CGPLUS

A Package Supporting the *CHARMM/GAMESSPLUS* Combination Package for Incorporating the Generalized Hybrid Orbital QM/MM Methods of *GAMESSPLUS* Into *CHARMM*

Users Manual

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Note: *CGPLUS*-v2008 is based on *CHARMM* version c30a1 and *GAMESSPLUS*-v2008 (which is based on *GAMESS* version March 24, 2007 (R6)].

CGPLUS Abstract

CGPLUS is a package supporting the *CHARMM/GAMESPLUSS* combination package for performing QM/MM calculations with the generalized hybrid orbital (GHO) boundary treatment at the *ab initio* HF level (GHO-AIHF). This package (*CGPLUS*) contains (1) utilities to prepare *GAMESSPLUS* for use with the *GAMESS* module of *CHARMM*, (2) modified *CHARMM* modules for carrying out GHO-AIHF calculations through the *CHARMM/GAMESSPLUS* interface, (3) instructions for compiling *CHARMM* with *GAMESSPLUS* as an integrated executable, and (4) a test suite for testing the GHO-AIHF QM/MM method.

Licensing

Introduction

To perform combined QM/MM calculations using the GHO boundary treatment at the HF level through the *CHARMM/GAMESSPLUS* interface, both the standard *CHARMM* and *GAMESSPLUS* require modifications to be compatible to each other. The modifications are made to enable the parsing of GHO related commands in *CHARMM*, to adjust the dimensionality in *GAMESSPLUS* for QM/MM calculations, to setup the basic master-slave module hierarchy for the combination package, and to resolve other conflicts to make the compilation of the two packages feasible. The *CGPLUS* package contains these modifications to be made and automates the modifying process for the installation of the *CHARMM/GAMESSPLUS* combination package by a script called "install_cgplus.com".

Besides the installation script "install_cgplus.com", the *CGPLUS* utility also contains seven modified *CHARMM* files, namely, blur.src, charmm_main.src, ddi.src, eintern.src, enefscal.src, gukini.src, update.src. The original *CHARMM* source files will be replaced by these modified ones by *CGPLUS* for compiling *CHARMM* and *GAMESSPLUS* into a single properly interfaced executable. In addition, sample make files for the compilation of the *CHARMM/GAMESSPLUS* combination package on IBM SP and IBM Regatta machines are provided in *CGPLUS*.

To verify the implementation of the GHO-AIHF algorithm in *GAMESSPLUS* and demonstrate the usage of the GHO-AIHF functionality through the *CHARMM/GAMESSPLUS* combination, a test suite containing 17 test runs has been included as part of the *CGPLUS* utility. Among these 17 test runs, 16 of them are designed to test the GHO functionality implemented in *CHARMM/GAMESSPLUS*. One

test run (in particular, test run 16) in *CGPLUS* is to illustrate the usage of the non-standard GHO keyword GLWD for the user-defined local Löwdin orthogonalization.

Referencing *CGPLUS*

CGPLUS is a package supporting the *CHARMM/GAMESPLUSS* combination package to incorporate the QM/MM calculations with generalized hybrid orbital (GHO) boundary treatment at the *ab initio* HF level (GHO-AIHF). This package contains (1) utilities to prepare *GAMESSPLUS* for use as a module of *CHARMM* and modified *CHARMM* routines for carrying out GHO-AIHF calculations through the *CHARMM/GAMESSPLUS* interface. A test suite containing 17 test runs for testing the GHO-AIHF QM/MM method is also included in the *CGPLUS* distribution. The recommended referencing for *CGPLUS* is as follows:

A) J. Chem. Phys. Format:

1. J. Pu, M. Higashi, J. Gao, and D. G. Truhlar, CGPLUS-version 2008, University of Minnesota, Minneapolis, 2008, CGPLUS-v2008, a package supporting the CHARMM/GAMESSPLUS combination program for incorporating the generalized hybrid orbital (GHO) QM/MM methods.
2. M. Higashi, A. C. Chamberlin, J. Pu, J. D. Thompson, J. D. Xidos, J. Li, T. Zhu, G. D. Hawkins, Y.-Y. Chuang, P. L. Fast, D. A. Liotard, D. Rinaldi, J. Gao, C. J. Cramer, and D. G. Truhlar, GAMESSPLUS–version 2008, University of Minnesota, Minneapolis, 2008, based on the General Atomic and Molecular Electronic Structure System (GAMESS) as described in M. W. Schmidt, K. K. Baldridge, J. A. Boatz, S. T. Elbert, M. S. Gordon, J. H. Jensen, S. Koseki, N. Matsunaga, K. A. Nguyen, S. J. Su, T. L. Windus, M. Dupuis, and J. A. Montgomery, J. Comput. Chem. **14**, 1347 (1993).
3. *Chemistry at HARvard Macromolecular Mechanics* (CHARMM) computer program, as described in B. R. Brooks, R. E. Bruccoleri, B. D. Olafson, D. J. States, S. Swaminathan, and M. Karplus, J. Comput. Chem. **4**, 187 (1983).

B) American Chemical Society Format:

1. Pu, J.; Higashi, M.; Gao, J.; Truhlar, D. G.; CGPLUS-version 2008, University of Minnesota, Minneapolis, 2008, CGPLUS-v2008, a package supporting the CHARMM/GAMESSPLUS combination program for incorporating the generalized hybrid orbital (GHO) QM/MM methods.
2. Higashi, M.; Chamberlin A. C.; Pu, J.; Thompson, J. D.; Xidos, J. D.; Li, J.; Zhu, T.; Hawkins, G. D.; Chuang, Y.-Y.; Fast, P. L.; Liotard, D. A.; Rinaldi, D.; Gao, J.; Cramer, C. J.; Truhlar, D. G. GAMESSPLUS–version 2008, University of Minnesota, Minneapolis, 2008, based on the General Atomic

and Molecular Electronic Structure System (GAMESS) as described in Schmidt, M. W.; Baldridge, K. K.; Boatz, J. A.; Elbert, S. T.; Gordon, M. S.; Jensen, J. H.; Koseki, S.; Matsunaga, N.; Nguyen, K. A.; Su, S. J.; Windus, T. L.; Dupuis, M.; Montgomery J. A. *J. Comp. Chem*. **1993**, *14*, 1347.

3. *Chemistry at HARvard Macromolecular Mechanics* (CHARMM) computer program, as described in Brooks, B. R.; Bruccoleri, R. E.; Olafson, B. D.; States, D. J.; Swaminathan, S.; Karplus, M. *J. Comput. Chem.* **1983**, *4*, 187.

C) Theoretical Chemistry Accounts Format:

1. Pu J, Higashi M, Gao J, Truhlar DG (2008) CGPLUS-version 2008, University of Minnesota, Minneapolis, 2008, CGPLUS-v2008, a package supporting the CHARMM/GAMESSPLUS combination program for incorporating the generalized hybrid orbital (GHO) QM/MM methods.
2. Higashi M, Chamberlin AC, Pu J, Thompson JD, Xidos JD, Li J, Zhu T, Hawkins GD, Chuang Y-Y, Fast PL, Liotard DA, Rinaldi D, Gao J, Cramer CJ, Truhlar DG (2004) GAMESSPLUS–version 2008, University of Minnesota, Minneapolis, 2008, based on the General Atomic and Molecular Electronic Structure System (GAMESS) as described in Schmidt MW, Baldridge KK, Boatz JA, Elbert ST, Gordon MS, Jensen JH, Koseki S, Matsunaga N, Nguyen KA, Su SJ, Windus TL, Dupuis M, Montgomery JA (1993) J. Comput. Chem. 14: 1347
3. Brooks, BR, Bruccoleri, RE, Olafson BD, States DJ, Swaminathan S, Karplus M (1983) J. Comput. Chem. 4: 187.

In addition, users should follow the user scientific publishing guidelines for referencing methods that are used.

The reference for GHO-AIHF is:

Pu, J.; Gao, J.; Truhlar, D. G. "Generalized Hybrid Orbital (GHO) Method for Combining *Ab Initio* Hartree-Fock Wave Functions with Molecular Mechanics", *J. Phys. Chem. A* **2004**, *108*, 632.

The original reference for the MIDI! basis set is:

Easton, R. E.; Giesen, D. J.; Welch, A.; Cramer, C. J.; Truhlar, D. G. "The MIDI! Basis Set for Quantum Mechanical Calculations of Molecular Geometries and Partial Charges" *Theor. Chim. Acta* **1996**, *93*, 281-301.

Utility for Modifying *CHARMM* and *GAMESSPLUS*

The *CGPLUS* utility will automatically (1) copy the *GAMESS* source code to the appropriate *CHARMM* directory (2) copy *GAMESSPLUS* modules to the appropriate *CHARMM* directory and replace some *GAMESS* modules by *GAMESSPLUS* modules (3) make changes to the source code of *GAMESSPLUS* so that *GAMESSPLUS* is called as a subroutine by *CHARMM* (4) make changes to some of the *CHARMM* source code to be compatible with GHO-AIHF calculations (5) prepare the make files necessary to compile the *CHARMM/GAMESSPLUS* combination package. When *CHARMM*, *GAMESS*, and *GAMESSPLUS* have been obtained, the integration of the code into a single executable as the *CHARMM/GAMESSPLUS* combination package is possible with the utility *CGPLUS*, which is available from the University of Minnesota (http://comp.chem.umn.edu/cgplus).

The *CHARMM/GAMESSPLUS* interface of *CHARMM* and *GAMESSPLUS* takes advantage of the modular nature of both programs, and, consequently, minimal modifications of *CHARMM*, *GAMESS*, and *GAMESSPLUS* were required. The *CHARMM* program is the main driver of the integrated program, which makes a FORTRAN call to the interface subprogram *GAMESSPLUS* to initiate the GHO QM/MM calculations by *GAMESSPLUS*.

Program Distribution

The *CGPLUS-v2008* program package consists of a compressed tar file called "cgplus.2008.tar.gz". The top-level directory of this file system is "cgplus-v2008"; the following is a list of the subdirectories and their contents:

cgplus-v2008	Contains the modified *CHARMM* modules, modified make files, an installation script

blur.src	charmm_main.src	ddi.src
enefscal.src	eintern.src	gamess.mk
gamint.mk	ghogms.fcm	gmscomp_ibmsp
gukini.src	install_cgplus.com	Makefile
Makefile_ibmsp	update.src	

ghohftest	Contains the test suite for testing GHO-AIHF
data/	
ghohf.topo	all topology files used in 17 test runs for GHO-AIHF
datadir.def	the file to specify data directory and scratch directory for *CHARMM*
Input/	
test*x*.inp	where $x = 1 – 17$
sto3g.str	the *GAMESSPLUS* input file for test*m*.inp ($m = 1 – 3$)
631gd.str	the *GAMESSPLUS* input file for test4.inp
midib.str	the *GAMESSPLUS* input file for test*n*.inp (n = 5, 6, 9 – 11, 13 – 17)
midib-.str	the *GAMESSPLUS* input file for test12.inp
midib-gho.bas	the file containing MIDI! basis set
uhf-midib.str	the *GAMESSPLUS* input file for test7.inp and test8.inp.
run_all.sh	a script to run the GHO-AIHF test suite
Output/	
test*x*.out	where $x = 1 – 17$

Description of the *CGPLUS* Installation Script "install_cgplus.com"

There are seven steps for *CGPLUS* to make the necessary modifications to the *CHARMM*, *GAMESS*, and *GAMESSPLUS* source files. For clarity, we denote the *CHARMM* directory as c30a1/, the *GAMESS* directory as gamess/, and *GAMESSPLUS* directory as gmsplus-v2008/, respectively.

Step 1:

CGPLUS copies all *GAMESS* source codes under gamess/source to the c30a1/source/gamint/gamess directory. This is required for *CHARMM* to compile *GAMESS* as its QM module.

Step 2:

CGPLUS copies *GAMESSPLUS* modules from the gmsplus-v2008/Code directory to c30a1/source/gamint/gamess directory. After this step, 24 *GAMESS* modules that were copied into the c30a1/source/gamint/gamess directory in step 1 will have been replaced by their corresponding *GAMESSPLUS* modules. This step modifies *GAMESS* to *GAMESSPLUS*, and puts the *GAMESSPLUS* source code in the appropriate location for *CHARMM*.

Step 3:

CGPLUS modifies the *GAMESSPLUS* main program to change *GAMESSPLUS* from a stand-alone program to a subroutine that can be called by *CHARMM*. The STOP statement in the *GAMESSPLUS* main program is changed to RETURN for returning control to *CHARMM*. A flag variable in *GAMESSPLUS* is turned on by replacing "KCHRMM=0" by "KCHRMM=1" to indicate the combined usage with *CHARMM*.

Step 4:

CGPLUS changes all occurrences of "MXCHRM=1" in *GAMESS/GAMESSPLUS* source files to "MXCHRM=25120". This dimensionality denotes the maximum number of MM atoms allowed to be included in a QM/MM calculation through the *CHARMM/GAMESSPLUS* combination package. This dimensionality variable has been set to 1 in the stand-alone *GAMESS or GAMESSPLUS* program for memory efficiency. For GHO QM/MM calculations, we set this maximum number of MM atoms to 25120.

Step 5:

CGPLUS comments out two dummy subroutines "CHGMIU" and "CHMDAT" in *GAMESS* source file iolib.src. The versions of these subroutines actually used in the *CHARMM/GAMESSPLUS* interface will be provided by *CHARMM* during the compilation.

Step 6:

CGPLUS changes "MAXGMS = 500" in c30a1/source/fcm/gamess.fcm to "MAXGMS = 2000" to be consistent with the corresponding parameter in *GAMESS* version March 24, 2007 (R6). This variable denotes the maximum number of atoms allowed in *GAMESS* calculation.

Step 7:

CGPLUS replaces the make files for compiling *CHARMM* by special make files (Makefile, Makefile.ibmsp, gamint.mk, and gamess.mk) compatible with *GAMESSPLUS*. This actually has two implications: (1) use compiler "xlf" instead of "mpxlf" for sequential compilation. (2) add sentences for compiling additional source files in *GAMESS* and *GAMESSPLUS* which is not covered by the *CHARMM* version c30a1 distribution.

Step 8:

CGPLUS removes parallel compiling options from the *CHARMM* file "pref.dat". This file is used to specify the control options for compiling *CHARMM*. For ibmsp machines, four parallel compiling options are removed by *CGPLUS*, namely, "*PARALELLE*", "*PARAFULL*", and "*SYNCHRON*".

Description of the Modifications of *CHARMM* Files Made by *CGPLUS*

There are seven *CHARMM* source files to be replaced by their modified version by *CGPLUS*. All modifications to these *CHARMM* files in *CGPLUS* have been marked by strings "CGPLUSSTR" and "CGPLUSEND". The description of the modifications made to each individual file is given as follows:

a) blur.src

The subroutine BLURIN has been modified to fix bugs in the c30a1 distribution. In c30a1 version of *CHARMM*, subroutine BLURIN contains three lines ending with a comma, which will incur compilation errors on IBM SP and IBM Regatta. To remove this problem, *CGPLUS* deletes those extra commas in BLURIN.

b) charmm_main.src:

The interfaces of *CHARMM* to *GAMESSUK* and *GAMESS(US)* have been combined into a single interface in *CHARMM* version c30a1. The initializations of both *GAMESSUK* and *GAMESS(US)* are handled by a subroutine called GUKINI. However, in the original charmm_main.src of version c30a1, the calls to the subroutine GUKINI is only compiled when *GAMESSUK* is used, but not for *GAMESS(US)*. For combining *CHARMM* with *GAMESSPLUS* [which is based on *GAMESS(US*)], charmm_main.src has

been modified in *CGPLUS* so that the calls to GUKINI are also compiled when *GAMESS(US)* is compiled with *CHARMM*.

c) ddi.src

A dummy subroutine DDI_OUTPUT has been added to ddi.src for compiling *CHARMM* together with *GAMESSPLUS*.

d) gukini.src

Modifications have been made for *CHARMM* to parse the GHO-related keywords, prepare the data structure for GHO-AIHF, and carry out the components of the analytical gradient calculations that derived from the basis transformations in GHO-AIHF.

e) einter.src

The MM energy for the A–B–X bending term is modified to incorporate the shift of the equilibrium angle for GHO-AIHF, where A denotes a frontier atom, B denotes a GHO boundary atom, and X denotes an MM atom bonded to B.

f) efscals.src

Similar modifications as in einter.src have been made. This is a fast version in *CHARMM* to calculate the MM internal energies.

g) update.src

The original *CHARMM/GAMESS* interface only checks the atom type for the central atoms in a dihedral, and if both them are QM atoms, that torsion term is not included in the total energy. According to this rule, terms Q–A–B–X in GHO-AIHF will be excluded, where Q denotes a fully QM atom, A denotes a frontier atom, B denotes a GHO boundary atom, and X denotes an MM atom bonded to B. However, such a term involves one MM atom, and therefore it should be included in the QM/MM total energy. The modified update.src tests the types of all four atoms in a dihedral term; if all of them are QM atoms (B is also treated as a QM atom in such test) it is skipped, therefore avoiding the exclusion of the above terms.

Description of the Make Files and Include File Provided by *CGPLUS*

a) gamess.mk

This make file in *CGPLUS* is the updated version of the gamess.mk in *CHARMM* version c30a1. This make file has been modified to be compatible with *GAMESSPLUS* version 2008 based on *GAMESS* version March 24, 2007 (R6).

b) gamint.mk

This make file in *CGPLUS* is the updated version of the gamint.mk in *CHARMM* version c30a1. This make file has been modified to include the compilation of the *gho* module in *GAMESSPLUS*. The *gho* module in *GAMESSPLUS* is written following the *CHARMM* programming convention, which utilizes include statements and conditional compiling. Therefore *CGPLUS* compiles the *gho* module as a part of the *CHARMM/GAMESS* interface library, which is controlled by the make file gamint.mk.

With this choice, *CHARMM/GAMESSPLUS* will treat the *gho* module by a *CHARMM* pre-processor (c30a1/tool/preflx) and convert it to a standard Fortran code following the same compiling procedure for *CHARMM* source files.

c) ghogms.fcm

This file contains all common block variables used for GHO-AIHF in the *CHARMM/GAMESSPLUS* combination package. This file will be copied to the c30a1/source/fcm directory (the *CHARMM* common block directory) by the *CGPLUS* installation script "install_cgplus.com".

Compiling *CHARMM* with *GAMESSPLUS*

Instructions for modifying *GAMESS* to create the *CHARMM/GAMESSPLUS* combination package to perform QM/MM calculations at the HF *ab initio* level with the GHO boundary treatment are summarized as follows (since the *CHARMM/GAMESSPLUS* combination package has only been compiled and tested on IBM SP and IBM Regatta machines, we describe the procedure for IBM SP machines as an example):

1. Obtain *CHARMM* (version c30a1, if possible) from Harvard University, obtain *GAMESS* from Iowa State University [March 24, 2007 (R6) version, if possible], obtain *GAMESSPLUS-v2008* and *CGPLUS-v*2008 from the University of Minnesota.

2. First execute "c30a1/install.com ibmsp medium Q" for a while, where the "c30a1" denotes the *CHARMM* root directory. This step is only used to obtain appropriate make files for *CHARMM* modules other than *gamss.mk* and *gamint.mk*, for which special treatment will be handled by *CGPLUS*. For this reason, this step of installation of *CHARMM* does not need to be completed. One may kill the installation job after it has been executed for a while.

3. Remove all files under the directory "c30a1/lib/ibmsp" to remove potential side effects that may have been introduced in the uncompleted installation in step 2.

4. Change the working directory to cgplus-v2008/, where "cgplus-v2008" denotes the *CGPLUS* home directory. Edit the script file *install_cgplus.com* to change the variables at the beginning of the script to point to the actual directories for *CHARMM*, *GAMESS*, *GAMESSPLUS*, and *CGPLUS*. For example:

```
set gamess = ~/gamess
set gmsplus = ~/gmsplus-v2008
set chmroot = ~/c30a1
set cgplus = ~/cgplus-v2008
```

5. Execute the *CGPLUS* installation script *install_cgplus.com*. This installation script will copy *GAMESS* file and *GAMESSPLUS* files to the appropriate *CHARMM* directory and prepare the special make files and compiling tools for compile *CHARMM* with *GAMESS* and *GAMESSPLUS* (see *CGPLUS User Manual* for a detailed description of the *install_cgplus.com* script). In the current version of

CGPLUS (version 2008), the make files are readily used for IBM SP and IBM Regatta machines in a serial compiling mode. For other machine types, no script is provided for modifications of these make files, but the modifications can be done in any convenient way. If any problems are encountered in this procedure, contact the *CGPLUS* developers for assistance (see http://comp.chem.umn.edu/cgplus for contact information).

6. Change to the *CHARMM* root directory c30a1/, type "install.com ibmsp medium Q" to compile the source codes of the combination package consisting of *CHARMM*, *GAMESS*, and *GAMSSPLUS*. The successful compilation will create the executable file `charmm` and put it into the directory of c30a1/exec/ibmsp.

Running *CHARMM/GAMESSPLUS*

For GHO-AIHF calculations, one needs to run the *CHARMM/GAMESSPLUS* combination package which is compiled as an integrated executable `charmm`. To start running a calculation with *CHARMM* input file $JOB.inp, type:

path`/charmm <$JOB.inp> $JOB.out`

where *path* is the directory path to the integrated `charmm` executable.

CHARMM/GAMESSPLUS Input for GHO-AIHF

For a QM/MM calculation carried by the *CHARMM*/*GAMESSPLUS* combination package, the GHO options are controlled by the *CHARMM* input file. In the *CHARMM* input, the keyword GAMEss is used to declare *GAMESSPLUS* calculations for the QM part (see *CHARMM* document 'gamess.doc' for a more detailed description). Note that in *CHARMM*, only four letters of a keyword are necessary. For example GAME is identical to GAMEss. In this manual, the redundant letters in a keyword are in lower case following the *CHARMM* documentation convention. The GHO-AIHF option is then turned on by the keyword GLNK on the GAMEss command line with following syntax:

GAMEss REMOve SELEction {QM atom-spec} GLNK SELEction {GHO atom-spec} - [GPROj] [GNDDao] [GHBOao] [GLLOfg] [GSCAle] [ASTS float] [ASTP float] - [APTS float] [APTP float] [CSTS float] [CPTP float] [CSTP float] [ABXS float]

The GHO boundary atoms are selected (using the *CHARMM* keyword SELE) after GLNK is specified. Four orthogonalization procedures are available for GHO-AIHF: (1) use the projected basis (specified by the keyword GPROj), (2) neglect diatomic differential overlap involving auxiliary orbitals (specified by the keyword GNDDao), (3) construct hybrid orbitals based on global Löwdin OAOs (specified by the keyword GHBOao), and (4) construct hybrid orbitals based on local Löwdin OAOs (specified by the keyword GLLOfg). The fourth method is a variation of the third, where only the GHO boundary atom, the QM frontier atom, and its QM neighbors (also called geminal atoms) are included into Löwdin orthogonalization in a local fashion, which is also denoted as the LLO:FG scheme. Note that GPROj, GNDDao, GHBOao, and GLLOfg are mutually exclusive.

Certain types of one-electron kinetic energy integrals involving the boundary orbitals can be scaled by user-specified scaling factors. To turn on the use of scaled integrals, the keyword GSCAle is required. Following GSCAle, various scaling integral keywords can be used for scaling a certain type of integrals. These scaling integral keywords include ASTS, ASTP, CSTS, CSTP, APTS, APTP, CSTS, CPTP, and CSTP.

To explain the meaning of these scaling integral keywords, we denote the valence *s* and *p* basis functions on the QM frontier atom A as s_A and p_A. In addition, the *s* and *p* orbitals on the GHO boundary atom B are denoted by s_B and p_B, respectively. The eight types of one-electron kinetic integrals to be scaled are labeled by keywords: ASTS for $(s_A|T|s_B)$, ASTP for $(s_A|T|p_B)$, CSTS for $(s_B|T|s_B)$, APTS for $(p_A|T|s_B)$, APTP for $(p_A|T|p_B)$, CSTS for $(s_B|T|s_B)$, CPTP for $(p_B|T|p_B)$, and CSTP for $(s_B|T|p_B)$. The scaling factor is then set by a floating point number following one of these integral-type keywords. The default values for all scaling factors are 1.0. Note that the sensitivity to these scaling factors and their optimum values are basis-set dependent. The recommended scaling factors for GHO-AIHF(LLO:FG)/MIDI! are (ASTS 0.9078, ASTP 1.0257, APTS 1.0806, APTP 1.0283, CSTS 0.9733, CPTP 0.9858, CSTP 0.9665). These values were obtained by parametrizing against a five-molecule training set to give good

gemoetries and charges. Examples of using scaling factors can be found in the directory cgplus-v2008/ghohftest/Input/test6.inp.

For a better description of the geometry, especially the bond angles near the GHO boundary, the MM parameters can also be adjusted. The keyword that can be used for such a modification is ABXS, where the A-B-X (A: the QM frontier atom, B: the GHO boundary atom, X: an MM atom bonded to B) equilibrium angle can be decreased by a few degrees specified by a floating point number following the ABXS keyword. The recommended A-B-X shift for the parametrized GHO-AIHF(LLO:FG)/MIDI! is 8 degrees.

Besides these standard options described above, *GAMESSPLUS-v2008* also provides more non-standard options and integral scaling keywords reserved for further development of the GHO method. Developers can refer to the section "*GHO status: Reserved Keywords for Developers*" in the *GAEMSSPLUS-v2008 Developer's Guide* for more information.

The QM/MM calculations carried out by *CHARMM*/*GAMESSPLUS* also require a *GAMESS* input file. One should read the *CHARMM* documentation file "gamess.doc" for the standard procedure to prepare these input files. Here we only comment on the special treatment for the *GAMESS* input file when GHO-AIHF calculations are carried. Because the GHO algorithm involves a modified SCF procedure, it does not work with all SCF convergence accelerators available in *GAMESSPLUS*. One should specify NOCONV=.TRUE. (an option in the $SCF namelist) in the *GAMESS* input file, to deactivate both the DIIS and SOSCF convergers during a GHO-AIHF calculation. If the NDDAO approximation is used (keyword GNDDao in *CHARMM* input file), INTTYP=HONDO must be used in the namelist $CONTROL. Another limitation of the GHO calculation with the NDDAO approximation is that it is incompatible with direct SCF; therefore one should avoid specifying DIRSCF=.TRUE. (the default is DIRSCF=.FALSE. in *GAMESSPLUS*) in the namelist $SCF.

Finally, we comment on the usage of external basis sets for GHO-AIHF calculations in *GAMESSPLUS*. Whenever a basis set that is internally stored in *GAMESSPLUS* is specified for the fully QM atoms, the STO-3Gv basis set is the default to represent the GHO boundary atom. Under these circumstances, the special treatment for the basis set on the GHO boundary atom is accomplished by the *GAMESSPLUS* code internally. However, sometimes one may prefer to use external basis sets for more flexibility. For example, the GHO-AIHF method has been parametrized for treating the QM fragment by HF/MIDI!, and this was shown to be able to provide accurate geometries and atomic charges. Because *GAMESSPLUS* does not provide MIDI! as an internal basis set, one must read the MIDI! basis set from an external file. For this situation, the STO-3Gv basis on the GHO boundary also needs to be read as an external basis. To avoid the conflict of the basis set used by a GHO boundary carbon and that for a fully QM carbon, the atomic label "Be" is used for a GHO boundary carbon. This is because the 1*s* core electrons on the GHO boundary carbon are not treated explicitly, therefore the effective nuclear charge are reduced to 4 as for "Be". Examples of inputting

MIDI! as an external basis set for GHO-AIHF calculations are available in cgplus-v2008/ghohftest/Input/, where an STO-3Gv basis set on a GHO boundary atom has to be given explicitly under the element labeled "Be" in a basis set file called *midib.bas*,. Furthermore, for *CHARMM/GAMESSPLUS* to locate the external basis set file, one also need to specify "envi extbas basis_filename" in the *CHARMM* input file.

Input Examples

Geometry optimization of ethane using GHO-AIHF/MIDI! with the local Löwdin orthogonalization treatment (LLO:FG) and scaled boundary orbital integrals.

CHARMM input file:

```
* Ethane: GHO-AIHF/MIDI!
*

if ?gamess .eq. 0  then stop
stream datadir.def

! -----------------
! molecule topology
! -----------------
OPEN READ FORMatted UNIT 1 NAME @0eth.topo
READ RTF CARD UNIT 1
CLOSe UNIT 1

! --------------
! parameter file
! --------------
OPEN READ FORMatted UNIT 1 NAME @1par_all22_prot.inp
READ PARAmeter CARD UNIT 1
CLOSe UNIT 1

! --------
! sequence
! --------
READ SEQUence CARD
* test ethane
*
 1
ETHA

GENERATE ETHA SETUP

IC PARAM
IC SEED 1 H11 1 C1 1 C2
IC BUILD
IC FILL
IC PURGE
PRINT IC

mini abnr nstep 2000 nprint 2000
```

```
define qm sele bynu 1:5 end

! -------------------
! GAMESS environment
! -------------------
envi input   "eth.str"
envi output  "scr/eth.gms"
envi punch   "scr/test.dat"
envi dictnry "scr/test.f10"
envi work15  "scr/test.f15"
envi aoints  "scr/test.ao"
envi dasort  "scr/test.f20"
envi extbas  "midib-gho.bas"

gamess remove noguess sele qm end glnk sele bynu 5 end
gllofg -
gscale -
    asts 0.90782 astp 1.02571 apts 1.08065 aptp 1.02825 -
    csts 0.97331 cptp 0.98583 cstp 0.96647 abxs 8

mini abnr nstep 200 tolgrd 0.01 nprint 1

print coor
```

Note: To illustrate the usage of the *CHARMM/GAMESSPLUS* combination package with the GHO keyword, we assume that the readers are familiar with the basic commands in *CHARMM*. For users who are not familiar with CHARMM data input and file manipulations, we strongly recommend reading the *CHARMM* documentation first to fully understand this example. In this example, *CHARMM* first reads in necessary topology files and parameter files to generate the sequence of residues (ethane in this case) and constructs internal coordinate data structures. A pure MM energy minimization is then carried out by *CHARMM* before the QM/MM calculation. Next, the atoms in the QM subsystem is labeled as "`qm`" by the command "`define qm sele bynu 1:5 end`". Note that the GHO boundary atom (atom number 5) is also required to be included as part of the QM subsystem atom selection. To establish the communication between *CHARMM* and *GAMESSPLUS*, values of a set environment variables are assigned in *CHARMM*. These environment variables will be used by *GAMESSPLUS* to locate the *GAMESSPLUS* input and output files, the external basis set file, and the scratch directory to store some intermediate results (see *GAMESS* documentation and *CHARMM* documentation "gamess.doc" for details). The major feature of GHO QM/MM calculations is controlled by the "`gamess`" command line, where the QM subsystem ("`sele qm end`") and the GHO boundary atom ("`sele bynu 5 end`") are defined. The local Löwdin orthogonalization scheme for GHO-AIHF is turned on by specifying "`gllofg`". Following the scaling integral

keyword "gscale", a set of scale factors are specified for GHO-AIHF/MIDI!. The keyword "abxs" is used to adjust the molecular mechanical parameter for A–B–X bond angles. Finally, the *CHARMM/GAMESSPLUS* combination program carries out a GHO-AIHF QM/MM energy minimization, and it prints out the final geometry at the end of the *CHARMM* output file.

GAMESSPLUS input file (the file "eth.str" referred by the *CHARMM* input file):

```
$CONTRL
     COORD=UNIQUE
     NOSYM=1
     ICHARG=0
     MULT=1
     SCFTYP=RHF
     RUNTYP=GRADIENT
     INTTYP=HONDO
     MAXIT=200
 $END
 $SYSTEM MEMORY=1000000 TIMLIM=100000 $END
 $BASIS
     ! use as an external basis
     GBASIS=MIDIBANG
     EXTFIL=.TRUE.
 $END
 $SCF
     NOCONV=.TRUE.
 $END
 $STATPT  NSTEP=100 OPTTOL=0.00000001 $END
 $DATA

 $END
```

Note: This example is a *GAMESSPLUS* input file for carrying out GHO-AIHF QM/MM calculations through the *CHARMM/GAMESSPLUS* combination package. In the $CONTRL namelist, variable RUNTYP is set to GRADIENT. This is because *CHARMM* is the main driver for the energy, gradient, and geometry optimizations. As a module of *CHARMM*, *GAMESSPLUS* only provides the QM energy, the electrostatic QM/MM interaction energy, and the corresponding gradient components, which will be incorporated into the total energy and gradients by *CHARMM*. The basis set specified in the *GAMESSPLUS* input file is used for fully QM atoms, but not for the GHO boundary atom. For a GHO boundary atom, a minimum valence basis set STO-3Gv is used. In this example, the MIDI! basis set is chosen and read in by *GAMESSPLUS* from an external file. The NOCONV variable in the $SCF namelist is set to .TRUE. to disable both

DIIS and SOSCF convergence accelerators, which conflict with the current implementation of the GHO-AIHF algorithm. The $DATA namelist is left empty for *CHARMM/GAMESSPLUS* combined calculations. The geometry of the molecule will be passed from *CHARMM* to *GAMESSPLUS* internally; therefore no explicit specification of the molecular geometry is needed in the *GAMESSPLUS* input file.

MIDI! basis set file (the file "`midib-gho.bas`" referred by the *CHARMM* input file):

```
H MIDIBANG
S   2
    1      4.5018000         0.0704520000
    2      0.6814440         0.4078260000
S   1
    1      0.1513980         1.0000000000

Be MIDIBANG
L   3
    1     2.9412494        -0.099967229187
    .155916274999
    2     0.6834831         0.399512826089
    .607683718598
    3     0.2222899         0.700115468880
    .391957393099

C MIDIBANG
S   3
    1    153.1722600         0.0707400000
    2     23.0730300         0.3953800000
    3      4.9232900         0.6633110000
S   2
    1      5.7255700        -0.0813800000
    2      0.4550400         0.5748530000
S   1
    1      0.1470700         1.0000000000
P   2
    1      4.2513100         0.1099310000
    2      0.8632700         0.4627130000
P   1
    1      0.2013500         1.0000000000
```

Note: The 8-character name of the MIDI! basis set is "MIDIBANG" in this external basis set file, which should match the value of GBASIS variable in the $BASIS namelist in the *GAEMSSPLUS* input file. The element name "Be" is used to label

a GHO boundary atom (a carbon atom without core electrons). As we mentioned above, the GHO boundary atom uses an STO-3Gv basis set, i.e., the valence basis functions in an STO-3G basis set for a carbon. Only necessary elements (C, H, GHO boundary atoms) are included in this example file for performing the GHO calculation for hydrocarbon systems, such as ethane. The complete MIDI! basis set containing all 12 elements for which it is defined: H, Li, C, N, O, F, Si, P, S. Cl, Br, I, and GHO boundary atoms, can be found at cgplus-v1.0/ghohftest/midib-gho.bas. Although current implementation for GHO-AIHF to read an external basis set is not applicable for a system containing a real "Be" atom, this does not present a problem for most practical uses of the method. It is worthwhile to point out that *GAMESSPLUS* does have this limitation when a basis set stored internally in *GAMESSPLUS* is used.

Test Suite for GHO-AIHF

CGPLUS contains 17 test runs to test the code and illustrate the use of the *CHARMM/GAMESSPLUS* combination package for QM/MM calculations with the GHO boundary treatment at the *ab initio* HF level. We strongly recommend that the user read the *CHARMM* document "gamess.doc" and the *GAMESSPLUS* document "*GAMESSPLUS-v2008 User Manual*" to understand these test jobs.

The test suite containing 17 test runs for testing the GHO-AIHF functionality in *GAMESSPLUS* has been collected in the directory cgplus-v1.0/Input. This test suite is designed to test the validity of the current GHO-AIHF implementation in *GAMESSPLUS* in various aspects, including (i) the basis set flexibility, (ii) GHO-AIRHF for a close-shell singlet, (iii) GHO-AIUHF for an open-shell doublet, (iv) four different orthogonalization schemes, (v) integral scaling factors, (vi) frontier atoms in different hybridization states, (vii) different functional groups near the boundary, (viii) systems in different charge states, (ix) multi-boundary systems, (x) user-defined local Löwdin orthogonalization, and (xi) analytical gradients. A description of the individual test runs is given next.

The first six test runs (Test 1 – 6) test the GHO-AIHF method for ethane with four different orthogoalization schemes, i. e., the projected basis (PROJ), the neglect of diatomic differential auxiliary overlap (NDDAO) approximation, the global Löwdin orthogonalization (GLO), and the local Löwdin orthogonalization (LLO:FG). In these test runs for ethane, STO-3G, 6-31G(d), and MIDI! basis sets are used. The scaled method for GHO-AIHF/MIDI! is tested for ethane in test run 6 with the LLO:FG treatment. Test run 7 tests GHO-AIUHF for ethyl radical based on GLO orthogonalization, which is identical to LLO:FG for ethyl, therefore the same integral scaling factors as those in test run 6 are applied. GHO-AIUHF (LLO:FG) with scaled integrals is tested against *n*-butyl radical in test run 8. Test runs 9 and 10 test the method against *n*-butane; test run 9 contains one GHO boundary atom and test 10 contains two GHO boundary atoms. Test run 10 represents the smallest realistic system containing more than one GHO boundary atoms for which the GLO orthogonalization is applicable. However, for LLO:FG orthogonalization, one frontier atom must be at least three bonds away from the other frontier atom in the current implementation to avoid the overlap of the geminal atoms for different boundary atoms. In Test run 11, we show that the LLO:FG othogonalization can be applied to such a system having more than one boundary, where two separate orbital orthogonalizations are involved, one localized near each boundary. Test run 12 tests the GHO-AIHF method for a system in a different charge state (negative ion). In test run 13, the GHO-AIHF method is tested for 1-butene, where an sp^2 hybridized carbon atom serves the frontier atom. Test runs 14 and 15 represent the applications of the method to a larger system and a biologically relevant molecule. Test run 16 test the non-standard keyword GLCLwd for user-defined local Löwdin orthogonalization including orbitals on boundary, frontier, geminal, and vicinal atoms. Test 17 carries out a single point energy calculation for propane, and tests the GHO analytical gradients against numerical ones. For clarity, the major feature of these 17 test runs for GHO-AIHF is summarized in the following table (the QM/MM division is given in column 2):

	System	QM basis	Orthogonalization	Scaling
Test 1	BH_3–AH_3	STO-3G	PROJ	No
Test 2	BH_3–AH_3	STO-3G	NDDAO	No
Test 3	BH_3–AH_3	STO-3G	GLO	No
Test 4	BH_3–AH_3	6-31G(d)	LLO:FG	No
Test 5	BH_3–AH_3	MIDI!	LLO:FG	No
Test 6	BH_3–AH_3	MIDI!	LLO:FG	Yes
Test 7	BH_3–$AH_2^{\bullet}$	MIDI!	GLO	Yes
Test 8	CH_3BH_2–$AH_2CH_2^{\bullet}$	MIDI!	LLO:FG	Yes
Test 9	CH_3BH_2–AH_2CH_3	MIDI!	LLO:FG	Yes
Test 10	BH_3AH_2–AH_2BH_3	MIDI!	GLO	No
Test 11	BH_3–$AH_2(CH_2)_2AH_2$–BH_3	MIDI!	LLO:FG	Yes
Test 12	CH_3BH_2–$AH_2CH_2O^-$	MIDI!	LLO:FG	Yes
Test 13	CH_3BH_2–$AH{=}CH_2$	MIDI!	LLO:FG	Yes
Test 14	Ethyl benzene	MIDI!	LLO:FG	Yes
Test 15	Alanine dipeptide	MIDI!	LLO:FG	Yes
Test 16	*n*-octane	MIDI!	LLO:FGV	Yes
Test 17	CH_3BH_2–AH_3	MIDI!	LLO:FG	Yes

Th test suite input files are available in the directory cgplus-v2008/ghohftest/Input. The necessary *CHARMM* topology files can be found in the directory cgplus-v2008/ghohftest/data cgplus-v2008. The test suite output files have been collected in the directory cgplus-v2008/ghohftest/Output (see chapter "*GHO-AIHF Test Results*"). *CGPLUS* also provides a Unix shell script called "run_all.sh" for running all 17 test runs. The "run_all.sh" script also creates a text file called "test.timings" containing the timing information about the test runs. You can compare them with the reference timings given in the chapter "*Test Runs Timing*".

GHO-AIHF Test Results

The results of the GHO-AIHF test suite been collected in the directory cgplus-v2008/ghohftest/Output. These reference test run output files, named "test##.out", were obtained on an IBM Regatta computer with Power4 processors running AIX 5.3 operating system. To verify the validity of the installation, users may use the UNIX command "diff" to compare the results of their calculations with these reference output files available in the *CGPLUS* distribution. Here we only give the output for one of the test runs for illustration. Note that the first 16 of the 17 test runs for GHO-AIHF all involve geometry optimization; therefore in 16 of these cases we only give the energy results of the last iteration and the QM/MM optimized geometries. For test run 17, we give the single point energy as well as the comparison between the GHO analytical gradients and numerical ones.

test1.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:         QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       48 -28038.86958       .00013       .16921       .00052
ABNR INTERN>          .09058      9.15538       .80001       .00000       .00000
ABNR EXTERN>         -.16896       .00000       .00000       .00000       .00000
ABNR QUANTM>   -28048.74659       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 1: ETHANE GHO-AIHF/STO-3G (PROJ, UNSCALED)
 TITLE>  *
    8
    1    1 ETHA C1     1.10147   -.02603   -.00021 ETHA 1       .00000
    2    1 ETHA H11     .01761   -.08464    .00001 ETHA 1       .00000
    3    1 ETHA H12    1.42300   -.59891   -.86397 ETHA 1       .00000
    4    1 ETHA H13    1.42305   -.59905    .86417 ETHA 1       .00000
    5    1 ETHA C2     1.60774   1.35758   -.00025 ETHA 1       .00000
    6    1 ETHA H21    2.70831   1.56927    .00002 ETHA 1       .00000
    7    1 ETHA H22    1.35504   2.06444   -.83187 ETHA 1       .00000
    8    1 ETHA H23    1.35498   2.06461    .83210 ETHA 1       .00000
```

test2.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:         QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       42 -28187.52117       .00028       .19742       .00078
ABNR INTERN>          .59934       .17277      3.70898       .00000       .00000
ABNR EXTERN>          .19650       .00000       .00000       .00000       .00000
ABNR QUANTM>   -28192.19876       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor
```

```
          COORDINATE FILE MODULE
 TITLE>  * TEST 2: ETHANE GHO-AIHF/STO-3G (NDDAO, UNSCALED)
 TITLE>  *
    8
    1    1 ETHA C1     1.15642    .12388   -.00001 ETHA 1       .00000
    2    1 ETHA H11     .07951    .14149    .00002 ETHA 1       .00000
    3    1 ETHA H12    1.51249   -.38292   -.88093 ETHA 1       .00000
    4    1 ETHA H13    1.51251   -.38286    .88100 ETHA 1       .00000
    5    1 ETHA C2     1.58851   1.30526    .00012 ETHA 1       .00000
    6    1 ETHA H21    2.72428   1.27776   -.00003 ETHA 1       .00000
    7    1 ETHA H22    1.20871   1.83233   -.93177 ETHA 1       .00000
    8    1 ETHA H23    1.20876   1.83232    .93160 ETHA 1       .00000
```

test3.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:        QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       29 -28049.66935       .00642       .16871       .00209
ABNR INTERN>         .03900       .05663       .97400       .00002       .00000
ABNR EXTERN>        -.16805       .00000       .00000       .00000       .00000
ABNR QUANTM>   -28050.57096       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 3: GHO-AIHF/STO-3G (GLO, UNSCALED)
 TITLE>  *
    8
    1    1 ETHA C1     1.07013   -.07625   -.00003 ETHA 1       .00000
    2    1 ETHA H11    -.00612   -.01738    .00001 ETHA 1       .00000
    3    1 ETHA H12    1.43220   -.56721   -.88853 ETHA 1       .00000
    4    1 ETHA H13    1.43221   -.56722    .88855 ETHA 1       .00000
    5    1 ETHA C2     1.65900   1.46047    .00001 ETHA 1       .00000
    6    1 ETHA H21    2.77616   1.46951    .00000 ETHA 1       .00000
    7    1 ETHA H22    1.31380   2.02267   -.90191 ETHA 1       .00000
    8    1 ETHA H23    1.31381   2.02267    .90190 ETHA 1       .00000
```

test4.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:        QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       43 -27807.92019       .00010       .17046       .00038
ABNR INTERN>         .18536      2.18761       .03763       .00000       .00000
ABNR EXTERN>        -.15541       .00000       .00000       .00000       .00000
ABNR QUANTM>   -27810.17539       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 4: ETHANE GHO-AIHF/6-31G(D) (LLO:FG, UNSCALED)
 TITLE>  *
```

```
    8
    1    1 ETHA C1     1.11110    .00000    .00000 ETHA 1       .00000
    2    1 ETHA H11     .02830    .01221    .00000 ETHA 1       .00000
    3    1 ETHA H12    1.46644   -.51410   -.88416 ETHA 1       .00000
    4    1 ETHA H13    1.46643   -.51404    .88411 ETHA 1       .00000
    5    1 ETHA C2     1.60383   1.34702    .00024 ETHA 1       .00000
    6    1 ETHA H21    2.72341   1.45711   -.00001 ETHA 1       .00000
    7    1 ETHA H22    1.29581   1.97955   -.87771 ETHA 1       .00000
    8    1 ETHA H23    1.29589   1.97950    .87754 ETHA 1       .00000
```

test5.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:        QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       39 -27930.12482       .00006       .17600       .00044
ABNR INTERN>         .08378      1.02848       .26762       .00000       .00000
ABNR EXTERN>        -.16401       .00000       .00000       .00000       .00000
ABNR QUANTM>   -27931.34070       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 5: ETHANE GHO-AIHF/MIDIBANG (LLO:FG, UNSCALED)
 TITLE>  *
    8
    1    1 ETHA C1     1.09395   -.04679    .00022 ETHA 1       .00000
    2    1 ETHA H11     .01410   -.00538   -.00002 ETHA 1       .00000
    3    1 ETHA H12    1.46255   -.53549   -.89057 ETHA 1       .00000
    4    1 ETHA H13    1.46248   -.53539    .89038 ETHA 1       .00000
    5    1 ETHA C2     1.62160   1.39590    .00008 ETHA 1       .00000
    6    1 ETHA H21    2.73953   1.47325   -.00001 ETHA 1       .00000
    7    1 ETHA H22    1.29848   2.00061   -.88590 ETHA 1       .00000
    8    1 ETHA H23    1.29850   2.00054    .88582 ETHA 1       .00000
```

test6.out

```
ABNER> Minimization exiting with gradient tolerance (  .2000000) satisfied.

ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:        QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       32 -27974.19232       .00059       .19641       .00092
ABNR INTERN>         .10835      3.29581       .03172       .00000     .00000
ABNR EXTERN>        -.15582       .00000       .00000       .00000     .00000
ABNR QUANTM>   -27977.47238       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 6: ETHANE GHO-AIHF/MIDIBANG (LLO:FG, SCALED)
 TITLE>  *
    8
    1    1 ETHA C1     1.10280   -.02242   -.00018 ETHA 1       .00000
```

```
    2    1 ETHA H11     .01994    .00928    .00001 ETHA 1       .00000
    3    1 ETHA H12    1.46770   -.52049   -.89000 ETHA 1       .00000
    4    1 ETHA H13    1.46775   -.52058    .89016 ETHA 1       .00000
    5    1 ETHA C2     1.62579   1.40681   -.00014 ETHA 1       .00000
    6    1 ETHA H21    2.74693   1.44038    .00001 ETHA 1       .00000
    7    1 ETHA H22    1.28016   1.97710   -.90169 ETHA 1       .00000
    8    1 ETHA H23    1.28012   1.97718    .90182 ETHA 1       .00000
```

test7.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:        QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       38 -27576.38145       .00023       .17644       .00072
ABNR INTERN>         .12609      3.02164       .00631       .19486       .00000
ABNR EXTERN>        -.11048       .00000       .00000       .00000       .00000
ABNR QUANTM>   -27579.61987       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 7: ETHYL GHO-AIUHF/MIDIBANG (GLO==LLO:FG, SCALED)
 TITLE>  *
    7
    1    1 ETHP C1     1.05807    .04118   -.11040 ETHP 1       .00000
    2    1 ETHP H11     .00185   -.05385    .06948 ETHP 1       .00000
    3    1 ETHP H12    1.49957   -.60196   -.85130 ETHP 1       .00000
    4    1 ETHP C2     1.62372   1.43703   -.02182 ETHP 1       .00000
    5    1 ETHP H21    2.74564   1.42882    .00301 ETHP 1       .00000
    6    1 ETHP H22    1.31535   2.06768   -.89836 ETHP 1       .00000
    7    1 ETHP H23    1.27731   1.96618    .90583 ETHP 1       .00000
```

test8.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:        QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       51 -51910.54551       .00322       .14651       .00236
ABNR INTERN>         .11472      2.79664       .13141       .04275       .00000
ABNR EXTERN>        -.31247      5.50935       .00000       .00000       .00000
ABNR QUANTM>   -51918.82792       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 8: BUTYL GHO-AIUHF/MIDIBANG (LLO:FG, SCALED)
 TITLE>  *
   13
    1    1 BUTP C1     1.04503    .10511    .15616 BUTP 1       .00000
    2    1 BUTP H11    -.00102   -.07983   -.01469 BUTP 1       .00000
    3    1 BUTP H12    1.65752   -.70530    .51000 BUTP 1       .00000
    4    1 BUTP C2     1.59559   1.51613    .06278 BUTP 1       .00000
    5    1 BUTP H21    1.26226   2.13271    .89541 BUTP 1       .00000
    6    1 BUTP H22    1.27354   2.00968   -.84931 BUTP 1       .00000
```

```
    7    1 BUTP C3     3.12479   1.55895    .07821 BUTP 1       .00000
    8    1 BUTP H31    3.58100    .97765   -.76866 BUTP 1       .00000
    9    1 BUTP H32    3.56045   1.11527   1.01431 BUTP 1       .00000
   10    1 BUTP C4     3.68079   2.98611   -.02544 BUTP 1       .00000
   11    1 BUTP H41    4.79014   2.96343   -.04918 BUTP 1       .00000
   12    1 BUTP H42    3.35386   3.58941    .84724 BUTP 1       .00000
   13    1 BUTP H43    3.31536   3.47379   -.95326 BUTP 1       .00000
```

test9.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:        QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       36 -52304.49070       .00024       .18456       .00100
ABNR INTERN>         .11340      2.96205       .14448       .03089       .00000
ABNR EXTERN>        -.37349      5.51368       .00000       .00000       .00000
ABNR QUANTM>   -52312.88170       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 9: BUTANE GHO-AIHF/MIDIBANG (LLO:FG, SCALED)
 TITLE>  *
   14
    1    1 BUTB C1     1.11205    .00060    .00000 BUTB 1       .00000
    2    1 BUTB H11     .02617   -.02557    .00000 BUTB 1       .00000
    3    1 BUTB H12    1.46614   -.53199    .87904 BUTB 1       .00000
    4    1 BUTB H13    1.46614   -.53199   -.87904 BUTB 1       .00000
    5    1 BUTB C2     1.62284   1.46932    .00000 BUTB 1       .00000
    6    1 BUTB H21    1.27788   2.00391    .87729 BUTB 1       .00000
    7    1 BUTB H22    1.27788   2.00391   -.87729 BUTB 1       .00000
    8    1 BUTB C3     3.14946   1.55146    .00000 BUTB 1       .00000
    9    1 BUTB H31    3.61214   1.05004   -.89266 BUTB 1       .00000
   10    1 BUTB H32    3.61214   1.05004    .89266 BUTB 1       .00000
   11    1 BUTB C4     3.67353   2.99559    .00000 BUTB 1       .00000
   12    1 BUTB H41    4.78285   3.00127    .00000 BUTB 1       .00000
   13    1 BUTB H42    3.31489   3.53434    .90240 BUTB 1       .00000
   14    1 BUTB H43    3.31489   3.53434   -.90240 BUTB 1       .00000
```

test10.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:        QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       40 -55117.45337       .00019       .16443       .00066
ABNR INTERN>         .13347      1.78566       .92019       .01146       .00000
ABNR EXTERN>        -.49637      3.26381       .00000       .00000       .00000
ABNR QUANTM>   -55123.07159       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 10: BUTANE GHO-AIHF/MIDIBANG (GLO, UNSCALED)
 TITLE>  *          TWO GHO BOUNDARY ATOMS
```

```
 TITLE>  *
   14
    1    1 BUTA C2     1.61218   1.46283   -.00001 BUTA 1       .00000
    2    1 BUTA H21    1.20242   1.94605   -.87690 BUTA 1       .00000
    3    1 BUTA H22    1.20241   1.94604    .87689 BUTA 1       .00000
    4    1 BUTA C3     3.18445   1.53773   -.00008 BUTA 1       .00000
    5    1 BUTA H31    3.59420   1.05453   -.87686 BUTA 1       .00000
    6    1 BUTA H32    3.59422   1.05450    .87693 BUTA 1       .00000
    7    1 BUTA C1     1.08243   -.00666    .00011 BUTA 1       .00000
    8    1 BUTA C4     3.71421   3.00722   -.00003 BUTA 1       .00000
    9    1 BUTA H11    -.03245   -.10180   -.00001 BUTA 1       .00000
   10    1 BUTA H12    1.41888   -.60140    .88671 BUTA 1       .00000
   11    1 BUTA H13    1.41892   -.60143   -.88679 BUTA 1       .00000
   12    1 BUTA H41    4.82908   3.10236    .00000 BUTA 1       .00000
   13    1 BUTA H42    3.37773   3.60198    .88677 BUTA 1       .00000
   14    1 BUTA H43    3.37774   3.60196   -.88674 BUTA 1       .00000
```

test11.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:        QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       32-103907.66990       .00101       .19756       .00136
ABNR INTERN>         .17984      6.25078       .15265       .01241       .00000
ABNR EXTERN>        -.52197      1.31084       .00000       .00000       .00000
ABNR QUANTM>  -103915.05446       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 11: HEXANE GHO-AIHF/MIDIBANG (LLO:FG, SCALED)
 TITLE>  *           TWO BOUNARY ATOMS CASE.
 TITLE>  *
   20
    1    1 HEXA C2     1.46387   1.35015   -.00008 HEXA 1       .00000
    2    1 HEXA H21    1.04754   1.83297   -.87839 HEXA 1       .00000
    3    1 HEXA H22    1.04752   1.83299    .87844 HEXA 1       .00000
    4    1 HEXA C3     3.01072   1.43654    .00004 HEXA 1       .00000
    5    1 HEXA H31    3.40045    .91696   -.87352 HEXA 1       .00000
    6    1 HEXA H32    3.40045    .91697    .87350 HEXA 1       .00000
    7    1 HEXA C4     3.49334   2.88475   -.00003 HEXA 1       .00000
    8    1 HEXA H41    3.10362   3.40433    .87352 HEXA 1       .00000
    9    1 HEXA H42    3.10362   3.40433   -.87350 HEXA 1       .00000
   10    1 HEXA C5     5.04020   2.97115    .00007 HEXA 1       .00000
   11    1 HEXA H51    5.45655   2.48830   -.87844 HEXA 1       .00000
   12    1 HEXA H52    5.45653   2.48832    .87839 HEXA 1       .00000
   13    1 HEXA C1      .95762   -.09834    .00006 HEXA 1       .00000
   14    1 HEXA C6     5.54645   4.41963   -.00005 HEXA 1       .00000
   15    1 HEXA H11    -.16026   -.16272    .00000 HEXA 1       .00000
   16    1 HEXA H12    1.31687   -.66099    .90063 HEXA 1       .00000
   17    1 HEXA H13    1.31689   -.66099   -.90066 HEXA 1       .00000
   18    1 HEXA H61    6.66433   4.48401    .00000 HEXA 1       .00000
   19    1 HEXA H62    5.18718   4.98228    .90066 HEXA 1       .00000
   20    1 HEXA H63    5.18720   4.98229   -.90063 HEXA 1       .00000
```

test12.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
```

```
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:        QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       32 -98594.55968       .00523       .17621       .00153
ABNR INTERN>         .10296      3.73141       .23813       .04104       .00000
ABNR EXTERN>        -.48883      5.54501       .00000       .00000       .00000
ABNR QUANTM>   -98603.72940       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 12: CH3BH2-AH2CH2O (-) (ANION)
 TITLE>  *          GHO-AIHF/MIDIBANG (LLO:FG, SCALED)
 TITLE>  *
   14
    1    1 BTOA C1     1.14692   -.05813    .07719 BTOA 1       .00000
    2    1 BTOA O1     1.55675   -.70068   1.14228 BTOA 1       .00000
    3    1 BTOA H11     .01744    .04514   -.08610 BTOA 1       .00000
    4    1 BTOA H12    1.46968   -.45657   -.94757 BTOA 1       .00000
    5    1 BTOA C2     1.64927   1.45483    .04290 BTOA 1       .00000
    6    1 BTOA H21    2.73708   1.46698    .07121 BTOA 1       .00000
    7    1 BTOA H22    1.28684   1.96799    .93149 BTOA 1       .00000
    8    1 BTOA C3     1.18381   2.23434  -1.19574 BTOA 1       .00000
    9    1 BTOA H31     .06802   2.28228  -1.29965 BTOA 1       .00000
   10    1 BTOA H32    1.52355   1.77944  -2.16307 BTOA 1       .00000
   11    1 BTOA C4     1.66478   3.69599  -1.23618 BTOA 1       .00000
   12    1 BTOA H41    2.77387   3.72131  -1.22504 BTOA 1       .00000
   13    1 BTOA H42    1.28705   4.23497   -.34306 BTOA 1       .00000
   14    1 BTOA H43    1.29531   4.19866  -2.15179 BTOA 1       .00000
```

test13.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:        QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       35 -51558.58268       .00013       .16699       .00067
ABNR INTERN>         .15512      3.09549       .04049      1.49750       .00000
ABNR EXTERN>         .20016      5.48577       .00000       .00000       .00000
ABNR QUANTM>   -51569.05722       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 13: BUTENE GHO-AIHF/MIDIBANG (LLO:FG, SCALED)
 TITLE>  *
   12
    1    1 BENE C1      .95819   -.04465   -.00680 BENE 1       .00000
    2    1 BENE H11    -.09707   -.05624   -.22206 BENE 1       .00000
    3    1 BENE H12    1.42200   -.99929    .16458 BENE 1       .00000
    4    1 BENE C2     1.65580   1.07112    .04813 BENE 1       .00000
    5    1 BENE H21    2.70790   1.05012    .26905 BENE 1       .00000
    6    1 BENE C3     1.07842   2.45389   -.17556 BENE 1       .00000
    7    1 BENE H31    1.56805   2.98242  -1.04060 BENE 1       .00000
    8    1 BENE H32    -.02168   2.42457   -.41632 BENE 1       .00000
    9    1 BENE C4     1.23932   3.36323   1.05139 BENE 1       .00000
```

```
   10    1 BENE H41     .70718   2.93440   1.92692 BENE 1       .00000
   11    1 BENE H42    2.31176   3.48732   1.31137 BENE 1       .00000
   12    1 BENE H43     .81266   4.36609    .83952 BENE 1       .00000
```

test14.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:        QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       36-146783.73998       .00015       .18854       .00079
ABNR INTERN>         .12235      4.96526       .00581       .92073       .00000
ABNR EXTERN>        -.09592      5.40393       .00000       .00000       .00000
ABNR QUANTM>  -146795.06214       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 14: ETHYL BENZENE GHO-AIHF/MIDIBANG (LLO:FG, SCALED)
 TITLE>  *
   18
    1    1 EBEZ CG     -.02899   -.03304   -.01439 EBEZ 1       .00000
    2    1 EBEZ HG     -.58062   -.95673   -.02183 EBEZ 1       .00000
    3    1 EBEZ CD1    1.35239   -.04861   -.01121 EBEZ 1       .00000
    4    1 EBEZ HD1    1.87838   -.98799   -.01526 EBEZ 1       .00000
    5    1 EBEZ CD2    -.69778   1.17573   -.00747 EBEZ 1       .00000
    6    1 EBEZ HD2   -1.77426   1.19334   -.00859 EBEZ 1       .00000
    7    1 EBEZ CE1    2.06142   1.13312   -.00359 EBEZ 1       .00000
    8    1 EBEZ HE1    3.13734   1.11576    .00025 EBEZ 1       .00000
    9    1 EBEZ CE2     .00638   2.36037    .00016 EBEZ 1       .00000
   10    1 EBEZ HE2    -.51912   3.29937    .00692 EBEZ 1       .00000
   11    1 EBEZ CZ     1.39411   2.34990    .00065 EBEZ 1       .00000
   12    1 EBEZ CB     2.17228   3.65292    .01343 EBEZ 1       .00000
   13    1 EBEZ HM1    3.15613   3.52276   -.51626 EBEZ 1       .00000
   14    1 EBEZ HM2    1.58971   4.45820   -.51346 EBEZ 1       .00000
   15    1 EBEZ C3     2.42719   4.07543   1.46289 EBEZ 1       .00000
   16    1 EBEZ H31    1.46837   4.22748   2.00281 EBEZ 1       .00000
   17    1 EBEZ H32    2.99639   5.02848   1.48683 EBEZ 1       .00000
   18    1 EBEZ H33    3.01718   3.30254   2.00004 EBEZ 1       .00000
```

test15.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:        QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       37-132654.77292       .00073       .15409       .00090
ABNR INTERN>         .35922      7.14048       .12197      3.26383       .02426
ABNR EXTERN>       -1.02543    -52.64309       .00000       .00000       .00000
ABNR QUANTM>  -132612.01416       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
```

```
 TITLE>  * TEST 15: ALANINE DIPEPTIDE
 TITLE>  *          GHO-AIHF/MIDIBANG (LLO:FG, SCALED)
 TITLE>  *
   22
    1    1 ALAD NR     4.37426   1.89522   -.08505 ALAD 1       .00000
    2    1 ALAD HR     3.97868   2.81259   -.18124 ALAD 1       .00000
    3    1 ALAD CR     5.80372   1.67468   -.23400 ALAD 1       .00000
    4    1 ALAD HR1    6.28110   2.63048   -.41219 ALAD 1       .00000
    5    1 ALAD HR2    6.00848   1.01118  -1.06794 ALAD 1       .00000
    6    1 ALAD HR3    6.21782   1.23065    .66510 ALAD 1       .00000
    7    1 ALAD CRP    3.54673    .85864    .14041 ALAD 1       .00000
    8    1 ALAD OR     3.90079   -.28386    .24309 ALAD 1       .00000
    9    1 ALAD CA     2.04978   1.26108    .26055 ALAD 1       .00000
   10    1 ALAD NL     1.26841    .08370    .24400 ALAD 1       .00000
   11    1 ALAD HL     1.73094   -.74527    .54761 ALAD 1       .00000
   12    1 ALAD HA     1.68871   1.87636   -.58065 ALAD 1       .00000
   13    1 ALAD CB     1.76312   2.07897   1.52625 ALAD 1       .00000
   14    1 ALAD HB1    2.02900   1.50201   2.43769 ALAD 1       .00000
   15    1 ALAD HB2    2.32372   3.03652   1.53059 ALAD 1       .00000
   16    1 ALAD HB3     .67716   2.31602   1.57645 ALAD 1       .00000
   17    1 ALAD CLP     .01168    .01106   -.20714 ALAD 1       .00000
   18    1 ALAD OL     -.60156    .98118   -.62863 ALAD 1       .00000
   19    1 ALAD CL     -.60996  -1.32999   -.17234 ALAD 1       .00000
   20    1 ALAD HL1   -1.63698  -1.26992   -.59290 ALAD 1       .00000
   21    1 ALAD HL2    -.66908  -1.69471    .87457 ALAD 1       .00000
   22    1 ALAD HL3    -.01222  -2.04209   -.77942 ALAD 1       .00000
```

test16.out

```
ABNR MIN: Cycle      ENERgy      Delta-E         GRMS    Step-size
ABNR INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ABNR EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ABNR QUANTUM:         QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ABNR>       32-152592.50070       .00127       .17073       .00153
ABNR INTERN>          .16379      6.04032       .24732       .01818       .00000
ABNR EXTERN>        -.53940       .25587       .00000       .00000       .00000
ABNR QUANTM>  -152598.68679       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 16: OCTANE GHO-AIHF/MIDIBANG (LLO:FGV, SCALED)
 TITLE>  *          USER-DEFINED LOCAL LOWDIN ORTHOGONALIZATION
 TITLE>  *
   26
    1    1 OCTC C2     1.64568   1.45880    .00000 OCTC 1       .00000
    2    1 OCTC H21    1.23347   1.95088   -.87523 OCTC 1       .00000
    3    1 OCTC H22    1.23347   1.95088    .87523 OCTC 1       .00000
    4    1 OCTC C3     3.20189   1.55373    .00000 OCTC 1       .00000
    5    1 OCTC H31    3.59182   1.03631    .87552 OCTC 1       .00000
    6    1 OCTC H32    3.59182   1.03631   -.87551 OCTC 1       .00000
    7    1 OCTC C4     3.68485   3.01346    .00000 OCTC 1       .00000
    8    1 OCTC H41    3.28505   3.52565    .87465 OCTC 1       .00000
    9    1 OCTC H42    3.28505   3.52565   -.87465 OCTC 1       .00000
   10    1 OCTC C7     7.25713   4.68055    .00000 OCTC 1       .00000
   11    1 OCTC H71    7.66934   4.18846   -.87523 OCTC 1       .00000
   12    1 OCTC H72    7.66934   4.18846    .87523 OCTC 1       .00000
   13    1 OCTC C6     5.70092   4.58562    .00000 OCTC 1       .00000
   14    1 OCTC H61    5.31099   5.10303    .87552 OCTC 1       .00000
```

```
   15    1 OCTC H62    5.31099   5.10303   -.87551 OCTC 1       .00000
   16    1 OCTC C5     5.21796   3.12588    .00000 OCTC 1       .00000
   17    1 OCTC H51    5.61776   2.61369   -.87465 OCTC 1       .00000
   18    1 OCTC H52    5.61776   2.61369    .87465 OCTC 1       .00000
   19    1 OCTC C1     1.09653    .01224    .00000 OCTC 1       .00000
   20    1 OCTC C8     7.80627   6.12710    .00000 OCTC 1       .00000
   21    1 OCTC H11    -.02236   -.02134    .00000 OCTC 1       .00000
   22    1 OCTC H12    1.44360   -.55680    .90080 OCTC 1       .00000
   23    1 OCTC H13    1.44360   -.55680   -.90080 OCTC 1       .00000
   24    1 OCTC H81    8.92517   6.16068    .00000 OCTC 1       .00000
   25    1 OCTC H82    7.45921   6.69614    .90080 OCTC 1       .00000
   26    1 OCTC H83    7.45921   6.69614   -.90080 OCTC 1       .00000
```

test17.out

```
ENER ENR:  Eval#     ENERgy      Delta-E         GRMS
ENER INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ENER EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
ENER QUANTUM:        QMELec        QMVDw
 ----------       ---------    ---------    ---------    ---------    ---------
ENER>        0 -27962.05020  27964.68930     10.85777
ENER INTERN>         .00795      1.70387       .01390       .00433       .00000
ENER EXTERN>        -.27613      5.41804       .00000       .00000       .00000
ENER QUANTM>   -27968.92216       .00000
 ----------       ---------    ---------    ---------    ---------    ---------

 CHARMM>

 CHARMM>    print coor

          COORDINATE FILE MODULE
 TITLE>  * TEST 17: PROPANE GHO-AIHF/MIDIBANG (LLO:FG, SCALED)
 TITLE>  *          SINGLE POINT ENERGY, TEST ANALYTICAL GRADIENT
 TITLE>  *
   11
    1    1 PROP C1     1.12683    .01344    .00000 PROP 1       .00000
    2    1 PROP H11     .01594   -.01433    .00000 PROP 1       .00000
    3    1 PROP H12    1.49194   -.52511    .90100 PROP 1       .00000
    4    1 PROP H13    1.49194   -.52511   -.90100 PROP 1       .00000
    5    1 PROP C2     1.62984   1.45778    .00000 PROP 1       .00000
    6    1 PROP H21    1.23582   1.98632    .89857 PROP 1       .00000
    7    1 PROP H22    1.23582   1.98632   -.89857 PROP 1       .00000
    8    1 PROP C3     3.15767   1.52739    .00000 PROP 1       .00000
    9    1 PROP H31    3.50151   2.58409    .00000 PROP 1       .00000
   10    1 PROP H32    3.56954   1.02369   -.90100 PROP 1       .00000
   11    1 PROP H33    3.56954   1.02369    .90100 PROP 1       .00000

 CHARMM>

 CHARMM>    test first tol 0.00 step 0.0005
 TESTFD: Parameters: STEP=    .00050  MASSweighting=   0
 TESTFD: The following first derivatives differ by more than TOL=     .000000
  DIM.         ATOM                 ANALYTIC        FINITE-DIFF     DEVIATION
    1 X ( PROP 1    PROP C1  )      -.31808672      -.31828984       .00020312
    1 Y ( PROP 1    PROP C1  )     32.92538287     32.92548105      -.00009818
    1 Z ( PROP 1    PROP C1  )       .00000000      -.00000001       .00000001
    2 X ( PROP 1    PROP H11 )    -20.70570991    -20.70552640      -.00018350
    2 Y ( PROP 1    PROP H11 )     -6.25333307     -6.25333076      -.00000231
    2 Z ( PROP 1    PROP H11 )       .00000000      -.00000004       .00000003
    3 X ( PROP 1    PROP H12 )      4.76105154      4.76105734      -.00000579
    3 Y ( PROP 1    PROP H12 )    -14.91708288    -14.91707465      -.00000823
    3 Z ( PROP 1    PROP H12 )     15.97124675     15.97115900       .00008774
```

4	X	(PROP 1	PROP H13)	4.76105154	4.76105729	-.00000575
4	Y	(PROP 1	PROP H13)	-14.91708288	-14.91707466	-.00000821
4	Z	(PROP 1	PROP H13)	-15.97124675	-15.97115898	-.00008777
5	X	(PROP 1	PROP C2)	17.84082701	17.84083549	-.00000849
5	Y	(PROP 1	PROP C2)	25.92580365	25.92561241	.00019125
5	Z	(PROP 1	PROP C2)	.00000000	.00000000	.00000000
6	X	(PROP 1	PROP H21)	-2.96784857	-2.96786753	.00001896
6	Y	(PROP 1	PROP H21)	-12.03327445	-12.03326652	-.00000793
6	Z	(PROP 1	PROP H21)	-3.66397293	-3.66396394	-.00000899
7	X	(PROP 1	PROP H22)	-2.96784858	-2.96786752	.00001895
7	Y	(PROP 1	PROP H22)	-12.03327445	-12.03326648	-.00000797
7	Z	(PROP 1	PROP H22)	3.66397293	3.66396393	.00000900
8	X	(PROP 1	PROP C3)	-2.92393558	-2.92400548	.00006990
8	Y	(PROP 1	PROP C3)	1.36785794	1.36790072	-.00004278
8	Z	(PROP 1	PROP C3)	.00000000	-.00000001	.00000001
9	X	(PROP 1	PROP H31)	.91492800	.91494444	-.00001645
9	Y	(PROP 1	PROP H31)	.56993380	.56993983	-.00000603
9	Z	(PROP 1	PROP H31)	.00000000	.00000001	-.00000001
10	X	(PROP 1	PROP H32)	.80278563	.80280398	-.00001836
10	Y	(PROP 1	PROP H32)	-.31746526	-.31748567	.00002041
10	Z	(PROP 1	PROP H32)	-.37500432	-.37502043	.00001611
11	X	(PROP 1	PROP H33)	.80278563	.80280394	-.00001831
11	Y	(PROP 1	PROP H33)	-.31746526	-.31748565	.00002039
11	Z	(PROP 1	PROP H33)	.37500432	.37502038	-.00001605

TESTFD: A total of 0 elements were within the tolerance

Platforms for which *CHARMM/GAMESSPLUS* Has Been Tested

Computer	Processor	Operating System	Compiler
IBM SP	Power 3	AIX 4.3	XL Fortran Compiler 7.1.12
IBM Regatta	Power 4	AIX 5.3	XL Fortran Compiler 7.1.12

Test run timings

The timings have been done using the UNIX time command (/bin/time). The User + System CPU times (s) for each test runs are given below:

	IBM SP	IBM Regatta
Test 1	42.4	13.4
Test 2	38.3	11.9
Test 3	25.7	7.5
Test 4	11.0	3.2
Test 5	15.2	5.0
Test 6	13.0	3.7
Test 7	13.9	3.4
Test 8	102.7	34.0
Test 9	81.3	27.2
Test 10	109.0	34.0
Test 11	606.8	204.9
Test 12	185.4	59.5
Test 13	47.1	14.7
Test 14	1013.5	343.8
Test 15	521.0	169.1
Test 16	1919.8	641.1
Test 17	27.5	7.8

Acknowledgment

The authors are grateful to Milan Hodoscek for helpful emails about the compiling of *CHARMM* with *GAMESS*.

Revision History and Extended Version Summaries

In the revision histories, for each version of *CGPLUS*, we list the authors of that version and we also list the versions of *CHARMM* and *GAMESSPLUS* which the *CGPLUS* was interfacing. The version of *GAMESS* which the *GAMESSPLUS* was based is also given for completeness.

***CGPLUS* Version 1.0 (January 2004)**
Authors: J. Pu, J. Gao, and D. G. Truhlar
CHARMM version: c30a1
GAMESSPLUS version: version 4.1, based on
GAMESS version: July 3, 2003 (R2)

This is the first version of *CGPLUS*.

***CGPLUS* Version 2008 (April 2008)**
Authors: J. Pu, M. Higashi, J. Gao, and D. G. Truhlar
CHARMM version: c30a1
GAMESSPLUS version: version 2008, based on
GAMESS version: March 24, 2007 (R6)

This version works with *GAMESSPLUS* version 2008 based on the March 24, 2007 (R6) version of *GAMESS*. ddi.src, gamess.mk, gmscomp_ibmsp and install_cgplus.com files has been modified.