Computational Physics II

WiSe 2014/15

Problem 1: Molecular dynamics with hard disks

Date: October 23, 2014 $\hspace{4cm}$ Deadline: November 13, 2014

Write a molecular dynamics program for N hard disks in a square box. Assume that all disks have the same radius and mass. Initial positions should be set randomly using a uniform distribution.

1. Make an animation of the disk trajectories for $N = 1, 2, 3$ to check your program visually.

2. Starting from a constant initial velocity ($|\vec{v}_i(t = 0)| = v > 0$ for $i = 1, \ldots, N$) and a uniform random distribution of directions $\vec{v}_i/v$, calculate and plot the velocity distribution (i.e., an histogram) as a function of time. Check that it converges toward the Maxwell distribution.

3. Starting from a velocity distribution at thermal equilibrium, calculate and plot the pressure as a function of temperature for several choices of box size and disk number N. Explain the deviations from the ideal gas law.