INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS (2)

Objectives:

- Integrate a second-order conservative ordinary differential equation numerically;
- Implement the velocity Verlet method;
- Identify whether a numerical integrator is sympletic;
- Transform an ordinary differential equation of order n into a system of n first-order differential equations;
- Integrate a system of coupled differential equations numerically;
- Solve a boundary value problem via the shooting method.

No list manipulation is allowed in this tutorial!

In this tutorial, we focus on problems which are relevant in Physics. In the first exercise, we study the dynamics of a material point in a conservative force field. In the second exercise, we study the fall of a cannonball in the gravity field in order to optimize its trajectory.

I. Motion of a material point in a conservative force field

Consider a material point of mass m in one dimension of space. This material point evolves in a conservative force field, which derives from a potential energy $V(x)$. The equation of motion of the particle is given by

$$m\ddot{x}(t) = -V'(x(t)). \tag{1}$$

This is a second-order autonomous Ordinary Differential Equation (ODE). If we introduce the linear momentum $p = m\dot{x}$ of the material point, the second-order ODE (1) is equivalent to a system of two couples first-order ODES:

$$\begin{cases} \dot{x}(t) = \dfrac{p(t)}{m}, \\ \dot{p}(t) = -V'(x(t)). \end{cases} \tag{2}$$

We recall that the motion of the material point is *conservative*, *i.e.*, the mechanical energy

$$E_{\mathrm{m}} = \frac{p^2}{2m} + V(x) \tag{3}$$

is conserved during the motion.

In the following, we consider the double-well potential

$$V(x) = \frac{\kappa}{4}(x-a)^2(x+a)^2, \tag{4}$$

and we work with rescaled units such that $m = 1$, $a = 1$, and $\kappa = 10$.

1. Choice of the numerical integrator

Question 1: Define two functions `potential(x)` and `force(x)` which respectively return the value of the potential energy and of the force.

Question 2: Plot the potential energy in the range $[-2, 2]$. Make a readable plot.

Question 3: Define a function `rk4(h, xi=0., pi=-1., ti=0., tf=10.)` which takes as an input the timestep h, implements the Runge-Kutta 4 method and returns three arrays `t_arr` (array of time values), `x_arr` (array of position values) and `p_arr` (array of linear momentum values). The other arguments represent the initial position `xi`, the initial linear momentum `pi`, the initial time `ti` and the final time `tf`. **You must take advantage of NumPy vectorization!**

Question 4: Define a function `verlet(h, xi=0., pi=-1., ti=0., tf=10.)` which takes as an input the timestep h, implements the velocity Verlet method and returns three arrays `t_arr` (array of time values), `x_arr` (array of position values) and `p_arr` (array of linear momentum values).

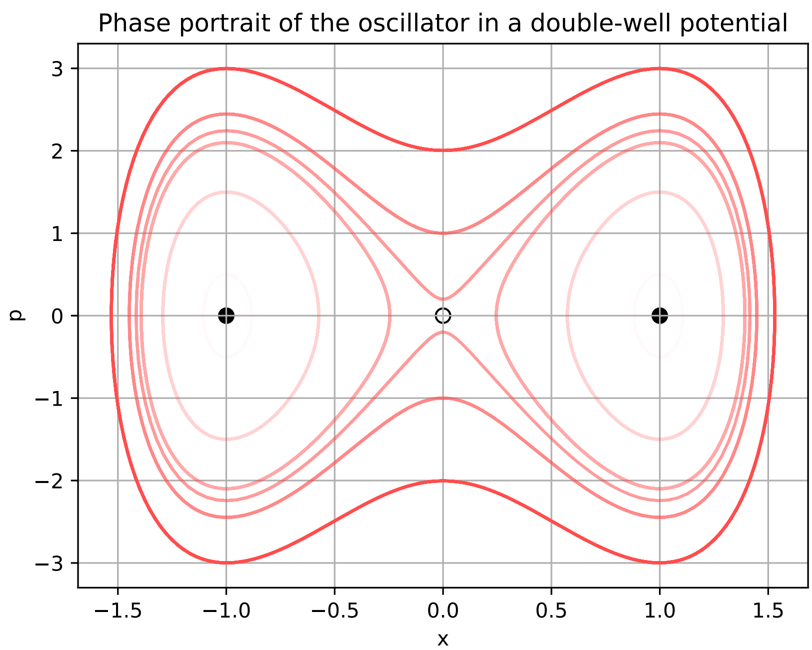
Question 5: Plot the time evolution of the position of the material point for the two methods for $h = 0.02$ (make a readable plot). Confront with the exact solution, which is given by the following function already written in Python. Which integrator provides the lowest global truncation error?

```
import scipy.special as spe
import numpy as np
def exact_sol(t):
    period = 2 * (2. / 15.) ** 0.25 * spe.ellipk(1. / (
    12. - 2. * np.sqrt(30.)))
    n = np.floor(t / period)
    tred = t - n * period
    return np.sign(tred - period / 2.) * np.sqrt((np.sqrt(6. / 5.) - 1.) * (
    1. / spe.ellipj(120 ** (1. / 4.) * tred, 0.5 + np.sqrt(30.) / 12.
    )[2] ** 2 - 1.))
```

Question 6: Plot the time evolution of the mechanical energy of the material point for the two methods for $h = 0.1$ and $t_{\text{f}} = 1000$ (make a readable plot). Which integrator approximately conserves energy?

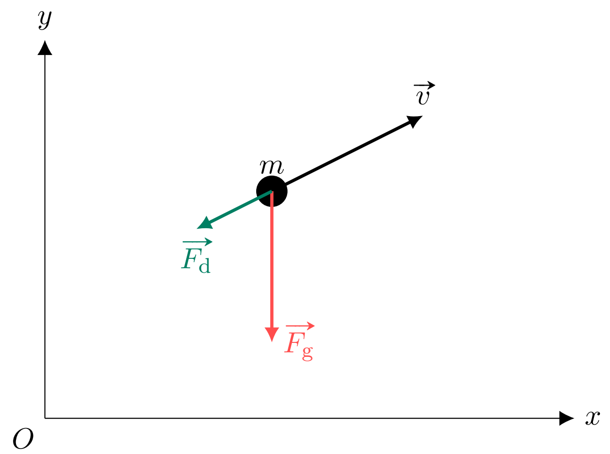
2. Phase portrait

Question 7: By changing the initial conditions, draw the phase portrait of the material point using the velocity Verlet algorithm. The figure should look like the one showed below, where the intensity of the color encodes the mechanical energy of the material point on the trajectory.



Question 8: Characterize in few words the different types of trajectories and of fixed points.

II. Ballistic trajectory of a cannonball



We consider a spherical cannonball of mass $m = 4.08\,\mathrm{kg}$ which is subject to the gravitational force $\vec{F_g} = -mg\vec{e_y}$ ($g = 9.81\,\mathrm{m.s^{-2}}$), and to a frictional force due to air drag (in the high-Reynolds number regime)

$$\vec{F_d} = -\frac{1}{2}\rho_a S_{cb} C \|\vec{v}\|\vec{v}. \quad (5)$$

In the above formula, $\rho_a = 1.21\,\mathrm{kg.m^{-3}}$ is the density of air, $S_{cb} = \pi r_{cb}^2$ is the cross-sectional area of the cannonball (with $r_b = 10.16\,\mathrm{cm}$ the radius of the cannonball), $C = 0.47$ is the drag coefficient of a sphere, and $\vec{v}$ is the velocity of the cannonball. The drag force has a magnitude $\|\vec{F_d}\| \propto \vec{v}^2$ and is always opposite to the velocity.

We start by formulating the problem mathematically. From the Newton's second law, one can easily derive that the equations of motion of the cannonball read

$$\begin{cases} \ddot{x} = -\alpha\dot{x}\sqrt{\dot{x}^2 + \dot{y}^2}, \\ \ddot{y} = -g - \alpha\dot{y}\sqrt{\dot{x}^2 + \dot{y}^2}, \end{cases} \quad (6)$$

with $\alpha = \dfrac{\rho_a \pi r_{cb}^2 C}{2m}$.

Question 1: Show that the above system (6) of two coupled second-order ODEs can be transformed into a system of four coupled first-order ODEs $\dot{\vec{Z}} = \vec{F}(\vec{Z})$, with:

$$\vec{Z} = \begin{pmatrix} x \\ y \\ v_x \\ v_y \end{pmatrix}, \quad \text{and} \quad \vec{F}\begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{pmatrix} = \begin{pmatrix} z_3 \\ z_4 \\ -\alpha z_3\sqrt{z_3^2 + z_4^2} \\ -g - \alpha z_4\sqrt{z_3^2 + z_4^2} \end{pmatrix}. \quad (7)$$

Why is it necessary to rewrite the problem like this?

Question 2: Define a function `rk4(h, vi, thetai, xi=0., yi=0., ti=0.)` which takes as an input the timestep h, the initial velocity magnitude v_i and the angle θ_i made by the initial velocity with $\vec{e_x}$, implements the Runge-Kutta 4 method and returns three arrays `t_arr` (array of time values), `x_arr` (array of x-coordinate values) and `y_arr` (array of y-coordinate values). The other arguments represent the initial x-coordinate `xi`, the initial y-coordinate `yi` and the initial time `ti`. Stop the integration when the cannonball hits the ground. **You must take advantage of NumPy vectorization!**
Hint 1: you should first define the function $\vec{F}$.

Hint 2: you do not know how many time steps are needed before the cannonball reaches the ground, but you can find a conservative upper bound by ignoring friction. Estimate the time of flight in the no-drag case to choose the array size.

Question 3: For an initial velocity $v_\mathrm{i} = 700\,\mathrm{m.s}^{-1}$, and starting from the origin ($x_\mathrm{i} = y_\mathrm{i} = 0$), compute the trajectories for initial angles $\theta_\mathrm{i} = 10°,\ 20°, \ldots,\ 80°$, and plot all of them on the same graph. Make a readable plot.

Question 4: The gunner located at $x_\mathrm{i} = y_\mathrm{i} = 0$ wants the cannonball to reach a target located at $x_\mathrm{t} = 1\,\mathrm{km}$ and $y_\mathrm{t} = 15\,\mathrm{m}$ (with a tolerance of $10\,\mathrm{cm}$). The initial speed $v_\mathrm{i} = 700\,\mathrm{m.s}^{-1}$ is imposed, but the gunner can freely choose the initial angle θ_i made by the velocity with $\vec{e_x}$.

a. From the figure drawn in the previous question, what are the two intervals of angles θ_min and θ_max such that $\theta_\mathrm{min} \leq \theta_\mathrm{i} \leq \theta_\mathrm{max}$.

b. Implement the bisection method to determine the two angles θ_i which allow the gunner to reach the target, and plot the two trajectories on the same graph.

c. Which trajectory corresponds to the higher kinetic energy at impact?