MM553/837 – Computational Physics – 2025

Lecturer:	Michele Della Morte	E-Mail: dellamor@qtc.sdu.dk
Tutor:	Samuel John Hindson	E-Mail: samhindson@imada.sdu.dk

Project 1

Submit before 21st of October.

This will be the first out of two projects, each project will count for 50% of the overall mark. Please prepare and submit (by e-mail, to `dellamor@cp3.sdu.dk`) the following before the 21st October 2024 (the deadline is at 22.00).

- Submit your codes, ideally as a single zip file with your name.
- Prepare and submit a short report (about 5 pages, max. 8 pages) about the project, your implementation and your findings. Feel free to include graphics from MATLAB.
- Prepare a short presentation (about 20 mins presentation + 10 mins for questions) to be presented (in teams of up to two) in week 43 of October during the lecture/exercise time slot.

As announced before, we allow for project submission in teams of two (at most). The idea is to exchange ideas and problem solutions rather than codes. Nevertheless, each team member has to submit the project report and the codes individually. Include your name and the name of your team partner (if applicable) in the header of every code file that you submit.

The project work is meant to be worked on during the next couple of exercises sessions, i.e., weeks 39, 40 and 41 (and as a homework, of course).

This project is about applying the techniques that we have developed for integrating the equations of motion to two bigger systems. Any of the algorithms we have discussed in class (and any of the corresponding code) can and may be used.

1) N particles in 1-dimension

The system consists of N particles moving in one dimension. These particles all have unit mass ($m = 1$) and interact with their immediate neighbors ($i-1$ and $i+1$) via a spring-like potential. Assume that the system has fixed boundary conditions so that particle N and particle 1 are always fixed to their equilibrium positions $x_1(t) = x_N(t) = 0$. The Hamiltonian (total energy) of the system is

$$H = E = \sum_{i=1}^{N} \frac{1}{2} p_i^2 + \sum_{\langle i,j \rangle} V(|x_i - x_j|),$$

$$V(|x_i - x_{i+1|}) = \frac{1}{2}(|x_i - x_{i+1}|)^2 + \frac{1}{3}(|x_i - x_{i+1}|)^3 + \frac{1}{4}(|x_i - x_{i+1}|)^4.$$

where x_i is the displacement of the ith particle from its equilibrium position and the sum in the potential term is over all adjacent pairs of particles $\langle i,j \rangle$. Note that each pair of particles is counted only once.

1. Find Hamilton's equations for this system (analytically by taking derivatives) and provide an expression for the force on a single particle i.
2. Decide on a value of N (larger than 100 but smaller than 1000, but more is always better!). Start the system in the configuration where all positions are fixed to 0, i.e.

   $$x_i(t = 0) = 0 \qquad \forall i$$

   so that the potential energy is zero and choose some random momenta in the range of -1 and 1 (excluding 0), i.e.

   $$p_i(t = 0) \in (-1, 0) \text{ or } (0, 1)$$

3. Implement the numerical integration of the N particles using the Euler-Cromer, Leap-Frog and RK2. Choose a small enough step size to ensure that the integration is accurate enough. Make a plot of the energy as time evolves. This should illustrate that the energy is approximately constant.
4. Run the system for some time to allow it to equilibrate, and then take measurements of the average velocity squared (in this setup the velocity v_i is equal to the momentum p_i):

   $$\langle v^2(t) \rangle = \frac{1}{N} \sum_{i=1}^{N} v_i^2(t)$$

   over all particles N at a fixed time t. Plot $\langle v^2(t) \rangle$ as a function of time.
5. Finally, take all of these individual measurements of the velocity at a single time and put them in a histogram to get an idea of how they are distributed. Statistical mechanics states that in equilibrium at a temperature T, the probability of finding a particular particle with velocity (magnitude) v is given by the Maxwell-Boltzmann distribution

   $$P_{\text{eq}}(v) = \sqrt{\frac{m}{2\pi k T}} \exp\left\{ -\frac{m\, v^2}{2\, k\, T} \right\}.$$

   Does your histogram look similar to this distribution?

2) Two planets around the sun in 2 dimensions

Consider a system of two planets (feel free to use more) that move around a big mass M at the origin. You can think about two planets moving around the sun. To keep things simple, we consider only two dimensions, i.e. all motion is in the x-y-plane. To simplify things even further, we place the big mass ("sun") at the origin of the coordinate plane and consider it as static, which means it does not move nor feel the gravity from the two smaller planets. Additionally, also we neglect the gravitational attraction between planets 1 and 2. For planetary motion, this is typically a valid approximation.

The Hamiltonian of such a system is given by

$$H = E = \frac{\langle \vec{p}_1, \vec{p}_1 \rangle}{2m_1} + \frac{\langle \vec{p}_2, \vec{p}_2 \rangle}{2m_2} - \frac{Gm_1 M}{r_1} - \frac{Gm_2 M}{r_2},$$

where the radius $r_i = \sqrt{x_i^2 + y_i^2}$ is the distance to the origin for particle i. In the following, we set $G = 1$ and $M = 1$. Make a choice for the masses of the planets that is $M \gg m_1 \neq m_2$.

1. Find Hamilton's equations for this system (analytically by taking derivatives) and provide the expressions for both planets. Please note that the results should be vectors, i.e. have an x- and a y-component.

2. Implement the numerical integration of the two planets using the Euler-Cromer, Leap-Frog and RK2. As before choose a small enough step size to ensure that the integration is accurate enough. Make a plot of the energy as time evolves. This should illustrate that the energy is approximately constant.

3. Choose an initial condition that produces an elliptic orbit for both planets. (You can simply try out different values and integrate them and see. Otherwise, you can look at the escape velocity $v_e = \sqrt{\frac{2\,G\,M}{r}}$ and choose a value that is smaller, but not too small).

4. Check Kepler's third law:
   "The ratio of the square of an object's orbital period with the cube of the semi-major axis of its orbit is the same for all objects orbiting the same primary."
   It can be written as

   $$\frac{a^3}{T^2} = \text{const.},$$

   where 'T' is the time for a full rotation around the sun and 'a' is half of the longest axis of the ellipse formed by the movement. Think about a way to determine T and a. And then check the ratio and look if it is roughly constant.

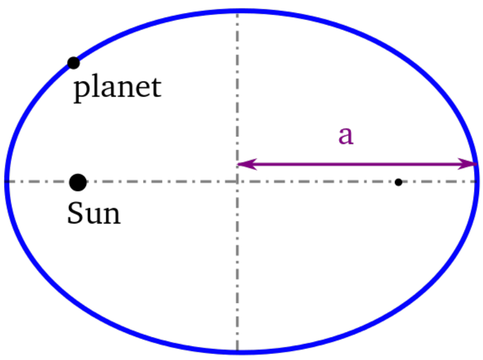

Figure 1: Illustration of a planetary motion