3650:350 **Modeling and Simulation** **Spring 2003**

Exercises #8
due: Wednesday, April 9, 2003

For additional information on this assignment, please read:
Rex and Thornton *Modern Physics*, Chapter 9 (Statistical Physics) pp 272–285
Giordano *Computational Physics* Chapter 8.3 (The Monte Carlo Method) pp 213-215
Giordano *Computational Physics* Chapter 9 (Molecular Dynamics) pp 232-252
The handouts from the books of D. C. Rapaport (The art of molecular dynamics simulations) and D. Chandler (Introduction to Modern Statistical Mechanics)

1. Monte Carlo simulations of a two-dimensional fluid
   The files *MC2dfluid.m* is the main program for a Monte Carlo simulation of a soft disk fluid. It calls the function files *fumlj.m*, *fconfigplot.m*, *fvirial.m*, and *fpairdist.m*.

   (a) Equilibration
   For this part, set the number of particles per row to `Nrow=5`, set the density to `density=0.5` and set the temperature to `Tred=1.0`. Set the illustration flag, `iflag` to 1, choose a small number of Monte Carlo steps, e.g `krun=50` and set the number of equilibration steps to zero, `kequ=0`. Run the program, compare the initial and final configuration of particles, and save all plots. Note the maximum displacement in a trial move, `dispmax`, and the acceptance rate. Change the maximum displacement to 0.2 times its original value, run the program again, note the acceptance rate and save all plots. Repeat with a maximum displacement of 5 times its original value. Compare the results. What is the trend here? Is there an optimum value for the maximum displacement? Can you confirm it? Use your best estimate for the following parts.

   Add a command to the program that plots the potential energy per particle `epot` as a function of Monte Carlo steps and note how the energy changes over the few steps. Increase the number of Monte Carlo steps to 500, run the program, and consider the plot of the internal energy and the plot of the energy correlation function. Estimate the correlation time for the internal energy from the time (in MC steps), where the correlation function goes to zero. Consider a time ten times as large for your equilibration time. Check your internal energy versus time plot to make sure that the internal energy at that time is no longer displaying obvious trends.

   (b) First production run
   Use your estimate for `kequ` from part (a), pick an observation time `kobs` that is about 4 times as long and divisible by 10 and set `krun` to `kequ+kobs`. Run the program, copy all figures into your word document, and note the final values for the pressure and its uncertainty.
   Note: if the uncertainty in the pressure is more than 10%, your run is probably too short.
   Consider the plot for the pair distribution function, can you tell whether the system is in the solid, liquid, or gas state?
   Note: it takes a very long run to obtain "smooth" pair distribution functions. For now,

a somewhat ragged function is alright, we will look at pair distribution functions in more detail in the last problem.

(c) Energy fluctuations
In the simulations, the temperature is fixed but the internal energy is allowed to fluctuate. Modify the program to determine the probability distribution for the internal energy by binning the results as in the previous homework assignment Run your program for the conditions in (a) and (b) and plot the probability distribution. What kind of probability distribution is it? What are its mean and standard deviation. Please also include block averaging for the total internal energy so that we can compare with MD simulation results later. Note: you may use either the potential or the total internal energy per particle, this will only change the mean.
Note: While you are working on the program, go back to short runs and set the state of the random number generator to a fixed value.

(d) Trial moves
The program "sweeps" through the particles, i.e. the particles are taken in turn when the trial moves are made. Change the program so that it picks the particles at random, instead. Run your program for the conditions in (a)–(c) and compare the results. Pay particular attention to the correlation time.

2. Molecular Dynamics simulations of a two-dimensional fluid
The files *md2dfluid.m* is the main program for a molecular dynamics simulation of a soft disk fluid. It calls the function files *fmdini.m*, *f2dfluid.m*, *fvdist.m*, *fconfigplot.m*, *fvirial.m*, and *fpairdist.m*

(a) Equilibration
For this part, set the number of particles per row to `Nrow=5`, set the density to `density=0.6` and set the target temperature to `Ttarget=1.0`. Set the illustration flag, `iflag` to 2, choose a small number of molecular dynamics steps, e.g `krun=52`, set the number of equilibration steps to `kequ=1`, and set `kgap=1`. Run the program and save all plots. Consider the plot that shows the trajectories (Figure(2)), can you identify collision events? (Note: please close this window before you start a new run.) Look at initial and final configurations, how much do they differ from each other? Consider the plot with the velocity distribution; is it close to the Maxwell distribution? Where is the maximum in the actual distribution and why?

Add plot commands to the program to plot the instantaneous temperature `tact` and the total energy per particle `etot` as a function of time and note how the temperature changes over the few steps. Does the total energy change too? If yes, by how much? Is that acceptable?

Increase the number `krun` of time steps until the temperature fluctuates about a mean value. Note that this is not the value of `Ttarget`. What is the reason for the change?
Once the temperature does not "drift" anymore, check the velocity distribution and make sure it is close to the Maxwell-Boltzmann velocity distribution. The values of the `H` function shown in the figure may help you quantify the effect. Use this time as your equilibration time.

(b) First production run
Use your estimate for `kequ` from part (a), pick an observation time `kobs` that is about 2 times as long and divisible by 10, then add 1 to `kobs` and set `krun` to `kequ+kobs+1`. Set `iflag=1`, run the program, copy all figures into your word document, and note the final values for the pressure and its uncertainty.
Note: if the uncertainty in the pressure is more than 10%, your run is probably too short.
Consider the plot for the pair distribution function, can you tell whether the system is in the solid, liquid, or gas state?

(c) Temperature fluctuations
In the simulations, the total energy is fixed but the kinetic energy and hence the temperature is allowed to fluctuate. Modify the program to determine the probability distribution for the temperature by binning the results as in the previous homework assignment. Run your program for the conditions in (a) and (b) and plot the probability distribution. What kind of probability distribution is it? What are its mean and standard deviation.
Note: While you are working on the program, go back to short runs and set the state of the random number generator to a fixed value.

(d) Non-zero total momentum
The file *fmdini.m* generates initial velocities in such a way that the total (linear) momentum is zero. This is done by considering the sums over the velocity components and adjusting the randomly generated velocities. Change the program in such a way that the total momentum is quite different from zero. Leave the other parameters as they were before, run the program and consider the velocity distribution. What has changed?
Please don't forget to change back to zero momentum for the rest of the exercises.

(e) Thermostat
As you noticed in (a), the temperature adjusts itself to a value different from the "target" value. If one wants to run MD simulations at a given temperature, adjustments are required. The theory of thermostats that act during the simulations is fairly complicated. However, temperature adjustments during the equilibration period are not as problematic. Since the temperature is closely related to the kinetic energy, rescaling the velocity is an obvious choice, see for example how the initial velocities are generated. However, in the Verlet algorithm, the velocities do not enter into the calculation of the configuration at the next time step, so that adjusting the velocities would have no effect. Describe a method that can be used to adjust the kinetic energy (and hence the temperature) in a Verlet algorithm.

3. Comparison of MD and MC simulations

(a) Perform MD simulations for the `Nrow=5` system at a density of $\rho = 0.5$ for target temperatures `Target=1,2,3,4` Record the results for the total energy per particle, the pressure and the temperature (include error estimates for temperature and pressure) and save the plots of the pair-distribution functions.
Note: Please make sure that the velocity distribution and the error estimates are acceptable, otherwise change your run and/or equilibration times.

(b) Perform MC simulations for the same system as in (a) using the actual average temperatures as your temperature for the MC simulation. Record the results for the pressure