NAMD 2.7 -
Key Features of Upcoming Release

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

What is NAMD?

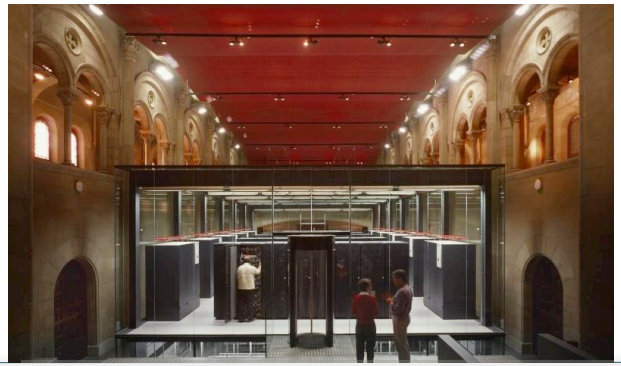
NAnoscale Molecular Dynamics

Based on Charm++ framework

Adaptable and Fast: Scales to 1000s of processors

Gordon Bell Award in supercomputing

NIH Funded Simulation Software



A few details ...

NAMD Setup

Free to download and use

Installed at all NSF supercomputing centers

Portable to virtually any platform with ethernet or MPI

C++ source code freely available via download or CVS access

Precompiled Binaries Available

AIX

BlueGeneP

Linux 32 and 64 bit on x86

Linux on SGI Altix

Mac-OSX Intel and PowerPC

Solaris on Sparc and 64 bit x86

Win XP, etc

Nightly build available for:

Linux x86_64 (Opteron, Athlon64, Intel EMT64)

Scalable Performance

Based on Charm++ parallel programming framework

Spatial and force decomposition

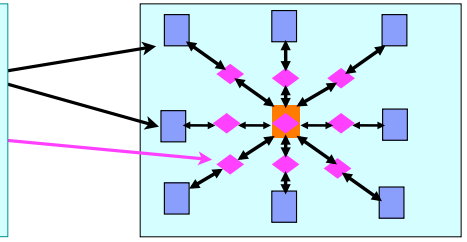
Message driven execution for latency tolerance on networks

Measurement-based load balancing - scales to 1000s of processors

Now capable of simulating 100 million atoms on as few as 16 cores

Hybrid of spatial and force decomposition:

- Spatial decomposition of atoms into cubes (called patches)
- For every pair of interacting patches, create one object for calculating electrostatic interactions
- Recent: Blue Matter, Desmond, etc. use this idea in some form



Model Building

VMD used to prepare molecular structure for simulation

Reads CHARMM, AMBER, GROMACS and X-PLOR input formats

Psfgen tool generates structure & coordinate files for CHARMM

Efficient conjugate gradient minimization

Fixed atoms and harmonic restraints

Thermal equilibration

What can NAMD do

Quick Summary of Features

~~What can NAMD do~~

…for me?

Basic Molecular Dynamics

Coarse-grain Simulations

Collective Variables Module

Alchemical Free Energy Module

User-Defined Forces Module

Accelerated Molecular Dynamics

Basic Molecular Dynamics

Constant temperature (Langevin)

Constant pressure (Berendsen or Langevin Nose-Hoover)

NVE, NVT & NPT ensembles

Particle mesh Ewald (PME) & full electrostatics for periodic systems

Symplectic multiple timestep integration

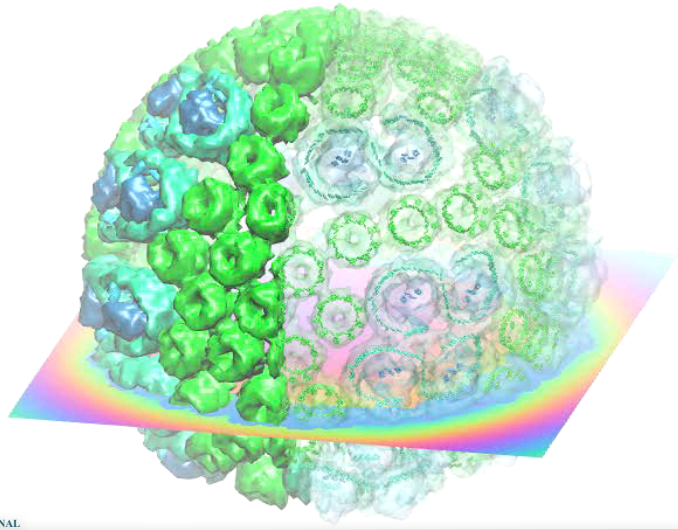
Rigid waters and bonds to hydrogen atoms (SHAKE, RATTLE)

Scriptable Interface allows user-control of simulations

Simulate Large Systems

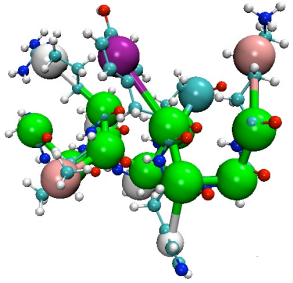
Routinely simulate 3 million atoms on 1000-3000 processors

100 million atoms on 16 processors with 128 GB memory

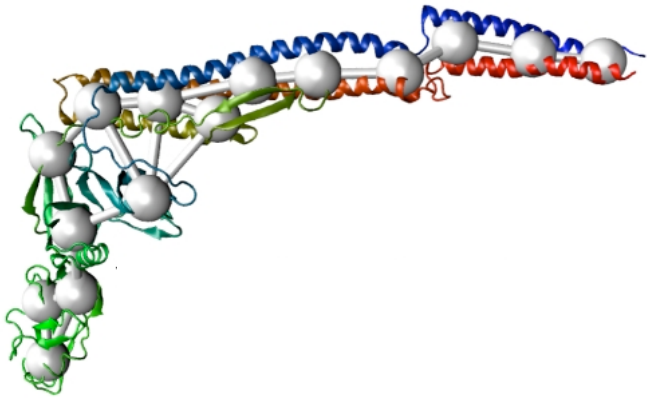


Coarse-grain your simulations

Residue-based (RBCG)



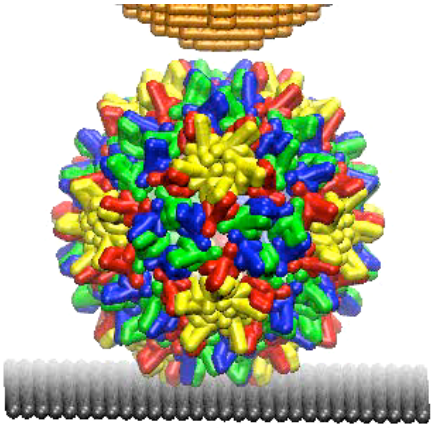
Shape-based (SBCG)

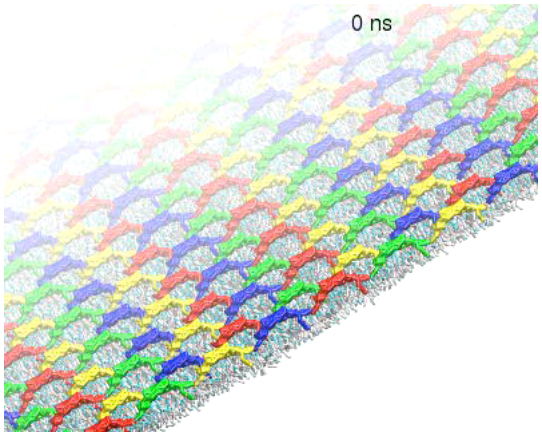


Coarse-grain your simulations

Residue-based (RBCG)

Shape-based (SBCG)





Collective Variables Module

Adaptive-biasing force (ABF) Metadynamics Harmonic Restraints

Degrees of Freedom

Bonds / Distances

Angles

Dihedrals

Collective Variables Module

Adaptive-biasing force (ABF) **Metadynamics** **Harmonic Restraints**

Degrees of Freedom

Bonds / Distances

Angles

Dihedrals

RMSd

alpha helicity

pi-stacking

domain-domain distance, angle, dihedral

....limited only by your creativity....

Collective Variables Module

Adaptive-biasing force (ABF) **Metadynamics** **Harmonic Restraints**

`distance`; `distanceXY`, `distanceZ` (relative to an axis)

`distanceDir` (value: unit vector)

`angle`, `dihedral`

`coordNum`: coordination number bw. atom groups

radius of `gyration`

`rmsd`: position RMSD from reference

`eigenvector`: displacement from ref. along given vector

`orientation` (best-fit rotation, value: quaternion)
can be used to restrain orientation of a molecule

`alpha`: α-helix content (H-bonds, angles)

suggestions and contributions welcome

Collective Variables Module

Adaptive-biasing force (ABF) **Metadynamics** **Harmonic Restraints**

```
colvarsTrajFrequency 2000
colvarsRestartFrequency 20000
```

general colvar module parameters

```
colvar {
  name d

  width 0.2
  lowerBoundary 2
  upperBoundary 32
  upperWallConstant 10.0

  distance {
    group1 {
      atomNumbers 1
    }
    group2 {
      atomNumbers {4 5 6 42}
    }
  }
}
```

defining one colvar

component: distance

```
colvar {
  name r

  width 0.05
  lowerBoundary  0.05
  upperBoundary 10.0

  rmsd {
    atoms {
      atomsFile trace.pdb
    }
    refpositionsfile beta-ideal.pdb
  }
}
```

second colvar

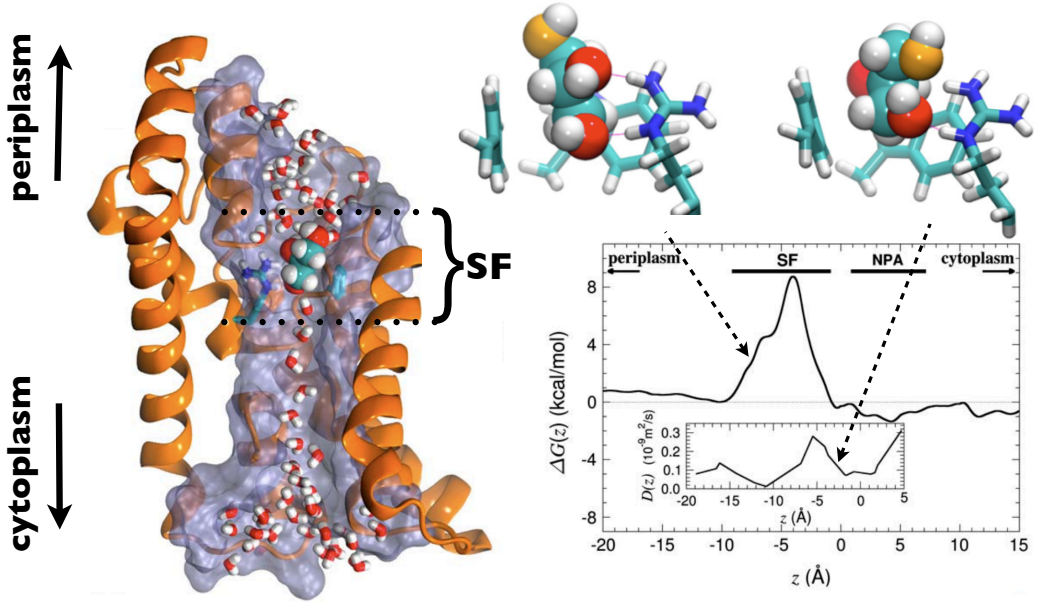
component: rmsd

```
abf {
  colvars d r
}
```

ABF bias (using default parameters)

Collective Variables Module

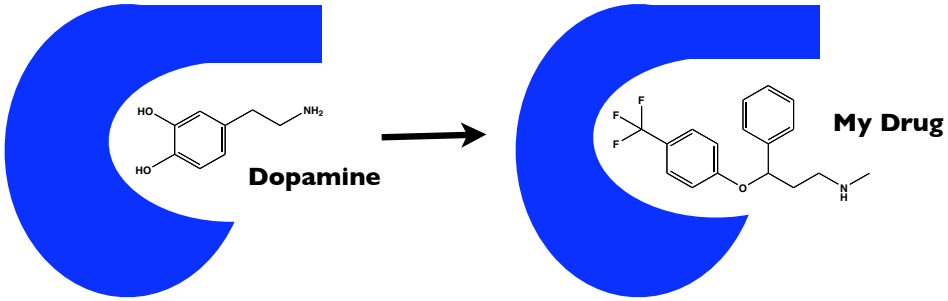
Adaptive-biasing force (ABF) **Metadynamics** **Harmonic Restraints**



Glycerol through *E. coli* Aquaglyceroporin GlpF

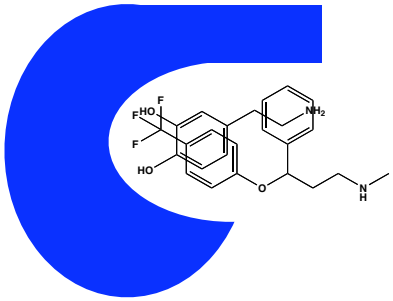
Alchemical Free Energy Module

Free Energy Perturbation **Thermodynamic Integration**



Alchemical Free Energy Module

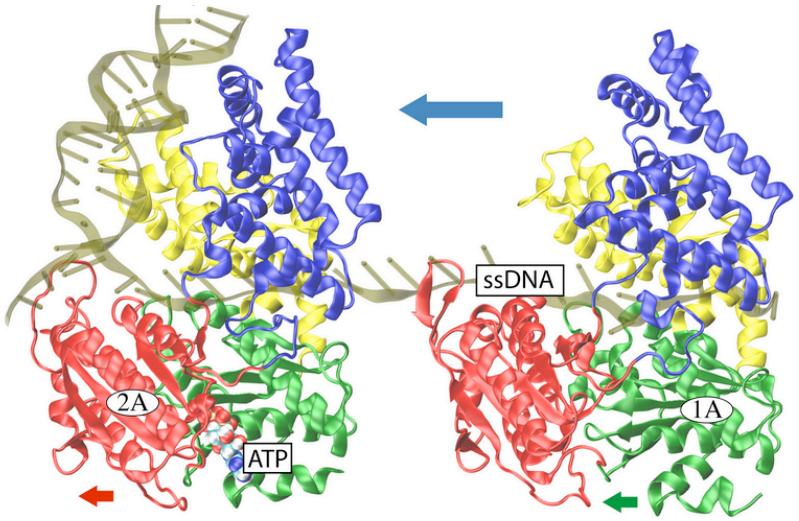
Free Energy Perturbation **Thermodynamic Integration**



Dopamine $\xrightarrow[dG]{}$ **My Drug**

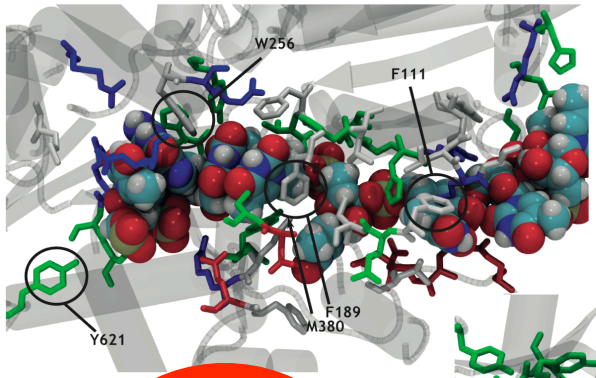
Alchemical Free Energy Module

Free Energy Perturbation **Thermodynamic Integration**



Alchemical Free Energy Module

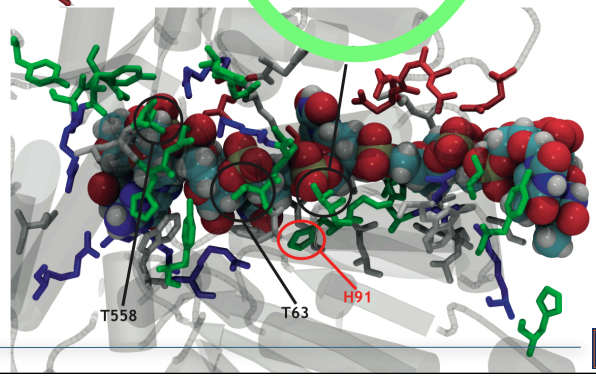
Free Energy Perturbation | **Thermodynamic Integration**



Y621
F189
W256

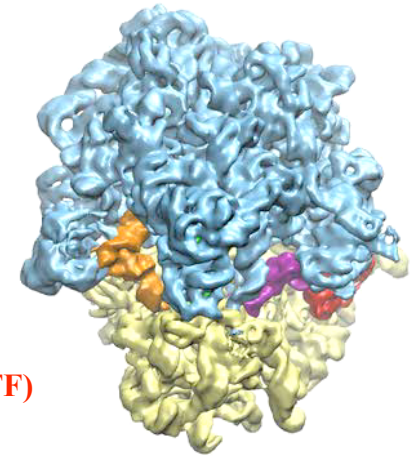
F11
M380

T558 T88
H91 T63



User-Defined Forces Module

Cryo-EM map of the *E. coli* ribosome at 6.7-Å resolution



Steered-molecular dynamics (SMD)

Targeted molecular dynamics (TMD)

Interactive molecular dynamics (IMD)

TclForces

GridForces

Molecular Dynamics Flexible Fitting (MDFF)

Accelerated Molecular Dynamics

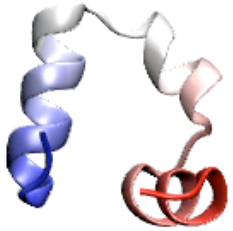
Locally Enhanced sampling (LES)

Replica-Exchange

Faster SHAKE & RATTLE for hydrogen and water

Enhanced load balancing & patch distribution

GPU based Molecular Dynamics



Accelerated Molecular Dynamics

Locally Enhanced sampling (LES)

Replica-Exchange

Faster SHAKE & RATTLE for hydrogen and water

Enhanced load balancing & patch distribution

GPU based Molecular Dynamics

Future Features ...

Places to go

To learn more / download NAMD:
http://www.ks.uiuc.edu/Research/namd

For suggestions to setup / compile NAMD:
http://www.ks.uiuc.edu/Research/namd/wiki/

The NAMD user community - for help using NAMD:
http://www.ks.uiuc.edu/Research/namd/mailing_list

For when you think you found a bug:
http://www.ks.uiuc.edu/Research/namd/bugreport.html