages, in terms of the computational time and accuracy, are presented in the attached benchmark simulation of the PMSM drive system. As a result, the object-oriented modeling via transmission elements provides a modular, easy-to-use scenario for the system development in the electric drive engineering, in which component developers may develop and test their component's models, system designers may then just use these as building blocks per drag and drop in *D&C Engine*'s GUI without detailed knowledge of the components. Along with the models for the power converters and the event-handling algorithm, the stable, efficient and numerically accurate simulation for such systems can be achieved.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

DEVELOPMENT OF A MULTI-RATE SIMULATION MODEL OF AN UNMANNED UNDERWATER VEHICLE FOR REAL-TIME APPLICATIONS

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Introduction. A propulsion system for an unmanned underwater vehicle (UUV) involving an electrical drive system presents many interesting design challenges and involves electronic, electrical, mechanical, thermal and fluid dynamic sub-systems. As with any other complex system, analysis of the behaviour of a system of this kind can be greatly facilitated by the use of computer simulation techniques. However, in applications of this kind, simulation-based investigations of the complete system can be computationally very demanding and investigations involving multi-run optimisation studies or real-time simulation can present difficulties.

In particular, difficulties can arise in the case of real-time simulation applications where the use of conventional variable step-length integration algorithms and discontinuity detection methods is not appropriate. One possible approach is to sub-divide the complete system model into sub-models having different dynamic ranges. Different time steps can then be used in different parts of the simulation model, giving a simulation which is capable of faster execution because the total number of calculations is smaller. This approach is known as *multiple frame rate* or *multi-rate simulation* and can be applied with many different types of integration algorithm.

The model and the associated multi-rate simulation. For the purposes of this investigation the six degrees of freedom equations of motion of an existing underwater vehicle (the U.S. Naval Postgraduate School (NPS) AUV II) were used. The specific equations and parameters relating to the NPS AUV II vehicle upon which the work is based are those given by Fossen [1], which are, in turn, based on information provided by Healey and Lienard [2]. Some important changes had to be introduced in order to get the simulation model to behave in a credible fashion for the range of open-loop conditions and manoeuvres needed in the proposed real-time simulation application. Modifications were made to the equations representing the propeller in order to allow the model to function correctly as the propeller speed dropped to zero. This involved adopting an approach, first suggested by Fossen [1], in which the original representation of the thrust generated by the propellers was replaced by a quadratic quasi-steady thrust equation relating the propeller speed and the surge velocity of the vehicle. The modifications made to the model also ensured that an undesirable situation involving a divide-by-zero condition that could occur with the original representation with zero initial propeller speed was eliminated. A power electronic and electrical drive system was incorporated into the UUV model and the combination of relatively fast events in the power electronic components and much slower dynamics of the vessel itself and of the battery source raised many issues in terms of potential real-time capability. For full mission simulation capability the model must be capable of representing accurately the high speed power electronic subsystem, with phenomena involving time intervals of less than 10 μs, over periods of time of the order of seconds, minutes or longer.

The simulation was implemented using the Virtual Test Bed (VTB), together with the VXE graphics software which can be used to display graphical and 3-D animations of model behaviour. Both of these software tools were developed at the University of South Carolina [3]. The main benefit of this approach is that the VTB provides a flexible simulation environment that allows sub-system models developed using different simulation tools to be combined.

Results. Although multi-rate simulation has been a familiar technique for many years and is a feature of a number of commercial simulation software packages, this application is notable because of the combination of an eventual real-time requirement and the need for very short frame times to handle part of the system. Through application of the multi-rate approach faster than real-time execution has been achieved on a typical laptop computer even when using the 3-D graphical output capability provided with the VXE. Work has also been carried out to develop non-real-time simulations of the system to allow detailed investigation of the effectiveness of the multi-rate approach, consider detailed issues of frame rates for different sub-systems and prepare the ground for real-time implementation.

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A Dynamic Hybrid Model Of A Vehicle Clutch For HIL Applications

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Introduction The purpose of the presented approach is to present a dynamic, hybrid model of a friction clutch of a hybrid vehicle for Hardware in the Loop (HiL) simulations. The HiL simulation is a new design technique to evolve existing vehicle concepts or even design new ones ([1], [2], [3]). This technique combines the advantages of both simulation (flexibility and adaptivity) and test bed experiments (significant and valid results). To perform those HiL tests two important elements are necessary: A suitable test bench environment to test a component and an accurate mathematical model of the system to be simulated.

Model features Figure 1 shows a simplified model of a real vehicle clutch in compound with the remainder of the vehicle's power train. Here the combustion torque M_c, generated by the engine acts on the simplified crankshaft inertia J_{CS}. The clutch itself is represented by two rotating plates with inertia J_{CL} as well as a spring-damper element (k, d), which represents the elastic stiffness of the clutch. The second clutch plate is coupled to the reduced inertia J_{GB} of the power train and the vehicle. The value of the inertia depends on the chosen gear in the gearbox.

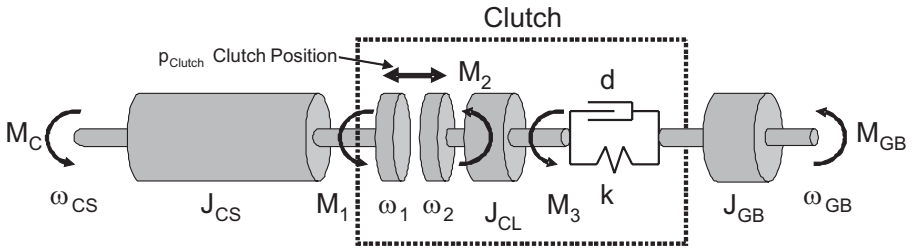

Figure 1: Model of the friction clutch

The dynamic model of the clutch is based on a hybrid state machine, which is defined by three discrete states: 'open', 'closed' and 'reopening'. All three states can be described by both algebraic and differential equations including a relative speed depending friction law. These equations as well as the transition conditions between the three states of the state machine are embedded into an external C function (static library) for Dymola. The model of the clutch is integrated into a complete model of a hybrid vehicle and tested in a simulation as well as on a hardware in the loop test bench. As a benchmark the standardized drive cycle 'NEDC' is used.

Conclusion In this contribution a new hybrid dynamic model of a vehicle clutch for online HiL simulation was presented. This new model is advantageous to previously published models since it is able to describe the real behavior of the clutch in an more accurate way, as the model incorporates a speed-depending friction coefficient as well as a rotational-damper-element.

Since the external function is programmed by using the standardized programming language C, the dynamic model of the vehicle clutch can be easily adapted to other simulation environments like MATLAB/Simulink and others. Another advantage of the presented approach is the high customisability of the clutch's behavior by adapting an individual but small set of clutch parameters.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELLING OF LATERAL DYNAMICS FOR AN ENDLESS METAL PROCESS BELT

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Introduction The meta belt is running over two cylindrical bend drums at each end (one of them being the driving drum) and can be supported by a number of supporting rollers. The main problem of this configuration is to guarantee perfect tracking of the belt utilizing swiveling drum axes, which guarantees a constant lateral position of the belt's edges under all process disturbances and geometric imperfections.

Mathematical models exist which are based on the assumption that the belt acts like a beam [1]. Those models were merely designed for the purpose to predict the lateral position of the belt off-line in the time domain [2, 3]. To this end geometric parameters of the process, material parameters of the belt, and a friction model for the contact between belt and drums have to be known and the transport delay for the duration of contact between belt and drum is neglected.

The model for lateral dynamics proposed here is more simple yet proves to be very accurate. Although only linear relations are utilized and a purely kinematic transport delay on the drums is assumed, the validation using experimental data from a test rig shows a much better fit to measured data for lateral dynamics than previous models.

Modeling The modeling approach presented here is partitioned into two parts: First, the static flexible deformation of the belt between the drums is derived from the geometric boundary conditions. Second, the kinematic transport of the belt on the drums is modeled assuming perfect adhesion between belt and drum. The final representation is dependent on the belt's spatial coordinate only. Starting out from the hypothesis that the lateral belt course speed is directly proportional to the crowd angles, the belt is modeled as a flexible beam [4]. Solving the respective system of equations finally gives a general expression for the beam's deflection only depending on the geometric boundary conditions. The resulting 4th-order linear state space system only contains the axle distance of the two drums as the single parameter. It explicitly contains the elastic deflection of both the upper and the lower belt and the transport effect on both drums; it does not contain time as independent variable, so the model is invariant to belt transport speed v.

Identification and Validation Step responses from an experimental test rig have been measured for a linear black-box identification and model validation. Since spatially measured data exhibit a marked periodic signal component due to irregularities during belt manufacturing, periodic parts had to be removed before the identification procedure. Additionally, outliers had to be detected and compensated by interpolation between correct data.

Utilizing step responses with increasing step sizes the region of linearity was experimentally evaluated. Only for very large control inputs a mild nonlinear transient effect was documented. Both non-parametric and parametric models have been identified from measured data using the MATLAB identification toolbox. A correlation analysis was performed for validating the system's transport delay. Best results for the black-box model were obtained with an ARX-model of 4th-order. Bode plots from the parametric ARX-model, the analytic model, and a non-parametric estimation show an excellent agreement between these models, and only the frequency and damping of the resonance peak is slightly offset in the simple analytical model.

Conclusion A simple analytic model which is linear, of 4th-order, and contains only two geometric parameters is presented. The transport delay of the drums is incorporated and a state space representation is given. Measurements from a test rig clearly show that the assumption of linear system behavior is justified up to very large control inputs, where nonlinear transient behavior was documented. It is further shown that both analytical and black-box models are consistent and capture the linearized dynamics of the process. Therefore, the presented analytical model can serve as a basis for design of a lateral position controller.

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MODELING AND SIMULATION OF THE DYNAMICS OF FUEL-CELL DRIVEN HYBRID POWERTRAINS

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In this contribution, modeling and simulation concepts of fuel cell-based hybrid powertrains for vehicles and other applications are presented. Mathematical models of fuel cells, DC/DC-converters, DC-Motor, and SuperCaps are derived and put together to simulate an arbitrarily load profile as well as driving cycles for vehicles with a fuel cell-based hybrid powertrain. The models are dynamical and, for the fuel cells, also include temperature effects. Further on, a power management algorithm is implemented and presented in the simulations.

The fuel cell system is modeled based on [1] and extended to include temperature effects as well as a dynamic DC-motor model in the compressor model. The same DC-motor model (with other parameters) is used as the drive motor in the hybrid system. Further on, a buck DC/DC-converter with a switch between the inductance and capacitance parts of the converter is modeled and implemented as controller for the DC-motor models. A sliding mode control approach is implemented for the motors. For the fuel cells, a continuous boost DC/DC-converter model is derived to control the bus voltage of the hybrid system at a constant level. Finally, a non-linear model of SuperCaps, which serve as energy buffer that can recuperate braking energy is modeled and validated. A load profile which include recuperation is implemented on the model and the results are shown in Figure 1.

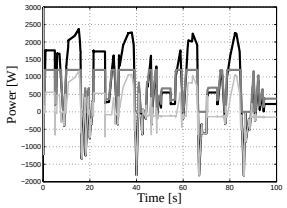

Figure 1: Simulation results for a given load profile. Dark Line - Power Electromotor, Grey Line - Power Fuel Cells, Bright Thin Line - Power SuperCaps

Two simulations were conducted; with and without power management. The power management has the task to distribute the available power between the components and affects directly the fuel cell life time. It also determines the ability of receiving regenerated power, the waste of unpredictable regenerative breaking due to fully charged SuperCaps, and the available power during sudden power peak demands. The power distribution between fuel cells and SuperCaps is calculated by choosing the actual SOC of the SuperCaps and split the power proportionally according to the rule $I_{max} = (1 - SOC) I_{maxdcdc}$, where $I_{maxdcdc}$ denotes the overall possible maximum current that can be withdrawn from the DC/DC-converters. The results are presented in Figure 2, where the difference between the power of the fuel cells with and without power management is seen. The high peaks and dynamics of the power for the fuel cells decrease their life time due to their sensitivity towards current, temperature, and humidity gradients. With power management the output power of the fuel cells becomes smoother and with lower gradients and hence, increases the life time of the fuel cells.

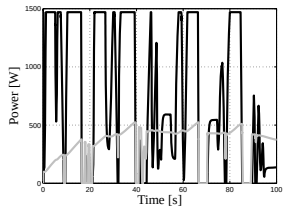

Figure 2: Difference in Fuel Cell power output with and without power management. Dark line - without power management, Bright line - with power management

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELLING, STABILITY ANALYSIS AND DYNAMIC RESPONSE OF A MULTI-DOMAIN MECHATRONIC SYSTEM

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Abstract. This paper presents methods for the modelling and simulation of a mechatronic system such as tilt mechanism. A complete mathematical model of tilt mechanism is developed including servo actuator dynamics and presented together with dynamic simulation in this paper. The dynamic response of mechatronic system based on conventional and bond graph modelling (BGM) techniques is determined. The modelling and simulation of the mechatronic system is carried out in order to establish the strength of the BGM for the solution of coupled multi-domain mechatronic systems in a unified approach. The conventional and BGM techniques were used to obtain the state space model of the mechatronic system. The tilt mechanism design is inherently stable verified by analysis of both approaches. The motion controllers are designed and used to obtain the desired dynamic response. The performance of the tilt mechanism actuator control system is examined with numerical simulation and verified. The BGM trend matched closely with conventional model. The settling time and percentage overshoot of conventional and BGM techniques were compared that revealed the effect of distributed mass. This effect is verified by numerical simulation based on state space model and BGM technique.

Content. The paper deals with the modelling, stability analysis and motion control of a mechatronic system for positioning or aiming a camera or laser. The design of a tilt mechanism is intended to perform a tracking task. The input is described in terms of desired angular position of the camera. It is a typical case of an inverse kinematics in the sense that given a predefined object (output), the input (reference) was determined by using image processing unit (image processing software on a computing unit), we want to determine the error signal and consequently amplified error signal to the motor of the tilt mechanism.

This paper focuses on the mechanism and actuator dynamics of the tilt mechanism. The dynamic response of pan mechanism is similar to tilt mechanism. To achieve these objectives and to verify results, two approaches are presented in this paper. First approach of this paper is mathematical modelling of the tilt mechanism using conventional approach. The second approach is based on BGM of the tilt mechanism. The conventional and BGM are applied to validate the response of the tilt mechanism. The gain and proportional-derivative (PD) controller were used with the models of tilt mechanism to achieve the desired response. The results are compared to validate the modelling techniques.

Result. Both the conventional and the bondgraph methods were used for the modelling and simulation of the physical system considered. The more accurate model of the tilt mechanism was obtained using the BGM. The effect of the load parameters (inertia and friction) of the mechanism on the actuation performance was explored using the BGM. In the conventional modelling, the load characteristics (J_L, f_v) were compensated in the actuator dynamics by finding the effective load and effective friction. The state space model of the tilt mechanism was obtained using the BGM. The stability of tilt mechanism was checked the system was found stable.

The efficacy of the BGM in dealing with the modelling and simulation of the mechatronic systems, that is, coupled multi-domain energy systems, has been effectively established in the application considered. This is in sharp contrast to the conventional methods which decouple the systems, or consider some average effect, thus masking the physics of the physical problem. Thus the BGM can be considered as the method of choice for the modelling and simulation of mechatronic system.

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FUZZY LOGIC IN POWER SYSTEM PERFORMABILITY

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Introduction. Performability modeling is an important topic of research in the area of fault-tolerant systems. Combining the structure state process (SSP) that describes the system evolution as influenced by failures and repair with the system performance in each state of the SSP means - composite performance-dependability analysis. In literature performance and dependability issues are dealt separately [1]. Combined performance-dependability studies give the performability model.

Content. A continuous-time Markov chains (MC) model or Stochastic Petri Nets (SPN) model equivalent to MC, it is easy to realize for SSP modelling [3]. We assume that the system reaches steady state in each of the structure state and use a performance model to compute the quantitative index of the system performance in a specific structure state (the reward associate with the structure state).

The model needs the performance measure for each of the SSP state. The structure state of the system changes due to its elements failure and repair as time progresses. For a power system the failure of an element is detected an isolated by the electric-power protection/automation system. If the electric-power protection/automation system is operational the failure is isolated and the transition to the next SSP state is possible. We propose to use the fuzzy Safety Transition (ST) due to the electric-power protection/automation system action as reward measure of each SSP state. A fuzzy logic system (FLS) is used for safety analysis of the electric power protection/automation system. The in FLS parameters are Occurrence and Severity of the failure and the out FLS parameter is Safety. Also an adequate rule based is elaborated [2].

The energy loss cost (ELC) due to system defaults is an important component in power system function. Performability of a power system must combine the results of the electric- power system dependability analysis with the results of the electric-power protection/automation system safety. The performability measure will be used for ELC evaluation considering the connected electric power- protection/automation system.

For protection/automation system safety is used the event-tree method. Event-trees examine sequences of events and their probability of occurrence. The tree - paths ranking evaluation is not enough for the electric - power protection system reliability calculation. A methodology to compute a quantitative index "General Safety Degree" (GSFD), for this kind of system, was developed in [2]. For electric power protection system safety evaluation an algorithm is proposed.

To elaborate the event tree and to use the proposed FLS on each path of the tree, a software tool "Fuzzy event-tree analysis" (FETA) was created. We can obtain a "Safety" fuzzy set on each path of the tree. All the evaluated "Safety" fuzzy sets are introduced in an algorithm to elaborate the fuzzy "General Safety" (SG) of the system. This measure is used as ST parameter due to the electric-power protection/automation system action.

Naval power plant is an isolated system, usually having a single sectioned busbar system. The fault tolerant power system has automatically coupled Diesel generators to different busbar sections, improving the system availability. The Diesel generators and the most important consumers are coupled to the main busbar (MB), with three sections, section S3 having the shore coupling board (SCB) system. The 220Vac consumers are coupled to the secundary busbar (SB). Two distinct alternatives, using four 800 KVA generators (A), or using six 500 KVA generators (b), can cover the most loaded stage of the system. The 220 Vac secundary busbar (SB) supply may by obtained in three different alternatives (1, 2, 3). The six NPP design alternatives A1, A2, A3, B1, B2, B3 need to be economically analyzed. Many terms are used in the economical analysis computing, but one of the most important is represented by energy loss cost due to system defaults. This term is obtained using the performability metrics, evaluated in the six design alternatives.

The performability measure (SEIR), for all six EP alternatives used in the proposed performability analysis, is a very important component of the economic comparative study. Alternative A performability is generally better than alternative B performability. For the same A or B alternative type, alternative A is better.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

FREE VIBRATION OF 3-D PIERCED SHEAR WALLS WITH CHANGES IN CROSS-SECTOIN USING CONTINUOUS CONNECTION METHOD

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The rapid growth of the urban population forces people to use the existing areas in the most economic way and also aim to be close to each other to avoid a continuous urban sprawl. For this purpose architects and engineers have to participate in the stages of the project in order to come up with economical buildings. The growth in modern tall building construction, during the last three decades, has been largely for commercial and residential purposes. However, the higher the buildings get, the more increased are the lateral loads, in addition to vertical ones. In multistory buildings made of reinforced concrete, the lateral loads are often resisted by specially arranged shear walls.

Shear wall components may be planar, are usually located at the sides of the building or in the form of a core which houses staircases or elevator shafts. Weakening of shear walls in tall buildings by doors, windows and corridor openings is generally unavoidable in structural engineering. When the coupling action between the piers separated by openings becomes important, some of the external effects are resisted by the internal forces and moments in the walls due to the increase in the stiffness of the coupled system by the connecting beams. Actually, the deformation of a pierced shear wall subjected to lateral loading is not confined to its plane. Studies considering in-plane, out-of-plane and torsional deformations in the investigation of pierced shear walls are called 3-D shear wall analyses. In 3-D pierced shear walls, both the flexural and torsional behaviours under external loading have to be taken into account in the analysis.

In this study, the free vibrations of 3-D pierced shear walls on rigid foundations are analyzed using the continuous connection method (CCM) and Vlasov's theory of thin-walled beams [1]. In the present work, the case of one vertical row of openings in a 3-D shear wall is considered as done in the static solution by Tso and Biswas [2]. The parts of the shear walls among the openings are considered as beams connecting the remaining parts of the shear walls. All geometric properties vary from region to region along the height. After finding the stiffness matrix of the structure employing the foregoing methods, the mass matrix is found with the lumped mass idealization ignoring their rotational stiffnesses. Then, the modal analysis is performed and the frequencies and the corresponding modes of vibration are determined. A computer program has been prepared in Fortran Language to implement the foregoing analysis. The structure is solved both by the present method using CCM and by the SAP2000 structural analysis program using the frame method. It is observed that the results obtained by the present method coincide with those of SAP2000 structural analysis program perfectly. This method is an effective method in terms of simplicity of its data and extremely short computation time for the predesign of high-rise buildings.

All of the dynamic analyses in the literature on perforated shear walls concern themselves with planar ones [3]. No study has been made, to the knowledge of the authors, concerning the dynamic analysis of 3-D pierced shear walls, so far.

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APPROXIMATION OF A DISSIPATIVE SYSTEM WITH DIRAC STRUCTURE CONSERVATION: CASE STUDY

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In this paper, we show that in a distributed parameter system, represented in a port-Hamiltonian form, we preserve the Dirac structure after a space discretization. Indeed, the conservation of the Dirac structure was shown only in the conservative case, without dissipation [2]. The study is applied to the case of a transmission line represented by the telegrapher's equations.

In the literature there are a number of results showing how port based network modelling of lumped and distributed parameter physical systems naturally leads to a geometrically defined class of systems, called port-Hamiltonian systems. The Hamiltonian approach starts from the principle of least action, use the Euler-Lagrange equations and the Legendre transformation, and arrive to the Hamiltonian equation of motion. The system behaviour is defined by a Dirac structure, which represents the power-conserving interconnection structure of the system, and the Hamiltonian, which is given by the total energy of the energy storing elements in the system. We can add energy-dissipating elements by terminating some of the system ports with resistive elements.

In the case of distributed parameter systems, an important problem is the incorporation into this framework of numerical methods for solving Partial Differential Equations (PDE) (finite elements and finite-differences for example). We have an infinite-dimensional system that we need to approximate with a finite-dimensional one. The existing numerical methods for solving PDEs assume that the boundary conditions are given. In the case of telegrapher's equations the boundary conditions are the voltage and the current at both ends of the line. But these values cannot be considered given because the transmission line is connected to the other dynamic systems of the electrical network. Therefore, we need to approximate the distributed-parameter system with a finite dimensional system while maintaining the power port structure [3].

We consider a transmission line where we define the energy variables as the charge density $q = q(t,x) \in \Lambda^1(\Omega)$ and the magnetic flux density $\varphi = \varphi(t,x) \in \Lambda^1(\Omega)$, where $\Lambda^1(\Omega)$ denotes the 1- forms space. In order to introduce the energy variables, we write the power balance of the transmission line starting with the total energy $H(q,\varphi)$. We introduce the conjugate energy variables flow $f_q(x,t),\ f_\varphi(x,t)$ (1-form) and effort $e_q(x,t), e_\varphi(x,t)$ (0-form) and obtain the following port-Hamiltonian system:

$$\begin{pmatrix} f_\varphi \\ f_q \end{pmatrix} = \begin{pmatrix} 0 & -d \\ -d & 0 \end{pmatrix} \begin{pmatrix} e_\varphi \\ e_q \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} f_{d\varphi} \\ f_{dq} \end{pmatrix},$$
$$\begin{pmatrix} f_{d\varphi} \\ f_{dq} \end{pmatrix} = \begin{pmatrix} r* & 0 \\ 0 & g* \end{pmatrix} \begin{pmatrix} e_\varphi \\ e_q \end{pmatrix}$$

$$e_{b0} = e_q(t,0),\ e_{b1} = e_q(t,1),\ f_{b0} = e_\varphi(t,0),\ f_{b1} = e_\varphi(t,1)$$

where *r* and *g* represent the resistance and the conductance density, respectively and where *d* is the usual exterior-derivative; b0 and b1 denote, the left and right boundary, respectively.

We make a spatial discretization and split the line in *m* cells. Due to spatial compositionality, we need to perform discretization to only one cell. We carry out a separation of variables and use the Whitney form, which make it possible to preserve the properties of the p-forms at the time of spatial discretization [1]. We show that the resulting structure satisfies all the conditions of the Dirac structure. It is known that the connection of two Dirac structures gives a Dirac structure. Thus, the entire transmission line can be reconstructed by connecting a fixed number of cells in advance.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

HYBRID MODELING OF A TWO-STAGE TURBOCHARGED DIESEL ENGINE AIR SYSTEM

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Introduction. Many contemporary diesel engines are equipped with turbochargers to simultaneously improve power and fuel efficiency by raising the boost pressure. In order to overcome the major disadvantage of exhaust-driven turbochargers, i.e. the lack of boost pressure at low engine speeds, the system of interest is equipped with two turbochargers, each one designed to be operated at either low or high engine speeds, respectively. Furthermore, a so-called exhaust-gas recirculation (EGR) is employed to lower nitrogen-oxide (NOx) emissions [2]. Due to the fact that EGR reduces the engine's power, it is usually only active if required by legislation. Hence, the system dealt with in this work is a two-stage turbocharged air system with cooled EGR and charge-air cooling (CAC) as depicted in Figure 1, whose working principle is as follows. Fresh air from the ambiance is consecutively compressed by the low- and high-pressure compressor (LPC and HPC), which are powered by the respective low- and high-pressure turbine (LPT and HPT) driven by exhaust gas from the internal combustion engine (ICE). Exhaust gas from the exhaust manifold (EM) is partly fed back into the intake manifold (IM) via the EGR. Having passed the LPT, the exhaust gas finally leaves the air system through the exhaust aftertreatment (EAT) system.

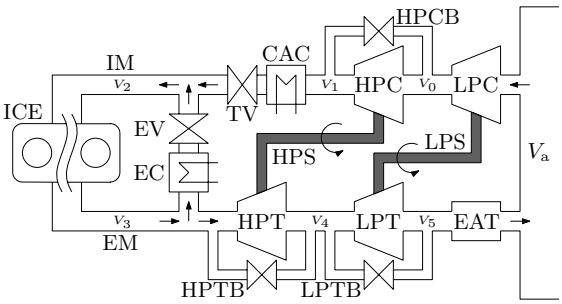

Figure 1: Sketch of the air system with high- and low-pressure compressor (HPC and LPC), charge air cooler (CAC), internal combustion engine (ICE), high- and low-pressure turbine (HPT and LPT), as well as EGR cooler (EC), valve (EV), and the exhaust aftertreatment (EAT).

Continuous-time dynamics. Assuming that the spatially distributed piping sections V_0-V_5 can be described by a lumped parameter model, the air system's continuous-time dynamics is given by a set of nonlinear ODEs for the respective thermodynamic states (e.g. pressures) and the mechanic states (turbocharger speeds) [2]. Since the basic modeling is the same for all piping sections, the overall air system model is set up in a modularized manner [3]. Thereby, algebraic coupling models determine mass and enthalpy flows between two adjacent chambers.

Hybrid characteristics. In addition to the continuous-time dynamics, the presence and absence of EGR in different operational regions of the engine as well as the employed turbocharging concept necessitate the consideration of different modes of air system operation. In particular, the EGR valve is opened and closed by the engine control scheme to realize a desired emission behavior and the HPC bypass is designed as a passive element opening and closing according to the pressure drop Δp_{HPC} over the HPC. In this work, the air system's operational modes are represented by the vertices of a finite state machine [4], while the corresponding switching rule is given by the respective edges. The graph for switchings caused by the HPCB is exemplarily given in Figure 2. It features two vertices (i.e. the discrete states) and two respective edges (i.e. the switching rule). From the inscription of the vertices it can further be seen that different sets of ODEs and different input vectors are associated with each operational mode. The air system model depicted in Figure 2, i.e. a discrete state machine driving a respective underlying continuous-time dynamics, is often referred to as hybrid automaton or hybrid system [1, 4]. The hybrid dynamical model of the state-of-the-art air system depicted in Figure 1 is presented in this work, including component modeling, parameter identification, and the setup of the discrete state machine. A simulation study demonstrates the suitability of the presented modeling concept.

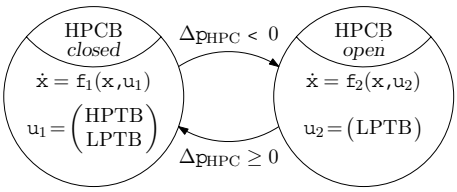

Figure 2: Hybrid automaton for HPCB switching in the diesel engine air system.

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MATHEMATICAL MODELLING OF TENDON MECHANICS

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Introduction. Tendon is a dense connective tissue, transmitting muscular forces to the skeleton, and is constituted by an organized hierarchical structure, from the molecular scale up to the macro one (i.e., the whole tendon) [1]. The mechanical behavior of tendons depends on the response of its constituents, primarily collagen fibers embedded in an extra-cellular matrix.

Collagen fibers are tilted, leading to a macroscopic planar crimped structure, aligned along the loading direction and their microstructure highly influences tendon mechanics. Moreover, recently a crucial role has been recognized to entropic processes occurring at the nano-scale within fibril structure [2].

Several constitutive models have been recently proposed for collagenous tissues, such as tendons, based on a continuum approach and involving a macroscopic mechanical description. Most of them are deduced from phenomenological evidences. Other approaches consider crimped linearly elastic collagen fibers but they lack a suitable experimental validation or they are based on model parameters obtained by parametric fitting of experimental data, ignoring any histological evidence. Moreover, they do not take into account the non-linear collagen constitutive behaviour deeply related to nano-scale entropic processes.

A multiscale mechanical model. In the present work, tendon mechanical behavior is modelled by a two-step homogenization technique, based on a multiscale approach. First a micromechanical homogenization procedure is employed in order to reduce a crimped fiber to an equivalent straight one, and then a classical homogenization approach is involved to reduce the tendon tissue to a one-dimensional homogeneous structure, subjected to uniaxial traction along the fiber direction. Moreover, a generalized version of the Worm-Like Chain (WLC) model, traditionally employed in DNA entropic elasticity, is proposed in order to describe the non-linear constitutive behaviour of collagen, in agreement with nano-scale evidences [3].

Tendons large-strain and large-displacement elastic response is numerically computed by an iterative algorithm, involving the solution of a sequence of linearized problems. Model parameters are related with measurable histological and geometrical properties and are consistent with reference values available in specialized literature.

Model validation. In order to show the effectiveness of the proposed multiscale nano-micro-macro approach, a tensile experimental test on a rat tail tendon is numerically reproduced. In Fig. 1, nano-micro-macro results are compared with both those obtained through a micro-macro formulation (i.e., neglecting collagen non-linearities) and experimental measures.

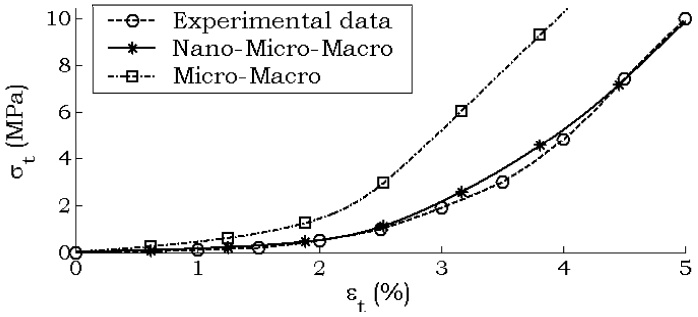

Figure 1: Experimental stress/strain response (○) for a rat tail tendon [4] compared with the numerical results obtained by the proposed model, considering both a micro-macro and a nano-micro-macro (∗) approach.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

OBJECT ORIENTED MODELLING AND SIMULATION OF ACUREX SOLAR THERMAL POWER PLANT

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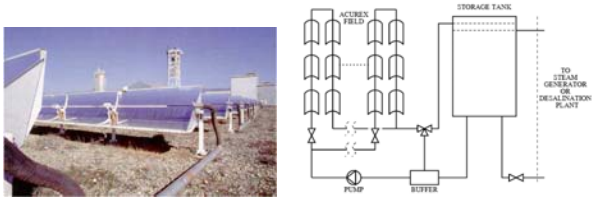
This paper presents the actual status of the research performed within the framework of modelling and simulation of Parabolic Trough Colectors (PTC) in the scope of Solar Power Plants. The work is mainly oriented to the development of dynamic models of solar energy plants, to be used in the design of automatic control systems aimed at optimizing global performance.

The system used as test-bed plant is the ACUREX facility, sited at Plataforma Solar de Almería (CIEMAT). It is an arrangement formed by ten rows of PTC's using oil as heat transfer fluid, working as an approximattely 1 MW_t solar power plant. The model presented in this paper is used in the design of hybrid model predictive control and intelligent control schemes to optimize plant performance, even under start-up and shutdown situations and in the presence of highly variable load disturbances due to the daily cycle of solar radiation and passing clouds. It is based on the works presented in [1] but including several new approaches due to the modelling technologies used.

An overview of the different operational configurations of ACUREX facility will be included, showing explicative diagrams and photographs (figures 1(a) and 1(b)). The operation of this kind of plants is based in the concentration of incoming direct solar radiation onto the absorber tube located in the geometrical focal line of a cilindrical-parabolic mirror. As the sun position changes during the day, each PTC of the facility has to change its orientation as the solar radiation vector does. The absorber tube in each PTC acts as an energy exchanger, receiving solar energy and transferring it to a thermo-hydraulic circuit with a heat transfer fluid (HTF) as medium. A comprenhensive review about this and newer PTC technologies is explained in [3]. The facility is composed in addition of the PTC's field by a storage tank, heat hexchangers, pumps, injectors and valves, although the modelling and simulation work will focus on those components used in the solar operation mode. In this operational mode the ACUREX field acts as a solar heater receiving oil from the storage tank and transporting the collected energy to a thermal load and/or the tank. A oil pump and an outlet controlled valve define boundary conditions for the field. The final objective of the model is to predict the transient behaviour of the thermodynamics variables associated to the thermo-hydraulic output power of the field and the tank (temperature, pressure, specific enthalpy,...), when the external disturbances (concentrated solar radiation, ambient temperature, wind speed and direction, ...) and controllable inputs change.



(a) ACUREX facility at PSA (b) Schematic diagram of ACUREX facility at PSA

Figure 1: Central receiver solar thermal power plant

The work analyzes each of the main components of the thermohydraulic circuits of oil and explains the modelling assumptions, trying to justify each one. Each one of the assumptions are oriented to get, by means of the symbolic manipulations that Dymola tool performs, a not high index DAE system for the complete model in which the number of nonlinear algebraic loops is minimized. For this purpose, all the components are classified, following the modelling methodology derived from the Finite Volume Method (FVM) [2].

Finally, simulation results are presented with boundary conditions (controlled variables and disturbances) similar to those imposed to the ACUREX plant.

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DETERMINATION OF THE DYNAMIC BEHAVIOR OF AN ELASTO-HYDRODYNAMIC BEARING

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Hydrodynamic bearings for industrial applications usually are highly dynamically loaded, like a roll bearing assembly in rolling mills in steel industry. Such applications require high positioning accuracy but are a dominant compliance in mechanical systems. Therefore, a good understanding of the dynamic behavior of such bearings becomes more and more important.

At high pressures in the lubricant and thin film thicknesses, the mechanical bearing components are significantly elastically deformed what leads to a change of the pressure distribution and the bearing dynamic. This nonlinear coupling is called Elasto-Hydro-Dynamic (EHD). This behavior has been investigated carefully and an EHD-bearing model has been set up. The model was used for the numerical determination of the dynamic model parameters at a defined operating point for being able to use the results in complex simulation models.

A structure of the developed EHD-bearing model was set up, which allows an independent calculation of the deformations of the mechanical components and the pressure of the lubricant inside the bearing gap. As shown in the figure below, the deformation of the contact surface with oil for both bearing rings is included, as well as the elastic deflection of the shaft, in particular for the trunnion.

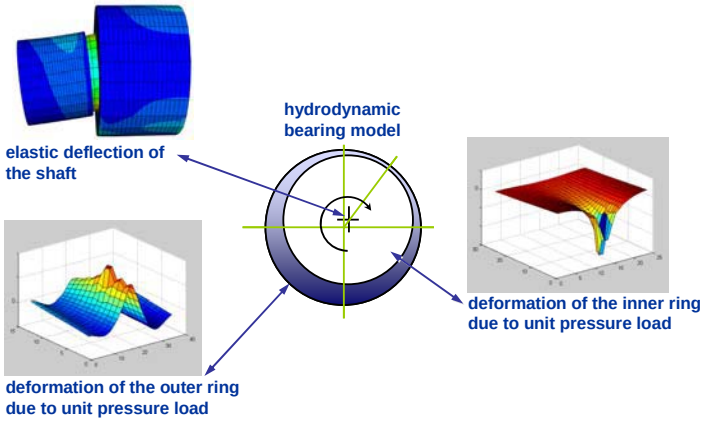

Figure. Structure of EHD-bearing with included deformation of the mechanical components.

With separate Finite Element models for the inner ring plus trunnion and the outer ring with the housing the deformation of the contact surfaces as reaction on the lubricant pressure will be calculated. The pressure distribution of the lubricant depends on the operating point and certainly on the size and geometry of the lubricant film what again depends on the surface deformation and has an influence on the load capacity.

As the pressure distribution can not be calculated explicitly for a general bearing geometry, iterative numerical methods have been used. In each iteration step, the complete deformation must be determined what causes very long computing times if the Finite Element model must be solved each time.

To avoid this, the method of influence functions has been used where the deformations have to be calculated only once. Herewith, a quick and efficient determination of the exact deformation of the bearing due to the pressure distribution can be done. This drastically reduces the overall computing time.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Fuzzy Systems – Modelling and Application

FUZZYPICS – A VISUAL APPROACH ON MODELING AND COMPUTING VAGUE KNOWLEDGE

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Introduction. In order to model vague human knowledge, it can be represented by the means of Fuzzy-Theory [3] (cp. [2]). In practical applications experts define Fuzzy-Sets of linguistic terms, combine the sets with rules and attach them to precise values or other Fuzzy-Sets. The concept of describing expert knowledge by using fuzzy sets is perfectly applicable to technical problems, where we apply grades of membership to unique values, such as speed or temperature. Not every sort of vague knowledge is possible to model, or there is a large lack of performance.

If one models variables like "Toothache" and "Fear from the dental drill" to decide if someone visits the dentist or not, there evolves a paradox in the set of rules, when both states of variables have the same linguistic-term, such is "severe". So, if "Toothache" and "Fear from the dental drill" are "severe", the decision depends on further information or can not be solved. If it is not possible to determine proper memberships functions for Fuzzy-Sets, or a well defined rule set for variables, one has to find other ways to model. The paper introduces a visual approach on modelling vague knowledge. The approach uses images, called Fuzzypics, to model human knowledge or generated models and supplies it directly as a computable bitmap.

Knowledge engineering. Suboptimal characteristics of common linguistic approaches are pointed out and lead to a formal definition of Fuzzypics and their use. In order to clarify the concept, examples of human decision making and technical problems are given. Knowledge engineering is done by visual means rather than linguistic terms to avoid inconsistencies in the Fuzzy-Rule sets and supply the holder of the knowledge with an intuitively understandable concept for knowledge representation. Therefore Fuzzypics do not require the explicit definition of Fuzzy-Sets but can handle them. The Fuzzypic can be filled by the expert using paper and pencil. The bitmap, once prepared for computation, works as the knowledge base for a computational reproduction of that knowledge. Further procedures of generating Fuzzypics are introduced, they cover extension with random values, completion of insufficient information as well as automated generation by calculation specifications.

Applications with Fuzzypics. The images can be arranged in sequences to allow sophisticated inference models. The presented concept can interlink between a crisp model and an extensive fuzzy model. The use of it is highly scalable. Since the inference procedure is a simple operation on the bitmap we buy computation rate at the expense of memory. Even thought the paper introduces the idea deduced from simulations of emotion driven decisions of humans, Fuzzypics can be applied to technical problems as well. The approach is a useful alternative to common ways of handling vague knowledge. Possible fields of use are automated Quality Control or general applications in simulation studies. The paper gives a overview of the concept of visual modelling with Fuzzypics. Due to the use of standard formats of the RGB Colour model (cp. [1], [4]) the use of Fuzzypics does not require a special set of tools. Creation and combinations do only require standard image processing tools.

Outlook. For a easy handling and improved communication the paper introduces formal definitions as well as examples. First operators, procedures and rules concerning the use are supplied. The concept could develop it strength at the point, where the use of Fuzzy-Logic is too costly, too complex to implement or just too slow, but fuzzy handling of data is preferable. It understands itself as a high-speed add-on to the wide range of possibilities to model and compute vague data. The idea holds large potential for further research.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

VALIDATING MEASUREMENT DATA BY QUALITY MEASURES USING FUZZY-APPROACHES

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Abstract. In many application situations, the researcher is confronted with the problem that there is a set of data sources available, e.g. measurements that refer to the same measured value, that substantially differ in data quality. Data quality in this context shall be defined along the criteria completeness (lost data, gaps, ...), scale (high – low), and precision (measurement error). Existing data explorations mostly concentrate on one of these criteria and offer proprietary solutions only. Those proprietary solutions are not capable to foster an integrative data interpretation that deals with measurements coming up from different data sources and measurement methods. However, putting together the data of different measurement approaches could bridge missing data and improve data reliability. The objective for this paper is to develop a data analysis and validation workflow that allows to combine the given strongly varying data sets to a common view on the resulting dimension.

To specify these tasks more precisely, the problem is formalized first giving every measured value an additional quality attribute. In consequence, the paper shows, how to use multiple measurements by different methods for improvement of the final result, how to incorporate the quality of the measurement into the mapping function, how to use fuzzy-methods for the classification task, and how to visualize the quality of the classification in the final 3D-representation.

Doing so, there are different levels of detail, the quality value can be specified: The most precise would be to attribute a distinguished value to every point (that means every tripel *(x,y,z)*) as implied by the formalism. For practical reasons, such an effort nor will be reasonable in respect to the time it would need to set a quality value for each point, neither it would be appropriate to the problem itself, because there is not that grade of differentiation in the measurements. Therefore, the level of differentiation will be determined by a common quality value for a certain measurement or even for the measurement method in general. This heuristic approach may be insufficient in respect to the granularity provided by the formalism and implies inaccuracies when different points are compared to each other within the data set of a single measurement, but for the overall interpretation of the data and in respect to the alternative interpretation pathways it is helpful to have a measure to compare the different data sets in regard on their contribution to the error minimization task in relation to the corresponding, competitive measurements. For practical reasons a general value for the measurement method will be pre-set that might be changed by the people who executed the measurements on level of measurement. For outliers the quality value can be overwritten explicitly on single point scale.

The paper provides in its first part the proper formalisation of the problem as sketched so far in this abstract, the second part will give a practical “to-do”-advice on the base of the MatLab Fuzzy-Toolbox and a self-developed collection of m-files and c-routines supporting the analysis and validating workflow to merge different measurements to an unique classification result.

MODELING AND IMPLEMENTATION OF COGNITIVE-BASED SUPERVISION AND ASSISTANCE

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Introduction. The safety of passing maneuver was already a focus in automotive history. In this work, an approach of automated supervision and driver assistance is introduced. The main advantage is that beside the supervision, the proposed underlying concept can also be used to fully autonomous driving.

The Situation-Operator-Modeling (SOM) approach. The core of the approach is the assumption that changes in the parts of the real world to be considered are understood as a sequence of effects modelled by scenes and actions. The item scene denotes a problem-fixed moment in time but independent from time, and the item operator denotes the action changing the scene. Both are connected by the underlying logic of action: the operator follows the scene and the following scene follows the operator, etc. The definitions of both items are coordinated in a double win. They are related to each other and therefore can also be used to relate the assumed structure of the real world to the structure of the database – called the mental model – of an intelligent system.

Concept of cognitive supervision and assistance. Using the Situation-Operator-Modeling, a related concept for automated supervision is developed and proposed in [1]. For the representational level as part of the cognitive approach, the SOM is used to model and structure the complex scene of the driver-vehicle-environment interaction. First, the scene is modeled as situation. Therefore, its characteristics have to be defined. Then, the set of actions which can be performed by the driver is specified and modeled as operators. The passing maneuver is chosen as an example because it provides enough complexity to demonstrate the approach, but on the other hand it is not too complex to get lost in details.

Implementation within an experimental environment. The implementation of the concept of automated supervision to a real vehicle was firstly realized within a cooperation between the Chair of Dynamics and Control (University of Duisburg-Essen) and the Institute of Transportation Systems (German Aerospace Cente, DLR) , which is described in [3] based on previous work [1, 2]. Here, sensor and video data of the ViewCar©, a test vehicle equipped with several sensors and cameras, is used to build a general model of the Driver-Vehicle-Interaction (DVI).

Within the DVI model, the logic of interaction is represented using the SOM approach. The sensor-based measurements of the vehicle are used as input of the model and are structured as a hybrid situation vector of the SOM-approach consisting of seven basic interpreted characteristics of different data types stated by a set of parameters, which are determined by actual scene presented by the sensor data. To obtain the characteristics from the sensor data, a number of prefilters is applied, including numerical calculations, data compressions, and other mathematical algorithms like fuzzy logics and neural networks etc. Furthermore, the actions of the driver are modeled as operators including a set of assumptions, which describe the relation of the operator to the initial situation. The assumptions are not fulfilled if the actual operator is not suitable to the current situation.

The implementation of this model is realized by a Java-Application, which enables the UDP-based communication between sensor system and a user interface. With the integrated prefilters and operator library, the application can provide online processing with raw sensor measurements from the database as input. The results of the analysis are fed back directly to the user interface, which displays the interpreted characteristics, operators matching the actual situation with respect to the assumptions, and the actual operator of the driver. Additionally, a warning message is shown if the actual operator does not match the actual situation.

Tests of the introduced DVI model was executed in both off-line and on-line mode, and finally in the real experimental ViewCar©. Results from the both experiments show that the off-line test has a better identification rate than the on-line mode because of the more complex driving environment and lack of more precise measurements support.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

INCREMENTAL CLASSIFICATION OF IMAGES AND LARGE DATA SETS BY INFORMATION COMPRESSION AND FUZZY SIMILARITY ANALYSIS

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Introduction. This paper proposes a two-stage computational scheme for classification of images and large process data sets [1] based on their similarity analysis. The procedure starts with a small number of known *core images* (or data sets) which form the initial size of the Image (Data) Base. During classification, the *dissimilarity degree* $0.0 \le D \le 1.0$ of every new (unknown) image is computed against each of the core images in the Image Base. As a result, depending on the preliminary given threshold *Th* for classification, the new image could be classified as belonging to a certain class (core image) in the Image Base, if $D < Th$ or could be "quite different" (if $D > Th$), thus forming a *new class* in the Image Base.

Information Compression. The first stage before the actual similarity analysis and classification of the images is to reduce the large amount of the "raw pixel information" contained in the original images. We call this step an *Information Compression*. From a computational viewpoint the information compression is a *transformation* of the original large data set: $\mathbf{x}_i = [x_{i1}, x_{i2}, ..., x_{iK}], i = 1,2,...,M$, consisting of *M* data in the *K*-dimensional input space into a respective *Neural Model* consisting of *N neurons* in the same space. Here $N << M$. and *CR = M/N* is the so called *Compression Ratio.* We use in the paper one modification of the popular unsupervised *Neural-Gas* learning algorithm [2] for such compression. The following figure illustrates the compression of the "raw" RGB pixel data from a test image into a smaller set, consisting of *62* neurons in the 3-dimenisonal space.

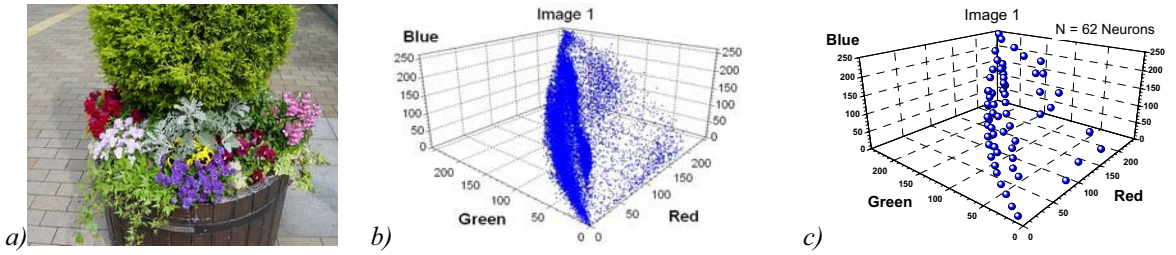

Figure. Example of *a)* Image; *b)* Raw Data (RGB pixels) and *c)* Compressed Information Model (CIM).

Fuzzy Similarity Analysis. As a second stage of the classification process we propose to use a special two-input fuzzy inference procedure $D = \mathbf{F}(P1, P2)$ for similarity analysis. First of all, we extract two important parameters (features) from each Compressed Information Model (CIM) that corresponds to a given image. These are the C*enter-of-Gravity* **CG** and the *Weighted Average Size WAS* of the CIM. Then for each pair of images {A,B} we compute the *distance* CGD between their centers-of-gravities as well as the *difference WSD* between their weighted average sizes and use them as input parameters *P1* and *P2* for the Fuzzy Inference, as follows:

$$P1 = CGD_{AB} = \sqrt{\sum_{j=1}^{K} [CG_j^A - CG_j^B]^2} \qquad P2 = WSD_{AB} = |WAS_A - WAS_B|$$

Example for image classification and results. A test example of *16* images of different flowers is given in the paper in order to illustrate and analyse the proposed classification scheme. *Four* different Image Bases, consisting of *3,4,5* and *6 core images* respectively were used for the classification with a predefined threshold *Th = 0.45*. The results are divided into two groups: *preliminary* classified images (based on the minimal dissimilarity *Dmin* only) and *finally* classified, that consider the given threshold *Th*. A comparison of these results with a human preference (human expert decision) is also made and discussed.

Conclusion. Important element of the proposed classification scheme is its ability to make *incremental classification*, which could be very useful in the cases of growing number of new images or data sets during time with a little initial information about the number of classes for classification. The need for a proper tuning of the Fuzzy Inference block, in order to obtain plausible similarity analysis results is also discussed in the paper.

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FAST FOURIER TRANSFORM AND AUTOREGRESSIVE ANALYSIS OF MITRAL VALVE DOPPLER SIGNALS AND CLASSIFICATION BY FUZZY CLUSTERING

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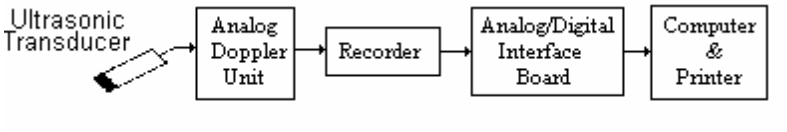
Today, quickly and trusty diagnosis of various diseases has great important. For this purpose, an additional diagnosis tool by artificial intelligence is developed to the aid of expert medical staff. In this work, cardiac Doppler signals recorded from mitral valve of 75 patients were transferred to a personal computer by using a 16 bit sound card. The fast Fourier transform (FFT) and Autoregressive (AR) method analysis was applied to the recorded signal from each patient. Further these values were classified by using Fuzzy clustering algorithm. Thus, an additional diagnosis tool is developed for the aid of expert medical staff.

The measurement system consists of five functional blocks as shown in Figure. These are 2.50 and 3.75 MHz ultrasound transducers, an analog Doppler unit (Toshiba Sonolayer 140A-Echo equipment), Sony recorder, an analog/digital interface board (Sound Blaster Pro-16 bit), and a personal computer.



Block diagram of measurement system

In order to take the FFT of a finite Doppler signal, it must be framed with the powers of 2, such as 64, 128, and 256. Windowing technique is used to evaluate the frequency spectrum for the corresponding frame. By using hanning windowing, the appearance of nonexisting frequency components in the spectrum is prevented. In addition, zero padding is applied to the same signal after the windowing process. This entails overhead on the process, although it increases the readability of spectrum. However, the performance of FFT method becomes insufficient for recording blood flow in the stenosis where the speed of blood is high thus causing turbulences. It is also observed that the spectrum becomes wider and frequency resolution decreases in these areas. The long frame length also makes FFT method insufficient in turbulent flow [1].

AR method is the most frequently used parametric method because estimation of AR parameters can be done easily by solving linear equations. Since Burg AR method is computationally efficient and yields stable estimates, PSD estimates of Doppler signals are obtained by using Burg AR method. The method is based on the minimization of the forward and backward prediction errors and on estimation of the reflection coefficient.

Clustering is the method of classifying data or objects within a data universe into different subgroups based on the similarities and the dissimilarities between objects. Clustering algorithms essentially perform two basic functions. They try to keep all objects, which are very close to each other in one subgroup or cluster. At the same time they try to maximize the dissimilarities between the clusters. Fuzzy *c*-means clustering (FCM) utilizes an objective function approach to allow formation of clusters in multi-dimensional space, where a data point is allowed to belong to more than one cluster, with different membership degree [2,3].

In this work, mitral valve Doppler signals which were recorded from aorta valve of 75 patients were used to Burg AR spectral analysis. The classification systems were developed with the application of FFT and AR parameters of mitral valve Doppler signals. Our finding demonstrated that 90.67% correct classification rate was obtained from fuzzy clustering with FFT parameters and 94.67% correct classification rate was obtained from fuzzy clustering with AR parameters.

These results demonstrate that the classification performance of fuzzy clustering with FFT parameters is lower than fuzzy clustering with AR parameters.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

INFERENCE TECHNIQUE BASED ON PRECEDENTS IN KNOWLEDGE BASES OF INTELLIGENCE SYSTEMS

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Abstract. The problem of a decision of the current problem on the basis of the precedents appears in the engineeringand in the medicine. So in the medicine the sick are treated for an illness on the basis of the precedents. In aviations when is using the group of airplanes for decision of the certain problem appears a necessary for the operative choice of strategies of their behaviors. For formalization of the previous successful experience are using:

- a description of the problem by situational vector (SV); the coordinates of the SV are linguistical variables;

- a presentation of the previous experience through the knowledge matrix - an ensemble of the precedents

that was using for the success decisions of the problem. Under operative use the formalized experience description problems is produced by situational vector with quantitative importance of the coordinates - a result of the measurements - a current situational vector. So in the medicine - current importance result analysis sick, in aviations - a results of the measurements, entering from on-board measuring device. On the current situational vector result by means of proposed mechanism pays the vector a priority precedent, recommended for decision of the concrete problem. The precedent with the maximum priority is recommended for use. The time of the arrival of the measurements is usually fixed (t1, t2, ,ti,). Change at time of the condition of the problem and mistakes of the measurement bring about unstable recommendation. For stabilization their is used procedure of the smoothing of the vector of the priorities of the precedents at a certain slithering time lag.

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MATHMOD 2009 Vienna
Abstract Volume

Modelling, Simulation and System Dynamics through E-Learning

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

E-CHO: MANAGING KNOWLEDGE THROUGH PERSONALIZED LEARNING ENVIRONMENT

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There is a rapid change in the concepts of software used for modern e-learning. Unlike the past, this change is not technology driven but by new ways of using modern technology, meaning communicating, collaborating, community building and generating content on behalf of end users [1]. It is expected that e-learning software in the future, such as LMS and other systems used are going to become less and less content delivery systems but more and more content authoring tools, where content and learning is going to be created. Systems used in e-learning will represent one of the nodes in the web network of content. These systems will not be applications installed and maintained by a target organization or company exclusively, but will become personal learning environments, a collection of interoperating systems, adapted to the learners' needs and interests [2]. At the same time need for knowledge management in the corporate and academic environments increases [3]. This calls for integration of additional structured and organized features into e-learning software used. Both tasks are contradictory and difficult to achieve.

At the first part of the paper, innovative aspects of the ICT supported knowledge management systems are described and commented upon. These are based on the Web 2.0 concept, enhancing user generated content as well as new content selection and filtering possibilities (e.g. RSS feeds). As the most popular internet video, blogging and other community based portals generated more digital content than ever before (e.g. YouTube has generated more content in two years than BBC in its entire history), there is a need of fostering quality assessment and content adaptation, so that it could be used for the wider audience, instead of the few selected users that created the content and have luck to find it. In the closed corporate or academic environments new knowledge management opportunities lay in the integration of the Learning Management Systems into existing knowledge resources or information systems of the target environment, thus creating a personalized learning environment for end users. The paper presents case study, based on the integration of the E-CHO Learning Management System into specific academic environment at the Faculty of Electrical Engineering in Ljubljana. At the end of the paper, future research and development work is presented, based on our experience and new learning paradigm, putting learners into the centre of the educational process.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

E-LEARNING GAME USING VIRTUAL AND REMOTE LABORATORY ENVIRONMENT

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Introduction. In the paper an approach to a study of multivariable system control is presented. It has been realized through an e-learning environment, which has been developed at the Faculty of Electrical Engineering, Ljubljana, Slovenia. The introduced e-learning ideas were implemented as a competition game in a frame of laboratory exercises at lectures Multivariable systems. The presented approach bases on E-CHO and Matlab software, which are used for communication with the users, as well as for running both virtual and remote real-time experiments using laboratory pilot plant. Experimental environment enables testing and evaluation of modelling and control design results. Direct extensions are possible in the sense of virtual and remote experiments.

Objective. The aim of this paper is to present a newly introduced e-learning environment in a frame of lectures Multivariable systems. Since for the past few years, the Faculty of Electrical Engineering in Ljubljana, Slovenia, is investing intensive efforts into the introduction of the Bologna study, the introduction of the e-learning platform also initiates the renovation of the lecture program. The main reason for developing the environment was to modify the existing lecture program to make it more interesting and to allow more freedom in students' work organization. The goal of students' work was to design an optimal control structure to achieve stable and satisfying operation of the virtual and real laboratory plant.

Hardware and software realization. For the development of the e-learning environment we used E-CHO framework software, which is in cooperation with Matlab software, responsible for the communication between the system and the users and also for running virtual and remote real-time experiments on a laboratory pilot plant. The pilot plant used in this environment was a Coupled Drive Apparatus TQ-CE108, which seamed to be appropriate for this kind of experiments, since it is complex enough for testing various control structures, but also fast enough to allow short response times. The low-level communication between the E-CHO and Matlab software is based on PHP and MySQL, which are used for setting up a waiting queue, handling execution requests and exchanging the data files. The environment was designed in a manner that allowed students to examine open-loop and closed-loop characteristics of the model and the pilot plant, using appropriate control structures. In this respect, students were given an opportunity to design the optimal control structure.

E-competition. To achieve more interest at the lectures and to stimulate the students to put more effort into the development of the controllers, the introduced e-learining experiment was designed as an e-competition, which consisted of 3 phases. The first phase required the students to answer some questions about the multivariable systems theory. The second and third phase required the students to design an efficient controller for tracking the reference signal on a virtual or a real plant, taking into account the limitations of the control signals. Students were allowed to repeat phases 2 and 3 as many times as they wanted to obtain the optimal control parameters. Each student's best controller was latter used for the final evaluation of their performance, to obtain the first, second and third place of the e-competition.

Future plans. Since the presented e-learning system has been successfully realized and well accepted among the students, further effort is invested into the development of similar systems with other laboratory pilot plants. The presented system is very adaptable and could be, with minimal modifications, used for running virtual and real-time experiments on other laboratory plants. Using several pilot plants and one supervisory computer, it would be possible to build a virtual laboratory, which would allow the students to access the experiments 24 hours a day, 7 days a week and reduce the load in the actual laboratory.

Conclusion. In the paper some ideas are presented regarding the sequential transition from classical to e-education possibilities in the field of multivariable control. The presented e-learning approach was accepted very well among the students, since it allows more freedom in study organization and stimulates the cooperation between the partners of the groups. Therefore, considering the students' response, it is reasonable to invest further effort into the development of such e-environments.

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CAS - BASED E-LEARNING FOR THE IMPROVEMENT OF REFRESHER COURSES IN MATHEMATICS

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Introduction. The sheer increase in scientific output the information age created brought number of serious challenges to university lecturers. Most scientific fields get more and more diverted. Like the ”natural philosophy” drifted apart in the 17th century, forming the various natural sciences of today, the classical disciplines in engineering start to split into sub- and sub-sub-domains, often blurring the borders.

The usual five years of an engineering program are therefore barely enough to teach the basic knowledge plus advanced knowledge for such a very small part of a certain engineering discipline. This leads to an even steeper learning curve, and often to a reduction in the basic subjects which are no direct part of the discipline, especially mathematics.

The lecturers have two choices left: Increasing the workload for the students and alienating them, opening the door for further cuts on the subject, or embracing the technology the 21st century has to offer to optimize their teaching.

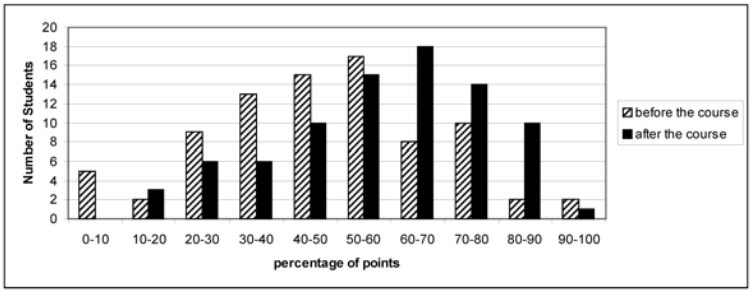
Content. Faced with the aforementioned problems, a new approach was devised at the Vienna University of Technology for students enrolling in the bachelor program for electrical engineering. The conventional lectures were changed to blended learning, and the Maple T.A. software package was introduced into the courses in two steps.

First, a refresher course in mathematics is offered. The content of this course is a balance between the level of the general qualification for university entrance, and the needs of the students in the electrotechnical subjects. It is held in the first three weeks of the first term, allowing students to fill the gaps in their knowledge that would hamper their understanding of the electrotechnical lectures.

The course was held as eight modules covering subjects ranged between basics like canceling of terms and advanced topics like integration. Each module consist of a short lecture, an exercise with a tutor in smaller groups, and a Maple T.A. topic which allows the students to practice on their own. After the first and last module, Maple T.A. was used to test the knowledge of the students. Very similar tests were used, allowing to study the progress of the students during the course.

After the refresher course, the Maple T.A. system is used in the exercises accompanying the mathematics lectures. Conveying calculation skill to the students is mainly done using this online system. This strategy saves valuable time for the lecturer and his or her assistants to instill understanding of the underlying principles into the students, rather then spending their time trying to figure out whether the solution of a particular computation was calculated or just transcribed from another student.

Results. The voluntary refresher course had a very wide acceptance - more then a hundred students attended it. The tests showed that the knowledge of the participants increased about fifty percent during the course, rising from an average score of 3.9 points at the first day to an average of 6 points after the last module, as also shown in the figure. Maple T.A. proved to be a very versatile tool, but showed a few shortcomings when trying to teach very basic subjects.



results of tests conducted with Maple T.A.

The course structure will be developed by creating further modules for other bachelor programs, allowing lecturers to put together courses with respect to the needs of a certain curricula by choosing the modules with the highest benefit for the students.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

E-TRAINING IN MECHATRONICS BY USING INNOVATIVE REMOTE LABORATORY

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Introduction. This paper describes e-training developed for teaching of the mechatronics. The mechatronics is relatively new engineering field which combines the electrical engineering, mechanical engineering, computer science and modern product design methods. However, the number of mechatronics specialists that have already finished a formal education, does not meet the needs of market in the most European countries. In order to at least partially fill that gap in Slovenia, e-training in mechatronics is introduced. The training was developed within the frame of Leonardo da Vinci life long learning programs and MeRLab project (Innovative Remote Laboratory in the E-training of Mechatronics).

Target group. The primary target group are the engineers or technicians who have already completed formal education in the field of mechanical, electrical engineering or other technical fields, but have no knowledge of mechatronics, although their job might require. Training is also suitable for the teachers of the secondary schools who want to pass this knowledge to their pupils, as well as for the regular students of mechatronics and automation in their first year. The training is performed by applying a distance education approach, which is most suitable for the primary target group of learners that are mostly employed in the industry.

E-learning platform and remote laboratory. For the training, special e-learning platform in the user friendly environment which is based on commercial eCampus and on the Moodle platform was built (shown in Figure). The complete materials in SCORM format with the animations, graphical presentations, tests and the utilities like discussion forums are offered to the registered user. Materials are available both in English and Slovene language. Also the remote laboratory experiments are available. The experiments are of crucial importance in the engineering education, since by executing the experiments the learners acquire some practical skills in operating the real systems. Therefore, in the e-learning approach, remote experiments are implemented instead of the hands-on laboratory exercises. In the remote laboratory, the learners operate real mechatronic devices, although they are not physically present at the laboratory. The connection between learner and the laboratory is established trough Web. The remote users can therefore conduct their experiments by accessing the lab at any time that fits their schedule and from any remote location.

Training. The training is divided to four modules: Introduction to mechatronics, Servo motor in mechatronics, Electrical circuits and Mechatronic devices. Each of the modules covers one important topic from the mechatronics and includes a remote experiment. The experiments are executed on various devices which include direct current servomotor, two degree of freedom SCARA robot, analogue passive filters and switched capacitors filters. All together the training lasts about 40 hours. For the evaluation of the training a pilot testing is conducted, which is accompanied with the usability testing.

MeRLab e-learning portal

A WEB-BASED E-LEARNING SYSTEM FOR TEACHING MATHEMATICS AND SIMULATION WITH MATLAB

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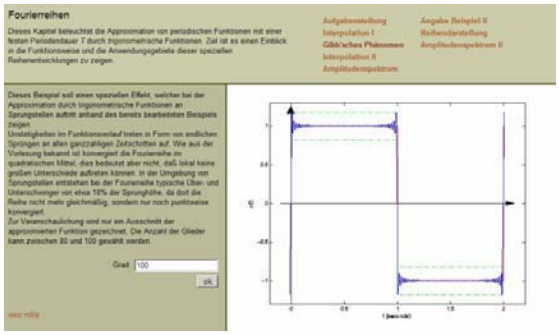
Task. The work presented in this paper deals with the development of a web-based e-learning system for teaching engineers in technical and applied mathematics as well as modelling and simulation of continuous and hybrid systems [1]. The first task and starting point of this system was the discussion, how to combine teaching in mathematics and applications with learning an adequate widespread programming language. The decision was than to use MATLAB because of its ability to solve algebraic problems as well as symbolic computation by using the *symbolic math toolbox* and also offering the feature of an interface for Webserver applications. The user interface is developed in PHP [2] and has a modular structure for fast example implementation and good usability.

Content. As known from theory "learning by doing" is one of the best options. That is why the department for analysis and scientific computing decided to implement an e-learning system for mathematicians and engineers. After a summary of the state of technology we decided to use the web server environment included in MATLAB 2006a. This decision was made because MATLAB is not only a computer algebra package, but has additional tools for symbolic computation and it is wide spread in industry and research.

One of the main goals is to present dynamical models with a praxis interrelationship, which will be explained during the lessons, but should also be available via a web interface for advanced learning at home. Another principle is based on mathematics and computer numeric. For example it is much more comprehensible for students that the associative and distributive laws working with floating point numbers are hurt, when the conclusion is confirmed by interactive examples. In this case it is also important to show the program code in a well known language or provide a description in pseudo code for the homework examples and programming tasks.
Due to licence agreement all students of Vienna University of Technology can buy a single user license. This assures that students can solve problems defined in the lessons on their personal computers. Additionally the lectures are planned in a way that the students learn mathematics and ways how to solve dynamic systems and simulate them, as well as programming in MATLAB. Therefore most blocks on the system include questions and in the practical part of the lectures they have to solve additional examples akin to the predefined. All students have direct access to the source code running on the server. They can download it and run the modified code on their own system.



Screenshot of one included example showing Gibb's phenomenon in subject to the degree of Fourier trigonometric polynomial

Because of a lack of readability of source code including a lot of queries about parameter limits, in our case in MATLAB, a PHP structure is included so that the check of boundaries of input parameters is excluded from the m-file; furthermore it is used for fast implementation of parameter input arrays in each example. The organisational structure of the system is defined in "chapters" as top level. This section comprises a global headline, the list of valid users and a short abstract. The second level is the single example, which is included in a chapter. As a reason of formatting we provide several files for the description text, the parameter arrays and their boundaries as well as for the global example name, the so called navigation label.

The system described in this work is in use for students in electrical engineering, surveying and mapping, mathematics and simulation. Current work focuses on a new server structure for the calculations and on a content management system for content providing.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A Content Management System for Courses on Analysis, Modelling and Simulation

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Introduction. This contribution deals with the developement of a content management system for web-based elearning applications and courses in the field of analysis and modelling and simulation. Our current remote learning system consists of a Matlab web server environment running MATLAB 2006a:

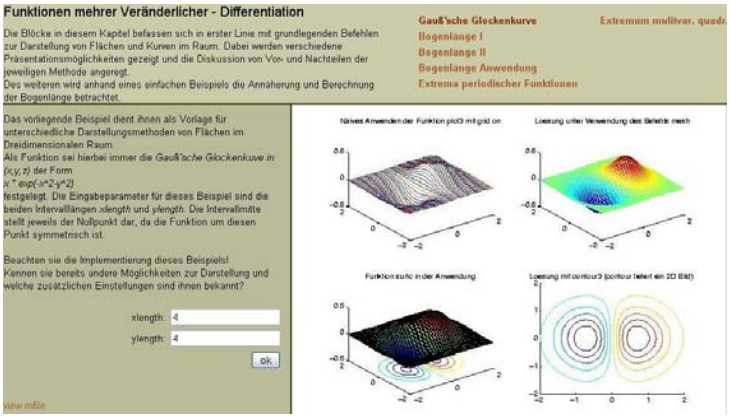

Figure: current MATLAB elearning environment - frontend view

The frontend is programmed in PHP using textfiles for configuration purposes. The examples provided are solely written in MATLAB. Examples can be administered by editing the PHP and configuration files. Access control and user management is realised with htaccess authentification. The environment is used to present courses and single examples mainly for students in electrical engineering, mathematics and simulation, computer engineering and surveying and mapping.

Content Management System. Current work in progress is a new content management frontend, which will improve the usability of the elearning environment. The frontend application is programmed in PHP using a PostgreSQL database for storing configuration data and examples. Adding new examples is possible directly via the web interface. Examples can easily be grouped in categories and courses to provide a structured view both for students and administrative users. User management and access control data is provided by the database structure.The right management system includes user rights as well as group rights. Rights can be granted for single examples as well as for whole categories of examples. The editing facilities used for managing the elearning content are simple and tailored to the specific needs of the system, e.g. parameter input, online editing of the examples source code. The editor provides basic formatting options. The integration of existing opensource editors, such as TinyMCE [2], has not been considered. The evaluated ones tended to have an overhead of functionality, e.g. emoticons and color formatting support, and do not fit most the systems core requirements, although most of them would be easy to integrate.

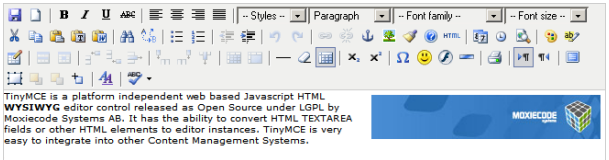

Figure: TinyMCE Panel- Java-based WYSIWYG Editor

Summary. The main task and requirement is to create a user-friendly content management environment, which allows editing and organising of elearning content.The content management frontend should not only support MATLAB content, but also examples and demonstration models written in other server-based programming languages, e.g. JAVA servlets, Octave and Maple content.

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[2] TinyMCE sourcecode and specifications: http://www.tinymce.moxiecode.com

TEACHING PHYSIOLOGICAL ENGINEERING USING A MATLAB-BASED WEB ENVIRONMENT

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Introduction. This contribution deals with the application of a web-based e-learning system in classes, during autonomous learning and as a presentation platform for mathematical models or algorithms. The applications available on our remote runtime environment are focused on the use of special methods or techniques in the field of modelling and simulation or demonstrate rather basic mathematical operations via graphical or textual output. Actually most of the remote programs are implemented in MATLAB and therefore also the programming of these examples can be of interest in education. The source code of all programs is available for students and can serve as basis for an introduction to the programming language. Furthermore the mathematics and techniques of modelling and their implementation are visible on the porgramming level.

Content. Based on the discussion of an example we present and define the aims and options of our system in education. This example is set in the area of physiology and consists in a compartment model for glucose regulation (blood sugar level). We discuss the process of building the model, implementation and simulation and in parallel also focus on aspects of these working stages in education i.e. during courses and autonomous learning.

The Model. Glucose – among other features – serves as energy carrier in many biochemical systems and is crucial for enzymatic reactions. Therefore concentration of carbohydrate is an important and carefully regulated physiological factor. In the human body especially two hormones are involved in the regulation of glucose, namely glucagon and insulin. A high level of glucose concentration leads to insulin production in the pancreas. Insulin favours the inclusion of glucose in the liver and muscles and accordingly serves as downregulator for the glucose concentration. A low level of glucose on the other side triggers glucagon production in the pancreas. Glucagon frees glucose, which has been enclosed in the liver and therefore is an upregulator. A very high concentration of glucose (hyperglycaemia) leads to direct expulsion through the kidney.

A classical formulation of these physiological processes is by a system of differential equations, which describes the concentration of glucose, glugacon and insulin over time. Due to the compartment structure of this model also an equivalent block model (using the SIMULINK environment) can be built.

Both approaches were implemented in order to be executable on the remote environment. Several scenarios concerning diseases and disfunctions of the physiological glucose regulation mechanism were analysed, documented and provided as seperate instances of this program.

Application in Education. As an example in education our model covers

- building and implementing a nonlinear model (ODEs) from a textual model description,
- using a model for dynamical simulation (disfunctions and countermeasures concerning glucose regulation),
- application and implementation of control and regulation mechanisms,
- generating a block diagram (SIMULINK) based on the analytic form (ODEs) and comparing both approaches,
- an example, which can serve as basis for tasks concerning programing, simulation and modelling, and
- an experiment (during courses) for motivating students and to spark interest in modelling and simulation.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

AN E-LEARNING APPLICATION ON CELL AND TISSUE ELETROPORATION

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Electroporation is an electrical increase in cell membrane permeability by means of local delivery of short and sufficiently intense voltage pulses to the target cells or tissues for biomedical and biotechnological purposes [1]. Electroporation is used as an effective technique for delivery of variety of therapeutic agents such as chemotherapeutic drugs, DNA or other molecules, which in normal conditions do not cross cell membrane, into many different cells either in vitro or in vivo. Electroporation is used in clinical electrochemotherapy of cutaneous and subcutaneous tumors, in non-viral gene electrotransfer for gene therapy and DNA vaccination purposes, in transdermal drug delivery and new medical applications are emerging at an increasing rate [2]. In this paper we present a web-based e-learning application which was developed in order to collect, organize and provide the knowledge and experience about cell and tissue electroporation as well as about its medical applications. The e-learning application is based on HTML, JavaScript, ASP and Macro-media Flash technologies and integrated into an interactive e-learning environment (E-CHO) developed at our institution. The E-CHO enables authentication of users, statistical analysis, network traffic measurement, support for video streaming, as well as the use of various types of communications among users, such as forums, e-mail correspondence and videoconferencing [3].

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[3] www.ltfe.org

DISTRIBUTED PROCESS CONTROL SYSTEM FOR DISTANCE LEARNING

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In the field of engineering education, practical experience plays an important role. With the increase in bandwidth through high speed communications, web-based distance experiments can play a significant role in supporting the learning process. Many institutions for engineering education are providing a web-based access to real experimental facilities to their students. Earlier systems, rely on custom software development e.g. cgi/Perl, Java/C++, etc. By those solutions a maintenance and upgrade of the codes become problematic. Furthermore, some system lack real-time streaming capabilities due to the client side control privilege. The more recent implementations of the web experiments are based on existing software platforms such as LabVIEW or Matlab [1], [2]. In this paper we present how the technologies of the remote and distributed control and Web-based SCADA can be exploited for distance learning of courses Instrumentation and Control, Process modelling and Process Identification. Web-based SCADA programs use the latest Internet technologies to help customers to increase plant floor productivities, to improve automation system flexibilities, and to minimize Supervisory Control and Data Acquisition (SCADA) system costs. On the client-side, only the web browser programme is needed to run the user interface (GUI) embedded in web browsers. This architecture ensures scalable and reliable access to our laboratory resources. The bridge between client and server side PCs consists of all professional programme modules and technologies, which are often used in industrial automation projects.

During an experiment session, users can normally change some parameters, observe the results and download data. To make the remote experiment sessions more stimulating a live webcam window is provided. Students can watch the real process in such window, having a most sense of presence in the laboratory. For video transmission, the web camera software is used, which can display on-line video, and it is not necessary for the user to install special software on the client side to perform this task. The user interface of such a remote laboratory experiment is presented in Figure 1.

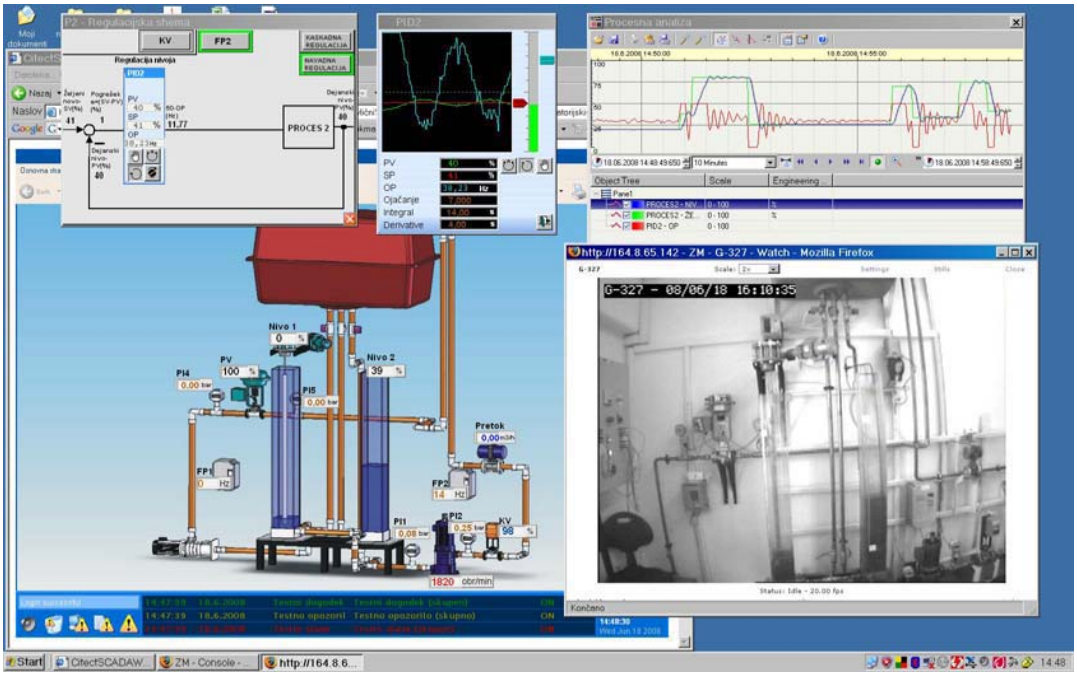

Figure 1. The user interface of remote laboratory experiment.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

E-LEARNING BASED M&S CURRICULUM TO ACHIEVE A SUSTAINABLE DEVELOPMENT OF HIGH QUALITY UNIVERSITY EDUCATION AS PART OF THE UNIVERSITY REFORM PROGRAM IN ETHIOPIA

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Introduction. In seeking to overcome poverty by 2015 – which is the so called MDG 1 (Millennium Development Goal), the "Ethiopian Industrial Development Strategy" (August 2003) stresses the need for industrial development. Capacity building has been identified as key factor in achieving this goal. Consequently a strategy for a comprehensive "Engineering Capacity Building Program" (ECBP) in Ethiopia has been developed by the Ethiopian government, represented by the Ministry of Capacity Building (MoCB). ECBP formulates a mission and corresponding objectives, and identifies four strategic areas of intervention, so called components, and lists key issues for each of these components. One of the four strategic areas of this ECBP, that has been developed and approved by the respective stakeholders, focus on the University Reform Component. Background for this component is a fundamental rethinking on all levels of higher education with the result that radical redesign of studies are necessary to achieve significant improvements in professional performance of university graduates.

As a result of several discussions of this ECBP University Reform Component on how to improve the nationwide education situation in a short time scale, it was decided to adopt the e-Learning concept. Henceforth, a project was initiated introducing e-Learning at the FOT´s of Ethiopian Universities with the target of awareness creation and trainings, to encourage instructors to deliver e-Learning courses and starting with the first steps towards institutionalization. As a result of a feasibility study this approach will not allow running e-Learning at a big scale within short time. It will be a process in slow motion. Henceforth, an additional strategic component was perceived being necessary to achieve the primarily target which take into account the possible use of already existing materials for e-Learning content and courses available on the web which fulfils the pre-accredited curricula at AAU FOT in order to identify international available e-learning courseware that can possibly be used. This emanates from a general agreement on leveraging the use of information and communication technology (ICT) in the learning and teaching process. Nevertheless, ICT-supported education or e-Learning, as ostensibly promising as its candid merits excels, requires also research through construction of models and simulating the scenarios as well as piloting realistic schemes.

Important didactical elements for the composition of content within an authoring and learning environment are simulation models.

The pivotal demands a simulation coupling within a learning environment must satisfy are:

- quality assurance of the models
- platform independency of the clients and a web-based access to the model
- customisation of the user interface and the level of detail depending on the learners background by the author
- multi-user access to models and a user specific administration of simulation runs and results

The advantages and disadvantages of typical solutions to integrate simulation models into e-Learning environments (reprogramming in a new programming language, using a terminal client, etc.) need a specific system architecture

Embedding simulation in a client/server architecture has proven to be the best solution and achieves the demands mentioned before for coupling simulation with a learning environment.

Identifying open courseware content and it's customization and reuse is an approach that allow running e-Learning at a big scale within short time. Integrating e-Learning with modeling and simulation is an ideal problem-oriented learning strategy.

WEB-BASED DISCRETE SIMULATION SERVICES FOR EDUCATION IN MODELLING AND SIMULATION

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Introduction. The radical increase in new web technologies have preluded a new era of web application programming using modular software libraries which distinguish between the content of a web application, its presentation, and its actual behaviour towards user interaction. The current common web browser generation is capable to deal with dynamic content and asynchronous parallel communication with these services. This paper introduces a software architecture for a discrete event oriented simulation environment which mainly gets its modelling input via a web browser. The idea is to develop a concept for modelling and simulation for e-Learning based academic lectures in terms of teaching simulation exercises.

Content. The features which modern web technlogies like AJAX (Asynchronous Javascript and XML) do provide are commonly referred as Web 2.0. Browsers which can deal with Javascript code based on the *XmlHttpRequest* programing interface can visualise and update data from a webserver without reloading the whole web page again. The application framework classifies four different modules:

- the user interface for human interaction
- the generation of data code which is transferred to the remote simulator
- the execution of asynchronous remote procedures over XML
- an embedded platform for human utilised resources like wikis, tutorials, screencasts, and WYSIWYG modelling graphical user interfaces.

The AJAX-based user interface for modelling, data manipulation, and controlling the simulation process is designed in Java using the UI-elements of the GWT (Google Web Toolkit). The goal is to minimize the effort and time the student/developer invests to be familiar with libraries and functions of a certain simulator. The parametrization of the model is allocated with the visual tools the web application creates on the client side. As the web client can exchange the modified data within the web server in the background the whole page has not to be reloaded at every request. Thus the user can easily design relationships between the entities of its model like cardinality, dependencies, etc. with a What You See Is What You Get (WYSIWYG) editor.

The objects which act in the simulation operation are translated to the semantic representation of the JSON (JavaScript Object Notation). Events and instances in discrete simulation can become very complex regarding their relationship towards each other. A formal description language is often bound to restrictions and regulations of the actual simulator working in the background. The translation of an Javascript object into its JSON format reduces the computational overhead which is created while parsing XML. Furthermore most of the common programming languages provide bindings to assimilate with JSON-encoded objects, so that cross-site simulators on different web servers can be integrated dynamically.

The interaction of the web client with the simulator is conducted in different steps. Besides the encapsulated encoding of the data the framework also qualifies to execute remote methods on the server via the XML-RPC (XML Remote Procedure Call) specification which is much faster and not so heavy-weighted like a SOAP infrastructure. Thus the web application remains fast and tiny which makes it applicatory for student labs where lots of users work simultaneously in the same networking environment. The data shipped to the application server is extracted and assigned to the according session of the simulator. A simulation translater which plays the role of a semantic middle layer generates callby messages and passes them on towards the simulation engine. This structure facilitates the compatibilty and commutability of different simlators.

E-Learning platforms are often attached with static artefact management: assignments, files and other resources are linked on webpages to offer teaching support. Now that this application service already includes the simulation interfaces with exportedability features, the student can analyse recorded simulation executions as part of a tutorial or debugging facility. Screencasts can introduce the student how to use the framework. And the teaching staff can remotely mark, examine, and comment on the simulation experiments.

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Modelling of Fuel Cells and Chemical Engineering Applications

DYNAMIC MODELING AND SIMULATION OF LOW DENSITY POLYETHYLENE PRODUCTION - A COMPARATIVE STUDY

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This study deals with the modelling and simulation of low density polyethylene (LDPE) production. LDPE is one of the most widely produced polymers which appears in the form of simple goods in our everyday life (eg. food and pharmaceutical packaging, carrier bags). It is produced in a complex industrial process which takes place under extreme operating conditions (at pressure between 2000-3000 bar). It can show intricate nonlinear dynamic behaviour due to the high exothermicity of the chemical reaction in combination with some internal recycle loops, which requires some stabilizing control.

Usually, such a plant receives the raw materials from upstream processes which may cause load changes in the LDPE plant. It is important to maintain the product quality in the face of such load changes. Furthermore, in such a plant, typically more than 15 different grades of product with different product properties (density, melt flow index etc.) may be produced. In order to follow frequently changing market demands it is necessary to follow an optimum grade transition policy during manufacturing different polymer while maintaining a profitable operation. These issues emphasize the significance of control tasks for the LDPE plant and subsequently the significance of suitable process models which can be employed for control purposes. Earlier works for optimization based control utilize steady state models only [1]. However more recently it is possible to use dynamic optimization methods within the framework of nonlinear model predictive control (NMPC) based on dynamic models. Although first steps have been made in this direction [2], the size of the mathematical model arising from the distributed nature of the LDPE plant remains a challenging issue.

The objective of this study is to provide a benchmark model of the LDPE plant with a reasonable model size which can be useful for optimal control approaches. Therefore first a detailed reference model developed in our group [3, 4] is reviewed and then possible model simplifications are introduced systematically. The reference model of the LDPE plant is represented by a distributed system with an external coordinate (reactor length) and various internal coordinates (the chain length of the polymer molecules, short and long chain branching and the number of double bounds), which can have strong effect on product properties. This model describes the heat transfer in detail in addition to including material recycles, both of which are shown to have influence on the plant dynamics. The experience gained on the process via reference model is used to make necessary model simplifications. The simulation with the suggested simple model are carried out to analyse the effects of heat transfer, the types of initiators and modifier on the state profiles and product properties. Results of the simple and reference models are compared and conclusions are drawn.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODEL REDUCTION TECHNIQUES FOR THE SIMULATION OF PARTICLE POPULATIONS IN FLUID FLOW

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Crystallization denotes the formation of solid particles from a solute dissolved in a liquid solvent. Crystallization is one of the most important processes in chemical and pharmaceutical industry. The majority of chemical products and even more than 90% of pharmaceutical agents are produced in crystalline form. Furthermore, crystallization is an intermediate step used for purification in many chemical production processes.

Usually crystal properties like characteristic size or shape determine the quality of crystalline products. Therefore the main task of design and control of crystallization processes is to generate particle populations with desired property distributions. Property distributions change due to various physical phenomena like nucleation, *i.e.* formation of new crystals, crystal growth, breakage or agglomeration. All these effects depend strongly on the interaction between fluid flow and particle phase. A realistic mathematical model of a crystallization process must account for transport processes in the liquid phase and in the solid phase as well as for the coupling between both phases. The model has to describe fluid dynamic effects in up to three space coordinates or external coordinates and in addition the development of particle populations along one or several internal coordinates like *e.g.* the characteristic particle size. The resulting high-dimensional models are very complex. For many applications in the field of model based process control such detailed models are hardly suitable. Instead, there is a need for low order models capable of predicting the key features of a crystallization process in the relevant operation window with reasonable accuracy. This work aims at developing such models.

The model reduction process consists of lumping in the external coordinates as well as in the internal coordinates. For both sets of coordinates reduction techniques are available in literature. As a new approach these techniques are combined in this work in order to make them applicable to particle population processes in fluid flow. For the reduction of internal coordinates, the method of moments is an established technique. For the external coordinates, Proper Orthogonal Decomposition (POD) is used. The POD method is a technique which can be used to obtain the overall behavior of a process system. The method yields a basis which represents simulation or experimental samples of a reference full-order model. The resulting basis can be considered as optimal in the sense that the first terms contain more "energy" than the same number of terms from any other basis. A reduced-order model can be constructed by a Galerkin method with a POD eigenfunctions basis. By varying the number of basis eigenfunctions, the order and the covered "energy" content of the reduced model may be specified.

As an application example for the described model reduction technique, a simple model of a urea crystallizer is used. The process is modeled by incompressible Navier-Stokes equations coupled with a mass balance for the dissolved urea and a population balance equation (PBE) for a dispersed phase distribution. With help of the method of moments the population balance equation has been reduced and converted to convective-diffusion equations for two moments μ_0 and μ_1 of the crystal size distribution. The reduced ODE system has 18 equations that corresponds to a system order reduction ≈ 500 times while reduction in the computation time reduction is about factor 5. The low computation time reduction can be explained by nonlinear terms for growth and nucleation that require projection to the reduced basis space for every evaluation of the right-hand side in an ODE solver. The resulting reduced low-order ODE model may be used further for control, optimization or parameter identification purposes.

Optimal Experimental Design and Model Selection by a Sigma Point approach

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Complex biological systems can be described and analysed by deterministic models. The process of model development requires not only knowledge about the model structure but also about related model parameters θ. Even with a suitable model structure, parameter identification can be a challenging task. Uncertainty about experimental data leads to uncertainty about estimated parameters $\hat{\theta}$, consequently, the estimates can be represented by confidence regions instead of single values. To get meaningful models these confidence regions should be as small as possible. For this purpose, Optimal Experimental Design (OED) provides new experimental conditions, e.g. the system stimuli $u(t)$, resulting in more precise estimates.

To define a cost function for Optimal Experimental Design, it is necessary to express the parameter uncertainties by mathematical terms, leading to the (co)variance matrix $C_{\hat{\theta}}$ and the mean $E[\hat{\theta}]$ of the estimated parameters. A frequently applied method for this is based on the inverse of the Fisher information matrix (FIM). However, this method leads in many cases to a poor approximation of the parameter (co)variances and does not provide any information about the mean. To find a more realistic approximation of the parameter statistics, methods have been developed, which are based on Monte Carlo simulation as the Bootstrap approach and the Global Sensitivity Analysis (GSA). These approaches have a very high computational effort, which prohibits their use in the framework of OED. A more suitable approximation can be achieved using the Sigma Point method [1], which has been introduced recently in the field of OED [2, 3]. Julier and Uhlmann suggested the use of the Sigma Points in order to determine the mean and (co)variance of a random variable $\eta \in \mathbb{R}^l$ from the mean and (co)variance of a random variable $\xi \in \mathbb{R}^f$, where η is related to ξ by the non-linear mapping $\eta = g(\xi)$. Adjusted to parameter identification, ξ represents all available measurement data[1], $g(\cdot)$ stands for the complete parameter identification process and η is the resulting vector of estimated model parameters. By using this analogy, the Sigma Point method can be applied directly to calculate the mean and the (co)variances of $\hat{\theta}$.

Moreover, the basic concept of the Sigma Point method enables the investigation of the influence of parameter uncertainties on simulation results $x(t)$. The determination of confidence regions of the dynamic states becomes possible and can be used to evaluate novel cost functions for the OED process. Beyond this, the confidence regions of the states provide an efficient and elegant way to take the imperfections of parameter estimation in the field of model selection into account. For this purpose, an overlap can be defined (Fig.1) that should be as small as possible to distinguish between competing model candidates (Fig.2). All aspects are demonstrated for a biological substrate uptake model.

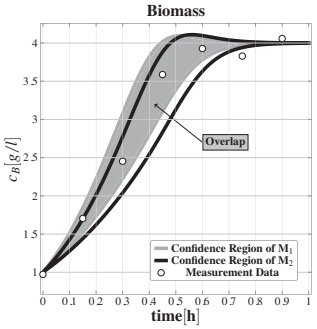

Figure 1: Unsuitable initial conditions for model selection lead to confidence regions of both model candidates M_1 and M_2 that cover nearly the same state space, i.e., large overlap.

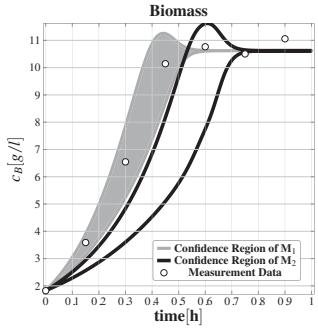

Figure 2: By minimising the overlap, the two model candidates M_1 and M_2 become distinguishable related to measurement data.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A 2+1D MODEL OF A PROTON EXCHANGE MEMBRANE FUEL CELL WITH GLASSY-CARBON MICRO-STRUCTURES

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Introduction. A PEM fuel cell transforms the chemical energy liberated during the electro-chemical reaction of hydrogen and oxygen to electrical energy. Physical processes in a PEM fuel cell include the transport of the gas species, water, heat, and electric charge. Oxygen is reduced on the cathode side, and hydrogen is oxidised on the anode side in the electro-chemical reactions. A comprehensive fuel cell model needs to take these coupled transport processes into account. Moreover, transport of the reactant gases (oxygen and hydrogen) to the catalyst layers is mostly established using flow-field channels of serpentine shape. This leads to a complex shape of the in-plane model domain of the fuel cell.

Modelling of the transport processes and the electro-chemical reactions results in a highly nonlinear coupled system of PDEs. There is a high aspect ratio between the in-plane dimensions and the through-plane dimensions. Therefore, discretising the cell geometry in three dimensions results in a very high number of DOF variables, and thus complicates parameter studies. In contrast, the "2+1D" approach presented in this paper significantly reduces the number of degrees-of-freedom (DOF) variables in comparison to a full 3D discretisation of the PDEs.

2+1D model approach. The gas flow channels and bipolar plates of the anode and cathode are discretised in two dimensions. Coupling between the anodic and cathodic side is established by a 1D model representing the membrane electrode assembly (MEA). Coupling between the 1D model of the MEA and the 2D models is achieved by using the values of the DOF variables of the 2D model as Dirichlet boundary conditions of the 1D model.

The 1D model of the MEA and the GDLs is created from the symbolic weak form expressions of the coupled transport phenomena. The integrands of the tangential element stiffness matrix and the element residual vector of the coupled FEM problem are computed analytically by the computer algebra software Mathematica. In this way we obtain a nonlinear system of equations that model the MEA. The expressions for the tangential stiffness matrix and for the residual vector are converted to the programming language C by Mathematica and used to assemble the system matrix. Finally, a nonlinear coupled 2+1D problem is solved for with our FEM code SESES [1].

Simulation. The 2+1D FEM model is applied to simulate a simplified micro polymer electrolyte fuel cell without gas diffusion layers with an active area of $1cm^2$. The gas flow-field of this fuel cell is made of micro-structured glassy carbon plates. Simulation results for operation at an average current density of $250mA/cm^2$ are presented. The electric current density of the 2D domains in the through-plane direction is shown in Fig. 1. This current density is predicted by the 1D model, that is, in the direction perpendicular to the cell area. The current density is lowest near the gas inlet (top right), it increases to a maximum value in the cell center, and decreases towards the gas outlet (top left). The minimum value near the gas inlet is due to a low value of the membrane water content, i.e. the protonic conductivity in this region is lowest here. An increase of the membrane water content is found in the cell center.

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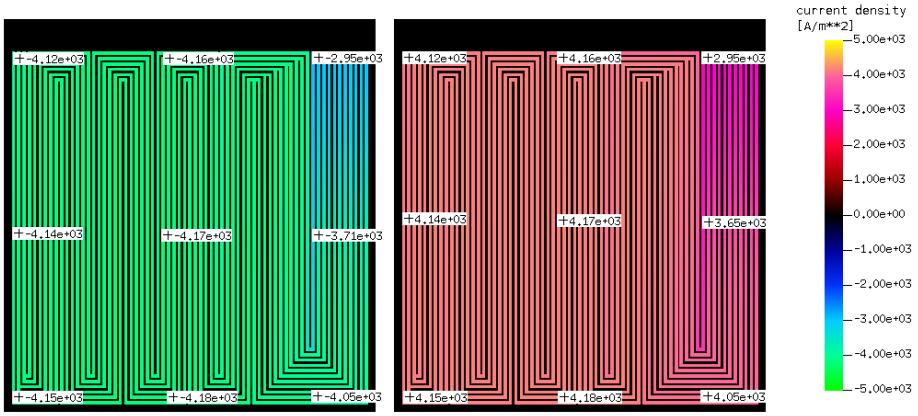

Figure 1: Electric current density of a micro PEM fuel cell in the through-plane direction (left: anode, right: cathode).

FASTER LOAD CHANGES FOR MOLTEN CARBONATE FUEL CELL SYSTEMS

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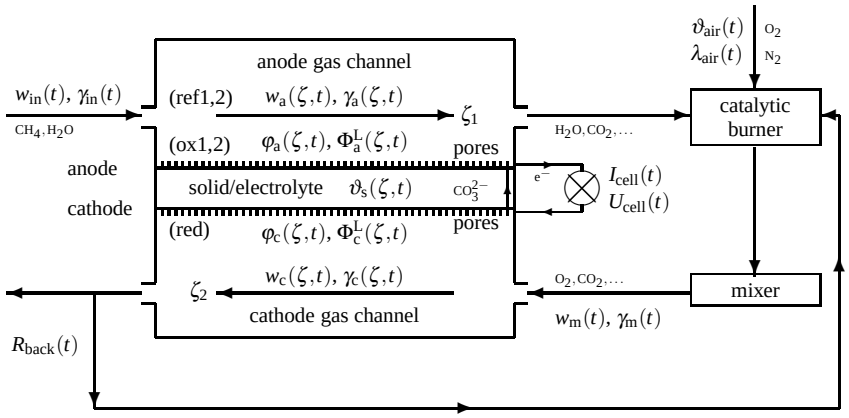
Molten carbonate fuel cell systems (MCFC) are an efficient and environmentally friendly technology for the simultaneous stationary production of electrical energy and heat (resp. cooling).

MCFC belong to the class of high temperature fuel cells. The operation temperature is about 600ºC. In contrast to low temperature fuel cells, the temperature is high enough to allow for internal reforming, i.e. to produce hydrogen internally in the cell system from different kinds of fuel gases (e.g. CH_4). Moreover, neither expensive catalysts nor expensive ceramics are needed for an efficient operation. Due to the high operating temperatures, it is difficult to operate MCFCs. One has to stay within a certain range of admissible temperatures. Chemical and electrochemical reactions decelerate in regions of low temperature, whereas in regions of high temperature fast catalyst degradation appears. Temperature gradients have to be moderate in order to avoid material corrosion due to temperature induced stresses. Therefore the cell temperatures are crucial for the system's performance and lifetime.

MCFC systems are being developed and tested by several companies around the world and can be expected to become competitive to classical power plants within the next few years. Nevertheless, efforts are necessary to increase their efficiency, to develop better control strategies, and to improve long time stability. Besides experimental validations, mathematical models are an indispensable tool to achieve these goals. Potentially dangerous or even disastrous control scenarios for real stacks of fuel cells can be safely simulated by means of mathematical models. Realistic mathematical models (Heidebrecht) based on *physical* and *chemical laws* have paved the road to apply mathematical optimization and optimal control techniques [2]. Moreover mathematical models allow to study the consequences of modified designs in advance such as crossflow versus counterflow designs or different (optimal) catalyst distribution.

We describe the mathematical model and the approach to compute numerical results. We present and discuss the steady state solution as well as an optimal controlled faster load change of the molten carbonate fuel cell. This is a hard problem, due to the dimension of the (degenerated) integro partial differential equation system and the different time scales of the variables.



(ref1) $CH_4 + H_2O \rightleftharpoons CO + 3H_2$ (ref2) $CO + H_2O \rightleftharpoons CO_2 + H_2$
(ox1) $H_2 + CO_3^{2-} \rightleftharpoons H_2O + CO_2 + 2e^-$ (ox2) $CO + CO_3^{2-} \rightleftharpoons 2CO_2 + 2e^-$
(red) $\frac{1}{2}O_2 + CO_2 + 2e^- \rightleftharpoons CO_3^{2-}$

Figure 1: 2D crossflow model of a molten carbonate fuel cell with variables $w = (\chi, \vartheta)$, χ =vector of molar fractions, ϑ =temperature, φ =vector of partial pressures, Φ =electrical potentials, U_{cell} =cell voltage, I_{cell} =cell current

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Modelling in Physics and Natural Sciences

A QUANTISTIC MODELLING OF WINE EVALUATION IN OENOLOGY– *PROBABILITY ANALYSIS*

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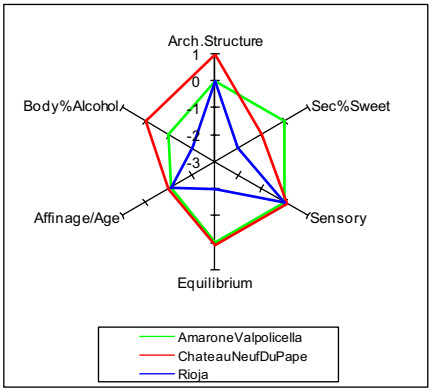
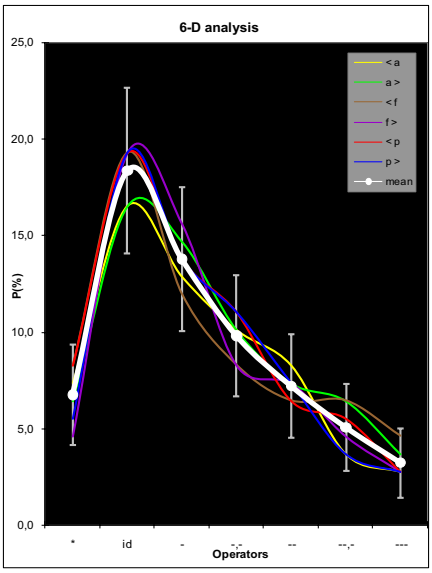
Executive summary. This paper describes a formalization of the essential organoleptic characteristics assessed in the wine evaluation process. A scalar quality metrics is associated and bound to 3 dimensions and 6 variables representing standard organoleptic wine features detected by mouth-tasting. The correlation existing between such wine characteristics is mathematically modelled by a matrix of operators' values acting on the corresponding variables. An algebraic notation is developed to express the multi-dimensional nature of the wine quality and to provide a measurement tool for the still subjective evaluation of a wine. Probability distributions are computed for the values measured on a sample of over 100 wines in order to test the metrics performance in terms of phase-space and bias. The statistical meaning of the empiric distributions obtained by applying such a wine evaluation metrics is analysed by benchmarking them versus well-known theoretical mathematical conditions: this reverse-engineering of the metrics allows the factorization of the intrinsic metrics features from the effects due to the interaction with the "observer" and his preferences. Finally, the relation between independent and correlated quantities for wine evaluation is emphasized, and a conditional probability model is proposed.



Graphical notation.

Definitions and metrics. Let us define Q to be a scalar expressing the overall quality of a wine by assuming the values: Q = [0.1; 0.2; 0.3; 0.4; 0.5; 0.6; 0.7; 0.8; 0.9; 1.0; 1*; 1**; 1***]. The range of Q can be transformed to an integers' space: Q = [-9 ; +3]. Let us define α, ϕ, π as 3 independent dimensions in the evaluation of wine characteristics: α = *Architecture* ; ϕ = *Finesse* ; π = *Power*. Each dimension holds two correlated signed directions and operators, identified as < and > , representing and valuing the organoleptic variables of the wine: $<\alpha$ = *Complex* ; $\alpha>$ = *Harmonious* ; $<\phi$ = *Sec* ; $\phi>$ = *Fined* ; $<\pi$ = *Sensory* ; $\pi>$ = *Bodied*. Let each operator apply the values [+1; 0; -1; -2; -3], also noted as [* ; *id* ; - ; -- ; ---], to the variables above. The correlations between the paired variables are modelled by constraining each of the α,ϕ,π dimensions to assume the patterns: [*X; X*; X; -X; X-; -X-; --X; X--; --X-; -X--; ---X; X---]. Hence the total number of allowed combinations by the metrics for expressing a wine evaluation is: 12^3=1728. The sum of the 6 operators on the three α,ϕ,π dimensions is contained in the range [-9;+3] and it coincides numerically with the Q value, thus binding a scalar measure to the multi-dimensional wine system. Example: Q=0.7 [*α -ϕ-- π-]. Such algebraic notation $[_i\alpha_j\ _i\phi_j\ _i\pi_j]$ maps to a graphical representation.



Probability for operators on α,ϕ,π.

Analysis and Probability. The statistical distribution of the scalar wine-quality measure is found to be quantitatively determined by a pure combinatorial effect (due to the binding to the organoleptic 6-dimensional system), superimposed by the effect of an observer-specific sampling of the wines phase space. The mathematical meaning of the interaction of the "observer" (human evaluating the wine subjectively), with the system represented by the sample of wines being "measured", is quantified and plotted in the figure. The probability of finding any of the values +1,0,-1,-2,-3 (or *, id, -, --, ---) on a side of α,ϕ,π, regardless what value appears on the opposite side, is: $P(i) = \sum_j[P(_iX_j)] = \sum_j[P(i\&j)]$, where: $X=\alpha,\phi,\pi$; i,j=+1,0,-1,-2,-3. A conditional probability model is developed to relate P(i) to the 12 operator patterns. Example: $P(\text{--}X) = P(\text{-- } \& \textit{ id}) = P(\textit{id}) \cdot P(\text{-- } | \textit{ id}) = P(\text{--}) \cdot P(\textit{id}) \cdot [1 - P(*) - P(\text{---})] \cdot [1 - P(*) - P(\text{--}) - P(\text{---})]^{-1}$. Such a modelling matches the empirical mean values in the figure with a precision at the level of few percent.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MATHEMATICS AND EGGS – DO THOSE TWO TERMS HAVE SOMETHING IN COMMON?

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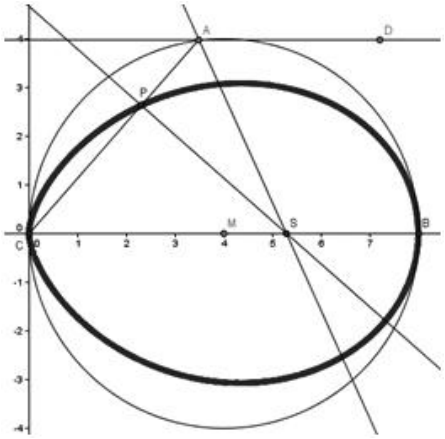
The importance of application-oriented contexts in mathematics education is without controversy.

Solving problems in proper application-oriented contexts is – contrary to vested problems – always completely or at least in parts connected to a modeling cycle. The concept of modeling in mathematics education is one of the fundamental ideas, which should be presented to students and discussed with them by using interesting problems, which can be found in students' life-world.

By modelling objects of daily life in mathematics education the subject mathematics could be experienced as a motivating and fascinating part in education. For this reason the paper shows a possibility, how an object which is common to all students in school, the egg, can be an item for an exciting discussion in schools.

Based on two mathematical definitions a figure is constructed with the help of dynamical geometry software (DGS). Following the definition the egg-curve can be constructed by using the dynamical options.



Egg-curve, constructed with DGS

Based on this fact the description in polar-coordinates and Cartesian implicit equations is developed.

By following the stepwise modelling cycle of Blum it can be shown, that the way of modelling of daily objects can be done in school and demands of curricula can be implemented.

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MODELLING OF THE DRIVING PROCESS OF L-SHAPED METAL SHEETS

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Introduction. The Driving process nowadays is based on an incremental method for sheet metal forming with significantly reduced investment expenses. This technique which has not yet had much relevance in scientific considerations is one of the oldest metal forming processes available and has been used for centuries. The Driving has a highly interactive process [2], in which material properties are changed by work hardening and where contact conditions are varied with every stroke. After a multitude of strokes, the shapes of the metal sheets suffer from accumulated inaccuracies. But in controlling or automating this forming process, an analytical model should be given to yield the corresponding parameters. Furthermore, such a model brings more knowledge of the internal forming procedures of the metal sheets, while FE model has not the ability to calculate the parameters due to its natural limitations and to be used in real-time control system. Hence, the driving process will be analytically modelled in this paper, although the high process interactions are mentioned in the above.

Modelling. Using the driving machine, the L-shaped metal sheets can be stretched or shrinked in processes by means of hammering strokes on the metal sheets. During every forming stroke, the tools clamp the sheet and transform the vertical stroke into horizontal movement and by that induce tensile (stretching) or compressive (shrinking) stress into the sheet. The forming force can be applied manually or automatically by tuning the stroke depth, which denotes the distance between the upper and the lower tool part. In this paper, only the stretching process will be modelled.

Geo-Model of the L-shaped Metal Sheets. The L-sheet has two flanks and the transition zone between the both. In the forming process, the material of the upper flank is extended in the plain at the stroke position but with different rates. The nearer the stroke point is located at the transition zone, the less the flank is elongated. For the geometry approximation of the L-sheet, it can be seen as the combination of the two flanks that have a common edge with a constant length and the transition zone is replaced with constraints.

Material Model. There are altogether six material models that can describe more or less the real forming process [3]. The often used, simple model is elastic-ideal plastic. But it is suitable for the mixture of the elastic-plastic forming. Furthermore, the elastic-real hardening model is employed for the pure material flow.

Tool Model. The tool has two parts that press the sheet together so as to transform the vertical force in the horizontal direction. Each part has two movable sections that can be pushed horizon-tally to the sides by the transition elements of the tool parts.

Model of the Forming. By a hammering stroke, the upper tool moves downwards to the upper surface of the L-sheet and brings the force into the L-sheet successively. There are three phases in the total process. In the first phase, the two flanks from the approximated geometry model of the sheets are formed till the flow limit of the material. The second phase indicates the material flow procedure that happens simultaneously in both parts. With the decreased force on the L-sheet, the two flanks spring back in the third phase, where the reverse bending can be caused in one of the flanks [1].

Results The model is evaluated under the experiments using standardized L-sheets. The force progression on stroke depth and the stress-strain curve are obtained through a force dynamometer and a flat drawing trial respectively. In comparison with the results of the experiments, the simulation results match very well and the difference of the bending angles lie actually in the tolerance band, although there exist many approximations in the modelling. This model can then be used in improv-ing FEM simulations, controlling of the production process or the other model based applications.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A TOOL FOR THE AUTOMATIC MODELING OF CAPACITIVE MEMS GYROSCOPES

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Introduction. Since Micro-Electro-Mechanical-Systems (MEMS) are complex devices, the systematic derivation of an appropriate mathematical model is a challenging task. In general, MEMS comprise components or sub-systems from different physical domains like rigid and elastic mechanical structures, capacitors, inductors, optical and fluidic elements. Therefore, one has to deal with the adequate laws of continuum mechanics, electromagnetism and thermodynamics in order to derive a suitable mathematical formulation.
The demands on the mathematical models vary strongly with the intended applications. In order to understand the basic mode of operation, typically lumped parameter models are used, which in general are insufficient in terms of accuracy. By means of the Finite Element Method (FEM) on the other hand it is possible to reproduce the dynamic behavior at a high level of detail, even if the geometry of the device is complex. Therefore, such models are used in a broad range of applications such as the analysis of elastic mechanical structures, the determination of thermodynamical interactions, the calculation of electrostatic and electromagnetic fields, etc. This method, however, has the disadvantage that the resulting system of differential equations is very large and therefore can neither be used for the controller design nor for transient simulations within reasonable time. For this reason, considerable research activity has been conducted in the field of model order reduction techniques. Thereby, lower order systems are derived still representing the essential dynamic behavior of the large scale finite element models with sufficient accuracy. The drawback of these techniques is that the systematic order reduction of non-linear systems, which we have to deal with when modeling capacitive actuators and sensors, is still an open issue. An alternative approach to receive a mathematical description with a reasonable number of state variables is to partition the device into functional components (e.g., rigid bodies, elastic bodies, lumped capacitors, etc.) before deriving the actual mathematical representation.
Although there are several commercially available simulation environments which cope with the mathematical modeling of MEMS, none of these tools is capable of extracting a symbolic representation of the device under consideration. In view of this shortcoming, a software is presented in this paper to derive the non-linear mathematical model of capacitive gyroscopes in a symbolic form from the geometry data available from CAD tools.

Mathematical Concept Based on the partitioning of the device under consideration into its functional components, i.e., rigid bodies $\mathscr{R}_\alpha$, elastic bodies $\mathscr{E}_\beta$ and capacitors $\mathscr{C}_\gamma$, the derivation of the equations of motion of the device will be introduced by means of the well known Lagrange formalism.

Software The proposed software tool is composed of two parts. The first part, *SimMEMS*, is implemented in the object oriented scripting language *Python* [3] and provides the functionality to extract the necessary information from the geometry data to represent the device under consideration with the introduced mathematical elements. To make the analysis steps comprehensible, all objects can be visualized in an integrated 3D viewer. Additionally, to make the software as flexible as possible an interactive interpreter and an editor frame have been added such that all objects can be arbitrarily changed and scripts for reusable tasks can be developed.

The second part, *ModelMEMS*, is implemented as a library in the commercial computer algebra system *Maple* [1] and provides a symbolic mathematical model of the introduced elements. Since *Maple* is used as the calculation engine, all calculation steps can be performed symbolically and/or, if desired, with arbitrary precision arithmetic. In general, a symbolic representation leads to a better understanding of the overall system behavior, prevents numerical inaccuracies and thus also preserves the mathematical symmetries found in these devices.

For the further controller design and simulation of the closed-loop behavior in MATLAB/Simulink [2], a *Level 2 C-Code S-Function* simulation model can be generated from the mathematical model by the integrated code generator.

Acknowledgments
This work was funded by the German BMBF as part of the EURIPIDES project RESTLES (project nr.: 16SV3579).

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CFD MODEL AIDED DESIGN OF PERSONALIZED AIR SUPPLY FOR AIRCRAFT CABIN SEAT

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Introduction. The Computer Fluid Dynamics (CFD) model presented in the paper has been developed in the framework of the FP 6 EU Project SEAT aimed, among other, at providing an optimal micro-environment for the individual passenger during long-distance commercial flights. The objective is to supply each of the aircraft passengers with fresh and humidified air to prevent them from possible health problems. Unlike the standard environment control systems commonly used in commercial aircrafts each of the seats in the aircraft cabin is supplied individually with a separated air flow which forms a personalized microclimate in the seat area.

Concept of personalized air distribution. The presented micro-environment control consists in supplying each of the aircraft passengers with "his/her own" ration of fresh and humidified air with the aim to prevent him/her from possible health problems [1]. Unlike the standard environment control systems commonly used in commercial aircrafts each of the seats in the cabin is supplied individually with a separated air flow which forms a personalized microclimate in the seat area. Focusing the personal air supply into the breathing area of the passenger is based on the principle of Penot nozzle [2].

CFD model based design The role of the CFD models was decisive in the research. From the model experiments with varying the air flows focused on the seated manikins it turned out that it is possible to provide each passenger with "his/her own" fresh air despite one half of the air supply is re-circulated.

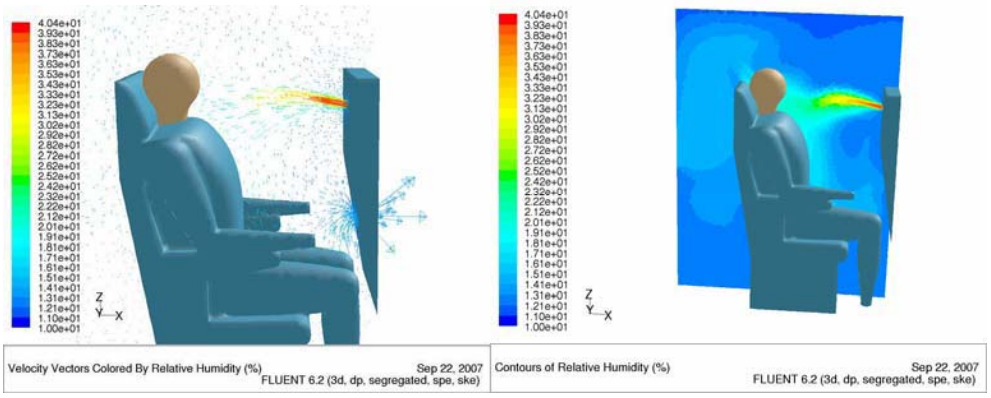

Figure Air velocity and relative humidity visualization in the personalized air distribution system, results of CFD models.

Conclusions The proposed concept of personalized air distribution in the aircraft cabin has been validated on laboratory experiments. The aim of separating the breathing areas of the passengers means considerable contribution from the point of view of passengers' health and comfort.

Acknowledgement: The presented research results have been achieved in the framework of the Project SEAT (Smart technologies for stress free air travel) sponsored by the European Commission DG H.3 Research, Aeronautics Unit under the 6th Framework Programme under contract Number: AST5-CT-2006-030958.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODEL-BASED DEVELOPMENT OF SELF-ORGANIZING EARTHQUAKE EARLY WARNING SYSTEMS

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A new approach for Earthquake Early Warning Systems (EEWS) is presented that uses wireless, self-organizing mesh sensor networks. To develop the prototype of such IT-infrastructures, we follow a model-driven system development paradigm. Structure and behaviour models of network topologies in specific geographic regions are coupled with wave signal analyzing algorithms, alarming protocols, convenient visualisations and earthquake data bases to form the basis for various simulation experiments ahead of system implementation and installation. The general objective of these studies is to test the functionality of an EEWS and to optimize it under the real-time, reliability and cost-depended requirements of potential end-users. For modelling a technology mix of SDL/ASN.1/UML/C++ is used to generate the code for different kind of simulators, and for the target platform (several node types). This approach is used for realizing a prototype-EEWS developed within the EU project SAFER (Seismic eArly warning For EuRope) in cooperation with the GeoForschungsZentrum Potsdam (GFZ).

The SAFER project aims to fully exploit the possibilities offered by the real-time analysis of the signals coming from seismic networks for a wide range of actions, performed over time intervals of a few seconds to some tens of minutes. These actions include the shutting down of critical systems of lifelines and industrial processes, closing highways, railways, etc., the activation of control systems for the protection of crucial structures, as well as supporting the rapid response decisions that must be made by emergency management (continuously updated damage scenarios, aftershocks hazard etc) [1][2]. The first operational area of that EEWS is preparation for Istanbul in a region threatened by strong earthquakes. However, first SOSEWIN model tests were realized by using historical earthquake data, recognized by a centralized seismometer network in Taiwan and synthetic sensor data generated by a tool based on the work of Wang.

The presented paper focuses on our adopted and developed tool-based modelling and data base techniques used in that project, that are general and flexible enough for addressing similar prototyping use cases of self-organizing sensor-based IT-infrastructures.

This architecture is based on OGC, OMG and ITU-T standards and combines different technologies for GIS, databases, behaviour modelling, code generation and simulation according to a special application domain by one integrated framework. So, it allows the evaluation of the real-time behaviour of projected earthquake monitoring and alarming systems and supports automatic code generation from evaluated structure and behavioural models. Modelling techniques, which we used here, are based on SDL and UML under special real-time requirements. Our prototyping infrastructure, implemented in C++, is used in the project SAFER for optimizing self-organizing seismic earthquake early-warning and rapid response systems, a real testbed is established in Istanbul.

An evaluation of the real-time behaviour of such complex systems is almost impossible or too expensive without prior modelling experiments, involving computer simulations. For that we identified several investigation goals supported by different simulators. This involves functional and performance evaluation of EEWS models by tuning topologies and parameters. Additionally to the model-based development our prototyping infrastructure supports also the installation, test, and operating of the network.

Currently the concepts of a cooperative signal analyzing are tested and the compiler technology reached a stable level. Now experiments have to evaluate and improve performance characteristics of the alarming protocol.

Although this contribution is naturally focussed on earthquake driven applications, the presented architecture of prototyping system may be adopted to those use cases where meshed sensor-based self-organizing infrastructures in combination with GIS are applied, such as in Heat Health Warning Systems [3].

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EFFICIENT DYNAMIC MODELLING OF A TRICKLE BED REACTOR FOR DESULPHURISATION OF BIOGAS

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Introduction Biogas is of great significance in the field of renewable energy while desulphurisation remains a major obstacle in the purification process. Trickle bed reactors working with microorganisms are a standard state-of-the-art method to remove hydrogen sulphide H_2S. However, varying H_2S concentrations and gas flows have a negative impact on the removal efficiency if no process control measures are taken. Also, subsequent biogas upgrading requires keeping the output concentration of oxygen in the treated biogas below certain limits.
The goal of this study was to develop a grey-box model of the H_2S degradation process in a trickle bed reactor using physico-chemical models and experimental data. Measurements were taken at the biogas plant in Bruck/Leitha (40 km outside of Vienna) with a maximum biogas capacity of 1000 m^3/h.

Modelling The structure of the mathematical model is based on the idea of an ideal local discretised plug flow reactor which performs like a stirred tank cascade with ten stages. For wastewater treatment there exist similar ideas, but Wik [1] and Janssen et al. [2] put their emphasis on the chemical and biological processes in the liquid phase and the biofilm. Wik actually neglects the gas phase and Janssen et al. control the oxygen regulation by controlling the redox potential. On the contrary, Deshusses et al. [3] concentrate on the gas phase, but do not deal with desulphurisation and oxygen addition. In this paper a different approach is proposed, which is better suited for the investigation of biogas desulphurisation. CFD-simulations in FLUENT show that the assumptions of an ideal plug flow inside the reactor are indeed fulfilled. The mass transfer between gas and liquid phase is accounted for by the two-film theory. By biochemical reactions H_2S is converted into elemental sulphur and sulphuric acid either by direct oxidation or by oxidation with elemental sulphur as intermediate. Because of unknown degradation processes of the microorganisms, a black-box term approximated by experimental data is added to the mass balance of O_2 in the liquid phase.

Simulation The mass balances were implemented in a non-linear dynamic model in Matlab/Simulink. Simulation results show that at O_2 input concentration steps the output behaves like a PT_n element with a cumulative dead-time which is typical for chemical plants.

Experimental validation The model is validated against one series of measurements of 5 hours (Figure 1). The left diagram in Figure 1 shows the correlation between the simulated and the measured H_2S output concentration. The right one describes the same for the O_2 output concentration.

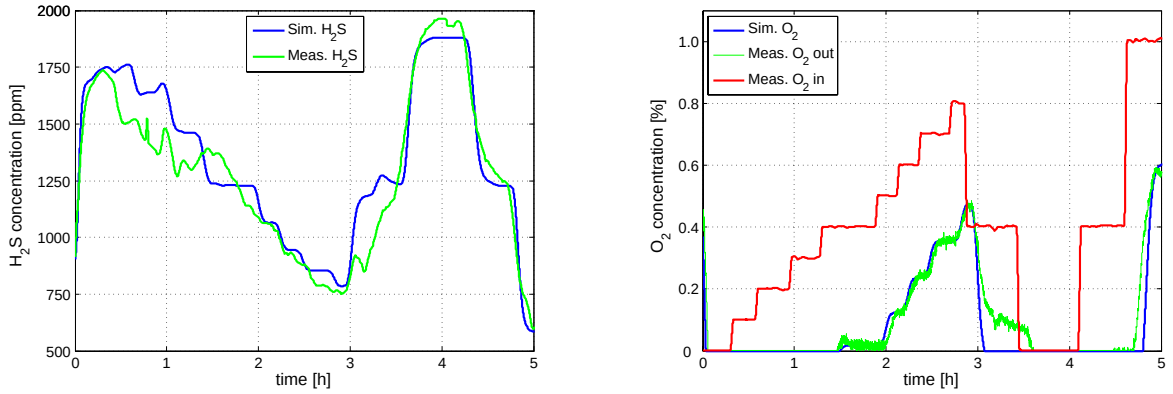

Figure 1: Correlation between simulated and measured output concentrations of H_2S and O_2. H_2S input concentration is between 1750 and 1950 ppm, $\dot{V}_g$ decreases from 710 to 610 and 455 m^3/h and O_2 input concentration changes in steps.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MATHEMATICAL MODELLING OF ENERGETIC PROCESSES IN REVERSE PULSE ELECTROPLATING

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For producing nano- and micro-crystalline materials the electrodeposition appears a versatile technique. Recently, much interest in electrodeposition has evolved due to (*i*) the low temperatures involved, which enable formation of highly crystalline deposits with low solubility in body fluids and low residual stresses, (*ii*) the ability to coat porous, geometrically complex or non line-of-sight surfaces, (*iii*) the ability to control the thickness, composition, and microstructure of the deposit, (*iv*) the possible improvement of the substrate/coating bond strength, and (*v*) the availability and low cost of equipment. This makes electrodeposition ideal for the synthesis of high performance metallic coatings for microelectronics, magnetic recording, and mechano-electromagnetic systems applications, where control of microstructure and texture over a wide range of length scales is essential. It is also worth noticing that today, nano-materials, in which dimensions are measured in billionths of a meter, are the foundations for a fast-growing approach to energy saving.

The research carried out in recent years shows that electrolytic processes consume more than 6% of the total electrical generating capacity of the world. Therefore, the field of electrodeposition, and allied electrochemical surface-modification techniques exhibit significant economic and strategic value. Despite the proven cost-effectiveness of these technologies, a significant proportion of potential energy efficiency improvements remain untapped due to numerous understanding barriers. Metal electrodepositions on high-end thin-layers and on other product in cutting-edge technologies were at the very limit of what DC processes could achieve, and it turned out periodic pulse reverse current (PPRC) technology could go beyond that. All major process studies concentrate currently around the PPRC electroplating technology and the general metal finishing products. This is common on rough parts or when a bright finish is required. By using pulse and reverse pulse plating for the production of electrodeposited surface layers, it is possible to obtain deposits with much more optimized properties than using DC plating, by adjusting the parameters of the pulse program.

The electrodeposition processes can be described by mathematical models derived from the Maxwell equations and mass balance equations. Such models have a two-fold purpose: first, they can account all the facts discovered experimentally, and second, they can be able predict the system behavior under various conditions. Starting from this general imperative, the elaboration of a model for the interface phenomena is performed by making a certain number of hypotheses which generally simplify the governing equations. Their form has been presented as a set of differential-algebraic equations. Relations developed with using the elaborated mathematical model have showed strong dependence between electrocrystallization products and forms of reverse pulse currents in connections with reactor parameters used for electrodeposition.

In this paper, a novel method was presented to improve the energy performance of surface layer depositing by periodic pulse reverse currents. The method is quite different from the traditional way of coating metallic particles itself with inorganic and organic compounds. First we introduced the periodic pulse reverse current supplying an electrolytic tank and then a mathematical model of the electrocrystallization process has been developed. The mathematical model of metal electrodeposition was formulated to explain why the process energy efficiency increases under periodic pulse reverse current conditions, proposing that the lowering of current efficiency was caused by the disproportion of periods of the supplied current waveform and the natural oscillations of the given electroplating reactor. Next, taking into account particular processes governing the electrocystallization the energy delivered to the electrolyser has been determined. The interrelationships between process operating conditions, product quality, and energy consumption are studied by means of model calculations. Conditions for matching the parameters of the electrocrystallization reactor to supplying pulse current source are established. It was found that the improvement of cycling performance is greatly ascribed to the good witching period of supplying current in accord to the given parameters of electrolyzer.

The technique of the present invention permits selection of the desired operating parameters for an electrode/electrolyte system thereby increasing electrode electrocatalysis and creating more efficient electrochemical systems. The one-period energy loops such that have been involved can provide new information which could not be obtained previously with traditional techniques such as measurement of the open circuit potential, the polarization resistance, recording of polarization curves and/or the electrochemical impedance spectroscopy. Using the established new tool it is possible to produce electrodeposited materials with the properties and functionalities which can importantly differ from those of similar material, i.e. with the same composition, but deposited by other means or manufactured in bulk.

ANISOTROPIC MODEL OF DAMAGE FOR GEOMATERIALS AND CONCRETE

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Geomaterials and concretes are regarded as isotropic and heterogeneous materials before any mechanical loading at a mesoscopic scale. The application of a mechanical loading allows onset of defects whose direction of propagation depends on the local stress field. Before any loading, these materials are characterized by a significant density of microscopic cracks that propagate in a direction normal to the tension but tend to close in the case of compression [1,2] with possibility of frictional slip on the lips of discontinuities.

The complete crack closure causes a recovering of the material rigidity. This phenomenon is called unilateral effect [3]. In addition one observes during a simple mechanical test that the cancellation of the loading leads to a more or less important irreversible strain. These effects are caused by frictions, which appear at the crack closure.

A mechanical modeling approach of these materials must describe the behaviors and associated phenomena described below. The damage mechanics constitutes a theoretical tool adapted to describe the complex mechanisms associated with damage and rupture under mechanical loading. Thus the formulation of the model must take account of the principal characteristics described which are summarized below:

(1) degradation of the properties of material by creation of defects in the structure

(2) an anisotropic behavior as a consequence of damage

(3) unilateral effect at the crack closure in the case of the application of compressive stresses.

(4) dissymmetry in behavior between tension and compression

(5) occurrence of irreversible deformation after total unloading.

Many research treats damage phenomenon in concretes and geomaterials. The production of several models is mainly imposed by the complexity and the variety of the behaviors observed. According to the type and the level of imposed loading, the response can evolve from a linear elastic behavior to a nonlinear behavior with development of a damage depending on the structure and mechanical properties as well as loading field. Some models take into account the unilateral effect (3) [1, 2] and the dissymmetry between tension and compression (4). Irreversible deformation (5) is rarely included in the formulation of the behavior laws [1, 2, 3].

The present model takes accounts of the various characteristics of behavior quoted above. Our approach is based on the formulation of a potential of free energy as a scalar function of the strain and damage tensors. This choice avoids singularity in the expression of the stress tensor obtained by derivation of the potential of free energy [1]. State variables are reduced to two rank symmetric tensorial variables $\underline{\underline{\varepsilon}}$ (strain variable) and $\boldsymbol{D}$ (damage variable). The model takes also account of dissymmetry between traction and compression and contains a term related to the residual effects. In last part we propose an application to the case of a tensile and then of a compression tests. A comparison with experimental results will be carried out to test the acuity of the model.

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Computational Micromagnetics

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

REDUCED MODEL IN THIN-FILM MICROMAGNETICS

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Introduction. Computing a minimizer of the Landau-Lifschitz free micromagnetic energy is a highly complex numerical task due to the different scales involved. For certain asymptotic regimes, however, reduced energy functionals have been derived in the literature. We consider the reduced model proposed in [3] which is consistent with the prior works [1] and [5] and is valid in a certain thin-film regime.

The Full Micromagnetic Energy Minimization Problem. The steady state of a magnetization $\mathbf{M}$ of a ferromagnetic sample was first described by Landau and Lifschitz as the solution of a minimization problem. For a uniaxial material with easy axis e_1, the bulk energy reads

$$E(\mathbf{M}) = d^2 \int_\Omega |\nabla \mathbf{M}|^2 \, dx + Q \int_\Omega \mathbf{M}_2^2 + \mathbf{M}_3^2 \, dx + \int_{\mathbb{R}^3} |\nabla U|^2 \, dx - 2 \int_\Omega \mathbf{F} \cdot \mathbf{M} \, dx. \tag{1}$$

The problem of micromagnetics is to find a local minimizer $\mathbf{M}^*$ of E, that satisfies the non-convex constraint $|\mathbf{M}| = 1$. Here, $\nabla \mathbf{M}$ denotes the Jacobian of $\mathbf{M}$ and $|\cdot|$ denotes the Euclidean norm for the matrix $\nabla \mathbf{M}$ and the vector ∇U, respectively.

The stray field involves the magnetostatic potential U which solves the magnetostatic Maxwell equation

$$\int_{\mathbb{R}^3} \nabla U \cdot \nabla V \, dx = \int_\Omega \mathbf{M} \cdot \nabla V \, dx, \quad \text{for all} \quad V \in \mathscr{D}(\mathbb{R}^3) \tag{2}$$

stated here in distributional form. Finally, the constants $d, Q > 0$ denote material dependant parameters and $\mathbf{F}$ denotes an applied exterior field.

Thin-Film Micromagnetics. Let $\omega \subseteq \mathbb{R}^2$ denote a bounded Lipschitz domain with diameter $\ell = 1$. This domain represents our ferromagnetic sample $\Omega = \omega \times [0,t]$, whose thickness $t > 0$ is neglected for simplicity. With an in-plane applied exterior field $\mathbf{f} : \omega \to \mathbb{R}^2$, we seek a minimizer $\mathbf{m}^*$ of the reduced energy

$$e(\mathbf{m}) = \frac{1}{2} \int_{\mathbb{R}^3} |\nabla u|^2 \, dx + \frac{q}{2} \int_\omega \mathbf{m}_2^2 \, dx - \int_\omega \mathbf{f} \cdot \mathbf{m} \, dx, \tag{3}$$

where the magnetic potential $u : \mathbb{R}^3 \to \mathbb{R}$ now solves

$$\int_{\mathbb{R}^3} \nabla u \cdot \nabla V \, dx = \int_\omega \mathbf{m} \cdot \nabla V(x,0) \, dx \quad \text{for all} \quad V \in \mathscr{D}(\mathbb{R}^3). \tag{4}$$

An extensive analysis has been performed in [2], where Γ-convergence of the Landau-Lifschitz problem (1) is proven for vanishing thickness $t \to 0$. The model is valid for sufficiently large and thin samples. We stress, that the constraint $|\mathbf{m}| = 1$ of the Landau-Lifschitz problem relaxes to the convex constraint $|\mathbf{m}| \leq 1$ in the thin-film limit. To discretize the ansatz and test functions we use Raviart-Thomas finite elements.

For a constant applied filed $\mathbf{f}$ and soft ferromagnetic samples where the energy contribution $\frac{q}{2} \int_\omega \mathbf{m}_2^2 \, dx$ may be neglected, the model problem even further simplifies and the solution only depends on the divergence $\nabla \cdot \mathbf{m}$ of the magnetization. This case has been studied in [4], where numerical experiments also show that for sufficiently weak applied field $\mathbf{f}$ the constraint $|\mathbf{m}|$ is not active.

We consider a more general case than the one mentioned above. First, we don't drop the anisotropic energy contribution and, second, we don't assume the applied field to be constant. Among others, we discuss the appropriate functional setting and well-posedness of the problem in thin-film micromagnetics (3).

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MIXED CONFORMING ELEMENTS FOR THE LARGE-BODY LIMIT IN MICROMAGNETICS

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We consider the large-body limit of the stationary Landau-Lifshitz minimization problem introduced by DESIMONE in 1993, cf. [2]: Find a minimizer $\mathbf{m} : \Omega \to \mathbb{R}^d$ with $|\mathbf{m}| \leq 1$ a.e. of the bulk energy

$$E(\mathbf{m}) = \frac{1}{2}\int_{\mathbb{R}^d} |\nabla u|^2\, dx + \int_\Omega \phi^{**}(\mathbf{m})\, dx - \int_\Omega \mathbf{f}\cdot\mathbf{m}\, dx. \tag{1}$$

Here, $\Omega \subset \mathbb{R}^d$, for $d = 2,3$, is the spatial domain of the ferromagnetic material, ϕ^{**} is the (convexified) anisotropy density, and $\mathbf{f} : \Omega \to \mathbb{R}^d$ is an applied exterior field. The magnetic potential $u : \mathbb{R}^d \to \mathbb{R}$ is related to the magnetization $\mathbf{m}$ by the magnetostatic Maxwell equation, which reads in distributional form

$$\operatorname{div}(-\nabla u + \mathbf{m}) = 0 \quad \text{in } \mathscr{D}'(\mathbb{R}^d). \tag{2}$$

In our discretization, we replace the entire space $\mathbb{R}^d$ in the energy functional E and in the potential equation (2) by a bounded Lipschitz domain $\widehat{\Omega}$ containing Ω and stipulate $u \in H^1_0(\widehat{\Omega})$ as the boundary condition on $\partial\widehat{\Omega}$. Moreover, we enforce the side constraint $|\mathbf{m}| \leq 1$ by a penalization strategy and arrive at a new formulation of (1) and (2): Find minimizer $(u,\mathbf{m}) \in X := H^1_0(\widehat{\Omega}) \times L^2(\Omega)$ of

$$E^{penal}(u,\mathbf{m}) := \frac{1}{2}\int_{\widehat{\Omega}} |\nabla u|^2 + \int_\Omega \phi^{**}(\mathbf{m}) - \int_\Omega \mathbf{f}\cdot\mathbf{m} + \frac{1}{2\varepsilon}\int_\Omega (|\mathbf{m}|-1)^2_+, \tag{3}$$

under the side constraint $u \in H^1_0(\widehat{\Omega})$ with

$$\operatorname{div}(\nabla u - \chi_\Omega \mathbf{m}) = 0 \quad \text{in } H^{-1}(\Omega). \tag{4}$$

The Lagrangean

$$\mathscr{L}(u,\mathbf{m};w) := E^{penal}(u,\mathbf{m}) + b(u,\mathbf{m};w), \quad \text{where} \quad b(u,\mathbf{m};w) := \int_{\widehat{\Omega}} (\nabla u - \chi_\Omega \mathbf{m})\cdot\nabla w,$$

leads us now to the corresponding (and equivalent) Euler-Lagrange equations in a so called saddle point formulation for $\mathbf{m}, u$, and the Lagrange parameter $w \in H^1_0(\widehat{\Omega})$:

$$\frac{\partial \mathscr{L}}{\partial(u,\mathbf{m})} = 0 \quad \text{and} \quad \frac{\partial \mathscr{L}}{\partial w} = 0. \tag{5}$$

We consider a mixed P^0-S^1_0-S^1_0 finite element discretization of $(\mathbf{m},u,w)$ for (5). Since conforming elements appear to be unstable for the pure Galerkin discretization (cf. [1]), we append to the Galerkin discretization the consistent stabilization term

$$||\operatorname{div}(\nabla u_h - \chi_\Omega \mathbf{m}_h)||_{H^{-1}(\widehat{\Omega})}.$$

In this talk, we discuss the well-posedness of the discrete problem and the corresponding *a priori* error analysis. We comment on the extension of the analysis to higher-order finite elements. Additionally, we discuss residual-based *a posteriori* error estimation and related mesh adaptivity for this discretization which appears to be necessary because of lack of smoothness of the (unknown) solution $(u,\mathbf{m})$ of (3) and (4). Finally, we address the question of how the full space equation (2) can be treated numerically using an appropriate FEM-BEM coupling.

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SIMULATION OF SPIN TORQUE OSCILLATORS USING FAST INTEGRAL METHODS

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Magnetization oscillations in nano-sized magnets can be driven a by spin polarized current. When the torque term cancels the Gilbert damping term the steady state solution of the LLG equation is accessed resulting in perodic oscillations of the magnetization. Spin torque oscillators may be used as microwave generators in wireless communication and microwave assisted magnetic recording.

The LLG equation augmented with the spin torque term [1] is solved for different magnetic nanostructures using fast integral methods for the calculation of magnetic fields. The total magnetic field is the sum of the Oersted field whose source is the current distribution and of the magnetostatic field which arises from the divergence of the magnetization. The equation of motion for the magnetization is solved with an implicit time stepping scheme with the magnetic fields computed self-consistently [2] from the distribution of the current and the distribution of the magnetization (see Figure 1).

The numerical results are compared with experimental data for prototype spin torque oscillators. Figure 2 shows the spin waves generated in a thin magnetic multilayer whereby a current is applied through two point contacts. The mutual interaction between the oscillation magnetization lead to phase locking resulting in a high output power [3]**.**

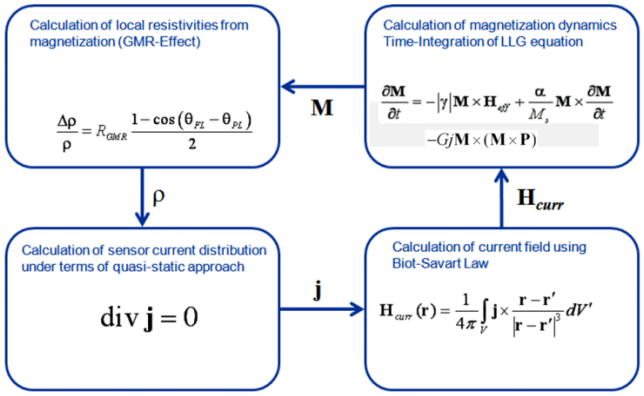

Figure 1: Fundamental equations solved using an implicit time integration scheme together with fast integral methods for field calculation.

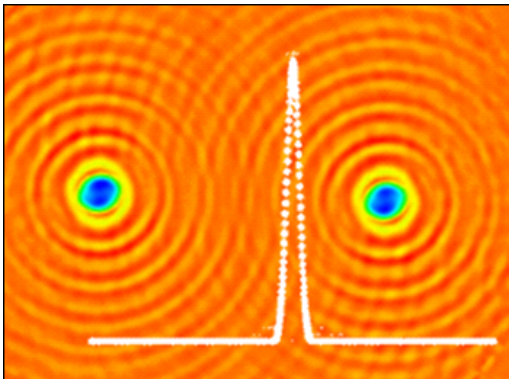

Figure 2: Spin waves generated in a double point contact spin oscillator. The dashed line is the power spectrum density of the oscillator.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MULTISCALE MODELING FOR ADVANCED MAGNETIC RECORDING DEVICES

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Continued growth of storage densities in the presence of instability of recorded data against thermal decay, often called the 'superparamagnetic effect', requires major breakthroughs in recording devices. In order to design highly functional magnetic recording materials reliable methods are required that are suitable to describe the recording process in detail. Our developed micromagnetic model allows for the calculation of the whole write process, including the current in the coils of the recording head, the magnetization processes in the yoke and in the pole tip close to the recording media. The recording head moves across the recording media, where the information is written. Finally also the read back signal can be calculated. In these fully integrated recording simulations various different length scales and times scales are involved that require sophisticated numerical methods, such as a hybrid finite element boundary element method, H-matrices for the compression of the boundary matrix and preconditioned time integration schemes. In order to estimate the thermal stability of the written bits switching times at large time scales have to be calculated. For this task the transition state theory is applied that requires the calculation of the saddlepoint that separates two stable states (bit 1 and bit 0). The nudged elastic band method was found to be an efficient tool to determine the saddle points numerical within the framework of micromagnetics. These models are applied to design advanced magnetic recording media. The talk will focus on exchange spring and a novell 3D storage concept that were recently proposed to postpone the superparamagnetic effect to higher densities.

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Tools for Modelling of Reaction Systems

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELLING BIOCHEMICAL REACTION NETWORKS WITH BIOCHAM EXTRACTING QUALITATIVE AND QUANTITATIVE INFORMATION FROM THE STRUCTURE

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Introduction. Recent advances in Biology have shown that the amount and heterogeneity of the (post-genomic) data now available call for new techniques able to cope with such input and to build high-level models of the complex systems involved.

Arguably two key open issues in this emerging area of Computational Systems Biology concern the integration of qualitative and quantitative models and the revision of such integrated models.

The purpose of the Biochemical Abstract Machine (BIOCHAM) modelling environment is to provide formalisms to describe biological mechanisms, including both the studied system and its properties, at different abstraction levels. Based on these formalisms it gives access to a set of tools, mostly focused around model-checking, that help the user in developing, curating, exchanging and refining his models.

We take as an example invariant computation of the Petri net representing a biological reaction system, and show both a new efficient method for this step, as resolution of a constraint problem, and also how this analysis brings both qualitative and quantitative information on the models, in the form of conservation laws, consistency checking, etc. ranging over all the above defined abstraction levels.

Related work. The Biochemical Abstract Machine (http://contraintes.inria.fr/BIOCHAM/) was built as a simplification of the process algebras like the π-calculus, using instead a simple rule-based language focused on reactions to describe biological systems. This point of view is shared with all the Systems Biology Markup Language (SBML) community and enables exchanging of models but also, as we shall see, reasoning at different levels on a same model. BIOCHAM also adds the use of Temporal Logics as a second formalism to encode the expected or observed properties of the system, from a purely qualitative view to a completely quantitative one. This allows to automatically check that the model behaves as specified through model-checking tools adapted to the considered level.

The use of Petri-nets to represent those reaction models, taking into account the difference between compounds and reactions in the graph, and make available various kinds of analyses is quite old, however it remains somehow focused towards mostly qualitative and structural properties. Some have been used for module decomposition, like (I/O) T-invariants, related to dynamical notions of elementary flux modes. However, there is, to our knowledge, very little use of P-invariant computation, which provides both qualitative information about some notion of module related to the "life cycle" of compounds or about reachability in the boolean or bounded views of the system, and quantitative information related to conservation laws and Jacobian matrix singularity for the continuous ODE based-view of the same system.

Our approach. After an illustration of the different views provided for a given reaction model, we present a very simple way to incorporate invariant computation into an existing biological modelling tool, using constraint programming with symmetry detection and breaking. We compare it to other approaches and evaluate it, for the case of P-invariants, on some examples of various sizes. This experimentation is done through an implementation of the described method in the BIOCHAM modelling environment and the Nicotine tool (http://contraintes.inria.fr/~soliman/nicotine/).

We detail this new method to efficiently compute invariants of a reaction network, based on Finite Domain constraint programming with a generalized notion of symmetry. It scales up well to the biggest reaction networks found and seems to show that structural problems for Petri-nets (invariants, sinks, attractors, etc.) can benefit from the know-how developed for finite domain CP solving, like symmetry breaking, search heuristics, etc. which leads to generalize our approach to other problems of this category.

P-invariants of a biological reaction model are not difficult to compute in most cases, but they do, however, carry information about conservation laws that is useful for efficient and precise dynamical simulation of the system, and provide some notion of module, which is related to the life cycle of molecules, and thus mix qualitative and quantitative information about the system.

We conclude by reinforcing our call for using reaction networks and reasoning about them at different levels in order to capture the available qualitative and quantitative information.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A FAST ALGORITHM FOR COMPUTING A MINIMAL DECOMPOSITION OF A METABOLIC FLUX VECTOR IN TERMS OF ELEMENTARY FLUX VECTORS

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The intracellular metabolism of living cells is usually represented by a metabolic network where the nodes represent the metabolites and the edges represent the metabolic fluxes. According to the quasi steady-state paradigm of metabolic flux analysis (MFA), the fluxes are assumed to be balanced at each internal node. This is expressed by the algebraic relation:

$$\mathbf{N}\mathbf{v} = \mathbf{0} \qquad \mathbf{v} \geqslant \mathbf{0} \tag{1}$$

where $\mathbf{v}$ is the m-dimensional column vector of fluxes and $\mathbf{N}$ is the $n \times m$ stoichiometric matrix of the metabolic network (m is the number of fluxes and n the number of internal nodes of the network). The set S of possible flux distributions is the set of vectors $\mathbf{v}$ that satisfy the linear system (1). This set S is a pointed polyhedral cone. This implies that there exists a set of elementary flux vectors $\mathbf{e}_i$ which are the edges (or extremal rays) of S such that any flux distribution $\mathbf{v}$ can be expressed as a non-negative linear combination of the vectors $\mathbf{e}_i$: $\mathbf{v} = \mathbf{E}\mathbf{w}$ with $\mathbf{w} \triangleq (w_1, w_2, \ldots, w_q)^T$ and $\mathbf{E}$ is the $m \times q$ non-negative matrix $\mathbf{E}$ with column vectors $\mathbf{e}_i$.

Metabolic flux analysis (MFA) is the exercise of calculating the admissible flux distributions $\mathbf{v}$ that satisfy the system (1) together with an additional set of linear measurement constraints

$$\mathbf{P}\mathbf{v} = \mathbf{v}_m \tag{2}$$

whith the measurements collected in the vector $\mathbf{v}_m$ and the matrix $\mathbf{P}$ being a given $p \times m$ full-rank matrix.

For any admissible flux vector $\mathbf{v}$ solution of (1)-(2) the decomposition of $\mathbf{v}$ in the convex basis $\{\mathbf{e}_i\}$ is **not** unique. Our aim is to determine minimal decompositions. We show that every admissible $\mathbf{v}$ has a minimal decomposition involving terms with $p \leqslant \leqslant (m-n)$. Furthermore there necessarily exist admissible vectors $\mathbf{v}$ having decompositions that include p terms only. Computing such decompositions may be very expensive at first sight since the number of distinct extremal rays $\mathbf{e}_i$ is not bounded by a polynomial in the sizes of $\mathbf{N}$ and $\mathbf{P}$ and may be very large because it increases combinatorially with the size of the metabolic network.

In this paper, our main conribution is then to present a fast algorithm that randomly computes admissible vectors $\mathbf{v}$ having a minimal decomposition from the sole knowledge of the stoichiometric matrices $\mathbf{N}$, $\mathbf{P}$ and the measurement vector $\mathbf{v}_m$ but without explicitely enumerating the extremal rays of the cone S (i.e. the columns of the huge matrix $\mathbf{E}$).

As a matter of illustration and motivation to the methodology presented above, we consider the example of chinese hamster ovary (CHO) cells cultivated in batch mode in stirred flasks in a serum-free medium. During the growth phase, we assume that the cell metabolism is described by a metabolic network involving the Glycolysis pathway, the Pentose-Phosphate pathway, the Krebs cycle, the amino-acid metabolism, the urea cycle as well as the metabolic reactions for nucleotide, protein and lipid synthesis

For this network we have $m = 82$ fluxes and $n = 53$ internal metabolites, and there are 65329 elementary flux vectors $\mathbf{e}_i$ (i.e the matrix $\mathbf{E}$ has 65329 columns) while the admissible flux distributions are expressed as a combination of p=22 elementary vectors only.

TWO DIFFERENT APPROACHES FOR MODELING BIOCHEMICAL REACTION NETWORKS WITH PROMOT

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Introduction. In recent years modeling of reaction systems tend to be more complex. Especially in systems biology researchers are faced with large-scale and highly interconnected networks that have to be mapped on various types of mathematical models. Handling of such systems requires efficient and flexible computing tools as well as a powerful modeling concept to describe the system under investigation. The modeling tool PROMOT provides an unique framework for setup, editing and visualization of systems which are relevant in chemical engineering and systems biology.
PROMOT is based on a modular modeling concept which is well suited to describe modular structures of technical and biological systems. This concept is based on network theory [1] that provides elementary modeling entities like compounds or single reactions. The elementary modeling entities can be aggregated to higher structural elements like chemical apparatus or overall pathways in systems biology. The modular modeling concept was originally applied to a quantitative modeling approach and also recently extended to include a qualitative modeling approach, frequently used in systems biology.
Setting up and managing models can be done using either a textual or diagrammatic user interface in PROMOT. In order to analyze or simulate models, PROMOT is tightly coupled with several simulation and analysis tools in order to get a closed environment which results in an optimized modeling workflow. PROMOT is also linked with many other tools via SBML, the standard exchange format in the area of systems biology.

Modeling based on DAE systems. The quantitative modeling approach in PROMOT has its origin in chemical engineering and is also capable to describe cellular processes in systems biology such as intracellular metabolic or signaling processes [2]. Elementary modeling entities are substance storages and substance transformers, representing single compounds and biochemical reactions, respectively. The resulting equations that allow to simulate the system are based on mass balances. However, in many cases, model reduction can be performed that allow to reduce the number of dynamic state variables by setting up algebraic relationships between the compounds. For instance the processes of signal transduction are in general much faster than the processes of protein synthesis and therefore its dynamics can be neglected. The resulting differential and algebraic equations (DAE systems) are provided automatically by PROMOT.
Models that are set up with PROMOT finally can be exported to various simulation engines such as MATLAB, DIVA or its successor Diana. Furthermore, a different set of kinetic parameters can be reloaded in PROMOT, e. g. after parameter estimation with DIVA.

Modeling based on a logical modeling formalism. Besides the quantitative approach PROMOT supports also a logical (Boolean) modeling formalism which results in a qualitative description of the system [3]. This approach is well suited to describe systems with a large number of components and considerably less information about the dynamics. In most cases there is a lack of kinetic parameters. Moreover, experimental data may be available only at discrete values ("a protein is present or not" or "if protein A is active then also protein B is active"). In this case, the approach of logical modeling is more appealing.
Substances, represented through compounds can be connected with logical gates like AND, OR and NOT to build up the logical network. Editing can be done in the PROMOT Visual Editor where predefined library elements can be placed using drag&drop functionality. Afterwards the elements can be connected by links. In order to analyze these logical models, PROMOT provides the export of the models to CELLNETANALYZER in the form of logical equations coupled with a graphical representation. The analysis results of CELLNETANALYZER can be re-imported in PROMOT and visualized in an intuitive way.
The approach is applied to a number of projects dealing with signal transduction networks (i. e. Epidermal Growth Factor Receptor, T-Cell Receptor Signaling). For a convenient and user-friendly setup of logical models, PROMOT provides a library containing the basic components, short-cuts for efficient and less error-prone work, validation for structural modeling errors while editing and special visual representations which are used to represent the logical model. This is of great value in order to interpret and discuss specific results in interdisciplinary teams.

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IGPE – A Novel Method for Efficient Global Parameter Estimation in Dynamical Systems

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

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Introduction. Mathematical models giving accurate predictions of physical phenomena are essential tools in engineering and scientific fields. However, these models often contain adjustable parameters (semi-empirical models), the values of which are to be determined from available experimental data to yield accurate predictions. Traditionally, parameter estimation is performed following a maximum likelihood approach. Both, the *sequential* and *simultaneous* approaches of dynamic optimization have been widely studied in this context. In the sequential approach, an integration routine is used to determine the state values for a given set of model parameters, which in turn allows for the evaluation of the objective function and its derivatives in a master nonlinear program (NLP). In the simultaneous approach, on the other hand, the dynamic system is converted into a set of algebraic equations, which are solved along with the model parameter values in a large-scale NLP.

The aforementioned approaches rely on local search methods and can, at best, achieve convergence to a local minimum. This deficiency to converge to a global minimum may have dramatic consequences. In the context of reaction kinetics, for instance, getting a bad fit (due to only locally optimal parameter values) may lead to the erroneous conclusion that a proposed kinetic model yields an incorrect description of the chemistry [1]; in other words, only a global minimum allows one to conclude that a proposed model structure is invalid.

Both *stochastic* and *deterministic global optimization* have been developed to increase the likelihood of finding a global minimizer. Stochastic search methods rely on probabilistic approaches. They are usually quite simple to implement and their efficiency has been demonstrated on many applications. Yet, they cannot guarantee locating a global solution in a finite number of iterations. Deterministic methods, on the other hand, can provide a level of assurance that the global optimum will be located in finite time. These sound theoretical convergence properties have stimulated the development of deterministic global optimization for problems with embedded differential equations [2]. Although tremendous progress has been achieved in recent years, global dynamic optimization methods are currently limited to problems containing no more than a few decision variables and still no general method has been proposed to rigorously address problems with DAEs embedded.

All of the foregoing parameter estimation approaches (be they local or global) fall into the scope of *simultaneous* identification (also called *integral* method), in the sense that *all* the adjustable model parameters are estimated simultaneously. Recently, the so-called *incremental* approach for model identification has been introduced by Marquardt and coworkers [3]. The key idea therein is to follow the steps that are usually taken in the development of model structures, thus yielding a sequence of algebraic parameter estimation problems, which are simpler than the original differential problem. Although incremental identification approaches do not share the same theoretical properties as simultaneous methods, namely they are neither unbiased nor consistent, their major advantage lies in the computational ease.

This paper proposes a novel methodology for global parameter estimation in dynamical systems. Building upon the incremental identification method, the original problem is split into 5 steps. The contribution of this paper is twofold. First, the incremental approach is extended to encompass general parameter identification problems in DAE systems, i.e., not necessarily reaction kinetic models. Second, deterministic global optimization is used in a systematic way for solving the (potentially nonconvex) algebraic estimation problems, hence the name *Incremental Global Parameter Estimation* (IGPE). The main advantage of IGPE, as compared to simultaneous global optimization, lies in a significant decrease of the overall computational time. The downside, of course, is that – in the presence of measurement noise – the global solution in the incremental approach will generally be different from the global solution in the simultaneous approach. However, the incremental solution can be used as a starting point in a local simultaneous estimation problem. In particular, our experience is that this heuristic procedure typically yields the global solution to the original problem.

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RapOpt - An Automation Tool for Production-Orientated Run-to-Run Model Evolution

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Mathematical models have been proven to be a key factor in optimizing production processes in recent years. However, in the case of biochemical processes the design is usually done using heuristics, since these systems show complex internal regulation mechanisms and strongly nonlinear behavior. This makes it difficult to find an appropriate model. In those cases, where a structured biochemical model has been successfully identified, the yield of the process can be increased significantly. Obtaining a suitable production model is usually a difficult and time consuming task, especially for biochemical systems.

In this contribution the concept for an automation tool is presented which starts with the few noisy measurements of initial experiments to perform a model evolution from run to run. For the first crude, unstructured model it is assumed that all substrates may influence the reaction rates of the specified states. Due to the difficult measurement situation in biochemical processes many different model candidates may show a similar fit to the data why it is unwise to focus on one model candidate for process design, only. Furthermore, the use of more than one model candidate for the design procedure represents a kind of robustness for the planning. Based on balance equations and conservation laws RapOpt will interchange individual reaction kinetics within this basic structure and thus create a multi-model system environment. All automatically created models constructing the model family and their corresponding parameter files will be coded by RapOpt in a MATLAB m-file for easy interpretable documentation as well as coded and compiled in *C* for accelerated simulation.

Even the first unstructured model candidates are already used for an optimal production-orientated process design (see Figure 1) whose realization will provide additional information about the dynamic behavior within the production area and therefore leading to new and improved model candidates. Repeating this cyclic procedure enables a run to run model evolution as well as an optimal production design corresponding to the available measurement information at any time.

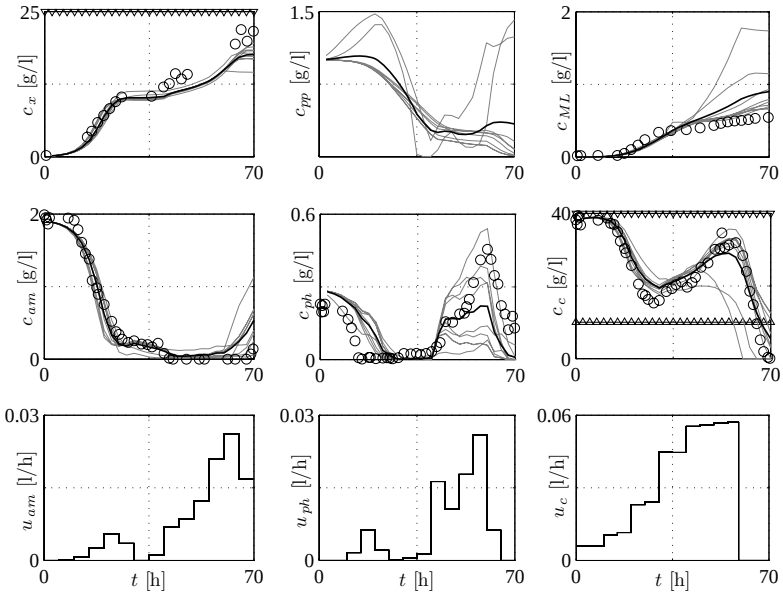

Figure 1: Optimized trajectories of the different models in a process design that considers nine models. Measurements of the concentration of biomass c_x, product c_{ML}, ammonium c_{am}, phosphate c_{ph} and glucose c_c are given by open circles, the different model simulations by grey solid lines. Third row: optimal feeding profiles used for ammonium, phosphate and glucose feed. Constraints are shown as lines with triangulars.

Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Numerics of Ordinary Differential Equations with Uncertainties

POLYNOMIAL CHAOS EXPANSIONS FOR ANALYSING OSCILLATORS WITH UNCERTAINTIES

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Mathematical modelling of dynamical processes often yields systems of ordinary differential equations (ODEs) or differential algebraic equations (DAEs). The systems include physical parameters, which may exhibit uncertainties. Consequently, we replace the relevant parameters by random variables on a probability space $(\Omega, \mathscr{A}, \mu)$. The solution of the ODEs or DAEs becomes a random process. If the stochastic model is resolved by quasi Monte-Carlo methods of related techniques, then often a large computational effort is required.

The strategy of the generalised polynomial chaos (gPC) provides a promising alternative in certain applications, see [1]. This concept can be applied to general systems of (partial) differential equations with random parameters. The idea is to expand the unknown random process in a series with orthogonal basis polynomials depending on the probability space. The unknown coefficient functions can be determined by stochastic collocation or a Galerkin approach, see the review [3]. We focus on the application of the Galerkin method.

In [2], forced oscillators, which are described by non-autonomous systems of DAEs, have been resolved via the gPC approach. Now we consider autonomous systems of the form

$$A(\mathbf{p})\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}(\mathbf{x}(t,\mathbf{p}),\mathbf{p}) \tag{1}$$

with parameters $\mathbf{p} \in Q \subseteq \mathbb{R}^q$ and solution $\mathbf{x} : [t_0, t_1] \times Q \to \mathbb{R}^n$. If the matrix $A(\mathbf{p}) \in \mathbb{R}^{n\times n}$ is singular, then the system (1) represents DAEs. Since we investigate oscillators, periodic solutions satisfying $\mathbf{x}(t+T(\mathbf{p})) = \mathbf{x}(t)$ have to be determined. In contrast to forced oscillators, the period $T(\mathbf{p})$ depends on the parameters in general. Hence we apply the transformation $\tilde{\mathbf{x}}(\tau,\mathbf{p}) := \mathbf{x}(\tau T(\mathbf{p}),\mathbf{p})$ and obtain the equivalent system

$$A(\mathbf{p})\dot{\tilde{\mathbf{x}}}(\tau,\mathbf{p}) = T(\mathbf{p})\mathbf{f}(\tilde{\mathbf{x}}(\tau,\mathbf{p}),\mathbf{p}) . \tag{2}$$

Periodic solutions are determined via the two-point boundary value problem $\tilde{\mathbf{x}}(0,\mathbf{p}) = \tilde{\mathbf{x}}(1,\mathbf{p})$. Since the period $T(\mathbf{p})$ is unknown a priori, an additional condition has to be imposed to identify an isolated solution.

In view of uncertainties, the parameters are substituted by random variables $\mathbf{p} : \Omega \to Q$. We apply the gPC expansions of the random process $\tilde{\mathbf{x}}$ as well as the random period T satisfying (2), i.e.,

$$\tilde{\mathbf{x}}(\tau,\mathbf{p}(\omega)) = \sum_{i=0}^{\infty} \mathbf{v}_i(\tau)\Phi_i(\mathbf{p}(\omega)) , \qquad T(\mathbf{p}(\omega)) = \sum_{j=0}^{\infty} w_j \Phi_j(\mathbf{p}(\omega)) \tag{3}$$

with a complete basis of multivariate polynomials $(\Phi_i)_{i\in\mathbb{N}}$. The gPC uses orthogonal polynomials with respect to the inner product of $L^2(\Omega)$. The coefficients $\mathbf{v}_i : [\tau_0, \tau_1] \to \mathbb{R}^n$ and $w_j \in \mathbb{R}$ represent unknowns of the problem. The coefficient functions inherit the periodicity condition $\mathbf{v}_i(0) = \mathbf{v}_i(1)$ for each i.

The infinite sums (3) are truncated to achieve numerical methods. Inserting the finite sums into (2) yields a residual. The Galerkin approach produces a larger coupled system of ODEs or DAEs, respectively, for the unknown coefficients of the finite gPC expansions (3) with periodic boundary conditions. The coupled system is underdetermined due to the unknown coefficients of the random period. We construct additional conditions to identify appropriate solutions. Thereby, the structure of a two-point boundary value problem is maintained.

In case of ODEs, the local stability of a periodic solution can be decided via the eigenvalues of the corresponding monodromy matrix. The monodromy matrix satisfies a linear system of differential equations. Generalisations to the case of DAEs are feasible. We analyse the local stability of periodic solutions of the coupled system from the Galerkin method. The resulting linear matrix differential equation exhibits a specific structure in case of autonomous oscillators.

Finally, we present numerical simulations of an electric circuit, where a mathematical modelling yields a system of the form (1). The results confirm that the techniques based on gPC resolve the stochastic model correctly. Moreover, the systems exhibit locally stable periodic solutions.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

APPLICATION OF THE POLYNOMIAL CHAOS EXPANSION TO THE NUMERICAL SIMULATION OF A BATCH REACTOR

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Introduction. The polynomial chaos expansion can reduce stochastic differential equations to deterministic differential equations by projecting this expansion onto the probability space. We use this feature to simulate the decomposition of acetylated castor oil ester in an isothermal batch reactor and to compare the deterministic and stochastic approach.

Isothermal batch reactor. We study the case of a batch reactor with no change in temperature. With the homogeneity assumption the dynamics of the system is given by a set of ordinary differential equations

$$\frac{d\eta_i}{dt} = R_i, \qquad i = 1, ..., N. \tag{1}$$

with η_i the molar concentration of species i and R_i the *overall reaction rate* for species i. This reaction rate depends on the molar concentrations of other reactants, which results on a system of coupled differential equations. If one or more parameters of the system are randomly distributed, we are faced with a system of stochastic differential equations. One way to solve this problem is via polynomial chaos.

Polynomial Chaos. Homogeneous chaos is defined as a span of Hermite polynomial functionals of a Gaussian process. The Fourier-Hermite series can approximate any functionals in L_2 and converges in the L_2 sense. So second-order random processes can be expanded in terms of orthonormal Hermite polynomials. A general second order random process $x(\theta)$, with θ being the random event, can be represented in the form

$$x(\theta) = \sum_{i=0}^{\infty} a_i \Psi_i(\xi). \tag{2}$$

The polynomial basis Ψ_i forms a complete orthonormal basis of the Hilbert space H and the coefficients a_i in (2) may be computed very efficiently by a multi-dimensional Gauss-Hermite quadrature. For an $n-$dimensional stochastic space, truncation of the expansion after

$$N+1 = \frac{(n+p)!}{n!p!} \tag{3}$$

terms yields an approximation of order p for the random variable x, [1]. For normal distributed random variables the exponential convergence of the homogeneous chaos expansion can be shown, [2].

Case Study. The decomposition of acetylated castor oil ester is simulated in an isothermal batch reactor. The temperature is assumed to be not deterministic but normal distributed. Comparison between the stochastic simulation of the process and the deterministic approach yields a relative error of 20% when neglecting variation in temperature.

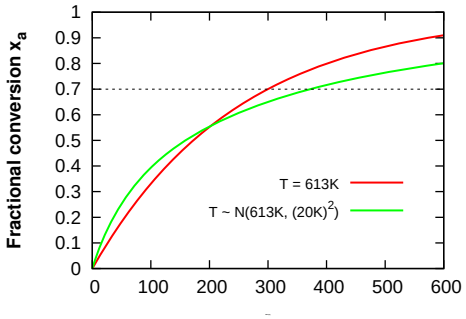

Figure 1: Comparison of fractional conversion for deterministic and normal distributed temperature.

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NUMERICS OF THE VAN-DER-POL EQUATION WITH RANDOM PARAMETER

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"I have a theory that whenever you want to get in trouble with a method, look for the Van-der-Pol equation" (P. E. Zadunaisky, 1982, [1]). The long-term integration of the random Van-der-Pol equation

$$\frac{d^2}{dt^2}y(t,p) + p(y(t,p)^2 - 1)\frac{d}{dt}y(t,p) + y(t,p) = 0$$

with uniformly distributed parameter $p \sim \mathscr{U}[1.9, 2.1]$ is a challenging problem. The random parameter p is related to the characteristics of a diode in an electrical circuit. Especially the problem of error reduction of the approximation of the stochastic behavior of the Van-der-Pol equation is within the scope of this work.

The method of Wiener-Askey expansion has proven to be a powerful method for dealing with uncertainty. The random behavior of the solution is approximated with exponential convergence of the truncated Wiener-Askey expansion, if a suitable probability measure P is chosen. But although the basic principles of applying this method are simple, its application to basic benchmark problems can be very capricious, see [3]. For example integration of ordinary differential equations with random parameters is known to lose accuracy at early times due to increasingly slow convergence.
For approximation of the random behavior of the solution of the Van-der-Pol equation, the Wiener-Askey procedure uses a fixed probability measure P at initial time and sets up the expansion with the corresponding orthogonal polynomials Ψ_i. Truncation leads to a numerically tractable problem in the context of stochastic Finite Elements Methods. Insufficient accuracy of the approximation is handled by MEgPC, or by adding more terms to the truncated Wiener-Askey expansion.
A major drawback of this method is that, except from a few cases, the estimation of the approximation error is still an open question. This problem is discussed by means of the Van-der-Pol equation. Following the work of P. Vos [2] y is approximated using a process adapted density.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

FILTERING NONLINEAR SYSTEMS WITH UNCERTAINTIES

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Problem. An important class of non-linear systems with uncertainties may be represented by a state model with process and measurement errors. In order to remove this errors in the model and to approximate the true state, a tool is needed which estimates this values on the basis of noisy observations.

Content. To handle problems of this kind, filters have been developed. This presentation illustrates how filters can be designed, which characteristics and limits they have, and how they differ from each other. This paper especially deals with non-linear problems and so particular attention is payed to non-linear filters.

At first the fundamentals of non-linear dynamic systems will be illustrated. Particularly we examine the observability and controllability of a system, since they have considerable influence on the efficiency of filters applied to such problems.

Since non-linear filters are based on linear approaches, we have to understand linear filters first. Pioneering work on this field was achieved by R.E. Kalman [1] with the Kalman Filter named after him. The filtering rules directly can be derived from the system equations. However this is only possible under the assumption that every variable is gaussian distributed. The Kalman Filter is proven to be an optimal state estimator for linear models in the mean square sense.

A widely spread filter for non-linear systems is the Extended Kalman Filter (EKF) which is based on succesive linearization. In contrast to its linear counterpart, the EKF is not an optimal estimator. One noteable disadvantage is the requirement to explicitly calculate Jacobians, which for complex functions can be a difficult task in itself, i.e. requiring complicated derivatives if done analytically or being computationally costly if done numerically. In spite of all these difficulties and inaccuracies, that result from highly non-linear equations and non-gaussian distributions, the EKF is still standard for many non-linear applications.

One useful and efficient option to the EKF for highly non-linear models is the Unscented Kalman Filter (UKF), which is based on the EKF but removes the requirement to calculate the Jacobians. It uses a deterministic sampling technique instead, which has been invented by S.J. Julier and J.K. Uhlmann as Unscented Transform [2], to pick a minimal set of sample points called Sigma Points around the mean. These Sigma Points are then propagated through the non-linear functions, and the estimate for the state variable is recovered.

Application. To illustrate applications and differences of non-linear filters, some examples will be discussed finally. Particularly this presentation deals with the predator-prey model. This system, also called Lotka-Volterra equations, is a pair of weakly non-linear equations frequently used to describe the dynamics of biological systems in which two species interact. If we treat this system as a model with uncertain parameters, we will see, that in spite of the weak non-linearity the EKF is not able to estimate the parameters. Thus we can demonstrate the advantage of UKF with this example.

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Stochastic Modelling

STOCHASTIC MODELS FOR INTERMITTENT DEMANDS FORECASTING AND STOCK CONTROL

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Introduction. Demand forecasting with regard to stock control is a central issue of inventory management. Serious difficulties arise for intermittent demands, that is, if there are slow-moving items demanded only sporadically. Prevalent methods then usually perform poorly as they do not properly take the stochastic nature of intermittent demand patterns into account. They often rely on heuristic assumptions and apply deterministic smoothing techniques. Stochastic models appear to be more appropriate for intermittent demands forecasting and stock control.

In practice, the most common forecasting technique is simple exponential smoothing (SES), that is forecasts are made by means of a weighted sum of past observations in that based on given time series data $x_1, \ldots, x_t$ a forecast $\hat{x}_{t+1}$ for the next data point x_{t+1} is computed recursively by $\hat{x}_1 = x_1$ and $\hat{x}_{t+1} = \alpha x_t + (1-\alpha)\hat{x}_t$ for $t > 0$ where $\alpha \in (0,1)$ is a smoothing constant that needs to be chosen appropriately. For intermittent demands, pure SES does not provide satisfactory forecasts for intermittent demands and Croston's method [1] is most widely applied.

Croston separates the time intervals between successive demands (interdemand times) and the number of units that are demanded (demand sizes). He argues that the time periods (days, weeks, or months) between successive demands as well as the demand sizes are independent and identically distributed (iid) random variables. He assumes the geometric distribution for the interdemand times and the normal distribution for the demand sizes. If a demand occurs, separate forecasts for the interdemand time and the demand size are updated according to SES using the same smoothing constant for both forecasts. Though specifically targeted to intermittent demands and often more accurate than SES, in some cases Croston's method and its various modifications do not provide proper forecasts and not even outperform SES. After all, there is still no satisfactory approach to intermittent demands forecasting.

Stochastic Modeling Approach. According to [2], deterministic SES as a forecasting technique is not consistent with stochastic models, because any underlying stochastic model must be non-stationary and defined on a continuous sample space with negative values, which does not match to the real properties of intermittent demand patterns. We believe that starting with a forecasting technique and building an according underlying model is exactly the reversed order of what is required. Consequently, we argue that one should first build an adequate stochastic model based on real data, then validate its goodness of fit and finally derive forecasts and stock control strategies.

We have developed a systematic procedure for model fitting to real industrial data. Initially, no independence assumptions are made but after computing comprehensive statistics, the independence is checked. Dependent on the outcome either the time series corresponding to interdemand times and demand sizes are fitted to autogressive moving average (ARMA) processes or to adequate probability distributions. This procedure has been applied to the demand patterns of different slow-moving items. In addition to model fitting for each of these items, similarities are identified in order to build an aggregated model that integrates as much slow-moving items as possible.

One of our main findings is that for almost all intermittent demand patterns the independence assumption is valid. Even for the two potentially critical items, the best fits to ARMA processes resulted in neglecting the MA part and low orders of the AR part, i.e. they were best fitted to purely autoregressive processes of order 2 and 4, respectively, which indicates a very weak dependence. Taking the data as independent and fitting to probability distributions resulted in very accurate fits. Hence, it seems reasonable to assume independence even for these critical items.

The focus was on discrete probability distributions since both the interdemand times (months in our case) and the demand sizes are integer numbers. The geometric distribution fits best for the interdemand times of all items studied. The logarithmic distribution fits best to the demand sizes in the majority of cases and at least fits well in all cases. Hence, Croston's interdemand time distribution has turned out to be appropriate and is now validated on the basis of real data. His assumption of normally distributed demand sizes has been substituted by the logarithmic distribution. This supports our belief that the weaknesses are mainly due to inappropriate forecasting techniques.

Once we have valid stochastic models, it is clear that deterministic point forecasts are not very meaningful but stock control strategies are possible which do not rely on simple point forecasts. Service level guarantees can be obtained in terms of probability bounds on stock out or item availability, respectively.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

DIFFERENCE EQUATIONS FOR SIZING INTERMEDIATE STORAGES IN DISCRETE STOCHASTIC MODELS AND THEIR MATHEMATICAL GENERALIZATIONS

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Intermediate storages play important role in improving the operating efficiency of processing systems, and fitting to each other the subsystems with different operational characteristics. The processing system consists of batch and continuous/batch subsystems which are connected by an intermediate storage where the batch units form the inputs of the storage while at the output the material is removed continuously or in batches. Two natural questions arise: how large the intermediate storage should be in order to avoid overflow, and how much initial amount is needed in order to avoid running out of material. The above two questions can be investigated separately as well. In this paper we deal with the problem of determining the appropriate size of the storage in order to avoid overflow. Most of the works dealing with these questions suppose stochastic operation conditions. If conditions concerning the operations assume random variables with continuous distribution functions concerning both the time values between consecutive fillings and the amount of the filled material, the functions describing reliability satisfy integro-differential equations. But in some cases the material arrives at the storage in discrete time points and the amount of material can also be given by random variables with discrete distributions. Such model will be investigated in this paper.

Let us consider the model investigated. The amount of material withdrawn from the storage during one time unit is constant and it is chosen the unit of the material. Let $t_0 = 0$ and $t_k \quad k = 1,2,3...$ be the intervals between the consecutive filling times (time of inputs), supposing them independent identically distributed random variables with discrete distribution. Similarly let $Y_k \quad k = 1,2,3...$ be the amount of material filled into the storage during *k*-th filling and they are also assumed to be independent identically distributed random variables with discrete distribution. Let denote $N(t)$ the number of fillings on the time interval $[0,t]$, which is a stochastic process. As the filled material can be expressed as the sum of the filled material during the fillings, the change of amount in the intermediate storage is $\sum_{k=1}^{N(t)} Y_k - t$. If the total volume of the storage is z_s and the initial amount of material is z_0, then, in order to avoid overflow the following inequality has to be held $z_0 + \sum_{k=1}^{N(t)} Y_k - t \le z_s \quad t \ge 0$, that is $\sum_{k=1}^{N(t)} Y_k - t \le z_s - z_0 \quad t \ge 0$. Taking into account that the appropriate values of Y_k and t_k are integer, if we would like to investigate the overflow probability and the overflow time, we have to consider $u(n) = P(\sum_{k=1}^{N(m)} Y_k - m > n \quad for \quad some \quad m = 0,1,2..)$ $n = 0,1,2,..$, furthermore $p_m^{(n)} = P(m - \sum_{k=1}^{N(m)} Y_k + n < 0 \quad \text{and} \quad s - \sum_{k=1}^{N(s)} Y_k + n \ge 0 \quad 0 \le s < m) \quad n = 0,1,2,..$, $m = 0,1,2,..$, which the probability that the first overflow happens at time point *m*. As a generalization we investigate the z transform of the sequence $p_m^{(n)}$, namely the function $\varphi^{(n)}(z) = \sum_{k=0}^{\infty} p_k^{(n)} z^{-k} \quad z \ge 1$. As $\varphi^{(n)}(1) = u(n)$, and $\left(\varphi^{(n)}\right)'(z)|_{z=1}$ equals the opposite of the expectation of the overflow time, it is suitable for investigating both overflow probabilities both overflow time. Using the theorem of probability theory we proved that function $\varphi^{(n)}(z)$ satisfies the following difference equation with $f(j) = P(t_k = j)$ and $g(i) = P(Y_k = i)$:

$$\varphi^{(n)}(z) = \sum_{j=0}^{\infty} \sum_{i=1}^{n+j} \varphi^{(n+i-j)}(z) f(j) g(i) z^{-j} + \sum_{j=0}^{\infty} \sum_{i=n+j+1}^{\infty} f(j) g(i) z^{-j} .$$

We analyse this equation, prove the existence and the uniqueness of the solutions for $z > 1$, and we prove its limit property $\lim_{n\to\infty} \varphi^{(n)}(z) = 0 \ , \ z > 1$. In special cases we determined its analytical solutions and used them for solving the original sizing problem.

DECISION MAKING WITH A RANDOM WALK IN A DISCRETE TIME MARKOV CHAIN

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Description of the problem. We consider the problem of evaluating alternatives in the early stages of an innovation process. In this application area alternatives need to be evaluated by several decision makers with respect to different criteria. There are possibly many alternatives that need to be considered; therefore it is necessary to make the evaluation process fast and simple. The following example describes the intended application. During an innovation workshop a large number of ideas are produced. Each idea is described only with a title and a short characterisation. An innovation team must identify the top ten ideas to bring them forward to the first stage of a stage-gate process [2]. Little or no quantifiable information is available about the ideas, therefore it is not possible to rank the ideas based on objective criteria. Instead, only subjective impressions are available at this stage, enabling decisions of the form “A is better than B” with respect to a given criterion.

The following questions need to be addressed: How to model an evaluation process and a decision process with the specified parameters? How to deal with inconsistent or non-transitive evaluations, which can occur due to the subjective nature of the evaluations? How to determine the top alternatives?

State of the art. In the field of multi-criteria decision making (MCDM) many methods have been developed for specialised applications. Two more general methods which can be used in the early stages of an innovation process are AHP (the Analytic Hierarchy Process) [3] and cost-benefit analysis (CBA) [1]. However, AHP and CBA are not directly applicable to the intended application. AHP does not support multiple decision makers and requires consistent transitive evaluations in order to compute a valid result. CBA needs measurable and quantifiable criteria to compute a valid result. Accordingly, AHP and CBA cannot be the preferred methods to evaluate alternatives under these circumstances.

New in our approach. Based on the assumption that little or no information about the alternatives is available, the evaluation process is implemented as pair wise comparisons between all alternatives, concerning all criteria. These comparisons only ask for a decision of the following form “is better than”. This solution allows comparisons according to non measurable evaluation criteria, such as taste or preference.

We assign weights to the decision makers according to their expertise and to the evaluation criteria according to their relevance, and scale these weights to sum up to one. We build a weighted directed graph, where each comparison adds an edge from the less preferred alternative to the better one. The edge weight results from the weight of the criterion and the decision maker. After adding the edges corresponding to the comparisons to the graph, we can scale the edge weights such that the sum of all outgoing edges of a node is one. The resulting graph is a discrete-time Markov chain, where the edges lead from the less preferred to the better alternatives.

We believe that the decision process then corresponds to a random walk on this resulting Markov chain. We assume that the sojourn time of better alternatives is larger than for inferior ones. To determine the preferred alternatives, the DTMC is solved, resulting in the steady state probability vector. The more incoming edges with large weights one node has, the more comparisons were made preferring that alternative. The more outgoing edges with large weights one node has, the fewer comparisons preferred that alternative. Consequently the better alternatives with more incoming edges have a larger probability in the result. The resulting probability vector is then interpreted as a ranking of the alternatives, where larger probabilities show a higher rank.

Advantages in our approach. The method allows quantifiable and soft evaluation criteria. The method enables decision makers to evaluate alternatives with little or no information available. The method combines a decision making problem with an established mathematical method (discrete-time Markov chains). By combining only some of the comparisons made, it is possible to compute intermediate results during the evaluation process. The method is simple to use, because we only ask for “better than” decisions. The method can easily represent levels of competence of the decision makers with respect to the criteria.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

THE OPTIMAL PORTFOLIO SELECTION: THE CASE OF INTEGRAL BUDGET

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In 1969 R.C. Merton used the dynamic programming for investigation of in order to study the optimal consumption and optimal portfolio selection problems in continuous-time on in efficient and arbitrage-free markets. Since that time, the task of optimal portfolio selection under uncertainty conditions (where the model of investors' budget is described by the stochastic differential equation (SDE)), is still a wide-studied problem.

It was proved that the normal distribution does not exactly describe the behavior of the stocks. One of the reason is that the economic time series "typically" exhibit cycles of all orders of magnitude, the slowest cycles having periods of duration comparable to the total sample size. The sample spectra of such series show no sharp "pure period", but a spectral density with sharp peak near frequencies close to the inverse of the sample size. So that, in this paper, we consider the financial market, characterized as a market with volatility growth, antipersistence or persistence, long-range or short-range dependencies and describe the investors' budget dynamics by SDE with fractional Brownian motion (FBM).

Let H be the Hurst parameter of FBM. If 0<H<1/2, the FBM exhibits a short-range dependence, and if 1/2<H<1, the stochastic process presents long-range dependence. Theoretically, the second case is much more easier to solve as far as, due to the trajectories features of FBM, one can use a pathwise approach to define integrals with respect to FBM and consequently obtain a stochastic control with respect to the FBM.

To avoid the usage of stochastic calculus in the optimal portfolio selection problem it is possible to use the state moment as a new state variable of the investor's budget equation. The link between fractional variational calculus, Hamilton-Jacoby equation and fractional dynamic programming was established in works of G. Jumarie. However, the solution to the problem subject to control constraints was not found. On the other hand stochastic maximum principle was used in the same problem, but again without control constraints.

In our paper, we consider the optimal portfolio selection problem, with the budget equation presented by SDE with FBM, replaced by weakly singular integral equation and subject to control constraints. So, we transformed the stochastic problem to a non-stochastic one. Therefore, our goal is to find a solution to the problem with integral object's equation (which corresponds to stochastic process with short-range), subject to control constraints. For this problem, we derive first order necessary conditions in the form of Euler-Lagrange equation, which is also called the "local maximum principle".

The paper is organized as follows: we formulate the optimal portfolio selection problem, derive necessary optimality conditions for the case of short-range dependencies, give an algorithm of numerical solution, and finally provide an application of the results in the problem of parameters estimation of selected stocks (to find an optimal portfolio allocation which maximizes the expected utility from terminal wealth).

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Modelling in Economics and Finance

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

COMMON-KNOWLEDGE RESOLVES MORAL HAZARD

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This article investigates the relationship between common-knowledge and agreement in multi-agent system, and to apply the agreement result by common-knowledge to the principal-agent model under asymmetric information. We treat the two problems: (1) how we capture the fact that the agents agree on an event or they get consensus on it from epistemic point of view, and (2) how the agreement theorem will be able to make progress to settle a moral hazard problem in the principal-agent model under asymmetric information. We shall propose a solution program for the moral hazard in the principalagents model under asymmetric information by common-knowledge. Let us start that the agents have the knowledge structure induced from an equivalence relation associated with the multi-modal logic **S5n**. Each agent obtains the membership value of an event under his/her private information, so he/she considers the event. Specifically consider the situation that the agents commonly know all membership values of the other agents. In this circumstance we shall show the agreement theorem that consensus on the membership values among all agents can still be guaranteed. Furthermore, under certain assumptions we shall show the moral hazard can resolve in the principal-agent model when all the expected marginal costs are common-knowledge among the principal and agents.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MATHEMATICAL RELATIONSHIP BETWEEN TRANSPORTATION & ECONOMIC GROWTH BY VECTOR AUTO-REGRESSION MODEL

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Abstract. Transportation as one of the effective factors on economic growth has a leading role in every country's policies. Facilitating the trade and business, the transportation sector provides both national and international growth and increases the accessibility grounds to national welfare and facilities. Thus, in the process of economic growth it has a very main and effective role while it is also affected by the process of economic growth and development. This study mainly aims at investigating the role of development of the transportation sector in economic growth of the country using the statistics within 1971-2004. For the empirical testing of the model, Vector Auto-Regression Model has been used. Investigating the stationary state and co-integration of the variables, the researcher has determined the collection degree of the variables of the model and then specified the number of optimal lags of the model. Next, the number of the co-integration vectors of the model is determined and then the desirable model is designated indicating that the development of the transportation sector has a positive and long-term effect on the country's economic growth. Furthermore, the effects of different shocks of the transportation sector on the economic growth over time as well as the degree of regression variances of the variable viz added value of transportation sector on economic growth are taken into consideration in this study by using the Analysis of Prognosis Error.

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Modeling of Decentralized Service Systems in Automation Technologies

MODELLING OF THE REQUIREMENTS FOR DECENTRALIZED BUILDING AUTOMATION SYSTEMS

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In modern building automation (BA), decentralized automation networks gradually replace hierarchic automation network structures. These building automation system (BAS) consist of up to 30000 different devices and are thus complex. In addition, many different manufacturers offer a large number of various devices each, and conformity is not guaranteed among devices of different manufacturers. Today, planners have to design such BAS manually, which requires huge effort. Besides this problem, they are confronted with the challenge of various assembly sections (AS), e.g. Heating, Ventilation, and Air Conditioning (HVAC), lighting and shading (room automation). Each device performs a certain task within an AS, and different tasks are often planned by different engineers. All these points lead to a huge effort within the Requirement-Elicitation phase. Today's elicitation of requirements for such a BAS, which is to be planned, depends on customers' requests and on planner knowledge. This procedure often leads to sub-optimal requirements for the further engineering phases Planning-Stage and Implementation-Planning. Especially, flaws in early phases of the engineering workflow lead to increased costs in later phases. Fundamental causes for this non-optimal requirements elicitation are e.g. that the building-owner and planner use different vocabularies, leading to misunderstandings, and that the planner cannot cope with all the functionalities and different types of devices. A new approach of automated Requirement Analysis within the AUTEG-Project [1] differs from the current elicitation of requirements in the application of an intelligent Requirement Analyzing Tool [2]. This Tool offers the possibility to fulfill the described problems by means of automated engineering mechanisms. These automated mechanisms can save costs [3]. A model to describe the requirements of a decentralized building automation system, which is to be planned, is mandatory for this intelligent requirement elicitation. Such a model allows defining consistent, semantically described requirements and their causal dependencies.

A short introduction defines the intention of building automation to clarify the complexity of modern decentralized building automation systems. A main topic of this paper is the modelling of the requirements for such automation systems, which are to be planned. Thereto, the Model Classes, e.g. Application Function-Controllers, Sensors and their Model Sub-Classes (devices and possible requirements respectively) e.g. Constant Light Control-Controller, Stairway Lighting-Controller, and Illuminance Sensor, are defined. The Model Sub-Classes are specified by Device Attributes, and if necessary by Functional Artifacts/Functions, and Nonfunctional Artifacts/Hardware Moduls. The Functional and Nonfunctional Artifacts are again specified by Artifact Attributes. Additionally, the possible causal dependencies between these Sub-Classes (e.g. Constant Light Control-Controller "requires" Illuminance Sensor) are presented. Closing this topic, a short example of modelling by using these requirement model classes is shown. Another main topic of this paper is the data exchange of the modelled requirements by using the Data Exchange Format for the Engineering of Building Automation Systems [4]. This Format is based on CAEX (Computer Aided Engineering eXchange) [5], which is a meta model for vendor- and tool-independent structuring and categorization of CAE data. Thus, CAEX does not define domain specific patterns. Hence, a specification of CAEX, also referred to as modelling, to the terminology of the requirement modelling is shown in this paper. The previous example is reused to explain the data exchange. Finally, this paper gives a summary of the deliverables, and an outlook declares advantages representing this requirement model and models in general by means of the Semantic Web Technology OWL (Ontology Web Language) [6].

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

ON SERVICE-ORIENTATION AS A NEW APPROACH FOR AUTOMATION ENVIRONMENTS

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Introduction. In the field of automation environments software has to fulfil many standards especially according to security and safety. Using such a standard and an engineering tool, an engineer is able to build up an application for controlling a process within a plant. This results in two limitations. The first one are the fixed (engineered) connections between the parts of the application. So a change of the plant would result in a complete new program, which has to be compiled and loaded. The second limitation is that an information, which has been evolved at the level of automation systems has to be forwarded via different interfaces to the higher management and enterprise levels, where it will be needed also.

A new approach should result in a more flexible and cost-effective plant to present innovative products in even shorter time to the market.

Todays automation architecture. During the past in the field of automation the costs for a reconfiguration of a plant are reduced by using a high standardization. This was also important to get the needed reliability and safety of a plant. This lead to the *level model of a corporation* as introduced e.g. by IEC 62264. Which results in the representation of the *automation pyramid*. The pyramid yields from the Enterprise Resource Planning (ERP) level on top to the Process Level at bottom. The levels are separated from each other.

The basic idea of recent inventions is that an automation system is a distributed and decentralized system. But nevertheless it is not possible to make changes to a running plant. Often from the sight of the process changes during runtime are possible and so the user did not want to stop the process due to the upcoming costs.

Service-orientation in automation environments. The term 'service oriented architecture' is here understood like it is presented by OASIS [2] as a paradigm for organizing and utilizing distributed interoperable systems. The requirements of a service-oriented system are scalability, reliability and flexibility.

The model of the architecture used here was introduced by Epple on the NAMUR Workshop 2008 [1]. The idea is the placement of a service system in parallel to the automation pyramid. Between both elements the service interfaces are placed to grant access to the services. In each level of the automation pyramid there may be a kind of functionality realized as a service. So by the usage of the service interface the service can be located and used.

The service system is an effort of the whole automation system and provides the resources to manage and to execute the services. A service system is available on all levels of the automation pyramid and a service is responsible for all levels.

A survey on possible classes of services and more concrete services follows here. First of all there are classic control services like archiving or reporting. Next theme are steering services e.g. for tuning of process parameters. Also monitoring is one possible service class to determine key performance indicators of a plant or an enterprise. Another often used functionality is maintenance e.g. to realize an asset management service. Other classes will follow and have to be discussed in official committees where users and vendors are both represented in order to get a widespread acceptance.

One assumption is that a plant consists of different components each reliable for one step in the production. So each component can be engineered independent from other components. The standardized functionalities of the components need not to be engineered any more due to the fact, that these functionalities are applicable by the service system. This results in reliable and more flexible systems with reduced engineering time and costs.

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A DECENTRALIZED FOUNDATION MODEL FOR AUTOMATION TECHNOLOGIES

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Motivation. For current automation systems a device failure yields to extensive costs and working time for bringing a replacement in production mode. Beside the physical replacement itself the setup procedure of the newly added device produces workload for several engineers before the device is in the position to fulfill the demand of the failed device – most likely a complete workflow needs to be established.

This paper presents an foundation approach addressing this and other current issues within the field of automation. The approach bases on ideas from second generation Peer2Peer systems [4], which main focus is decentralization. Where some second generation Peer2Peer networks still have a central point within their overlay network – e.g. for authentification – this one is completely decentralized thus a resulting system would be more complex in terms of design but even more flexible and reliable.

Foundation Model. The approach introduces the service-oriented architecture principle (SOA) [3] for these kind of systems, thus proposes to see an overlay Peer2Peer network as an foundation for a various range of decentralized applications consist of services, which could depend on each other as well as interact. The approach proposes an abstract architecture model including the application interface as one main part providing information about the current Peer2Peer network and its changes to the high level applications on top of the foundation. By abstracting from the concrete implementation as well as the management of data within the foundation this interface makes it possible to customize the approach to various application scenarios.

For realization one needs to define so called flavors, which concretize the model by defining specific plug points, which need to fit together in a way that the whole system fulfills the concrete requirements. As an example one plug point is *Neighborhood* describing a set of peers, which are monitored by a peer – meaning through this peer the network recognizes and thus could react on a failure of the monitored devices. Different flavors would have different performance advantages as well as penalties. Like in all information technology systems the developer has the choice between speed (meaning less communication for Peer2Peer networks) and using more memory by defining an appropriate flavor.

Within the prototype of the foundation model, a very simply flavor was designed and realized. For demonstrating the capabilities of this approach, this flavor assumes as plug point for the neighborhood the system to be rather small thus all peers could know each other. Other flavors address larger networks or systems not providing enough memory to store a whole view of the network. These flavors would on demand of their upper layer services retrieve information about the base network. As an example of this foundation model implementation the *Zero-Config* scenario is presented, which addresses the failure-replacement-workflow mentioned at the beginning. By storing the configuration data within the application *Distributed Data* as well as monitoring failures, the application *Self-Config* could retrieve information about past failures upon startup of the device and (potentially) decide which replacement the device is for. After acknowledge of the operator, the device could retrieve the configuration data and directly go to production mode. The prototype realization bases on the ACPLT Technologies as described in [1].

Conclusion. The presented model yields to a new way of device communication at the automation. It enables a complete decentralization by providing a migration path due to the fact that – as shown within the prototype – configuration could be implemented using the approach without interfacing the traditional system, which could be in operation like before. Other scenarios as heterogeneous peers [2] including discovery capabilities are planed to be adopted to this approach.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

DECLARATIVE RESOURCE DISCOVERY IN DISTRIBUTED AUTOMATION SYSTEMS

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Introduction. Engineering is the major cost factor in the construction of state of the art industrial systems. Automation equipment features a multitude of parameters that need to be configured and parameterized during commissioning of a plant. Additionally, the environment is highly heterogeneous with multiple equipment vendors and product versions. Finally the recent demand from customers to build more flexible, easier to customise and fully integrated manufacturing systems adds to the complexity.

A key problem is the so called point to point dilemma, i.e., the tight coupling of automated functions and resources. Today systems are designed statically by directly specifying end-to-end communication. For example, sensor S delivers data to motor M. If M is replaced, or other units are interested in data generated by S, each new connection needs to be configured end-to-end. Thus an enormous conglomeration of static communication links is the result. Besides being expensive to configure, the static interweaving of automation equipment prevents flexible execution of control software.

In this paper, we present an architecture capable of de-coupling individual automation equipment. We propose a robust and self-organising system to discover resources at runtime in a networked automation system using declarative resource discovery. We use Peer-to-Peer (P2P) and Grid computing technology originally designed for the Internet and advance them such that they can be implemented on even resource constraint equipment. P2P systems such as Chord and CAN provide the foundation for loosely coupled systems in the Internet. However, both their code complexity as well as stabilisation effort, i.e. the intensity of required communication, suggest cost intensive realisations and hence those approaches are rather unlikely to emerge in industrial products. We therefore investigate how a lightweight algorithm can provide similar features albeit being less capable in an Internet scale, i.e., millions of users, scenario.

Content. We address the point to point dilemma by designing automation systems as loosely coupled orchestrations of automation assets. Similar approaches are taken in service oriented architectures (SOA) such as sensor Grids or similar Grid computing applications. In SOA, assets are described by the service, i.e. the function, they provide. Services encapsulate resources which execute the functions provided by the service via a service interface which in turn provides a consistent view on the resource. Besides the service interface, a service description provides information about the interface as well as qualities of operation and management. In order to use a service, a service consumer states his interest in a service query and issues the query at a service registry which maintains all available service descriptions. Once found, the service consumer binds to the service first and then executes the desired functions. A key advantage of the service oriented approach are the different temporal options for service binding. Early binding is referred to at design time when requirements are mapped to service descriptions. Late binding, in contrast, renders a system more flexible as the service consumer binds the service at runtime. Ultra-late binding takes the concept one step further as applications are created by composing services dynamically for each invocation and removing services from the application after they are no longer needed.

In order to support late and ultra-late binding paradigm, the service registry must provide efficient means to process the service query and match it to service descriptions accordingly. Solutions for this service discovery process range from simple keyword searches to evaluation of fuzzy logic and semantic reasoning. While the expressiveness of keyword searches is often not sufficient for complex service descriptions, the resource demand for semantic matching prohibits cost efficient solutions. A flexible compromise is provided by complex declarative queries, common in most database systems. Query languages like the standard query language (SQL) provide rich semantics to express complex interests yet they can be implemented efficiently.

While centralised registries can be implemented efficiently, they are additional infrastructure components that need to be integrated and maintained. Distributed registries, however, use already existing resources of the networked assets. They are further more robust and scale dynamically with the number of networked assets. We describe a generic service oriented architecture for loosely coupled automation devices. Being a key component, we emphasis in the description of a distributed service registry with support for declarative queries. The approach is evaluated through extensive simulations which demonstrate benefits and applicability of the proposed architecture.

Proceedings
MATHMOD 2009 Vienna
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Numerical Methods in Quantum Simulations

A MODULAR GREEN'S FUNCTION METHOD FOR QUANTUM TRANSPORT THROUGH GRAPHENE

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Introduction Advances in the preparation of carbon-based two-dimensional thin films have made available a monoatomic, hexagonal grid of carbon atoms in the plane [1]. This novel material, called graphene, has already given rise to remarkable discoveries as, e.g., the first observation of the integer quantum Hall effect at room temperature. The transport properties of graphene are determined by the Schrödinger and, in limiting cases, the Dirac equation of quantum mechanics. The latter limit has caused excitement as it may allow to explore relativistic physics in a low energy regime. However, solving the corresponding wave equations is very challenging. To compare with experiments, additional contributions due to rough edges or lattice defects have to be included. The resulting problems require a flexible, powerful technique that can cope with these requirements. We adapted the modular recursive Green's function method (MRGM) for this purpose [2].

Technique Our approach is based on a tight-binding discretization on the hexagonal graphene lattice [3]. The key idea is to break down a large device into separable, rectangular modules, each of which can be computed very efficiently. To illustrate our technique, we consider a graphene-based nanoribbon. In a first step, an eigenvalue problem is solved on a one-dimensional chain of carbon atoms [see Fig. 1(a)] to obtain its Green's function. Periodic repetition of this chain creates a half-infinite ribbon of graphene [see Fig. 1(b)], the Green's function of which allows to separate off a rectangular module by way of a Dyson equation [see Fig. 1(c)]. By combining several rectangular modules, a complex scattering geometry can be realized [see Fig. 1(d)]. The key advantage of this strategy is that the computing time is independent of the length of the rectangular module, scaling only with the width W of the ribbon. Large scattering geometries of realistic dimensions can therefore be assembled without major effort.

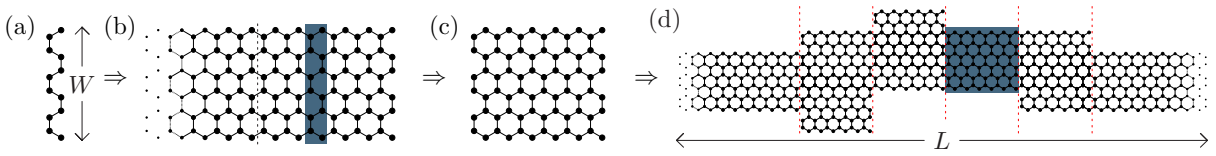

Figure 1: (a) Single graphene block made of a one-dimensional chain of atoms. (b) A half-infinite waveguide is assembled by periodic repetition of (a) (see shaded area). (c) A finite-length rectangular module is cut off from (b), which is then used to assemble a large-scale scattering structure (d).

Conclusion The MRGM allows us to treat a wide variety of different device geometries in a numerically efficient way. We calculate both the scattering matrix and individual scattering states. We find that transport is strongly suppressed by deviations from a perfect graphene lattice, which are not included in models based on the Dirac equation. Furthermore, lattice defects result in localization of the wavefunction, that can be directly visualized in the scattering state. For very long ribbons ($L \approx 3\mu$m, over 12000 blocks) we observe exponential (Anderson) localization of the wavefunction densities over eight orders of magnitude. Finally, our method is not restricted to graphene: any periodic lattice geometry (including an artifical quadratic lattice to model continuum equations) can be treated as well.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

HOW MATHEMATICS CAN SPEED UP QUANTUM MECHANICAL CALCULATIONS OF SOLIDS

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Introduction. Today rather complex materials can be simulated applying different methods according to the corresponding length scale. At the atomic scale, where the electronic structure plays the dominant role, calculations are mostly done with density functional theory (DFT) and often with the WIEN2k program package (see www.wien2k.at) that has been developed during the last 28 years and is used worldwide by more than 1400 users in academia and industry [1]. Mathematics can contribute a lot to achieve high efficiency; some important aspects are:

Material sciences. A solid (or surface) is represented by a unit cell and periodic boundary conditions. The cell is defined by its shape and the atoms it contains, which may be 1 or over 1000, where each atom is specified by its atomic number and the position in the cell. The properties vary from insulators, metals to magnets.

Electronic structure requires quantum mechanics, e.g. DFT leading to one-electron Schrödinger-type Kohn-Sham equations, which need to be solved iteratively within self-consistent field (SCF) cycles. From an input density one generates a potential leading to wave functions which define an output density. A clever mixing between input and output density (using a better than Broyden's mixing) can reduce the number of cycles. The wave functions are expanded in basis functions, which - in our case - are given in linearized augmented plane waves (LAPW). In order to find the expansion coefficients (according to the variational scheme) a general eigenvalue problem must be solved that is rather computing intensive (scales with n^3). The matrix size can be above n=50000. For the SCF cycles only the occupied states are needed and thus one can use a subspace and a modified Davidson solver using information from the previous cycles to find the necessary eigenstates.

Structure optimization. The atoms can move to their equilibrium positions till the forces acting on them vanish. A rough estimate of the Hessian (using results from previous steps) can reduce the number of steps towards the equilibrium geometry of the system.

Mathematics can provide efficient algorithms for the various tasks as indicated above. The mathematician must consider the specific needs of materials sciences but also the available computer architecture. In addition the numerical precision must often be very high, since the quantity of interest (e.g. the total energy) may vary in the eleventh decimal place.

Hardware and software. The rapid improvements in terms of in memory, communication, libraries, parallelization, etc need to be optimally utilized.

Summary. A high efficiency can only be gained by combining the expertise in all these fields. Optimization must consider which parts of matrices are dominant, how previous information can be reused but also numerical precision, convergence, data locality, band width, parallelization etc. These issues need to be addressed with proper algorithms, which recently were found to be very successful.

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Proceedings
MATHMOD 2009 Vienna
Abstract Volume

Short Paper Abstracts

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

λ-Scale Convergence Applied to the Stationary Heat Conduction Equation with Non-Periodic Thermal Conductivity Matrix

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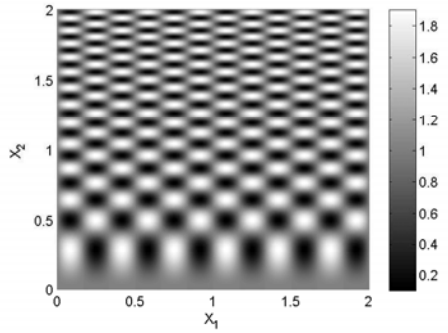
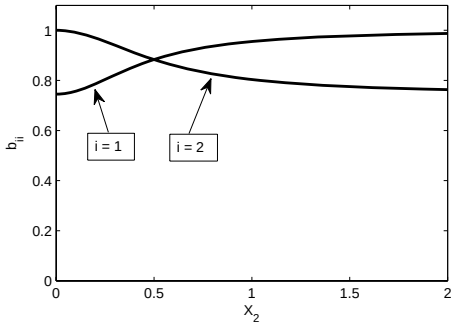
Homogenization theory makes sense to use whenever the microscopical behaviour of a partial differential equation can not be seized by numerical solution methods. In this contribution we examine a sequence of stationary heat conduction equations with homogeneous Dirichlet boundary data,

$$\begin{cases} -\nabla\cdot\left\{(A\circ\alpha^h)\nabla u^h\right\} = f & \text{in } \Omega, \\ u^h = 0 & \text{on } \partial\Omega, \end{cases} \tag{1}$$

as $h\to\infty$, where A is Y-periodic. We see that $\{\alpha^h\}$ yields a sequence of possibly non-periodic thermal conductivity matrices $\{A\circ\alpha^h\}$. To obtain the homogenized limit we utilize the recently developed λ-scale convergence technique [3], which is a generalization of classical periodic two-scale convergence [2], but a special case of scale convergence [1]. Under certain restrictions, especially the property of $\{\alpha^h\}$ being asymptotically uniformly distributed on Ω, it is implied that the λ-scale convergence is achieved for both the sequence of solutions $\{u^h\}$ and the corresponding sequence of gradients $\{\nabla u^h\}$ (spawning an extra term in the limit), which is the main key to homogenize the stationary heat conduction problem (1). The concept of type-H_X^Π sequences is tailor-made in order to formulate a main theorem on the homogenization of the problem. The original part of the contribution commences by introducing a simple two-dimensional "toy model" defined by $\alpha^h(x) = \left(hx_1, hx_2|x_2|\right)$ on $\mathbb{R}^2$, and an open interval Ω strictly included in the first quadrant of the $\mathbb{R}^2$-plane. We show that the "toy model" sequence $\{\alpha^h\}$ satisfies the conditions of the aforementioned main theorem on the homogenization, which is then used to express the main original result of the contribution where we claim an explicit formula for the homogenized thermal conductivity matrix B and a local problem in Y (parametric over Ω). The contribution is concluded by numerically computing B with $\Omega = (\delta,2)^2$ (where $\delta \gtrsim 0$) and an A on the form $A(y) = \left(1+\frac{9}{10}\sin 2\pi y_1 \sin 2\pi y_2\right)I$, $y\in\mathbb{R}^2$, such that the scalar factor of the composition with α^h is given according to the left figure below. In this case, the homogenized thermal conductivity matrix B turns out to have vanishing off-diagonal entries and non-vanishing diagonal entries according to the right figure below. The simple but illuminating "toy model" studied in this contribution clearly shows that it is possible to homogenize problems of the type (1) with respect to sequences of sufficiently well-behaved non-periodic thermal conductivity matrices. The results here open up a wide range of more "realistic" stationary heat conduction problems to examine.



The scalar factor of $A\circ\alpha^h$ for $h=3$.



The diagonal entries of B.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A COMPARISON OF FEATURE NORMALIZATION TECHNIQUES FOR PCA-BASED PALMPRINT RECOGNITION

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The term *biometrics* refers to a scientific discipline which involves automatic methods for recognizing (verifying or identifying) people based on their physical and/or behavioral characteristics. Many biometric systems, i.e., systems which exploit these methods to establish identity, have already been presented in the literature; among them, systems which make use of biometric characteristics such as fingerprints, face, voice, iris, retina, hand-geometry, signature or palmprints are the most common [3].

While a considerable research effort is directed towards the development of efficient, fast, robust and user-friendly biometric systems, there are still some major problems that need to be tackled before they can be deployed on a larger scale. One of the main challenges, which has yet to be solved, includes increasing the recognition performance of biometric systems. Towards this end, a trend has emerged in recent years, namely, the employment of multi-modal biometric systems which establish identity either by considering several biometric modalities (e.g., the face, the iris, palmprints, voice etc.) or by combining the recognition results of several algorithms performed on the same biometric sample. While such an approach is a valid solution for the problem of recognition performance, it commonly decreases the user-convenience, as it requires a greater effort from the user to operate the system or it increases the time needed to process a single user. From this point of view, other solutions capable of increasing the recognition rates and not influencing the convenience of using the biometric systems should be sought.

One possibility of increasing the recognition performance is to closer examine feature normalization techniques, which hold the potential to greatly decrease the error rates of biometric systems, but have so far been largely neglected in most research papers on the subject of biometrics. Commonly, only a sentence or two is devoted to the employed normalization technique, even though feature normalization represents a crucial step in the design of a biometric system. Feature normalization techniques have a great impact on the procedure of constructing user templates (or models), i.e., mathematical representations of the feature vectors extracted from several measurements of the biometric characteristic (e.g., palmprints) during user enrollment stage, and consequently on the way how user-specific biometric characteristics are modeled. They represent a fast and efficient way of boosting the recognition performance of biometric systems which does not significantly increase the processing time of a user.

In this paper we present an empirical evaluation of the following feature normalization techniques: unit-length normalization (UL), zero-mean and unit-variance normalization (MV), linear scaling to unit-range (SC), rank normalization (RN) and gaussianization (GS), which we apply to feature vectors extracted from palmprint images by means of principal component analysis (PCA) [2]. We report comparative results with the recognition performance of raw palmprint features, i.e, features without normalization (WN), and assess their performance in conjunction with the nearest neighbor classifier and three popular similarity measures, namely, the Euclidian distance, the City Block distance and the cosine similarity measure.

Experimental results obtained on the publicly available PolyU palmprint database [6] show the the choice of an appropriate normalization technique greatly influences the performance of the palmprint-based authentication system and can result in error rate reductions of more than 30%. In particular, the results suggest that gaussianization of the feature component distribution is the best normalization technique among the tested ones and ensures consistent improvements regardless of the similarity measure used in the matching stage.

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A DEVELOPMENT OF AN ANALYSIS FOR ENERGY AND FLUID CONVECTION USING THE THERMAL DISCRETE BOLTZMANN EQUATION WITH AN ANALYTICAL SOLUTION OF A RELAXATION EQUATION

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Summary. In this paper the new time integral method for the discrete Boltzmann equation (DBE) is introduced. It is based on the exact solution of the relaxation equation, and it is achieved to stable, good accurate and rapid calculating method for fluid simulation using DBE. To describe the effectiveness of this method, the rid-driven flow and the natural convection in a square cavity are calculated. The results of these problems have good accuracy to compare with the past researches. Then the numerical method is effective for the computation of fluid and temperature using DBE, and it is expected to apply the high Reynolds number flow field or the high Rayleigh number flow field.

Introduction. In this paper, the new time integral method is proposed for the Discrete Boltzmann Equation (DBE). The numerical experience for fluids using the Lattice Boltzmann Method (LBM) [1] is attended, because the analysis is simple and it has good effect for complex fluids or complex boundary. But, LBM is allowed to the computation with staggered lattices. Then, the approach of the dissipation for the weakness of LBM is suggested. It is that the basic equation, namely DBE of LBM is discretized using the Finite Volume Method [5] or the Characteristics Galerkin Method [6] for space. However, a new problem is appeared. It is about stability. On the simulation with LBM, calculation is executed completely stable, but there is unstable region yield to depend on the time integral method by DBE. On the computational fluid dynamics (CFD), there are two approaches to solve unsteady problem. The one is to use the exact solution of a differential equation, and another is to add the stability term. We stand on using the exact solution of a relaxation equation. This is achieved to realize stable form. And more this formulation makes the calculation time be less than the conventional time integral metho. This formulation is named as the Semi-Analytical Method.

The Semi-Analytical Method is performed to the rid-driven flow and the natural convection in square cavity. The result of the rid-driven flow is compared with the numerical result by Ghia et al [4], and the natural convection in the square cavity is calculated using thermal DBE suggested by He et al [2] and is compared with the result by de Vahl Davis [3].

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A METAMODEL FOR EVALUATING NEW KEY PERFORMANCE INDEXES ON TOP PRODUCTS SELLING IN RETAIL FASHION: METHODOLOGY AND CASE STUDY.

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Abstract. the concept of enterprise resource management, evolved in its larger extents of ECC and SOA, is nowadays very popular, and most of medium-large companies in the world have implemented an integrated information system to manage operations and data. One of the targets of such companies is to improve their performances in terms of revenues, costs, competitiveness on the market through the integration of such information systems. But for the retail-fashion companies (especially luxury brands) is not so easy to evaluate the earnings and savings deriving from such costly operations as implementing a new enterprise management system, because traditional literature of KPIs do not offer a very exhaustive cockpit of indexes for retail fashion to keep in control business and its development, mostly for evaluating typical fashion-related effects, such as seasonal products impact, must-have effects, special requirements from customers etc.

Based on a series of requests coming from some possible ERP customers in the fashion area, that are making a software selection, the Authors have created some models to evaluate and forecast specific retail-fashion effects, in order to be implemented in the ECC system and to be integrated with materials management and production planning applications.

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A METHOD FOR MINIMIZATION OF PRONUNCIATION-LEXICON FINITE-STATE MODEL FOR AUTOMATIC SPEECH RECOGNITION

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Introduction. The common mathematical model of the human speech communication process comprises two major components. The low-level component is called the acoustic model and is related to the acoustic realization of human spoken language. This model incorporates general phonetic and psycho-acoustic knowledge about the human speech production and perception system. It is used to model the sequences of acoustic speech observations. The well-known hidden Markov models (HMMs) [3] and artificial neural networks (ANNs) are normally used for this purpose.

The high-level component of the whole speech model is called the language model. This model comprises several sub-components, like pronunciation lexicons, context-free and/or stochastic grammar models, and semantic models. This part of the joint model is related more to the phonological and linguistic aspects of human spoken language. The language model is commonly represented as a finite-state machine, or more precisely, as a deterministic or non-deterministic finite-state network (FSN) [1].

When HMMs are used for the acoustic model, the joint speech model can be represented as a unified multi-level probabilistic FSN (directed graph). This approach reduces the problem of ASR to the problem of searching for the most probable path through such a network, given an acoustic speech observation sequence [2].

Optimisation problem. The performance of large-vocabulary automatic speech recognition (LV-ASR) systems, which are based on the above modelling concept, critically depends on the size of the used FSN. Due to the limited computational performance of current computer systems, all implementation of LV-ASR systems require certain optimization of the network in terms of its size and algorithmic complexity. The concept of WFSTs provide a general representation and algorithmic framework for such an optimization that can be achieved using general algorithms for model composition, weighted determinisation and minimization, and weight pushing [2].

Research goal. One of our main research goals is the development of our own state-of-the art LV-ASR system. The main motivation for this is our research commitment to develop such a system for our mother tongue, the Slovenian language. Our language is richly inflected with a grammar that is similar to that of other Slavic languages. It has certain distinctive characteristics, like dual grammatical number, two accentual norms, and abundant inflection. Although Slovene is basically a subject-verb-object language, word order is very flexible, often adjusted for emphasis or stylistic reasons. These characteristics provide a good reason, why we should not strictly follow the concepts that are used for the less inflected languages with less flexible word order, like English or German. We also have ambition to develop a single-pass LV-ASR system that requires certain adaptations of the system structure.

LV-ASR System. In order to provide more flexibility, we divided our LV-ASR system into three major components that can be developed and optimized separately. In this paper we briefly present work-in-progress on the system. Especially, we focus on the lexicon level, embedded between the acoustic and grammar level. We also present the concept of a single-pass token-passing algorithm that performs multi-level search for the most probable sequences of words, given an input acoustic speech observation sequence. Finally, we present a simple method for dynamic minimization of a deterministic FSN that is used for the modelling of pronunciation lexicons.

Results The presented FSN optimisation algorithm proved to be as good as the general optimization algorithms that are defined with the concept of WFSTs. These algorithms are implemented in the well-known AT&T FSM library. In the experiment, we constructed several pronunciation-lexicon FSNs from a list of 35k word pronunciations using different algorithms. For the optimization that was achieved using the AT&T FSM library, we had to run a whole sequence of algorithms. On the other hand, the presented algorithm runs in a single backward-forward pass for each added word pronunciation that is optimally merged with the existing pronunciation lexicon FSN.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A Probability Model for TCP Slow Start

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Abstract

This paper presents one approach of probability modelling of TCP connection during the slow start phase. Such modelling can be used for TCP connection analysis with reduced simulation time compared to the packet-level simulators. Proposed model is validated by packet simulations obtained by ns-2 simulator.

Application protocols mainly used on the Internet, such as HTTP or SMTP, use TCP protocol for reliable transport [1]. TCP connection performance analysis can be carried out in two different ways. First one is simulation of TCP connection at the packet-level. This approach leads to accurate results but also requires long simulation time. Alternative approach is to model the TCP behavior analytically, significantly reducing simulation time while simultaneously keeping accuracy at an acceptable level. One way to abstract the TCP behavior through mathematical tools is to use differential equations. The second approach is based on probability analysis. In this approach, statistical formulas are used to model the TCP behavior in different stages.

TCP is a reliable connection-oriented transport protocol for packet-switched networks. Reliability is achieved by employing acknowledgments (ACKs) [2]. Using ACKs and sequence numbers, the transmitter keeps the track on packets that are successfully delivered to the receiver. TCP operates by going through different stages, such as Slow Start, Congestion Avoidance, Fast Retransmission, Fast Recovery and Timeout. Transition between stages is determined by packet loss or acknowledgment of predefined number of packets. The window size determines the maximum number of packets that a transmitter may send before receiving the first acknowledgement. In the Slow Start phase, window size is incremented with every received ACK. The window size varies with the rate of the packet loss in the network. Hence, the packet loss probability increases with the number of sent packets due to the congestion in the network.

There are two approaches for creating probability models of TCP behavior. The source centric model assumes that packets leave the source with a certain loss probability [3]. The assumption taken by the second model is that the network generates loss probabilities for each packet [4]. Thus, the arrival process is represented by Poisson random process. In [3], the slow-start phase is modeled for time intervals called *rounds*, lasting from the moment when the first packet in the window is sent until the last packet in the window is acknowledged. The model further takes the following assumptions: when one packet in the round is lost, all the remaining packets in the round are also lost; packet loss occurs only in forward direction; packet losses are independent of window size.

Based on the source-centric model [3], we derived the expected value of the number of packets sent in the slow start phase as a function of packet loss probability p, the initial size of congestion window w_i and the number of packet acknowledged by one ACK. The model is based on assumption that packet loss is detected by three duplicated ACKs and timeouts. We further distinguished the two boundary cases related to the position where packet was lost. The first case is characterized by the packet loss occurring at the beginning of the round. For the second case, the packet loss occurs at the end of the round. The actual number of packets sent during the slow-start stage lies in the interval defined by these two limits. Assuming uniform distribution of the lost packet position, we derived formula for estimated value of window size in the round *'i'* , when packet is lost. Our analysis is confirmed by a large number of simulations using packet-level simulator ns-2.

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A PROJECTED NON-LINEAR CONJUGATE GRADIENT METHOD FOR INTERACTIVE INVERSE KINEMATICS.

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Introduction. Inverse Kinematics is used in both Graphics and Robotics. Recently attempts at solving the inverse kinematics problem using optimization techniques have been performed [1, 2, 3]. The problem can be formulated as a general problem and arbitrary optimization methods may be used to solve the problem. Not all of these methods are optimal in interactive applications and it is therefore of interest to identify the methods best suited for this particular problem type. We want an iterative method which has an acceptable compromise between performance and accuracy. Experience in Graphics indicate that the Conjugate Gradient method have worked very well in similar conditions, for example interactive cloth simulation [4]. Therefore Non-linear Conjugate Gradient method may be a feasible choice for Inverse Kinematics.

We present a novel method based on the Non-linear Conjugate Gradient method [5] combined with a projected line-search, inspired by the projected gradient method [6]. This box-constrained optimization approach is tested on a human figure using motion captured data as a reference. Results show that the method has better accuracy and is faster than the Jacobian Transpose method for Inverse Kinematics. Further the Non-linear Conjugate Gradient method does not suffer from oscillating behavior exhibited by the Jacobian Transpose or Jacobian Inverse methods. Altogether making the Non-linear Conjugate Gradient method with a projected line-search a more suitable choice for interactive Inverse Kinematics.

Projected Non-linear Conjugate Gradient The main difference between our approach and an unconstrained Non-linear Conjugate Gradient method is the projected line-search. Our focus in this paper is to explain the addition of the projected line-search to the unconstrained method. The Non-linear Conjugate Gradient method is described sufficiently elsewhere [5]. The projected line-search can be explained as a very effective specialization of an active set approach. Instead of adding and removing constraints from an active set one by one, the entire active set is recalculated in each iteration. This is only possible if the constraints are independent of each other and thus the projected line-search can only be performed where constraints are bounds on individual variables. Fortunately, this is often the case.

Results The Projected Non-linear Conjugate Gradient method has been implemented in the OpenTissue Library where it is possible to test Inverse Kinematics against motion captured data references. This makes it possible to test performance with regards to accuracy as well as time expenditure. We show how the Projected Non-linear Conjugate Gradient method compares to two Quasi–Newton methods as well as the Steepest Descent and the traditional Jacobian Transpose methods. Our results imply that the Projected Non-linear Conjugate Gradient method provides a desirable compromise between performance and accuracy, suitable for real time Inverse Kinematics.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A SYSTEM DYNAMICS MODEL OF HEALTH INSURANCE FINANCING IN AUSTRIA

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Summary. As the financial situation of the health care system in Austria is an important issue, a dynamic model of receipts and expenditures of a public health insurance can give important insights into possible future behavior and the outcome of various policies. Therefore such a model is developed using System Dynamics (as defined by Jay W. Forrester) and the software Vensim. Based on a dynamic population model, income and expenses are simulated, where the income results mainly from contributions to and expenses on medical attendance and prescribed drugs, which are calculated from occurring illnesses. Policy and scenario testing can be done very easily with such a model.

Motivation. In Austria, health care is organized primarily in public health insurances (see for example Hofmarcher et al. [1]). Most of them have been under great financial pressure during the last few years, so decisions have to be made in order to reform their structure. However, the health system is apparently complex, and impacts of new policies cannot be predicted easily as the system has various dynamic feedback loops with different delay – for example if one considers the long-term effects of disease prevention programs, which might be costly for the short term, but pay off later. Thus a dynamic cost model of a public health insurance is useful for getting better insight into resulting problems and the suitability of possible solutions. Furthermore it is possible to simulate various scenarios and get qualitative insights.

The chosen approach. A model of a public health insurance is created using the System Dynamics methodology and the Software Vensim (a similar approach was chosen by Groesser [2] for modeling the German Health Insurance System, but in less detail). Its basis is a dynamic population model, consisting of 5-year age compartments for both sexes and the flows between them. The population generates the insured persons of the health insurance. It was chosen to model a regional insurance because there is exactly one in every federal state and most people are covered in them. Aside from this, only special occupational groups are insured in other insurances. With help of the demographic structure of the insured persons, the main goal of the model – calculating income and expenses of the health insurance – is achieved. On the one hand, contributions of the various insured persons are a large part of the insurance's income. On the other hand, the most important matters of expense are ambulatory and stationary medical attendance as well as prescribed drugs. Therefore these parts are modeled in detail.

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A TEST PROBLEM FOR MODELS OF THE URINE CONCENTRATING MECHANISM

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Introduction. The kidney is one of the most important organs in our body and is responsible for: regulating the volume and composition of the extracellular fluid; excreting metabolic waste (as urine) and foreign substances; and also producing some hormones. Different models of the kidney (most of them steady-state) can be found on the literature, either multinephron or shunted, central core or vasa recta based. Our goal is to develop a transient version of the WKM model ([3]) which includes anatomical features (such as possible exchange between adjacent structures), something that has been found to be a key question on the process of concentration. However, to study numerical issues arising from these systems a simpler model is needed as a test model.

The kidney and the urine concentration. In a normal adult, each kidney (Figure **1**) is about 11 *cm* long and about 5 *cm* thick, weighing 150 grams. The *nephron* (Figure **1**) is the functional unit of the kidney and there are a million in each of them. Each nephron contains a tuft of capillaries called the *glomerulus*, through which large amounts of fluid are filtered from the blood, and a long *tubule* in which the filtered fluid is converted into urine on its way to the pelvis.

Model and equations. The model described here, which differs from a more realistic model as no Loops of Henle are included, only includes one part of the nephron (the collecting duct,CD) and the vasa recta (VR) (see [1] for a more detailed model of the VR only). With these settings we can represent mainly the key factors that will appear in a more detailed model, such as the presence of turning loops, the presence of a tube (the ascending vasa recta) that plays the role of the interstitium and also a tube where, at the papillary tip, fluid leaves the system to the bladder as final urine.

The equations describing the system are based on conservation of volume mass within the tubes (Equation (1)) and also conservation of volume and mass for the medulla as a whole (Equation (2)).

For the descending vasa recta and collecting duct

$$\frac{dF_v^j}{dx} = -J_v, \qquad \frac{\partial C^j}{\partial t} = \frac{1}{A^j}\left(-\frac{\partial F_s^j}{\partial x} - J_s^j\right) \tag{1}$$

For the ascending vasa recta

$$\sum_j F_v^j(x) = F_v^{CD}(L), \qquad \sum_j F_s^j(x) = F_s^{CD}(L) \tag{2}$$

where C represents the concentration of solute at each tubule j, F_v^j and F_s^j are tubular flows of volume and solute, different J^j represents transmural fluxes due to membrane transport (osmosis, diffusion, solvent drag and active transport) and A^j represents the cross-sectional area of each tube j. Boundary conditions are known at $x = 0$ for volume flows and concentrations entering the descending structures, and for $x = L$ (where L represents the papillary tip of the medulla) continuity conditions are imposed.

Numerical methods and solutions. The boundary value problem corresponding with the steady formulation of Equations (1) and (2) is solved by collocation while the transient formulation is solved by the numerical method of lines. Initial conditions are considered to be constant along the tube (equal to flows entering). Solutions presented show concentration profiles at the steady state as well as the different stages through time until this is reached.

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ALGORITHMS OF CONSTRUCTION OF ADEQUATE MATHEMATICAL DESCRIPTION OF DYNAMIC SYSTEM

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Abstract. The main problem of mathematical modeling is the construction (synthesis) of mathematical model (MM) of motion of real dynamic system which in aggregate with model of external load (MEL) z gives the adequate to experimental observations the results of mathematical modeling. It is formally possible to write as an inequality for dynamic systems with the concentrated parameters

$$\left\| A_p z - B_p x_\delta \right\|_U \le \varepsilon , \qquad (1)$$

where A_p is an operator of the certain structure which is carrying out the connection of chosen MEL and the response u_δ of MM on this MEL $(u_\delta = B_p x_\delta)$; x_δ is experimentally obtained reactions of real dynamic system on real external load (EL); B_p – linear operator; $\varepsilon - const, \varepsilon > 0$ is a required accuracy of the coincidence of experiment with results of mathematical modelling; $x_\delta \in X$, $u_\delta \in U$, $z \in Z$; X, U, Z – functional spaces, $\|\cdot\|_U$ is a norm in U.

Characteristic feature for problems of a considered type is that the operator A_p is compact operator [4]. The vector-function x_δ is obtained from experiment with a known error δ:

$$\left\| x_T - x_\delta \right\|_X \le \delta ,$$

where x_T is an exact responses of dynamic system on real EL.

It is obvious that in the case of performance of inequality (1) operators A_p and function z are connected. It is easy to show, that at the fixed operator A_p in (1) exists infinite set of various among themselves functions z, which satisfy the inequality (1) [4]. And, on the contrary, at the fixed function z there are infinite many various operators for which an inequality (1) is valid. It was shown that the criterions of choice of good model of mathematical model of dynamic system separately from choice of right model of external load do not exist.

At research of concrete dynamic systems the structure of the mathematical model is fixed as a rule. However the parameters of dynamic systems are given approximately.

Two basic approaches to this problem are selected:

1) MM is given a priori with inexact parameters and then MEL is being determine for which the inequality (1) is valid [2];
2) Some MEL is given a priori and then MM is being choose for which the inequality (1) is satisfy [3].

Within of first approach some algorithms are offered which allow receive adequate results of mathematical modeling. The different variants of choosing of models which are depending from final goals of mathematical modeling (modeling of given motion of system, different estimation of responses of dynamic system, modeling of best forecast of system motion, the most stable model to small change of initial data, unitary model) are considered. These problems are incorrect problems by their nature and so for their solution are being used the regularization methods [1,2]. For increase the exactness of approximate solution the method of choice of special mathematical models was suggested. The test calculation was executed [1,2].

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AN EFFECTIVE NUMERICAL ALGORITHM FOR SOLVING THREE-DIMENSIONAL REACHABILITY PROBLEMS[1]

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The construction of *reachable sets* which consist of all states reachable with some of the available controls is a key problem in mathematical theory of controlled processes. In particular, they allow to solve the *problem of control synthesis*. Reachable sets are well studied for linear control systems. Developed are many numerical methods for their approximation through unions or intersections of simpler standard-shape domains, such for example, as ellipsoids or parallelotopes. For *nonlinear* control systems the reachability problem is much more complicated, though it is known to be reducable to appropriate problems of dynamic optimization ([1]). Here we introduce the value function $V(t,x)$ being a generalized solution to the corresponding Hamilton-Jacobi equation, such that the reachable set $X[t] = X(t,t_0,X^0)$ from initial states $x(t_0) = x^0 \in X^0$ is a level set of $V(t,x)$ ([1]). Hence the problem is how to find the value function. This may be done by numerical methods for the Hamilton-Jacobi equation, such for example, as the *level set methods*. But these methods may firstly be very sensitive to the discretization rate in time and state space and even to the choice of the corresponding grids (especially those around the nonsmooth points of $V(t,x)$). Secondly, we may have too many mesh points in these grids in large spatial dimensions.

It is thus reasonable to concentrate on the reachability problem for special classes of nonlinear control systems when it may be possible to construct more regular and simpler numerical methods. Here we discuss a simple numerical algorithm for the exact reachability problem aimed at a particular class of control systems rather than at a general kind. Namely, we consider a certain subclass of the next systems *linear* in the control parameters:

$$\dot{x}(t) = G(x(t))u(t), \qquad x(t) \in \mathbb{R}^n,\ u(t) \in \mathscr{P} \subset \mathbb{R}^m,\ t \in [t_0,T]. \tag{1}$$

Here we assume that the matrix-valued function $G : \mathbb{R}^n \to \mathbb{R}^{n\times m}$ is smooth enough and that $\mathscr{P}$ is a strongly convex compact with smooth boundary and zero in its interior, for instance, an ellipsoid. We assume also that $m > 1$, hence, the boundary of $\mathscr{P}$ is connected. We suppose that (1) is *controllable*, hence, set $X[t]$ is of full dimension, and also that $\partial X[t]$ is connected. Certain additional properties that provide *regularity* of the reachability problem are also supposed to be fulfilled. These may be checked directly through the equations of control system.

The algorithm is based on using the *Cauchy characteristics* for the Hamilton-Jacobi equation related to the reachability problem. The equations of these characteristics coincide with those of *L.S.Pontryagin's maximum principle* when $x[t] \in \partial X[t]$ ([2]). Under the regularity assumptions of the above, when we are within the *non-singular* control modes of the maximum principle, the boundary $\partial X[t]$ may be presented as a subset of the end points of characteristics parameterized by the vector $\alpha \in \mathbb{R}^{n-1}$. But it is known that even if the parametrization $x(t,\alpha)$ is smooth, $\partial X[t]$ may be nonsmooth at some points since the surface obtained through this parametrization may be *self-intersecting*. This effect is analogous to the notion of *cut locus* known in variational calculus when several characteristics corresponding to different values of α may pass through the same point. In the latter case it follows that for all future instants of time these characteristics depart from $\partial X[t]$ and are in the interior of $X[t]$. Thus, $\partial X[t]$ may be presented as the closure of its *smooth* points that are end points of some characteristics that do not pass through cut loci. The algorithm discussed in this paper selects the necessary characteristics numerically.

At the end of the talk some examples for several *three-dimensional control systems* are envisaged to be given. They illustrate some possible situations that may occur when the algorithm works successfully. Here all the considered control systems are bilinear (i.e. matrix $G(x)$ of (1) is *linear* in x) with equations taken from [3], and with singularities caused by nonsmoothness of $\partial X[t]$. They here consist either of several distinct points, or of several cuts diffeomorphic to closed segments which do not divide the set of smooth points of $\partial X[t]$ into separate components, or of closed curves dividing the set of smooth points into separate disconnected components.

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[1]This work is supported by Russian Foundation for Basic Research (grant 06-01-00332). It has been realized within the programs "State Support of the Leading Scientific Schools" (NS-4576.2008.1) and "Development of Scientific Potential of the Higher School" (RNP 2.1.1.1714).

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

COMMUNICATION WITHIN AN INTEGRATED BATCH CONTROL

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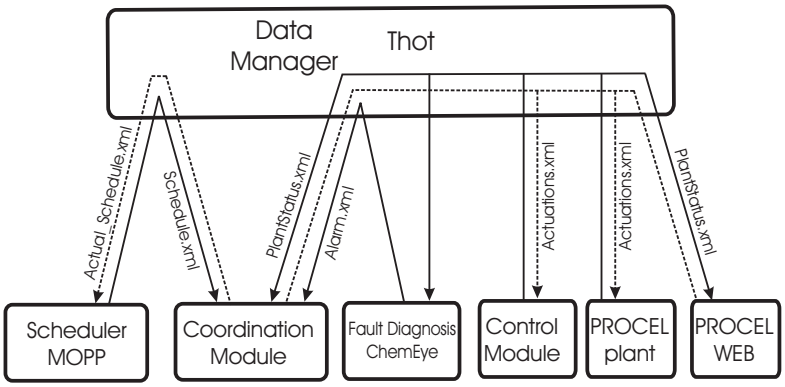
Introduction. It is not an easy task to deal with the complexity of batch processes and to meet the high-quality requirements of control software for batch-process control according to the ISA standards [1]. Until recently this has not been possible due to technological limitations. Nowadays, computing power and powerful memory systems make this possible, however, achieving an integrated framework for operational tasks is still quite complex. Problems of task integration include not only the consideration of information flow and timing for a continuously changing environment, but also the integration of various problem-solving methodologies.

Integrated Batch Control. The work is based on general area of batch control. In batch production, a recipe that contains all requisite information for manufacturing, the product determines the products processes. In batch processes it is supposed there are three different types of control: basic control, procedural control and co-ordination control.

The integrated batch control system that is being developed by the group of CEPIMA from UPC is made up of various components where each generates and requires information to perform different functions [2]. These components handle various aspects of the process control within the flexible system to support decisions. All these components have to be able to exchange information and to coordinate their implementation in order to operate as an integrated application. The MOPP planner generates and sends a production plan. This plan is later translated by the Coordination module into control actions. Control module receives instruction for control actions and performs them at the plant. In the case of anomalous situation Fault Diagnosis system detects that and sends an alarm to Coordination module. Coordination module receives also the data about the plant status. Based on this data Coordination module recalculates the control actions and inform MOPP scheduler about the actual schedule. This integrated control system is being implemented in the pilot plant PROCEL that has been built at the CEPIMA department. The PROCEL WEB is web interface used to control and supervise the plant, i.e., SCADA system. All the communications are done trough the data manager Thot. Components of the integrated system and the information flows are depicted in the next figure.



System components

Today, a sustainable effort has been devoted to establish standards that solve the problems of heterogeneous components integration. One of them is the representation of the data. This can be a complex structure, defined as an object where data specified compose the object and the methods to manage it. Within this work communication should be defined based on XML messages and should be synchronized in a common distribution system. Messages should follow the standards of the scheme defined by ISA S95 [3] and S88 [4]. Their implementation proposed by the World Bach Forum (WBF) was used at this work to define messages.

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COMPARING TWO NEW ECOEPIDEMIC MODELS OF THE SALTON SEA

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Abstract

In the Salton Sea, botulism bacteria can grow and produce toxins very easily. Fish then get infected and rise to the water surface thus becoming an easy prey for fish eating birds, like the pelicans. In turn the latter get affected by feeding on diseased prey and die in large numbers as well. This situation in the literature has been considered according to different biological viewpoints. Most of the models classify the fish as susceptible or infected, and assume that either the birds feed just on infected fish, or the predation functional responses for the susceptible and the infected prey are different. This assumption may not always be realistic in the Salton sea context. Pelicans may in fact feed on both susceptible and infected fishes with the same functional responses.

The choice of which functional response type best fits the description of a particular situation is not an easy task, especially in case of theoretical studies. To shed some light on this question, here two new models are proposed for studying the eco-epidemiology of infections among fish and pelicans in the unique environment of the Salton sea, in which the prey hunting is respectively modeled as a simple Holling type II and a ratio-dependent functional response. We compare their predictions to better understand under which assumptions the model becomes more realistic.

To describe real world situations the Holling type II functional response is the most commonly used among the prey dependent functional responses, but, when predators have to share food or compete for it, a higher predator density leads to more frequent encounters between predators, causing a fall in predating efficiency due to the predators interference among each other. A more suitable predator-prey theory should then be based on the ratio-dependent theory, as field and laboratory experiments support it. Its meaning lies therefore in the fact that the per capita predator growth rate is a function of the ratio of prey to predator abundance.

We consider then two models. In the first model, we assume Pelicans to feed on both sound and infected fish sub-populations with the same functional response: the sound prey contribute to the growth of the birds population, while the infected ones instead kill them. In the second model we refine the choice of the feeding functional response by taking it to be ratio-dependent instead of a simple Holling type II function.

Our results indicate that a small probability for the occurrence of the origin and the interior coexistence equilibrium is possible for the second model, while the first one gives probability zero for these to occur. Thus the second model therefore appears to be more realistic, since it allows the probable existence of an interior equilibrium.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

CONSTRAINED NONLINEAR OPTIMIZATION WITHOUT DERIVATIVES

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Mathematical programming has been used for the study and real understanding of many problems and phenomena's, in engineering, economy, medicine, etc. Optimization problems are abundant, where it is necessity to determine the best suitable solutions for a given reality. The techniques or strategies used in each method depends on the amount of usable information, the efficiency and robustness of the algorithm , the easiness of implementation, and, obviously, the properties of the problem to solve.

In real optimization problems, usually the analytical expression of the objective function is not known, nor its derivatives, or they are complex. In these cases it becomes essential to use optimization methods where the calculation of the derivatives, or the verification of their existence, is not necessary: the Direct Search Methods.

When the problem has constraints (Constrained Nonlinear Programming Problems), the Direct Search Methods are not enough, because they only solve unconstrained nonlinear problems.

Traditionally, this kind of problems are solved using penalty or merit functions, that are a linear combination of the objective function and a measure of the constrained violation. These functions transform the original problem in a sequence of other problems, derived from the initial, all without constraints. Becomes possible to solve constrained Nonlinear Problems by means of methods that are usually used for unconstrained problems. Unfortunately the choice of suitable penalty parameters are, frequently, very difficult, because most of the strategies for choosing them are heuristics strategies.

The difficulties of choosing appropriate values for the penalty parameters in penalty methods caused nonsmooth penalty methods to fall out of favor during the early 1990's. It led to the development of filter methods which do not require a penalty parameter.

So as an alternative to penalty function appeared the filter methods which are introduced by Fletcher and Leyffer. A filter algorithm introduces a function that aggregates the constrained violations and constructs a bi-objective problem. In this problem the step is accepted if it either reduces the objective function or the constrained violation. This implies that the filter methods are less parameter dependent than a penalty function.

Afterwards, a new approach for updating the penalty parameter, the Dynamic Penalty Methods, promised to solve these difficulties, because they automatically increase the penalty parameter and overcome this undesirable behaviour. These methods adjust the penalty parameter at every iteration to achieve a prescribed level of linear feasibility. Consequently the choice of the penalty parameter becomes an integral part of the step computation.

Our goal is to create a Web Application able of solving any Constrained or Unconstrained Nonlinear Problem. It will have a computation engine, to solve the problems and Web Interface, available to clients using a Web Browser. Clients will interact with the computation engine using and Web page. The methods are being implemented using Java Technology. It is an multi-platform technology, that has a rich variety of classes that abstracts the Internet protocols like HTTP, FTP, IP, TCP-IP, SMTP, DNS, making it suitable for networked applications. In fact it was the Internet that made it so popular, embeded in applets, running in web pages.

Thus, in this work, we present a synopsis of the existing techniques to solve optimization problems with continuous, discrete and mixing constraints, without using derivatives or approximations of them, we briefly present the general structure of our future Web Application, that will be able of solving these problems. Then we describe summary some results that were achieved through the implementation that has been made in Java Technology.

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CONVECTION IN A VOLCANIC CONDUIT

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Introduction. A common feature of basaltic volcanoes is that they can exhibit periods of persistent degassing, which can last from years to millennia (e.g. Stromboli, Izu-Oshima). During these degassing periods there is a constant flux of gas released to the atmosphere with relatively negligible volumes of magma being discharged. Deep below the earth's surface large pressures ensure that all volatile species are dissolved in the silicate melt. When a volatile-rich magma ascends towards the surface, a decrease in hydrostatic pressure causes gas exsolution and bubble formation. The bubbly mixture will then rise buoyantly to the surface and these gases will be released into the atmosphere. What becomes of the degassed magma? One possibility is that it solidifies and is stored at shallow levels. However, this would lead to the endogeneous growth of the volcanic edifice and since flank deformation is not always observed, [3], this indicates that the degassed magma must be transported elsewhere. In fact, the degassed magma will be heavier and more dense (and more viscous) than the nondegassed magma and as a result will descend back to the chamber along the conduit walls and displace the gas-rich magma there. This creates a convective circulation within the conduit driven by the density difference between the degassed and nondegassed magmas. This proposed mechanism of continuous passive degassing has been considered in many studies in the literature, see for example [1], [2] and [3]. A simple model for basaltic magmas consists of Poiseuille flow in a concentric double walled pipe, where nondegassed magma ascends in the center and heavier degassed magma descends in the outer annulus and the flow is driven by the density difference between the ascending and descending magmas. These conduit convection models are simplistic and ignore the effects of bubbles, simply assuming a change in density when gases are released at the top of the conduit. Bubbles will cause buoyancy effects to increase as the magma ascends and the resultant density difference between degassed and nondegassed magma is in actuality a function of height above the chamber. Increased buoyancy, in turn, leads to an increased magma ascent velocity. A particularly important consequence of conduit convection models is the transport of heat from the chamber to the conduit which can prevent the magma from cooling by offsetting the heat loss to the surrounding rock en route to the surface. Expanding the idea of these conduit convection models we construct a comprehensive two-phase flow theory to examine the process of convective overturn in a conduit.

The Mathematical Model. We consider a two-dimensional model for flow in the conduit. We assume the presence of a single gas species, which we take to be water vapor. Our magma consists of a low viscosity silicate melt with dissolved H_2O and a separate gas phase is also present. We assume that the rapid rise speed of the two-phase mixture hinders the formation of crystals and we neglect their effect on the viscosity of the melt. The density of the magma will depend on the individual phase densities and the volume fraction of gas via the relationship

$$\rho = \alpha\rho_g + (1-\alpha)\rho_l\,,$$

where the subscripts g and l indicate gas and liquid respectively. However, the volatile species can be present in the magma as both a gas and dissolved in the liquid phase. Thus, the liquid density will vary with dissolved gas content, which has mass fraction c. A homogeneous two-fluid model is used where the mixture has a single velocity $\mathbf{u}$ and there is no relative motion between the phases. At a given depth the solubility of water in the melt is given as a function of pressure by Henry's law

$$c = K\sqrt{p}\,,$$

where K depends on magma composition. Mass of both phases is conserved and, in addition, the total mass of water, both dissolved in the melt and present as a gaseous phase, is conserved. We assume the gas phase obeys the ideal gas law and, taking a Boussinesq approach, we allow the liquid density to vary with temperature,

$$\rho_l = \bar{\rho_l}[1-\beta(T-\bar{T})]\,,$$

where β is the coefficient of thermal expansion. Density variations are neglected except in the gravity terms of the momentum equation. The dimensionless model is essentially standard thermal convection depending on the dimensionless Prandtl and Rayleigh numbers. However, the gas volume fraction replaces temperature in the body force term, and thus exsolution of gases as a result of depressurisation drives convection within the conduit.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

DESIGN AND PERFORMANCE SIMULATION OF THE MATHEMATICAL MODELS IN CLUSTER SYSTEMS – *FINAL ABSTRACT* FOR SHORT PAPER

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Introduction. The power of simulation is that a uniform model execution technique can be used to solve a large variety of systems. An important aspect of the simulation technique is that one builds a simulation model to replicate the actual system. A precision of the system modeling with a hybrid approach using both closed-form methods and simulation on the parallel computer systems.

1 Preface

Simulation is often essential in the following cases: 1) the model is very complex with many variables and interacting components; 2) the underlying variables relationships are nonlinear; 3) the model contains random variates; 4) the model output is to be visual as in a 3D computer animation [1].

The necessity of high fidelity modeling in the design process is often conflicting with the requirement of short turn around time. A way to reduce this time is to use powerful parallel computer systems.

2 Computer simulation

Computer simulation is the discipline of designing a model of an actual or theoretical physical system, executing the model on a digital computer, and analyzing the execution output. Simulation embodies the principle – to learn about the system we must first build a model of some sort and then operate the model.

To simulate something physical, you will first need to create a *mathematical model* which represents that physical object. You can also execute (i.e., simulate) the program on a massively parallel computer.

3 Performance and validity of simulation

So on the hand, performance can be expected to improve with reduced complexity. On the other hand, reducing the resolution simulator often entails a loss of validity of the model. Of course, has to be measured within an experimental frame of interest. We see, conceptually depicted, performance increasing while validity decreases as the resolution product is decreased [3].

4 Simulation of mathematical model

The architecture of models based on objects communicating via message sending allows us to combine different modeling tools must somehow support the object-oriented style of communication via message sending.

The mathematical models increase of angle trajectory of aircraft is defined [2]:

$$\Delta\theta(s) = -W_{\theta}^{\delta_T}(s)\Delta\delta_T(s) - W_{\theta}^{\delta_B}(s)\Delta\delta_B(s). \tag{1}$$

The most used parallel systems are based on either shared memory, distributed memory or hybrid distributed-shared memory systems.

5 Performance and measurement

The parallel performance is analyzed in terms of computational performance and parallel efficiency on four processors cluster ‘EvaOne’.

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FAULT ISOLABILITY STUDY OF NONLINEAR SYSTEMS BY REDUNDANT GRAPH

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The operation principle of a fault detection and isolation (FDI) system is the comparison between reference models with process observations from which diverse symptoms o residuals can be inferred. This operation could be established if exists a redundancy between process properties which are modified if a fault occurs and are insensitive to disturbance and faults of no interest.

The FDI system design is tackled by the control community dividing it in two tasks: the first associated with the detection and the second with the isolation of faults. This separation simplified the detection task; however the impossibility to get a solution for the isolation issue cannot be analyzed from the beginning with the tasks division. This fact motivated the search of *a priori* existence conditions for the detectability and isolability of faults.

The conditions for a residual generator for analytical models of dynamics non linear system using the geometric approach are derived by De-Persis [2]. Simultaneously to this contribution the Frank's school determined by algebraic tools the existence conditions of robust observer with unknown inputs for a residual generation [3]. Other option to address the FDI issue is the design of structured residuals using parity relations with numerical values [4].

The test of the solution conditions for a FDI issue in large scale or non linear system is not an easy task because models are not precise and the relations between variables are complex. Moreover, if the conditions cannot be satisfied the settling of sensors or data which could solve the issue is not trivial.

Taking into account that the variables coupling describes a process behavior, the Staroswiecki's school proposed the structural framework with graphs to analyze the diagnosticability in fault conditions without numerical models [1]. This idea generates diverse procedures to study generic FDI capabilities of a process using graph theory. The casuals models, Bondh graphs, Petri nets, structural linear models. The advantage of these tools is the possibility to include different levels of knowledge about faults during the analysis and since numeric values are ignored, the conservatism of the results is the main drawback.

To study the faults detectability and isolability of a system with graph tools, this paper introduces the concept of *redundant graph* between known signals in the framework of Blanke's school [1]. This concept is equivalent to the analytical redundant relation and allows to

- systematize the search of redundancy between known signals $\mathscr{K}$ in a system;
- to maximize the isolability with short paths between known variables;
- to clarify explicitly the dynamic aspect of the graph;
- to reduce the conservatism of the structural analysis considering specific excitation signals in the system.

The start point of the analysis is the over-constrained part of the Dulmage-Mendelsohn decomposition of the incidence matrix of unknown variables. Its advantages are shown with an Hessenberg system in which the absence of a solution for the diagnosis is easily justified and the candidate sensors to improve the isolability are straightforward identified.

Acknowledgement. This contribution includes results of project IN112208 that is supported by the DGAPA-UNAM.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

FRACTIONAL ORDER MODEL OF WIEN BRIDGE OSCILLATORS CONTAINING CPES

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Current technological needs and trends include technology development and transfer, manufacturing and deployment, implementation and testing, modelling and characterization, design and optimization, simulation and analysis of complex nano- and micro-scale devices such as, for instance, molecular computers, logic gates and switches, actuators and sensors, digital and analogue integrated circuits, etc. The diversity of materials produced in nano-engineering has led to spectacular progress in functionality of such electronic devices as oscillators, filters, antennas, etc. It is central to understanding the relationship between the structure and properties of naturally occurring and synthetic materials, which is at the root of current technological development and innovations.

The microstructures of such aggregate materials as nano- and micro-crystalline surface deposits can be successfully modelled by fractal sets rather than traditional geometric sets. The dimension of the fractal sets used to model these structures is also of primary importance as it determines the scaling, and ultimately the sizing effects for that particular material. Fractional calculus is deemed appropriate and necessary for the study of these models as ordinary integer order calculus is ill-equipped to differentiate the fractal functions at work. One of advantages is that we have more degrees of freedom in the model. The next advantage is that we have a 'memory' in the model. The fractional order systems have unlimited memory, being broaden with respect to integer-order systems exhibiting always limited memory.

Fractional calculus is concerned with the development and application of differential equations of non-integral order α with $m\text{-}1 < \alpha < m$ (m is the nearest integer number), and the methods for their solution. The attraction in using a constitutive description based on fractional calculus for modelling micro-structure devices is their potentially superior accuracy, and the possibility of correlating the hierarchical structure of physical systems to the fractional order α.

This contribution is a continuation of the author previous works and deals with the time domain mathematical description and analysis of fractional-order oscillation systems. Main emphasis is put on the mathematical modeling of fractional-order Wien bridge oscillators build up with constant phase elements (CPEs) and classical resistors and Op-Amps. We present results of simulations of such oscillators with the aim to investigate the circuit stability. The basic elements of this circuit are the appropriate impedances Z_1 and Z_2 – so called fractances in the feedback, which define the fractional-order (FO) of the differential operator describing the whole configuration. The function of the amplifier stage is to determine the required gain of the resulting FO operator or to compensate the gain of the feedback stage.

Applying the Kirchhoff current and voltage laws and assuming identical CPEs and resistors in the voltage divider we have determined solutions of the factorial Wien bridge oscillator mathematical model. The fractional oscillation equation was derived from the classical equations for linear dynamical circuits by introducing a fractional derivative of order 2α. For practical reasons we studied the solutions with $1 < 2\alpha \leq 2$ and natural angular frequency $\omega_0 = 1$rad/s. Several properties of this type of corresponding functions are presented and discussed. Results of performed simulations are reported for $\alpha \in \{0.9; 0.95; 1.0\}$. It is worth noting that for $\alpha \leq 0.95$ the oscillations attenuate and for $\alpha \geq 0.95$ oscillations remain practically sinusoidal. By changing the resistor and CPE values in the positive feedback network, the output frequency can be changed. With proper maintenance of the bridge configuration its oscillations can go on indefinitely. For $0.95 < \alpha \leq 1$ the oscillations are quite well tuned and thus they contradict commonly adopted point of view that frequencies above 1MHz are unachievable with the Wien bridge oscillator.

The analysis carried out in this short paper has attested possibilities of using supercapacitors as suitable CPEs for realization of fractional Wien bridge oscillators. Fractional calculus is deemed appropriate and necessary for the study of these models as ordinary integer order calculus is ill-equipped to differentiate the fractal functions at work. As has been demonstrated, the idea of fractional calculus requires one to reconsider dynamic system concepts that are often taken for granted. Thus, changing the order of a system from integer to fractional, we can also move from two-dimensional system to the infinite dimension.

The goal of this paper is not only to expose the reader to the basic concepts of fractional calculus, but also to whet his/her appetite with scientific and engineering applications. It is also worth noticing that some alternative types of mathematical description and methods of solution of the fractional-order dynamical systems are under development. The benefits of using of fractional-order models of real dynamical objects and processes become more and more obvious and numerous examples of applications in various fields of science and technology will appear in the near future.

Free Analytical Vibrations of Smart Beams using Distributed Transfer Function Analysis

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The modal Effective Electromechanical Coupling Coefficient (EMCC) is known as a critical parameter in justifying the performance of piezoelectric materials since it describes the efficiency of converting mechanical strain to electric charges and vice versa. For a vibrating structure, the EMCC is defined by [1]

$$k_r^2 = \frac{(\omega_r^{oc})^2 - (\omega_r^{sc})^2}{(\omega_r^{sc})^2}$$

Where ω^{oc} and ω^{sc} are the natural frequencies of the structure under the open-circuit (OC) and short-circuit (SC) boundary conditions for the *r*th mode. The equations of motion are first derived for the three segments of a thin elastic beam with single bonded piezoelectric patch as shown in the figure. The equations are then transformed to the Laplace domain and cast into a state space form [2]

$$\frac{\partial}{\partial x} Y_i(x,s) = F_i(s) Y_i(x,s), \qquad i = 1,2,3$$

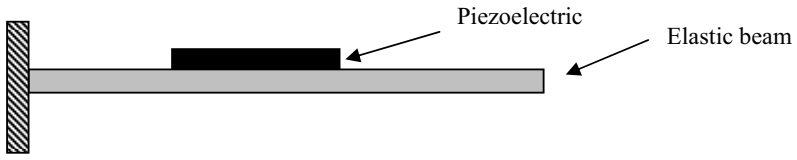
Where the state vector is made of the deformation vector $D(x,s)$, and the strain vector

$$Y_i(x,s) = \begin{Bmatrix} D(x,s) \\ P_i(x,s) \end{Bmatrix}, \; D(x,s) = \begin{Bmatrix} u_i, & w_i, & \dfrac{\partial w_i}{\partial x} \end{Bmatrix}^T, \; P_i(x,s) = \begin{Bmatrix} \dfrac{\partial u_i}{\partial x}, & \dfrac{\partial^2 w_i}{\partial x^2}, & \dfrac{\partial^3 w_i}{\partial x^3} \end{Bmatrix}^T$$

The essential displacement continuity conditions are cast also in matrix equations

$$M_i Y_i(x_{i-1}, s) + N_i Y_i(x_i, s) = \gamma_i(s)$$

And the solution becomes $Y_i(x,s) = e^{F_i x} \left[M_i e^{F_i x_{i-1}} + N_i e^{F_i x_i} \right]^{-1} \gamma_i(s)$, where $\gamma_i(s)$ is a vector satisfying the last both equations. Upon application of the force continuity condition, a dynamic stiffness matrix is derived such that $K(s)\gamma_2(s) = 0$ and frequencies are calculated by setting det(K) = 0. The OC boundary conditions are implemented by updating the dynamic stiffness matrix based on vanishing surface charges.



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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

IMPROVED ROLL TO ROLL MODELLING FOR ELASTIC WEBS

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Introduction. The systems transporting thin and flexible materials such as fabric, paper, polymer or metal sheets are very common in the industry. The key points in the web handling industry are to increase the web transport velocity as much as possible while controlling the tension of the web. The main concern is the coupling existing between web velocity and tension.

Modelling and control of web handling systems have been studied for several decades [4]. However, increasing requirement on control performance and better handling of elastic web material have led to search for more sophisticated robust control strategies [4][2] and therefore for more precise roll to roll modelling [4]. Especially control strategies based on phenomenological models (for example feedforward control) require precise plant modelling [2][3].

The nonlinear model of a web transport system is built from the classical equations describing the web tension behaviour between two consecutive rolls and the velocity of each roll. The web elasticity is described by the Hooke's law. The viscosity effects can also be included (for example the Maxwell or Voigt models). The web is assumed perfectly flexible with no bending stiffness. Moreover, one major hypothesis is that there is no sliding between web and rolls. The established model was identified on an experimental bench [1].

In the published models, the elastic web strain between two consecutive rolls (and therefore the web tension) is considered as positive. Nevertheless, the case of negative web strain can appear in transient phases when low web tension is required. A new dynamic web model is presented in this paper which includes the influences of web slacks.

Content. The nonlinear model of a web transport system is built from the equations describing the web tension behaviour between two consecutive rolls and the velocity of each roll. This model was identified on an experimental bench [1]. The dynamics of web tension between two rolls of web transport systems is based on three laws [4]: the *Hooke's law*, the *Coulomb's law* and the *Equation of Continuity*. The last equation applied to the web between two driven rolls, yields:

$$L\,\frac{d}{dt}\left(\frac{1}{1+\varepsilon_k}\right)=\frac{V_{k-1}}{1+\varepsilon_{k-1}}-\frac{V_k}{1+\varepsilon_k} \tag{1}$$

where ε is the web strain, k is the span number, L is the distance between two consecutive rolls, V the velocity of each roll.

The strain dynamic of the web can be described with equation (1). For flexible webs, negative web strain can not appear in a real plant and consequently this equation is useful only for positive strain (and positive web tension). Classically, the resolution of equation (1) includes a saturation that eliminates negative strains. The drawback is that the web slack is not taken into account. A new approach including the web slack calculation and the effects of the slack has been established. The modifications of equation (1) are given in the paper. The results have been applied on a 3-motor plant and a new simulator has been built in Matlab/Simulink software environment. Simulation results show the improvements of this new model compared to the classic one including a saturation.

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INTRODUCING A MODEL FOR ROAD PRICING

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Abstract. In the present paper, a very condensed overview of the "Identification, Investigation, and Comparison of Road Pricing and Valuing Softwares" project is presented. This paper was defined and carried out as a research project and a guide to identify roads valuation and pricing models. This paper, roughly speaking, is a survey research on the literature and comparative analysis. To this end, a research including the 4 phases. With the exception of the first chapter which includes generalities and research methodology, the present study has embedded the above-mentioned issues in the following structure within three chapters. In Chapter 2 scientific and practical experiences of both Iran and other countries have been reviewed. Furthermore, the framework of the software utilized for the application and execution of road pricing models in other countries is presented. The main components of valuation models include database of road infrastructures (information about roads), amount of investment and road cost price, economical parameters regarding interest rate, rate of capital restoration, inflation rate and so on and so forth, road erosion calculation method, the method of engaging road maintenance and rehabilitations, the method of engaging renewed road investment and its development, and finally the method of depreciation calculation. All in all, the value of roads network which is considered as the major property of Ministry of Roads and Transportation should be obtained with respect to the current conditions. These issues have been dealt with in Chapter 2. In Chapter 3 road evaluating and pricing models are compared with each other. In this chapter, the comparison and benchmarking of the existing models and software are dealt with, and the best and the most appropriate model with regard to Iran's conditions is identified; then, the way it is performed is briefly explained. At the end of this chapter, the conclusions of the research are presented.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

LEARNING ORDER INVARIANT AGGREGATION FUNCTIONS WITH RECURRENT NEURAL NETWORKS

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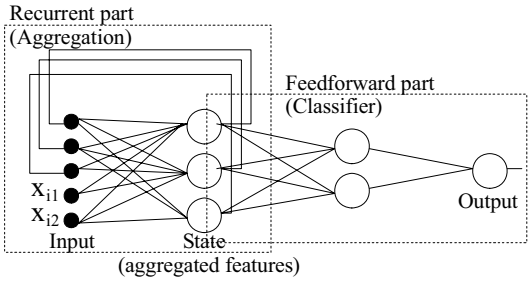
Numerous applications benefit from parts-based representations resulting in sets of feature vectors. To apply standard machine learning methods, these sets of varying cardinality need to be aggregated into a single fixed-length vector. Since, per-se, no order is imposed on the set elements the aggregation function has to be order invariant.

Related Work. Some work has been done on classification of structures containing an unknown number of elements [1], where the authors propose to use *generalized recursive neurons* to represent the structure of a graph. The problem is similar to ours in that the number of input elements can vary, however their approach uses the structure present in the input to deduce the order in which to present the elements to the network. Recently kernel functions have been proposed operating on sets of features [2]. These approaches either assume that direct correspondences exist between the elements of sets or require sets of equal cardinality.

Approach. We propose using Recurrent Neural Networks (RNNs) to perform both aggregation and classification of the sets of feature vectors. The n input vectors $x_1, x_2, \ldots, x_n$ will be processed by the network as if they were a time sequence. The classification result will be available at the output after n "time steps". However, since this sequence of vectors has no inherent ordering special methods for achieving invariance of the RNN have to be applied. Order invariance of RNNs is realized by reshuffling of the data during training: The sequence of the feature vectors in the set will be randomly permuted after each training epoch of the network. The neural network should thus learn to be order-invariant. Another option is sorting as a pre-processing step that establishes order invariance among the set elements. For dimensions greater than 1 sorting is non-trivial and requires problem-specific order relations.



Evaluation. We have compared the performance three common RNN architectures, Elman, Williams&Zipser and Long Short Term Memory (LSTM) [3] networks, in approximating eight different aggregation functions of varying complexity. Data sets have been produced by applying aggregation functions to sets of scalar entries $x_{i,j} \in \mathbb{R}$. We have trained each network using both sorted and shuffled representations of these data sets. The accuracy of the approximation is assessed by the Pearson correlation coefficient R of the network's output with the target value on test data not presented during training. On most of the data sets Elman, Williams & Zipser and LSTM networks perform similarly for both the sorted and shuffled case, indicating that order invariance can be achieved through training with shuffled data.

On the most difficult to approximate function only the LSTM network can be trained to perform order invariant. This function computes the minimum distance (`MinDist`) between any two elements when interpreted as points in Euclidean space. While the earlier architectures fail to approximate the `MinDist` function, the LSTM network achieves 40% correlation – too low for practical applications but certainly better than random.

Further investigation into the state-space behaviour of the LSTM network reveals that for `MinDist` it is actually only approximating a function dependent on the element count of the sets. Due to the distribution of the test data this simplification still yields 40% correlation. This behaviour has been verified by using a modified version of `MinDist` where any correlation between target value and input length has been removed.

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LONG TERM BEHAVIOUR OF AGENT BASED EPIDEMIC SIMULATION OF STREPTOCOCCUS PNEUMONIAE - A MATHEMATICAL STATUS REPORT

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Introduction. Streptococcus Pneumoniae is a bacterium that causes several infections like pneumonia, otitis media, meningitis and sepsis. The purpose of this thesis is to develop an agent based SIS-model that is able to simulate an epidemic like Streptococcus Pneumoniae and analyze vaccination strategies for the PCV-7 vaccination which covers seven frequent of about 90 serotypes. Also profound data search has to be done to understand the whole system and identify the model parameters as well as possible.

Streptococcus Pneumoniae and vaccination. The real system seems to be very complex; additionally many different medical studies report different results. Fact is that a significant part of the population is infected with Streptococcus Pneumoniae and can infect other people while only a non-significant part falls sick with it. All the other people get rid of it after a while and do not even realize that they have been infected. Because of the small number of sick people it must be possible to simulate a relatively large population.

Especially two phenomena that are only presumed but not proven yet should be examined. One is serotype replacement which means that vaccinated people get infected with other serotypes instead of the covered ones. If such a behavior occurs and is too strong it can reduce the effect of the vaccination dramatically. The other phenomenon is herd immunity which means that only a part of the population is vaccinated while non-vaccinated people benefit too because of the lower total number of infected individuals.

The model. The agent based model consists of three parts: The population part, the social part and the infection part. The agents in this model are single persons with attributes age, gender, infection state and pregnancy for women only. In the population part the population is calculated, people get older and die and babies are born using real life data for Austria from *Statistik Austria*. The detailed population part is important to do long-term simulation with a changing population. For the spread of an epidemic people have to meet each other. The social model is realized in the social part. Instead of simulating households, workplace, family, friends and random acquaintances only connections between people are stored in a list in the social part. These connections are varied every time step by resolving old and finding new connections using different algorithms. New connections are found randomly, within circles of friends, where all connected people considered as friends and within groups. In the infection part all healthy people that are connected to infected agents are infected with an individual probability depending on the own age and the number of infected friends and their pathogens.

The behavior of the model. While simulating one pathogen only the model behaves very predictable. Depending on infection probability and recovery time the number of infected and healthy persons reaches, independent of the start values, a constant level. Things become more difficult when simulating two or more pathogens. If both pathogens are equally strong (that means that they have the same parameters) the behavior will be completely random until one pathogen becomes extinct, then the system continues in the stable one-pathogen system. If one pathogen is stronger (higher infection probability and recovery time) the weaker pathogen will become extinct very soon.

Results. The model shows a good protection from vaccinated serotypes even if only a part of the population is vaccinated. But it also shows that vaccinated people are more often infected with non-vaccinated serotypes so that the total number of infected people stays at a more or less constant level, this means we get a nearly complete serotype replacement.

Outlook. Now another approach for the infection part of the model is being developed to achieve a more predictable and stable behavior for multi-pathogen simulations. With the adopted model it should be possible to simulate stable multi-serotype systems. Then we can expect some more reliable results about serotype replacement and herd immunity.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MANAGING DATA IN AN RFID APPLICATION

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Introduction. A Radio frequency identification (RFID) is playing an essential role with systems deployed in a number of industries [1]. In the future, it can be expected, that many retailers, also in food production, will use RFID systems to track their products to the point of sale. At present, no individual food products have RFID tags attached and no encoding formats for custom data exist. Because of that, the companies would be able to define their own encoding formats. To design and to implement an RFID application dealing with food products identification to perform inventory we needed to define our own data base of food products with suitable encoding model to determine RFID tags custom data.

Many home appliance producers tend to build RFID systems in their products, where the fridge is the one which will use the possibility of food identification. The information from each individual food product would be possible to use at home in many kinds of applications. It becomes also very important in food industry to improve customer service and to bring benefits of reduced exposure to safety risks [2]. Additionally, a traceability system would define the types of data that should be collected and transferred to each state of the supply chain management and also to interested customers.

Data encoding models. The radio frequency identification (RFID) application will perform an inventory of food products with attached RFID tags (I-CODE SLI Smart label IC with 1024 bits EEPROM memory). It will predict the lunch menu based on the recipes saved in a data base. The information about food products is saved in a custom part of RFID tag's memory defined with next data fields: Food product type, Food product name, Price, Currency, Production date, Expiration date, Measure value and Measure type. The information is saved in tag's memory considered as a matrix of encoded bytes organized in blocks which are transfered in RFID system during the read or write cycle. Readers normally return the binary or hexadecimal representation of data. For UID part of data a special encoding format that depends on the particular RFID tag is used which is not the case for custom data of food products in our application.

Two different encoding formats were analysed. The first one, ASCII (American Standard Code for Information Interchange) encoding is simpler to represent the information but at the same time it can be very complex which can enable the overload of data in the transmission process between the reader and RFID tags attached to the products. The second analysed is BCD (Binary-Coded Design) encoding which requires far less memory space, the transmission of data demands less time but additional encoding tables are needed to obtain the information.

Comparison of ASCII and BCD encoding. An example of two RFID tags in ASCII and BCD encoding formats are presented in 'Table 1' as raw hexadecimal data records. The encoded information obtained by RFID application defines: Food product type: Milk product, Food product name: Whole milk, Price: 0,78, Currency: Euro, Production date: $12-11-2008$, Expiration date: $23-01-2009$, Measure value: 1000, and Measure type: mililitre.

Data format	UID	Custom data
ASCII	E0040100 158C0C12	4D696C6B 2070726F 64756374 57686F6C 65206D69 6C6Bxxxx 302C3738 4555524F 31322D31 312D3230 3038xxxx 32332D30 312D3230 3039xxxx 31303030 6D696C69 6C697472 65xxxxxx
BCD	E0040100 158C0BD0	0061xxxx 02301192 00007801 12112008 23012009 00100004

Table 1: RFID data define the whole milk product in ASCII and BCD encoding. Each UID consists of two blocks and is defined with RFID tag's encoding format (2^{nd} column). ASCII encoding format uses 18 blocks of custom data, and BCD encoding uses only 6 blocks of custom data. Value x represents a part of field not used in encoding.

In the comparison we show the advantages of having a smaller RFID tag's memory when using BCD encoding and the feasibility of organising two fields of data into the same block. It was tested in an application that runs on the experimental RFID system where we analysed the benefits of the proposed encoding format which improves identification rate and the time in read/write operations due to less data that is transmitted.

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MATHEMATICAL MODELING OF MECHANICAL BEHAVIOUR OF LAYERED STRUCTURES USING A CONTINUUM APPROACH

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For material consisting of a large number of layers a continuum approximation approach seems appropriate to describe its mechanical behaviour. In the framework of this approach the real structured media are replaced with a homogeneous continuum possessing some effective properties. In case a uniform external stress such a homogeneous medium may be treated just as an anisotropic elastic one. The general solution of the problem of the effective elastic characteristics determination for such a medium is well known as obtained by Lifshitz and Rozentsveig [1]. However, if the medium allows relative sliding of the layers, then bending may occur at the places of stress gradients. The bending is accompanied by such effects as the violation of the shear stress parity rule and the moment stresses appearing. A similar situation may take place even in the case of the perfect cohesion between the layers, if one group of the layers is sufficiently compliant to be considered as slippery interfaces. Various variants of models accounting for this effect were suggested by many researches starting with the pioneer work [2]. Some modifications and generalizations were suggested by the authors.

Various types of continuum models were derived as follows. At the fine scale (of the order of layer thickness) a set of independent kinematics variables, such as displacements, are introduced and approximated by a set of parameters. Then using a variational principle the corresponding potential (energy) is written down in terms of the introduced independent variables. The equations of motion (equilibrium) and natural boundary conditions are obtained from this potential by the standard variation procedure. In the classical continuum mechanics, due to the assumption that there exists a limit of the energy of the medium at decreasing the volume element down to zero, the influence of high-order derivatives of independent field vanishes. For the structured media, such as layered media in question, this assumption is omitted (the representative volume element may not be less then element of the structure), and the set of the parameters, introduced to characterize the field within the volume element may include high-order derivatives of independent field and the additional degrees of freedom of the model. Various types of continuum models were obtained, which were divided into three groups: classical models of effective elastic media (CM), models accounting for additionally bending of layers (universal models, UM), and models supposing that bending prevails (BM).

The FEM code was built incorporating various continuum models and various types of elements, namely: 3-point simplex element, 6-point element, 3-point element with conjugated gradients.

As an example layered structure bending problem was addressed. The results obtained by various continuum models using FEM simulation and simplified Ritz method were compared with the results of direct FEM simulation accounting for individual layers.

For the addressed problem the ranges of applicability of three specified groups of models (CM, UM, BM) were specified. They were determined by the parameter, characterizing relative rigidity of the layers. It was shown that CM is applicable for high and moderate relative rigidity of the soft layers; BM does for extremely low relative rigidity of the soft layers; UM does for any value of rigidity of the soft layers. The results obtained by various variants of UM are very close to each other not allowing choosing the best.

The results obtained with the simplified Ritz method were also in a very good agreement with the direct FEM modelling. However the direct application of this approach is restricted with very simple geometries.

The comparison of using various types of finite elements leads to the following conclusions. Using 3-point simplex element is inappropriate for these kinds of models, because this requires too many elements (comparable to the number of elements in the direct modelling) for the good convergence to the exact solution; 6-point elements and 3-point element with conjugated gradients yield good convergence.

An example of a graphite plate deformation is considered. It was shown that calculating deformations of small plates CM could yield errors, and UM are preferable.

This work was supported by the Program of Fundamental Research of Presidium of the RAS N11.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MECHANICAL MODELING OF OXYGEN-CONTAINING PRECIPITATES IN SILICON WAFERS

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Introduction. The effective tool for eliminating of the negative influence of the defects within the silicon wafers is the formation of different sinks for point defects (including intrinsic and impurity defects) and dislocations within the silicon wafers. The internal sink for the defects is usually called getter and the process of the internal getter formation is called gettering process. The silicon wafers with build-in internal getter are used in the modern VLSICs manufacturing technology. The getter is formed as a result of the controlled decomposition of the oversaturated solid oxygen solution in the silicon and consists of the oxygen-containing precipitates. Depending on the precipitate sizes and the features of external loading the precipitates can be either sinks for the defects or sources of the defects nucleation. Therefore the modeling of the mechanical behaviour of the silicon wafers containing oxygen-containing precipitates is an actual problem.

In the paper the continuum modeling of the isolated oxygen-containing precipitate within a silicon wafer is performed. The precipitate is modeled as an elastic inclusion in the shape of spheroid buried in an elastic silicon matrix and undergoing the uniform eigenstrains [1]. The elastic inclusion is assumed to be isotropic (polycrystalline phase of silicon dioxide) and the silicon matrix is assumed to be anisotropic with the cubic type of anisotropy. Moreover, the stress state far away from the precipitate is supposed to be uniform and corresponding to the uniform external loading of the silicon wafer. The problem of the stress-deformation state searching for is solved analytically for the considered precipitate model in the framework of elasticity.

To perform the numerical analysis of the stress-deformation state in real silicon wafers it is necessary to know the numerical values of the precipitate eigenstrains. In this connection, two different approaches for the precipitate eigenstrains evaluation are developed. Fist approach is based on the analysis of the geometric characteristics of the oxygen-containing precipitate – dislocation loops complexes formed on the later stages of the silicon wafers multistage thermal treatments. The eigenstrains are determined from the condition of equilibrium of the precipitate – dislocation loops complex [2]. More specifically, this means that the force acting on the first dislocation loop in the complex from the precipitate should be opposite and equal to the force acting on it from the second dislocation loop in the complex. The second method proposed in the paper is deferent and based on the analysis of the conditions of the dislocation loop nucleation in the vicinity of the precipitate. The eigenstrains of the precipitate are determined from the requirement of equivalence of the model calculations and the experimental data related to the dislocation loop nucleation conditions. The numerical estimates of precipitate eigenstrains obtained by using different methods are approximately the same and equal to 6%.

The obtained estimate of the precipitate eigenstrains and the solution of the problem on searching for the stress-deformation state within the framework of the proposed oxygen-containing precipitate model are used for the numerical modeling of the mechanical behaviour of the isolated precipitate in the silicon wafer taking into account the silicon matrix anisotropy.

This study was supported by the Russian Foundation for Basic Research (Project No.08-02-01080).

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MINIMIZING QUEUING CONSTRAINS IN SERVICE DELIVERY ON ENTERPRISE COMMUNICATION&COMPUTING PLATFORM

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The key objective of the enterprise communication&computing platform is to deliver services at anytime, anywhere, to any device. And, the responsibility of the service delivery environment is to provide the services over the enterprise communication platform to the end users [1]. The service providers are in critical need for the agile service delivery, to succeed in highly concurrent e-services business market. Thus, regardless of many similarities between the service delivery models used by different providers, the customization is highly desired to enable communications within diverse operations and business support systems (OSS/BSS) and niche-market developments [2].

The Internet Service Providers (ISPs) and Mobile Virtual Network Operators (MVNOs) as well as IT departments of large companies face various problems when designing, building/implementing, and engineering/managing their enterprise infrastructures. They struggle mostly because of inflexible legacy networks in the face of accelerating technological growth and increasing business and customer demands. Integrated infrastructure solutions are extremely complex to design, support, and manage. Besides, the enterprise communication&computing platform must be able to adapt quickly, to support new technologies that enable rapidly evolving business processes [1]. Furthermore, the services and providers continue to converge and bring in many different types of services, such as wireless, broadband media, and voice ones.

Also, computing centres are now distributed across the world, as there are devices and clients that they support. And, the situation totally cannot be comparable with the past, where computing centres typically supported limited number long-term services, for instance - a single server ran the same application for its lifecycle of operation. The little changes were made, networks were static, often flat to ease administration, and network security was confined to just a few points within the implementation.

But, designing networks and architectures for millions of users, transactions, and diverse content types requires an approach that differs from that of standard infrastructure designs. These infrastructures must support convergent services, with high levels of reliability and performance, while maintaining manageability as well as security. The computing architectures and applications must be designed to support ubiquitous access. Flexibility is required to support new or evolving business and technical requirements with agile respond to business conditions and competitive pressures. The “always-on” access has become a requirement whether services are accessed over the Internet, intranet or extranet [1, 2].

The solution for all the difficulties enterprise communication&computing platform faces cannot be simple and whole, done in once. It can be efficient only if it is modular and includes differentiated features. As an answer to this complex dilemma - we split different problems into different sub-areas, and apply certain customized solutions to the certain kind of challenges.

We take also into consideration that an analytical performance evaluation is crucial for the justification of the effectiveness of the modelling of different operational conditions in delivering of high-quality services [3]. Consequently, in this paper, we apply a mathematical model into the monitoring of services delivery in two interconnected systems in tandem on the enterprise communication&computing platform. We consider here a queuing network model used to represent a series of 2 single-server queues, each with unlimited waiting space and the FIFO service discipline [4]. And, we develop our model in order to obtain feasible values of main performance features. Also, we present in this work a practical area of the implementation of our model.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODEL DRIVEN CONCEIVED / DATA DRIVEN TUNED CONTROL SYSTEMS

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Summary. Three approaches for control system design are faced on this paper and the role played by the plant model highlighted. On one side we have the well known Model-Based Control (MBC), that is further extended to the Model-Driven Control (MDC) conception of a control system and, finally, embedded within the Data-Driven Controller (DDC) approach for design. The advantages of conceiving the overall control system as a MDC are raised and the possibility of doing the design of the controller as a DDC overcomes the sometimes imposed constraint of suitable low complexity (linear) models.

Content. Model-Based Control (MBC) is a well known and accepted approach for the conception and design of feedback control systems. The disposal of a model as a meaningful representation of the real world (in fact the plant we are to control), allows to simulate, predict and design a suitable controller to determine its behavior. This is the route taken by modern control approaches where a controller is computed on the basis of the plant model. However, the finally deployed controller, even computed on the basis of a plant model does not explicitly contains the plant model. In this sense, the approach is *model-based*.

On the other hand, within a Model-Driven Control (MDC) formulation the plant model is explicitly used as a part of the controller.Perhaps the more well known example of MDC architecture is the *Internal Model Control* (IMC) proposed by [4]. This structure has some interesting features, basically from the formulation of controller design problem point of view. All these features are extensively discussed in [4]. One of the cornerstones of the IMC formulation is that when the model is precise ($G(s) = G_n(s)$) the feedback signal vanishes. Therefore the IMC controller $C(s)$ operates in open-loop. In other words, the proposed control action is basically a feedforward controller and the feedback signal is generated (therefore used) only when necessary ($G(s) \neq G_n(s)$ or $d \neq 0$). Being the main drawback of the IMC formulation the need for the plant to be stable, in [6] a general formulation was proposed where no need for open-loop stability is required. The resulting structure is also model-driven and several advantages of the explicit use of the model on the controller feedforward components have been recently reported. See [5] and [2].

From a completely different perspective, during the last decade, the relationship between system modelization and system control has been analyzed. Nowadays, it has become clear that the good- ness of a model is dependent of how useful it becomes in the control design task (see introduction in [3]). This concept leads to a broad classification of control synthesis approaches as: Model-based Control and Data-based Control. Data-based, or Data-Driven controllers refers to the family of methods which founds the controller directly from data and never attempts to determine a model. See for example [1].

What is presented in this paper is the conjunction of the advantages of MDC system conception but by using a DDC approach for tuning. Among other advantages it is seen that what really matters is the inclusion of the plant information into the controller. In some situations the need for a simplified model for controller design implies to loose valuable information. The paper presents a concrete formulation that lays down the IMC-*style* decoupling of the feedback and feedforward components; provided by the fact of being a MDC.

The controller components that are structured on the basis of the plant model and that operate in feedforward mode, are designed under a DDC approach. Therefore directly translating the available plant information to the (explicitly) model dependent controller terms. Several advantages with respect to the other existing DDC formulations (but acting on a MBC) are highlighted.

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MODEL OF A HYBRID DRIVE TRAIN FOR BOATS

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Abstract

Hybrid drivelines have been proposed over decades for road vehicles. However, they are not yet as popular in ships and boats, up to some special uses, mostly purely electrical, like in submarines or other essentially military applications, see [2] for one of the few examples. This is surprising, because they could strongly improve the environmental acceptance in harbours or inland waterways, and also offer dynamic advantages during acceleration phases. Indeed, during acceleration, fast boats go through a series of changes of assets which cause a reduction of the acceleration in a certain time interval which is perceived negatively by the passengers (see **Fehler! Verweisquelle konnte nicht gefunden werden.**, where the yellow curve shows the acceleration with the clearly distinguishable drop between 12 and 20 seconds).

Additionally, hybrid drives can be used to supply current for other uses on the boat, and can allow a purely electrical operation in suitable places. In order to obtain a smoother performance during acceleration, two elements are needed: a peak torque supply unit, in this case an electrical motor able to supply an additional torque for few seconds, and a model based control strategy able to control it. The figure below shows the hybrid system used together with the test boat. The control setup is different from standard road applications, on one side for the different emission regulations, but even more for the difficult repeatability on water with respect to the road (besides the lack of a fixed coordinate system) and the small number of production lots which makes the determination of extensive physical models hardly viable.

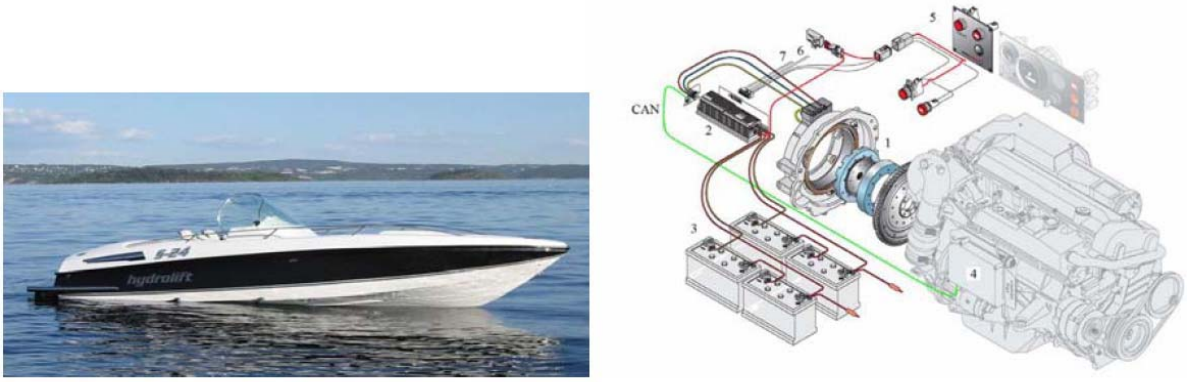

Figure 1: Test boat and structure of the hybrid unit

This paper is concerned with the modelling of the system using easily available physical understanding, but using as much identification as possible, as this strongly reduces the time demand for modelling and is more suitable to the bad variants/performance ratio of ship industry. To improve this aspect, the model is build up modularly and uses torque estimators to determine parameters during the actual boat operation.

The result is a multi-physics modular model with a constant engine and changing boat design and use profile, which has been used to design a compensation law which allows to use the available boost power of the electrical motor. The model has been designed as a combination of physical understanding, experiments and/or data on components (in particular the combustion engine and the electrical drive) and dynamical identification steps.

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MODELING OF NONLINEAR INDUCTANCE IN DYNAMIC TRANSIENT SIMULATIONS

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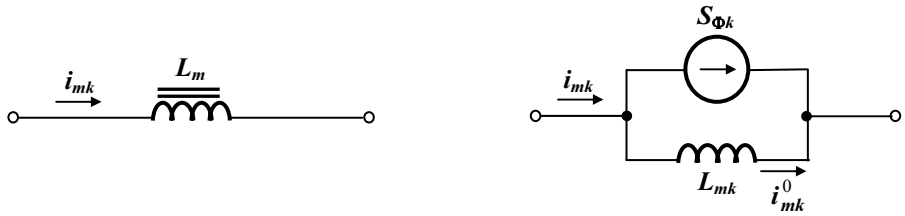
The modeling of nonlinear electrical elements in electrical simulations can be done by using analytical function or by using piecewise linear representation of nonlinear curve. Linearizing of nonlinear curve compared to using analytical function has advantage and disadvantage. A control of numerical stability properties of applied numerical methods is the main advantage. Another advantage is improved simulation speed of nonlinear algebraic-differential equation systems. Piece-wise linearization has basic disadvantage related to negative overshooting effects or jumping of certain linear segments. The piecewise linearizing of nonlinear elements is preferred in this paper. The following relation is valid for nonlinear inductance:

$$i_{m_k} = \frac{1}{L_{m_k}}\Phi + \mathrm{sgn}(\Phi)\cdot I_{m_k} = \frac{1}{L_{m_k}}\Phi + S_{\Phi_k}$$

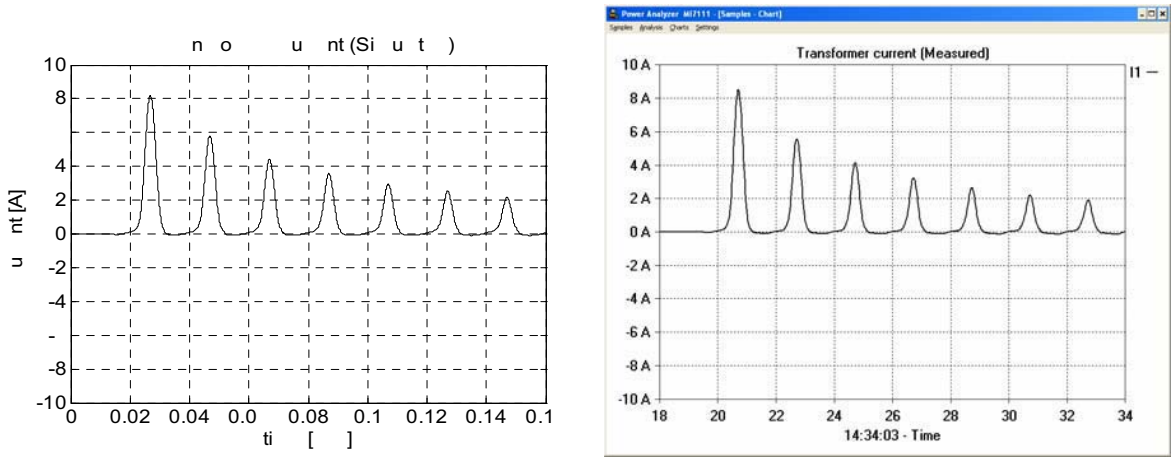
It is possible to create an equivalent model for representing the nonlinear inductance using a linear inductance and a corresponding current source, Figure:



(a) (b)

Figure (a) Non-linear inductance, (b) equivalent model

Differential equation systems, which are used to describe the behaviour of transformer electromagnetic transients, written in a state space form, are usually stiff or very stiff. Stiff systems require being solved using A and L-stable numerical methods, to ensure numerical stability. Backward Differential Formulas (BDF) is preferred in this paper. Developed model of nonlinear inductance is tested on the simple example of single-phase transformer energization. The next Figure shows measured and simulated result of transformer inrush currents obtained by developed model of nonlinear inductance.



(a) (b)

Figure Transformer inrush current: (a) measured and (b) simulated

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MODELING OF SHIP STABILITY DURING CHANGABLE REGIME OF SAILING

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Abstract. The paper deals with dynamic analysis of automatic ship steering gear systems utilizing complex controls that function according to the principle of proportional, integral and derivation regulators. The analysis involves a system dynamic simulation modeling methodology as one of the most suitable and effective means of dynamic modeling of complex non-linear, natural, organizational and technical systems. The paper discusses system dynamics simulation models being used in qualitative (mental-verbal, structural) and quantitative (mathematical and computer) simulation models on ships equipped with trailing steering systems and PID regulator. Authors suggest using the presented models for designing and constructing new steering systems, for diagnosing existing constructions and for education in Universities. *The results presented in the paper have been derived from the scientific research project „New Technologies in Diagnosis and Control of Marine Propulsion Systems“ supported by the Ministry of Science, Education and Sports of the Republic of Croatia.*

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELLING AND REAL-TIME SIMULATION OF HELIOSTAT FIELDS IN CENTRAL RECEIVER PLANTS

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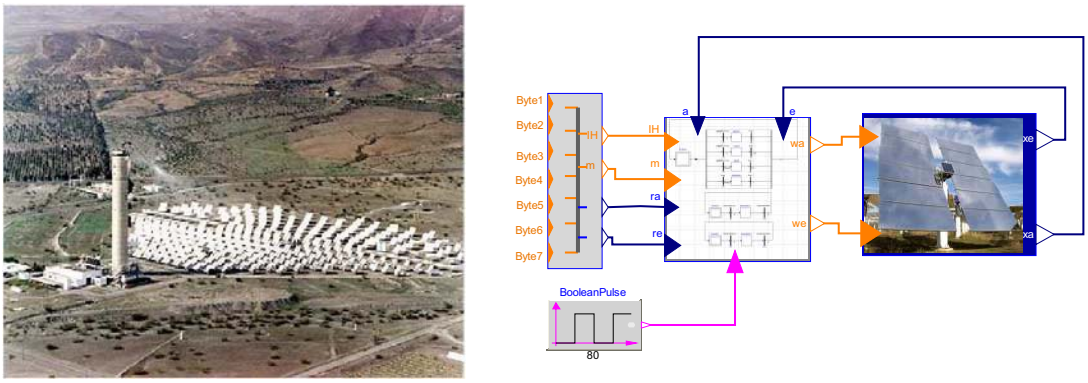
Design and development of dynamic models for simulation and control system design purposes, is getting importance in solar thermal industrial processes. One example is the deployment of advanced control systems that optimize the overall performance of central receiver solar thermal power plants. It is in fact nowadays that this task is a priority research line at CIEMAT National Labs (Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas - Research Centre for Energy, Environment and Technology), public organism owned by the Spanish Ministry of Science and Innovation.

The modelling and simulation activities object of this work are focused on the CESA-I facility, a central receiver solar thermal power plant belonging to CIEMAT, and located at the Plataforma Solar de Almería (PSA), South-East of Spain. This test-bed plant can be seen in 1(a), and it is a experimental prototype for electricity generation among other research projects. It is worthy mentioning [1] as previous research in this area.

During the last years a tough effort has been devoted to the development of control systems for solar thermal power plants, making an important part of the experiences directly against the real plant. These real tests have increased the resources needed for the development, some of which are expensive and scarce, as the experimentation time in the real facility. This fact has motivated the development of a dynamic model for the CESA-I heliostat field plant, mainly aimed as a tool for the enhancement of advanced control algorithms.



(a) The real plant at the PSA

(b) The hybrid one-heliostat model

Figure 1: Central receiver solar thermal power plant

This paper presents a heliostat field simulator, based on a hybrid model, using Modelica as the modelling language. Modelica is a standard unified modelling language with many advantages for modelling dynamic systems because it is both an object-oriented and acausal language. Dynamic behaviour and numerical aspects are taken into account in Modelica, because it provides equation sections and event modelling [2].

The hybrid field model is mainly composed of a differential equation system which determines each heliostat orientation in two axes, azimuth and elevation and the state of each heliostat in the field, using the *StateGraph* [3] Modelica library. The hybrid Modelica heliostat component is shown in 1(b).

The developed simulator is the union of the hybrid model and a wrapped model which handles the real-time simulation and communication issues. This simulator is communicated with a control system application [4] which is in charge of manipulating the heliostat field.

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MODELLING AND SIMULATION OF ROLLING BEARINGS USING ADVANCE SOFTWARE TOOLS

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Introduction. Rolling bearing represents an assembly that is typical and common in lot of engineering applications and it consists of a few components such as inner ring, outer ring and rolling elements. In aim to increase rolling bearings quality and reliability, it is necessary to improve an estimation, construction and technology of rolling bearing manufacturing process. This kind of an approach in modelling is very important, because starting from a mathematical model of load distribution in a mechanical system, we attend to achieve particular objective in Engineering practice and application.

Bearing load distribution. The especially important place in rolling bearings estimation and optimization is taking a problem of load distribution between rolling elements. The internal bearing geometry has may be the major influence on the load distribution between elements in bearing assembly. For this reason, the load distribution for two the most used types of rolling bearing (deep groove ball bearing and cylindrical roller bearing) is analyzed in this paper. For further development of mathematical model it is supposed that bearings are loaded by constant radial external load, parts of bearing assembly are rigid and made absolute accurate and in a load less condition there is a clearance between rolling elements and internal ring equal to half of a total internal radial clearance. Bearing load distribution in the loaded zone is unequal, caused by number of rolling elements participating in transfer of external load, as well as degree of their engagement in load distribution. Because of large number of the influence factors and complexity of their influence on load distribution, the load distribution factor used to be involved into the mathematical model. This factor represents the ratio of rolling element load and external load. Based on the load distribution factor analysis supported by diagrams it is possible to explain character of load distribution between rolling elements depending on the various influence factors. The carried out analyze can be used for more precise determination of load carrying capacity, stiffness, service life and other performances of rolling bearings, such as an excellent base for bearing modelling and simulation.

Modelling and simulations. Based on mathematical model and results of bearing load distribution analysis, corresponding models of rolling bearings are performed using software CATIA V5, as a modern and advanced engineering software tool. Modelling process is conducted In “Part design module” of this software, where bearing models are made in their original size and with standard performances. Using main bearing parameters, with some correlations and formulas between them, it is possible to make series of bearings by parametric modelling method in aim to find the best solution for demanding conditions. For above mentioned bearing models, CATIA V5 as an advance software tool gives an opportunity to make several simulations. The first is the simulation of kinematics, which means motion simulation of bearing elements in work, which is possible to make in CATIA V5 module for DMU Kinematics. Besides, it is very important to make also simulation of the bearing under the real load conditions. It allows us to analyze the unequal load distribution of the bearing, stress values such as displacements of every part in bearing assembly. As an example, a figure shown in the full paper present Von Misses stress values of a loaded bearing caused by unequal load distribution. Conducted simulation is made based on FEM method and for relevant finite element is selected to be linear elastic tetrahedron. As an approach in a simulation of the bearing dynamic behavior is to analyze the frequency content of the simulated system. This kind of simulation problems is also possible to conduct in CATIA V5 structure analyzes module with set of dominant self frequencies as a result. Based on presented simulation results, this advance software tool allow us to solve also some optimization problems, but this aspect of analyzes exceed simulation topic and it is not presented in this paper.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELLING CONSERVATION QUANTITIES USING CELLULAR AUTOMATA

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Introduction. Cellular automata (CA) have been proven to be a suitable tool in modelling tasks, specially, when the underlying procedures are difficult to express in mathematical terms. This might be due to the lack of a mathematical theory for the specific problem or too many unknown parameters. Thus, CA are often used as some kind of soft tool which might have not same modelling accuracy as classic methods (white box-models). CA are rather black box-models, wherby the inner structure of the system can't often be described in detail, but the behaviour or interactions of the system are well known.

Choosing CA. The underlying dynamics of a complex system like the migration of pollutants (actinoides) in contaminated soil is not known in detail. Indeed, the most important migration processes like diffusion and convection can be described mathematically very well by PDEs. But there're also other processes which influence the migration ability of pollutants significantly, like sorption or matrix diffusion. These processes are well observed, but a suitable underlying mathematical description is still missing. Thus, modelling the migration of pollutants in contaminated soil is far too imprecise for a white box-model. A black box-model like CA would be more suitable. Due to the fact, that there existed an area, where the modelling results were to be compared to an actual contaminated area the modelling technique of CA was chosen. Contaminated areas have to be characterised by a systematic sampling strategy, followed by spectrometric analyses. In order to define a sampling strategy a sampling grid has to be defined, and on every node of the grid a sample is taken. CA are quite similar, they also work on the basis of a grid, whereby the spaces between the nodes a defined as cells.

Implementation. The underlying problem of the migration behaviour of actinoides in soils was implemented on the basis of the transport equation in the form of an automata rule to MATLAB. The transport equation, a PDE first became discretised and then adapted to the observed behaviour of the pollutants. Thus, the discretised transport equation was extended by retardation factors due to sorption towards certain barriers and matrix diffusion. Because of the fact that actinoides are radioactive nuclides, the radioactive decay process and the created progenies of the pollutants have also to be considered in the spreading.

Summarising all these different facts an automata rule was defined for 3-dim migration of pollutants in soil. Due to different emphasis on the two basic mechanisms, diffusion and convection, the *von-Neumann neighbourhood* was chosen for the comparatively weak process of diffusion, while the *Moore-neighbourhood* was chosen for the comparatively strong process of convection. The migration problem itself was implemented by the mentioned conditions in MATLAB. The contaminated area itself and the spreading of every single nuclide (americium-241, plutonium-241, plutonium-238, plutonium-239+240, neptunium-237, uranium-234) was implemented in the form of matrices of same dimensions. Therefore, a certain cell a_{ij} was at the same position in all of these matrices, but in probably different states. Thus, if that cell keept a certain amount of a particular actinoide and a certain amount of another particular actinoid, it was easy to calculate the total amount of pollutants in that cell which represents the area.

In order to track the migration behaviour of pollutants through the model, a certain amount of particles (pollutants) was released in the matrix which represents the contaminated area. The spreading in space and time was observed. The migration of pollutants particles as well as the spreading of their progenies due to radioactive decay were summarised all time at all cells. Soon it was seen that the total amount of pollutants present on the surface was always constant. Due to the strong ability of matrix manipulation, MATLAB was of big help for the checking of the conservation of the amount of substance (particle counting). Considering the amount of substance and molar masses of the concerning nuclides, conservation of mass can also be shown in this model.

Conclusion. Observing the migration model it was easily seen that CA are also capable to handle conservation quantities like amount of substance and mass. The only precondition is that the quantity to be conserved has to be discretised prior its implementation to the automata rule. Also conservation quantities like momentum, energy, angular momentum and spin become can be modelled by CA as long as they can be reasonable discretised or at lest reasonable subdivided into smaller parts for the automata rule.

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MODELLING DYNAMICS OF TWO-SIDED WEDGE MECHANISM WITH VARYING CONTACT

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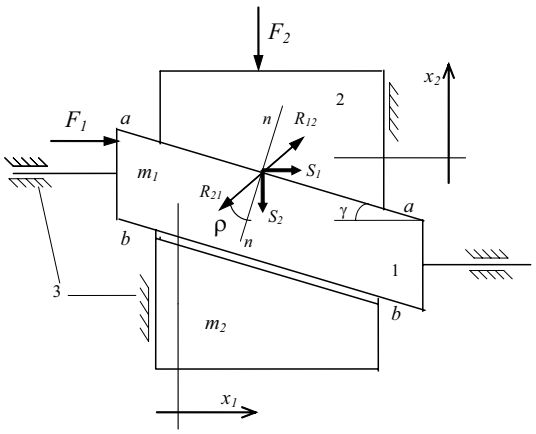
This paper is the result of research in multi-body contact dynamics emphasising the discontinuity approach for the analysis of varying force constraints and efficiency problems of the worm gear drive systems by the special developed physical model called as Two-Sided Wedge like Mechanism.



Two-Sided Wedge Mechanism. Design Dynamic Model in Plane

The discontinuity approach has been clarified the dynamically variable regimes of motion deals with worm gearmesh contact properties that covering sliding friction and backlash occurs between the worm and the mating gear. A set of the force ratio (called as force transfer function) according to the type of active contact line and direction of friction forces describes different relationships between internal tangential forces and efficiency of torque multiplication for different contact surface. The two dynamical regimes of motion called as tractive and inverse-tractive are accepted for modelling.

The qualitative force constraints analysis deals with the instantaneous changes of varying contact-cases and appropriate dynamical regimes that exhibit jump discontinuous events within continuous simulation process. The model configuration is presented by partitioning co-ordinates, which includes kinematics, force and inertial systems parameters. All parameters are reduced to the reference contact point by regular well known manner depends from gear geometry. The kinematic and force constraint equations are deduced from kinetostatic analysis at equilibrium Systems State.

The residual form of mathematical model formulation has been presented by ODEs with Discontinuity kernel in the right-hand side. The numerical integration scheme for monitoring the possible switching events (or discontinuities) within continuous ODE solver has been carried out via additional construction of switching function and control conditions using a technique known as zero-crossing detection. The problem is that to locate discontinuities accurately within standard ODE solver. Different aspects of that numerical problem are well discussed in [1,2]. The numerical example that illustrates the developed methodology is given for motor operated valve with worm gearbox. The performed investigation allows determining the influence of worm gear geometry, inertial and external forces of the drive mechanical system on internal forces ratio, and designing an efficiency factors in dynamically different regimes of motion.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MODELLING OF HIERARCHICAL MANPOWER SYSTEMS AND DETERMINATION OF CONTROL STRATEGIES

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Introduction. Due to the disturbances in the economic environment, the hierarchical manpower system should be steered to the new desired structure. According to stated trajectory one should provide acceptable strategy to achieve target values. The model should be accepted by the user therefore the System Dynamics methodology was applied. In order to perform numerical optimization discrete state space of the model was used.

Methodology. In previous research [1] it has been indicated, that the bare numerical approaches give little insight into the structure of gained solution. One major factor that impacts low acceptance of optimization methods in manpower planning is low undestanding of the system structure. Successful application of sophisticated optimization approaches to the manpower planning depends on the user understanding of the process considered. In this regard System Dynamics [2, 3] has been identified as proper approach to modelling hierarchical manpower system. Formulation of the system in discrete space where $\Delta t = 1$, takes a form of:

$$\begin{cases} \mathbf{x}(k+1) &= \mathbf{A}\mathbf{x}(k) + \mathbf{B}\mathbf{u}(k) \\ \mathbf{y}(k) &= \mathbf{C}\mathbf{x}(k) \end{cases} \tag{1}$$

Trajectory function, which describes the way in which particular goal value should be attained is defined by the following rule:

$$g(t) = x_T + \frac{(x_0 - x_k)(k-t)}{k} e^{-pt} \tag{2}$$

where x_0, x_T represent initial and terminal state, k is simulation time and $p \in [0, \infty]$ importance factor. The set of curves which attain goal value in prescribed final time is dependant on the value of importance factor, which determine how fast the target value is achieved. In order to achieve prescribed trajectory, the minimization of the distance to the target function is defined by Eq. (2):

$$J = \mathscr{A}\left(\min_{u,r,f}\left[\sum_{k=1}^{t_k} \mathbf{w}\left(\mathbf{z}(k) - \mathbf{x}(k)\right)^2\right]\right) \tag{3}$$

subject to constraints in parameters of matrix $\mathbf{A}$; $\mathbf{u}$, $\mathbf{r}$ and $\mathbf{f}$. $\mathscr{A}$ represents applied automaton which is used to classify acceptable strategies by elimination oscillations in rates. The set of states is $S = \{S_0, S_1, S_2, S_3, S_4, S_5\}$, the comparison alphabet is $A = \{l, e, g\}$, the initial state is $i = \{S_0\}$ and the set of terminal states is $T = \{S_0, S_1, S_2, S_3, S_4, S_5\}$. The transition function of $\mathscr{A}$, $\delta : S \times A \rightarrow S$ is defined by the transition table selecting the proper strategy which should not examine oscillations in rate elements. $\mathbf{w}$ is time–invariant vector of weights reflecting the importance of holding deviations for rank n as small as possible, $\mathbf{z}(k)$ represents goal trajectory of the system defined by Eq. 2. Constraints of parameters are prescibed as: $\mathbf{u}_{min}(k)$ and $\mathbf{u}_{max}(k)$, vectors of lower and upper boundary for recruitment in rank x_1 respectively, $\mathbf{r}_{min}(k)$ and $\mathbf{r}_{max}(k)$, vectors of lower and upper boundary for transitions between ranks x respectively, $\mathbf{f}_{min}(k)$ and $\mathbf{f}_{max}(k)$, vectors of lower and upper boundary for fluctuations in rank x respectively. Note that all boundaries are time dependant which increases the complexity of addressed optimization problem. Minimization was realized by Pattern Search with GPS Positive Basis search method and GPS Positive Basis 2N Pool method.

Results and Discussion. Developed method, which include discrete state space model, Finite Automata, trajectory function and Pattern Search provides effective determination of proper strategies to gain desired target structure of hierarchical manpower system. System Dynamics methodology has been successfully applied at the user interaction with the system which is important for successful application of developed approach. Developed methodology could be transferred to other similar hierarchical systems such as supply chains or chain production systems.

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Modeling the impact of childhood vaccination on the spreading of pneumococcal diseases in Austria: Differences between a Markovian and ODE approach.

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Abstract

In Austria pneumococcal bacteria cause over 25000 serious illnesses each year[6]. The most common are meningitis, septicaemia, bacteraemic pneumonia. Furthermore there are other illnesses where only a certain proportion is caused by identified serotypes (e.g. otitis media). Most infections occur among children, especially those younger than 2 years and people older than 60 years[6,3]. There is a vaccine that protects against 23 pneumococcal serotypes (of approximately 90) which can only be used for people over 2 years, but also a 7-valent conjugate vaccine for children which can already be used for 2-months-old babies and is licensed in the European Union and other developed countries[1]. This vaccine is under discussion of being introduced in Austria's child immunization program and is already in use for about 10 percent of all children, for example premature babies. The aim is to create a model to simulate the pneumococcal illnesses and estimate the possibility of preventing the disease by vaccination with the 7-valent vaccine. Therefore a Markovian model has been developed to be compared with existing models. We look at a single birth-cohort and each time-step covers 6 months. The structure of the Markovian model does not allow a deeper insight into the spreading of the illnesses and dynamic feedback due to the Markovian Properties. With this model it is not possible to represent dynamical nonlinear effects like herd-immunity in other age groups. Therefore afterwards a system of differential equations is created to get a deeper insight on these phenomena. The system is very sensitive to costs that illnesses and long-term sequelae cause. Another factor of uncertainty is serotype shifting where different studies contradict each other. Therefore it is a borderline decision if vaccination is really cost-efficient and by now different studies result in different conclusions.

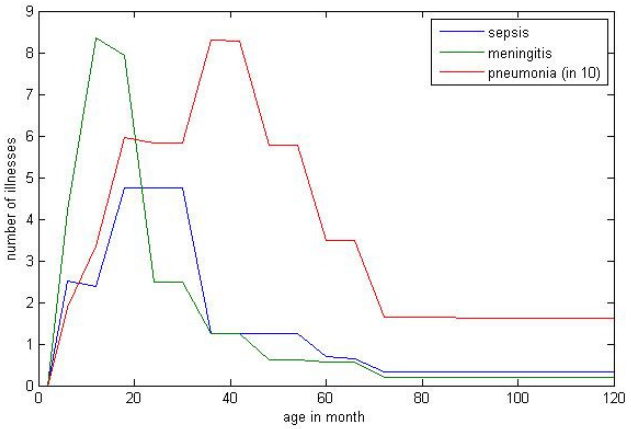

Figure: Number of illnesses in a single birth cohort.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

NONLINEAR MODELING AND ANALYSIS OF AIRCRAFT GROUND DYNAMICS

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Summary. The ground dynamics of passenger aircraft are influenced by nonlinear characteristics of components, especially aerodynamic surfaces and tyre properties. We present a mathematical model of a mid-sized passenger aircraft that captures these effects and apply dynamical systems tools to its study. Specifically, we present a two-parameter bifurcation analysis where we vary the steering angle and taxiway friction coefficient as parameters. Solutions are represented as surfaces that allow us to draw conclusions on the robustness of ground operations under varying operating conditions.

Abstract. The primary goal for commercial aircraft taxiing between terminal and runway is to do so quickly and safely. The desire to understand how this can be achieved reliably motivates the study of aircraft ground dynamics. Computer modeling can be used to gain useful insights into operational procedure of existing aircraft and help with the design of future aircraft at relatively low cost. Indeed, computer simulation has previously been used to study the dynamics of aircraft on the ground; examples are, a study of a linearised bicycle model [1] and a study of a model implemented in the multibody systems package SIMPACK that includes nonlinear effects [2]. Nonlinearities play a significant role in the dynamics of aircraft, specifically in components such as the tyres and aerodynamics. Therefore, in the development of a computer model, it is important to incorporate and evaluate nonlinearities inherent in the various components. A previous study by the authors [3] used a nonlinear model implemented in the multibody systems package SimMechanics. In contrast to existing work, the system was analysed with tools from nonlinear dynamics, specifically, a bifurcation analysis was performed.

In order to improve computational efficiency and functionality with tools used for bifurcation analysis we present here a fully mathematical description in the form of a tricycle model of a typical medium sized single aisle aircraft in which the nose wheel is used for steering. The equations of motion are given in terms of a set of ordinary differential equations, where the aircraft is modeled as a rigid body with six degrees of freedom. The forces applied to the body by components such as the tyres and aerodynamics are modeled from real test data. The model has been fully validated against the well established industry tested model used in our previous study [3].

To illustrate the use of nonlinear modeling and dynamical systems tools in the study of aircraft ground dynamics we present a bifurcation analysis with the continuation package AUTO[4]. Specifically, we investigate the effect that differences in taxiway surface condition have on the lateral stability of turning. The results are presented in terms of two-parameter bifurcation diagrams in which the solutions are represented as surfaces. The results confirm that turns made in low friction (wet) conditions can result in a loss of lateral stability at lower velocities. However, at high velocities where aerodynamic effects play a more significant role, we find that, counter intuitively, regions of stability may be extended in low friction conditions.

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NONSYMMETRIC FINITE INTEGRAL TRANSFORMATIONS AND THEIR APPLICATION IN THERMOVISCOELASTICITY

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A finite integral transformation method for the solution of initial-boundary value problems for hyperbolic systems of PDEs recently proposed by Y. Senitskii is generalized to nonselfadjoint case. The new method is applicable to dissipative non-symmetrical visco- and thermovisco-elastic dynamic problems for which classical approaches apparently fail. The obtained solutions are of the form of spectral expansions based on complete biorthogonal sets of eigenfunctions and associated functions, corresponding to adjoint pairs of matrix operator pencils. The co-ordinate functions of mentioned expansions, namely transforms, one can obtain by applying the special integral transformation with the matrix kernel, thus reducing the problem to the sequence of initial problems for ODEs. The usability of suggested method for the analysis of the non-stationary, high frequency loadings is elucidated.

Let $\mathbf{f}(\mathbf{x},t)$ and $\mathbf{y}_0^{(i)}(\mathbf{x})\,(i=0,\ldots,m-1)$ be the square integrable vector-functions defined in $V\times[0,\infty[$ and V respectively; $V\subset\mathbb{R}^n$. Assume that V is compact. Let $\mathcal{A}_i\,(i=0,\ldots,m)$ be the nonselfadjoint differential operators in the Hilbert space L^2_μ with scalar product $\langle\mathbf{v},\mathbf{w}\rangle=\int_V\mathbf{v}^{\mathrm{T}}\mu\,\overline{\mathbf{w}}\,dV(\mathbf{x})$, where μ is the metric matrix-function. Consider the following initially-boundary value problems (IBVP):

$$\sum_{i=0}^{m}\mathcal{A}_i\frac{\partial^i}{\partial t^i}\mathbf{y}(\mathbf{x},t)=\mathbf{f}(\mathbf{x},t),\quad \frac{\partial^i}{\partial t^i}\mathbf{y}(\mathbf{x},t)\,\Big|_{t=0}=\mathbf{y}_0^{(i)}(\mathbf{x}),\quad i=0,\ldots,m-1,\quad \mathbf{y}(\mathbf{x},t)\in\mathcal{D},\tag{1}$$

where $\mathcal{D}=\{\mathbf{y}|\mathbf{y}\in L^2_\mu\cap C_x^{(n)}\wedge\mathcal{B}(\mathbf{y})=0\}$, $\mathcal{B}$ is the boundary operator, defined by prescribed boundary conditions.

The obtained solutions of IBVP (1) are of the form of spectral expansions based on complete biorthogonal sets of eigenfunctions and associated functions, corresponding to the conjugate pairs of matrix operator pencils $\mathcal{L}_\nu$, $\mathcal{L}^*_{\overline{\nu}}$:

$$\mathcal{L}_\nu=\sum_{i=0}^{m}\nu^i\mathcal{A}_i,\ \mathcal{L}^*_{\overline{\nu}}=\sum_{i=0}^{m}\overline{\nu}^i\mathcal{A}_i^*,\quad(\mathbf{u}\in\mathcal{D}\wedge\mathbf{v}\in\mathcal{D}^*)\Leftrightarrow(\langle\mathcal{L}^*_{\overline{\nu}}\mathbf{u},\mathbf{v}\rangle-\langle\mathbf{u},\mathcal{L}_\nu\mathbf{v}\rangle=0).\tag{2}$$

Here $\mathcal{A}_i^*$ are conjugate to $\mathcal{A}_i$ differential operators, defined in the domain $\mathcal{D}^*$, that defined by boundary operator $\mathcal{B}^*$ conversely. The proposed method is applicable to analysis of dissipative dynamic systems, particular for dynamic viscoelastic and coupled dynamic thermoelastic nonselfadjoint IBVP.

As illustrative example the coupled dynamic thermoviscoelastic problem for a finite cylinder is solved. Some types (torsional, dilative, bending and prportional) of eigenfunctions in 3D representation are shown on Fig.1.

It is important to note, that, unlike well-known transformation technique (Laplace transform, etc.), that uses numerical approach for inversion, proposed method admit to obtain solution in closed analytical form and to develop effective algorithmic realization of computer simulation [1,2].

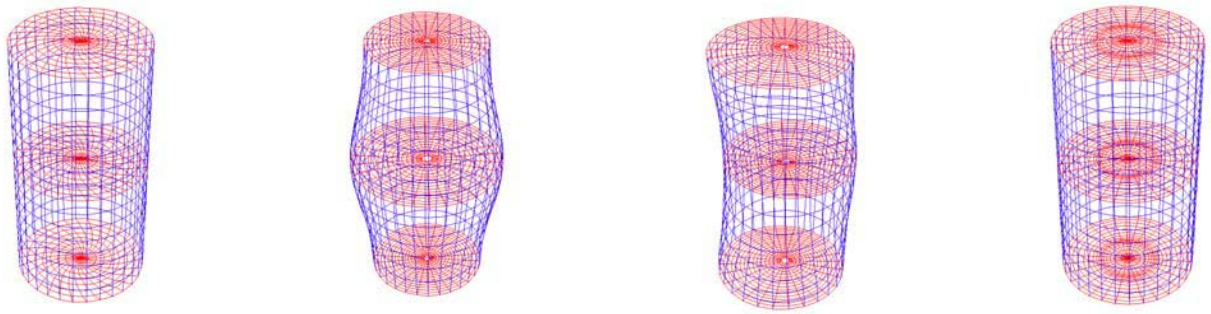

Fig. 1. 3D representation of the real parts of eigenfunctions.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

NOVEL DELAY-DEPENDENT STABILITY CRITERION FOR UNCERTAIN DYNAMIC SYSTEMS WITH INTERVAL TIME-VARYING DELAYS

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Since many industrial systems such as neural networks, chemical processes, network control systems, laser models, large-scale systems, and etc, can be modelled as time-delay systems, a great deal of effort has been done to the stability analysis or stabilization of time-delay system [1]. It is well known that the occurrence of time-delay deteriorate the system performance, cause oscillation.

Recently, delay-dependent stability analysis, which provides an maximum upper bound of delay for guaranteeing asymptotic stability, has been extensively investigated. In this field, an important index for checking the conservatism of stability criterion is the maximum allowable value of time-delay. Therefore, how to choose Lyapunov-Krasovskii functional and derive the time derivative of this with appropriate free-weighting matrices play key roles to increase the delay bounds for guaranteeing stability. To do this, various Lyapunov-Krasovskii's functionals and techniques in obtaining an upper bound of time-derivative value of Lyapunov-Krasovskii's functionals are proposed recently [2]-[6]. In this regard, Park [2] proposed a new bounding technique of cross terms and showed that the proposed stability criteria of time-delay systems have larger maximum allowable delay bound. Yue *et al.* [3] introduced neutral model transformation to get new stability criteria. Parameter neutral model transformation was used to reduce the conservatism of stability criteria [4]-[5]. Park and Ko [6] increase delay bounds by including all possible information of states when constructing some appropriate integral inequalities proposed in [2]. However, there are still room for reducing the conservatism of stability criterion yet.

Consider the following uncertain dynamic systems with interval time-varying delays:

$$\begin{aligned} \dot{x}(t) &= (A+\Delta A(t))x(t)+(A_d+\Delta A_d(t))x(t-h(t))\,, \\ x(s) &= \phi(s)\,, s\in[-h_U\,,\,0]\,. \end{aligned} \tag{1}$$

Here, $x(t)\in\mathscr{R}^n$ is the state vector, $A\in\mathscr{R}^n$ and $A_d\in\mathscr{R}^n$ are known constant matrices, $\phi(s)\in\mathscr{C}_{n\,h_U}$ are vector-valued initial functions, $h(t)$ means time-varying delays which satisfy $0\le h_L\le h(t)\le h_U$ and $\dot{h}(t)\le h_D$, $\Delta A(t)$, and $\Delta A_d(t)$ are the uncertainties of system matrices of the form

$$\left[\begin{array}{cc} \Delta A(t) & \Delta A_d(t) \end{array}\right] = DF(t)\left[\begin{array}{cc} E & E_d \end{array}\right], \tag{2}$$

in which the time-varying nonlinear function $F(t)$ satisfies

$$F^T(t)F(t)\le I\,,\ \forall\, t\,. \tag{3}$$

The purpose of this paper is to present a delay-dependent stability criterion for system (1). In order to derive less conservative results, a new Lyapunov functional which divides delay interval is proposed and different free-weighting matrices in divided delay intervals are included in taking upper bounds of integral terms of time-derivative Lyapunov functionals. Then, a novel condition for delay-dependent stability criterion is established in terms of LMIs (Linear Matrix Inequalities) which can be solved efficiently by various convex optimization algorithms [7]. Numerical examples will be included to show the effectiveness of the proposed method.

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NUMERICAL MATRIX EXPONENTIAL FUNCTION DERIVATIVE VIA LAPLACE TRANSFORM APPROACH

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Introduction. The paper deals with a method how to determine a derivative of a matrix exponential function with respect to a parameter inside a matrix of the exponent. The considered technique is based on a Laplace transform approach when, in the transform domain, the derivative is easily stated. To get a result in the original domain, however, it is necessary to use some numerical technique of an inverse Laplace transform (NILT). In the paper, two such methods are presented. To ensure numerical stability of the computation the NILT method is always preceeded by scaling to decrease a Euclidean norm of the matrix below a predefined value, and followed by squaring to return it to the original value. The method finds its practical application in various fields of the electrical engineering, e.g. for a sensitivity analysis in systems with multiconductor transmission lines (MTL).

Principle of the method. The matrix exponential function will be formulated as

$$\mathbf{\Phi}(\gamma, x) = e^{\mathbf{M}(\gamma)x} \ ,$$

with x standing for any real parameter, and $\mathbf{M}(\gamma)$ generally as a complex square matrix. To obtain its derivative $\partial\mathbf{\Phi}(\gamma,x)/\partial\gamma$, a q–domain image is first found, then differentiated, and finally inverted back into the x domain. Using a commutativity property of an integration and a differentiation, and doing some arrangements, a result is

$$\frac{\partial\mathbf{\Phi}(\gamma,x)}{\partial\gamma} = \mathbb{L}_x^{-1}\left\{\frac{\partial}{\partial\gamma}\mathbb{L}_x\left\{\mathbf{\Phi}(\gamma,x)\right\}\right\} = \mathbb{L}_x^{-1}\left\{\frac{\partial}{\partial\gamma}\left(q\mathbf{I}\text{-}\mathbf{M}(\gamma)\right)^{-1}\right\} = \mathbb{L}_x^{-1}\left\{\left(q\mathbf{I}\text{-}\mathbf{M}(\gamma)\right)^{-1}\frac{\partial\mathbf{M}(\gamma)}{\partial\gamma}\left(q\mathbf{I}\text{-}\mathbf{M}(\gamma)\right)^{-1}\right\} \ ,$$

when the derivative $\partial\mathbf{M}(\gamma)/\partial\gamma$ can already easily be determined. The inverse Laplace transform has to be done numerically in general. To guarantee the sufficiently fast convergence the scaling and squaring are applied [1]. The derivative is found for a transformed matrix exponential function $\mathbf{\Phi}(\gamma,x/r)$, for such the r in order to meet the Euclidean norm $\|\mathbf{M}(\gamma)x/r)\| < 0.5$. This temporal result is transformed back to get the original derivative. Hence, considering a formula $\mathbf{\Phi}(\gamma,x) = \mathbf{\Phi}^r(\gamma,x/r)$, then if $r = 2^M$, M integer, a restoring $\mathbf{\Phi}(\gamma,x)$ from $\mathbf{\Phi}(\gamma,x/r)$ can fast be performed by a squaring process as $\mathbf{\Phi}(\gamma,x/2^{m-1}) = \mathbf{\Phi}^2(\gamma,x/2^m)$, successively for $m = M, M\text{-}1,\ldots,1$. Then, a recursive formula to restore $\partial\mathbf{\Phi}(\gamma,x)/\partial\gamma$ from $\partial\mathbf{\Phi}(\gamma,x/r)/\partial\gamma$ has a form

$$\frac{\partial\mathbf{\Phi}(\gamma,x/2^{m-1})}{\partial\gamma} = \frac{\partial\mathbf{\Phi}(\gamma,x/2^m)}{\partial\gamma}\mathbf{\Phi}(\gamma,x/2^m) + \mathbf{\Phi}(\gamma,x/2^m)\frac{\partial\mathbf{\Phi}(\gamma,x/2^m)}{\partial\gamma} \ .$$

NILT techniques considered. In case of above stated scaling an inverse Laplace transform is solved for $x = 1$. Two NILT methods are considered in the paper. First one generalizes methods in [2] enabling to invert complex images, and is based on a transform core e^{qx} approximation. One of three possible formulae has a form

$$\hat{f}_s(x) = \frac{e^a}{2x}\left\{\hat{F}\left(\frac{a}{x}\right) + \sum_{n=1}^{\infty}(-1)^n\left[\hat{F}\left(\frac{a}{x} + jn\frac{\pi}{x}\right) + \hat{F}\left(\frac{a}{x} - jn\frac{\pi}{x}\right)\right]\right\} \ ,$$

leading to a predictable error if an Euler transform is utilized to accelerate a convergence of the infinite series. Second NILT method results from a Bromwich integral numerical integration and can advantageously be applied to get originals on whole grids of points by using IFFT and FFT algorithms [3]. Its formula has a form

$$\hat{f}_I(kX) = C_k\left(\sum_{n=0}^{N-1}\hat{F}_n z_k^n + \sum_{n=0}^{\infty}\hat{G}_n z_k^n + \sum_{n=0}^{N-1}\hat{F}_{-n} z_k^{-n} + \sum_{n=0}^{\infty}\hat{G}_{-n} z_k^{-n} - \hat{F}_0\right) \ ,$$

leading again to a predictable error if either an epsilon (ε) or a quotient-difference (q-d) algorithm is utilized to accelerate a convergence of the infinite series. Both methods seem to be stable and accurate enough for practice.

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Acknowledgments. This work was supported by the Czech Ministry of Education under the MSM 0021630503 Research Project MIKROSYN.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

ON CERTAIN CONTINUAL AND DISCRETE CONVOLUTION OPERATORS

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If we consider the Calderon-Zygmund operator

$$(Ku)(x) = \text{v.p.} \int_{\mathbf{R}^m} K(x-y)\,u(y)\,dy, \quad x \in \mathbf{R}^m,$$

where the kernel $K(x) \in C^\infty(\mathbf{R}^m \setminus \{0\})$, $\mathbf{R}^m$ is homogeneous of order $-m$, and has vanishing mean value on the sphere S^{m-1}, then it is well known, the spectra of such operator is same as image of its symbol [1], $K : L_2(\mathbf{R}^m) \to L_2(\mathbf{R}^m)$.

Let $\mathbf{Z}_h^m \subset R^m$ be a cubic lattice in R^m consisting of points of type

$$\tilde{e} = \sum_{k=1}^{n} a_k \tilde{e}_k,$$

where $\tilde{e}_k$, $k = 1,\ldots,m$, be standard basis of R^m , $a_k \in \mathbf{Z} \pmod h$. Given kernel $K(x)$ we construct discrete function$K_h(\tilde{x})$, $\tilde{x} \in \mathbf{Z}_h^m \setminus \{0\}$, and for discrete functions $u_h(\tilde{y})$ define discrete Calderon-Zygmund operator

$$(K_h u_h)(\tilde{x}) = \sum_{\tilde{y} \in \mathbf{Z}_h^m \setminus \{0\}} K_h(\tilde{x}-\tilde{y})\,u_h(\tilde{y})\,h^m$$

The symbol $\sigma_h(\xi)$ of such operator K_h can be treated as multivariable discrete Fourier transform [2] of its kernel $K_h(\tilde{x})$ in principal value sense

$$\sigma_h(\xi) = \lim_{N \to \infty} \sum_{\tilde{x} \in \mathbf{Z}_h^m \setminus \{0\}} e^{i\tilde{x}\cdot\xi} K_h(\tilde{x})\,h^m, \quad \tilde{x} \in Q_h^N$$

where Q_h^N is cube of a lattice with side Nh.

It is easily shown the function $\sigma_h(\xi)$ is defined and continuous on $\left[-\frac{\pi}{h}, \frac{\pi}{h}\right]^m \setminus \{0\}$, and periodical on R^m, and the spectra of operator $K_h : L_2\left(\mathbf{Z}_h^m\right) \to L_2\left(\mathbf{Z}_h^m\right)$ is the same as image $\sigma_h(\xi)$.

But the next is more impressible.

Proposition. Images $\sigma(\xi)$ and $\sigma_h(\xi)$ are the same for all $h \in (0;+\infty)$.

The last property can be useful for approximating infinite singular discrete convolution operator by finite-difference operator and explanating approximate solution of multivariable singular integral equations.

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ON DISCRETE-TIME SAMPLED-DATA MODELS FOR NONLINEAR SYSTEMS

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Introduction. Most research in modeling and control of nonlinear systems is devoted to continuous time systems, the discrete time models being not well defined and difficult to handle. In this paper, an attempt to obtain equivalent discrete time models for sampled data nonlinear system is presented. Although the class of nonlinear systems is restricted to the so called sampled data computable nonlinear systems, it is also shown how broad the class of systems suitable to be expressed by this form is.

Content. Recently [1], an approach for the discretization of CT NL models has been presented. The approach is only valid for models expressed as a set of ordinary differential equations affine in the input signal, and by using the so called normal form. The SD exact discretization is only achieved for a restricted class of systems but the modeling errors are bounded and related to the relative degree of the original CT system.

The purpose of this paper is to study the DT modeling of NL systems to be controlled by digital controllers. Of course, a particular class of NL systems, those systems which open-loop step response is analytically computable, will be considered. This class of NL systems, as shown in the paper, includes a number of other previously defined classes, like finite discretizable systems [2], and do cover a wide range of NL systems reported in the literature.

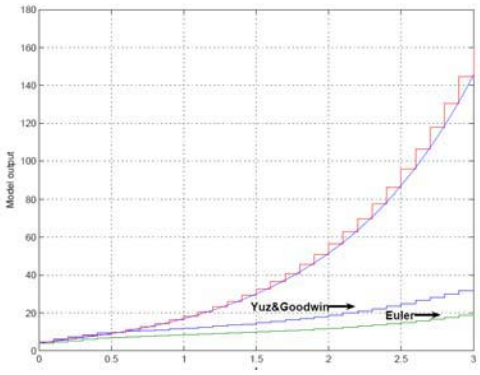
A chained and modular structure is assumed in the global system. Each subsystem is nonlinear in the input, although its input may be external or coming from precedent-in-the-line subsystems. Some subsystems may have the same, different, or none external input. Our first purpose is to obtain SD NL models of these systems, that is, DT equivalent models for piecewise-constant input functions, under some special form of the nonlinearities. These DT models will allow a direct discrete simulation of the systems, as a basis for further SD NL process models.

For instance, a CT *nonlinear in the input feedforward system* (NIF) is defined by r blocks

$$\begin{aligned} \dot{x}_i(t) &= A_i x_i(t) + B_i g_i(x_1, x_2, \ldots, x_{i-1}, u_i), \\ & \quad i = 1, \cdots, r \end{aligned} \tag{1}$$

where $x_i \in \mathbb{R}^{n_i}$ and $u_i \in \mathbb{R}^{m_i}$. Assuming, for any inner subsystem, i, the nonlinear function $g_i(x_1(t), \ldots, x_{i-1}(t), u_i(t))$ is a polynomial function in the state variable arguments, and $u_i(t) = u_i(k\Delta)$, $\forall t \in [\Delta k, \Delta(k+1))$, being constant in the sampling period, the nonlinear function $g_i(t, u_i(k\Delta))$ will be also a vector field of generalized exponential functions, easy to compute, their coefficients being obtained after matrix exponential computations.

Example. In Figure 1, the sampled data model of a continuous nonlinear NIF system is computed and compared for different discretization methods. From $x_0 = [2 \quad 3 \quad 4]^T$, the x_3 state variable response for constant inputs, ($u_1(t) = 1, \forall t \geq 0$, $u_2(t) = -4, \forall t \geq 0.4s$) computed by the exact solution and the different approximated ones, with sampling period $\Delta = 0.1$ s, are shown.



$$\Sigma : \begin{cases} \dot{x}_1 = -x_1 + u_1 \\ \dot{x}_2 = -2x_2 - u_2 \\ \dot{x}_3 = x_3 + x_1 + x_2 u_2 \end{cases}$$

Figure 1: State variable x_3 time response

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

ON EXACT/APPROXIMATE REDUCTION OF DYNAMICAL SYSTEMS LIVING ON PIECEWISE LINEAR PARTITION

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Most of the methods that are proposed so far for control and analysis of hybrid and switched systems are compelling of suffer from high computational burden when dealing with large-scale dynamical systems. Because of the weakness of nonlinear model reduction techniques and also pressing needs for efficient analysis and control of large-scale dynamical hybrid and switched systems; it is essential to study model reduction of hybrid and switched systems in particular. This fact has motivated the researchers in hybrid systems to study model reduction. Model reduction problem for dynamical systems which are defined on piecewise linear partitioning is addressed in this paper. This problem is motivated by control of piecewise linear hybrid system. To our knowledge the only available study in this context in the literature is the work done by Habets and Schuppen [1] which has considered the problem of the exact reduction due to non-observability [1]. Our presented work is generalization and modification of the method in [1]. It is easy to show that in our method if we restrict our attention just to reduction due to non-observability the method also provides the same results as [1].The technique presented is based on the transformation of affine dynamical systems inside the cells to a new structure and it can be applied for both exact reduction and also approximate model reduction. In this method both controllability and observability of the affine system inside the polytopes are considered for reduction purpose. The goal is to drive conditions and method for exact/ approximate reduction of affine dynamical systems living on full dimensional cells of linear partition associated to a quadruple (E,K,U,S), where E is a polyhedral set (a polytope) in $\mathbb{R}^n$, K is a piecewise affine partition of E, U is a polyhedral set (of admissible inputs) in $\mathbb{R}^m$, and $S=\{s_p : P \in K_n\}$ is a family of piecewise affine systems: $s_p : \dot{x} = A_p x + B_p u + a_p,\ y = C_p x + D_p u$. In exact reduction input/output behaviour must be preserved but in approximate reduction the goal is to keep the input/output behaviour approximately close to the original system while we reduce the order. In the following we first transform s_p into the structure which contains input/output information which is important from reduction viewpoint and also is suitable to apply linear reduction methods and can be retransformed to the original structure after reduction. If we introduce the new input vector $W_p =: \begin{bmatrix} u^T & a_p^T \end{bmatrix}^T$,the transformed system will be: $s_p : \dot{x} = A_p x + [B_p \quad I]W_p,\ y = C_p x + \begin{bmatrix} D_p & O \end{bmatrix} W_p$. Transformation to this structure makes sense because the reduction procedure has nothing to do with the vector of inputs and it is obvious that based on the dimension of a_p we can recover the new constant vector in the reduced system. The next step is to find a way to embed the switching information to the structure; in other words information of the cell in which our affine system is defined $P \equiv \{x \in \mathbb{R}^n : Nx \le a\}$, this will help us to pay attention to the importance of the states which are probably not important from local input/output maps but they are actively involved the switching conditions. The idea is to define new output and using the advantage of exact/approximate preservation of input-output behavior in model reduction. To do this we define a new output as: $Y_{new} := \begin{bmatrix} y^T & (Nx)^T \end{bmatrix}^T$. In this structure we have new system matrices in terms of matrix N and the old system matrices. The reduced system can easily be changed into the original structure by partitioning after reduction. Transformed LTI systems contain state contribution in local input/output behaviour and their contribution to the switching actions. At this point, we are in position to use several results from linear system theory regarding conditions for exact reduction and also methods to find appropriate projection for exact/ approximate reduction. In the case of exact reduction, applying ordinary controllability/observability tests for LTI systems on the aforementioned transformed system provide us with conditions for exact reducibility. In these propositions for exact reduction we have conditions on the rank of controllability/observability matrices of the transformed system and consequently conditions on affine system matrices and N .One can also approach the problem using Grammians which leads the same results. It is also straightforward to find appropriate projection to remove the states due to non-observability or noncotrollability [2]. In the case of approximate reduction after transformation of the affine system to the aforementioned structure one can use different reduction techniques such as balanced reduction techniques and then it is possible to recover the original structure of the system by partitioning the system based on old output and input. Although this method provides satisfactory approximate results but in approximate reduction a lot of other issues arise which needs more investigations and further research in this context.

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ON THE DETERMINATION OF EFFECTIVE PROPERTIES OF CERTAIN STRUCTURES WITH NON-PERIODIC TEMPORAL OSCILLATIONS

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We study an evolution process in a heterogeneous material possible to model by a parabolic equation, e.g. heat conduction. Consider the equation

$$\begin{aligned} \partial_t u^h(x,t) - \nabla \cdot (a(hx,\beta^h(t))\nabla u^h(x,t)) = f(x,t) \quad &\text{in } \Omega \times (0,T)\,, \\ u^h(x,t) = 0 \quad &\text{on } \partial\Omega \times (0,T)\,, \\ u^h(x,0) = u^0(x) \quad &\text{in } \Omega\,, \end{aligned}$$

where Ω is an open bounded set in $\mathbb{R}^N$ and the function a is periodic in both arguments with respect to the unit cube Y in $\mathbb{R}^N$ and $(0,1)$, respectively. We assume that the material coefficient

$$a^h(x,t) = a(hx,\beta^h(t))$$

and hence may develop in a non-periodic fashion in time while the structure is periodic in space with period $\varepsilon = h^{-1}$ for each fixed t and h. Under certain assumptions on a the sequence of solutions u^h will converge (as $h \to \infty$) towards a limit function u, which solves an equation of the same type as above with identical boundary and initial data but with a coefficient b which is constant. This equation is called the homogenized problem. This means that the effective property of a material as described above, for ε small, will be close to that of a material whose properties does not vary in space or time.

For the special case of periodic homogenization, where we have periodic time oscillations according to

$$\beta^h(t) = h^r t\,, \tag{1}$$

we arrive at three different types of so-called local problems for $0 < r < 2$, $r = 2$ and $r > 2$ respectively, which make it possible to determine the limit coefficient b. For $0 < r < 2$ this coefficient turns out to have the entries

$$b_{ij} = \int_0^1 \int_Y a_{ij}(y,s) + \sum_{k=1}^N a_{ik}(y,s)\partial_{y_k} z_j(y,s)\, dyds\,,$$

where z_j is Y-periodic in the first argument and $(0,1)$-periodic in the second and solves the local problem

$$-\nabla_y \cdot (a(y,s)(e_j + \nabla_y z_j(y,s))) = 0 \quad \text{in } Y \times (0,1)\,,$$

see e.g. [BLP].

Under some uniformity assumptions on $\{\beta^h\}$, cf. [Si], and in particular the assumption

$$h^{-2}\partial_t \beta^h(t) \to 0 \quad \text{in } L^\infty(0,T),$$

it turns out that the homogenized problem for the non-periodic case coincides with that of the periodic case (1) for $0 < r < 2$. Thus it is possible to determine the limit coefficient also in certain non-periodic cases, where the key criterion concerns the rate of change of the function β^h. Our approach is based on a generalization of the two-scale convergence method by Nguetseng, see [Ng], which covers also non-periodic structures, see [Si].

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

ONE-DIMENSIONAL SIMULATION OF BLOOD FLOW IN ARTERIES USING FINITE ELEMENTS

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Introduction. In many developed countries diseases of the cardiovascular system are the most common cause of death, which makes research in that domain particularly important. Among this research work, the modelling and simulation of the cardiovascular system is of great importance. Due to numerical simulations it is possible to study the effects of pharmaceuticals, develop non-invasive measuring methods or investigate the effects of surgeries before the real surgical operation.

This work deals with the modelling and simulation of blood flow in major arteries. Starting from a few assumptions, concerning among others the geometry of the vessel, a one-dimensional model for the blood flow is derived. This model will be integrated in a controlled model for the cardiovascular system of the entire human body.

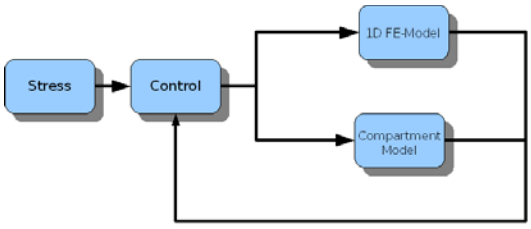
Derivation of the model. The model is based on the Navier-Stokes equations for incompressible fluids. A cylindrical domain is considered in which the Navier-Stokes equations are valid. The domain boundary changes with time due to the movement of the vessel wall caused by the flow. Further assumptions (axial symmetry, radial displacement of vessel wall, constant pressure, neglect of body forces, dominance of axial velocity) are made to reduce the model. In order to get a one-dimensional system, the Navier-Stokes equations are integrated over a generic cross-sectional area.

The resulting system consists of two equations with three state variables: the cross-sectional area, the averaged volume flow, and the averaged pressure. With the help of an additional algebraic equation taken from a mechanical model for the vessel wall displacement it is possible to solve the system.

Discretization, implementation and simulation. In order to solve the equations of the one-dimensional model, a Finite Element Method, more precisely a Taylor-Galerkin scheme of second order, is used. It is necessary to provide suitable boundary values for every time step. The characteristic variables of the system are used to calculate the required boundary conditions.

With the derived model, the blood flow in single arteries as well as at bifurcations of the arterial tree is studied. The system is solved numerically with Matlab. To verify the implementation, several experiments including different pressure functions as test inputs are performed.

Integration in controlled model. With the help of the model described above, blood flow and pressure in a part or in the whole network of larger arteries of the human body can be simulated. For that purpose the vascular system is modelled approximately with straight pipe segments. The network model can be coupled with a model for the control of the cardiovascular system. In this way, influences like physical strain and their impact on pressure conditions in particular parts of the arterial tree can be studied. A simulation scheme is illustrated in the following figure.



Scheme of a simulation of the cardiovascular system

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OPTIMIZATION METHODS FOR INDIVIDUAL-BASED MODEL PARAMETER ESTIMATION IN PREDICTIVE MICROBIOLOGY

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Introduction. The aim of predictive microbiology is to predict the evolution of a microbial population under specific conditions once the initial state has been determined. In order to build proper mathematical models that describe the systems under study, it is essential to accurately define their variables and precisely delimit the values of their parameters.

Individual-based Models in microbiology. In the framework of microbiology, Individual-based Models (IbMs) are discrete models in which the main entities are microbes. These models define rules for the individual cells' behaviour (e.g., uptake, metabolism and cell cycle, among others) and for the processes that take place in the environment (e.g., nutrient diffusion and medium heating, among others). Once they are implemented in a computer, simulations show the evolution of an initial population that is following individual and local rules. Two examples of IbM simulations that have provided varied and interesting results in microbiology are BacSim [2] and INDISIM [1].

The use of IbM simulations as 'virtual experiments' to predict the evolution of a population under specific conditions requires an accurate setting of the parameters involved. Most of them are related to individual characteristics of the microbes (e.g., individual mean growth rate, individual mean uptake rate and individual mean mass to initiate the reproduction cycle, among others). Thus, they are difficult (if not impossible) to assess experimentally. They must be indirectly estimated by fitting the output simulations with the related experimental measurements at the population scale, by means of an objective function that assesses this likelihood. Several methods for parameter estimation have been developed within the framework of continuous modelling. However, they are not usable with IbM because they are generally based on gradient methods, which are not applicable in IbM because of their discrete nature.

Methods for IbM parameter estimation. The classic method for estimating the parameters of an Individual-based Model is the grid search: each parameter is discretized in a certain interval where its best value is assumed to lie, and the resulting grid (different combinations of parameters to be evaluated) is explored to find the best point. This method involves great time expenditure, since it requires an enormous number of simulations. In this study we adapted and tested two optimization methods for an IbM parameter estimation: the Nelder-Mead Threshold Accepting (NMTA) [3] and the NEWUOA [4]. Both of them were implemented in Matlab and used to estimate one-, two- and three-parameter of BacSim and INDISIM, providing similar results.

Results. We present here the results of INDISIM parameter estimation: (i) the one-parameter estimation (mean individual uptake rate, u_{max}) was performed by means of a grid search, NMTA method and NEWUOA; (ii) the two-parameter estimation (u_{max} and mean individual biomass to initiate the reproduction cycle) was performed by means of a grid search and the NEWUOA method; and (iii) the three-parameter estimation (u_{max} and two parameters of the initial biomass distribution) was tested with NEWUOA. NMTA and NEWUOA methods presented no convergence problems, and the best results in terms of time expenditure where for NEWUOA method.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

OPTIMIZATION OF PARAMETERS BY USING TAGUCHI'S DESIGN OF EXPERIMENTS APPROACH

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Introduction The paper discusses applying Taguchi Design of Experiments approach for robust design i.e. selection of suitable parameters for various segments of fault detection and isolation (FDI) systems to achieve better operation, e.g. less false alarms, quick response and ability to handle small faults (sensor bias, drift) under close loop conditions. Fault detection and isolation systems (FDI) are becoming widely used in many modern systems mainly due to evolved industrial IT equipment, which is raising the level of automation in various technical systems. However, poorly designed FDI system can cause more damage if false alarms are produced which reduces the credibility of the FDI scheme.

Auto-associative neural networ s by Taguchi DoE Among many data-driven methods, statistical methods have many benefits nevertheless neural networks remain their main competition. In 1991, Kramer [1] presented nonlinear principle component approach where he proposed an auto-associative neural structure along with recommendations how to select optimal number of mapping layers. Such one-factor representation does not take all the key factors under consideration therefore also number of bottleneck nodes, transfer function, learning algorithm, should be included into design. Instead of Kramer's approach a Taguchi DoE [2] was tested where experimental results determine which combination of the structure and parameter settings are optimal for desired study case. In the Table 1, variations of process variables were planned and defined by orthogonal array L_{27} (3^{13}). If a classic design of experiments (trial-and-error) would be used, 5^3 experiments would be necessary to conduct. To complete the task by Taguchi DoE, only 27 experiments were conducted a few times (3x27=81 experiments) in random order to achieve mean values of respective results. It is a subjective decision or case dependent how factors are entered into OA, as this defines the ability to detect correlation (interaction) between variables. After conducting experiments, robustness measure in the form of Signal-to-Noise (S/N) ratio was calculated. Since a good process model is needed, neural network with smaller training error is preferred (S/N type "Smaller is better", [6]). Fig. 1 shows calculation of S/N ratios, upon which best parameter selection can be achieved. Further analysis of cross-correlation and interaction between process variables is possible (ANOVA) and it depends how the data was inserted into OA (adequate columns).

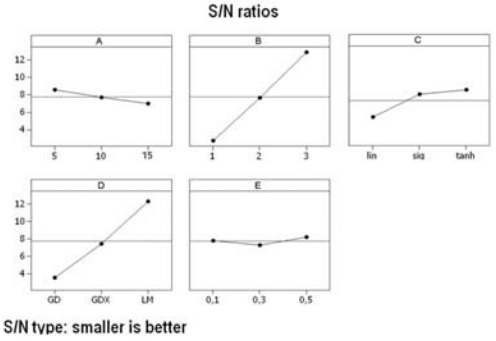

Figure . Calculated S/N ratios (right)

Factor	*Level 1*	*Level 2*	*Level 3*
A	5	10	20
B	1	2	3
C	Lin	Sig	Tanh
D	LM	GD	GDX
E	10%	30%	50%

Table . Planned variations of parameters and respective levels

Factor A: number of hidden neurons in encoding/decoding layer; Factor B: number of neurons in bottle-neck layer; Factor C: transfer function; Factor D: back-propagation learning method: LM (Levenberg-Marquardt), GD (gradient descent), GDX (momentum gradient descent with adaptation); Factor E: size of learning data against size of complete data

Conclusion The neural network model was used in the FDI scheme to be able to detect small faults under closed loop control. By properly setting the isolation parameters of FDI scheme shift detection on the level sensors was achieved capable of detecting small faults e.g. 4% variation of the measured signal. Also a test for sensor drift was conducted, where it proved that drifts could be detected even under close loop conditions. Many factors such as noise and unpredicted disturbances on measured signals can always produce unwanted responses in the system however sensitivity, reliability and accuracy of the FDI system can be greatly improved if suitable design is used. The same technique can be used in many different optimization or design tasks therefore an on-going research will discuss also the selection of parameters for optimal observer based FDI scheme, controller design, selection of the number of principle components, etc.

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PARAMETER STUDIES OF MODE INTERACTIONS IN NOSE LANDING GEAR SHIMMY

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Shimmy oscillations are a classical vibration problem in wheeled vehicles that is caused by a variety of structural and tyre flexibilities [1, 2]. These oscillations are undesirable because of their adverse effects on vehicles and their passengers. Shimmy oscillations are observed in cars, motorcycles, and indeed aircraft. In this work we study their nature in an aircraft nose landing gear. Namely, we consider the interaction between different vibrational modes of a nose landing gear that contribute to shimmy oscillations. To this end, we investigate a mathematical model of a nose landing gear that includes torsional and lateral bending vibrational modes. This model also includes the relevant effects of a non-zero rake angle — which is the angle made by the gear strut with the vertical. To analyze the dependence of the dynamics on parameters, we perform a bifurcation analysis of the model equations with the software package AUTO, where the parameter values used are typical for a midsize passenger aircraft. Specifically, we present two-parameter bifurcation diagrams in the plane of forward velocity and vertical force on the gear. These diagrams contain different bifurcation curves that indicate stability changes in their corresponding vibrational modes [3]. When bifurcation curves intersect, a complicated mixed-mode response involving frequencies of more than one vibrational mode may arise.

The bifurcation diagrams allow one to identify regions in parameter space that correspond to different types of shimmy oscillations in terms of the dominant vibrational mode. In an aircraft nose landing gear they can occur during taxiing, takeoff or landing. During each of these maneuvers the relationship between the forward velocity of the aircraft and the vertical force on the gear has a different and typical profile. To study the stability of the gear under different operating conditions, the associated curves can be overlaid onto the two-parameter bifurcation diagrams in the plane of forward velocity and vertical force. We also investigate the effect of geometric parameters, such as the length of the landing gear or the torsional damping, on the two-parameter bifurcation diagram. This type of sensitivity study may help enhance the design and evaluation of a nose landing gear over the entire relevant range of operating parameters.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

PROPERTIES OF THE NONSTATIONARY BALANCE-BASED MODELLING

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Introduction From the model-based control point of view, the most important feature of the model is its ability to follow the variations of the controlled output in the presence of the changes of the disturbances, when there is a large uncertainty on the description of the physical phenomena taking place. This ability should be obtained with possibly simple form of the model, which ensures simple form of the resulting control law. Practically, it is impossible to meet these requirements without nonstationary modelling.

Content In this paper, the simplified balance-based model is suggested. It is mainly dedicated as a basis for the model-based controller design. This model benefits from the general and unified balance-based form:

$$\textit{rate of accumulation} = \textit{(measurable) inflow} - \textit{(measurable) outflow} \pm \textit{(unknown)}\ R_Y, \tag{1}$$

as well as from the fact that in the advanced control system there is usually a number of measurable disturbances that provide the feedforward action. However, the feedback from the measurement data can be applied not only for this action, but also as a source of information for nonstationary modeling. Thus, in the above model, the measurable signals are included as the *(measurable) inflow* and the *(measurable) outflow* and these terms represent the so-called balance-based part. The parameter R_Y, which is also included in the model, is a positive or negative time-varying term and its description is assumed to be unknown. It represents one global reaction including all reversible and/or irreversible reactions or heat exchange and/or production with nonlinear and unknown kinetics. In other words, in the suggested form of the model (1) all the known and measurable quantities are included in the measurable terms while all the fluxes, for which the description must be considered as unknown, are represented by one time-varying parameter R_Y.

The simplified model (1) can be always satisfied since it is always possible to find the value of R_Y that satisfies the equation (1) at the particular moment of time. When we assume that the value of R_Y can vary in time, it is obvious that we can ensure that the model can be satisfied at each moment of time by the appropriate choice of the current value of R_Y. This value is easily estimated on-line by the RLS method. The generality of the suggested approach results from the fact that there is always only one parameter to estimate and that the estimation procedure is based on the discretised form of the model (1). Thus, the estimation procedure has a scalar form, which provides some very interesting properties. Namely, this form ensures that the estimation always converges, even when the system is in the steady state. There is no need to apply any additional external excitation signals that are usually necessary to guarantee the persistence of excitation for the on-line multiparameter identification. It is hard to overestimate this property in the case when the continuous external excitation is not possible, which usually takes place in the control loop.

In the paper, the most important properties of the suggested model are investigated by the simulation with the application of the simplified example process. The simulation experiments show high modelling accuracy in the presence of the following uncertainty and the emergency cases:

- different (higher than 1) order of a process, especially the presence of not modelled time delay in the system,
- the variations of the measurable disturbances,
- failure of the sensors for disturbing input.

The results show that due to the nostationary form and compensating properties of the estimation procedure, the model follows the variations of a controlled output very accurately, despite of its simplified form. In our opinion, the conclusion is that the suggested approach is an interesting possibility of the general nonstationary modelling for model-based control, which provides high modelling accuracy without the detailed knowledge on the nonlinear description of a process.

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QUATERNIONIC METHODS IN MATHEMATICAL PHYSICS

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Introduction. Quaternionic analysis has become an important tool in the analysis of partial differential equations and their application in mathematical physics and engineering. In particular fluid flow problems, Maxwell equations and equations in 3D-elasticity has been considered. The main goal of my talk is to offer an (almost) complete quaternionic modelling and solution theory including analytical and numerical investigations. The talk reflects the meaning and the importance of quaternionic operator methods for the treatment of boundary value problems and initial boundary value problems of stationary and non-stationary linear and some non-linear equations in fluid dynamics.

Content. We will give a survey on problems which can be successfully dealt with quaternionic methods. The scope of these problems reachs from classical Navier–Stokes equations for Newtonian fluids up to viscous fluids under the influence of temperature or field induction and problems in elasticity and electro-magnetism. A corresponding discrete calculus exists and is worked out in ([2]). The technique is demonstrated for the stationary Benard's problem.

Aside this problem the technique is suitable for Navier–Stokes equations, shallow water wave equations etc.) also fluid flow problems on the sphere (forecasting equations) and through porous media (Galpern-Sobolev equations) can be studied in the same way. (cf. ([4])).

The essential new element in this approach is the use of a quaternionic operator calculus, which is generated by three operators: an algebraical integral operator the so called Teodorescu transform, an algebraical differential operator the so called generalized Dirac operator and an initial-value operator, which is identified with a Cauchy–Fueter operator.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

RECONSTRUCTION OF THE AQUIFER HISTORY OF GRAN CANARIA

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We perform a study on the recent history and current state of the aquifer in the Island of Gran Canaria (Canary Is., 28ºN, 15ºW). Until the 1950's, traditional agricultural practices and small population were able to keep the aquifer in a constant state, even though at the beginning of the 20th Century culture of several water-consuming species was introduced on a commercial basis due to the relative proximity of the Canaries to continental Europe and to the possibility of more than one yearly harvest due to the subtropical climate. Well digging reached depths of more than 300m in many cases, and a chronic hydraulic deficit appeared together with the spoiling of vast coastal areas of the aquifer through intrusion of brackish water. In the mid 1960's, coincident with the apex of agricultural exploitation because of high prices of fruits and vegetables, massive tourism entered the scene. This new activity eventually has become a substitute for Agriculture, attracting more new labour force to the island, and the main result has been a very fast population growth. Moreover, new water use practices are now common. As a consequence, the main causes for the aquifer decline are the simultaneous fast population growth and extensive Agriculture practices in use during the last half of the 20th Century.

The study computes the net water balance by comparing the time series of rainfall with the one describing the joint evolution of agricultural and human water consumption in the last 60 years. Little rainfall is a constant of the canarian climate: 300mm/yr on average (466 cuHm /yr, cuHm = cubic Hectometer) over Gran Canaria, from which some 60% is lost into the sea through runoff because of the steep topography and the imperviousness of volcanic rocks. Therefore, population growth with changing water-consuming habits prevents the recovery of the aquifer, even though Agriculture is no longer so water greedy as it used to be.

The human consumption series takes into account the evolution from 70 l/day to 200 l/day in less than 30 years, and the fact that population is the sum of resident inhabitants and a number of tourists, in a ratio 7/1. The agricultural consumption series has been obtained through proxy measurements on exportation data of the main export products, like tomatoes, cucumbers and bananas. Rainfall series were obtained from the AEMet (Spanish Met Agency) and analysed for trends and periodicities.

In average, the actual hydraulic deficit has been computed yielding 268 cuHm/yr, while desalination plants produce only up to 240 cuHm/yr. Therefore, there is still a water shortage preventing aquifer recovery. The future scenarios of Climate Change announcing a drier climate make it difficult to forecast whether the aquifer can be ever recharged to the pre-1960 levels.

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REPITCHING OF YEAST IN BEER FERMENTATIONS: INDIVIDUAL-BASED MODEL SIMULATIONS

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The industrial production of beer reuses yeast cropped at the end of fermentation in subsequent fermentation. This process, known as serial repitching, is unique to brewery fermentations [1]. The fermentation performance of brewer's yeast strains is dependent on their ability to adapt to changes, particularly during batch brewery fermentation. It has recently been suggested that the distribution of the cells' age on cropping may affect both the immediate and the long term fermentation performance. The yeast *Saccharomyces cerevisiae* has a limited replicative lifespan. Each cell within a population is only capable of a finite number of divisions prior to senescence and death. Replicative ageing depends on the number of divisions undergone by each cell, and can be determined by counting the number of bud scars on the wall of the mother cell. As a consequence of senescence, yeast cells are subject to morphological, metabolic and genetic modifications [5,6].

The aim of this paper is to present the preliminary simulation results from a study designed to explore the influence of cell ageing on the fermentation process, carried out with the individual-based simulator INDISIM-YEAST [3,4] developed from the generic simulator INDISIM [2]. The study was developed by following the cell cycle of a virtual population of the yeast *S. cerevisiae*, up to the point when the production of ethanol flattens out. Cells of different genealogical ages are then cropped. For instance, one yeast cell which has not undergone cell division is cropped, a second showing 1 scar, a third with 2 scars, and so on up to 10 or12 scars. Then individual-based model simulations are performed for each case, in order to study the influence of the initial age of each cell on the increase in population, the rate of glucose uptake and ethanol production. The simulator INDISIM-YEAST is discrete in space and time. It is rule-based and uses stochastic variables to account for cell variability. The physical domain where the virtual fermentation takes place is divided into spatial cubes. The yeast cells grow under batch conditions in a liquid medium, with glucose particles as the main nutrient, and with ethanol, the excreted product, as the only metabolite. The temporal evolution of the population is divided into equal intervals associated with computer or time steps. The web page htpps://aneto.upc.es/simulacio/hoja-portada presents a basic interactive version of INDISIM-YEAST [4]. The virtual system models the behaviour of each yeast cell with the following actions: motion, glucose uptake, maintenance energy, new biomass production, ethanol excretion, budding reproduction and cellular viability [3,4]. Each cell is characterized by its biomass, genealogical age, state in the reproductive cycle and survival time. During the implementation of the program, the simulator takes into account the number of scars left on the membrane of the parent cells, the chemical stresses on the cells, the increase of biomass and the varying duration of the two cycle stages (unbudded phase and budding phase). Simulation results show the time evolution of the number of viable cells, with details of the initial growth and the full time evolution of the system. These results show that, in the case of a virgin cell as inoculum, the lag phase is much longer than in the other cases, as it needs to reach a "critical" biomass in order to start reproducing. Moreover, the maximum number of viable cells are displaced towards a larger number of time steps with lower genealogical ages. A similar picture emerges when the time evolutions of the ethanol particles are depicted. The results show that, in broad agreement with experiments, the initial age of the seed yeast cell not only influences the population growth, but also the rate of nutrient uptake and ethanol production. In other words, the individual features of the initial inoculums influence yeast fermentation performance.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

SENSITIVITY ANALYSIS APPLIED TO A TEST RIG MODEL

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Introduction. The detection of critical parameter variations is a major objective in robust design analyses. Tolerances of parameters lead to scattering system properties. It must be assured that these properties are within a given range. Numerical simulation is one method to investigate the consequences of parameter variations. It is assumed that the technical system to be investigated, in this case an elastomer test rig, can be modelled by a set of DAEs. Sensitivity analysis is used to determine parameters which highly affect the system behaviour. The knowledge of the relation between parameters and system characteristics can also help to determine parameter ranges. As a general approach a Taylor series approximation using an appropriate order can be applied. First-order sensitivities are widely used, while typically higher order sensitivities are applied less. Approaches to determine second-order sensitivities will be discussed in this paper.

Mathematical Model. The equations of motion of the considered systems are given by a differential-algebraic system of equations (DAEs)

$$F(x, \dot{x}, p, t) = 0\,, \tag{1}$$

where $x(t) \in \mathbb{R}^n$ are implicitly defined waveform values (state variables) and $p \in \mathbb{R}^m$ summarises the real-valued parameters p_i. Applying implicit function rules, the system to determine first-order parameter sensitivities $\frac{\partial x}{\partial p_i}(t)$ for all p_i with $i=1,\ldots,m$ can be established [1] as

$$\frac{\partial F}{\partial x}\frac{\partial x}{\partial p_i} + \frac{\partial F}{\partial \dot{x}}\frac{\partial \dot{x}}{\partial p_i} = -\frac{\partial F}{\partial p_i}\ . \tag{2}$$

In the same way, the second-order parameter sensitivities $\frac{\partial^2 x}{\partial {p_i}^2}(t)$ can be determined. It is obvious that higher order sensitivity equations depend on the state variables of the original system (1) and the vectors of lower order sensitivities. Therefore, the adjoint sensitivity approach cannot be applied directly to higher order sensitivity analysis. Thus, we apply algorithms to determine first-order sensitivities on a combination of (1) and (2) using the DAE solver DASPK [2] and the simulator Dymola. An alternative method for a special implementation to determine higher order sensitivities is a staggered solution of (1) and the sensitivity systems.

Interpretation of Sensitivity Results. The sensitivities were computed to detect critical parameters regarding the model of an existing test rig for elastomer bushings, whereas the DAE system of the elastomer test rig is described by 3 equations of motion with 3 state variables $\tilde{x}(t)$, *y(t)* and $\alpha(t)$ as well as 23 system parameters. Parameters with a significant influence to the interesting variable $\tilde{x}$ are single component masses. Concerning sensitivities of *y* also masses have an influence as soon as parameters with a significant influence to α are single inertias. The same critical parameters can be identified by Monte Carlo simulation. However, the effort is much more higher if the Monte Carlo simulation runs are carried out using the original system. The Taylor series approach using second-order sensitivities was compared to the result of solving the system's equation directly. The comparison of the parameter varied (+10%) nominal solution of a special displacement and the solution using first-order Taylor approach as well as second-order Taylor approach shows obviously, that the Taylor approach of second order is a good approximation for the solution of the DAE system of the elastomer test rig and that the second-order Taylor approach represents a better approximation as the first-order Taylor approach.

Conclusion. Sensitivities are well qualified to detect critical parameters of a system. In order to describe a nonlinear relation between parameters and system's characteristics at least second-order sensitivities should be considered. These sensitivities can be determined in parallel to the solution of the original system to reduce the computational effort. Sensitivities of second order allow a good approximation of the solution and yield a reduction of computational effort compared to MC methods. The potential of this approach was investigated using the model of an existing test rig for automotive applications.

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SIMULATION MODEL OF CE108 COUPLED DRIVES APPARATUS

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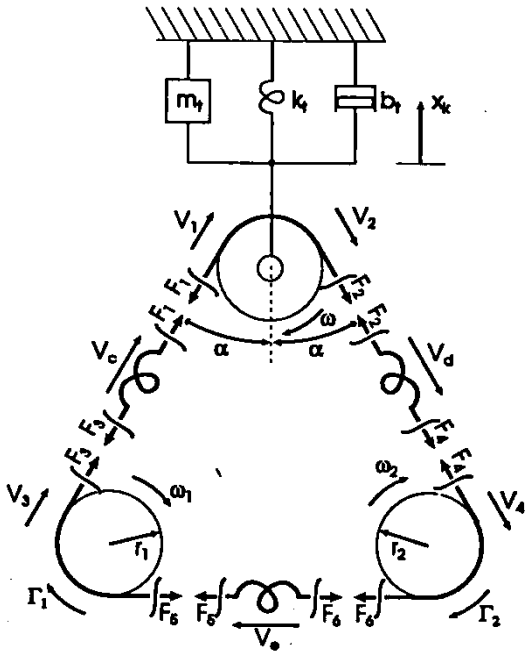
Abstract Creating mathematical models of real objects in purpose of modelling and simulation is one of the most important phases of identification and control of real processes. The paper deals with the model of CE108 Coupled Drives Apparatus created in MATLAB-SIMULINK. The model was created in purpose to test the chosen identification and control algorithms which aimed to be verified at CE108 Coupled Drives Apparatus in the laboratory. CE108 Coupled Drives Apparatus is manufactured by TecQuipment. The model was created in the form of Simulink block having two inputs and four outputs in accordance with the real apparatus. The model was verified by simulation, the model is based on the data measured by Perutka and Dolezel (2006).

The CE108 Coupled Drives Apparatus is fully described in the manual provided by the producer. The principal scheme of apparatus [2] is shown in the figure. Let us suppose the both parts of the belt have the same angular deflection α from vertical line. Moreover, let us suppose the small change of turn angle of the moving jib in purpose to apply the distance x_k. The belt can be divided into linear parts of stiffness k_c, k_d and k_e, where wheel 1 and wheel 2 have inertia momentum and coefficient of rotation friction I_1, b_1, and I_2, b_2 respectively. The speed of belt parts is marked as v with the corresponding indexes. Let us view on the system as the one described in figure. Let us suppose no rotation friction of wheel proving $F_1 = F_2 = F$.

The future work will be directed to the verification of the proposed control on the simulation model before it is verified on the apparatus.



Scheme of CE108 laboratory apparatus

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

SIMULATION OF ATMOSPHERIC POLLUTION DISPERSION

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Introduction. The modeling of atmospheric pollution has a great importance in the case of prediction of pollutant behaviour throw the atmosphere. It has gone big journey in the last century. One of the first model was so called Gaussian plume model which was first proposed by Pasquille and others in sixties of 20th century. It was firstly used for modeling of a pollution dispersion from a point source, however, it was soon applied to line and area sources as well. It matched with the observations and became a standard in every industrial country. The concern shifted to studying of dispersion phenomena, namely dry dispersion, that is to pollutant behavior above the ground and studying of its causalities. Consequently, a new full form of diffusion equation was formulated, which contains diffusivity, advection, deposition, emission and chemistry term. Since that time, no new general model was proposed and until know it is focused to solute this full atmospheric equation.

In our work we are concentrated so far on a model consisting of advection, diffusion and deposition terms [1]:

$$\frac{\partial C}{\partial t} = -u_x \frac{\partial C}{\partial x} + D_y(x)\frac{\partial^2 C}{\partial y^2} + D_z(x)\frac{\partial^2 C}{\partial z^2} + W\frac{\partial C}{\partial z} \tag{1}$$

where the C is concentration in time-space domain (t, x, y, z), u_x is a wind size in x direction, D_y and D_z diffusion coefficients in appropriate axes and W is a deposition rate or deposition velocity.

Model approximation. In our work we have chosen a method of lines as a method for solving PDE. It is based on finite differences where the variables (spatial) are discretized except for one (time variable). This procedure gives us a system of ordinary differential equations (ODE), which can be solved by numerous explicit or implicit methods such as Euler, Runge-Kutta and others. Within this model, we have made a numerical stability analysis and we have verified it by experiments. The conditions for a case of Euler explicit integration scheme are of the form:

$$d_y + d_z \le \frac{1}{2},\ c_x + c_z \le (1 - d_z)d_z,$$

where

$$c_x = \frac{u_x \Delta t}{2\Delta x},\ c_z = \frac{W\Delta t}{2\Delta z},\ d_y = \frac{D_y \Delta t}{\Delta y^2},\ d_z = \frac{D_z \Delta t}{\Delta z^2}.$$

The accuracy is another important property of the approximation. The larger errors are arisen near the source when the steady state equation is approximated [2]. This is caused due to the fact that source strength is only approximated and a large gradient appears there. However, when the time derivative is added this kind of error disappears during a time. The second place where the error was relatively large is near the ground, where the terrain boundary condition is applied. The solution has a tendency to oscillate around the proper value. While in a case of a stable solution the oscillations are damped, in a case of an almost unstable solution (near the border of stability) the error remains far away from the source.

The problem of oscillation of numerical solution is well known and thus many propositions have been made. In recent years the generalized characteristics method that combines Eulerian (time-space domain) and Lagrangian (domain of characteristics) methods is being developed for transport-disperse problems [6]. It turns out that it greatly reduces the numerical anomalies and it can incorporate the boundary conditions naturally within its definition. Therefore it can be inspiring for further development of this work. The investigation of possible incorporation of reaction terms into ADE as well as testing of non-constant coefficients will be other stages of the project. The latter is especially important in this field, because every physical variable in the ADE is changing during a time and space in a real world.

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STUDY OF THE EFFECT OF THE iSCSI PARAMETERS ON THE PERFORMANCE

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Summary: This paper is simulation of iSCSI protocol. iSCSI helps for the transferring the block level data over the network. Simulation offers a flexible way to study the iSCSI – based storage systems. We wish to study a storage area network, which uses iSCSI Protocol to exchange data between its various nodes.

We are looking into the performance issues of the iSCSI protocol. So, we have tuned the different parameters of iSCSI protocol. Tuning is done by Simulation of iSCSI protocol in NS2.

Demands for more storage in the industry has increased beyond that the traditional storage mechanisms can supply and thus, the concept of Storage Area Networks (SANs) has evolved.

This has resulted in the design of iSCSI (Internet SCSI) protocols that have SCSI

Commands and allow data transfer to take place over the network. Fiber channel protocol was the first such protocol that used Gigabit per second links to carry commands over long distances. The iSCSI Protocol maps the SCSI block oriented storage data over TCP/IP and enables storage devices to be accessed over standard Ethernet based TCP/IP networks, With the development of Gigabit Ethernet and the iSCSI protocol, reduction in costs and a uniform network infrastructure can be achieved.

This study will help us in understanding how iSCSI works in a storage area network.

We have used ns2 for our simulation work. We have simulated an iSCSI initiator and an iSCSI target, which communicate through iSCSI. iSCSI lies upon TCP Protocol. R/W requests are made by the iSCSI initiator and data exchange takes place depending on these requests. The throughput is calculated and graph is plotted.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

SNAPSHOT–BASED PARAMETRIC MODEL ORDER REDUCTION

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During the last decades, Krylov subspace projection based Model Order Reduction (MOR) proved as a practical way to reduce the state space dimension of large scale dynamical systems [1]. With state space dimensions reaching magnitudes of $10^5 \dots 10^7$ in models of micro- or nanoscale devices, time domain simulations become impossible without MOR, especially when the coupling of several large scale subsystems is required for system level simulation. Thus, MOR has become an essential step in model generation and simulation of integrated circuits and heterogeneous systems such as micro electrical mechanical systems (MEMS).

Confronted with a growing demand for tools incorporating manufacturing tolerances during simulation and design, Fraunhofer started a joint research project named CAROD (Computer–Aided Robust Design) [3]. One of its subgoals is the integration of Parametric Model Order Reduction (PMOR) methods into Electronic Design Automation (EDA) software. This should give a significant speedup for the computation of parameter sweeps needed for optimization tasks and sensitivity calculations.

Despite a considerable amount of PMOR methods being proposed by different authors, there is major side–issue in our setting that makes these methods inapplicable at first glance: Resulting from the fact that tools for the generation of the system matrices behave like black boxes, the analytical relationship between parameter values and resulting system matrices is unknown. As a workaround, we start with generating a series of *snapshots* of the full order model at fixed parameter values using tools like ANSYS or the partial element equivalent circuit (PEEC) discretization method [2].

With the help of finite differences, the resulting series of linear time invariant descriptor systems is then transformed into a parameter dependent system of the form

$$\left.\begin{aligned} \mathbf{M}(\mu)\ddot{\mathbf{x}} + \mathbf{D}(\mu)\dot{\mathbf{x}} + \mathbf{K}(\mu)\mathbf{x} &= \mathbf{B}^{\text{in}}(\mu)\mathbf{u} \\ \mathbf{y} &= \mathbf{B}_1^{\text{out}}(\mu)\mathbf{x} + \mathbf{B}_2^{\text{out}}(\mu)\dot{\mathbf{x}} + \mathbf{F}(\mu)\mathbf{u} \end{aligned}\right\} \tag{1}$$

with the system matrices $\mathbf{M}, \mathbf{D}, \mathbf{K} \in \mathbb{R}^{n\times n}$; $\mathbf{B}^{\text{in}} \in \mathbb{R}^{n\times p}$; $\mathbf{B}_1^{\text{out}}, \mathbf{B}_2^{\text{out}} \in \mathbb{R}^{q\times n}$; $\mathbf{F} \in \mathbb{R}^{q\times p}$ being polynomials in the parameter vector $\mu \in \mathbb{R}^k$ with matrix–valued coefficients.

Finally, implicit moment matching is achieved with a modified rational Block–Arnoldi method, yielding a parameter dependent reduced order system with the same structure as (1) but smaller state space dimension n.

As a second issue, the introduction of parameters renders passivity preservation more complicated than with classical MOR methods. But under certain assumptions, passivity can still be preserved in practice.

We will present two application examples from nanoscale IC design and MEMS design respectively, where passivity is preserved within a certain parameter range and where the reduced systems give a good approximation of the original systems over a wide frequency range.

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STOCHASTIC MODELING IN THE TASK OF BIOCHEMICAL OXYGEN DEMAND MONITORING

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The environmental monitoring, analysis, forecast and control are very important and highly complicated problems as far as ecological systems show stochastic nature and high dimensionality. So, the choice of a suitable mathematical model depends on the available data and consequently on a estimation method.

The analysis and forecast of biochemical oxygen demand (BOD) are essential in assessing the effects of water pollution. Moreover, the process, which corresponds to BOD, is the repetitive one and usually measurements are presented by panel data.

Using analogies with signal processing, we selected the stochastic differential equation as a model of BOD process and focused our investigation on this model parametric estimation. We developed the identification method, which gives unbiased estimates, and presented the analytic expression for the mean squared error of the forecast. Several computational experiments as well as the results for BOD monitoring in Omega Bay of Sevastopol (Ukraine) are given.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

SYNCHRONIZATION OF A GENERAL CLASS OF NEURAL NETWORKS WITH STOCHASTIC PERTURBATION

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During the last decade, neural networks are widely studied, because of their immense potentials of application prospective in a variety of areas such as signal processing, patten recognition, associative memory and combinatorial optimization [1]. Since significant time delays are ubiquitous both in neural processing and in signal transmission, it is necessary to introduce delays into communication channels which lead to delayed neural networks (DCNNs) model. Recently, it has been revealed that if neural network's parameters and time delays are appropriately chosen, the DCNNs can exhibit some complicated dynamics and even chaotic behaviors. Hence, it has attracted many scholars to study the synchronization of chaotic DCNNs [2]. In real nervous systems, synaptic transmission is a noisy process brought on by random fluctuations from the release of neurotransmitters [3]. Therefore, it is of practical importance to study the stochastic effects on the stability property of delayed neural networks [4]. In Li and Cao [5], the synchronization problem for DCNNs with stochastic perturbation has been investigated. On the other hand, due to the complicated dynamic properties of the neural cells in the real world, the existing neural network models in many cases cannot characterize the properties of a neural reaction process precisely. It is natural and important that systems will contain some information about the derivative of the past state to further describe and model the dynamics for such complex neural reactions [6].

This paper considers neural networks of neutral type with stochastic perturbation. To date, the synchronization problem for neural networks of neutral type with stochastic perturbation has not been investigated fully.

Consider a class of neural networks with time-varying delays

$$d[x(t)-Cx(t-h(t))] = \Big[-Ax(t)+W_0 f(x(t))+W_1 f(x(t-h(t)))+J\Big]dt, \tag{1}$$

where $x(t)=[x_1(t),x_2(t),...,x_n(t)]^T \in \mathscr{R}^n$ is the neuron state vector, n denotes the number of neurons in a neural network, $f(x(t))=[f_1(x_1(t)),...,f_n(x_n(t))]^T \in \mathscr{R}^n$ denotes the neuron activation function, $A=diag\{a_i\}$ is a positive diagonal matrix, $W_0=(w_{ij}^0)_{n\times n}$, $W_1=(w_{ij}^1)_{n\times n}$, and $C=(c_{ij})_{n\times n}$ are the interconnection matrices representing the weight coefficients of the neurons, $J=[J_1,J_2,...,J_n]^T$ means a constant input vector, and $h(t)$ is time-varying delay. In this Paper, it is assumed that $0\le h(t)\le h$ and $\dot{h}(t)\le h_d < 1$, and the matrix C satisfies $\rho(C) < 1$.

The activation functions, $f_i(x_i(t)), i=1,2,...,n$, are assumed to be nondecreasing, bounded and globally Lipschitz; that is, $|f_j(\xi_j)|\le|l_j(\xi_j)|, \forall\,\xi_j\neq 0$, $j=1,...,n$, where l_i is known real constant.

For synchronization problem, let us take system (1) as a drive network, then, we construct the response networks as follows:

$$\begin{aligned} d[y(t)-Cy(t-h(t))] = \Big[&-Ay(t)+W_0 f(y(t))+W_1 f(y(t-h(t))) \\ &+J+u(t)\Big]dt+[H_0(y(t)-x(t))+H_1(y(t-h(t))-x(t-h(t)))]\,d\omega(t), \end{aligned} \tag{2}$$

where $y(t)=[y_1(t),y_2(t),...,y_n(t)]^T \in \mathscr{R}^n$ is the state vector of response network, $u(t)$ is the control input for achieving synchronization, H_0 and H_1 are known constant matrices with appropriate dimensions, $\omega(t)$ is a scalar Wiener Process (Brownian Motion) on $(\Omega,\mathscr{F},\{F_t\}_{t\ge 0},\mathscr{P})$ which satisfies $\mathbf{E}\{d\omega(t)\}=0$ and $\mathbf{E}\{d\omega^2(t)\}=dt$. This type of stochastic perturbation can be regarded as a result from the occurrence of external random fluctuation and other probabilistic causes.

The goal of this short paper is to present a criterion for synchronization between (1) and (2).

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THE ALGORITHMIC BEAUTY OF PLANT ROOTS

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Summary The simulation of plant root growth is an important tool when analysing plant and soil interaction within the rhizosphere. In this work we deal with the visualisation of plant root systems. Exploiting the self similarity of root systems by using L-Systems, we gain a very compact algorithmic description of underlying root geometry. This makes it possible to create two-dimensional geometries of plant root systems and compare them to images of root systems such as the drawings of Lore Kutschera [1] who made hand drawings of root systems of a multitude of European plants. We think that these images have both scientific as well as artistic value.

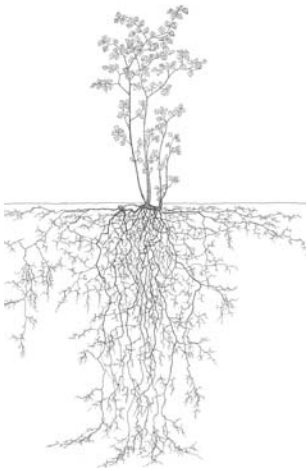
Introduction In modelling and simulation of plant-soil interactions, accurate root growth models are of major importance. In this work we emphasize the visual and artistic aspect of them and do not focus on the continuous elongation of the root systems. The self similar structure of plant roots can be described by using L-Systems. L-Systems are often used in computer graphics to describe the complex geometry of plants and can derive amazing images from simple production rules (see [2]).

L-systems are rewriting systems. All letters of an initial word usually denoted as ω are replaced according to production rules. The production rules are applied to each letter of the word, this is performed recursively n times to achieve a L-system of the n^{th} generation. The resulting string is interpreted graphically. For example the initiator ω and the production rule for X

$$\omega = X, \quad X \to F - [\,[\,X\,] + X\,] + F\,[\,+\,F\,X\,] - X$$

creates a simple tree like structure. Note that the letters $F, +, -, [$, and $]$ are replaced by themselves and are used for the graphical interpretation of the string.

We use parametrized L-System to include effects of gravitropism on root system development. In this way it is possible to describe root geometry that is visually comparable to the images of Lore Kutschera, see figure. We are flattered that our work can be considered as algorithmic art by definition of Vlatko Ceric [3].



The root system of Hasel [1]

Acknowledgements This work was supported by the Vienna Science and Technology Fund (WWTF, Grant No.: MA07-008) and the Austrian Science Fund (FWF, Grand No.: T341-N13). Andrea Schnepf is a Hertha-Firnberg Research Fellow. Tiina Roose is a Royal Society University Research Fellow.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

THE MULTIPHYSICS MODEL OF THE GAS-DAMPED MICROMIRROR FOR THE MEMS-BASED OPTICAL SWITCH

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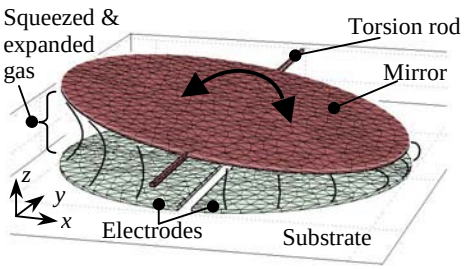
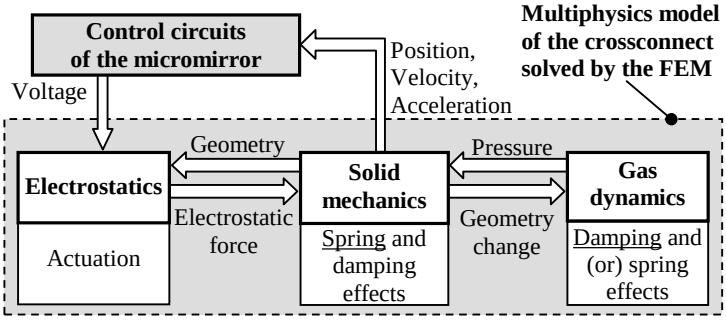
The multiphysics model with distributed parameters of a gas-damped micromirror and its solution by the finite element method (FEM) is presented. Moreover, the model is valid for any electrostatically actuated MEMS device. Thus, it can be used for the modeling of gas-damped parallel plate or comb drive actuators. Presented model and its solution by the FEM are suitable for practical writing of the own simulation software, which is capable to model and simulate the described problem. The simulation results are not included in the paper.

The model is a useful tool for advanced micromirror design and optimization (i.e., the optimization of the shape and dimensions of the micromirror, and its control circuits). The MEMS-based micromirrors have been already fabricated and can be used in the optical crossconnects in all-optical high-throughput interconnection networks [1–3]. Many researchers and companies labour for reducing switching time of the switch because for useful application in all-optical networks it is necessary to achieve short switching time as much as possible, i.e. the micromirror have to adopt new steady-state position in minimal time. Our approach is based on the presence of suitable gas (see figure (a)), which can cause aperiodic transient response and thus improve the properties of the switch. In this point, it is very interesting and challenging to model and simulate the switching process in the switch. The incidence of the gas can be numerically modeled by the squeeze film damping effect. Nevertheless, the Navier-Stokes equations in the conservative form should to be used for more precisely results.

The model of the crossconnect, as shown in figure (b), is divided into two parts, the model of control circuit, and the multiphysics model of the crossconnect. The model of control circuit is the model with concentrated parameters, whereas the multiphysics model is the model with distributed parameters. Our attention in this paper is concentrated only on the multiphysics model of the crossconnect. The multiphysics model is represented as a system of partial differential equations. The model consists of three parts, an electrostatics part described by the Poisson equation, a solid mechanics part described by the Newton equations, and a gas dynamics part decscribed by the Navier-Stokes equations. Simultaneous interaction between these three physical areas can model all essential processes in the crossconnect. The interaction is based on the coupled boundary conditions (e.g. through interactively acting forces on the boundaries, geometry conditions, etc.), which are computed in each time step.



(a) Tilting of the micromirror in the crossconnect



(b) Multiphysics model of the crossconnect of the switch in block diagram with their interaction with control circuits

Figure. The model of the crossconnect of the switch

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THE SIMULATION METHOD USED TO SOLVE ENGINEERING INVERSE PROBLEMS

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Introduction In this paper a special numerical method used to solve engineering inverse problems is presented. This method named the Simulation Method because computer simulations are applied to aid the process of construction computational algorithms and to estimate coefficients in regularization procedure. Under consideration is taken a system appearing frequently in practice which is described by partial differential equation called the Poisson equation. To solve this equation the 2-D discrete models are used for the use of special computational tools constructed on bases of objects from modern combinatorics and principles standing in physics. From various inverse problems the identification of field sources was chosen to detail studies. From the engineering point of view inverse problems involve identification, system synthesis and controlling. To identification problems belong all problems aiming at the reconstruction of information on a mathematical model of the system from data come from measurements. Within various identification problems the identification of field sources was chosen to study because its solution is of importance in engineering and technology. It should be pointed that there is no general method which can solve the great number of parameter and source identification problems for 2-D systems. The choice of adequate method may depend on the kind of real system, its mathematical formulation, the number of data available for measurements, nature of the parameters (constant or space-varying) or nature of the measurements (noisy of noiseless).

System description. In the considerations is taken the system appears frequently in practice described by the following partial differential equation called the Poisson equation

$$\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2} = f(x,y), \qquad u|_{\Gamma} = 0,$$

where:
$x \in (0, \mathrm{r})$, $y \in (0, \mathrm{s})$, $u=u(x, y) \in R^2$ - potential function, $f= f(x, y) \in R^2$ - field sources' function, Γ - boundary.

The zero boundary conditions is assumed to simplify notation without loss of generality it is assumed. In the aim to use numerical method a discretization was done by using a five point differences scheme and the method of separation of discrete variables.

Idea of the Simulated Method. To solve the above equation the 2-D discrete models are used for the use of special computational tools constructed on bases of objects from modern combinatorics. These objects are the non-zero monic power polynomials of the second kind $P(q)$ which coefficients generated by special modified numerical triangle. The $P(q)$ polynomials are defined by the recurrence

$$P_{n+2}(q) = (2+q)P_{n+1}(q) - P_n(q), n = 0, 1, 2, \ldots \qquad P_0(q) = 0, P_1(q) = 1,$$

Using the polynomial approach the inverse problem solution can be express by the formula

$$F_l(k) = \frac{U_{l+1}(k) - P_{l+1}(q_k)U_1(k) - \sum_{i=1}^{l-1} P_{l+1-i}(q_k)h^2 F_i(k)}{P_l(q_k)h^2}.$$

Conclusions In this paper there was presented special numerical method named the Simulation Method used to solve engineering inverse problems. This method uses special computational tools based on objects from combinatorics or on principles standing in physics. Especially the idea of construction computational algorithms was presented. Special computational tools and regularization procedures were described in detail. Also it was pointed that the Simulation Method may be applied to solve inverse problems for reduced measurement data as well as optimization problems with the use of the power functional.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

THE SOLUTION OF IMPLICIT DIFFERENTIAL EQUATIONS VIA A LOBATTO IIIC RUNGE-KUTTA METHOD

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Introduction. This paper considers the numerical solution of the implicit differential equations (IDEs) $\Phi(y,\dot{y},t) = 0$, where the scalar t is the time, $y(t) \in \mathscr{R}^n$ is the state, $\dot{y}(t) \in \mathscr{R}^n$ is the state derivative, and $\Phi(y,\dot{y},t) \in \mathscr{R}^n$. It is assumed that the initial conditions $y(t_0)$, $\dot{y}(t_0)$ at time $t = t_0$ are consistent, i.e., $\Phi(y(t_0), \dot{y}(t_0), t_0) = 0$.

In this paper we design an implement a composite implicit Runge-Kutta method described by the Butcher tableau

$$\begin{array}{c|c} \bar{c} & \bar{A} \\ \hline & \bar{b}^T \\ & \hat{b}^T \end{array}, \quad \bar{A} = \frac{1}{2}\begin{bmatrix} A & 0 \\ eb^T & A \end{bmatrix}, \quad \bar{b} = \frac{1}{2}\begin{bmatrix} b \\ b \end{bmatrix}, \quad \bar{c} = \frac{1}{2}\begin{bmatrix} c \\ c+e \end{bmatrix},$$

where $e = [1,1,\cdots,1]^T \in \mathscr{R}^s$. A, b, and c are the coefficients of the $s = 3$-stage Lobatto IIIC method. The coefficients $\hat{b}$ are determined using an approach similar to the ideas of [1]. Here we find a $\hat{b}$ that yields a third order L-stable error estimator.

A MATLAB implementation of the algorithm (`l3cide` [2]) is used to solve some benchmark test problems that involve index-3 differential-algebraic equations written in stabilized index-1 form. We compare the performance our implementation with the MATLAB program `ode15i`, as well as the MATLAB program `ride`, which solves implicit differential equations using the three stage Radau IIA method [3].

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THEORETICAL ISSUES FOR CAD SUPPORT OF FOOTWEAR MANUFACTURING

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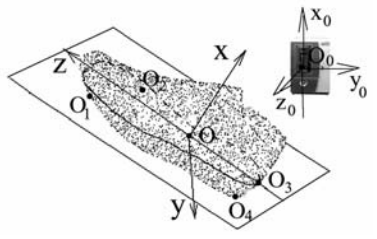
To a great extent, the design of shoes and their comfort are determined by the shape of the last. We propose a mathematical model of a shoe-last consisting of the base part and the forepart. The forepart exercising the functions of design and depending on fashion tendencies is determined by a set of parameters and is designed in a reference coordinate system with due regard for the client's requirements. The base part of the last is designed on the basis of large-scale measuring of feet, averaging, dynamical correction of the averaged foot shape, the properties of the set of materials, the product storage and operation conditions [1]; it is standardized until the next period of large-scale measuring of the population's feet and determining a new averaged foot in each territorial sex-age group. The reference coordinate system (the RCS) is a constant value for a specific type of last because it is based on anthropometric constants on the surface of a foot.

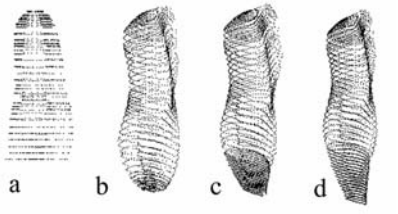
The purpose of the RCS introduction is to create an algorithm of constructing a mathematical model of a last in a coordinate system not connected with a specific device. For that purpose, the authors propose to use four points whose position is stable for any last – the heel curve point O_3, the mass centre of the whole last O (the RCS centre) and specific points O_1 and O_2 on the footprint edge (see Figure).

If we draw a straight line through points O and O_3, we obtain an unambiguous and invariable axis for constructing a coordinate system in the last. Two other axes are located in the plane being perpendicular to this straight line. Points O_1 and O_2 located in the same plane but at a definite distance from point O_4 on the edge curve are used for aligning these axes.

The style of a last is defined by the shape of its forepart as far as the footprint outline and longitudinal profile are concerned. The authors propose to divide the surface of the last in two parts: the basic zone characterized by its stability (0D – 0.9D) and the forepart (starting with 0.9D) subject to the influence of fashion. This method allows vary the length and shape of the last forepart without altering the shape of its carcass and does not bring about any negative consequences for the interior shape of the shoes. As the authors analyzed the shape of the basic parts of the lasts, they detected peculiarities the lasts form change for different sex-age groups of the population [2]. In the process of designing the last forepart, authors accept as the axial line the one passing through the aggregate of the mass centers of the toe cap sections. The forepart is fully determined by three invariant parameters (its length, twist and curvature), the section profile taper and form alteration factors.



The reference coordinate system and the specific points on the last



The basic part of the last itself (a) and with the foreparts (b, c, d) having different form change and taper parameters

The RCS is intended for the purposes of standardization, coordination and accrued sectoral data exchange. A specially convenient feature of the proposed system is the standardization of the set of the lasts' basic parts on the basis of moulds of average feet typical for various territorial sex-age groups for mass-produced shoes. The basic part of the last is not subject to the influence of fashion, unlike its forepart starting with the section 0.9D; this part is calculated by altering parameters or modified manually by a designer in a computer-aided design system separately from the basic part (see Figure).

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

TOWARDS DYNAMIC STRUCTURE HYBRID DEVS FOR SCIENTIFIC AND TECHNICAL COMPUTING ENVIRONMENTS

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Introduction. This Paper presents our current research on an extension of Discrete Event System Specification (DEVS) and corresponding modelling and simulation algorithms. Focus is put on the suitability for engineering problems and integration into software environments engineers are familiar with. Modelling and simulation of dynamic structure hybrid systems still poses a challenge for today's engineers. A dynamic structure system in this context is a modular hierarchical system whose structure changes during simulation time. Dynamic structure here does not mean switching between differential equation systems. Hierarchical models are composed of two system types, atomic and coupled models. Coupled models consist of other coupled models and/or atomic models. The dynamic behaviour of a system is reflected in atomic models, while dynamic structure is defined at the coupled system level. Dynamic structure changes are e.g. creation, deletion and exchange of models. Hybrid means that besides discrete model fractions, continuous model parts are contained, as well. There are two ways to approach those kinds of systems, resulting from the two general worldviews. One approach starts from the continuous modelling and simulation worldview and therefore extends a continuous model to a hybrid one. Discrete events are expressed as root-finding problems. The model is then simulated by a continuous simulation engine, i.e. it is processed by an ODE solver with discontinuity detection and localisation. Usually, in modular hierarchical modelling and simulation environments, the model structure is flattened before execution. Hence, hierarchical structure information is partly not available during simulation time and dynamic structure behaviour needs to be elaborately modelled at atomic system level. It seems to be more promising to gain access to the problem through the second worldview, the discrete event worldview. Among descriptions for discrete event system models and their simulators, we have chosen and enhanced the DEVS approach. An overview of the formalisms that underpin and extend DEVS theory is given by Zeigler et al. in [3]. One of several extensions of the basic DEVS formalism is the hybrid DEVS formalism introduced by Praehofer [2].

Dynamic Structure Hybrid DEVS. In hybrid DEVS formalisms and associated simulator concepts the continuous part of the model causes events to occur in the DEVS part. The model is simulated by a modified discrete event simulation engine which calls an ordinary differential equation (ODE) solver during simulation cycles. Structure information of the hybrid modular hierarchical model remains available during simulation time. Thus, the design and simulation of dynamic structure hybrid models becomes imaginable. Computation algorithms for modular hierarchical DEVS models involving dynamic structure and hybrid system extensions were established in [3, 2, 1]. The key idea is to map a model specification to interacting program objects to reflect the system components and their coupling relations. Problems arise for the effective calculation of continuous model parts if they are distributed over different program objects. Current approaches work with the Euler method and do not support the use of other ODE solvers. However, engineers ask for advanced ODE solvers with implicit integration methods, predictor/corrector integration methods and automatic step width control to solve e.g. stiff systems. Our paper introduces the Dynamic Structure hybrid DEVS (DSDEVS-hybrid) formalism. DSDEVS-hybrid comprises new data structures and methods which automatically generate the description of the continuous model equations and continuous state vectors of all components in a closed form. This closed description is prerequisite for the efficient use of advanced ODE solver methods. Currently only ordinary differential equations are supported; the algorithms do not work for differential algebraic equation (DAE) solvers. Unlike other modelling methodologies for discrete event systems such as Petri nets or state charts, DEVS formalisms have not been widely accepted by engineers, although they are to be seen as powerful tools to solve engineering problems. To help eliminating this lack of acceptance we propose the employment of programmable scientific and technical computing environments (SCEs). SCEs provide a large number of predefined advanced ODE solvers which can be involved to compute the continuous parts of hybrid models. Moreover, a SCE provides an adequate prototyping environment for the evolution of the DEVS approach itself.

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Student Poster Abstracts

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A CELLULAR AUTOMATA MODEL OF A SOCCER GAME IN JAVA

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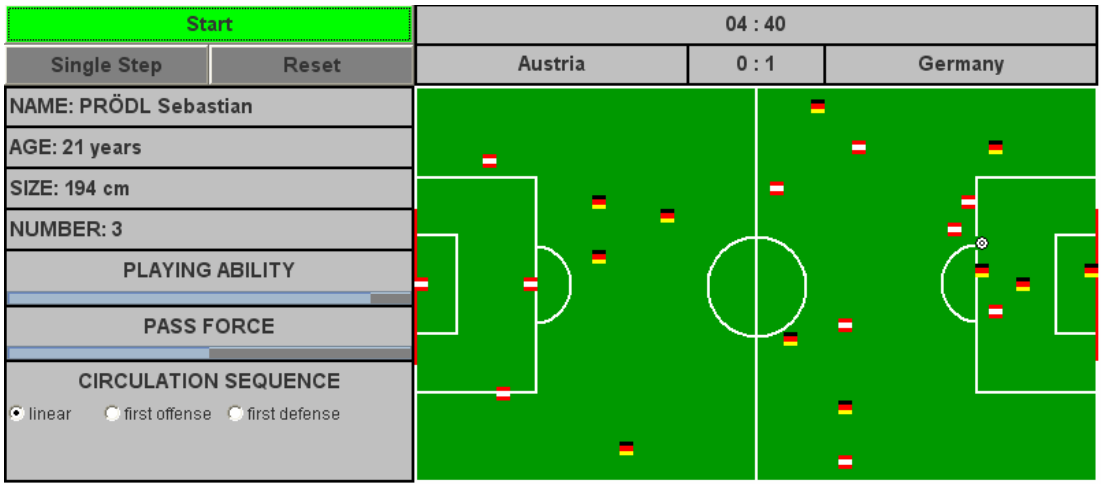
Introduction. "The Goal" of this work is to define a *Cellular Automata Model* of a simple *Soccer game*. There are - not surprisingly - 22 players, including two Goalkeepers, one ball and two goals. Rules as foul play or offside will be ignored. Out balls are avoided by introduce a 'board' where the ball is rebounded. The model was introduced to test the modelling of different strategies of team line up and was influenced by holding the 2008 UEFA European Football Championship in Austria and Switzerland. The model is realized as a JAVA Applet.

The Model. The Cellular Automata consists of 50x29 Cells. As neighbourhood the Moore neighbourhood (8-neighboring Cells) was chosen. In order to limit the movement of the player the playing field was divided in three parts and each player was allocated by one part. Computing the cells every "non-empty" cell will be classified. Either it is occupied with a player of one of the teams or with the ball. The analysis includes affiliation, possession of ball, defending or offending team player, goal keeper or field player. For every different type different rules for the Cellular Automata are implemented. The characteristics of each player (age, name, weight...) as well as the "Game Strength" (dribbling) and "Strength of pass" (length of passes) are stored in a text files. For example a Player can decide wether he shoots or passes depending on distance to goal and other informations. To implement realistic correlations the ball is computed twice within a players circle. Different special situations like duels are computed in case of appearance.

Advantages/Disadvantages of the system. Changes in the model are very simple to implement by changing the transitional function, in our case by adding or omit individual rules. For this reason different strategies can be tested and compared. So the virtual manager can compare the advantages or disadvantages of 4-4-2 versus 3-4-3 with his – limited – pool of players. So it can be shown, that some strategies only work with players like Ronaldo and not with Prödl and so the strategies can be adjusted to the pool of players As a common problem in using Cellular Automata the 'simultaneous application of the cells' is scarcely feasible in practice of a Game of Soccer. The state of the cells is also depending on the processing sequence of the cells.

The User Interface. The picture above shows the Model which is implemented in a Java applet. The Screenshot shows the model during the situation of a pass between German Forwarders.



Austria loosing vs. Germany

Information about the players shown on the left side, can be achieved by clicking on the player. The only user changes in the computing of the model can be done in the succession of computing of the different cells. "*linear*" means the succession from top left to bottom right in a "classical" way, "*first offense*" means that the field will be run through twice - first only the offending team will be processed, the defending team afterwards. "*first defense*" is analogue in reversed order.

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[2] Golder W., *Beziehungskiste aka Party-Planer*, http://www.golder.de/psion/bkiste/main.htm

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

A MATLAB/SIMULINK ENVIRONMENT FOR BLENDED LEARNING IN A TELECOMMUNICATION COURSE

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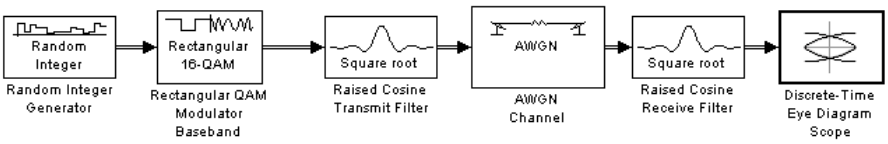
Introduction. In the academic studies of Electrical Engineering at the Technical Universitiy of Vienna an introducing course for telecommunication is scheduled. After receiving the bachelor's degree, the students choose one of five Master Studies (Automatisation, Computer-Technique, Microelectronics, Power-Engineering and Telecommunications).
The telecommunication course gives a complete survey of telecommunications and is addressed to all students of Electrical Engineering. As the course gives an overview, it also specializes in several specific issues (i.e. transmission, coding, detection, etc.). Simulations should supplement the theoretical lecture as well as the exercises. Therefore Matlab and Simulink is used. Especially Simulink is proper to display single technical methods, because of the block-oriented structure, and Matlab for the analysis and presentation of diagrams.

Content. A great number of methods in telecommunications can be shown in diagrams. However each printed diagram is static. Indeed many single diagrams can be produced, but only with an increased effort and a worse clearness. In this process computer based learning is helpful as a new generation of a diagram is done by a click on a button.
Furthermore it can be the case that different functionalities in different diagrams, which are linked, have to be shown. A change in one diagram has an unavoidable effect on the other diagram. This connection between these is also better shown with a computer based system.

An example for this is the raised-cosine filter. It has both, characteristics which are observed in the frequency domain and characteristics which are observed in the time domain. The quality of the raised-cosine filter depends on an important parameter, the so called roll-off factor.
A modification of the roll-off factor leads to a changing in both diagrams, in time as well as in frequency. This dependency is well shown via a graphical user interface (GUI) in Matlab. A controller can be implemented in the GUI and by shifting the controller the value is changed and the effects are immediately shown in the diagrams.
In communication systems, especially the filter and many other components are very important. In a big system the roll of all components can be easily shown by Simulink. In Simulink the function, which was first observed in Matlab, is represented by a block and displayed in an interaction between all components (see figure).



Simulink model: transmission through a additive white Gaussian noise (AWGN) channel with raised-cosine filter

Summary. For test purposes a kind of blended learning (see [1]) was used in one lesson of the telecommunication course. The aim was to visualize the interactions of different topics in this course. In a course evaluation which is done after each term, the use of blended learning was well accepted and positively remarked by students. This acceptance on the part of students shows that the use of a blended learning system increases the outcome of teaching.

[1] John G. Proakis, Masoud Salehi, Gerhard Bauch, *Contemporary Communication Systems using Matlab and Simulink*. Thomson Press, 2003.
[2] Josef Hoffmann, *MATLAB und SIMULINK in Signalverarbeitung und Kommunikationstechnik*. Addison-Wesley, 1999.

BLACK-BOX IDENTIFICATION OF WHEEL FORCES OF A RAILWAY VEHICLE USING ASYNCHRONOUSLY SAMPLED DATA

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Introduction. Data-based techniques are widely used for identification purposes of dynamic systems [1]. In case of a limited number of measurement channels, signals are divided into multiple measurement systems, which are utilized for data recording. As identification algorithms require synchronously and uniformly sampled data in terms of independently measured input and output data, a synchronization process becomes necessary.

The aim of this investigation was to identify a dynamic model, which describes the relation between track geometry and vertical wheel forces of a railway car. Track geometry and wheel forces have been recorded of different railway cars by independent measurement setups.

In addition to the well established cross-correlation method a linear model-based iterative algorithm was used to enhance synchronization of data sets as well as model quality [2, 3]. Subsequently, artificial neural networks (NARX) were trained to improve prediction quality and synchronization of the data sets.

Synchronization and Identification. Data sets are recorded in spatial domain according to the wheel circumference. Thus, approximation of rolling radii by the nominal value and the non-linear shaped running tread leads to non-uniformly and asynchronously sampled input and output data. Since both data sets are distorted, the geometric track signals, gauge and cant, are assumed to be free of any distortions and jitter due to the measurement principle. The corresponding output signal, which is shifted to the input by a relative shift function, is the difference of vertical wheel-forces.

The relative shift function can be split up into a constant, a linear and a zero-mean non-linear term. The constant shift is caused by independent starting points of the measurement setups or dead-time. Cross-Correlation methods cannot distinguish between these cases. Additionally, a left shift (acausal) in consequence of the measuring setup can be detected. The linear shift component leads on average to a relative shift of the wavelengths of the output and input data respectively. Thus, a biased model would be identified. In order to avoid large errors of the identified model poles, the linear relative shift between input and output primerily has to be removed by cross-correlation.

The model-based iterative algorithm is performed in two steps. First, a model, which is capable of reproducing the input-output dynamics on average (prediction error method) is identified. Next, a windowed cross-correlation function between output and simulated output is calculated and the detected shift is corrected by resampling the output data by applying cubic-splines.

Results and Conclusion. The model-based iterative algorithm enhances the synchronizity of the data sets compared to the cross-correlation method as a result of strongly pronounced extrema in the cross-correlation function caused by the high frequency content in the simulated and measured output.

A high-order output error model was identified, which leads to high prediction quality in the low and middle frequency range. The model predicated on the presented algorithm outperfoms other models, which are identified by application only cross-correlation techniques in the prediction quality by cross-validation. Artificial Neural Networks show no enhancement regarding prediction accuracy compared to linear models.

[1] L. Ljung. *System Identification - Theory for the User 2nd Edition*. Prentice Hall PTR, 1999.
[2] M. Kozek. Input-output sychronization with non-uniformly and asynchronously sampled output data. In *Proc. IEEE Conference on Decision and Control*, volume 4, pages 3926–3931, December 1999.
[3] M. Tiefenbacher. Identifikation der Radkräfte eines Eisenbahnwagons bei asynchron gesampelten Messdaten. Master's thesis, TU Wien, December 2007.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

DATABASE EVALUATION FOR LECTURE ROOM PLANNING AT VIENNA UNIVERSITY OF TECHNOLOGY

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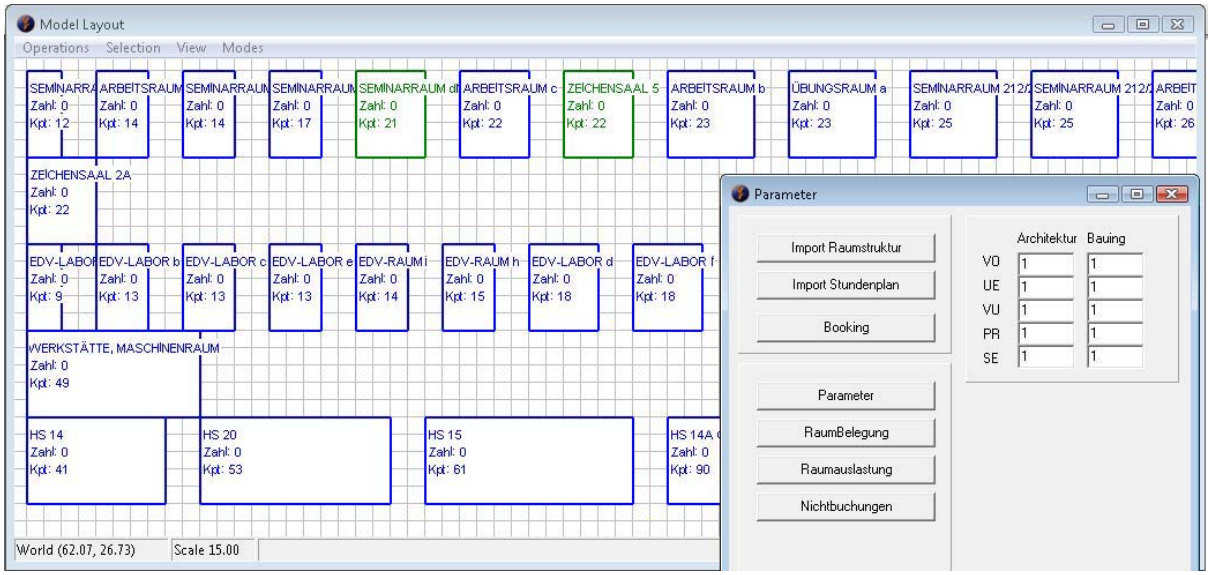
The Problem. Generating a model of a simple system using specialized libraries and a simulator with drag-and-drop environment is not too hard of a task. This process of course becomes more and more challenging as the systems grows in size and complexity. Besides encountering the common obstacle of lacking predefined objects as they get more specific, large-scale problems with a changing structure will make it excessively trying to adjust the model to such an ever differing structure. Which is the case in the present problem — creating a model for the allocation of lecture rooms at the Vienna University of Technology (TU Vienna) during its reconstruction period.

This work is based on the project <more-space> in which a tool is being developed to conquer the sketched challenge. As the reconstruction and relocation of departments are taking place parallel to daily business the task is not a simple one. This becomes further evident when looking at the university's dimensions with more than 3.000 employees and over 20.000 students.

Approach to Solution. A possible solution to cope with such a task lies within database-driven automated model generation. For this approach two requirements are fundamental. First one needs to be able to translate the stored information from a database into a functional model. The second requirement lies within the provided data and is twofold itself. On one hand the data needs to be treated and prepared in order to be automatically processable and on the other hand data needs to be gathered at all — one of the principle problems of real-life modeling.



Screenshot of room structure and GUI for data-import

The Data. The research group *"Mathematical Modelling and Simulation"* developed a module for automated model generation, thus in this work we shall focus on the data aspect explained above. As the model is being generated in Enterprise Dynamics data could be accessed and stored in various different formats. Because of good pre- and post-processing options Microsoft Excel was chosen as primary "database" with the option of later migration to MS Access.

As the model will be used to simulate various scenarios for the lecture room planning at TU Vienna different data-sets need to be prepared an made available. Most of the required data was available over the universities internal information system (TUWIS++). Since this data has not been complete it had to be completed we will also focus on this procedure.

Results. Finally we will compare the input- and output-data (results) of the simulations. Some of the relevant findings will be presented. For example the influence of a modified room structure on the number of failed booking attempts. A recommendation regarding this finding is the utilization of flexible rooms (e.g. partition walls to separate and connect lecture rooms into smaller or bigger units, respectively).

DEVELOPING OF MAPLE T.A. EXAMPLES FOR LECTURE EXERCISES

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Introduction. For students of Electrical Engineering it is an absolute necessity to master the basic techniques of higher mathematics. After the successful integration of the Maple T.A. system in the refresher courses it seemed to be obvious to use the system for further mathematical courses too. Especially for the exercises accompanying the lectures the system would be an interesting alternative to the common way of teaching.

Maple T.A. (abbr. for Testing and Assessment) is a web-based system for creating tests and assignments. The system combines the benefits of the widespread mathematical software Maple and an online platform that is accessible from all over the world. The Maple engine does the computation and the web-interface assumes the presentation.

Content. The aim was the creation of several examples for each topic of the introductive mathematical courses. To avoid the chance of transcription one of the key features of the Maple T.A. system was used. It is possible to set parameters for each question, and initialize them with random values. So every student gets exercises with varying parameters and therefore varying solutions. For the author in most cases it is not necessary to know the solution for each question. The computation is the task of the Maple engine. In some exercises it is essential to generate plots. Whether a 2D-plot or a 3D-plot is needed Maple T.A. can do this in the usual Maple manner.

With the Maple T.A. Question Bank Editor authors are able to create questions of several types. This allows the author to choose the appropriate type of questions for each exercise. For example if the author wants to create an exercise for curve sketching, he can take advantage of these possibilities provided by the system.

First of all he creates a randomized function within given borders, then plot several functions and let the students pick the right plot out of the given answers (Multiple Choice). After that he may ask for the derivatives of this function. The student has to type the correct mathematical formulas in a text field. These examples of the usage can be extended forever more.

Maple T.A. also provides from "fill in the blanks"-questions, true/false-questions, questions with numeric answers to complete essays, that unfortunately can not be assessed automatically and request a further review by a proctor of the assignment. Actually nearly every imaginable type of question can be implemented, with more or less effort.

Results. The Maple T.A. system is a very useful tool to simplify the process of assignments and to improve skills in basic mathematical exercises. A student is able to practice his calculation skills on his own and gets immediate corrections for his performances. For the lecturer and the assistants it is a comfortable and effective way to determine the level of the skills of the students. The questions are created automatically and assessed immediately.

Nevertheless the usability of the platform is still improvable. Sometimes it is rather difficult to generate questions with a higher grade of complexity without losing the overview.

From the student's point of view you have to get familiar with the Maple syntax. A complex mathematical formula can get confusing really fast within a single text field. Maybe the whole answer to a question is wrong, because of a simple typing error.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

DEVELOPMENT OF EXAMPLES FOR BLENDED LEARNING WITH SIMULINK

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Introduction. Visualisation is an important part in a modern academic teaching and learning process. It helps the students to get a deeper understanding of the matter. Unlike static visualisations, dynamic generated graphics can show dependences on various parameters. This interactive type of learning enables the students to get a feeling for the meaning behind the numbers directly. Matlab Simulink is a widely spread simulation environment and so a good choice for implementing such examples into a learning platform. In the following we will discuss the implementation of concrete examples which were realized.

Content. Matlab Simulink is a tool for modelling and simulating dynamic systems. It consists of a library of functional blocks, which can be combined to a complex system. Furthermore every Matlab program can be used in the Simulink environment. That's why it is possible to use it for wide area of applications such as mechanics, electro-techniques or biomedicine. Because of the designing concept as a graphical user interface, building a Simulink model is possible nearly for everyone, even without advanced programming skills.

In the following we will show the implementation process with a concrete example. The example deals with an electrical class-E power amplifier. For the beginning we need to derive differential equations from the given schematic diagram with help of the Kirchhoff voltage and current laws. Then these differential equations have to be converted into a Simulink model. The next task is to compute the eigenvalues of the system in the on- and off-state respectively. This can be done by a build-in Matlab function. Here the students can experience how a change to the component values affects the behaviour of the eigenvalues. Then the system is simulated over a particular time interval and time curves of the state variables are plotted. In this visualisation students can learn how the initial state affects the characteristics of the solution.

This existing model can be exported as a .m file. Due to the fact that it is possible to run Matlab on a web server we have the possibility to make the example accessible for everyone who is connected to the server.

Summary. We see, with the help of Matlab Simulink, it is quite simple to illustrate complicated correlations and make them identifiable for students. Thanks to the wide spread applicability of Simulink it is possible to use this system in nearly every technical field of studies.

[1] N.O. Sokal, A.D. Sokal: *Models, Methods, Experiments – Modern aspects of simulation languages*. In: Proc. 2nd European Simulation Conference, Antwerpen, 1986, SCS, San Diego, 1986, 195–199.

DYNAMIC NEURONAL NETWORK MODEL SIMULATION IN TIME OPTIMAL SERVOMECHANISM CONTROL

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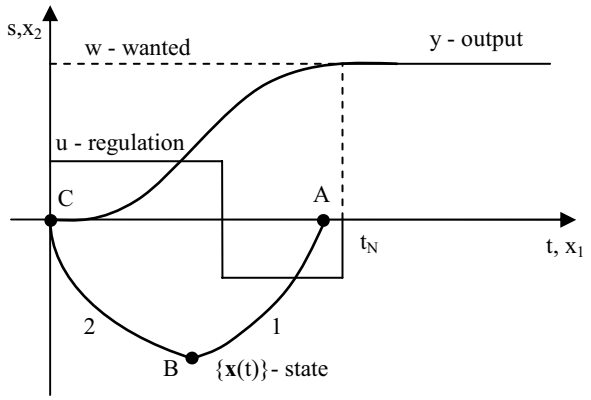
Introduction. The main task of time optimal control is to get controlled object from its initial state $\boldsymbol{x}(t_0)$ to another terminal state $\boldsymbol{x}(t_N)$ – wanted – in the shortest time. Its behaviour in state plane can be described with trajectories 1 and 2 on the picture. The problem is to find the switching point B. There are several possibilities to do that used by my predecessors, e.g. classical sliding mode approach; you can combine it with neuronal networks to get the model of this system [1] or with state estimator to compute utilizable switching curve [2]. But main weakness of these methods is that they need at least one run to learn and set up the control. My task is to provide time optimal control using neuronal networks even in the first run of the control process by use of today's easily available multi-core computers. This technology enhances neuronal networks control method with its performance and parallelism.



T-optimal control with control trajectory in state space.

Algorithm. As you can see on the picture while servomechanism speeds up we are traversing through the state space along the trajectory 1 from point A – initial state – to point B – switching point. In this part we're using data measured from the servomechanism as training data for inverse neural network model. It's obvious that we have to get to the point C so our neuronal network model should start its work in this point and simulate traversing the state space in reverse direction – to the point B. At the same time as we are moving along the trajectory 2 we need to simulate switching in various points of generated switching curve (trajectory 2) to find a point on the x_1 axis which would correspond with the initial state (point A). We have only short time to make this whole process until controlled process doesn't reach this point on its own. For example if the regulated process under the certain conditions will in worst case last 5 seconds, we have to switch the polarity in e.g. 3,2nd second to get required result, so we have maximally 3,2 seconds to do all the calculations to get the switching point. Therefore it's important to make the best account of available resources provided by the computer. When we find switching point value soon enough, our task is fulfilled. Now we have only to wait until real servomechanism traverses its representative point along the trajectory 1 to point B and just in that time to switch maximum input voltage to opposite polarity. This will lead to deceleration represented by moving along the trajectory 2. As the wanted position will be reached it is needed to disconnect this input voltage to prevent another movement of the servomechanism.

Acknowledgement. This contribution is prepared under the project VEGA 1/0808/08 "Self Tuning and Learning Algorithms for Automatic Control".

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[2] Kráľ M.: *Aplikácia učiaceho sa algoritmu pri suboptimálnom riadení servomechanizmu.* Graduation thesis, University of Žilina, Žilina, 2008.

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

ELECTRONICAL MACHINES – AN APPLICATION FOR MODEL ORDER REDUCTION

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Introduction The division "Industry – Drive Technologies – Large Drives" (I DT LD) of the Siemens AG is one of the world leading manufacturers and developers of large-scale drives. The segment "Special Machines" develops and optimizes machines according to the demands of their costumers. A major part of this work is the modeling and simulation of such machines with complex finite element analysis. For these 2nd order systems more then 10^5 variables and several weeks for time-transient calculations are not unusual. Besides the high number of variables the systems are often partially non-linear, leading to additional computational efforts.

Currently, within Siemens no model order reduction methods are used, because to best of our knowledge no application software is available, that considers the specifics of rotor dynamic systems. This illustrates the need of adapted model order reduction algorithms. The aim of the presented work is to investigate the mathematical structure of the finite element models of large drives. First of all the calculation of the natural frequencies is shown followed by a view to the gyroscopic moment.

Natural frequencies of a rotor The first step at the dimensioning of a motor is the modeling of the rotor and the calculation of the bending and torsion vibrations. The system is described by the following equation:

$$\begin{aligned} M\ddot{x} + D\dot{x} + Sx &= Bu \\ y &= Cx. \end{aligned} \tag{1}$$

In this connection M is the inertia matrix, D describes the damping of the system, S is the stiffness matrix, B the input matrix and C the measurement matrix. The vector x describes the state of the system, which means in this case the oscillation and rotation at the nodes. The input vector is u and y the output vector. Possible inputs can be unbalances, external forces or moments of a torque.

For a rotor system the matrixes M, D, S are describable in a band structure [1] because only the elements in the neighborhood are influencing each other. Therefore these calculations are less time consuming.

Gyroscopic moment For a more realistic description of the system one has to consider the gyroscopic moment, which describes the force against a tilt of the rotation axis. Even though the tilt angle caused by the bending of the rotor is very small, the gyroscopic moment cannot be neglected because of the high mass and rotation speed of the rotor. With the gyroscopic matrix G the equation (1) changes to:

$$\begin{aligned} M\ddot{x} + D\dot{x} + G\dot{x} + Sx &= Bu \\ y &= Cx. \end{aligned} \tag{2}$$

The gyroscopic matrix G leads to a coupling of the oscillation with the bending of the nodes. In the mathematic model this results in a non-band structure. For such systems the numerical calculations take much more time. As mentioned above the gyroscopic moment depends on the rotation speed Ω in such a way, that the equation (2) can also be written as [1]:

$$\begin{aligned} M\ddot{x} + \left(D + \Omega\overline{G}\right)\dot{x} + Sx &= Bu \quad ,\Omega\overline{G} = G \\ y &= Cx. \end{aligned} \tag{3}$$

This means for the dimensioning of a motor the whole system has to be calculated for different rotation speeds. From the rotor model one can deduce the model to calculate the whole machine.

Complete electromechanical system Due to the rising requirements it becomes more and more important to simulate and calculate the whole machine, including the case and the bed plate, for certain operating scenarios. For instance, if the nominal rotation speed of a motor is higher than the first natural bending frequency, it is necessary to simulate the run up. These simulations provide an insight into the behavior during the run through of the critical rotation speed region around the natural bending frequency. This is very important, because in every rotor there are small unbalances and therefore running through the natural frequencies may cause a critical vibration.

According to the customer requirements and the construction of the drive it is also possible that the differential equations become non-linear. One example for such non-linearitys are ship engines where sudden strokes to the case have to be simulated. Another example are friction clutches where the physical behavior of the so called Stick-Slip-Effect produces strong non-linearity. Obviously it is necessary to establish model order reduction to these systems.

[1] R. Gasch, R. Normann, H. Pfützner. *Rotordynamik.* Springer, Berlin, 2006.

IS A ONE-DIMENSIONAL SIMULATOR SUFFICIENT TO EVALUATE ALGORITHMS FOR SWARM ROBOTICS

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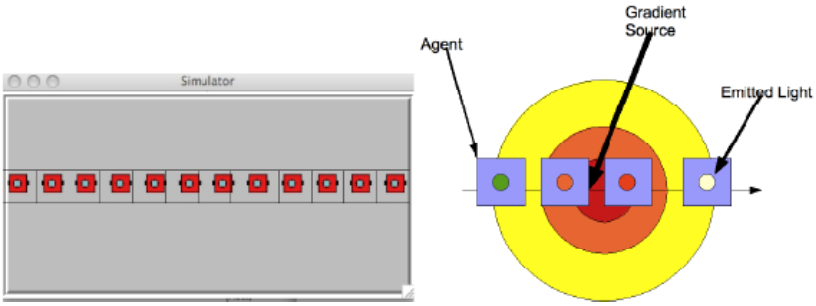
Introduction The task is to develop a test-scenarion for multilayer neural networks which should be able to control a swarm robot. Therefore the network must be able to detect and recognize environmental signals and memorize the activation of past patterns. The memorizing capabilities are implemented with context layers, which are used additionally to normal layers. A part of the task includes the evaluation and implementation of some interesting neurobiological features and their influence on the processing abilities of the network.

Definition of the Standard Problem The standard problem used for evaluation of the processing capabilities of a network is simple one dimensional world including an environmental pattern (e.g. a light gradient). A group of agents (robots) aligned along a line(See fig. 1). The robots are only able to move along this line. Additionally they are equipped with a LED that allows them to emit light with changeable wave lengths and therefore different colors.The problem that must be solved by the robots is to build a line in which every robot emits a color. No color should be reused, and therefore every robot must emit light in a different color. The robots are also equipped with a sensor which is able to detect measurands which are emitting radiations (e.g. heat). The robots are using the intensity of the radiation to decide what color should be emitted. Therefore the robots are able to coordinate their light signals without direct communication.

The Networ To demonstrate our standard problem we implemented a feedforward neural network. It has an input layer, one to n hidden layers and context layers and one output layer. The context layers are able to persist past activation results and feed them to the current activation process of the neural network.The addition of context layers enabled the network to flashback in time and therefore to learn time-based functions and also to recognize steps in the future. In our paper we will show the detailed function and the advantages of our presented standard problem.



Screenshot Sceem of implementation of agent in our one-dimmensional environment

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MATHEMATICAL METHODS IN D NAMIC PROJECT MANAGEMENT WITH ECONOMIC RIS S TA EN INTO ACCO NT

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The purpose of the research is creation of methodological principles and imitating-mathematical toolkit of adaptive risk management. The toolkit is necessary for estimation of risk indicators and project key parameters (the investment sums - taking into account possibilities of the investor and real terms of financing, the size of an insurance covering in case of failure) in conditions when the most developed methods including – quantitative are based on heuristics and do not consider realities of the transients arising during realization of the project. Such estimations should be carried out at a preliminary stage – during a choice of a variant of the project, and during its realization – in a project management mode.

As a result of the research the following problems are solved:

- realization of the preliminary analysis of variants on a basis of a stage-by-stage procedures of a “decision tree”;
- realization of the trends research of fiscal effects receive during capital investment project realization;
- receive of a management efficiency criterion of investment process and stability indicator of this process for acceptance of corresponding decisions;
- creation of economic-mathematical toolkit of a choice iterative estimation of the investment project, definition of the investment sum and parameters of selective risk.

The object of the research is project (investment) activity in various economy branches, carried out in the conditions of uncertainty and risks. The subject of the researches is adaptive risk management of capital investment projects. Risk management of the projects, which realization is stretched for significant terms, should have property of adaptation. It is necessary to bring the specified concept of stability considering dynamism of management, and not just interests of participants of the project as it is done at the financial analysis of the project.

The research is based on applied directions of the system analysis, the theory of risks, the theory of adaptive management of complex systems, methods of processes simulation modeling connected with material and financial streams in economy objects, information technologies and a cross section analysis of information systems.

During research the scientific problem of methodological bases receive and imitating-mathematical toolkit of projects adaptive management with allowance for investors’ risks and financing dynamics, intended for the estimation of parameters of capital investment project (the invested sums and a possible insurance cover), the sums and risk indicators has been raised and solved.

The method of a preliminary choice of an investment object by means of a decision tree is offered. As a criterion during the choice of strategy of actions of the investor company the concept «advantage of a concrete condition of the economic environment» is used.

The analysis of realization process of a capital investment project by means of logistical curves is carried out. The corresponding expressions describing trends of investment transient are members of some temporal row. The basic trends are revealed and the possible reasons of occurrence of additional trends are shown.

The analytical expression, allowing to estimate stability of investment process with Mihaylov criterion application is received. It is proved that irrespective of money sums transfer tactics by the investor and from additional trends occurrence this expression does not change (numerical factors change only).

The exponent of the investor risk, having monotonous connection with probability of risk event is offered. It is possible to develop iterative procedure of parameters estimation of a capital investment project, taking into account this monotonous interdependence. By means of such procedure in "a game" interactive mode it is possible to determine volumes of the investment, the expected monetary estimation, expected value of exact information and tactics of money transfers.

Mathematical modelling of economic processes

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Economic processes in a society flow past in the conditions of a complicated interlacing of the diversified factors - social and economic, biological, geographical, etc. Therefore research of economic processes demands handling of great volumes of the information. Complexity of research of economic system is that if not to use special mathematical methods it is impossible to assume in advance as this system will lead itself as a result of exterior action. And it in turn demands enough good mathematical preparation of the contributor.

The modelling singularity in economy is that in an economic science is not enough possibilities for application of controllable experiments. For research of influence of many factors and detection of distinctions in economic processes the science is necessary on statistical and economic-mathematical methods of the analysis. The study of these rationes leads to the major in the mathematics to concept of connection or rationes between variables.

It is necessary to distinguish causal and functional connections. Causal relationship in economic processes is such connection which assumes detection of one or several reasons leading to some consequence. Functional connection expresses association of one magnitudes on others in the course of their modification and concerns purely to external relations and serves only as the form of display of a causal connetions. Therefore always it is necessary to fill study of functional connection not from mathematical operations, but from penetration into essence of an appearance, from an establishment of its causal relationships. Especially it is important, when for research of economic processes use mathematical modelling.

The mathematical model represents the equation or a set of equations describing correlations, happening in a pre-image. Creation of models of real processes considerably facilitates carrying out of the economic analysis and economical calculations, and also allows to study economy in real conditions in which it is very difficult, and is frequent and it is absolutely impossible to realise economic researches by traditional methods. At mathematical modelling always it is necessary to start with a being of economic rationes, from the qualitative analysis of economic relations, instead of to postulate at first model, and then to give them economic explanation.

In economy economic-statistical and economic-mathematical models are widely applied. The economic-statistical model represents the correlative equation of connection dependent and the several independent factors defining quantitative value of the dependent factor. In economic-mathematical model parametres are usually given in the form of the table of the numbers connected in uniform system of the functional equations of various type and there are two types of these models : deterministic and stochastic.

To deterministic models in which the outcome completely and is univalently defined by a gang of explanatory variables concern. Usually these models are under construction on the basis of rules of linear algebra and is represented as the set of equations, outcomes jointly solved for deriving. Stochastic models describe the casual processes submitting to laws of a probability theory. Studied process is conditionally considered as deterministic, but elements of an estimation of probabilities of deriving of outcomes are included into model. To the stochastic are refered the models based on principles of smoothing of statistical rows and they describe a variation number is integrated by means of a gang of distribution parametres characterising it or by means of graphs of normal distribution. Distinctive line of stochastic model is that the effect variable always serves average, instead of univalent performance of factors influencing it.

Mathematical modelling of economic processes and creation of economic-mathematical model consists basically of some consecutive stages: study of economic process. Changing initial conditions of a problem and criteria of optimality, it is possible to calculate some variants of a solution. Then do the economic analysis of these variants and choose the most expedient project of the optimum plan. However, the project head at a choice of a definitive variant uses criteria which it is impossible to present in the formalized aspect.

As an example we will consider simple two-parametre mathematical model of activity Bank Austria in segment report Q12007-Q12008 for Central and Easten Europe[1]: association Total revenues (Y, € m) from net-interest (x, € m). If the amount of unknowns not so is a lot of and investigated process is monotone than by means of simple criterion it is possible to choose one of nine functions (Y=a+b*x; Y=a+b*lnx; Y=a+b/x; Y=a*b^x; Y=a*x^b; Y=exp (a+b/x); Y=1 / (a+b/x); Y=1 / (a+b*lnx); Y=x / (a+b*x); a, b-const.) which optimum describes an investigated appearance. Unknown constants are calculated by means of a method of least squares. For their determination it is necessary to transform beforehand the necessary equation to a linear aspect.

As a result of the conducted researches it is received the optimum formula in the form of Y=23,221+1,502*x. Quality received regression equation can be estimated by means of factor of determination R^2=0,882. The found dependence with certain accuracy, allows to predict the most probable value of the estimated parametre Y.

[1] - http://www.bankaustria.at/informationspdfs/IR_Segment_reporting_Q1_2007_-_Q1_2008.pdf

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

MATHEMATICAL SWARM MODEL FOR NANOROBOTIC COMMUNICATION

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Summary This paper proposes a framework for mathematical modeling of swarms of micro-scopic robots that may one day be useful in medical applications. While such devices do not yet exist, the modeling approach can be helpful in identifying various design trade-offs for the robots and be a useful guide for their eventual fabrication. Specifically, we examine microscopic robots that reside in a fluid, for example, a bloodstream, and are able to detect and respond to different chemicals. We present the general mathematical model of a scenario in which robots locate a chemical source. We solve the scenario in one-dimension and show how results can be used to evaluate certain design decisions.

Introduction This mathematical approach is particularly useful for preliminary evaluation of design trade-offs for robots that cannot yet be built and will operate in poorly characterized envi-ronments. As one such application, robots with sizes comparable to bacteria (“nanorobots”) could provide many novel capabilities through their ability to sense and act in microscopic environ-ments. Of particular interest are medical applications, where robots and nanoscale-structured materials inside the body could significantly improve disease diagnosis and treatment. Our work complements other theoretical studies of microscopic robots by providing a methodology for studying collective swarm behavior.

For our modeling implementations, we use SesAm software. In this media, we consider the nano-robots as mobile agents and the tumor cell as the target that releases chemical signals according to table1. Using Ant colony algorithm, the communication signals shown as fermon and the RBCs as random mobile obstacles. Limitations of this approach are its underlying assumptions, namely that to determine relevant collective swarm behaviors the occupancy numbers are a sufficient descrip-tion of the individual robots and fluctuations are small so the averages over many independent instances of the swarm are close to the actual observed behaviors in most of those instances. More broadly, this approach connects average, aggregate behavior with local robot controllers rather than providing specific details of individual robots. For applications involving large populations of microscopic robots, the law of large numbers will ensure behaviors are usually close to average

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NUMERICAL PROPERTIES OF SOME ANALYTICAL COUPLED CONSOLIDATION MODELS

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Summary The numerical properties of the analytical solutions of some pile consolidation models (i.e. point-symmetric coupled consolidation models in the 2D and the 3D space) are analysed in the function of some prescribed initial conditions and various boundary conditions. Results depend on the "distance" of the specified solution from the zero solution in terms of the norm of the initial condition and, on the size of the displacement domain.

Motivation The one dimensional coupled linear coupled consolidation models for space dimensions 2 and 3 are used for the evaluation of the CPTU dissipation test. If the penetration is partly drained then the initial pore water pressure may decrease very rapidly with the radial distance to zero. It would be good to know whether this extreme case can acceptably be described by the analytical solutions.

Methods The numerical properties of analytical solution of the one dimensional point-symmetric linear coupled consolidation models (see the Table) are analysed in the function of n, the space dimension of the displacement domain, the initial condition and the size of the displacement domain.

1D point-symmetric consolidation models [1]

V or ε boundary condition	1D (Oedometric models)
No (uncoupled)	Terzaghi (1923) [2]
v-v (coupled 1)	Imre (1997-1999) [3]
v-ε (coupled 2)	Biot (1941) [4]

2D point-symmetric consolidation models

v or ε boundary condition	2D (Cylindrical pile models)
No (uncoupled)	Soderberg (1962) [5]
v-v (coupled 1)	Imre et al (1987), Imre & Rózsa (1998) [1], [6]
v-ε (coupled 2)	Randolph at al (1979) [7]

3D point-symmetric consolidation models

v or ε boundary condition	3D (Spherical pile models)
No (uncoupled)	Torstensson (1975) [8]
v-v (coupled 1)	Imre & Rózsa (2002) [9]
v-ε (coupled 2)	Imre & Rózsa (2005) [10]

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

SMURF - A WEB-BASED REVIEWING AND COLLABORATION TOOL FOR PUBLICATIONS IN SIMULATION NEWS EUROPE - SNE

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Introduction. The journal series of SNE - Simulation News Europe - informs about developments in modelling and simulation by technical articles, software notes and comparisons. The comparisions presented in the SNE journal series give a comprehensive overview on on current research and implementations in the application field of simulation and modelling techniques. In addition to that SNE is also the official membership journal of EUROSIM and SCS Europe simulation societies. Therefore news and reports from this two simulation societies and events from International Simulation Societies and Simulation Groups are published within the SNE journal volumes,too.

The current reviewing and collaboration process of documents and articles intended to be part of an SNE journal volume is primarily managed by email and various types of mobile data storage media, e.g. USB sticks: Authors deliver their articles to the editor in chief and certain pre-selected reviewers. The reviewers send their comments and reply usually via email to the authors and to the editors.

The System. The developed application, which bears the working title SMURF (Simply Manufactured Unseen Reviewing Facility), provides a web-based working environment, where authors can upload and update their documents and reviewers have the possibility to give feedback in a structure and predefined way. The editors in chief are able to assign reviewers to articles and select articles for SNE volumes via the collaboration platform.

Figure: Graphical User Interface showing an overview table

The application consists of four core components:
The main component is the business logic, which is implemented in Java and thus, in principle, platform-independent. The business logics task is to control the workflows and processes of the overall system. The graphical user interface has been developed with Google Web Toolkit (GWT)[1].
The application uses an JBOSS application server [2] as base component for its web features. Another component is the mail system: SMURF uses email as a supportive communication channel for general notifications and direct transmitting different kind of user-relevant information to improve the collaboration processes and level of knowledge. The task of the MySQL database component is storing data structures and relationships of articles, authors, issues and reviewers. The information saved within the database includes review data, access rights, user privileges and system settings and the system news. The documents are available via a separate storage system to ensure that the MYSQL database remains slim and efficient. A so called concurrent versioning system (CVS) holds the documents' content and has a build-in versioning functionality. The CVS can be accessed through the web applications interfaces as well as directly via SSH protocol.

Workflow and User Roles. Registered and authorized users upload their SNE contributions via the graphical user interface component. The editor in chief assigns the uploaded documents to one or more reviewers per document. If the review is done, the authors get their review feedback and status information directly on the software platform. Additional mail notifications are send, if certain events or status changes occur. Depending on the review feedback the articles have to be revised and updated by their corresponding authors. If contributions are accepted and released, the editor in chief can assign and group the articles to issues.

Summary. The aim and main requirement was to create a user-friendly and web-based reviewing and collaboration facility and production environment for SNE publications. The developed JAVA (J2EE) software outcome is a user-friendly and straightforward approach, with a strong focus on simplifying and optimizing the review, contribution and editoring workflows of SNE journal contributions.

[1] Google Web Toolkit source code and documentation: http://code.google.com/intl/de-AT/webtoolkit/
[2] JBOSS installation files and documentation: http://jboss.org/

GENERALIZATIONS OF SEMICONDUCTOR ENERGY-TRANSPORT MODELS: LATTICE TEMPERATURE EFFECTS AND HIGHER-ORDER MOMENTS

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Overview. As a result of the miniaturization in modern semiconductor devices, it is essential to study models which consider temperature effects. One well-known example is the energy-transport model which is given in the scaled drift-diffusion formulation by

$$\begin{aligned} &\partial_t g_1 - \operatorname{div}_x J_1 = -R, && J_1 = \nabla_x g_1 - \frac{g_1}{T}\nabla_x V, \\ &\partial_t g_2 - \operatorname{div}_x J_2 = -J_1\cdot\nabla_x V + W - \frac{g_2}{g_1}R, && J_2 = \nabla_x g_2 - \frac{g_2}{T}\nabla_x V, \end{aligned} \qquad \lambda^2\Delta_x V = g_1 - Dop.$$

Here g_1, g_2, J_1, and J_2 denote the electron and energy densities and their respective current densities, V is the potential and T the electron temperature. The energy term $W(g_1,T)$ models collision processes, R generation and recombination effects, Dop describes the doping profile, and λ is a scaling constant.

Lattice temperature effects. One problem encountered in the design of modern ICs is the production of heat. The *heat equation* is given by

$$\rho_L c_L \partial_t T_L - \operatorname{div}_x\left(\kappa_L \nabla_x T_L\right) = H$$

where ρ_L ist the density, κ_L the heat conductivity, and c_L the heat capacity. The heat transport depends $\propto T^3$ of lattice vibrations, while it only depends $\propto T$ of electrons. However, in nanoscale devices the electron temperature can be several thousands Kelvin. From physical principles and under certain simplifications (e. g. neglect the temperature dependence of the energy bands) the following coupling term can be derived:

$$H = -W + R\left(E_g + \tfrac{3}{2}k_B T\right).$$

For the *boundary conditions* in the drift-diffusion model second-order Robin-type BCs can be derived from the Boltzmann equation, which model non-uniform electron injection velocities. In the heat equation empirical Robin-type BCs are used. For the non-conducting parts homogeneous Neumann-BCs are used.

So far 1-d transient computations have been made, the goal are 2-d and 3-d calculations as well as the derivation of higher-order BCs for the ET model.

Higher-order moments. For the derivation of a higher-order model we start with the *Boltzmann equation*

$$\alpha^2\partial_t f_\alpha + \alpha(u\cdot\nabla_x f_\alpha + \nabla_x V\cdot\nabla_p f_\alpha) = Q(f_\alpha).$$

This is a PDE in the distribution function $f_\alpha(x,p,t)$, where $u = \nabla_p\varepsilon$ denotes the group velocity, ε the energy band, Q the collision operator, and $0 < \alpha \ll 1$ the ratio between phonon and electron energy. For the *thermal equilibrium* we search a function M_f that maximizes a certain entropy $f \mapsto H(f)$ under the constraints

$$\left\langle \kappa_i f(x,\cdot,t)\right\rangle := \int \kappa_i(p) f(x,p,t)\,\mathrm{d}p = m_i(x,t) \quad \forall x,t,i$$

for given *moments* $m_i(x,t)$ and *weight functions* $\kappa_i(p)$.

We insert the *Chapman-Enskog expansion* $f_\alpha = M_{f_\alpha} + \alpha g_\alpha$, assume $Q = Q_1 + \alpha^2 Q_2$, and obtain

$$\partial_t m_i - \operatorname{div}_x J_i = \left\langle G\nabla_p\kappa_i\right\rangle\cdot\nabla_x V + \left\langle Q_2(M_{f_\alpha})\kappa_i\right\rangle$$

after $\alpha\to 0$ with the current densities $J_i := -\langle\kappa_i G u\rangle$ and $G := \lim_{\alpha\to 0} g_\alpha$. For a special case we choose $\kappa_i = \varepsilon^i$. Then the balance equations simplify to $\partial_t m_i - \operatorname{div}_x J_i = -iJ_{i-1}\cdot\nabla_x V + W_i$ (confer the model in the overview), and the current densities can be expressed in terms of a positive definite *diffusion matrix*.

As a novelty, this approach defines a hierarchy of many models including the classical drift-diffusion and energy-transport and Grasser's higher-order model. The work in progress is to implement a finite-element-Gummel algorithm for numerical simulations and to generalize the Maxwell to the Fermi-Dirac statistics.

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

USING CONSTRAINED OPTIMAL CONTROL TO MODEL A SOCIAL-SUSTAINABLE FISHERY

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The used model for a renewable resource harvesting is known as the sole-owner-case. Let $y(t)$ be the accumulated capital (in $[0,t]$) of some fishermen, which we want to maximize within the given time interval $[0,T]$. Further let $x(t)$ be the biomass of the fish stock and $u(t)$ the fishing effort. So we get the following optimal control problem, where the harvesting effort $u(t)$ is the control:

$$\max_u y(T) \tag{1}$$

with:
$$\dot{x} = rx\left(1-\frac{x}{G}\right) - ux \qquad x(0) = x_0 \tag{2}$$

$$\dot{y} = ux - \frac{1}{2}u^2 \qquad y(0) = 0 \tag{3}$$

$$u(t) \geq 0 \qquad t \in [0,T] \tag{4}$$

The capital function $y(t)$ is composed of the income (the harvesting success $u \cdot x$) and a quadratic cost term. The biomass of the fish population $x(t)$ is expected to follow the logistic growth (determined by parameters r, G), while the harvesting success decreases the growth. In comparison to the primal model (published amongst others in Clark [1]) we neglect several parameters, which do not change the qualitative behavior of the solution.
Solving (1) - (4) for a small initial value x_0 (only few fishes at the beginning), shows that there is a certain time without fishing. As the fishermen would have no income in this period (see fig. 1), this should be avoided by introducing appropriate constraints.
One possibility is to claim, that the capital function $y(t)$ is strictly monotonic increasing, so the first derivative has to be positive ($\dot{y}(t) \geq K_1 > 0$) for all time $t \in [0,T]$:

$$\dot{y}(t) = u(t)x(t) - \frac{1}{2}u(t)^2 \geq K_1 \qquad \Longrightarrow g(x(t),u(t)) = u(t)x(t) - \frac{1}{2}u(t)^2 - K_1 \geq 0 \qquad t \in [0,T] \tag{5}$$

This approach leads to a global mixed constraint.
An alternative is to discretize the planning interval $[0,T]$ by N timepoints τ_i and to claim the capital stock $y(t)$ to increase in every interval $[\tau_i, \tau_{i+1}]$ at least with the value K_2, so we get $N-1$ isolated inequality constraints:

$$y(\tau_{i+1}) - y(\tau_i) \geq K_2 \qquad i = 1,\ldots,N-1 \qquad (\tau_i \in [0,T],\ i = 1,\ldots,N) \tag{6}$$

For the two resulting constrained optimal control problems we derived the necessary conditions (according to Hartl et al. [2]) and used an iterative method to calculate the harvesting effort in several examples. In fig. 1 a comparision of the computed capital functions $y(t)$ are shown. The unconstrained solution yields the highest end capital but in the first year the income vanishes. The globally constrained solution increases linear with K_1 as long as constraint is active and faster afterwards. In the pointwise constrained case appear again several periods without fishing but obvious shorter than in the unconstrained case.

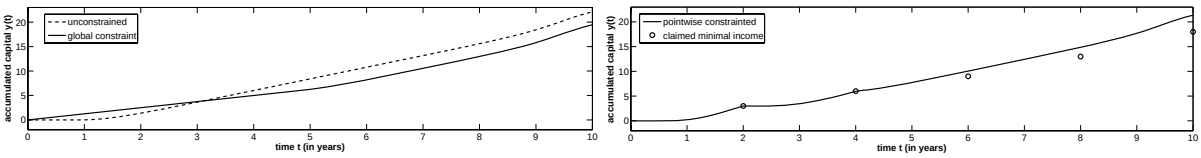

Figure 1: Comparison of the calculated capital functions $y(t)$ ($T = 10$ (years), $r = 1, G = 10, x(0) = 2$):
left figure: dashed line – without a constraint the fisherman have in $[0,1]$ no income but achieve a higher terminal capital $y(T)$; solid line – the global constraint $u(t)x(t) - \frac{1}{2}u(t)^2 \geq K_1 = 1.25$ is active for $t \in [0,5]$;
right figure: solid line – the point constraints $y(i) - y(i-1) \geq K_2 = 3$ ($i = 2,4,6,8,10$) are in the first 4 years active, whereas short periods with no income appear (the circles mark the claimed minimal income at i)

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I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6

I. Troch, F. Breitenecker, eds. ISBN 978-3-901608-34-6


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