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

- 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/ccuv/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} 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 'paiblas' or 'none':"

expect Enter your envice of this of actual of actual of pylotas of notion 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}/\${gamess}/ddi sed -i -e 's/MAXCPUS=32/MAXCPUS=1024/' -e 's/MAXNODES=1024/MAXNODES=2/' compddi csh ./compddi mv ddikick.x ../ cd \${work}/\${gamess} # patch -p0 < \${patch_compall}</pre> ./compall ./lked #-----chmod -R o-rwx source object find . -name "src" | xargs chmod -R o-rwx #-----

patch -p0 < \${patch_rungms}</pre>