

NAMD 3.0b7 - SMP+CUDA (single node)

Webpage

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

Version

3.0b7

Build Environment

- GCC 8.5.0
- Intel MKL 2024.1
- CUDA 12.4 Update 1

Files Required

- NAMD_3.0b7_Source.tar.gz
 - tcl and tcl-threaded are obtained from <http://www.ks.uiuc.edu/Research/namd/libraries>
 - fftw of MKL is used

Build Procedure

```
#!/bin/sh

VERSION=3.0b7
CHARM_VERSION=7.0.0
WORKDIR=/gwork/users/${USER}
SOURCEDIR=/home/users/${USER}/Software/NAMD/${VERSION}
NAME=NAMD_${VERSION}_Source

TARBALL=${SOURCEDIR}/${NAME}.tar.gz

LIBURL=http://www.ks.uiuc.edu/Research/namd/libraries
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_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 mkl/2024.1
module -s load cuda/12.4u1

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-v${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 ../

tar xzf ${TARBALL_TCL}
mv ${TCL} tcl
tar xzf ${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-single-node-cuda

cd Linux-x86_64-g++

make -j${PARALLEL}
make release
# install contents of Linux-x86_64-g++/NAMD_3.0b7_Linux-x86_64-multicore-CUDA.tar.gz into /apl/namd/3.0b7-smp-cuda
```

Notes

- Failed to build with gcc11, 12, and 13 (syntax error).
 - This is probably due to the implementation of new features and bug fixes.
- Gcc10 can build the executable without problem. However, the performance of GPU runs is slightly worse than gcc8 version.
 - (For the performance of CPU part, gcc10 version is better than gcc8 one.)
 - The overall performance is comparable or very slightly worse than the previous build [β.0b6](#)).