Configuring and Running NAMD Simulations

Jim Phillips
Theoretical Biophysics Group
Beckman Institute, UIUC

NAMD Basics

- NAMD is a batch-mode program.
- A text configuration file controls all options for input, output, and simulation methods.
- NAMD is portable to a variety of platforms.
- Command line flags and the command used to launch parallel jobs are not uniform.
- Some platforms have multiple versions.

Charm++, Converse, and MPI

- NAMD is built on Charm++/Converse.
- Charm++ is a parallel programming system based on message-driven objects and C++.
- Converse is a parallel runtime providing message driven execution which can use several underlying messaging protocols.
- MPI is a standardized messaging system.

Running on Supercomputers

- Use MPI version for >8 CPUs on Origin:

  mpirun –np X namd2 config.namd
- Otherwise just use:

  namd2 +pX config.namd
- For T3E:

  mpprun –n X namd2 config.namd

  (See release notes for full details.)

Running on Clusters

- Need no password access to all hosts!
  - Can use ssh: setenv CONV_RSH ssh
- Create a nodelist or ~/.nodelist file:

```
group main
   host romeo
   host juliet
```

- charmrun namd2 config.namd

(See release notes for full details.)

Cluster Command Line Options

- Number of nodes to run on: +pX
- Just run on localhost: ++local
- Which group in nodelist: ++nodegroup X
- Which nodelist file: ++nodelist X
- Diagnose startup errors: ++verbose
- View stdout in xterm: ++in-xterm
- List all options: ++help

Directories and Paths

- Full paths to binaries may be needed:

  ~/bin/charmrun ~/bin/namd2 bpti.namd
- All paths in the config file are relative to the directory which contains the config file:

  charmrun namd2 /home/jim/test/bpti.namd
- Unless the cwd parameter is given:

  “cwd /home/jim/research/bpti”

Configuration File Format

- NAMD is case insensitive (Tcl isn't).
- All options follow: <name> <value>
- Some options may appear several times.
- Some options contain scripts inside { }.
- Everything following '#' is a comment.
- Include other files with "source <file>".
- If you know Tcl, use print rather than puts.

Quick Intro to Tcl

- Basic assumption: Everything is a string.
- Terminate commands with newline or ;
- Comments are just the command #
- Setting variables: set temp 300
- Using variables: langevinTemp $temp
- Math: set temp [expr $temp + 50]
- See http://dev.ajubasolutions.com/scripting/primer.html

Molecular System Configuration

- Structure (.psf) file:

  "structure protein.psf"

  Must be X-PLOR style, not CHARMM.

  (CHARMM can generate this format.)

- Coordinates (.pdb) file:

  "coordinates protein.pdb"

  Must be X-PLOR style, only ATOM records.

Periodic Cell Configuration

- 1-3 basis vectors and a center point

  “cellBasisVector1 60.23 0 0”

  “cellBasisVector2 0 46.31 0”

  “cellBasisVector3 0 0 30.42”

  “cellOrigin 0 0 0”

- May also be read from restart file with

  “extendedSystem restart.xsc”

Energy Function Configuration

- Parameter file(s):

  "parameters param19.pro"

  Default is X-PLOR format, or may use

  "paraTypeCharmm on"

- Also need exclusion policy:

  "exclude scaled1-4"

  "1-4scaling 0.4" (see parameter file)

Nonbonded Cutoff Configuration

- Generally want the following (values vary):
  - “switching on”
  - “switchdist 7.5”
  - “cutoff 8”
  - “pairlistdist 9.5”
  - “stepspercycle 10”
- All needed even with full electrostatics.

Minimization Configuration

- Conjugate gradient minimization:

  "minimization on"
- Efficient, self-tuning, and very robust.
- In case of initial instability, reduce this:

  "minTinyStep 1.0e-6"
- In case of later instability, reduce this:

  "minBabyStep 10.e-2"

Integrator Configuration

- Uses Verlet, basic configuration:

  "timestep 1.0"
- Optional rigid water model:

  "rigidBonds water"
- Longer timesteps with all bonds to H rigid:

  "rigidBonds all"

  "timestep 2.0"
- Additional rigidBonds options in manual.

Initial Velocities

- Obtained from Boltzmann distribution:

  "temperature 300"
- Or from restart file:

  "velocities restart.vel"
- Center of mass motion is subtracted.

Number of Steps

- Based on a continuing simulation model to allow log files to be concatenated.
- First give the numer of steps already done:

  "firstTimestep 30,000" (defaults to 0)
- Then the final step wanted in this run:

  "numsteps 40,000" (must be >= firstTimestep)
- In the above 10,000 more steps will be run.

Log Printout

- Configuration options and energy logs are send to standard output.
- Reduce amount of energy output:

  "outputEnergies 20" (default is 1, every step)
- Print out periodic performance data:

  "outputTiming 100" (default is 0, never)
- Also options for momenta and pressure.

Restart & Trajectory Output

- Periodic restart files and final configuration:
  - "outputName run1" (generates run1.coor, etc.)
  - "restartFreq 1000" (save every 1000 steps)
- See manual for info on binary formats!
- Generate a DCD trajectory file:
  - "DCDFreq 500" (one frame every 500 steps)
- Existing files renamed to .BAK

Wrapping Coordinates

- Water, etc. drifts “outside” of periodic cell.
- Visualization programs don’t handle well.
- Old option “wrapWater on” for water.
- New option “wrapAll on” for all clusters.
- New option “wrapNearest on” wraps to, e.g., hexagon rather than parallelogram.

Advanced Tcl Scripting

- Complex protocols can be written in Tcl:

```
minimize 1000
for { set t 100 } { $t <= 500 } { incr t 50 } {
   reinitvels $t;  run 10000
   checkpoint
   minimize 1000;  output min_$t
   revert
}
```

Diagnosing Problems

- Check the output log for:
  - Misspelled parameters which are ignored.
  - Abnormally high initial energies. (Minimize!)
  - Warnings that may be related.
- Check the input structure and coordinates:

  vmd -psf bpti.psf -pdb bpti.pdb
- Email namd@ks.uiuc.edu.