

NAMD-2.9

Webpage

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

Version

2.9

Tools for Compiling

- ▶ Intel Composer XE 2011 sp1.8.273
- ▶ Intel MPI 4.0.2.003

Necessary Files for Compiling

- ▶ NAMD_2.9_Source.tar.gz
- ▶ fftw-linux-x86_64.tar.gz
- ▶ tcl8.5.9-linux-x86_64.tar.gz

Procedure of Compiling

```
#!/bin/csh -f
umask 022
set file_namd=/home/users/${USER}/build/namd29/NAMD_2.9_Source.tar.gz
set work=/work/users/${USER}
set file_fftw=/home/users/${USER}/build/namd29/fftw-linux-x86_64.tar.gz
set file_tcl=/home/users/${USER}/build/namd29/tcl8.5.9-linux-x86_64.tar.gz
#-----
cd ${work}
if (-d NAMD_2.9_Source) then
  mv NAMD_2.9_Source NAMD_2.9_Source-erase
  rm -rf NAMD_2.9_Source-erase &
endif
tar xzf ${file_namd}
cd NAMD_2.9_Source
tar xf charm-6.4.0.tar
cd charm-6.4.0
patch -p1 <<PATCH
diff -uNr charm-6.4.0-orig/src/scripts/charmc charm-6.4.0/src/scripts/charmc
--- charm-6.4.0-orig/src/scripts/charmc 2011-05-14 04:47:47.000000000 +0900
+++ charm-6.4.0/src/scripts/charmc 2012-04-09 14:39:09.247996000 +0900
@@ -997,11 +997,11 @@
  Debug "set 4"
  if [ "${OPTIMIZE_MODE}" = "true" ]
  then
  - OPTS_CC="\${CMK_C_OPTIMIZE} \${OPTS_CC}"
  - OPTS_CXX="\${CMK_CXX_OPTIMIZE} \${OPTS_CXX}"
  - OPTS_F90="\${CMK_F90_OPTIMIZE} \${OPTS_F90}"
  - OPTS_LD="\${CMK_C_OPTIMIZE} \${OPTS_LD}"
  - OPTS_LDXX="\${CMK_CXX_OPTIMIZE} \${OPTS_LDXX}"
  + OPTS_CC="\${CMK_C_OPTIMIZE} -xhost \${OPTS_CC}"
  + OPTS_CXX="\${CMK_CXX_OPTIMIZE} -xhost \${OPTS_CXX}"
  + OPTS_F90="\${CMK_F90_OPTIMIZE} -xhost \${OPTS_F90}"
  + OPTS_LD="\${CMK_C_OPTIMIZE} -xhost \${OPTS_LD}"
  + OPTS_LDXX="\${CMK_CXX_OPTIMIZE} -xhost \${OPTS_LDXX}"
  fi

  # Pick up per-architecture production mode settings
  diff -uNr charm-6.4.0-orig/src/arch/mpi/charmrun charm-6.4.0/src/arch/mpi/charmrun
  --- charm-6.4.0-orig/src/arch/mpi/charmrun 2011-05-14 04:46:38.000000000 +0900
  +++ charm-6.4.0/src/arch/mpi/charmrun 2012-04-09 15:23:55.191226000 +0900
  @@ -36,11 +36,11 @@
  +p*)
  pes="echo \${1} | awk '{print substr(\$1,3)}'"
  ;;
  - -machinefile)
  - machinefile=\${2}
  - args=" \${1} " \${2} " \${args}
  - shift
  - ;;
  +# -machinefile)
  +# machinefile=\${2}
  +# args=" \${1} " \${2} " \${args}
  +# shift
```

```

+# ;;
*)
  args=\$args" "$1
  ;;
@@ -83,7 +83,7 @@
  mpirun -np \$pes \$args
  # mpdallexit
  else # normal case
-   test -z "\$machinefile" && args=-machinefile" "\$PBS_NODEFILE" "\$args
+#   test -z "\$machinefile" && args=-machinefile" "\$PBS_NODEFILE" "\$args
  echo mpirun -np \$pes \$args
  mpirun -np \$pes \$args
  fi
PATCH
setenv MPICXX mpiicpc
setenv MPICC mpiicc
setenv MPIF90 mpiifort
setenv MPIF77 mpiifort
./build charm++ mpi-linux-x86_64 smp --no-build-shared --with-production -j8
cd ..
#-----
tar xzf ${file_fftw}
mv linux-x86_64 fftw
tar xzf ${file_tcl}
mv tcl8.5.9-linux-x86_64 tcl
./config Linux-x86_64-icc --charm-arch mpi-linux-x86_64-smp --cxx-opts '-xhost -i-static -O3 -ip -fno-rtti' --cc-opts '-xhost -i-static -O3 -ip -fno-rtti'
cd Linux-x86_64-icc
make -j 8
#-----
cd ${work}/NAMD_2.9_Source
rm -rf Make.charm Make.depends Makefile arch charm-6.4.0.tar charm-6.4.0 config fftw psfgn src tcl ug
cd Linux-x86_64-icc
mv charmrn flipbinpdb flipdcd namd2 psfgn sortreplicas ..
cd ..
rm -rf Linux-x86_64-icc

```