Lecture 3: Verlet Method & Hamiltonian Systems

Solutions of the D-exercises

September 24, 2026

Exercise D1

Problem: Consider the one-dimensional case ($d = 1$), $H = H(p, q)$. Using the chain rule, show that the energy remains constant along solutions of the system:

$$H(p(t), q(t)) = \text{constant}$$

Solution: Using the chain rule for a function of two variables $p(t)$ and $q(t)$:

$$\frac{dH}{dt} = \frac{\partial H}{\partial p}\frac{dp}{dt} + \frac{\partial H}{\partial q}\frac{dq}{dt}$$

From Hamilton's equations, we have:

$$\dot{p} = \frac{dp}{dt} = -\frac{\partial H}{\partial q} \quad \text{and} \quad \dot{q} = \frac{dq}{dt} = \frac{\partial H}{\partial p}$$

Substituting these equations into the chain rule expression yields:

$$\frac{dH}{dt} = \frac{\partial H}{\partial p}\left(-\frac{\partial H}{\partial q}\right) + \frac{\partial H}{\partial q}\left(\frac{\partial H}{\partial p}\right) = 0$$

Since the time derivative is zero, $H(p(t), q(t)) = \text{constant}$ along the trajectories.

Exercise D2

Problem: Show that for small displacements x, the equations of motion simplify to $\dot{x} = y, \dot{y} = -x$. Verify the solution $x(t) = \cos(t), y(t) = -\sin(t)$ for $x(0) = 1, y(0) = 0$. Describe the phase plane trajectory and find the energy H.

Solution:

1. **Simplification:** For small x, we apply the Taylor approximation $\sin(x) \approx x$. The system $\dot{x} = y, \dot{y} = -\sin(x)$ simplifies to:
$$\begin{cases} \dot{x} = y \\ \dot{y} = -x \end{cases}$$
2. **Verification:** Checking the differential equations:
$$\dot{x}(t) = \frac{d}{dt}\cos(t) = -\sin(t) = y(t) \quad \checkmark$$
$$\dot{y}(t) = \frac{d}{dt}(-\sin(t)) = -\cos(t) = -x(t) \quad \checkmark$$
Checking the initial conditions:
$$x(0) = \cos(0) = 1, \quad y(0) = -\sin(0) = 0 \quad \checkmark$$

3. **Phase Plane Trajectory:** Since $x(t)^2 + y(t)^2 = \cos^2(t) + \sin^2(t) = 1$, the trajectory in the x-y plane is a **unit circle centered at the origin**, traversed clockwise.

4. **Energy Expression:** The energy for this simplified harmonic oscillator is:

$$H(x, y) = \frac{1}{2}y^2 + \frac{1}{2}x^2 = \frac{1}{2}(x^2 + y^2)$$

Evaluating along the solution gives $H(t) = \frac{1}{2}(\cos^2(t) + \sin^2(t)) = \frac{1}{2}$ (constant).

Exercise D3

Problem: Derive the equations of motion for two mutually attracting bodies with Hamiltonian:

$$H(p_1, p_2, q_1, q_2) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}$$

Solution: Using Hamilton's equations $\dot{q}_i = \frac{\partial H}{\partial p_i}$ and $\dot{p}_i = -\frac{\partial H}{\partial q_i}$ for $i = 1, 2$:

- **Position derivatives:**

$$\dot{q}_1 = \frac{\partial H}{\partial p_1} = p_1, \qquad \dot{q}_2 = \frac{\partial H}{\partial p_2} = p_2$$

- **Momentum derivatives:** Rewriting the potential term as $U(q_1, q_2) = -(q_1^2 + q_2^2)^{-1/2}$ and taking partial derivatives with the chain rule:

$$\dot{p}_1 = -\frac{\partial H}{\partial q_1} = -\left(-\frac{1}{2}(q_1^2 + q_2^2)^{-3/2} \cdot 2q_1\right) = -\frac{q_1}{(q_1^2 + q_2^2)^{3/2}}$$

$$\dot{p}_2 = -\frac{\partial H}{\partial q_2} = -\left(-\frac{1}{2}(q_1^2 + q_2^2)^{-3/2} \cdot 2q_2\right) = -\frac{q_2}{(q_1^2 + q_2^2)^{3/2}}$$

Exercise D4

Problem: Show using Taylor expansion that:

$$\ddot{q}(t^n) = \frac{q^{n+1} - 2q^n + q^{n-1}}{(\Delta t)^2} + F_1, \quad \text{where } F_1 = -\frac{1}{12}(\Delta t)^2 \frac{d^4 q}{dt^4}$$

Solution: Expanding $q(t^{n+1}) = q(t^n + \Delta t)$ and $q(t^{n-1}) = q(t^n - \Delta t)$ around t^n:

$$q^{n+1} = q^n + \Delta t \dot{q}^n + \frac{(\Delta t)^2}{2}\ddot{q}^n + \frac{(\Delta t)^3}{6}q^{(3)}(t^n) + \frac{(\Delta t)^4}{24}q^{(4)}(t^n) + \mathcal{O}((\Delta t)^5)$$

$$q^{n-1} = q^n - \Delta t \dot{q}^n + \frac{(\Delta t)^2}{2}\ddot{q}^n - \frac{(\Delta t)^3}{6}q^{(3)}(t^n) + \frac{(\Delta t)^4}{24}q^{(4)}(t^n) + \mathcal{O}((\Delta t)^5)$$

Adding these two expansions eliminates the odd-order derivative terms:

$$q^{n+1} + q^{n-1} = 2q^n + (\Delta t)^2 \ddot{q}^n + \frac{(\Delta t)^4}{12}q^{(4)}(t^n) + \mathcal{O}((\Delta t)^6)$$

Rearranging terms to solve for $\ddot{q}(t^n)$:

$$\frac{q^{n+1} - 2q^n + q^{n-1}}{(\Delta t)^2} = \ddot{q}^n + \frac{(\Delta t)^2}{12}q^{(4)}(t^n) + \mathcal{O}((\Delta t)^4)$$

Isolating $\ddot{q}(t^n)$ gives:

$$\ddot{q}(t^n) = \frac{q^{n+1} - 2q^n + q^{n-1}}{(\Delta t)^2} - \frac{1}{12}(\Delta t)^2 \frac{d^4 q}{dt^4} + \dots$$

Hence, the leading error term is $F_1 = -\frac{1}{12}(\Delta t)^2 \frac{d^4 q}{dt^4}$.

Exercise D5

Problem: Express $(x^{n+1})^2 + (y^{n+1})^2$ as a function of $(x^n)^2 + (y^n)^2$ for Euler Forward (EF), Euler Backward (EB), and the Implicit Midpoint Method.

Solution:

1. Euler Forward (EF)

The scheme is $x^{n+1} = x^n + \Delta t y^n$ and $y^{n+1} = y^n - \Delta t x^n$.

$$(x^{n+1})^2 + (y^{n+1})^2 = (x^n + \Delta t y^n)^2 + (y^n - \Delta t x^n)^2$$

$$= (x^n)^2 + 2\Delta t x^n y^n + (\Delta t)^2 (y^n)^2 + (y^n)^2 - 2\Delta t x^n y^n + (\Delta t)^2 (x^n)^2$$

$$= (1 + (\Delta t)^2) \left((x^n)^2 + (y^n)^2 \right)$$

Since $1 + (\Delta t)^2 > 1$, the numerical energy **increases** at each step.

2. Euler Backward (EB)

The scheme is $x^{n+1} = x^n + \Delta t y^{n+1}$ and $y^{n+1} = y^n - \Delta t x^{n+1}$. In matrix form:

$$\begin{pmatrix} 1 & -\Delta t \\ \Delta t & 1 \end{pmatrix} \begin{pmatrix} x^{n+1} \\ y^{n+1} \end{pmatrix} = \begin{pmatrix} x^n \\ y^n \end{pmatrix} \implies \begin{pmatrix} x^{n+1} \\ y^{n+1} \end{pmatrix} = \frac{1}{1 + (\Delta t)^2} \begin{pmatrix} 1 & \Delta t \\ -\Delta t & 1 \end{pmatrix} \begin{pmatrix} x^n \\ y^n \end{pmatrix}$$

Taking the square magnitude:

$$(x^{n+1})^2 + (y^{n+1})^2 = \frac{1}{(1 + (\Delta t)^2)^2} \left((x^n + \Delta t y^n)^2 + (-\Delta t x^n + y^n)^2 \right)$$

$$= \frac{1 + (\Delta t)^2}{(1 + (\Delta t)^2)^2} \left((x^n)^2 + (y^n)^2 \right) = \frac{1}{1 + (\Delta t)^2} \left((x^n)^2 + (y^n)^2 \right)$$

Since $\frac{1}{1+(\Delta t)^2} < 1$, the numerical energy **decreases** at each step.

3. Implicit Midpoint Method

The scheme is:

$$x^{n+1} - x^n = \frac{\Delta t}{2}(y^n + y^{n+1}), \qquad y^{n+1} - y^n = -\frac{\Delta t}{2}(x^n + x^{n+1})$$

Multiplying the first equation by $(x^{n+1} + x^n)$ and the second by $(y^{n+1} + y^n)$:

$$(x^{n+1})^2 - (x^n)^2 = \frac{\Delta t}{2}(y^n + y^{n+1})(x^{n+1} + x^n)$$

$$(y^{n+1})^2 - (y^n)^2 = -\frac{\Delta t}{2}(x^n + x^{n+1})(y^n + y^{n+1})$$

Adding both equations together:

$$\left((x^{n+1})^2 + (y^{n+1})^2 \right) - \left((x^n)^2 + (y^n)^2 \right) = 0 \implies (x^{n+1})^2 + (y^{n+1})^2 = (x^n)^2 + (y^n)^2$$

The numerical energy **remains strictly constant**.