

GAMESS-2017Apr20 for UV2000

Webpage

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

Version

Apr 20, 2017

Tools for Compiling

- ▶ Intel Compiler 17.0.2.174
- ▶ Intel MKL 2017.2.174

Necessary Files for Compiling

- ▶ gameess-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_gameess=/home/users/${USER}/build/gameess2017Apr20/gameess-2017Apr20.tar.gz
set work=/work/users/${USER}
source /opt/intel/compilers_and_libraries_2017.2.174/linux/bin/compilervars.csh intel64
set gameess=gameess2017Apr20
set patch_compall=/home/users/${USER}/build/gameess2017Apr20/compall.patch
set patch_rungms=/home/users/${USER}/build/gameess2017Apr20/ccuv/rungms.patch
#-----
cd ${work}
if (-d ${gameess}) then
  mv ${gameess} ${gameess}-erase
  rm -rf ${gameess}-erase &
endif
#-----
tar xzf ${file_gameess}
mv gameess ${gameess}
cd ${work}/${gameess}
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"
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 "sockets\r"
expect "Do you want to try LIBCCHEM"
send "no\r"
expect eof
```

```
EXPECT
#-----
cd ${work}/${games}/ddi
sed -i -e 's/MAXCPUS=32/MAXCPUS=1024/' -e 's/MAXNODES=1024/MAXNODES=2/' compddi
csh ./compddi
mv ddikick.x ./
cd ${work}/${games}
# patch -p0 < ${patch_compall}
./compall
./lked
#-----
chmod -R o-rwx source object
find . -name "src" | xargs chmod -R o-rwx
#-----
patch -p0 < ${patch_rungms}
```
