GAMESS-2017Apr20 for PRIMERGY

Webpage

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

Version

Apr 20, 2017

Tools for Compiling

- Intel Compiler 17.0.2.174
- Intel MPI 2017.2.174
- Intel MKL 2017.2.174

Necessary Files for Compiling

- gamess-2017Apr20.tar.gz (from GAMESS webpage)
- rungms.patch (See patched 'rungms'.)

Attention

The test "exam13.inp" cannot pass in parallel execution. The higher electrostatic moments cannot be calculated in parallel execution due to its bug.

Procedure of Compiling

```
#!/bin/csh -f
umask 022
set file_gamess=/home/users/${USER}/build/gamess2017Apr20/gamess-2017Apr20.tar.gz
set work=/work/users/${USER}
source /opt/intel/compilers_and_libraries_2017.2.174/linux/bin/compilervars.csh intel64
set gamess=gamess2017Apr20
set patch_compall=/home/users/${USER}/build/gamess2017Apr20/compall.patch
set patch_rungms=/home/users/${USER}/build/gamess2017Apr20/ccpg/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/EXTRAOPT -warn/EXTRAOPT -xHost -warn/' comp
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 "\r"
expect "GAMESS build directory?"
send "\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."
send "\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 ${work}/${gamess}/ddi
./compddi
cd ${work}/${gamess}
# patch -p0 < ${patch_compall}
./compall
./lked
#------------------------------------------------------------------------
chmod -R o-rwx source object
find . -name "src" | xargs chmod -R o-rwx
#------------------------------------------------------------------------
patch -p0 < ${patch_rungms}
```