

Computational Science 1

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Seminar Exercises

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Exercise 8 (16.1.2014):

Qualitative properties of a liquid and a gas

from *An Introduction to Computer Simulation Methods*,
Chapter 8, Problem 8.7+8

- a) Modify the example `LJParticlesApp`. Generate an initial configuration using `setRectangularLattice` with $N = 64$ and $Lx = Ly = 12$ and an initial temperature of 2.0. What is the density? Modify your program so that the values of the temperature T and pressure P are not stored until the system has reached equilibrium. Check that the average values of T and P over finite time intervals do not drift with time.
- b) Choose a value of the time step Δt so that the total energy is conserved to the desired accuracy and run the simulation for a sufficient time to estimate the equilibrium pressure and temperature. Compare your estimate for the ratio PV/NkT with its value for an ideal gas. (We have written V for the area of the system, so that the ideal gas equation of state has a familiar form.) Save the final configuration of your simulation in a file.
- c) One way of starting a simulation is to use the positions saved from an earlier run. The simplest way of obtaining an initial condition corresponding to a different density, but the same value of N , is to rescale the positions of the particles and the linear dimensions of the cell. How do you expect P and T to change when the system is compressed? Gradually increase the density and determine how PV/NkT changes with increasing density. Can you distinguish the different phases?
- d) The temperature can be changed to the desired value by rescaling the velocities of the system. Run your program to create an equilibrium configuration for $Lx = Ly = 12$ and $N = 64$ and determine $T(E)$, the energy dependence of mean temperature, in the range $T = 1.0$ to $T = 1.2$. Rescale the velocities by the desired amount over some time interval.
- e) Use your data for $T(E)$ to plot the total energy E as a function of T . Is T a monotonically increasing function of E ? What percentage of the contribution to the heat capacity $C_V = (\delta E / \delta T)_V$ is due to the potential energy? Why is an accurate determination of C_V difficult to achieve?
- f) A way of determining C_V is to relate it to the fluctuations of the kinetic energy.

$$C_V = \frac{dNk}{2} \left[1 - \frac{2}{dN} \frac{(\langle T^2 \rangle - \langle T \rangle^2)}{(k\langle T \rangle)^2} \right]^{-1}. \quad (1)$$

Method `getHeatCapacity` determines C_V from (1). Compare your results obtained using (1) with the determination of C_V in part (e). What are the advantages and disadvantages of determining C_V from the fluctuations of the temperature compared to the method used in part (e)?