NAMD 3.0 - SMP+CUDA (single node)

ウェブページ

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

バージョン

3.0

ビルド環境

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

ビルドに必要なファイル

- NAMD_3.0_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

VERSION=3.0
CHARM_VERSION=8.0.0
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

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 ../

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-single-node-cuda
cd Linux-x86_64-g++

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

メモ

- 3.0b6 の導入手順を踏襲