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Molecular dynamics Calculations in NAMD

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NAMD

NAMD web page: http://www.ks.uiuc.edu/Research/namd/
Documentation: http://www.ks.uiuc.edu/Research/namd/2.7/ug/
http://www.ks.uiuc.edu/Training/Tutorials/namd/namd-tutorial-win.pdf

NAMD is ia 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.

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Before you start…

Example files location on ARCHIE-WeSt:
/users/cwb08102/NAMD_Training

Load the modules:
module load /apps/bin/vmd/1.9.1
module load /mpi/gcc/openmpi/1.4.5
module load /libs/gcc/fftw2/float-mpi/2.1.5
module load /apps/gcc/namd/mpi/2.8

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Simulations in NAMD

Now we will follow the manual and will run sample simulations remotely on ARCHIE-WeSt.