# NAMD-2.1.3 with GPU support for LX

## ウェブページ

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

## バージョン

2.13

## ビルド環境

- Intel Parallel Studio 2017 update8
- CUDA 9.1.85

## ビルドに必要なファイル

- NAMD_2.13_Source.tar.gz
- charmrun.patch

```
--- src/arch/mpi/charmrun.org    2018-11-26 16:02:00.000000000 +0900
+++ src/arch/mpi/charmrun    2018-11-26 16:04:16.000000000 +0900
@@ -37,11 +37,11 @@
    +p[0-9]*)
       pes=`echo $1 | awk '{print substr($1,3)}'`
       ;;
-      -machinefile)
-      machinefile=$2
-      args=" "$1" "$2" "$args
-      shift
-      ;;
+#      -machinefile)
+#      machinefile=$2
+#      args=" "$1" "$2" "$args
+#      shift
+#      ;;
    ++quiet)
       QUIET=1
       args=$args" "$1
@@ -88,7 +88,7 @@
       mpirun -np $pes $args
       #    mpdallexit
     else   # normal case
-      test -z "$machinefile" && args=-machinefile" "$PBS_NODEFILE" "$args
+       #test -z "$machinefile" && args=-machinefile" "$PBS_NODEFILE" "$args
       test $QUIET -eq 0 && echo mpirun -np $pes $args
       mpirun -np $pes $args
     fi
```

- (以下スクリプト内で取得)
  - tcl8.5.9-linux-x86_64.tar.gz
  - tcl8.5.9-linux-x86_64-threaded.tar.gz

## ビルド手順

```
#!/bin/sh

VERSION=2.13
CHARM_VERSION=6.8.2
WORKDIR=/work/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

PATCH0=${SOURCEDIR}/charmrun.patch

PARALLEL=12

#------------------------------------------------------------
umask 0022

export LANG=""
export LC_ALL=C
```

```
module purge
module load intel_parallelstudio/2017update8
module load cuda/9.1

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}
patch -p0 < ${PATCH0}
sed -i -e "s/_OPTIMIZE/_OPTIMIZE -xHost/" src/scripts/charmc

export CC=icc
export CXX=icpc
export F90=ifort
export F77=ifort

./build charm++ multicore-linux-x86_64-iccstatic \
      --no-build-shared --with-production -j${PARALLEL}
cd multicore-linux-x86_64-iccstatic/tests/charm++/megatest
make pgm
mpirun -np ${PARALLEL} ./pgm
cd ../../../../
cd ../

wget ${TCL_URL}
tar zxf ${TCL}.tar.gz
mv ${TCL} tcl
wget ${TCL_THREADED_URL}
tar zxf ${TCL_THREADED}.tar.gz
mv ${TCL_THREADED} tcl-threaded

NEWOPTS="-xHost -static-intel -O3 -ip -fp-model fast=2 -DNAMD_DISABLE_SSE"
./config Linux-x86_64-icc \
      --charm-arch multicore-linux-x86_64-iccstatic \
      --with-mkl \
      --with-python \
      --with-cuda \
      --cuda-prefix /local/apl/lx/cuda-9.1 \
      --cuda-gencode "arch=compute_60,code=sm_60" \
      --cuda-gencode "arch=compute_70,code=sm_70" \
      --cuda-dlink "arch=compute_60,code=sm_60" \
      --cuda-dlink "arch=compute_70,code=sm_70" \
      --cxx-opts "$NEWOPTS" \
      --cxx-thread-opts "$NEWOPTS" \
      --cxx-noalias-opts "$NEWOPTS -fno-alias" \
      --cc-opts "$NEWOPTS"
cd Linux-x86_64-icc
make -j${PARALLEL}
make release
```