

ウェブページ

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

バージョン

Apr 20, 2017

ビルド環境

- Intel Compiler 17.0.2.174
- Intel MKL 2017.2.174

ビルドに必要なファイル

- gamess-2017Apr20.tar.gz (GAMESSのウェブページからダウンロードしたもの)
- rungms.patch (長いので割愛します。パッチ適用後のrungmsをご覧ください)

注意事項

exam13.inpのテストを並列実行するとFailedとなる。並列計算時に高次のElectrostatic Momentsが結果不正となるバグ（開発元に報告済み）が原因です。

ビルド手順

```
#!/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 'papiblas' or 'none':"
```

```

expect Enter your choice of MKL or atlas or acml or pgblas 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}

```