

NAMD2 INSTALL GUIDE ON NKSTARS

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ABSTRACT. To install namd2 in parallel cluster environment, Libraries using MPICH, GM, etc, with compiler icc.

1. NAMD 2.5

- (1) Download Namd2.5 source from Namd website.
- (2) Download tcl and fftw libraries, namd plugins from namd website too.
- (3) Uncompress namd2.5.tar.gz using: `tar -xzf namd2.5.tar.gz`; uncompress tcl and fftw using `tar -xzf` too. Change directory to namd 2.5 source directory and uncompress charm-5.9 archive, using: `tar -xvf charm-5.9.tar`. (namd 2.5 use a old version of charm, you should remove the charm.tar in the source directory and download a new version of charm, like charm-5.9 etc.
- (4) Change directory to charm source directory, edit file: `src/arch/mpi-linux/conv-mach.sh`, add the mpich lib directory, gm lib directory, pthread lib to the "CMK_LIBS" variable, like: `CMK_LIBS='-lckqt -L/usr/local/mpich/1.2.6..13a/gm-2.1.3aa2nks3/smp/intel32/ssh/lib -lmpich -L/opt/xcat/gm/lib/ -lgm -lpthread'`
- (5) build the mpi-linux version charm++: `./build charm++ mpi-linux gm icc -incdir /usr/local/mpich/1.2.6..13a/gm-2.1.3aa2nks3/smp/intel32/ssh/include -incdir /opt/xcat/gm/include -libdir /usr/local/mpich/1.2.6..13a/gm-2.1.3aa2nks3/smp/intel32/ssh/lib -libdir /opt/xcat/gm/lib -O -DCMK_OPTIMIZE`.
- (6) change directory to NAMD source. edit `arch/Linux-i686.tcl` to point to the location of tcl libraries; edit `arch/Linux-i686.tcl` to point to the fftw libraries; edit the `arch/All-linux.plugins` to point to the location of plugins

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files. edit the Make.charm file to point out the location of charm directory.

edit arch/Linux-i686-MPI.arch, change "mpi-linux" to "mpi-linux-gm-icc".

- (7) Use this to creat a namd compile directory: ./config tcl fftw plugins Linux-i686-MPI.
- (8) enter the Linux-i686-MPI directory, make.
- (9) Done!

2. NAMD 2.6

- (1) Download source files as section 1.
- (2) build mpi-linux version as section 1.
- (3) build build namd2, with version Linux-i686-MPI-icc, as section one.
- (4) Done!