TUTORIAL: INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS

I. Harmonic oscillator

We want to integrate the equation of motion of a harmonic oscillator of angular frequency ω:

$$\frac{\mathrm{d}x^2}{\mathrm{d}t^2} = -\omega^2 x, \tag{1}$$

with initial conditions: $x(0) = 1$ and $\mathrm{d}x/\mathrm{d}t(0) = 0$. We try several algorithms to integrate Eq. (1) up to time t_f.

Question 1: How should you choose t_f with respect to ω?

Question 2: We start with the Forward Euler method.

a. Implement the method.

b. Solve Eq. (1) for $\omega = 2$ and for different values of the time step $h \in [10^{-4}, 0.2]$. Plot the solution. What do you observe?

c. Plot the time series of the energy per unit mass

$$E = \frac{1}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 + \frac{1}{2}\omega^2 x^2. \tag{2}$$

Comment. How does $E - \omega^2/2$ at the end of the integration scale with h?

d. Conclude on the feasibility of simulating a harmonic oscillator using the Forward Euler method.

Question 3: We now consider the Runge-Kutta 4 method. Repeat the above questions in this case.

II. A simplified model of Human crowds dynamics (a stiff ODE)

We want to solve the following Cauchy problem, which corresponds to an oversimplified model of Human crowds dynamics:

$$\begin{cases} \dfrac{\mathrm{d}x}{\mathrm{d}t} = -80x + 9y\,(x\sin t - y\cos t) + 1440\cos t, \\ \dfrac{\mathrm{d}y}{\mathrm{d}t} = -80y - 9x\,(x\sin t - y\cos t) + 1440\sin t, \\ x(0) = y(0) = 9, \end{cases} \tag{3}$$

for which the exact solution is known:

$$x(t) = 9\sqrt{2}\cos\left(t + \frac{\pi}{4}\right), \qquad y(t) = 9\sqrt{2}\sin\left(t + \frac{\pi}{4}\right). \tag{4}$$

Question 1: We first try to solve the problem with the Runge-Kutta 4 method.

a. Implement the method.

b. Solve up to $t = 100$ for $h = 0.01$ and $h = 0.1$. Plot the numerical solution and the exact solution on the same graph. Comment.

Question 2: The above Cauchy problem is stiff (can you see why?). We thus turn to the Backward Euler method.

a. We denote by $x_n^{(h)}$ and $y_n^{(h)}$ the numerical estimates of the solutions $x(t)$ and $y(t)$ at time $t_n = nh$. Write the recurrence relations for $x_{n+1}^{(h)}$ and $y_{n+1}^{(h)}$. Show that they take the form

$$G_1\left(x_{n+1}^{(h)}, y_{n+1}^{(h)}\right) = G_2\left(x_{n+1}^{(h)}, y_{n+1}^{(h)}\right) = 0, \tag{5}$$

with

$$\begin{cases} G_1(x,y) = x(1+80h) - x_n^{(h)} - 9hy\left(x\sin t_{n+1} - y\cos t_{n+1}\right) - 1440h\cos t_{n+1}, \\ G_2(x,y) = y(1+80h) - y_n^{(h)} + 9hx\left(x\sin t_{n+1} - y\cos t_{n+1}\right) - 1440h\sin t_{n+1}. \end{cases} \tag{6}$$

b. Compute the Jacobian matrix

$$J = \begin{pmatrix} \dfrac{\partial G_1}{\partial x} & \dfrac{\partial G_1}{\partial y} \\ \dfrac{\partial G_2}{\partial x} & \dfrac{\partial G_2}{\partial y} \end{pmatrix}. \tag{7}$$

c. Question **2.a.** shows that $x_{n+1}^{(h)}$ and $y_{n+1}^{(h)}$ are the roots of $G_1(x,y)$ and $G_2(x,y)$. By using the result of question **2.b.**, implement the Newton root-finding method to compute $x_{n+1}^{(h)}$ and $y_{n+1}^{(h)}$. This requires to solve linear systems involving J: you can first use pen and paper to invert J or directly use Python to solve the linear systems.

d. Solve the Cauchy problem (3) with the Backward Euler method up to $t = 100$ for $h = 0.01$ and $h = 0.1$. Plot the numerical solution and the exact solution on the same graph. Comment.

III. Ballistic trajectory

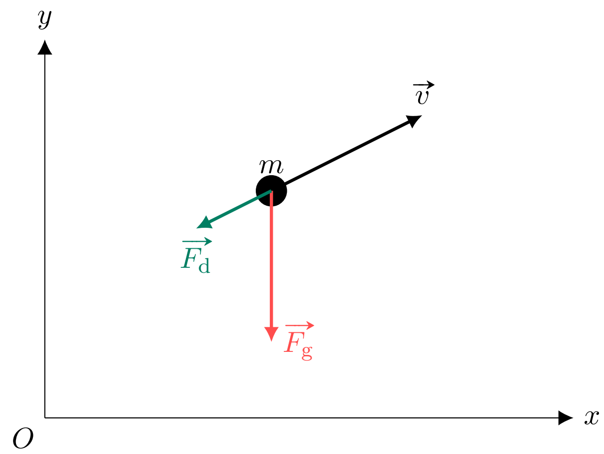

Figure 1: **Forces acting on a cannonball.** We have represented the cannonball of mass m and velocity $\vec{v}$, along with the gravitational force $\vec{F_\text{g}}$ and the drag force $\vec{F_\text{d}}$ acting on it.

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

$$\vec{F_\text{d}} = -\frac{1}{2}\rho_\text{a} S_\text{cb} C \|\vec{v}\|\vec{v}, \tag{8}$$

see Fig. 1. In the above formula, $\rho_\text{a} = 1.21\,\text{kg.m}^{-3}$ is the density of air, $S_\text{cb} = \pi r_\text{cb}^2$ is the cross-sectional area of the cannonball (with $r_\text{b} = 10.16\,\text{cm}$ 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 $\|\vec{F_\mathrm{d}}\| \propto \vec{v}^2$ and is always opposite to the velocity.

Question 1: We start by formulating the problem mathematically.

a. Show that the equations of motion of the cannonball can be written

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\alpha \frac{\mathrm{d}x}{\mathrm{d}t}\sqrt{\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}t}\right)^2}, \quad \frac{\mathrm{d}^2 y}{\mathrm{d}t^2} = -g - \alpha \frac{\mathrm{d}y}{\mathrm{d}t}\sqrt{\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}t}\right)^2}. \tag{9}$$

Express α as a function of C, m, ρ_a, r_b.

b. Transform the above equations of motion into a system of four first-order ODEs.

Question 2: Implement a Runge-Kutta 4 method to integrate the above system of ODEs. Stop the integration when the cannonball hits the ground ($y = 0$).

Question 3: For an initial velocity $v_\mathrm{i} = 250\,\mathrm{m.s}^{-1}$, an initial angle $\theta_\mathrm{i} = 20°$ between $\vec{v}$ and $\vec{e_x}$, and starting from the origin ($x_\mathrm{i} = y_\mathrm{i} = 0$), compute and plot the trajectory. Plot on the same graph the trajectory in the absence of the drag force. Comment.

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 made by the velocity with $\vec{e_x}$ between $0°$ and $45°$.

a. Implement the bisection method to determine the angle θ_t which allows the gunner to reach the target.

b. What is the value of the speed of the cannonball at the impact?

IV. Simulation of two repulsive particles in a harmonic potential

We consider two particles 1 and 2 of equal mass m in a two-dimensional harmonic potential of stiffness κ, corresponding to a potential energy $(1/2)\kappa\vec{r_a}^2$ (for $a = 1, 2$). The two particles also interact repulsively with an interaction potential $-\delta\ln(\|\vec{r_1} - \vec{r_2}\|)$.

Question 1: We start by formulating the problem mathematically.

a. Show that the equations of motion for the two particles are

$$\begin{cases} m\dfrac{\mathrm{d}^2\vec{r_1}}{\mathrm{d}t^2} = -\kappa\vec{r_1} + \dfrac{\delta}{\|\vec{r_1} - \vec{r_2}\|^2}(\vec{r_1} - \vec{r_2}), \\ m\dfrac{\mathrm{d}^2\vec{r_2}}{\mathrm{d}t^2} = -\kappa\vec{r_2} - \dfrac{\delta}{\|\vec{r_1} - \vec{r_2}\|^2}(\vec{r_1} - \vec{r_2}). \end{cases} \tag{10}$$

b. We want to make the above equations non-dimensionalized. For that we express the time t in units of t_0 and define a non-dimensionalized time $\tilde{t} = t/t_0$ (with t_0 having the dimension of time). Similarly, we express all lengths ℓ in units of ℓ_0 and define non-dimensionalized lengths $\tilde{\ell} = \ell/\ell_0$ (with ℓ_0 having the dimension of length). Find ℓ_0 and t_0 such that the above equations read

$$\begin{cases} \dfrac{\mathrm{d}^2\vec{x_1}}{\mathrm{d}\tilde{t}^2} = -\vec{x_1} + \dfrac{\vec{x_1} - \vec{x_2}}{\|\vec{x_1} - \vec{x_2}\|^2}, \\ \dfrac{\mathrm{d}^2\vec{x_2}}{\mathrm{d}\tilde{t}^2} = -\vec{x_2} - \dfrac{\vec{x_1} - \vec{x_2}}{\|\vec{x_1} - \vec{x_2}\|^2}, \end{cases} \tag{11}$$

with $\vec{x_a} = \vec{r_a}/\ell_0$ (for $a = 1, 2$).

c. Justify that the non-dimensionalized energy

$$\Xi = \frac{1}{2}\left(\frac{\mathrm{d}\vec{x_1}}{\mathrm{d}\tilde{t}}\right)^2 + \frac{1}{2}\left(\frac{\mathrm{d}\vec{x_2}}{\mathrm{d}\tilde{t}}\right)^2 + \frac{1}{2}\vec{x_1}^2 + \frac{1}{2}\vec{x_2}^2 - \ln\|\vec{x_1} - \vec{x_2}\|. \tag{12}$$

and the non-dimensionalized total angular momentum

$$\vec{\Lambda} = \vec{x_1} \times \frac{\mathrm{d}\vec{x_1}}{\mathrm{d}\tilde{t}} + \vec{x_2} \times \frac{\mathrm{d}\vec{x_2}}{\mathrm{d}\tilde{t}}. \tag{13}$$

are conserved quantities, *i.e.*, they remain constant with time.

Question 2: We propose to use a velocity Verlet algorithm to solve Eq. (11) numerically.

a. Implement the algorithm.

b. For initial conditions

$$\vec{x_1}(0) = \vec{e_y}, \quad \frac{\mathrm{d}\vec{x_1}}{\mathrm{d}\tilde{t}}(0) = -\vec{e_x}, \quad \vec{x_2}(0) = \vec{e_x}, \quad \frac{\mathrm{d}\vec{x_2}}{\mathrm{d}\tilde{t}}(0) = \vec{e_y}, \tag{14}$$

run the dynamics up to $\tilde{t} = 100$ for a time step $\tilde{h} = 0.01$. Plot the time series of the energy and of the total angular momentum. Check that the two quantities are approximately conserved.

Question 3: In simulations, energy is said to be conserved if its relative fluctuations are smaller than 10^{-4}. Relative energy fluctuations are defined as the standard deviation of the energy during the simulation (quantifying energy fluctuations) divided by its mean.

a. Run different simulations up to $\tilde{t} = 100$ with the initial conditions given by Eq. (14) for several values of time steps $\tilde{h} \in [10^{-3}, 1]$. Plot the relative energy fluctuations as a function of $\tilde{h}$ in a loglog plot. How do the relative energy fluctuations scale with $\tilde{h}$?

b. How should you choose $\tilde{h}$ such that energy is conserved?

Question 4: We now consider the initial conditions

$$\vec{x_1}(0) = \frac{1}{2}\left(\vec{e_x} + \vec{e_y}\right), \quad \frac{\mathrm{d}\vec{x_1}}{\mathrm{d}\tilde{t}}(0) = \vec{v_0}, \quad \vec{x_2}(0) = -\frac{1}{2}\left(\vec{e_x} + \vec{e_y}\right), \quad \frac{\mathrm{d}\vec{x_2}}{\mathrm{d}\tilde{t}}(0) = \vec{0}. \tag{15}$$

a. Run the dynamics for $\vec{v_0} = \vec{0}$. Plot the trajectories of the two particles on the same graph. Can you rationalize what you observe?

b. Now, run the dynamics for $\vec{v_0} = 0.1(\vec{e_x} + \vec{e_y})$. Plot the trajectories of the two particles on the same graph and comment.

c. Finally, run the dynamics for $\vec{v_0} = 0.1(\vec{e_x} - \vec{e_y})$. Plot the trajectories of the two particles on the same graph and comment.

V. Kinetics of an allosteric protein (another stiff ODE)

We consider a protein X which can have two conformations X_1 and X_2. We denote by x_1 and x_2 their respective concentrations in the medium as a function of time. This protein can be involved in different reactions depending on its conformation.

1. X can self-degrade with a conformation-dependent rate:

$$\begin{cases} \mathsf{X}_1 \xrightarrow[k_1]{} \emptyset, & \dfrac{\mathrm{d}x_1}{\mathrm{d}t} = -k_1 x_1, \\ \mathsf{X}_2 \xrightarrow[k_2]{} \emptyset, & \dfrac{\mathrm{d}x_2}{\mathrm{d}t} = -k_2 x_2. \end{cases} \tag{16}$$

2. The protein in conformation X_1 can react with a reactant Q to release a protein in conformation X_2. A molecule of Q and a protein in conformation X_1 are also by-products of the reaction:

$$\mathsf{X_1 + Q} \underset{k_3}{\longrightarrow} \mathsf{X_1 + Q + X_2}, \qquad \frac{\mathrm{d}x_2}{\mathrm{d}t} = k_3 x_1. \tag{17}$$

3. In the presence of a catalyst R, the protein X can switch from conformation X_2 to conformation X_1:

$$\mathsf{X_2 + R} \underset{k_4}{\longrightarrow} \mathsf{X_1 + R}, \qquad \begin{cases} \dfrac{\mathrm{d}x_1}{\mathrm{d}t} = k_4 x_2, \\ \dfrac{\mathrm{d}x_2}{\mathrm{d}t} = -k_4 x_2. \end{cases} \tag{18}$$

4. Proteins in both conformations are injected periodically in the medium at the same period but with a phase shift and different injection rates:

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} = j_1 \sin(\omega t), \qquad \frac{\mathrm{d}x_2}{\mathrm{d}t} = j_2 \sin\left(\omega t + \frac{3\pi}{4}\right). \tag{19}$$

We want to study the dynamics of the two concentrations x_1 and x_2.

Question 1: We start by formulating the problem mathematically.

a. Show that the above problem is equivalent to the system of coupled ODEs:

$$\begin{cases} \dfrac{\mathrm{d}x_1}{\mathrm{d}t} = -k_1 x_1 + k_4 x_2 + j_1 \sin(\omega t), \\ \dfrac{\mathrm{d}x_2}{\mathrm{d}t} = k_3 x_1 - (k_2 + k_4) x_2 + \dfrac{j_2}{\sqrt{2}} \left[\cos(\omega t) - \sin(\omega t)\right]. \end{cases} \tag{20}$$

b. In the following, we express times and concentrations in SI units without specifying their unit. In these units, the value of the reaction rates read $k_1 = 2$, $k_4 = 1$, $k_2 = k_3 = a - 1$ (with $a > 0$). Finally, we impose the following initial conditions: $x_1(0) = 2$ and $x_2(0) = 3$, and the following injection properties: $\omega = 1$, $j_1 = 2$ and $j_2 = \sqrt{2}a$. The mathematical description of the kinetics of the allosteric protein X then becomes equivalent to the following Cauchy problem:

$$\begin{cases} \dfrac{\mathrm{d}x_1}{\mathrm{d}t} = -2x_1 + x_2 + 2\sin t, \\ \dfrac{\mathrm{d}x_2}{\mathrm{d}t} = (a-1)x_1 - a x_2 + a(\cos t - \sin t), \\ x_1(0) = 2, \\ x_2(0) = 3. \end{cases} \tag{21}$$

c. Check analytically that the solution to the above Cauchy problem is independent of a and reads

$$x_1(t) = 2e^{-t} + \sin t, \qquad x_2(t) = 2e^{-t} + \cos t. \tag{22}$$

Question 2: We now want to integrate numerically the above ODE.

a. Implement the trapezoidal method with a predictor-corrector scheme.

b. Apply the method with $h = 0.001$ up to $t = 100$, first for $a = 2$ and then for $a = 999$. For each value of a, plot the numerical solution and the exact solution on the same graph. Check that you recover the exact solution.

c. Integrate for the same values of a but with $h = 0.01$. For each value of a, plot the numerical solution and the exact solution on the same graph. Comment.

d. By analyzing the different timescales involved in the problem, justify that Eq. (21) corresponds to a stiff ODE.

Question 3: To solve Eq. (21), we implement an implicit trapezoidal method.

a. We denote $x_{1,n}^{(h)}$ and $x_{2,n}^{(h)}$ the estimates of the solutions of the ODE at time $t_n = nh$. Show that the estimates of the solutions of the ODE at step $n+1$ are the solutions of the linear system

$$\begin{pmatrix} 1+h & -\dfrac{h}{2} \\ -\dfrac{h}{2}(a-1) & 1+\dfrac{ah}{2} \end{pmatrix} \begin{pmatrix} x_{1,n+1}^{(h)} \\ x_{2,n+1}^{(h)} \end{pmatrix} = \begin{pmatrix} x_{1,n}^{(h)} + \dfrac{h}{2}\left(-2x_{1,n}^{(h)} + x_{2,n}^{(h)} + 2\sin t_n + 2\sin t_{n+1}\right) \\ x_{2,n}^{(h)} + \dfrac{h}{2}\left[(a-1)x_{1,n}^{(h)} - a x_{2,n}^{(h)} + a\left(\cos t_n - \sin t_n + \cos t_{n+1} - \sin t_{n+1}\right)\right] \end{pmatrix}. \tag{23}$$

b. Implement the implicit trapezoidal method. You can first use pen and paper to solve analytically the above system, or you can solve it directly with Python.

c. Integrate Eq. (21) for $a = 2$ and $a = 999$ and vary the time step $h \in [0.001, 0.1]$. Plot the exact solution and the numerical solution on the same graph. What do you observe?