

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-bininput.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-bininput.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 zxf `${GA_TARBALL}`
cd ga-`${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_CXCOPT="-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 zxf `${MOLPRO_TARBALL}`
cd `${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.