

NAMD-2.11 for PRIMERGY

Webpage

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

Version

2.11

Tools for Compiling

- ▶ Intel Compiler 16.0.2.181
- ▶ Intel MPI 5.1.3

Necessary Files for Compiling

- ▶ NAMD_2.11_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/${USER}/build/namd211/NAMD_2.11_Source.tar.gz
set work=/work/users/${USER}
set file_fftw=/home/users/${USER}/build/namd211/fftw-linux-x86_64.tar.gz
set file_tcl=/home/users/${USER}/build/namd211/tcl8.5.9-linux-x86_64.tar.gz
#-----
cd ${work}
rm -rf NAMD_2.11_Source
tar xzf ${file_namd}
cd NAMD_2.11_Source
tar xf charm-6.7.0.tar
cd charm-6.7.0
patch -p1 <<PATCH
diff -uNr charm-6.7.0-orig/src/scripts/charm charm-6.7.0/src/scripts/charm
--- charm-6.7.0-orig/src/scripts/charm 2011-05-14 04:47:47.000000000 +0900
+++ charm-6.7.0/src/scripts/charm 2012-04-09 14:39:09.247996000 +0900
@@ -997,11 +997,11 @@
Debug "set 4"
if [ "${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-6.7.0-orig/src/arch/mpi/charmrun charm-6.7.0/src/arch/mpi/charmrun
--- charm-6.7.0-orig/src/arch/mpi/charmrun 2011-05-14 04:46:38.000000000 +0900
+++ charm-6.7.0/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} " \${sargs}
- shift
- ;;
+# -machinefile)
+# machinefile=\${2}
+# args=" \${1} " \${2} " \${sargs}
+# shift
+# ;;
*)
args=\${sargs} " \${1}
;;
@@ -83,7 +83,7 @@
mpirun -np \${pes} \${sargs}
```

```
# mpdallexit
else # normal case
- test -z "$machinefile" && args=-machinefile "$PBS_NODEFILE" "$sargs
+# test -z "$machinefile" && args=-machinefile "$PBS_NODEFILE" "$sargs
echo mpirun -np $pes $sargs
mpirun -np $pes $sargs
fi
PATCH
setenv MPICXX mpiicpc
setenv MPICC mpiicc
setenv MPIF90 mpiifort
setenv MPIF77 mpiifort
./build charm++ mpi-linux-x86_64 --no-build-shared --with-production
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 --cxx-opts '-xhost -static-intel -O2 -ip -no-vec' --cxx-noalias-opts '-xhost -static-intel -O2 -fno-alias -ip -no-vec' --cc-opts '-xhost -static-intel -O2 -ip -no-vec'
cd Linux-x86_64-icc
make -j 8
make release
```
