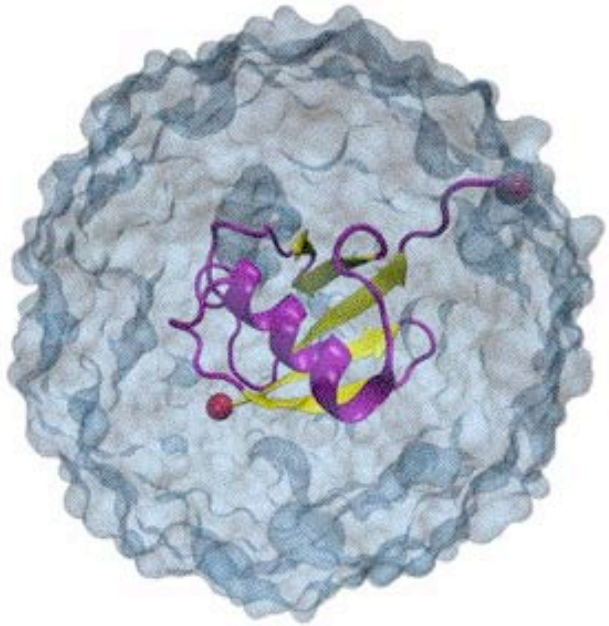
NAMD TUTORIAL

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*

Received 14 December 2004; Accepted 26 May 2005
DOI 10.1002/jcc.20289
Published online in Wiley InterScience (www.interscience.wiley.com).

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


# 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
```

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

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

The NAMD Configuration File / 5

Controlling temperature

```
{\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

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

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

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

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

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

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

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

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

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

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

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

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.
```

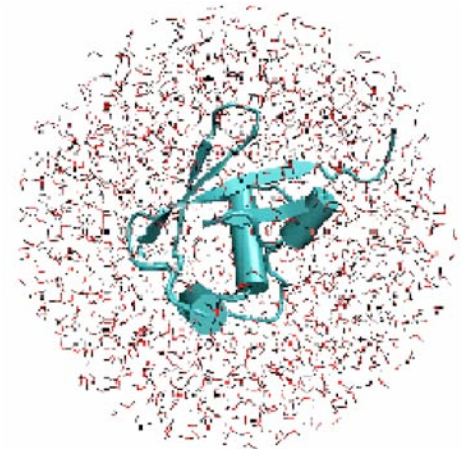
The NAMD Experience / 1

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

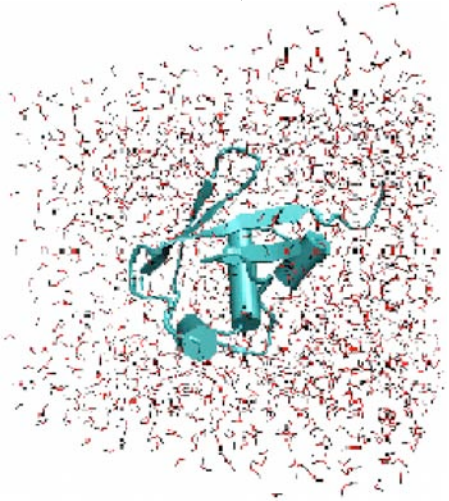
Generating a Protein Structure File (PSF)

- 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**