Time evolution:

Coupled ODE's: (discretized PDE's for instance!)

$$\dot{z} = f(z)$$

$$\vec{z} = \begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix}$$

Aim: Given $z(t=0)$, find $z(t)$.

Method of choice: timestepping

$$\vec{z}(t_1) = M(\vec{z}(t_0))$$

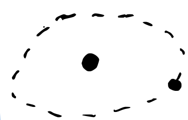
$$\vec{z}(t_2) = M(\vec{z}(t_1))$$

$$\dots$$

M: some map (algorithm!)

Today: learn from examples

① Orbit in a radial potential



$$V(r) = -\frac{\lambda}{\sqrt{x^2+y^2}}$$

EoM:

$$\dot{p}_x = -\frac{\partial V}{\partial x} = -\frac{\lambda x}{\sqrt{x^2+y^2}} \equiv K_x(x,y)$$

$$\dot{p}_y = -\frac{\partial V}{\partial y} = -\frac{\lambda y}{\sqrt{x^2+y^2}} \equiv K_y(x,y)$$

$$\dot{x} = p_x$$

$$\dot{y} = p_y$$

$$H = \frac{p_x^2}{2} + \frac{p_y^2}{2} - \frac{\lambda}{\sqrt{x^2+y^2}}$$

$$L = x p_y - y p_x$$

Energy and angular momentum are conserved $\Rightarrow$

$$r(\theta) = \frac{-L^2}{1+e\cos(\theta)}, \quad e = \sqrt{1+2EL^2}$$

Attempt # 1: "Forward Euler" (FE)

$$\frac{df}{dt} \simeq \frac{f(t+\Delta t) - f(t)}{\Delta t}$$

$$\Rightarrow \quad \vec{p}(x+\Delta t) = \vec{p}(t) + \Delta t\, \vec{K}(x(t), y(t))$$

$$\vec{x}(x+\Delta t) = \vec{x}(t) + \Delta t\, \vec{p}(t)$$

See julia notebook

FE does not preserve L cons.

Notation: $f(t+\Delta t) \equiv f^{+1}$ $\quad f(t) \equiv f$

$$K(x(t+\Delta t), y(t+\Delta t)) = K^{+1}$$

$$L^{+1} = x^{+1} p_y^{+1} - y^{+1} p_x^{+1}$$

$$x^{+1} p_y^{+1} = x p_y + \Delta t\, p_x p_y + \Delta t\, K_y\, x + \Delta t^2 K_y p_x$$

$$\Rightarrow L^{+1} = L + \Delta t\,(\overbrace{K_y x - K_x y}^{=0}) + \Delta t^2 (K_y p_x - K_x p_y) \quad + \Delta t^2 (K_x p_y - K_y p_x)$$

Suggests:

$$\begin{cases} \vec{p}^{+1} = \vec{p} + \Delta t\, \vec{K} \\ \vec{x}^{+1} = \vec{x} + \Delta t\, \vec{p}^{+} \end{cases}$$

Semi-implicit Euler

See julia notebook

Take home: Physics $\rightleftarrows$ algorithms

Built an algorithm that preservos the conservation laws ("symplectic")

$\downarrow$

Good for Hamiltonian systems

H: $H(x, p_x)$ $\{x, p\} = 1$

Poisson bracket: $\{f, g\} = \frac{\partial f}{\partial x}\frac{\partial g}{\partial p_x} - \frac{\partial f}{\partial p_x}\frac{\partial g}{\partial x}$

Symplectic : Preserves $\{\cdot, \cdot\}$

$\Updownarrow$

Preserves conservations laws

Some algorithm's properties:

- $\boxed{\text{Explicit}}$ vs implicit

  + cheaper — More expensive

  − less stable + More stable

- Order of convergence

  ~ $\overset{\text{exact}}{X(t)} - X(t) = O(\Delta t^{\ell})$

  ~ Δconserved $= O(\Delta t^{\ell})$

- For Hamiltonian systems: symplectic vs non-symplectic

Higher orders #1 : Verlet

Combine symplectic steps !

Semi-implicit Euler

V1

$$\begin{cases} \vec{p}^{\,+1} = \vec{p} + \Delta t\, \vec{K} \\ \vec{x}^{\,+1} = \vec{x} + \Delta t\, \vec{p}^{\,+1} \end{cases}$$

V2

$$\begin{cases} \vec{x}^{\,+1} = \vec{x} + \Delta t\, \vec{p} \\ \vec{p}^{\,+1} = \vec{p} + \Delta\, \vec{K}^{+1} \end{cases}$$

Add 1/2 time step and alternate V1/V2

Velocity - verlet : (VV)

$$\vec{p}^{\,+1/2} = \vec{p} + \frac{1}{2}\Delta t\, \vec{K}$$

$$\vec{x}^{\,+1} = \vec{x} + \Delta t\, \vec{p}_{1/2}$$

$$\vec{p}^{\,+1} = \vec{p}_{1/2} + \frac{1}{2}\Delta t\, \vec{K}_{1/2}$$

Position verlet : (PV)

$$\vec{x}^{\,+1/2} = \vec{x} + \frac{1}{2}\Delta t\, \vec{p}$$

$$\vec{p}^{\,+1} = \vec{p} + \Delta t\, \vec{K}_{1/2}$$

$$\vec{x}^{\,+1} = \vec{x}_{1/2} + \frac{1}{2}\Delta t\, \vec{p}_{+1}$$

Can also generalize it to higher order (Δt^{10} in CL !)

See julia notebook

Staggered Leapfrog :

PV but don't stop at $\vec{x}_{+1}$!

$$\vec{x}^{\,+1/2} = \vec{x}^{\,-1/2} + \Delta t\, \vec{p}$$

$$\vec{p}^{\,+1} = \vec{p} + \Delta t\, \vec{K}_{1/2}$$

⚠ Need to compare quantities at same times.

Higher orders #2: Runge-Kutta (RK)

Directly write higher order discret. of the ODE.

→ Not symplectic but works for non-Hamiltonian systems

(Verlet needs kicks to be momentum independent)

For instance: **Modified Euler (RK2)**

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

$$\vec{p}^{+1} = \vec{p} + \frac{\Delta t}{2}\left(\vec{K}^{(1)} + \vec{K}^{(2)}\right)$$

$$\vec{p}^{(1)} = \vec{p} \qquad \vec{K}^{(1)} = \vec{K}(\vec{x}, \vec{p})$$

$$\vec{p}^{(2)} = \vec{p} + \Delta t\, \vec{K}^{(1)} \qquad \vec{K}^{(2)} = \vec{K}(\vec{x} + \Delta t\, p^{(1)}, p^{(1)})$$

See julia notebook

RK4:

$$\vec{x}^{+1} = \vec{x} + \frac{\Delta t}{6}\left(p^{(1)} + 2p^{(2)} + 2p^{(3)} + p^{(4)}\right)$$

$$\vec{p}^{+1} = \vec{p} + \frac{\Delta t}{6}\left(k_1^p + 2k_2^p + 2k_3^p + k_4^p\right)$$

$$p^{(1)} = \vec{p}, \qquad k_1^p = \vec{K}(\vec{x}, \vec{p})$$

$$p^{(2)} = \vec{p} + \frac{\Delta t}{2} k_1^p, \qquad k_2^p = \vec{K}(\vec{x} + \tfrac{\Delta t}{2} p^{(1)}, p^{(1)})$$

$$p^{(3)} = \vec{p} + \frac{\Delta t}{2} k_2^p, \qquad k_3^p = \vec{K}(\vec{x} + \tfrac{\Delta t}{2} p^{(2)}, p^{(2)})$$

$$p^{(4)} = \vec{p} + \Delta t\, k_3^p, \qquad k_4^p = \vec{K}(\vec{x} + \Delta t\, p^{(3)}, p^{(3)})$$

See julia notebook.

Summary:

- Time evolution through time-stepping
- Physics of the problem informs on algorithm
- Accuracy of solver matters

② (1+1) Wave equation:

Almost the same!

$$-\partial_t^2 \varphi(x,t) + \partial_x^2 \varphi(x,t) = 0$$

① Discretize in space (see lecture 1)

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

$$\equiv \Delta_x^2 \varphi(n,t)$$

② Reduce to coupled 1^{st} order ODEs

$$\partial_t \varphi(n,t) \equiv \pi(n,t)$$

$$\Rightarrow \quad \partial_t \pi(n,t) = \Delta_x^2 \varphi(n,t)$$

$$\partial_t \phi(n,t) = \pi(n,t)$$

$2N$ ODE's. Use the same methods as before!

$\uparrow$

number lattice points

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Comments: • Memory usage can be an issue $\rightarrow$ Verlet / leapfrog only 1 copy of fields

vs

RK, more than 1.

• CFL condition

$$\Delta t < \frac{1}{\sqrt{\text{dimension}}} \Delta x$$

Idea of proof: Take $f(x,t) = e^{ikx - i\omega t}$

Gain ansatz: $f(x, t + \frac{\Delta t}{2}) = G\, f(x,t)$

$$f(x, t + \Delta t) = G^2 f(x,t)$$

Position - Verlet:

$$f(x, t + \tfrac{\Delta t}{2}) = f(x,t) + \frac{\Delta t}{2} p(x,t)$$

$$p(x, t + \Delta t) = p(x,t) + \Delta t\, \Delta_x^+ f(x,t)$$

$$f(x, t + \Delta t) = f(x, t + \Delta t/2) + \frac{\Delta t}{2} p(x,t)$$

Using: $\Delta_x^+ f(x,t) = \dfrac{(2\cos(k\Delta x) - 1)}{\Delta x^2} f(x,t)$

Find eq. for G. $\dfrac{\Delta t^2}{\Delta x^2} < 1$ imposes

$|G| \leq 1 \Rightarrow$ stable.