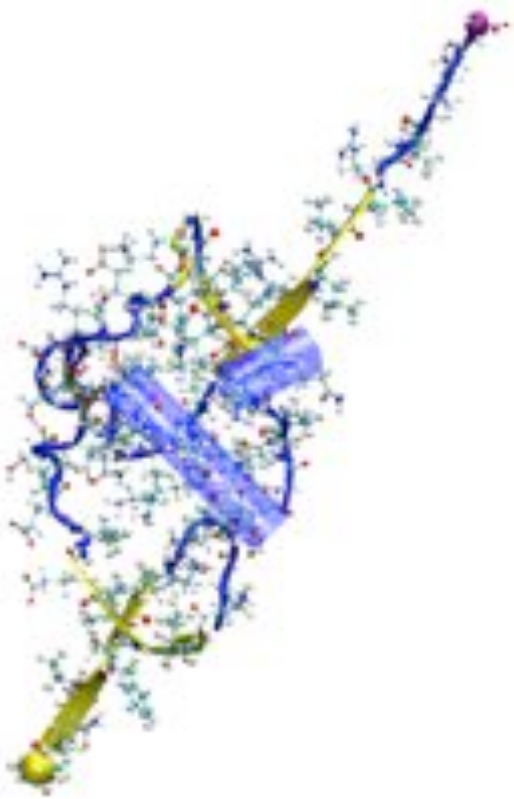
NAMD TUTORIAL



NAMD Developer: James Phillips

Timothy Isgro
James Phillips
Marcos Sotomayor
Elizabeth Villa

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
```

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

```
{\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

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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 Kale et al., J. Comp. Phys. 151:283-312 (1999)
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.
```

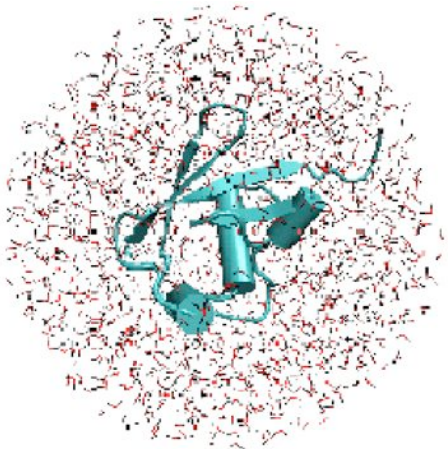
The NAMD Experience / 1

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

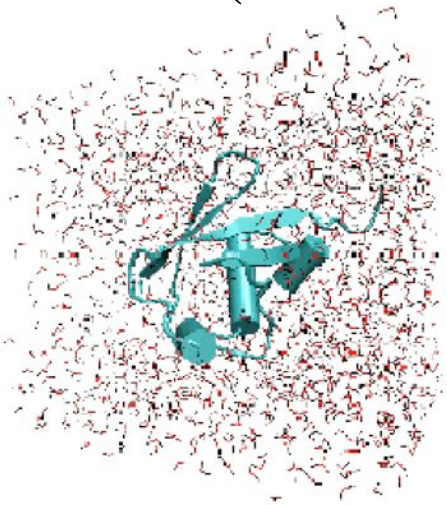
Generating a Protein Structure File (PSF)

- 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**