

## GAMESS 2022R2 (2022Sep30)

(this version will be installed on Mar 6, 2023)

## Webpage

<https://www.msg.chem.iastate.edu/gamess/index.html>

## Version

2022R2 (2022Sep30)

## Build Environment

- Intel oneAPI Compiler Classic 2022.2.1
- Open MPI 3.1.6

## Files Required

- gamess-current.tar.gz (2022R2)
- gmsnbo.i8.a (NBO7.0)
- rungms\_rccs\_openmpi3 (please check installed rungms)
- exam43.patch

```
--- tests/standard/exam43.inp.orig 2018-03-13 11:58:15.322187865 +0900
+++ tests/standard/exam43.inp 2018-03-13 11:58:32.049289234 +0900
@@ -48,7 +48,7 @@
! geometry in $DATA, although this is not necessary.
!
$contrl scftyp=rhf runtyp=g3mp2 $end
- $system timlim=2 mwords=2 memddi=5 $end
+ $system timlim=2 mwords=30 memddi=5 $end
$scf dirscf=.true. $end
$data
Methane...G3(MP2,CCSD(T))
```

- pbs\_remsh

```
#!/bin/sh
host="$1"
shift
/usr/bin/ssh -n "$host" env PBS_JOBID="$PBS_JOBID" pbs_attach $*
```

## Build Procedure

```
#!/bin/sh

VERSION=2022Sep30
DIRNAME=gamess${VERSION}
INSTDIR=/apl/gamess/2022R2

# files and patches
MYROOT="/home/users/${USER}/Software/GAMESS/gamess${VERSION}"
GAMESS_TARBALL="${MYROOT}/gamess-current.tar.gz"
GAMESS_NBOI8A="${MYROOT}/gmsnbo.i8.a"
PATCH_EXAM43="${MYROOT}/exam43.patch"
RUNGMS_RCCS="${MYROOT}/rungms_rccs_openmpi3"
PBS_REMSH="${MYROOT}/pbs_remsh"

PARALLEL=12

#-----
umask 0022
```

```

export LANG=C
export LC_ALL=C

module -s purge
. ~/intel/oneapi/compiler/2022.2.1/env/vars.sh
. ~/intel/oneapi/mkl/2022.2.1/env/vars.sh
module -s load openmpi/3.1.6/intel2022.2.1

OMPIDIR=/apl/openmpi/3.1.6/intel2022.2.1

cd ${INSTDIR}
if [ -d gamess ]; then
    mv gamess gamess-erase
    rm -rf gamess-erase &
fi

tar xzf ${GAMESS_TARBALL}
mv ${INSTDIR}/gamess/* .
rm -rf ${INSTDIR}/gamess # maybe already empty

for f in comp compall config lked gms-files.csh runall ddi/compddi \
    tools/remd.csh tools/localgms tools/libxc/download-libxc.csh \
    tools/mdi/download-mdi.csh; do
    sed -i -e "1s/.*/#\!\bin\csh -f/" $f
done

patch -p0 < ${PATCH_EXAM43}
cp ${PBS_REMSH} .

expect << EXPECT
spawn csh -f ./config
expect "After the new window is open"
send "\r"
expect "please enter your target machine name:"
send "linux64\r"
expect "GAMESS directory?"
send "${INSTDIR}\r"
expect "GAMESS build directory?"
send "${INSTDIR}\r"
expect "Version?"
send "\r"
expect "Please enter your choice of FORTRAN:"
send "oneapi-ifort\r"
expect "hit <ENTER> to continue to the math library setup."
send "\r"
expect "Enter your choice of 'mkl' or 'atlas' or 'acml' or 'libflame' or 'openblas' or 'pgiblas' or 'armpl' or 'none':"
send "mkl\r"
expect "MKL pathname?"
send "${MKLROOT}\r"
expect "MKL version (or 'proceed')?"
send "proceed\r"
expect "Hit <ENTER> to continue to the GAMESS DDI communications setup."
send "\r"
expect "Hit <ENTER> to set up your network for Linux clusters."
send "\r"
expect "communication library ('serial','sockets' or 'mpi' or 'mixed')?"
send "mpi\r"
expect "Enter MPI library"
send "openmpi\r"
expect "Please enter your openmpi"
send "${OMPIDIR}\r"
expect "Optional: Build LibXC interface?"
send "yes\r"
expect "Hit <ENTER>"
send "\r"

```

```

expect "Optional: Build MDI support?"
send "yes\r"
expect "Hit <ENTER>"
send "\r"
expect "Optional: Build Michigan State University CCT3 & CCSD3A methods?"
send "yes\r"
expect "Do you want to try LIBCCHEM"
send "no\r"
expect "Build GAMESS with OpenMP thread support?"
send "yes\r"
expect "Optional: Build GAMESS with VeraChem's VM2 library? (yes/no):"
send "no\r"
expect "Optional: Build GAMESS with TINKER plug-in? (yes/no):"
send "no\r"
expect "Optional: Build GAMESS with VB2000 plug-in? (yes/no):"
send "yes\r"
expect "Optional: Build GAMESS with XMVB plug-in? (yes/no):"
send "no\r"
expect "Optional: Build GAMESS with NEO plug-in? (yes/no):"
send "yes\r"
expect "Optional: Build GAMESS with NBO plug-in? (yes/no):"
send "yes\r"
expect "Please enter the full file name of your NBO library (being careful about your choice of i4 or i8 integers):"
send "${GAMESS_NBOI8A}\r"
expect eof
EXPECT

# ?
sed -i -e "s/MDI_INSTALL/GMS_3RD_PATH/" Makefile.in
sed -i -e "s/mdi.mod/mdi*.mod/" Makefile.in

make ddi
# do libxc first (according to the installation guide)
csh -f ./tools/libxc/download-libxc.csh
make -j ${PARALLEL} libxc
csh -f ./tools/mdi/download-mdi.csh
make -j ${PARALLEL} libmdi

/bin/cp -f 3rd-party/mdi/objdir/MDI_Library/*.mod 3rd-party/include/mdi
/bin/cp -f 3rd-party/mdi/objdir/MDI_Library/*.mod object/

make modules
make -j ${PARALLEL}

mv rungms rungms.orig
cp ${RUNGMS_RCCS} ./rungms

chmod -R o-rwx source object libccchem
chmod -R o-rwx ddi/src ddi/server ddi/kickoff
find . -name "src" | xargs chmod -R o-rwx

# localgms may need this env variable
export GMSPATH=${INSTDIR}

sed -i -e "s/tools/localgms/rungms/" \
    -e "/RUNGMS/s/VERSION)/VERSION) \$(NCPUS)/" \
    Makefile.in

export OMP_NUM_THREADS=8
make checktest
make clean_exams

export OMP_NUM_THREADS=1

TEST_LIST="eda qmefpea efp-ci standard"

```

```
# Excluded tests
# cim: does not run with parallel, and ksh not avail
# efmo: not enough memory? problem of input?
# excitatino: no avail test for parallel?
# neb: too long
for tp in $TEST_LIST; do
    make checktest NCPUS=8 EXAM_PATH=$tp
done

ipcrm -a
```

## Tests

- Even when "setenv OMPI\_MCA\_mpi\_yield\_when\_idle 1" is done, oversubscribing processes do not improve performance.
  - (please don't use ncpus=32:mpiprocs=64. ncpus=32:mpiprocs=32 would be better.)
  - Single node performance is comparable to sockets version. (I don't know why.) For multinode runs, this MPI version shows better performance than sockets one.
  - HPC-X 2.11 version failed with UCX error. Probably because UCX bundled with HPC-X does not support multi-thread. As a result, multi node performance is quite bad.
    - ~~(The error is caused by hcoll. Therefore, disabling hcoll may change the situation (not yet tried). Error messages disappeared, but the performance and the log (using -x UCX\_LOG\_LEVEL=data) didn't show significant changes.~~
    - UCX used in Open MPI 3.1.6 is multi-thread enabled.
- Intel MPI version failed if number of MPI processes becomes large.
  - (This may be due to libhcoll. Disabling libhcoll may solve this problem.)