

## 3.320 Atomistic Modeling of Materials Spring 2005

### Problem set 4: Molecular Dynamics

Due date: 4/21/05

In this problem set, we will examine some of the common features of molecular dynamics calculations (MD). First, we will examine the key features of the different integrators which form the basis of any MD engine. Our first exercise will focus on timestep selection as well as the stability and accuracy of a variety of different integration methods.

In this problem set, we will also look at Kr using MD with a Lennard-Jones energy model. In particular, we will be studying the melting behavior of Kr.

In addition, we will discuss the scalability of simulations with system size. We will also look at the fluctuation of temperature in a MD and how it changes with the system size.

#### **Problem 1. Accuracy of different Integrators (20 pts)**

Newton's equations of motion are at the core of any classical MD calculation. While different ensembles may use different dynamics, all MD calculations require accurate and stable integrators in order to solve the equations of motion. In class, we discussed some Verlet algorithms and briefly mentioned some predictor-corrector algorithms. In this exercise, we will examine the accuracy and stability of different integrators as they apply to an EAM model of Ni.

- A.) Using GULP's MD capability, examine the average total energy as a function of timestep size using the leapfrog Verlet integration method. Do all of these calculations at 300K. Plot your results.
- B.) On the same plot, show the average total energy as a function of timestep size using both the velocity Verlet and the Gear Predictor-Corrector algorithms.
- C.) Now plot the standard deviation of the average total energy for the three different algorithms as a function of timestep size.
- D.) For a timestep of 0.001 ps, plot the instantaneous energy of the three algorithms
- E.) Comment on your results with respect to which algorithm is most stable, which is most accurate, and which is most computationally expensive.

#### **Problem 2. Melting temperature of bulk Kr (60 pts)**

In this problem, we find the melting temperature of bulk Krypton by two methods, 1) direct annealing and 2) two-phase simulation method. We will use Lennard-Jones potential in this problem.

- A.) Find the melting temperature of solid Kr by performing MD of the crystal at different temperatures. (45 pts) You have to find a suitable timestep for the simulations and system size. What ensemble do you use? Analyze your data with several techniques to determine the melting temperature (i.e. mean-square displacement, etc.) You should also mention other ways of determining melting which are conceptually easy but difficult without writing new analysis routines. Make sure to record all of your simulation parameters (such as time step, cell size, equilibration time, sampling time, ensemble used,

and so on). Would this method overestimate or underestimate the melting temperature? Why?

**Two phase simulation method:**

This method was first introduced by F. Ercolessi et. al. Surf. Sci. Lett. **258**, L676 (1991).  
B) Read the paper by Morris et. al. Phys. Rev. B **49**, 5 (1993). Describe the method in the paper. Calculate the melting temperature of Kr using two phase simulation method. (15 pts)

**Problem 3. Scalability of MD Systems (10 pts)**

Consider a bulk material simulation using periodic boundary conditions and large supercells.

- A.) For an fcc material, how many atoms are contained in a supercell consisting of  $N \times N \times N$  unit cells?
- B.) How many force calculations are required for each timestep if all atoms are considered? How many force calculations are required if a potential cutoff is implemented? How many times must you calculate the distance between atoms?
- C.) Rank the following force calculations in terms of the CPU time required: Hartree-Fock methods, Lennard-Jones pair potentials, EAM pair functional potentials, and Density Functional Theory. Explain your choices.
- D.) For simple forms of empirical potentials, most of the computation time is spent calculating the distance between atoms. Can you think of any ways of reducing the amount of time spent calculating distances?

**Problem 4. Temperature fluctuation in a MD and how it changes with system size (10 pts)**

You may notice, when doing problem 1, the production run temperature fluctuates around its average value. In this question, we will explore the change in this fluctuation as we increase the system size.

- A.) Go back to the output file in Problem 1 (Velocity verlet method, timestep = 0.001 ps), plot the instantaneous temperature of the production run as a function of time.
- B.) Run the MD with bigger system size (cell = 4, 5, 6 etc) and plot the instantaneous temperature on the same graph. Remember to use the same integration method and timestep.
- C.) Explain the changes in fluctuation of the temperature with the system size.
- D.) What is the mathematical relation between the standard deviation of the temperature and the system size (ie. number of atoms)? Verify this with your data in part C.

### **Extra Credit Opportunities**

#### **(20pts): Building your own tool**

Write your own molecular dynamics code from scratch. This task is really not very hard if you stick to the basics but can quickly increase in difficulty as you add features.

The easy parts: (5 pts)

- 1.) Include a force calculation routine
- 2.) Include an integrator
- 3.) Output atomic positions

A bit harder: (5 pts)

- 1.) Include an Input/Output mechanism for handling different configurations
- 2.) Report total energy, kinetic energy, and potential energy
- 3.) Incorporate periodic boundary conditions
- 4.) Include a velocity rescaling equilibration stage

Even a bit harder: (5 pts)

- 1.) Include neighborlist tracking
- 2.) Report pressure and temperature
- 3.) Calculate mean squared displacements and radial distribution functions

Much harder: (5 pts) (very advanced topics, which may be useful if you intend to get more involved with these calculations)

- 1.) Include other thermodynamic ensembles besides microcanonical (Andersen, Parrinello & Rahman methods)
- 2.) Include cell-bin list counting
- 3.) Allow for multiple potential forms
- 4.) Parallelize your code using MPI calls

Alternate programming opportunity: (Hard!, but you'll have my gratitude as well as the satisfaction of knowing future generations will use your code.)

Modify the MOLDY code to handle pair functional potentials as well as standard pair potentials.

(10pts): Use GULP MD to study the melting of the provided EAM Ni using direct heating.