NAMD 3.0b6 - SMP(single node)

Webpage

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

Version

3.0b6

Build Environment

- GCC 12.1.1 (gcc-toolset-12)
- Intel MKL 2024.0

Files Required

- NAMD_3.0b6_Source.tar.gz
  - tcl, tcl-threaded are obtained from http://www.ks.uiuc.edu/Research/namd/libraries
  - MKL was used for FFTW

Build Procedure

```
#!/bin/sh

VERSION=3.0b6
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
#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/12
module -s load mkl/2024.0

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 \
      --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 \
       --with-mkl \
       --with-python
cd Linux-x86_64-g++

make -j${PARALLEL}
make release
# install contents of Linux-x86_64-g++/NAMD_3.0b6_Linux-x86_64-multicore.tar.gz into /apl/namd/3.0b6-smp manually
```

Notes

- GCC12 binary shows a slightly better performance than Intel oneAPI 2023 Compiler (Classic) one.
- For multi-nodes runs, please use MPI version.
- Acceleration by AVX-512 is not available for EPYC Milan CPUs.
    - Please consider to use single node cuda version for higher performance.