

ウェブページ

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

バージョン

Dec 5, 2014

ビルド環境

- Intel Compiler 15.0.2.164
- Intel MPI 4.1.0.030
- Intel MKL 2015.2.164

ビルドに必要なファイル

- gamess-2014Dec05.tar.gz (GAMESSのウェブページからダウンロードしたもの)

ビルド手順

```
#!/bin/csh -f
umask 022
set file_gamess=/home/users/${USER}/build/gamess2014Dec05/gamess-2014Dec05.tar.gz
set work=/work/users/${USER}
source /opt/intel/composer_xe_2015.2.164/bin/compilervars.csh intel64
set gamess=gamess2014Dec05
#-----
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 "15\r"
expect "hit <return> to continue to the math library setup."
send "\r"
expect "Enter your choice of 'mkl' or 'atlas' or 'acml' or 'none':"
send "mkl\r"
expect "MKL pathname?"
send "/opt/intel/composer_xe_2015.2.164/mkl\r"
expect "MKL version (or 'skip')?"
send "skip\r"
expect "hit <return> after you have digested this warning."
send "\r"
```

```
setenv \
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, mvapich2, mpt, sockets):"
send "impi\r"
expect "Please enter your impi's location:"
send "/opt/intel/impi/4.1.0.030\r"
expect "Do you want to try LIBCCHEM"
send "no\r"
expect eof
EXPECT
#-----
cd ${work}/${games}/ddi
./compddi
cd ${work}/${games}
./compall
./lked
#-----
chmod -R o-rwx source object
find . -name "src" | xargs chmod -R o-rwx
```

rungmsの変更点

変更点は多数あるため、以下のファイルをコピーして使って下さい。

```
/local/apl/pg/games2014Dec05/samples/rungms
```