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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Distribution site: http://comp.chem.umn.edu/cgplus
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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/GAMESSPLUS* 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.

**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/GAMESSPLUS** 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:**

B) **American Chemical Society Format:**
C) **Theoretical Chemistry Accounts Format:**


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

The reference for GHO-AIHF is:


The original reference for the MIDI! basis set is:

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
ghoftest 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/
testx.inp  where x = 1 – 17
sto3g.str  the GAMESSPLUS input file for testm.inp (m = 1 – 3)
631gd.str  the GAMESSPLUS input file for test4.inp
midib.str  the GAMESSPLUS input file for testn.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/
testx.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 games.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-v2008 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 'gameess.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} -
[GPProj] [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, CPTP, APTS, APTP, CSTP, 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 $(p_A | T | p_B)$, CSTP 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 GAMESSPLUS-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 1s 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-AIH/MIDI! with the local Löwdin orthogonalization treatment (LLO:FG) and scaled boundary orbital integrals.

CHARMM input file:

```plaintext
* Ethane: GHO-AIH/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 apts 1.02825 -
  csts 0.97331 cstp 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
  EXTFL= .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-AHF 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  0.155916274999
  2  0.6834831
  0.399512826089  0.607683718598
  3  0.2222899
  0.700115468880  0.391957393099

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 orthogonalization 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 orthogonalization 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):

<table>
<thead>
<tr>
<th>Test Run</th>
<th>Feature Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 – 6</td>
<td>Test GHO-AIHF method for ethane with different orthogonalization schemes</td>
</tr>
<tr>
<td>7</td>
<td>Test GHO-AIUHF for ethyl radical based on GLO orthogonalization</td>
</tr>
<tr>
<td>8</td>
<td>Test GHO-AIUHF (LLO:FG) with scaled integrals against <em>n</em>-butyl radical</td>
</tr>
<tr>
<td>9, 10</td>
<td>Test the method against <em>n</em>-butane, one GHO boundary atom, two GHO boundary atoms</td>
</tr>
<tr>
<td>11</td>
<td>Test LLO:FG orthogonalization for multiple boundary systems</td>
</tr>
<tr>
<td>12</td>
<td>Test the GHO-AIHF method for a system in a different charge state</td>
</tr>
<tr>
<td>13</td>
<td>Test GHO-AIHF method for 1-butene</td>
</tr>
<tr>
<td>14, 15</td>
<td>Test applications of the method to larger systems and biologically relevant molecule</td>
</tr>
<tr>
<td>16</td>
<td>Test GLCLwd keyword for user-defined local Löwdin orthogonalization</td>
</tr>
<tr>
<td>17</td>
<td>Single point energy calculation for propane, test analytical gradients against</td>
</tr>
</tbody>
</table>

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):
<table>
<thead>
<tr>
<th>Test</th>
<th>System</th>
<th>QM basis</th>
<th>Orthogonalization</th>
<th>Scaling</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BH₃–AH₃</td>
<td>STO-3G</td>
<td>PROJ</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>BH₃–AH₃</td>
<td>STO-3G</td>
<td>NDDAO</td>
<td>No</td>
</tr>
<tr>
<td>3</td>
<td>BH₃–AH₃</td>
<td>STO-3G</td>
<td>GLO</td>
<td>No</td>
</tr>
<tr>
<td>4</td>
<td>BH₃–AH₃</td>
<td>6-31G(d)</td>
<td>LLO:FG</td>
<td>No</td>
</tr>
<tr>
<td>5</td>
<td>BH₃–AH₃</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>No</td>
</tr>
<tr>
<td>6</td>
<td>BH₃–AH₃</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>Yes</td>
</tr>
<tr>
<td>7</td>
<td>BH₃–AH₂⁺</td>
<td>MIDI!</td>
<td>GLO</td>
<td>Yes</td>
</tr>
<tr>
<td>8</td>
<td>CH₃BH₂–AH₂CH₂⁺</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>Yes</td>
</tr>
<tr>
<td>9</td>
<td>CH₃BH₂–AH₂CH₃</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>Yes</td>
</tr>
<tr>
<td>10</td>
<td>BH₃AH₂–AH₂BH₃</td>
<td>MIDI!</td>
<td>GLO</td>
<td>No</td>
</tr>
<tr>
<td>11</td>
<td>BH₃–AH₂(CH₂)₂AH₂–BH₃</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>Yes</td>
</tr>
<tr>
<td>12</td>
<td>CH₃BH₂–AH₂CH₂O⁻</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>Yes</td>
</tr>
<tr>
<td>13</td>
<td>CH₃BH₂–AH=CH₂</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>Yes</td>
</tr>
<tr>
<td>14</td>
<td>Ethyl benzene</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>Yes</td>
</tr>
<tr>
<td>15</td>
<td>Alanine dipeptide</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>Yes</td>
</tr>
<tr>
<td>16</td>
<td>n-octane</td>
<td>MIDI!</td>
<td>LLO:FGV</td>
<td>Yes</td>
</tr>
<tr>
<td>17</td>
<td>CH₃BH₂–AH₃</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>Yes</td>
</tr>
</tbody>
</table>

The 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-AHF 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**

<table>
<thead>
<tr>
<th>Cycle</th>
<th>ENERGY</th>
<th>Delta-E</th>
<th>GRMS</th>
<th>Step-size</th>
</tr>
</thead>
<tbody>
<tr>
<td>48</td>
<td>-28038.66958</td>
<td>.00013</td>
<td>.16921</td>
<td>.00052</td>
</tr>
<tr>
<td>9.15538</td>
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<tr>
<td>1.42305</td>
<td>-.59905</td>
<td>.86397</td>
<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td>1.60774</td>
<td>1.35758</td>
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<td>.00000</td>
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<tr>
<td>2.70831</td>
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<td>1.35504</td>
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</table>

**test2.out**

<table>
<thead>
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<th>Delta-E</th>
<th>GRMS</th>
<th>Step-size</th>
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<td>42</td>
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<td>1.72777</td>
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</tr>
<tr>
<td>1.00000</td>
<td>ETHA 1</td>
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</tr>
<tr>
<td>1.35498</td>
<td>2.06461</td>
<td>ETHA 1</td>
<td>.00000</td>
<td>.00000</td>
</tr>
</tbody>
</table>
COORDINATE FILE MODULE
TITLE>  * TEST 2: ETHANE GHO-AIHF/STO-3G (NDDAO, UNSCALED)

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

CHARMM>
CHARMM>    print coor
CHARMM>

COORDINATE FILE MODULE
TITLE>  * TEST 3: GHO-AIHF/STO-3G (GLO, UNSCALED)

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

CHARMM>
CHARMM>    print coor
CHARMM>

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

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
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<thead>
<tr>
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<th>1 ETHA H11</th>
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<th>.00928</th>
<th>.00001</th>
<th>ETHA 1</th>
<th>.00000</th>
</tr>
</thead>
<tbody>
<tr>
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<td>1 ETHA H12</td>
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<td>-.89000</td>
<td>ETHA 1</td>
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</tr>
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<td></td>
<td>1 ETHA H13</td>
<td>1.46775</td>
<td>-.52058</td>
<td>.89016</td>
<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td></td>
<td>1 ETHA C2</td>
<td>1.62579</td>
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<td>-.00014</td>
<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td></td>
<td>1 ETHA H21</td>
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<td>1.44038</td>
<td>.00014</td>
<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td></td>
<td>1 ETHA H22</td>
<td>1.28016</td>
<td>1.97710</td>
<td>-.90169</td>
<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td></td>
<td>1 ETHA H23</td>
<td>1.28012</td>
<td>1.97718</td>
<td>.90182</td>
<td>ETHA 1</td>
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</tr>
</tbody>
</table>

**test7.out**

<table>
<thead>
<tr>
<th>ABNR MIN: Cycle</th>
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<th>Delta-E</th>
<th>GRMS</th>
<th>Step-size</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABNR INTERN:</td>
<td>BONDS</td>
<td>ANGLES</td>
<td>UREY-b</td>
<td>DIHEDRALS</td>
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<tr>
<td>ABNR EXTERN:</td>
<td>VDWaals</td>
<td>ELEC</td>
<td>HBONds</td>
<td>ASP</td>
</tr>
<tr>
<td>ABNR QUANTUM:</td>
<td>QMELec</td>
<td>QMVDw</td>
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<td>ABNR QUANTM:</td>
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<td></td>
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</tr>
</tbody>
</table>

**CHARMM>**

**print coor**

**COORDINATE FILE MODULE**

**TITLE>** * TEST 7: ETHYL GHO-AIUF/MIDIBANG (GLO==LLO:FG, SCALED)

|   | 1 ETHP C1     | 1.05807 | .04118 | -.11040 | ETHP 1 | .00000 |
|   | 1 ETHP H11    | .00185  | -.05385| .06948  | ETHP 1 | .00000 |
|   | 1 ETHP H12    | 1.49957 | -.60196| -.85130 | ETHP 1 | .00000 |
|   | 1 ETHP C2     | 1.62372 | 1.43703| -.02182 | ETHP 1 | .00000 |
|   | 1 ETHP H21    | 2.74564 | 1.42882| .00301  | ETHP 1 | .00000 |
|   | 1 ETHP H22    | 1.31535 | 2.06768| -.89836 | ETHP 1 | .00000 |
|   | 1 ETHP H23    | 1.27731 | 1.96618| .90583  | ETHP 1 | .00000 |

**test8.out**

<table>
<thead>
<tr>
<th>ABNR MIN: Cycle</th>
<th>ENERGY</th>
<th>Delta-E</th>
<th>GRMS</th>
<th>Step-size</th>
</tr>
</thead>
<tbody>
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<td>ABNR INTERN:</td>
<td>BONDS</td>
<td>ANGLES</td>
<td>UREY-b</td>
<td>DIHEDRALS</td>
</tr>
<tr>
<td>ABNR EXTERN:</td>
<td>VDWaals</td>
<td>ELEC</td>
<td>HBONds</td>
<td>ASP</td>
</tr>
<tr>
<td>ABNR QUANTUM:</td>
<td>QMELec</td>
<td>QMVDw</td>
<td></td>
<td></td>
</tr>
<tr>
<td>------------------</td>
<td>--------</td>
<td>---------</td>
<td>------</td>
<td>-----------</td>
</tr>
<tr>
<td>51</td>
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<td></td>
</tr>
</tbody>
</table>

**CHARMM>**

**print coor**

**COORDINATE FILE MODULE**

**TITLE>** * TEST 8: BUTYL GHO-AIUF/MIDIBANG (LLO:FG, SCALED)

|   | 1 BUTP C1     | 1.04503 | .10511 | .15616  | BUTP 1 | .00000 |
|   | 1 BUTP H11    | -.00102 | -.07983| -.01469 | BUTP 1 | .00000 |
|   | 1 BUTP H12    | 1.65752 | -.70530| .51000  | BUTP 1 | .00000 |
|   | 1 BUTP H21    | 1.59559 | 1.51613| .06278  | BUTP 1 | .00000 |
|   | 1 BUTP H22    | 1.26226 | 2.13271| .89541  | BUTP 1 | .00000 |
|   | 1 BUTP H23    | 1.27354 | 2.00968| -.84931 | BUTP 1 | .00000 |
ABNR MIN: Cycle ENERgy Delta-E GRMS Step-size
ABNR INTERN: BONDs ANGLEs UREY-b DIHEdral IMPRoper
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)

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

ABNR MIN: Cycle ENERgy Delta-E GRMS Step-size
ABNR INTERN: BONDs ANGLEs UREY-b DIHEdral IMPRoper
ABNR EXTERN: VDWaals ELEC HBONds ASP USER
ABNR QUANTUM: QMElec QMVdW

---------- --------- --------- --------- ---------
ABNR>  40  -55117.45337  .00019  .16443  .00066
ABNR INTERN>  .13347  1.78536  .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)

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

CHARMM>
CHARMM>  print coor

COORDINATE FILE MODULE

TITLE>  * TEST 10: BUTANE GHO-AIHF/MIDIBANG (GLO, UNSCALED)

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
### test11.out

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### test12.out

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<td>3.36323</td>
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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> -1.09592    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)

CHARMM>

COORDINATE FILE MODULE

---

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  1.83952 BENE 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
| 1  | ALAD NR | 4.37426 | 1.89522 | -0.08505 | ALAD 1 | .00000 |
| 2  | ALAD HR | 3.97868 | 2.81259 | -0.18124 | ALAD 1 | .00000 |
| 3  | ALAD CR | 5.80372 | 1.67468 | -0.23400 | ALAD 1 | .00000 |
| 4  | ALAD HR1| 6.28110 | 2.63048 | -0.41219 | ALAD 1 | .00000 |
| 5  | ALAD HR2| 6.00848 | 1.01118 | -1.06794 | ALAD 1 | .00000 |
| 6  | ALAD HR3| 6.21782 | 1.23065 | .66510   | ALAD 1 | .00000 |
| 7  | ALAD CRP| 3.54673 | .85864  | 1.4041   | ALAD 1 | .00000 |
| 8  | ALAD OR | 3.90079 | -.28386 | .24309   | ALAD 1 | .00000 |
| 9  | ALAD CA | 2.04978 | 1.26108 | .26055   | ALAD 1 | .00000 |
| 10 | ALAD NL | 1.26841 | .08370  | .24400   | ALAD 1 | .00000 |
| 11 | ALAD HA | 1.68871 | 1.87636 | -.58065  | ALAD 1 | .00000 |
| 12 | ALAD CB | 1.76312 | 2.07897 | 1.52625  | ALAD 1 | .00000 |
| 13 | ALAD HB1| 2.02900 | 1.50201 | 2.43769  | ALAD 1 | .00000 |
| 14 | ALAD HB2| 2.32372 | 3.03652 | 1.53059  | ALAD 1 | .00000 |
| 15 | ALAD HB3| .67716  | 2.31602 | 1.57645  | ALAD 1 | .00000 |
| 16 | ALAD CLP| .01168  | .01106  | .20714   | ALAD 1 | .00000 |
| 17 | ALAD CL  |-.60156 | .98118  | -.62863  | ALAD 1 | .00000 |
| 18 | ALAD CL  |-.60996 | .91296  | -.17234  | ALAD 1 | .00000 |
| 19 | ALAD HL1| -1.63698| -1.26992| -.59290  | ALAD 1 | .00000 |
| 20 | ALAD HL2| -.66908| -1.69471| .87457   | ALAD 1 | .00000 |
| 21 | ALAD HL3| -.01222| -2.04209| -.77942  | ALAD 1 | .00000 |

**test16.out**

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**CHARMM>**

print coor
ENER ENR: Eval#     ENERgy      Delta-E         GRMS
ENER INTERN:          BONDs       ANGLes       UREY-b    DIHEdralS    IMPRopers
ENER EXTERN:        VDWaals         ELEC       HBONdS          ASP         USER
ENER QUANTM:        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     -.15541   -.90511    .90100 PROP 1       .00000
4 1 PROP H13     1.49194   -.52511    .90100 PROP 1       .00000
5 1 PROP H21    1.23582   1.98632    .90857 PROP 1       .00000
6 1 PROP H22    1.23582   1.98632    .90857 PROP 1       .00000
7 1 PROP H23    1.23582   1.98632    .90857 PROP 1       .00000
8 1 PROP H32    3.56954   1.02369    .90100 PROP 1       .00000
9 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=    .00000
DIM.  ATOM  ANALYT   FINITE-DIFF  DEVIATION
  1   X ( PROP 1    PROP C1  )    -.31808672    -.31828984       .00020312
  1   X ( PROP 1    PROP H11 )    32.92538287    32.92548105       .00009818
  1   X ( PROP 1    PROP H12 )    -.00000000   -.00000001       .00000001
  1   X ( PROP 1    PROP H13 )    32.92538287    32.92548105       .00009818
  1   X ( PROP 1    PROP H21 )    -.00000000   -.00000001       .00000001
  1   X ( PROP 1    PROP H22 )    32.92538287    32.92548105       .00009818
  1   X ( PROP 1    PROP H23 )    32.92538287    32.92548105       .00009818
  1   X ( PROP 1    PROP H32 )    32.92538287    32.92548105       .00009818
  1   X ( PROP 1    PROP H33 )    32.92538287    32.92548105       .00009818

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**TESTFD:** A total of 0 elements were within the tolerance.
Platforms for which CHARMM/GAMESSPLUS Has Been Tested

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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:

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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.