# NAMD Best Practices

HPC ADVISORY COUNCIL
NETWORK OF EXPERTISE
BEST PRACTICES

## 1. Introduction:

The following best practices document is provided as courtesy of the HPC Advisory Council.

## 2. Application Description:

NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. Based on Charm++ parallel objects, NAMD scales to hundreds of processors on high-end parallel platforms and tens of processors on commodity clusters using gigabit ethernet. NAMD uses the popular molecular graphics program VMD for simulation setup and trajectory analysis, but is also file-compatible with AMBER, CHARMM, and X-PLOR. NAMD is distributed free of charge with source code. For further information, see http://www.ks.uiuc.edu/Research/namd

## 3. Version Information:

NAMD Version 2.7 (b1)

Download from:

http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=NAMD

## 4. Prerequisites:

4.1 Hardware:

The instructions from this best practice have been tested on the HPC Advisory Council, Dell PowerEdge R730 32-node cluster.

- Intel® Xeon® 14-core CPUs E5-2697 V3 @ 2.60 GHz
- Mellanox ConnectX®-3 VPI 56Gb/s FDR InfiniBand HCA (Driver: MLNX_OFED 2.3-2.0.5)
- Mellanox SwitchX SX6036 36-Port 56Gb/s FDR InfiniBand switch

4.2 Software:

a. OS: Red Hat Enterprise Linux 6.5

b. GNU Compilers 4.4.6, Intel® C and C++ Compiler; composer_xe_2015.1.133

c. Libraries:

- tcl-8.5.17 (compiled by Intel® compiler)
- FFTW 2.1.5 (compiled by Intel® compiler)
- charm++ 6.6.1 (compiled by Intel® compiler)
- HPC-X version 1.2.0

## 5. Building FFTW and Charm++

If NAMD will be compiled by Intel Compiler, FFTW and Charm++ also need to be built by Intel compiler.

For Intel Compilers:

module use /opt/hpcx-v1.2.0-318-icc-MLNX_OFED_LINUX-2.3-2.0.5-redhat6.5/modulefiles

module load hpcx

For GNU Compilers:

module use /opt/hpcx-v1.2.0-318-gcc-MLNX_OFED_LINUX-2.3-2.0.5-redhat6.5/modulefiles

module load hpcx

5.1 Building FFTW 2.1.5:

Download fftw from http://www.fftw.org/fftw-2.1.5.tar.gz

./configure --prefix=/home/namd/fftw-2.1.5-intel F77=ifort CC=icc CFLAGS=-O3 FFLAGS="-O3 --enable-shared --enable-threads" --enable-float --enable-type-prefix

5.2 Building Charm++ 6.6.1:

rm -rf charm-6.6.1

tar xfp charm-6.6.1.tar

cd charm-6.6.1

For Intel Compilers

./build charm++ mpi-linux-x86_64 mpicxx ifort --no-shared -O3 -DCMK_OPTIMIZE=1

For GNU compilers:

./build charm++ mpi-linux-x86_64 mpicxx gfortran --no-shared -O3 -DCMK_OPTIMIZE=1

5.3 Building tcl8.5.17:

Download tcl from http://prdownloads.sourceforge.net/tcl/tcl8.5.17-src.tar.gz.

tar xvfz tcl8.5.17-src.tar.gz

cd unix

./configure F77=ifort CC=icc CFLAGS=-O3 FFLAGS=-O3 --enable-64bit --prefix=/home/namd/tcl-8.5.17-intel

make

make install

## 6. Building NAMD:

6.1 Modify architecture file:

cp -fr arch/Linux-x86_64-icc.arch arch/Linux-x86_64-MPI-icc.arch

Modify it using:

sed -e "s/-i-static/-static-intel/g" -i arch/Linux-x86_64-MPI-icc.arch

Update arch/Linux-x86_64.fftw and arch/Linux-x86_64.tcl to reflect current directory.

6.2 Run NAMD configure:

./config Linux-x86_64-MPI-icc --charm-arch mpi-linux-x86_64-ifort-mpicxx

6.3 Compile NAMD For Intel Compilers:
cd Linux-x86_64-MPI-icc
export MPICH_CXX="icpc"
export MPICH_CC="icc"
export MPICH_F77="ifort"
export MPICH_F90="ifort"
make
For GNU Compilers:
CXX = g++ -m64 -O3
CXXOPTS = -fexpensive-optimizations -ffast-math
CC = gcc -m64 -O3
COPTS = -fexpensive-optimizations -ffast-math

## 7. Running NAMD:

7.1 Download a benchmark file from:

http://www.ks.uiuc.edu/Research/namd/utilities/apoa1.tar.gz

7.2 Untar the data files:

tar -vzxf apoa1.tar.gz

7.3 Run the benchmark:

mpirun -np <number of procs> -hostfile <hostfile> Linux-x86_64-MPI-icc/namd2 apoa1/apoa1.namd

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