Computational Science 1

http://www.tu-chemnitz.de/physik/THUS/de/lehre/CSM_WS1819.php

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Seminar
Exercises

Exercise 9 (8.1.2019):

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.

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

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)?