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分享·交流·学习

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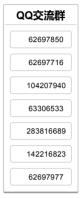
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```
#
#  The archiver and the flag(s) to use when building archive (library)
#  Also the ranlib routine.  If your system has no ranlib, set RANLIB = echo
#

ARCH         = ar
ARCHFLAGS    = cr
RANLIB       = ranlib

#
```

```
⬛ Tested with: GFortran 4.9.2, MPICH 3.1, LAPACK 3.5.0, ScaLAPACK 2.0.2
CC         = gcc
CPP        =
FC         = mpif90
LD         = mpif90
AR         = ar -r
ACML_INC   = /opt/acml5.3.1/gfortran64/include
ACML_LIB   = /opt/acml5.3.1/gfortran64/lib
FFTW_INC   = /opt/fftw/include
FFTW_LIB   = /opt/fftw/lib
LIBINT_INC = /opt/libint/include
LIBINT_LIB = /opt/libint/lib
LIBXC_INC  = /opt/libxc/include
LIBXC_LIB  = /opt/libxc/lib
DFLAGS     = -D__FFTW3 -D__LIBINT -D__LIBXC2 -D__MPI_VERSION=3\
             -D__LIBINT_MAX_AM=7 -D__LIBDERIV_MAX_AM1=6 -D__MAX_CONTR=4\
             -D__parallel -D__SCALAPACK

CPPFLAGS   =
FCFLAGS    = $(DFLAGS) -O2 -ffast-math -ffree-form -ffree-line-length-none\
             -fopenmp -ftree-vectorize -funroll-loops\
             -mtune=native\
             -I$(ACML_INC) -I$(FFTW_INC) -I$(LIBINT_INC) -I$(LIBXC_INC)
LDFLAGS    = $(FCFLAGS) -static-libgfortran
LIBS       = /opt/scalapack/libscalapack.a\
             /opt/acml5.3.1/gfortran64/lib/libacml.a\
             /opt/fftw/lib/libfftw3.a\
             /opt/fftw/lib/libfftw3_threads.a\
             /opt/libxc/lib/libxcf90.a\
             /opt/libxc/lib/libxc.a\
             /opt/libint/lib/libderiv.a\
             /opt/libint/lib/libint.a
►http://www.cndba.cn/shuye100
```

```
make -j 8 ARCH=Linux-x86-64-gfortran VERSION=psmp
```

```
MPILE_REVISION="\"svn:17462\"" -D__DATA_DIR="\"/root/cp2k-4.1/data\"" -static-libgfortran -L/root/cp2k-4.1/lib/Linux-x86-64-gfortran/psmp -o ./
Linux-x86-64-gfortran/cp2k.psmp cp2k.o  -lcp2kstart -lcp2kmc -lcp2kswarm -lcp2kmotion -lcp2kthermostat -lcp2kemd -lcp2ktmc -lcp2keri
x -lcp2khfxbase -lcp2ksubsys -lcp2kxc -lcp2kao -lcp2kinput -lcp2kpw -lcp2kfft -lcp2kdbcsrwrap -ldbcsr -ldbcsrarnoldi -ldbcsrvec -ldbcsrmm -ldb
ck -ldbcsrbdist -ldbcsrbase -ldbcsrdata -ldbcsrerr -lmicsmm -lclsmm -lcp2kacc -lcp2kaccmic -lcp2kaccopencl -lcp2kfm -lcp2kcommon -lcp2kmpiwrap
base /opt/scalapack/libscalapack.a /opt/acml5.3.1/gfortran64/lib/libacml.a /opt/fftw/lib/libfftw3.a /opt/fftw/lib/libfftw3_threads.a /opt/libxc
opt/libxc/lib/libxc.a /opt/libint/lib/libderiv.a /opt/libint/lib/libint.a
mpif90 -D__FFTW3 -D__LIBINT -D__LIBXC2 -D__MPI_VERSION=3 -D__LIBINT_MAX_AM=7 -D__LIBDERIV_MAX_AM1=6 -D__MAX_CONTR=4 -D__parallel -D__SCALAPACK
ffree-form -ffree-line-length-none -fopenmp -ftree-vectorize -funroll-loops -mtune=native -L/opt/acml5.3.1/gfortran64/include -L/opt/fftw/inclu
include -L/opt/libxc/include -D__COMPILE_ARCH="\"Linux-x86-64-gfortran\"" -D__COMPILE_DATE="\"Mon Jan 16 20:54:13 EST 2017\"" -D__COMPILE_HOST=
MPILE_REVISION="\"svn:17462\"" -D__DATA_DIR="\"/root/cp2k-4.1/data\"" -static-libgfortran -L/root/cp2k-4.1/lib/Linux-x86-64-gfortran/psmp -o ./
Linux-x86-64-gfortran/cp2k_shell.psmp cp2k_shell.o  -lcp2kstart -lcp2kmc -lcp2kswarm -lcp2kmotion -lcp2kthermostat -lcp2kemd -lcp2ktmc -lcp2kma
-lcp2kminimax -lcp2khfxbase -lcp2ksubsys -lcp2kxc -lcp2kao -lcp2kinput -lcp2kpw -lcp2kfft -lcp2kdbcsrwrap -ldbcsr -ldbcsrarnoldi -ldbcsrvec -ld
-ldbcsrbblock -ldbcsrbdist -ldbcsrbase -ldbcsrdata -ldbcsrerr -lmicsmm -lclsmm -lcp2kacc -lcp2kaccmic -lcp2kaccopencl -lcp2kfm -lcp2kcommon -l
kgrid -lcp2kbase /opt/scalapack/libscalapack.a /opt/acml5.3.1/gfortran64/lib/libacml.a /opt/fftw/lib/libfftw3.a /opt/fftw/lib/libfftw3_threads.
libxcf90.a /opt/libxc/lib/libxc.a /opt/libint/lib/libderiv.a /opt/libint/lib/libint.a
mpif90 -D__FFTW3 -D__LIBINT -D__LIBXC2 -D__MPI_VERSION=3 -D__LIBINT_MAX_AM=7 -D__LIBDERIV_MAX_AM1=6 -D__MAX_CONTR=4 -D__parallel -D__SCALAPACK
ffree-form -ffree-line-length-none -fopenmp -ftree-vectorize -funroll-loops -mtune=native -L/opt/acml5.3.1/gfortran64/include -L/opt/fftw/inclu
include -L/opt/libxc/include -D__COMPILE_ARCH="\"Linux-x86-64-gfortran\"" -D__COMPILE_DATE="\"Mon Jan 16 20:54:13 EST 2017\"" -D__COMPILE_HOST=
MPILE_REVISION="\"svn:17462\"" -D__DATA_DIR="\"/root/cp2k-4.1/data\"" -static-libgfortran -L/root/cp2k-4.1/lib/Linux-x86-64-gfortran/psmp -o ./
/Linux-x86-64-gfortran/libcp2k_unittest.psmp libcp2k_unittest.o  -lcp2kstart -lcp2kmc -lcp2kswarm -lcp2kmotion -lcp2kthermostat -lcp2kemd -lcp2
lcp2keri_mmc -lcp2kminimax -lcp2khfxbase -lcp2ksubsys -lcp2kxc -lcp2kao -lcp2kinput -lcp2kpw -lcp2kfft -lcp2kdbcsrwrap -ldbcsr -ldbcsrarnoldi -
mm -ldbcsrops -ldbcsrbblock -ldbcsrbdist -ldbcsrbase -ldbcsrdata -ldbcsrerr -lmicsmm -lclsmm -lcp2kacc -lcp2kaccmic -lcp2kaccopencl -lcp2kfm -
mpiwrap -lcp2kgrid -lcp2kbase /opt/scalapack/libscalapack.a /opt/acml5.3.1/gfortran64/lib/libacml.a /opt/fftw/lib/libfftw3.a /opt/fftw/lib/libf
pt/libxc/lib/libxcf90.a /opt/libxc/lib/libxc.a /opt/libint/lib/libderiv.a /opt/libint/lib/libint.a
/bin/ld: Warning: size of symbol `build_deriv1_eri' changed from 10368 in /root/cp2k-4.1/lib/Linux-x86-64-gfortran/psmp/libcp2kmain.a(hfx_libin
048 in /opt/libint/lib/libderiv.a(init_libderiv.o)
/bin/ld: Warning: size of symbol `build_eri' changed from 19208 in /root/cp2k-4.1/lib/Linux-x86-64-gfortran/psmp/libcp2kmain.a(hfx_libint_wrapp
/opt/libint/lib/libint.a(init_libint.o)
/bin/ld: Warning: size of symbol `build_deriv1_eri' changed from 10368 in /root/cp2k-4.1/lib/Linux-x86-64-gfortran/psmp/libcp2kmain.a(hfx_libin
048 in /opt/libint/lib/libderiv.a(init_libderiv.o)
/bin/ld: Warning: size of symbol `build_eri' changed from 19208 in /root/cp2k-4.1/lib/Linux-x86-64-gfortran/psmp/libcp2kmain.a(hfx_libint_wrapp
/opt/libint/lib/libint.a(init_libint.o)
/bin/ld: Warning: size of symbol `build_deriv1_eri' changed from 10368 in /root/cp2k-4.1/lib/Linux-x86-64-gfortran/psmp/libcp2kmain.a(hfx_libin
048 in /opt/libint/lib/libderiv.a(init_libderiv.o)
/bin/ld: Warning: size of symbol `build_eri' changed from 19208 in /root/cp2k-4.1/lib/Linux-x86-64-gfortran/psmp/libcp2kmain.a(hfx_libint_wrapp
/opt/libint/lib/libint.a(init_libint.o)
[root@cp2k makefiles]# shuye100
```

最后会在~/cp2k-4.1/exe/Linux-x86-64-gfortran/目录下面生成N多个psmp文件包含cp2k.psmp

刚刚开始写博客,也得不清楚或有问题的地方还请多多指正,QQ:86427461

标签：hpc cp2k

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用户评论

[   ]

* 以下用户言论只代表其个人观点，不代表CNDBA社区的观点或立场

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