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 a recipient of the 2002 Gordon Bell Award (HPC and networking field) and a 2012 Sidney Fernbach Award (established in 1992 in memory of high-performance computing pioneer Sidney Fernbach. This Award recognizes outstanding contributions in the application of high-performance computers using innovative approaches).

The NAMD reference paper in September 2014 had over 4,000 citations

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NAMD Features

- **Dynamics Simulation Options**:
  - Periodic boundary conditions
  - Energy minimization
  - Fixed atoms, rigid waters, rigid bonds to hydrogen, harmonic restraints, spherical or cylindrical boundary restraints, constant energy dynamics
  - Constant temperature dynamics via:
    - Velocity rescaling,
    - Velocity reassignment,
    - Langevin dynamics,
  - Constant pressure dynamics via:
    - Berendsen pressure coupling,
    - Nosé-Hoover Langevin piston,

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VMD

VMD web page: http://www.ks.uiuc.edu/Research/vmd/
Documentation: http://www.ks.uiuc.edu/Research/vmd/current/docs.html

VMD is designed for **modeling, visualization, and analysis** of biological systems such as proteins, nucleic acids, lipid bilayer assemblies, etc. It may be used to view more general molecules, as **VMD can read standard Protein Data Bank (PDB)** files and display the contained structure. VMD provides a wide variety of methods for rendering and coloring a molecule: simple points and lines, CPK spheres and cylinders, licorice bonds, backbone tubes and ribbons, cartoon drawings, and others. **VMD can be used to animate and analyze the trajectory of a molecular dynamics (MD) simulation**. In particular, VMD can act as a graphical front end for an external MD program by displaying and animating a molecule undergoing simulation on a remote computer.

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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

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