Universität Freiburg – Institut für Physik
Applied Theoretical Physics
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Exercise 1 for '*Computational Physics - Material Science*', SoSe 2023

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Please provide a well documented submission of your solution. Your submission should include

- A pdf file containing the solution to the questions with the corresponding equations that are implemented in your codes. Figures must contain axis titles with corresponding units and a caption.
- The source codes should be commented, and the equations given in the pdf file have to be referenced in the source codes.

Exercise: The Planets in the Solar System

In this exercise, a code for calculating the trajectories of the planets in the solar system for a finite number of years needs to be written. The masses of the sun and the planets, M_i, are provided in the data file *m*ass.dat. While the sun is initially located at (0,0,0) with no initial velocities, the initial positions, $\vec{r_i}$, and velocities, $\vec{v_i}$, of all nine planets (we also consider Pluto) are provided in the data file *p*lanets.dat. The potential energy between two planets i and j, $V_{ij}(r_{ij})$, is given by the gravitational interaction energy, which writes

$$V_{ij}(r_{ij}) = -G\frac{M_i M_j}{r_{ij}} \,,$$

where $G = 6.67408 \times 10^{-11}$ m^3 kg^{-1} s^{-2} is the gravitational constant, and r_{ij} is the (center-of-mass) distance between two planets. In the implementation, planet-planet and planet-sun interactions have to be included.

a) Demonstrate analytically that the Verlet and Velocity-Verlet integration schemes lead to the same trajectories. Which initial conditions are needed to use (i) the Verlet, and (ii) the Velocity Verlet integration schemes? Given the initial positions, $\vec{r_i}$, and the initial velocities, $\vec{v_i}$ at time t, define the initial conditions to be used by the Verlet integration scheme.

b) Using a time-step of half a day, use the Velocity-Verlet integration scheme to predict the trajectory of the solar system in the next 500 years. Plot the location of the planets in 50 years and 100 years (see below a format to save the trajectory in a format readable by the visualisation software Ovito). Plot the trajectory of Pluto over the next 100 years. What is the orbital period of Pluto around the Sun? (*Hint: the total energy of the system is conserved using the Velocity Verlet integration scheme*).

c) Implement the Verlet integration scheme. Is the trajectory of Pluto similar to the one obtained in the previous question? What is the orbital period of Mars around the Sun?

d) Implement the Euler integration scheme. Is the total energy (potential energy U, kinetic energy K, and $E = U+K$) conserved? Is the trajectory of Pluto similar to the one obtained in the previous questions?

e) In your opinion, how realistic is this model? How does the elliptic axes of Mercury compare to the real one? What could be reasons for deviations in the realistic system?

Output format for trajectory readable by the visualisation software Ovito

ITEM: TIMESTEP
timestep t
ITEM: NUMBER OF ATOMS
natoms (nplanets)
ITEM: BOX BOUNDS
xlo xhi xlo xhi
ylo yhi ylo yhi
zlo zhi zlo zhi
ITEM: ATOMS id type x y z
id_1, $type_1$ x_1 y_1 z_1
. . . . .
id_i, $type_i$ x_i y_i z_i
. . . . .
ITEM: TIMESTEP
timestep $t+n_{save}\ \delta t$
...
...

The lines starting with the keyword ITEM should not be changed. The text written in italic should be replaced with its numerical values. In the current tutorial, the box bounds should be large enough to include all the planets. In the section 'ITEM: ATOMS', the 'id' number ranges between 1 and 10, and each planet should have a different 'type'.

Hints and suggestions: Take care to consider which quantities need to be computed, stored, and updated each time-step. It would be extremely useful to write the codes in this exercise in easily readable and modular formats for the exercises to follow.

Overview of Time Integration Schemes:

a) Euler Algorithm:
The position $\boldsymbol{r}_i$ of a particle i at the time $t + \Delta t$ can be obtained by computing

$$\boldsymbol{r}_i(t+\Delta t) = \boldsymbol{r}_i(t) + \Delta t \boldsymbol{v}_i(t) + \frac{\Delta t^2}{2m_i}\boldsymbol{f}_i(t) + \mathcal{O}(\Delta t^3)\,,$$

where $\boldsymbol{v}_i(t)$ is the velocity vector of the particle at time t and $\boldsymbol{f}_i(t)$ is the force acting on the particle of a mass m_i with $\boldsymbol{f}_i(t) = m_i\boldsymbol{a}_i(t)$. The velocity $\boldsymbol{v}_i(t+\Delta t)$ writes

$$\boldsymbol{v}_i(t+\Delta t) = \boldsymbol{v}_i(t) + \frac{\Delta t}{m_i}\boldsymbol{f}_i(t) + \mathcal{O}(\Delta t^2)\,.$$

b) Verlet algorithm:

The Verlet scheme allows propagation of the position through

$$\boldsymbol{r}_i(t+\Delta t) = 2\boldsymbol{r}_i(t) - \boldsymbol{r}_i(t-\Delta t) + \frac{\Delta t^2}{m_i}\boldsymbol{f}_i(t) + \mathcal{O}(\Delta t^4)\,.$$

The velocity at time t is subsequently calculated by taking the previous and the future time steps. It writes

$$\boldsymbol{v}_i(t) = \frac{\boldsymbol{r}_i(t+\Delta t) - \boldsymbol{r}_i(t-\Delta t)}{2\Delta t} + \mathcal{O}(\Delta t^3)\,.$$

c) Velocity-Verlet algorithm:
The Velocity-Verlet scheme allows calculating the position according to

$$\boldsymbol{r}_i(t+\Delta t) = \boldsymbol{r}_i(t) + \boldsymbol{v}_i(t)\Delta t + \frac{\Delta t^2}{2m_i}\boldsymbol{f}_i(t) + \mathcal{O}(\Delta t^3)\,,$$

and the velocity

$$\boldsymbol{v}_i(t+\Delta t) = \boldsymbol{v}_i(t) + \frac{\Delta t}{2m_i}\left[\boldsymbol{f}_i(t) + \boldsymbol{f}_i(t+\Delta t)\right] + \mathcal{O}(\Delta t^3)$$

at time $t + \Delta t$ at the same time.