

NAMD-2.13 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 Compiler 18.0.5 (from Intel Parallel Studio 2018 update4)
- Intel MKL 2018.0.4 (from Intel Parallel Studio 2018 update4)
- Open MPI 3.1.0 (intel18 version)

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
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/18.0.5
module load mpi/openmpi/3.1.0/intel
module load mkl/2018.0.4

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/charm.c

export CC=icc
export CXX=icpc
export F90=ifort
export F77=ifort
export MPICXX=mpicxx
export MPICC=mpicc
export MPIF90=mpif90
export MPIF77=mpif90

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

wget ${FFTW_URL}
tar zxf ${FFTW}.tar.gz
mv linux-x86_64 fftw
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 mpi-linux-x86_64-iccstatic \  
--with-mkl \  
--with-python \  
--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
```

メモ

- バージョン 2.11 の方が速度が出るケースがありそうです。一度ご自身のインプットでもご検証下さい。
- (2022/6/29) fftw を取得する部分が抜け落ちていました。申し訳ありません。