

CSE 498/598k: Homework #1

Due: 09/21/04

1. Complete Chapter 1 and Chapter 2 (through Section 2.1, page 47) of the NAMD tutorial available online at:

<http://www.ks.uiuc.edu/Training/SumSchool/labs.html>

It is listed under the item: *Tue, 6/3: Statistical Mechanics of Proteins*. You can work through it online in html or download the pdf. Note that you will also need the *input files*, under the same heading. Since this file is rather large, I have placed a local copy in our course web space on AFS.

Because this exercise is a basic follow-the-directions type, I expect that each person will individually work through it. That is not to say that you can not work together, but that each person is responsible for completing the assignment.

In order to run namd2 on the Linux cluster machines, you will need to first load the module. This can be done with the following command:

```
% module load namd/2.5
```

Unfortunately, VMD is not installed in AFS, but you can run it from my directory. I have versions for both Sun and Linux. For working in the cluster, I suggest adding the following lines to your .cshrc (.tcshrc) file:

```
alias vmd    '/afs/nd.edu/user8/shampton/usr/bin/vmd-linux'  
alias vmds   '/afs/nd.edu/user8/shampton/usr/bin/vmd'
```

As long as you can get to AFS, you can run either version of VMD. I would try to avoid running VMD through an SSH connection if at all possible.

In the tutorial, the authors suggest making modifications with a program called `nedit`. This is installed in AFS, but you are not required to use this. You may use any text editor that you are comfortable with. I prefer `vim`.

2. For the one dimensional harmonic oscillator (ODHO) given in class, ($\dot{x} = p$, $\dot{p} = -x$), apply the Backward Euler method:

$$y^{n+1} = y^n + \Delta t f(y^{n+1}), \quad y' = f$$

to obtain the propagation matrix E , where $y^{n+1} = E y^n$. Find the determinant of E and explain what it means. For extra credit, find the stability condition.

3. Write a small program that implements the Euler method and Leapfrog method for the ODHO of the previous problem. Run your program for various Δt and N . Plot the total, kinetic and potential energies, as well as phase space for each method.
4. Answer the following questions based on the assigned papers.

“A Test Set for Molecular Dynamics Algorithms”

- (a) Which test systems, as described in the paper, would be valid to solve the following problems:
 - i. You want to validate correctness of bond and angle calculations in your MD program.
 - ii. You want to validate correctness of dihedral calculations in your MD program.
 - iii. You want to observe different conformations.
 - iv. You want to produce a Ramachandran plot.

- v. You want to simulate protein folding.
- vi. You want to compare MD vs. experimental data on an Argon system.

“Molecular Dynamics Simulations”

- (a) What is an example of a disease associated mechanism that has been studied with MD?
- (b) What was the name and size of the first simulated protein? What name and size do the authors suggest is a recently simulated protein?

“Validation of Molecular Dynamics Simulation”

- (a) Why do the authors argue against non constant pressure, constant temperature simulations?
- (b) What are the five validation criteria listed?
- (c) What is meant by equilibration of a system?
- (d) How can MD software itself be validated and tested?
- (e) What is suggested for people writing and using MD software?
- (f) How would open software contribute towards validation of simulations?

What to turn in:

1. An RMSD plot of Ubiquitin.
2. Plot of the energies and temperature during a simulation.
3. Plot of the Maxwell-Boltzmann energy distribution.