

GAMESS-2017Nov11 for LX

Webpage

<http://www.msg.ameslab.gov/GAMESS/GAMESS.html>

Version

2017 Nov 11 R3

Tools for Compiling

- Intel Compiler 17.0.4.196
- Intel MPI 2017.4.196
- Intel MKL 2017.4.196

Necessary Files for Compiling

- gamess-2017Sep30.tar.gz (from GAMESS webpage)
- rungms.patch (See patched 'rungms'.)

Procedure of Compiling

```
#!/bin/csh -f
umask 022
set file_gamess=/home/users/${USER}/build/gamess2017Nov11/gamess-2017Nov11.tar.gz
set work=/work/users/${USER}
set gamess=gamess2017Nov11
set prefix=/local/apl/lx/$gamess
set patch_compall=/home/users/${USER}/build/gamess2017Nov11/compall.patch
set patch_rungms=/home/users/${USER}/build/gamess2017Nov11/cclx/rungms.patch
#-----
cd ${work}
if (-d ${gamess}) then
  mv ${gamess} ${gamess}-erase
  rm -rf ${gamess}-erase &
endif
#-----
tar xzf ${file_gamess}
mv gamess ${gamess}
cd ${work}/${gamess}
sed -i "s/GMS_OPENMP='false'/GMS_OPENMP='true'/" config
sed -i "s/EFP_OPENMP='false'/EFP_OPENMP='true'/" config
sed -i "s/MAKEFP_OPENMP='false'/MAKEFP_OPENMP='true'/" config
sed -i "s/RIMP2_OPENMP='false'/RIMP2_OPENMP='true'/" config
sed -i "s/EXTRAOPT -warn/EXTRAOPT -xHost -warn/" comp
sed -i "s/ext=log/ext=gamess/" tests/standard/checktst
expect <<EXPECT
spawn ./config
expect "After the new window is open"
send "\r"
expect "please enter your target machine name:"
send "linux64\r"
expect "GAMESS directory?"
send "$prefix\r"
expect "GAMESS build directory?"
send "$prefix\r"
expect "Version?"
send "\r"
expect "Please enter your choice of FORTRAN:"
send "ifort\r"
expect "Version?"
send "17\r"
expect "hit <return> to continue to the math library setup."
```

```

expect "\r"
send "\r"
expect "Enter your choice of 'mkl' or 'atlas' or 'acml' or 'pgiblas' or 'none':"
send "mkl\r"
expect "MKL pathname?"
send "$MKLROOT\r"
expect "MKL version (or 'proceed')?"
send "proceed\r"
expect "please hit <return> to compile the GAMESS source code activator "
send "\r"
expect "please hit <return> to set up your network for Linux clusters."
send "\r"
expect "communication library ('sockets' or 'mpi')?"
send "mpi\r"
expect "Enter MPI library (impi, mpich, mpich2, mvapich2, mpt, sockets): "
send "impi\r"
expect "Please enter your impi's location:"
send "$I_MPI_ROOT\r"
expect "Do you want to try LIBCCHEM"
send "no\r"
expect eof
EXPECT
#-----
cd ${work}/${gamsess}/ddi
./compddi
cd ${work}/${gamsess}
#patch -p0 < ${patch_compall}
./compall
./lked
#-----
chmod -R o-rwx source object
find . -name "src" | xargs chmod -R o-rwx
#-----
patch -p0 < ${patch_rungms}
#-----
setenv OMP_NUM_THREADS 8
cd tests/standard
../runtest $prefix/rungms 00 1
./checktst # All tests are OK.
setenv OMP_NUM_THREADS 4
../runtest $prefix/rungms 00 8
./checktst # FAILED but OK: exam05, 32, 39, 42, 45, 46, 4
ipcrm -a

```