

# Computational Science 1

[http://www.tu-chemnitz.de/physik/THUS/  
lehre/CSM\\_WS1213.php](http://www.tu-chemnitz.de/physik/THUS/lehre/CSM_WS1213.php)

## Seminar Exercises

**Prof. M. Schreiber**

[schreiber@physik.tu-chemnitz.de](mailto:schreiber@physik.tu-chemnitz.de)  
Room 2/P302, Phone 21910

**Dr. P. Cain**

[cain@physik.tu-chemnitz.de](mailto:cain@physik.tu-chemnitz.de)  
Room 2/P310, Phone 33144

## Exercise 8 (13.12.2012):

### Qualitative properties of a liquid and a gas

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

- 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.
- Choose a value of the time step  $\Delta t$  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.
- 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?
- 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.
- 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?
- 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)?