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
The code and manual are copyrighted, 2004-2008.

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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/GAMESPLUSS* 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.

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**Introduction**

To perform combined QM/MM calculations using the GHO boundary treatment at the HF level through the *CHARMM/GAMESPLUSS* 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/GAMESPLUSS* 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/GAMESPLUSS* 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/GAMESPLUSS* 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/GAMESPLUSS*. 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/GAMESPLUS combination package to incorporate the QM/MM calculations with generalized hybrid orbital (GHO) boundary treatment at the \textit{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/GAMESPLUS 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) \textbf{J. Chem. Phys. Format:}


B) \textbf{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

<table>
<thead>
<tr>
<th>blur.src</th>
<th>charmm_main.src</th>
<th>ddi.src</th>
</tr>
</thead>
<tbody>
<tr>
<td>enefscal.src</td>
<td>eintern.src</td>
<td>gameess.mk</td>
</tr>
<tr>
<td>gamint.mk</td>
<td>ghogms.fcm</td>
<td>gmscomp_ibmsp</td>
</tr>
<tr>
<td>gukini.src</td>
<td>install_cgplus.com</td>
<td>Makefile</td>
</tr>
<tr>
<td>Makefile_ibmsp</td>
<td></td>
<td></td>
</tr>
<tr>
<td>update.src</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

glohftest  Contains the test suite for testing GHO-AIHF
data/
gphoonf.topo  all topology files used in 17 test runs for GHO-AIHF
dataadir.def  the file to specify data directory and scratch directory for CHARMM

Input/
testx.inp  where $x = 1 \rightarrow 17$
sto3g.str  the GAMESSPLUS input file for test$m$.inp ($m = 1 \rightarrow 3$)
631gd.str  the GAMESSPLUS input file for test4.inp
midib.str  the GAMESSPLUS input file for test$n$.inp ($n = 5, 6, 9 \rightarrow 11, 13 \rightarrow 17$)
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 $x = 1 \rightarrow 17$
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 DDL_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) efs.cals.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:
   ```bash
   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 \( (p_A|T|p_B) \), CSTP for \( (s_B|T|p_B) \), 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 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-AIH 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:

```plaintext
* 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 aoin    "scr/test.ao"
envi dasort  "scr/test.f20"
envi extbas  "midib-gho.bas"

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

mini abnr nstep 200 tolg 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 "games" 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 "gilofg". 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
   RUNTP=GRADIENT
   INTTYP=HONDO
   MAXIT=200
$END
$SYSTEM MEMORY=1000000 TIMLIM=100000 $END
$BASIS
   ! use as an external basis
   GBASIS=MIDIBA
   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 RUNTP 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  0.6633100000
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 GAMESSPLUS 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-s-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/Inpu. 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 sp² 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 tests 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</th>
<th>System</th>
<th>QM basis</th>
<th>Orthogonalization</th>
<th>Scaling</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>BH$_3$–AH$_3$</td>
<td>STO-3G</td>
<td>PROJ</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>BH$_3$–AH$_3$</td>
<td>STO-3G</td>
<td>NDDAO</td>
<td>No</td>
</tr>
<tr>
<td>3</td>
<td>BH$_3$–AH$_3$</td>
<td>STO-3G</td>
<td>GLO</td>
<td>No</td>
</tr>
<tr>
<td>4</td>
<td>BH$_3$–AH$_3$</td>
<td>6-31G(d)</td>
<td>LLO:FG</td>
<td>No</td>
</tr>
<tr>
<td>5</td>
<td>BH$_3$–AH$_3$</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>No</td>
</tr>
<tr>
<td>6</td>
<td>BH$_3$–AH$_3$</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>Yes</td>
</tr>
<tr>
<td>7</td>
<td>BH$_3$–AH$_2$*</td>
<td>MIDI!</td>
<td>GLO</td>
<td>Yes</td>
</tr>
<tr>
<td>8</td>
<td>CH$_3$BH$_2$–AH$_2$CH$_2$*</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>Yes</td>
</tr>
<tr>
<td>9</td>
<td>CH$_3$BH$_2$–AH$_2$CH$_3$</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>Yes</td>
</tr>
<tr>
<td>10</td>
<td>BH$_3$AH$_2$–AH$_2$BH$_3$</td>
<td>MIDI!</td>
<td>GLO</td>
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</tr>
<tr>
<td>11</td>
<td>BH$_3$–AH$_2$(CH$_2$)$_2$AH$_2$–BH$_3$</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>Yes</td>
</tr>
<tr>
<td>12</td>
<td>CH$_3$BH$_2$–AH$_2$CH$_2$O$^-$</td>
<td>MIDI!</td>
<td>LLO:FG</td>
<td>Yes</td>
</tr>
<tr>
<td>13</td>
<td>CH$_3$BH$_2$–AH=CH$_2$</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>CH$_3$BH$_2$–AH$_3$</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-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**

<table>
<thead>
<tr>
<th>ABNR MIN: Cycle</th>
<th>ENERgy</th>
<th>Delta-E GRMS</th>
<th>Step-size IMPRopers</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABNR INTERN:</td>
<td>BONDs</td>
<td>ANGLes UREY-b DIHEdrals IMPRopers</td>
<td></td>
</tr>
<tr>
<td>ABNR EXTERN:</td>
<td>VDWaals ELEC HBONds ASP USER</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ABNR QUANTUM:</td>
<td>QMElec QMVDw</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ABNR&gt;</td>
<td>-28038.86958 .00013 .16921 .00052</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ABNR INTERN&gt;</td>
<td>.09058 9.15538 .80001 .00000 .00000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ABNR EXTERN&gt;</td>
<td>-.16896 .00000 .00000 .00000 .00000</td>
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<td></td>
</tr>
<tr>
<td>ABNR QUANTM&gt;</td>
<td>-28048.74659 .00000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHARMM&gt;</td>
<td>print coor</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**test2.out**

<table>
<thead>
<tr>
<th>ABNR MIN: Cycle</th>
<th>ENERgy</th>
<th>Delta-E GRMS</th>
<th>Step-size IMPRopers</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABNR INTERN:</td>
<td>BONDs</td>
<td>ANGLes UREY-b DIHEdrals IMPRopers</td>
<td></td>
</tr>
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<td></td>
</tr>
<tr>
<td>ABNR QUANTUM:</td>
<td>QMElec QMVDw</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ABNR&gt;</td>
<td>-28187.52117 .00028 .19742 .00078</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ABNR INTERN&gt;</td>
<td>.59934 .17277 3.70898 .00000 .00000</td>
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<td></td>
</tr>
<tr>
<td>ABNR EXTERN&gt;</td>
<td>.19650 .00000 .00000 .00000 .00000</td>
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<td></td>
</tr>
<tr>
<td>ABNR QUANTM&gt;</td>
<td>-28192.19876 .00000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHARMM&gt;</td>
<td>print coor</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
COORDINATE FILE MODULE

**TEST 2: ETHANE GHO-AIHF/STO-3G (NDDAO, UNSCALED)**

<table>
<thead>
<tr>
<th>No.</th>
<th>Atom 1</th>
<th>Atom 2</th>
<th>Atom 3</th>
<th>Atom 4</th>
<th>Atom 5</th>
<th>Atom 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ETHA C1</td>
<td>1.15642</td>
<td>.12388</td>
<td>-.00001</td>
<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td>2</td>
<td>ETHA H11</td>
<td>.07951</td>
<td>.14149</td>
<td>.00002</td>
<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td>3</td>
<td>ETHA H12</td>
<td>1.51249</td>
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<td>-.88093</td>
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</tr>
<tr>
<td>4</td>
<td>ETHA H13</td>
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</tr>
<tr>
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<td>ETHA C2</td>
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</tr>
<tr>
<td>6</td>
<td>ETHA H21</td>
<td>2.72428</td>
<td>1.27776</td>
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<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td>7</td>
<td>ETHA H22</td>
<td>1.20871</td>
<td>1.83233</td>
<td>-.93177</td>
<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td>8</td>
<td>ETHA H23</td>
<td>1.20876</td>
<td>1.83232</td>
<td>.93160</td>
<td>ETHA 1</td>
<td>.00000</td>
</tr>
</tbody>
</table>

**TEST 3: GHO-AIHF/STO-3G (GLO, UNSCALED)**

<table>
<thead>
<tr>
<th>No.</th>
<th>Atom 1</th>
<th>Atom 2</th>
<th>Atom 3</th>
<th>Atom 4</th>
<th>Atom 5</th>
<th>Atom 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ETHA C1</td>
<td>1.07013</td>
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<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td>2</td>
<td>ETHA H11</td>
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<td>-.01738</td>
<td>.00001</td>
<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td>3</td>
<td>ETHA H12</td>
<td>1.43220</td>
<td>-.56721</td>
<td>-.88853</td>
<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td>4</td>
<td>ETHA H13</td>
<td>1.43221</td>
<td>-.56722</td>
<td>.88855</td>
<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td>5</td>
<td>ETHA C2</td>
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</tr>
<tr>
<td>6</td>
<td>ETHA H21</td>
<td>2.77616</td>
<td>1.46951</td>
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<td>ETHA H22</td>
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</tbody>
</table>

**TEST 4: ETHANE GHO-AIHF/6-31G(D) (LLO:FG, UNSCALED)**

<table>
<thead>
<tr>
<th>No.</th>
<th>Atom 1</th>
<th>Atom 2</th>
<th>Atom 3</th>
<th>Atom 4</th>
<th>Atom 5</th>
<th>Atom 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ETHA C1</td>
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<td>-.00003</td>
<td>ETHA 1</td>
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<tr>
<td>2</td>
<td>ETHA H11</td>
<td>-.00612</td>
<td>-.01738</td>
<td>.00001</td>
<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td>3</td>
<td>ETHA H12</td>
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<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
<td>4</td>
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<td>-.56722</td>
<td>.88855</td>
<td>ETHA 1</td>
<td>.00000</td>
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<tr>
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<td>ETHA C2</td>
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<td>1.46047</td>
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<td>.00000</td>
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<tr>
<td>6</td>
<td>ETHA H21</td>
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<td>1.46951</td>
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<td>ETHA 1</td>
<td>.00000</td>
</tr>
<tr>
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<td>ETHA H23</td>
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<td>2.02267</td>
<td>.90190</td>
<td>ETHA 1</td>
<td>.00000</td>
</tr>
</tbody>
</table>
test5.out

ABNR MIN: Cycle      ENERgy      Delta-E     GRMS      Step-size
ABNR INTERN:        NDNs      ANGLes      UREY-b     DIHEdrams  IMPRopers
ABNR EXTERN:        VDWaals      ELEC      HBONds      ASP      USER
ABNR QUANTUM:        QMELec      QMVDr
-----------  ------------  ------------  ------------  ------------  ------------
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)

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 .00000 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

test6.out

ABNR> Minimization exiting with gradient tolerance (.2000000) satisfied.

ABNR MIN: Cycle      ENERgy      Delta-E     GRMS      Step-size
ABNR INTERN:        NDNs      ANGLes      UREY-b     DIHEdrams  IMPRopers
ABNR EXTERN:        VDWaals      ELEC      HBONds      ASP      USER
ABNR QUANTUM:        QMELec      QMVDr
-----------  ------------  ------------  ------------  ------------  ------------
ABNR>       32 -27974.19232       .00059       .19641       .00092
ABNR INTERN>        .08355      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)

8

1 1 ETHA C1  1.10280 -.02242 -.00018 ETHA 1 .00000
<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>2</td>
<td>1 ETHA H11</td>
<td>.01994</td>
<td>.00928</td>
<td>.00001 ETHA 1</td>
</tr>
<tr>
<td>3</td>
<td>1 ETHA H12</td>
<td>1.46770</td>
<td>-.52049</td>
<td>-.89000 ETHA 1</td>
</tr>
<tr>
<td>4</td>
<td>1 ETHA H13</td>
<td>1.46775</td>
<td>-.52058</td>
<td>.89016 ETHA 1</td>
</tr>
<tr>
<td>5</td>
<td>1 ETHA C2</td>
<td>1.62579</td>
<td>1.40681</td>
<td>.00001 ETHA 1</td>
</tr>
<tr>
<td>6</td>
<td>1 ETHA H21</td>
<td>2.74693</td>
<td>1.44038</td>
<td>.00001 ETHA 1</td>
</tr>
<tr>
<td>7</td>
<td>1 ETHA H22</td>
<td>1.28016</td>
<td>1.97710</td>
<td>-.90169 ETHA 1</td>
</tr>
<tr>
<td>8</td>
<td>1 ETHA H23</td>
<td>1.28012</td>
<td>1.97718</td>
<td>.90182 ETHA 1</td>
</tr>
</tbody>
</table>

**test7.out**

<table>
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<th>Step-size</th>
</tr>
</thead>
<tbody>
<tr>
<td>38</td>
<td>-27576.38145</td>
<td>.00023</td>
<td>.17644</td>
<td>.00072 ETHA 1</td>
</tr>
<tr>
<td>12609</td>
<td>2.79664</td>
<td>.13141</td>
<td>.04275</td>
<td>.00000 ETHA 1</td>
</tr>
<tr>
<td>-.31247</td>
<td>5.50935</td>
<td>.00000</td>
<td>.00000</td>
<td>.00000 ETHA 1</td>
</tr>
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</table>

**test8.out**

<table>
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<th>GRMS</th>
<th>Step-size</th>
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</thead>
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<tr>
<td>51</td>
<td>-51910.54551</td>
<td>.00322</td>
<td>.14651</td>
<td>.00236 ETHA 1</td>
</tr>
<tr>
<td>11472</td>
<td>2.79664</td>
<td>.13141</td>
<td>.04275</td>
<td>.00000 ETHA 1</td>
</tr>
<tr>
<td>-.31247</td>
<td>5.50935</td>
<td>.00000</td>
<td>.00000</td>
<td>.00000 ETHA 1</td>
</tr>
</tbody>
</table>

**COORDINATE FILE MODULE**

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

**COORDINATE FILE MODULE**

**TITLE> * TEST 8: BUTYL GHO-AIUHF/MIDIBANG (LLO:FG, SCALED)**
### test9.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>36</td>
<td>-52304.49070</td>
<td>.00024</td>
<td>.16443</td>
<td>.00066</td>
</tr>
</tbody>
</table>

**ABNR INTERN:**

- **BONDs**: .13140
- **ANGLES**: 2.96205
- **UREY-b**: .87729
- **DIHEDrals**: .01146
- **IMPRopers**: .00000

**ABNR EXTERN:**

- **VDWaals**: .00000
- **ELEC**: .00000
- **HBONds**: .00000
- **ASP**: .00000
- **USER**: .00000

**ABNR QUANTM:**

- **QMELec**: -52312.88170
- **QMVDw**: .00000

### test10.out

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<th>Delta-E</th>
<th>GRMS</th>
<th>Step-size</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>-55117.45337</td>
<td>.00019</td>
<td>.01146</td>
<td>.00000</td>
</tr>
</tbody>
</table>

**ABNR INTERN:**

- **BONDs**: .13347
- **ANGLES**: 1.78566
- **UREY-b**: .92019
- **DIHEDrals**: .00000
- **IMPRopers**: .00000

**ABNR EXTERN:**

- **VDWaals**: .00000
- **ELEC**: .00000
- **HBONds**: .00000
- **ASP**: .00000
- **USER**: .00000

**ABNR QUANTM:**

- **QMELec**: -55123.07159
- **QMVDw**: .00000

---

**CHARMM> print coor**

**COORDINATE FILE MODULE**

**TITLE> * TEST 9: BUTANE GHO-AIHF/MIDIBANG (LLO:FG, SCALED)**

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

**TITLE> * TWO GHO BOUNDARY ATOMS**
<table>
<thead>
<tr>
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<th>Delta-E</th>
<th>GRMS</th>
<th>Step-size</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.61218</td>
<td>1.46283</td>
<td>-.00001</td>
<td>BUTA 1</td>
</tr>
<tr>
<td>2</td>
<td>1.20242</td>
<td>1.94605</td>
<td>-.87690</td>
<td>BUTA 1</td>
</tr>
<tr>
<td>3</td>
<td>1.20241</td>
<td>1.94604</td>
<td>.87689</td>
<td>BUTA 1</td>
</tr>
<tr>
<td>4</td>
<td>3.18445</td>
<td>1.53773</td>
<td>-.00008</td>
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</tr>
<tr>
<td>5</td>
<td>3.59422</td>
<td>1.94604</td>
<td>.87689</td>
<td>BUTA 1</td>
</tr>
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<td>6</td>
<td>1.08243</td>
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<td>.00011</td>
<td>BUTA 1</td>
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<tr>
<td>7</td>
<td>3.71421</td>
<td>3.00722</td>
<td>-.00003</td>
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<tr>
<td>8</td>
<td>-.03245</td>
<td>-.10180</td>
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<td>BUTA 1</td>
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<tr>
<td>9</td>
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<td>3.10236</td>
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<td>10</td>
<td>4.2908</td>
<td>3.10236</td>
<td>.00000</td>
<td>BUTA 1</td>
</tr>
<tr>
<td>11</td>
<td>4.2908</td>
<td>3.10236</td>
<td>.00000</td>
<td>BUTA 1</td>
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**test11.out**

<table>
<thead>
<tr>
<th>ABNR MIN: Cycle</th>
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<th>Delta-E</th>
<th>GRMS</th>
<th>Step-size</th>
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<tbody>
<tr>
<td></td>
<td>32</td>
<td>103907.66990</td>
<td>.00101</td>
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<td></td>
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<td>103915.05446</td>
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**test12.out**

<table>
<thead>
<tr>
<th>ABNR MIN: Cycle</th>
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<th>GRMS</th>
<th>Step-size</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>4.2908</td>
<td>3.10236</td>
<td>.00000</td>
<td>BUTA 1</td>
</tr>
</tbody>
</table>
ABNR EXTERN: VDWaals ELEC HBONds ASP USER
ABNR QUANTUM: QMElec QMVDw

---

ABNR> 32 -98594.55968 0.00523 0.17621 0.00153
ABNR INTERN> 0.10296 3.73141 0.23813 0.04104 0.00000
ABNR EXTERN> -0.48883 5.54501 0.00000 0.00000 0.00000
ABNR QUANTM> -98603.72940 0.00000

---

CHARMM>
CHARMM> print coor
COORDINATE FILE MODULE

TITLE> * TEST 12: CH3BH2-AH2CH2 (ANION)
TITLE> * GHO-AIHF/MIDIBANG (LLO:FG, SCALED)

14 1 1 BTOA C1 1.14692 -.05813 .07719 BTOA 1 0.00000
2 1 BTOA O1 1.55675 -.70068 1.14228 BTOA 1 0.00000
3 1 BTOA H11 .01744 .04514 -.08610 BTOA 1 0.00000
4 1 BTOA H12 1.46968 -.45657 -.94757 BTOA 1 0.00000
5 1 BTOA C2 1.64927 1.45483 .04290 BTOA 1 0.00000
6 1 BTOA H21 2.73708 1.46698 .07121 BTOA 1 0.00000
7 1 BTOA H22 1.28684 1.96799 .93149 BTOA 1 0.00000
8 1 BTOA C3 1.18381 2.23434 -1.19574 BTOA 1 0.00000
9 1 BTOA H31 .06802 2.28228 1.29965 BTOA 1 0.00000
10 1 BTOA H32 1.52355 1.77944 -2.16307 BTOA 1 0.00000
11 1 BTOA C4 1.66478 3.69599 -1.23618 BTOA 1 0.00000
12 1 BTOA H41 2.77387 3.72131 -1.22504 BTOA 1 0.00000
13 1 BTOA H42 1.28705 4.23497 -.34306 BTOA 1 0.00000
14 1 BTOA H43 1.29531 4.19866 -2.15179 BTOA 1 0.00000

test13.out

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

---

ABNR> 35 -51558.58268 .00013 1.6699 .00067
ABNR INTERN> .15512 3.09549 .04049 1.49750 0.00000
ABNR EXTERN> .20016 5.48577 0.00000 0.00000 0.00000
ABNR QUANTM> -51569.05722 0.00000

---

CHARMM>
CHARMM> print coor
COORDINATE FILE MODULE

TITLE> * TEST 13: BUTENE GHO-AIHF/MIDIBANG (LLO:FG, SCALED)

12 1 1 BENE C1 .95819 -.04465 -.00680 BENE 1 0.00000
2 1 BENE H11 -.09707 -.05624 -.22206 BENE 1 0.00000
3 1 BENE H12 1.42200 -.99929 .16458 BENE 1 0.00000
4 1 BENE C2 1.65580 1.07112 .04813 BENE 1 0.00000
5 1 BENE H21 2.70790 1.05012 .26905 BENE 1 0.00000
6 1 BENE C3 1.07842 2.45389 -.17556 BENE 1 0.00000
7 1 BENE H31 1.56805 2.98242 -1.04060 BENE 1 0.00000
8 1 BENE H32 -.02168 2.42457 -.41632 BENE 1 0.00000
9 1 BENE C4 1.23932 3.36323 1.05139 BENE 1 0.00000
### test14.out

<table>
<thead>
<tr>
<th>Cycle</th>
<th>Energy (kcal/mol)</th>
<th>Delta-E (kcal/mol)</th>
<th>GRMS</th>
<th>Step-size</th>
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<tbody>
<tr>
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<table>
<thead>
<tr>
<th>Step</th>
<th>Bond Lengths (Å)</th>
<th>Angle (°)</th>
<th>Torsion (°)</th>
<th>Improper Angles (°)</th>
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<tbody>
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<table>
<thead>
<tr>
<th>Step</th>
<th>VDW Energies (kcal/mol)</th>
<th>Electrostatic Energies (kcal/mol)</th>
<th>H-Bond Energies (kcal/mol)</th>
<th>Other Energies (kcal/mol)</th>
</tr>
</thead>
<tbody>
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### test15.out

<table>
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<tr>
<th>Cycle</th>
<th>Energy (kcal/mol)</th>
<th>Delta-E (kcal/mol)</th>
<th>GRMS</th>
<th>Step-size</th>
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<th>Step</th>
<th>Bond Lengths (Å)</th>
<th>Angle (°)</th>
<th>Torsion (°)</th>
<th>Improper Angles (°)</th>
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<table>
<thead>
<tr>
<th>Step</th>
<th>VDW Energies (kcal/mol)</th>
<th>Electrostatic Energies (kcal/mol)</th>
<th>H-Bond Energies (kcal/mol)</th>
<th>Other Energies (kcal/mol)</th>
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CHARMM>

CHARMM> print coor

COORDINATE FILE MODULE

---

CHARMM>

CHARMM> print coor

COORDINATE FILE MODULE
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<td>19</td>
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<tr>
<td>20</td>
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<td>6.12710</td>
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<tr>
<td>21</td>
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<tr>
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<td>-0.02134</td>
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**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 QUANTM:  QMELec QMVdW

---

ENER>  0  -27962.05020  27964.68930  10.85777
ENER INTERN>  .00795  1.70387  0.01390  0.00433  0.00000
ENER EXTERN> -2.27613  5.41804  0.00000  0.00000
ENER QUANTM> -27968.92216  0.00000
---

CHARMM>
CHARMM>    print coor
COORDINATE FILE MODULE
TITLE>  * TEST 17: PROPANE GHO-AIHF/MIDIBANG (LLO:FG, SCALED)
TITLE>  * SINGLE POINT ENERGY, TEST ANALYTICAL GRADIENT

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 .00000000 .00000000
2 X ( PROP 1 PROP H11 ) -20.70570991 -20.70552640 .00018350
2 Y ( PROP 1 PROP H11 ) -6.25333307 -6.25333307 .00000231
2 Z ( PROP 1 PROP H11 ) .00000000 .00000000 .00000000
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 .0008774
```
|   | PROP 1 | PROP H13 |   | PROP 1 | PROP C2 |   | PROP 1 | PROP H21 |   | PROP 1 | PROP H22 |   | PROP 1 | PROP C3 |   | PROP 1 | PROP H31 |   | PROP 1 | PROP H32 |   | PROP 1 | PROP H33 |   |
|---|--------|---------|---|--------|--------|---|--------|---------|---|--------|---------|---|--------|--------|---|--------|---------|---|--------|---------|---|--------|---------|
| 4 | X      | 4.76105154 | 4.76105729 | -0.0000575 |
| 4 | Y      | -14.91708288 | -14.91707466 | -0.0000821 |
| 4 | Z      | -15.97124675 | -15.97115898 | -0.0008777 |
| 5 | X      | 17.84082701 | 17.84083549 | 0.0000849 |
| 5 | Y      | 25.92580365 | 25.92561241 | 0.0019125 |
| 5 | Z      | 0.00000000 | 0.00000000 | 0.0000000 |
| 6 | X      | -2.96784857 | -2.96786753 | 0.0001896 |
| 6 | Y      | -12.03327445 | -12.03326652 | -0.0000793 |
| 6 | Z      | -3.66397293 | -3.66396394 | -0.0000899 |
| 7 | X      | -2.96784858 | -2.96786752 | 0.0001895 |
| 7 | Y      | -12.03327445 | -12.03326648 | -0.0000797 |
| 7 | Z      | 3.66397293 | 3.66396393 | 0.0000900 |
| 8 | X      | -2.92393558 | -2.92400548 | 0.0006990 |
| 8 | Y      | 1.36785794 | 1.36790072 | -0.0004278 |
| 8 | Z      | 0.00000000 | 0.00000001 | 0.0000001 |
| 9 | X      | 0.91492800 | 0.91494444 | -0.0001645 |
| 9 | Y      | 0.56993380 | 0.56993983 | -0.0000603 |
| 9 | Z      | 0.00000000 | 0.00000001 | 0.0000001 |
| 10 | X    | 0.80278563 | 0.80280398 | -0.0001836 |
| 10 | Y    | -0.31746526 | -0.31748567 | 0.0002041 |
| 10 | Z    | -0.37500432 | -0.37502043 | 0.0001611 |
| 11 | X    | 0.80278563 | 0.80280394 | -0.0001831 |
| 11 | Y    | -0.31746526 | -0.31748565 | 0.0002039 |
| 11 | Z    | 0.37500432 | 0.37502038 | 0.0001605 |

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

<table>
<thead>
<tr>
<th>Computer</th>
<th>Processor</th>
<th>Operating System</th>
<th>Compiler</th>
</tr>
</thead>
<tbody>
<tr>
<td>IBM SP</td>
<td>Power 3</td>
<td>AIX 4.3</td>
<td>XL Fortran Compiler 7.1.12</td>
</tr>
<tr>
<td>IBM Regatta</td>
<td>Power 4</td>
<td>AIX 5.3</td>
<td>XL Fortran Compiler 7.1.12</td>
</tr>
</tbody>
</table>

**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:

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

**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.