

NAMD 3.0.2 - MPI

ウェブページ

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

バージョン

3.0.2

ビルド環境

- GCC 14.2.1 (gcc-toolset-14)
- Intel MKL 2025.3
- Open MPI 4.1.8

ビルドに必要なファイル

- NAMD_3.0.2_Source.tar.gz
 - tcl, tcl-threaded は <http://www.ks.uiuc.edu/Research/namd/libraries> より取得
 - fftw については MKL を利用

ビルド手順

```
#!/bin/sh
set -e

#=====
# USER CONFIGURATION SECTION
#=====
# NAMD version settings
VERSION=${NAMD_VERSION:-3.0.2}
CHARM_VERSION=${CHARM_VERSION:-8.0.0}

# Directory settings
WORKDIR=${NAMD_WORKDIR:-/gwork/users/${USER}}
SOURCEDIR=${NAMD_SOURCEDIR:-/home/users/${USER}/Software/namd/${VERSION}}

# TCL library settings
TCL_VERSION=${TCL_VERSION:-8.6.13}
TCL_THREADED_VERSION=${TCL_THREADED_VERSION:-8.6.17}

# Build settings
PARALLEL=${NAMD_PARALLEL:-12}
ARCH=${NAMD_ARCH:-Linux-x86_64-g++}
CHARM_ARCH=${CHARM_ARCH:-mpi-linux-x86_64}

# Module settings
GCC_MODULE=${GCC_MODULE:-gcc-toolset/14}
MKL_MODULE=${MKL_MODULE:-mkl/2025.3}
MPI_MODULE=${MPI_MODULE:-openmpi/4.1.8/gcc14}

# Python settings
PYTHON_PREFIX=${PYTHON_PREFIX:-/usr}

NAME=NAMD_${VERSION}_Source
TARBALL=${SOURCEDIR}/${NAME}.tar.gz
LIBURL=http://www.ks.uiuc.edu/Research/namd/libraries
TCL=tcl${TCL_VERSION}-linux-x86_64
TCL_URL=${LIBURL}/${TCL}.tar.gz
TCL_THREADED=tcl${TCL_THREADED_VERSION}-linux-x86_64-threaded
TCL_THREADED_URL=${LIBURL}/${TCL_THREADED}.tar.gz
TARBALL_TCL=${SOURCEDIR}/${TCL}.tar.gz
TARBALL_TCL_THREADED=${SOURCEDIR}/${TCL_THREADED}.tar.gz
```

```

#-----
umask 0022
export LANG=""
export LC_ALL=C

# Load modules
module -s purge
module -s load ${GCC_MODULE}
module -s load ${MKL_MODULE}
module -s load ${MPI_MODULE}

# Prepare build directory
cd ${WORKDIR}
if [ -d ${NAME} ]; then
mv ${NAME} namd_erase
rm -rf namd_erase &
fi

# Extract NAMD
tar xzf ${TARBALL}
cd ${NAME}

# Build Charm++
tar xf charm-${CHARM_VERSION}.tar
cd charm-${CHARM_VERSION}

export CC=gcc
export CXX=g++
export F90=gfortran
export F77=gfortran
export MPICXX=mpicxx
export MPICC=mpicc
export MPIF90=mpif90
export MPIF77=mpif90

./build charm++ ${CHARM_ARCH} \
    --no-build-shared --with-production -j${PARALLEL}

# Extract TCL libraries
cd ../
tar xzf ${TARBALL_TCL}
mv ${TCL} tcl
tar xzf ${TARBALL_TCL_THREADED}
mv ${TCL_THREADED} tcl-threaded

# Configure and build NAMD
./config ${ARCH} \
    --charm-arch ${CHARM_ARCH} \
    --with-mkl \
    --with-python \
    --python-prefix ${PYTHON_PREFIX}

cd ${ARCH}
make -j${PARALLEL}
make release

```

メモ

- 3.0.1 と同一の手順です。