Examples

The equations of motion have been reduced to

$$\frac{d\bar{\omega}}{dt} = f(\bar{\omega}, t)$$

$$\bar{\omega} = (\bar{x}, \bar{v}) \quad ; \quad \frac{d\bar{\omega}}{dt} = (\dot{\bar{x}}, \dot{\bar{v}}) = \left(\frac{\partial H}{\partial \bar{v}}, -\frac{\partial H}{\partial \bar{x}}\right) = f(\bar{x}, \bar{v}, t) = f(\bar{\omega}, t)$$

If one has a differential equation ($f \equiv$ scalar / 1D)

$$\frac{df}{dt} = G(f, t)$$

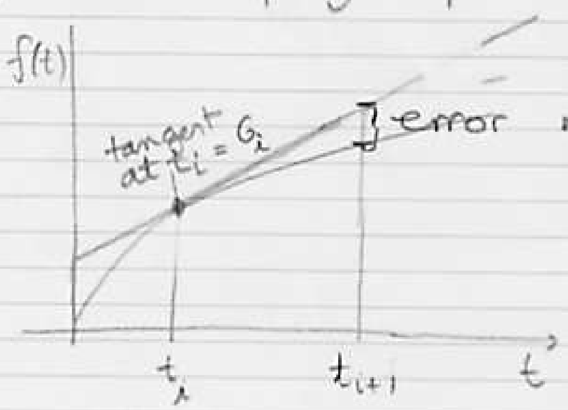
finite differences

$$\frac{\Delta f}{\Delta t} = \frac{f(t_{i+1}) - f(t_i)}{t_{i+1} - t_i} = \frac{f_{i+1} - f_i}{t_{i+1} - t_i} = G(f_i, t_i)$$

$$\therefore \boxed{f_{i+1} = f_i + \Delta t \cdot G(f_i, t_i)}$$

EULER SCHEME

one may obtain step by step the solution



This is essentially like making a Taylor expansion

$$f(t_{i+1}) \sim f(t_i) + \Delta t\, f'(t_i) + \frac{\Delta t^2}{2} f''(t_{i+\epsilon}) + \dots$$

Therefore the local error made is

$$\epsilon_{local} = f(t_{i+1}) - f_{i+1} = \frac{\Delta t^2}{2} f''(t_{i+\epsilon}) \quad \propto \Delta t^2$$

The global error after many steps:

$$\epsilon_{tot} \propto \sum_{i=1}^{N} \Delta t^2 \sim N \Delta t^2 = \frac{T_f - T_0}{\cancel{\Delta t}} \cdot \Delta t^{\cancel{2}} \propto \Delta t$$

→ so this method is only accurate to first order

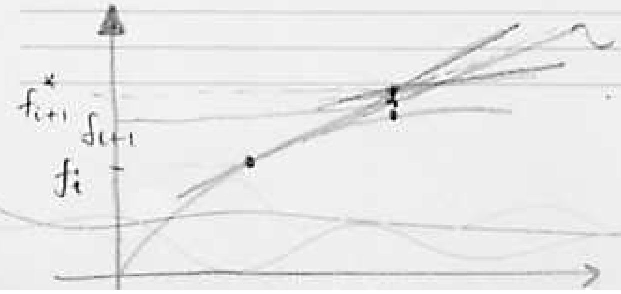
Modified Euler scheme

The idea is to use more information than just the value of the derivative at the initial position.

For example,

$$f_{i+1} = f_i + \Delta t * \frac{G_i + G^*_{i+1}}{2}$$

where $G^*_{i+1} = G(t_i + \Delta t, f_i + \Delta t\, G_i)$ $\boxed{\text{TRIAL STEP}}$



$\sim \dfrac{G_i + G^*_{i+1}}{2} \equiv$ average slope

The idea is

i) $f^*_{i+1} = f_i + \Delta t \cdot G_i$ (Euler)

ii) measure $G^*_{i+1} = G(t_{i+1}, f^*_{i+1})$

iii) $f_{i+1} = f_i + \Delta t \underbrace{\dfrac{G_i + G^*_{i+1}}{2}}_{\text{average slope}}$

In this case, the error made

$$f(t_{i+1}) = f(t_i) + f'(t_i)\Delta t + f''(t_i)\frac{\Delta t^2}{2} + f'''(t_i)\frac{\Delta t^3}{3!}$$

$$\epsilon = -\Delta t \left[\frac{G_i + G^*_{i+1}}{2}\right] + f'(t_i)\Delta t + f''\frac{\Delta t^2}{2} + f^{(3)}\frac{\Delta t^3}{3!}$$

To first order $G^*_{i+1} = G_i + \Delta t\, G'(t_i) = f'(t_i) + \Delta t\, f''(t_i)$

Therefore

$$\epsilon = -\Delta t \left\{ \cancel{\frac{f'(t_i)}{2}} + \cancel{\frac{f'(t_i)}{2}} + \frac{\Delta t}{2} f''(t_i) \right\} + \cancel{f'(t_i)\Delta t} + f''\frac{\Delta t^2}{2} + f^{(3)}\frac{\Delta t^3}{3!}$$

$$\sim -\frac{\Delta t^2}{2} f'' + \frac{\Delta t^2}{2} f'' + f^{(3)}\frac{\Delta t^3}{3!} = f^{(3)}\frac{\Delta t^3}{3!}$$

Therefore the error is smaller (because we have used additional information)

LEAP FROG

$$\boxed{f_{i+1} = f_i + \Delta t \, G_{i+1/2}}$$

More widely used

→ 2nd order accurate

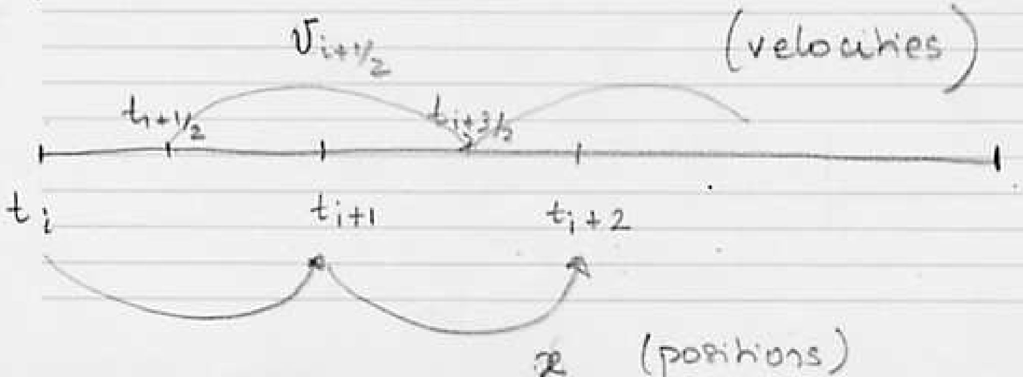
→ symmetric and hence time-reversible
(guarantees energy conservation)

$$\frac{dx}{dt} = v \qquad \frac{dv}{dt} = G(x)$$

≡ just like the eq. of motion in Hamiltonian dynamics.

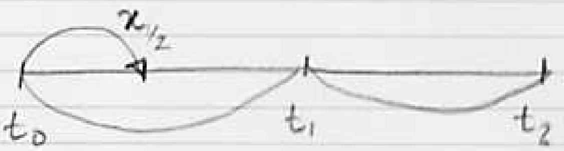
The recipe applied to this case is

$$\begin{cases} x_{i+1} = x_i + \Delta t \, v_{i+1/2} \\ v_{i+3/2} = v_{i+1/2} + \Delta t \, G(x_{i+1}) \end{cases}$$



Therefore the positions and velocities are updated out of phase:

→ jumpstart



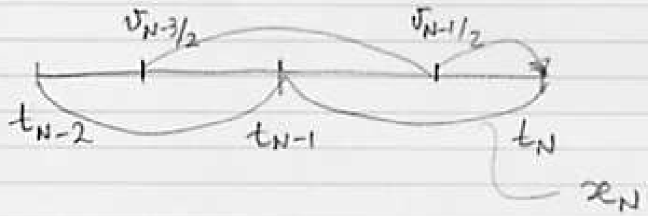
$$\boxed{\begin{aligned} &\text{pos:} \quad x_1 = x_0 + \Delta t \, v_{1/2} \\ &\text{vel:} \quad v_{1/2} = v_0 + \frac{\Delta t}{2} G(x_0) \end{aligned}}$$

(no jump)

(are shifted ahead)

But typically we want to know the positions <u>and</u> the velocities at a given time (output)

<u>Output</u> : <u>Resynchronization</u>



$$\boxed{v_N = v_{N-1/2} + \frac{\Delta t}{2} G(x_N)}$$

Time-reversibility

an extremely useful property of the leap-frog is the time-reversibility:

$$x_{i+1} = x_i + \Delta t\, v_{i+1/2}$$

$$v_{i+3/2} = v_{i+1/2} + \Delta t\, F(x_{i+1})$$

Suppose now we want to go from the current position to the previous one $(x_{i+1}, v_{i+3/2}) \rightarrow (x_i, v_{i+1/2})$

According to the algorithm (reversing Δt)

$$v_{i+1/2} = v_{i+3/2} - \Delta t\, F(x_{i+1})$$

$$x_i = x_{i+1} - \Delta t\, v_{i+1/2}$$

But this is exactly what we did before in reverse order - This implies that if we reverse the velocities and the timestep we would arrive at the same place where we started.

For example in the modified Euler

$$f^*_{i+1} = f_i + \Delta t\, G_i$$

$$G^*_{i+1} = G(t_{i+1}, f^*_{i+1})$$

$$f_{i+1} = f_i + \frac{\Delta t}{2}\left(G_i + G^*_{i+1} \right)$$

If we want to go from $(f_{i+1}, t_{i+1}) \to (f_i, t_i)$

$$f_i^* = f_{i+1} - \Delta t \; G(t_{i+1})$$

$$G_i^* = G(t_i, f_i^*)$$

$$\tilde{f}_i = f_{i+1} - \frac{\Delta t}{2}\left(G_{i+1} + G_i^*\right)$$

Therefore $\tilde{f}_i \neq f_i$

$$\cancel{f_{i+1}} - \cancel{\frac{\Delta t}{2}}\left(G_{i+1} + G_i^*\right) \neq \cancel{f_{i+1}} - \cancel{\frac{\Delta t}{2}}\left(G_i + G_{i+1}^*\right)$$

$$G(f_{i+1}, t_{i+1}) \neq G(f_i, t_i)$$

$$G(f_i + \Delta t\, G_i) \qquad G(f_{i+1} - \Delta t\, G_{i+1})$$

No systematic error in E