Computational Physics - PHYS 410/510
Spring 2025

Department of Physics - Northern Illinois University
Prof. Andreas Glatz www.aglatz.net/teaching/compphys_S2025

Homework HW 4

due *2025-03-18*

Info	midterm task:	**March 25-27, 2025**
	final project presentation:	**Thursday, April 24, 2025**, *9:30* (will be assigned beginning of April.)
	Program codes should be mailed to: aglatz@niu.edu (see also website). Other problem solutions can be handed in or mailed as well. Problems with points marked by * are for extra credit.	

I. MOLECULAR DYNAMICS *[10+10+12+10+10 PTS]*

Write a molecular dynamics code with the help of the following instructions.You can use either the leap-frog or the velocity Verlet algorithm. We consider the following system:

- There are $N = 100$ particles in a two-dimensional box with side length $L = 30$. The boundaries at the bottom, at the left- and at right-hand side are considered as reflecting. The top of the box is regarded as open (no periodic boundary condition or reflecting boundary is imposed).
- The particles interact through a Lennard-Jones potential, where ϵ and σ define the interaction.
- Furthermore, a gravitational force $F_{ext} = -mg\hat{e}_y$ acts on each particle, where m is the particle's mass, g is the acceleration due to gravity, and $\hat{e}_y$ denotes the unit vector in y-direction.
- As an initial condition, the particles can be placed within the box on a regular lattice, where the distance between the particles is the characteristic distance according to the Lennard-Jones potential, i.e. ϵ. The form and position of this lattice is arbitrary.

We measure the velocities and the positions of all particles. Use $\epsilon = \sigma = 1$. Illustrate the results of the simulations graphically. Other typical simulation parameters are: $m = 1$, $g = 9.81$, $\Delta t = 10^{-3}$, $N_t = 5000$ (number of time steps, can be larger), unless otherwise stated. Perform the following analysis:

a) Determine the temperature T from the kinetic energy as discussed in the lecture. Plot $T(t)$. Plot $\tilde{T}_n$, which is the averaged temperature $T(t)$ over ~ 100 time steps, the index n determines the averaging time interval, e.g. $[100n\Delta t; 100(n+1)\Delta t]$. Note that in this particular case we do not demand that $v_{tot} = 0$!

b) Try different initial conditions. For instance, set the initial velocity equal to zero and stack the particles in different geometric configurations (rectangle, triangle, . . .). The nearest neighbor distance between the particles can be set equal to ϵ. Choose one configuration and place it at different positions in the box. What happens?

c) Set in the initial condition to the inter-atomic distance of $2^{1/6}$. (Why?) Vary the gravitational acceleration g in order to simulate different states of matter. The reference program developed solid behavior for $g \approx 0$, liquid behavior for $g \approx 0.1$ and gaseous behavior for $g > 1$. Explain this behavior!

d) Measure the particle density $\rho(h)$ as a function of the height h. You should be able to reproduce the barometric formula:

$$\rho(h) \propto \exp(-\gamma h/T)\,, \quad \gamma > 0\,.$$

For this, discretize the y-direction in small intervals (~ 100) and count particles in these intervals, average over time (as $\tilde{T}_n$, which you can use here for comparison to barometric formula), disregard the initial equilibration phase.

e) Determine the momentum distribution ($p_i = mv_i$) of the particles and demonstrate that it follows a Maxwell-Boltzmann distribution

$$p(|v|) \propto |v|^2 \exp(-\gamma |v|^2/T)\,, \quad \gamma > 0$$

with the Euclidean norm $|v| = \sqrt{v_x^2 + v_y^2}$ (speed). Follow similar considerations as in d) (with discretization of the speed and time averaging in the steady state only).

II. STATIONARY HEAT EQUATION *[12+15 PTS]*

Implement a Gaussian Elimination solver (or simplified version or this case here) for the stationary inhomogeneous heat (diffusion) equation given in the lecture and solve for $N = 10, 100, 1000$ grid points:

a) use the Gaussian profile and parameters given in the lecture.

b) use a rectangular heat sink in the center with depth θ and width a, for $T_0 < T_N$, $T_0 > T_N$, $T_0 = T_N$ and study the influence of the width a of the heat sink on the temperature profile.

Other typical parameters are: $L = 10$, $\kappa = 1$, $\Theta = -0.4$, $\ell = 1$, $T_0 = 0$, $T_N = 2.0$.