PH509 Computational Physics
2025-26 Semester-II
Lab Sheet – 2

Instructions

Submit a `.ipynb` notebook or a well-documented `.py` script. Use only `numpy`, `scipy` (optional), and `matplotlib`. All plots must have labeled axes and legends where appropriate.

Goal. Implement Euler and RK2 methods for ODEs, compare with exact solutions, study error and stability, and understand step-size limitations.

Problem 1: Averaged Derivatives in RK2 and RK4

Consider the scalar initial value problem

$$\frac{dy}{dt} = f(y,t), \qquad y(t_0) = y_0,$$

and a single time step from t_n to $t_{n+1} = t_n + h$.

In this problem we will show that both RK2 and RK4 may be interpreted as using an *averaged derivative* over the interval $[t_n, t_{n+1}]$, and we will visualize this effective slope as in Figures 2.4(a,b) of Wang's textbook.

(a) RK2 as an average of endpoint derivatives

The RK2 method in Eq. (2.17) is

$$k_1 = h\, f(y_n, t_n), \qquad k_2 = h\, f(y_n + k_1,\, t_n + h),$$
$$y_{n+1} = y_n + \tfrac{1}{2}\,(k_1 + k_2).$$

1. Show that this update may be written in the form

   $$y_{n+1} = y_n + h\, \bar{f}_n^{(2)},$$

   and derive the explicit expression

   $$\bar{f}_n^{(2)} = \tfrac{1}{2}\Big[f(y_n, t_n) + f(y_n + k_1,\, t_n + h)\Big].$$

2. Take $f(y,t) = -y$, $y(0) = 1$, $t_n = 0$, and $h = 1$. On a single, clearly–labelled figure:
   - plot the exact solution $y(t) = e^{-t}$ for $0 \le t \le 1$;
   - mark the point (t_n, y_n);
   - draw two short tangent arrows at t_n and t_{n+1} with slopes $f(y_n, t_n)$ and $f(y_n + k_1, t_{n+1})$;
   - at $t_{n+1/2} = t_n + h/2$, draw a single tangent arrow whose slope is $\bar{f}_n^{(2)}$.

   This arrow represents the "effective" derivative used by RK2 over the step.

(b) RK4 as a weighted averaged derivative

The fourth–order Runge method in Eq. (2.18) is

$$k_1 = h\, f(y_n, t_n),$$
$$k_2 = h\, f\big(y_n + k_1/2,\, t_n + h/2\big),$$
$$k_3 = h\, f\big(y_n + k_2/2,\, t_n + h/2\big),$$
$$k_4 = h\, f\big(y_n + k_3,\, t_n + h\big),$$
$$y_{n+1} = y_n + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6}.$$

1. Show that this update may be written in the same form

$$y_{n+1} = y_n + h\,\bar{f}_n^{(4)},$$

where the averaged derivative is

$$\bar{f}_n^{(4)} = \frac{1}{6} f(y_n, t_n) + \frac{1}{3} f\big(y_n + k_1/2,\, t_n + h/2\big) + \frac{1}{3} f\big(y_n + k_2/2,\, t_n + h/2\big) + \frac{1}{6} f\big(y_n + k_3,\, t_n + h\big).$$

2. Using the same test problem $f(y,t) = -y$, $y(0) = 1$, $t_n = 0$, $h = 1$, produce a figure showing:
   - the exact curve $y(t)$ on $[0,1]$;
   - the four RK4 slope evaluations corresponding to $k_1, \dots, k_4$, drawn as tangent arrows at their respective times $(t_n,\, t_n + h/2,\, t_n + h/2,\, t_{n+1})$;
   - at $t_{n+1/2}$, a single arrow whose slope is $\bar{f}_n^{(4)}$.

(c) Comparison

On a separate plot, place the RK2 and RK4 averaged–slope arrows for the same step $[0,1]$. In a short comment (2–3 sentences), compare:

- the number and location of derivative evaluations used to construct $\bar{f}_n^{(2)}$ and $\bar{f}_n^{(4)}$;
- how the differing weights and evaluation points affect the "shape" of the effective slope.

Problem 2: Euler and Euler–Cromer for the Nonlinear Pendulum

We consider the undamped, undriven nonlinear pendulum of length ℓ in a uniform gravitational field of strength g. The equation of motion is

$$\theta''(t) + \frac{g}{\ell}\,\sin\theta(t) = 0,$$

where primes denote derivatives with respect to physical time t.

Introduce the angular velocity $\omega(t) = \theta'(t)$, so that

$$\theta' = \omega, \qquad \omega' = -\frac{g}{\ell}\,\sin\theta.$$

(a) Time scale and non-dimensionalization

1. Identify the natural time scale of the pendulum. (Hint: use the small-angle approximation $\sin\theta \approx \theta$, and compare with $\theta'' + \Omega_0^2\theta = 0$.)
2. Introduce a dimensionless time variable

$$\tau = \frac{t}{T_0}, \qquad \frac{d}{dt} = \frac{1}{T_0}\frac{d}{d\tau},$$

   where T_0 is the characteristic time you identified. Show that with a suitable choice of T_0 the pendulum equation becomes

$$\frac{d^2\theta}{d\tau^2} + \sin\theta = 0.$$

3. Rewrite the system in dimensionless first-order form:

$$\frac{d\theta}{d\tau} = \tilde{\omega}, \qquad \frac{d\tilde{\omega}}{d\tau} = -\sin\theta,$$

   and explain how $\tilde{\omega}$ relates to the physical angular velocity ω.

For the remainder of the problem we drop tildes and work with $\theta(\tau)$ and $\omega(\tau)$.

(b) Numerical schemes

Let $\tau_n = nh$.

Euler method.

$$\theta_{n+1} = \theta_n + h\,\omega_n, \qquad \omega_{n+1} = \omega_n - h\,\sin\theta_n.$$

Euler–Cromer method.

$$\omega_{n+1} = \omega_n - h\,\sin\theta_n, \qquad \theta_{n+1} = \theta_n + h\,\omega_{n+1}.$$

(c) Diagnostics: energy and phase portrait

$$E(\tau) = \frac{1}{2}\omega(\tau)^2 + \big(1 - \cos\theta(\tau)\big), \qquad E_n = \frac{1}{2}\omega_n^2 + \big(1 - \cos\theta_n\big).$$

(d) Tasks

Use initial conditions $\theta(0) = \theta_0$, $\omega(0) = 0$.

1. Consider a small-angle case ($\theta_0 = 0.2$) and a large-angle case ($\theta_0 = 2.5$). For each case integrate up to $\tau_{\max} = 200$ using at least two step sizes (e.g. $h = 0.05$ and $h = 0.02$).
2. For each method and each (θ_0, h), produce:
   - a time series of $\theta(\tau)$;
   - a phase portrait (θ_n, ω_n);
   - an energy drift plot E_n vs. τ_n.
3. Compare Euler and Euler–Cromer focusing on:
   - long-time stability,
   - whether the motion remains bounded,
   - the behaviour of the energy drift.
4. Convert back to physical time for $\ell = 1\,\mathrm{m}$, $g = 9.81\,\mathrm{m/s^2}$ and estimate the physical oscillation periods for $\theta_0 = 0.2$ and $2.5\,\mathrm{rad}$. Do you see any difference in the time period of the pendulum for small and large amplitudes? Explain what you see and explain the reason behind it.

Problem 3: Self–Study and Implementation of the Leapfrog Method

In this problem you will study, implement, and test the leapfrog (velocity–Verlet) integrator for the nonlinear pendulum. A detailed description of the method, its derivation, and its geometric properties is provided in the attached document (pp. 101–108).[1]

(a) Background reading

From the document, carefully study:

- the three–step leapfrog update shown in Eqs. (2.41)–(2.43);
- the geometric interpretation of the algorithm as a phase–space transformation (Fig. 2.6);
- the discussion of area preservation and time reversibility;
- the phase–space comparison of Euler, RK2, and leapfrog (Fig. 2.7).

(b) Apply leapfrog to the nonlinear pendulum

Consider the non-dimensionalized pendulum equation

$$\frac{d\theta}{d\tau} = \omega, \qquad \frac{d\omega}{d\tau} = -\sin\theta.$$

Using the leapfrog structure described in the reading, derive the update rules in the form:

$$\theta_{n+\frac{1}{2}} = \theta_n + \frac{h}{2}\,\omega_n, \qquad \omega_{n+1} = \omega_n - h\,\sin(\theta_{n+\frac{1}{2}}), \qquad \theta_{n+1} = \theta_{n+\frac{1}{2}} + \frac{h}{2}\,\omega_{n+1}.$$

[1] See the uploaded material on the leapfrog method: :contentReference[oaicite:0]index=0

(c) Implementation

Write your own leapfrog solver for the system above. Use initial conditions

$$\theta(0) = \theta_0, \qquad \omega(0) = 0,$$

with both a small–angle case ($\theta_0 = 0.2$) and a large–angle case ($\theta_0 = 2.5$). Use two step sizes, for example $h = 0.05$ and $h = 0.02$.

(d) Diagnostics

For each run, compute the discrete energy

$$E_n = \tfrac{1}{2}\,\omega_n^2 + \big(1 - \cos\theta_n\big),$$

and record:

- a plot of $\theta(\tau)$ vs. τ;
- a phase–space plot (θ_n, ω_n);
- E_n vs. τ_n (or $(E_n - E_0)/E_0$ vs. τ_n).

(e) Comparison with other solvers

Using the same initial conditions and step sizes, integrate the system with:

- Euler,
- Euler–Cromer,
- RK2 (midpoint).

Overlay all their phase–space trajectories on a single figure.

In 5–6 sentences, comment on:

- whether the trajectories spiral outward or inward,
- whether the curves remain approximately closed,
- the degree to which phase–space area is preserved,
- the behaviour of numerical energy over long times,
- why the leapfrog method performs differently from RK2 despite having the same formal order of accuracy.

(f) Reflection

Using the geometric argument presented in the reading (parallelogram area mapping on p. 103), explain in your own words why the leapfrog method preserves phase–space area and is time reversible. Relate these structural properties to your numerical results.

(g) Time step as a phase–space coordinate transformation

For a fixed step size h, each one–step numerical integrator defines a discrete–time dynamical system on phase space. In other words, instead of viewing the solution as a continuous trajectory

$$(\theta(\tau), \omega(\tau)), \qquad \tau \in \mathbb{R},$$

we view it as the orbit of a *map*

$$(\theta_n, \omega_n) \longmapsto (\theta_{n+1}, \omega_{n+1}), \qquad n \in \mathbb{Z},$$

where $\tau_n = nh$ is a discrete time coordinate. The pair $(\theta_{n+1}, \omega_{n+1})$ is obtained from (θ_n, ω_n) by a coordinate transformation in phase space that depends on h.

In this part you will treat the Euler and Euler–Cromer schemes as such transformations, and analyse their Jacobians.

1. For the dimensionless pendulum system

$$\frac{d\theta}{d\tau} = \omega, \qquad \frac{d\omega}{d\tau} = -\sin\theta,$$

the explicit Euler method is

$$\theta_{n+1} = \theta_n + h\,\omega_n, \qquad \omega_{n+1} = \omega_n - h\,\sin\theta_n.$$

View this as a map

$$F_{\mathrm{E}} : (\theta, \omega) \mapsto (\Theta, \Omega) = \big(\theta + h\omega,\ \omega - h\sin\theta\big).$$

Compute the Jacobian matrix

$$J_{\mathrm{E}}(\theta, \omega) = \begin{pmatrix} \dfrac{\partial\Theta}{\partial\theta} & \dfrac{\partial\Theta}{\partial\omega} \\ \dfrac{\partial\Omega}{\partial\theta} & \dfrac{\partial\Omega}{\partial\omega} \end{pmatrix},$$

and show that

$$\det J_{\mathrm{E}}(\theta, \omega) = 1 + h^2\cos\theta.$$

Interpret this determinant as the local area scaling factor for the Euler map in the (θ, ω) plane. Explain why $\det J_{\mathrm{E}} \neq 1$ in general implies that phase–space area and energy are not conserved, and relate this to the spiralling trajectories seen for Euler.

2. The Euler–Cromer method is

$$\omega_{n+1} = \omega_n - h\,\sin\theta_n, \qquad \theta_{n+1} = \theta_n + h\,\omega_{n+1}.$$

Write this as a single phase–space map $F_{\mathrm{EC}} : (\theta, \omega) \mapsto (\Theta, \Omega)$ by eliminating ω_{n+1} in favour of (θ, ω), and show that

$$\Theta = \theta + h\omega - h^2\sin\theta, \qquad \Omega = \omega - h\sin\theta.$$

Compute the Jacobian $J_{\mathrm{EC}}(\theta, \omega)$ and prove that

$$\det J_{\mathrm{EC}}(\theta, \omega) = 1 \quad \text{for all } (\theta, \omega).$$

Conclude that Euler–Cromer is exactly area–preserving in (θ, ω), even though it is only first order in h.

3. Comment briefly on the following points:
   - how the determinants $\det J_{\mathrm{E}}$ and $\det J_{\mathrm{EC}}$ quantify the "distortion" of the time step h when viewed as a coordinate transformation along the discrete orbit;
   - why $\det J = 1$ is a discrete analogue of Liouville's theorem for Hamiltonian flows;
   - how these Jacobian properties explain the qualitative difference between Euler and Euler–Cromer phase–space trajectories observed in your simulations.