

Molpro2015.1-pl44

Webpage

<http://www.molpro.net/>

Version

2015.1.44

Build Environment

- ▶ Intel Parallel Studio 2017 update 8
- ▶ GCC 4.9.2 (may not be necessary?)
- ▶ Global Arrays Toolkit 5.7

Files Required

- ▶ molpro.2015.1.44.tar.gz
- ▶ ga-5.7.tar.gz
- ▶ patch files
 - ▶ (see files in /local/apl/lx/molpro2015.1.44/patches directory for details)
 - ▶ (most of them are meant to modify parameters. these patches do not change test results.)
 - ▶ work.patch
 - ▶ patch-argos-binput.F
 - ▶ patch-common-cconf
 - ▶ patch-common-cconf1
 - ▶ patch-common-cref
 - ▶ patch-forces-forces_drv.F
 - ▶ patch-mrci-ciref.F
 - ▶ patch-util-zmatrix.F
 - ▶ patch-make-molver.mk
 - ▶ patch-cic-ltfFortranInt.h
- ▶ token

Build Procedure

```
#!/bin/sh
GA_VERSION=5.7
MOLPRO_VERSION=2015.1-pl44
MOLPRO_DIRNAME=molpro.2015.1.44
PARALLEL=12
BASEDIR=/home/users/${USER}/Software/Molpro/2015.1.44
MOLPRO_TARBALL=${BASEDIR}/molpro.2015.1.44.tar.gz
TOKEN=${BASEDIR}/token

WORKDIR=/work/users/${USER}
INSTALLDIR=/local/apl/lx/molpro${MOLPRO_VERSION}

GA_TARBALL=/home/users/${USER}/Software/GlobalArrays/5.7/ga-5.7.tar.gz
GA_INSTALLDIR=${WORKDIR}/ga-temporary
GA_INC=${GA_INSTALLDIR}

PATCH0=${BASEDIR}/work.patch
PATCH1=${BASEDIR}/patch-argos-binput.F
PATCH2=${BASEDIR}/patch-common-cconf
PATCH3=${BASEDIR}/patch-common-cconf1
PATCH4=${BASEDIR}/patch-common-cref
PATCH5=${BASEDIR}/patch-forces-forces_drv.F
PATCH6=${BASEDIR}/patch-mrci-ciref.F
PATCH7=${BASEDIR}/patch-util-zmatrix.F
PATCH8=${BASEDIR}/patch-make-molver.mk
PATCH9=${BASEDIR}/patch-cic-ltfFortranInt.h

#-----
umask 0022
ulimit -s unlimited
export LANG=C

cd $WORKDIR
if [ -d ga-${GA_VERSION} ]; then
  mv ga-${GA_VERSION} ga_tmp
  rm -rf ga_tmp &
fi
if [ -d ga-temporary ]; then
  mv ga-temporary ga_tmp_tmp
  rm -rf ga_tmp_tmp &
fi
if [ -d ${MOLPRO_DIRNAME} ]; then
```

```

mv ${MOLPRO_DIRNAME} molpro_tmp
rm -rf molpro_tmp &
fi

module purge
module load scl/devtoolset-3
module load intel_parallelstudio/2017update8

tar xzf ${GA_TARBALL}
cd ga-${GA_VERSION}

export CFLAGS="-pc80"
export FFLAGS="-pc80"
export FCFLAGS="-pc80"
export CXXFLAGS="-pc80"

export F77=mpiifort
export F90=mpiifort
export FC=mpiifort
export CC=mpiicc
export CXX=mpiicpc
export MPIF77=mpiifort
export MPIF90=mpiifort
export MPICC=mpiicc
export MPICXX=mpiicpc
export GA_FOPT="-O3 -ip -w -xHost"
export GA_COPT="-O3 -ip -w -xHost"
export GA_CXXOPT="-O3 -ip -w -xHost"

./configure --with-blas8 \
  --enable-i8 \
  --prefix=${GA_INSTALLDIR}

make -j ${PARALLEL}
#make check
make install
cp config.log ${GA_INSTALLDIR}

cd ../
tar xzf ${MOLPRO_TARBALL}
cd ${MOLPRO_DIRNAME}
patch -p0 < ${PATCH0}
patch -p0 < ${PATCH1}
patch -p0 < ${PATCH2}
patch -p0 < ${PATCH3}
patch -p0 < ${PATCH4}
patch -p0 < ${PATCH5}
patch -p0 < ${PATCH6}
patch -p0 < ${PATCH7}
patch -p0 < ${PATCH8}
patch -p0 < ${PATCH9}

export PATH="${GA_INSTALLDIR}/bin:$PATH" # where ga-config exists
CPPFLAGS="-I${GA_INSTALLDIR}/include" \
LDLFLAGS="-L${GA_INSTALLDIR}/lib" \
./configure --prefix=${INSTALLDIR} \
  --enable-mpp=ga-config \
  --enable-integer8 \
  --enable-slater

sed -i -e "s/pc64/pc80/g" CONFIG

LD_LIBRARY_PATH_ESC=`echo $LD_LIBRARY_PATH | sed -e 's/\/\///g'`
sed -i -e "s/^VERBOSE.*$/VERBOSE=" \
  -e "s/^LD_ENV=.*/LD_ENV=$LD_LIBRARY_PATH_ESC/" CONFIG
unset LD_LIBRARY_PATH_ESC

make -j ${PARALLEL}
cp $TOKEN lib/.token

make tuning

## manually modify tuning parameters!
#sed -i -e "s/tuning-mindgm.*/tuning-mindgm 0001/" \
# -e "s/tuning-mindgc.*/tuning-mindgc 0001/" \
# -e "s/tuning-mindgr.*/tuning-mindgr 0001/" \
# -e "s/tuning-mindgl.*/tuning-mindgl 0001/" \
# -e "s/tuning-mindgv.*/tuning-mindgv 0001/" lib/tuning.rc

MOLPRO_OPTIONS="" make quicktest
MOLPRO_OPTIONS=-n2 make test
#make install # do it manually

```

Notes

- ▶ Sep 7 update: originally installed version was the serial version. We have added --enable-mpp=ga-config and reinstalled the parallel version on Sep 6.

- ▶ All the tests in serial quicktest and parallel (2-MPI) test are passed without any problem.
 - ▶ -pc80 is added as in the later version of molpro.
 - ▶ Intel17 version is slightly faster than gcc9 version.
 - ▶ To compile with gcc, fortran functions qexp, qabs, and qfloat should be replaced with exp, abs, and real(arg,kind=kind(real*16 varname)), respectively.
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