

NAMD 2.14 (GPU)

Webpage

<http://www.ks.uiuc.edu/Research/namd/>

Version

2.14

Build Environment

- GCC 10.3.1 (gcc-toolset/10)
- Intel MKL 2022.2.1
- CUDA 11.6

Files Required

- NAMD_2.14_Source.tar.gz
- tcl8.5.9-linux-x86_64.tar.gz
- tcl8.5.9-linux-x86_64-threaded.tar.gz
 - obtained from <http://www.ks.uiuc.edu/Research/namd/libraries>
 - For fftw, MKL was used.

Build Procedure

```
#!/bin/sh

VERSION=2.14
CHARM_VERSION=6.10.2
WORKDIR=/gwork/users/${USER}/namd-gnu
SOURCEDIR=/home/users/${USER}/Software/NAMD/${VERSION}
NAME=NAMD_${VERSION}_Source
TARBALL=${SOURCEDIR}/${NAME}.tar.gz

#LIBURL=http://www.ks.uiuc.edu/Research/namd/libraries
#FFTW=fftw-linux-x86_64
#FFTW_URL=${LIBURL}/${FFTW}.tar.gz
TCL=tcl8.5.9-linux-x86_64
#TCL_URL=${LIBURL}/${TCL}.tar.gz
TCL_THREADED=tcl8.5.9-linux-x86_64-threaded
#TCL_THREADED_URL=${LIBURL}/${TCL_THREADED}.tar.gz

#TARBALL_FFTW=${SOURCEDIR}/${FFTW}.tar.gz
TARBALL_TCL=${SOURCEDIR}/${TCL}.tar.gz
TARBALL_TCL_THREADED=${SOURCEDIR}/${TCL_THREADED}.tar.gz

PARALLEL=12

#-----
umask 0022

export LANG=""
export LC_ALL=C

module -s purge
module -s load gcc-toolset/10
module -s load mkl/2022.2.1
module -s load cuda/11.6

cd ${WORKDIR}
if [ -d ${NAME} ]; then
  mv ${NAME} namd_erase
  rm -rf namd_erase &
```

```
fi

tar zxf ${TARBALL}
cd ${NAME}
tar xf charm-${CHARM_VERSION}.tar

cd charm-${CHARM_VERSION}

export CC=gcc
export CXX=g++
export F90=gfortran
export F77=gfortran

./build charm++ multicore-linux-x86_64-gcc \
  --no-build-shared --with-production -j${PARALLEL}
cd multicore-linux-x86_64-gcc/tests/charm++/megatest
make pgm
../../bin/charmrun ./pgm +p${PARALLEL}
cd ../../../../
cd ../

tar zxf ${TARBALL_TCL}
mv ${TCL} tcl
tar zxf ${TARBALL_TCL_THREADED}
mv ${TCL_THREADED} tcl-threaded

./config Linux-x86_64-g++ \
  --charm-arch multicore-linux-x86_64-gcc \
  --with-mkl \
  --with-python \
  --with-cuda
cd Linux-x86_64-g++

sed -i -e "/PYTHONLIB/s/lib64/lib64 -lpython3.9/" Make.config

make -j${PARALLEL}
make release
```