

# Computational Physics - PHYS 410/510

## Spring 2023

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www.aglatz.net/teaching/compphys\_S2023

### Homework

# 4

HW

due 2023-03-21

Info

midterm task: **March 20-22, 2023**  
final project presentation: **Tuesday, May 2, 2023, 9:30** (tentatively)  
(will be assigned beginning of April.)

Program codes should be mailed to: [aglatz@niu.edu](mailto: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  $\epsilon$  and  $\sigma$  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.  $\epsilon$ . 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  $\sim 100$  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  $\epsilon$ . 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 ( $\sim 100$ ) 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:

- use the Gaussian profile and parameters given in the lecture.
- use a rectangular heat sink in the center with depth  $\theta$  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:  $L = 10$ ,  $\kappa = 1$ ,  $\Theta = -0.4$ ,  $\ell = 1$ ,  $T_0 = 0$ ,  $T_N = 2.0$ .