NAMD TUTORIAL
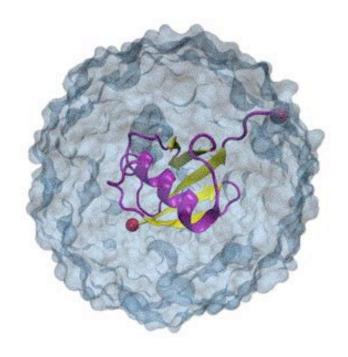## Unix/MacOSX Version

---

NAMD Developer: James Phillips

Timothy Isgro

James Phillips

Marcos Sotomayor

Elizabeth Villa

February 2006

Scalable Molecular Dynamics with NAMD

JAMES C. PHILLIPS,[1] ROSEMARY BRAUN,[1] WEI WANG,[1] JAMES GUMBART,[1]
EMAD TAJKHORSHID,[1] ELIZABETH VILLA,[1] CHRISTOPHE CHIPOT,[2] ROBERT D. SKEEL,[3]
LAXMIKANT KALÉ,[3] KLAUS SCHULTEN[1]

[1]*Beckman Institute, University of Illinois at Urbana–Champaign, Urbana, Illinois 61801*
[2]*UMR CNRS/UHP 7565, Université Henri Poincaré,*
54506 Vandœuvre-lès-Nancy, Cedex, France
[3]*Department of Computer Science and Beckman Institute, University of Illinois at*
Urbana–Champaign, Urbana, Illinois 61801

Abstract: NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. NAMD scales to hundreds of processors on high-end parallel platforms, as well as tens of processors on low-cost commodity clusters, and also runs on individual desktop and laptop computers. NAMD works with AMBER and CHARMM potential functions, parameters, and file formats. This article, directed to novices as well as experts, first introduces concepts and methods used in the NAMD program, describing the classical molecular dynamics force field, equations of motion, and integration methods along with the efficient electrostatics evaluation algorithms employed and temperature and pressure controls used. Features for steering the simulation across barriers and for calculating both alchemical and conformational free energy differences are presented. The motivations for and a roadmap to the internal design of NAMD, implemented in C++ and based on Charm++ parallel objects, are outlined. The factors affecting the serial and parallel performance of a simulation are discussed. Finally, typical NAMD use is illustrated with representative applications to a small, a medium, and a large biomolecular system, highlighting particular features of NAMD, for example, the Tcl scripting language. The article also provides a list of the key features of NAMD and discusses the benefits of combining NAMD with the molecular graphics/sequence analysis software VMD and the grid computing/collaboratory software BioCoRE. NAMD is distributed free of charge with source code at www.ks.uiuc.edu.

The NAMD Configuration File / 1

Files needed:

```
structure              mypsf.psf
coordinates            mypdb.pdb
```

Define temperature

```
set temperature    310
     ;# target temperature used several times below
```

Starting simulation with random velocities

```
# starting from scratch
temperature             $temperature
     ;# initialize velocities randomly
```

The NAMD Configuration File / 2
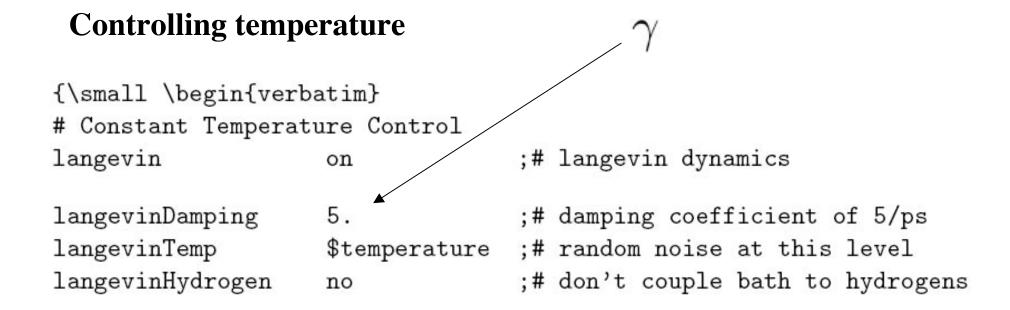
Continuing a simulation with positions and velocities from previous run

```
# continuing a run
set inputname       myinput            ;# only need to edit this in one place!
binCoordinates      $inputname.coor    ;# coordinates from last run (binary)
binVelocities       $inputname.vel     ;# velocities from last run (binary)
extendedSystem      $inputname.xsc     ;# cell dimensions from last run
firsttimestep       50000              ;# last step of previous run
numsteps            100000             ;# run stops when this step is reached
```

The NAMD Configuration File / 3

Organizing output

```
outputName            myoutput
      ;# base name for output from this run

restartfreq               500        ;# 500 steps = every 1ps
dcdfreq                   500
xstFreq                   500

outputEnergies        100        ;# 100 steps = every 0.2 ps
outputTiming        1000
      ;# shows time per step and time to completion
```

Here we assume an integration time step of 2 fs, to be defined below.

The NAMD Configuration File / 4

```
# Force-Field Parameters
paraTypeCharmm        on
parameters            par_all27_prot_lipid.inp

# These are specified by CHARMM
exclude               scaled1-4
1-4scaling            1.0
switching             on

# You have some freedom choosing the cutoff
cutoff                12. ;# may use smaller, maybe 10., with PME
switchdist            10. ;# cutoff - 2.

# Promise that atom won't move more than 2A in a cycle
pairlistdist          14. ;# cutoff + 2.
stepspercycle         10   ;# redo pairlists every ten steps
```

> 12A cutoff is official standard for CHARMM forcefield but smaller is OK when using full electrostatics

```
# Integrator Parameters
timestep            2.0   ;# 2fs/step
rigidBonds          all   ;# needed for 2fs steps
nonbondedFreq       1     ;# nonbonded forces every step
fullElectFrequency  2     ;# PME only every other step
```

> Energy drifts if too large, but smaller requires more steps per ns.

The NAMD Configuration File / 5

Controlling temperature

γ

```
{\small \begin{verbatim}
# Constant Temperature Control
langevin               on              ;# langevin dynamics

langevinDamping        5.              ;# damping coefficient of 5/ps
langevinTemp           $temperature    ;# random noise at this level
langevinHydrogen       no              ;# don't couple bath to hydrogens
```

Underlying Langevin equation for all atoms

$$m_i \frac{d^2 x_i(t)}{dt^2} = F_{i,\text{ff}} - \gamma m_i \frac{dx_i(t)}{dt} + R_i(t)$$

$$\langle R_i(t)\, R_i(t') \rangle = 2 k_B T_{\text{target}} \gamma_i\, \delta(t - t')$$

The NAMD Configuration File / 6

Using periodic boundary conditions
(avoids surface effects; permits Particle-Mesh-Ewald (PME) electrostatics; permits pressure control)

```
# Periodic Boundary conditions
cellBasisVector1     31.2    0.    0.    ;# vector to the next image
cellBasisVector2      0.    44.8   0.
cellBasisVector3      0.     0    51.3
cellOrigin            0.     0.    0.    ;# the *center* of the cell


wrapWater            on                 ;# wrap water to central cell
wrapAll              on                 ;# wrap other molecules too
wrapNearest          off                ;# use for non-rectangular cells
```

The NAMD Configuration File / 7

Particle-Mesh-Ewald electrostatics
(avoids cut-off of long-range Coulomb forces)

```
#PME (for full-system periodic electrostatics)
PME                        yes
PMEGridSizeX               32   ;# 2^5, close to 31.2
PMEGridSizeY               45   ;# 3^2 * 5, close to 44.8
PMEGridSizeZ               54   ;# 2 * 3^3, close to 51.3
```

The NAMD Configuration File / 8

Pressure Control

```
# Constant Pressure Control (variable volume)
useGroupPressure       yes ;# needed for rigid bonds
useFlexibleCell        no  ;# no for water box, yes for membrane
useConstantArea        no  ;# no for water box, maybe for membrane

langevinPiston         on
langevinPistonTarget   1.01325      ;# pressure in bar -> 1 atm
langevinPistonPeriod   100.         ;# oscillation period around 100 fs
langevinPistonDecay    50.          ;# oscillation decay time of 50 fs
langevinPistonTemp     $temperature ;# coupled to heat bath
```

Underlying Langevin-Hoover barostat equation for all atoms

$$\frac{d^2V(t)}{dt^2} = -\frac{1}{W_{bs}}\left[P(t) - P_{\text{target}}\right] - \frac{1}{\tau_{\text{bs}}}\frac{dV(t)}{dt} + R_{\text{bs}}(t)$$

$$P = \rho k_B T + \frac{1}{Vd}\sum_{i<j}\langle r_{ij}\frac{dU_{tot}(r_{ij})}{dr_{ij}}\rangle \qquad d = \text{dimension}$$

$$\langle R_{\text{bs}}(t)\,R_{\text{bs}}(t')\rangle = \frac{2\,k_{\text{B}}\,T_{\text{target}}\,\delta(t-t')}{W_{\text{bs}}\,\tau_{\text{bs}}} \qquad W_{\text{bs}} = d\,N_{\text{atoms}}\,k_{\text{B}}T_{\text{target}}\,\tau^2_{period}$$

The NAMD Configuration File / 8

Pressure Control

```
# Constant Pressure Control (variable volume)
useGroupPressure        yes ;# needed for rigid bonds
useFlexibleCell         no  ;# no for water box, yes for membrane
useConstantArea         no  ;# no for water box, maybe for membrane

langevinPiston          on
langevinPistonTarget    1.01325       ;# pressure in bar -> 1 atm
langevinPistonPeriod    100.          ;# oscillation period around 100 fs
langevinPistonDecay     50.           ;# oscillation decay time of 50 fs
langevinPistonTemp      $temperature  ;# coupled to heat bath
```

Underlying Langevin-Hoover barostat equation for all atoms:
Equations solved numerically in NAMD

$$\dot{\mathbf{r}}_i = \mathbf{v}_i + s\mathbf{r}_i \qquad\qquad \dot{\mathbf{v}}_i = \mathbf{F}_i / m_i - s\mathbf{v}_i$$

$$\dot{V} = dVs \qquad \dot{s} = dV(P - P_{\text{target}})/W - s/\tau_{\text{bs}} + R(t)$$

d - dimension

The NAMD Configuration File / 9

Fix atoms

```
fixedAtoms          on
fixedAtomsFile      myfixedatoms.pdb   ;# flags are in this file
fixedAtomsCol       B                  ;# set beta non-zero to fix an atom
```

The NAMD Configuration File / 10

Energy-minimize structure (T=0) , reset temperature T, run:

```
minimize              1000              ;# lower potential energy for 1000 steps
reinitvels            $temperature      ;# since minimization zeros velocities
run 50000 ;# 100ps
```

The NAMD Output File / 1

Preamble

```
Info: NAMD 2.5b2ss03 for Linux-i686-Clustermatic
Info:
Info: Please visit http://www.ks.uiuc.edu/Research/namd/
Info: and send feedback or bug reports to namd@ks.uiuc.edu
Info:
Info: Please cite Phillips et al., J. Comp. Chem. 26: 1781-1802 (2005)
Info: in all publications reporting results obtained with NAMD.
Info:
Info: Built Fri May 30 13:09:06 CDT 2003 by jim on umbriel
Info: Sending usage information to NAMD developers via UDP.
Info: Sent data is: 1 NAMD  2.5b2ss03  Linux-i686-Clustermatic 47 umbriel jim
Info: Running on 47 processors.
```

The NAMD Output File / 2

Energies

ETITLE:	TS	BOND	ANGLE	DIHED	IMPRP
	ELECT	VDW	BOUNDARY	MISC	KINETIC
	TOTAL	TEMP	TOTAL2	TOTAL3	TEMPAVG
	PRESSURE	GPRESSURE	VOLUME	PRESSAVG	GPRESSAVG
ENERGY:	1000	0.0000	0.0000	0.0000	0.0000
	-97022.1848	9595.3175	0.0000	0.0000	14319.5268
	-73107.3405	300.2464	-73076.6148	-73084.1411	297.7598
	-626.5205	-636.6638	240716.1374	-616.5673	-616.6619

The NAMD Output File / 1

Writing out trajectories

$\vdots$

```
OPENING COORDINATE DCD FILE
WRITING COORDINATES TO DCD FILE AT STEP 1000
```

$\vdots$

Performance information

```
Info: Benchmark time: 47 CPUs 0.0475851 s/step 0.275377 days/ns 13540 kB memory

TIMING: 1000  CPU: 18.35, 0.01831/step  Wall: 50.1581, 0.0499508/step, 6.92374
hours remaining, 14244 kB of memory in use.
```

Warnings

```
Warning: Pairlistdist is too small for 1 patches during timestep 17.
Warning: Pairlists partially disabled; reduced performance likely.
Warning: 20 pairlist warnings since previous energy output.
```
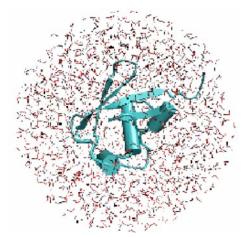
The NAMD Experience / 1

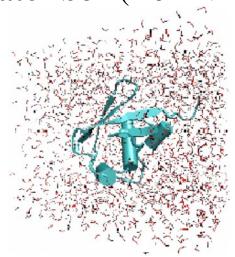**You will first simulate ubiquitin in a water sphere and water box:**

Generating a Protein Structure File (PSF)
- Go to 1-1-build directory
- Open VMD, choose extension TkCon
- Make from 1UBQ.pdb a structure without hydrogens, ubqp.pdb
- Create psf file for ubqp.pdb: ubq.pdb and ubq.psf
- Check if files exist

Solvate the protein in a water sphere (from VMD)

Solvate the protein in a water box (from VMD)

The NAMD Experience / 2

- RMSD value for equilibration
- Atomic RMSD values of equilibrated protein
- Velocity distribution
- Temperature distribution
- Specific heat
- Diffusion of whole protein
- Heat diffusion
- Temperature Echoes