Computational Physics

Lecture-22

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Contents

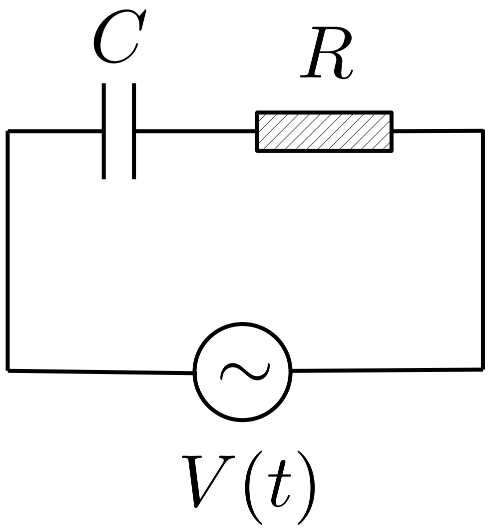
Ordinary Differential Equation

- Initial Value Problem

First Order ODE

$$\frac{q}{C} + R\frac{\mathrm{d}q}{\mathrm{d}t} = V(t)$$

$$q(t = t_0) = q_0$$

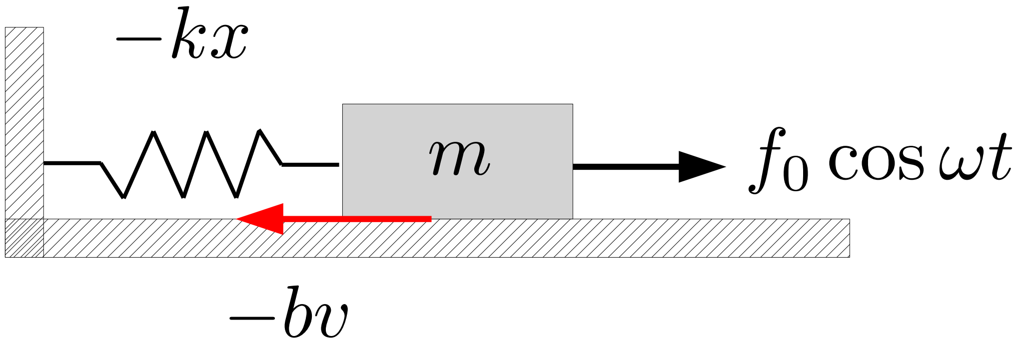


Second Order ODE

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -kx - bv + f_0 \cos \omega t$$

$$x(t = t_0) = x_0, \quad v(t = t_0) = v_0$$

$$v = \frac{\mathrm{d}x}{\mathrm{d}t}$$

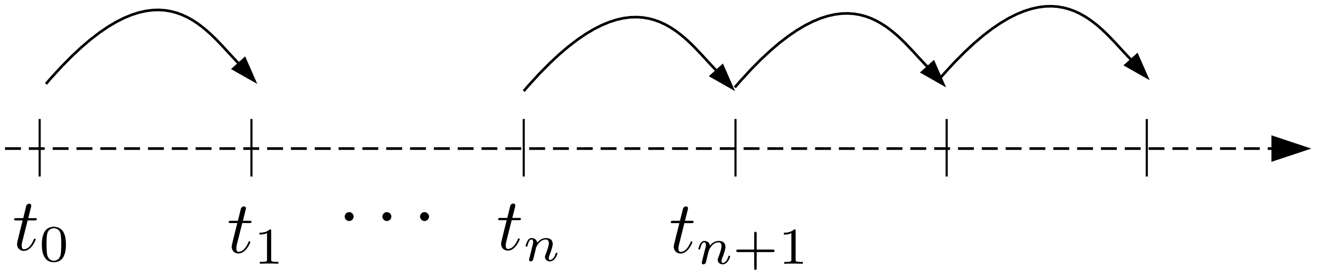


• **Ordinary Differential Equation** (Initial Value Problem)

• Euler Method (Explicit Method)

$$\dot{y} = f(y, t), \quad y(t = t_0) = y_0$$

First Order ODE



$$t_n = t_0 + n\Delta t$$

$$\dot{y}_n = f(y_n, t_n)$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(y, t) \Rightarrow \mathrm{d}y = f(y, t)\mathrm{d}t : \quad y_{n+1} = y_n + \int_{t_n}^{t_{n+1}} f[y(t'), t']\mathrm{d}t'$$

• Ordinary Differential Equation (Initial Value Problem)

• Euler Method (Explicit Method)

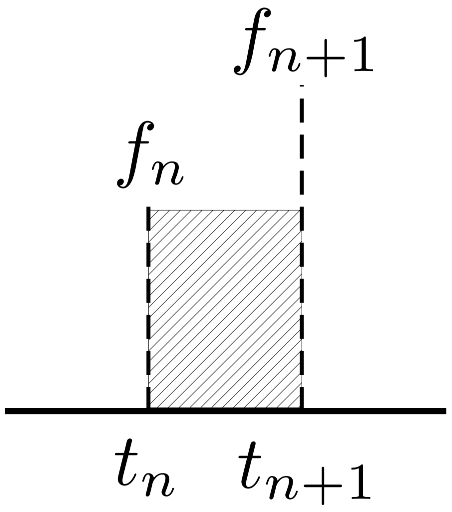
First Order ODE

$$\dot{y} = f(y,t), \quad y(t=t_0) = y_0$$

$$y_{n+1} = y_n + \int_{t_n}^{t_{n+1}} f[y(t'), t'] \mathrm{d}t'$$

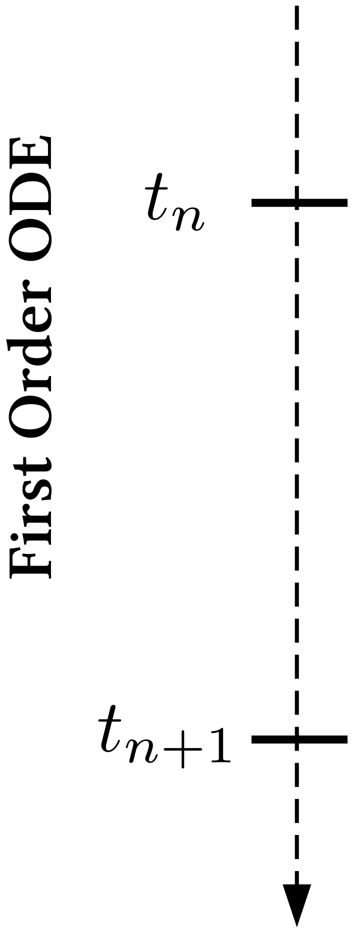
$$y_{n+1} = y_n + f_n \Delta t + O(\Delta t^2)$$

$$f_n = f(y_n, t_n)$$



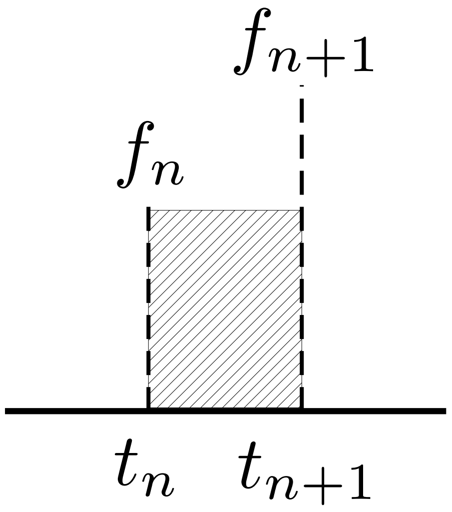
• Ordinary Differential Equation (Initial Value Problem)

• Euler Method (Explicit Method)



$$f_n = f(y_n, t_n)$$

$$y_{n+1} = y_n + f_n \Delta t$$



• **Ordinary Differential Equation** (Initial Value Problem)

• Stability of Euler Method (Explicit Method)

First Order ODE

$$y_{n+1} = y_n + \Delta t f(y_n, t_n)$$

$$y_{n+1} \rightarrow y_{n+1} + \delta y_{n+1}$$

$$y_n \rightarrow y_n + \delta y_n$$

$$\underbrace{y_{n+1} + \delta y_{n+1}}_{y_{n+1}} = \underbrace{y_n + \delta y_n}_{y_n} + \Delta t f(\underbrace{y_n + \delta y_n}_{y_n}, t_n)$$

• Ordinary Differential Equation (Initial Value Problem)

• Stability of Euler Method (Explicit Method)

First Order ODE

$$y_{n+1} = y_n + \Delta t f(y_n, t_n)$$

$$y_{n+1} + \delta y_{n+1} = y_n + \delta y_n + \Delta t \boxed{f(y_n + \delta y_n, t_n)}$$

$$\boxed{f(y_n + \delta y_n, t_n)} = f(y_n, t_n) + \left(\frac{\partial f}{\partial y}\right)_n \delta y_n + O(\delta y_n^2)$$

$$y_{n+1} + \delta y_{n+1} = y_n + \delta y_n + \Delta t f(y_n, t_n) + \Delta t \left(\frac{\partial f}{\partial y}\right)_n \delta y_n$$

$$y_{n+1} + \delta y_{n+1} = y_n + \Delta t f(y_n, t_n) + \left[1 + \Delta t \left(\frac{\partial f}{\partial y}\right)_n\right] \delta y_n$$

• **Ordinary Differential Equation** (Initial Value Problem)

• Stability of Euler Method (Explicit Method)

First Order ODE

$$y_{n+1} = y_n + \Delta t f(y_n, t_n)$$

$$y_{n+1} + \delta y_{n+1} = \underbrace{y_n + \Delta t f(y_n, t_n)}_{y_{n+1}} + \left[1 + \Delta t \left(\frac{\partial f}{\partial y}\right)_n\right] \delta y_n$$

$$\cancel{y_{n+1}} + \delta y_{n+1} = \cancel{y_{n+1}} + \left[1 + \Delta t \left(\frac{\partial f}{\partial y}\right)_n\right] \delta y_n$$

$$\delta y_{n+1} = \left[1 + \Delta t \left(\frac{\partial f}{\partial y}\right)_n\right] \delta y_n$$

• Ordinary Differential Equation (Initial Value Problem)

• Stability of Euler Method (Explicit Method)

First Order ODE

$$y_{n+1} = y_n + \Delta t f(y_n, t_n)$$

$$\delta y_{n+1} = \left[1 + \Delta t \left(\frac{\partial f}{\partial y}\right)_n\right] \delta y_n$$

Growth Factor: $\dfrac{\delta y_{n+1}}{\delta y_n} = 1 + \Delta t \left(\dfrac{\partial f}{\partial y}\right)_n, \quad \left|\dfrac{\delta y_{n+1}}{\delta y_n}\right| \leq 1$ Stability Condition

$$\left|1 + \Delta t \left(\frac{\partial f}{\partial y}\right)\right| \leq 1$$

• Ordinary Differential Equation (Initial Value Problem)

- Stability of Euler Method (Explicit Method)

First Order ODE

$$y_{n+1} = y_n + \Delta t f(y_n, t_n)$$

$$\left| 1 + \Delta t \left(\frac{\partial f}{\partial y} \right) \right| \leq 1$$

Stability Condition

Example: $y' = -ky, \quad y(0) = y_0, \quad k > 0$

$$|1 - k\Delta t| \leq 1$$

• Ordinary Differential Equation (Initial Value Problem)

• Picard Method (Implicit Method)

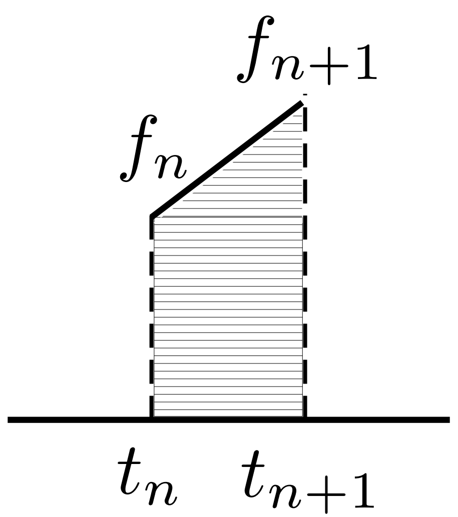
First Order ODE

$$\dot{y} = f(y,t), \quad y(t=t_0) = y_0$$

$$y_{n+1} = y_n + \int_{t_n}^{t_{n+1}} f[y(t'),t']\mathrm{d}t'$$

$$y_{n+1} = y_n + \frac{1}{2}(f_n + f_{n+1})\Delta t + O(\Delta t^3)$$

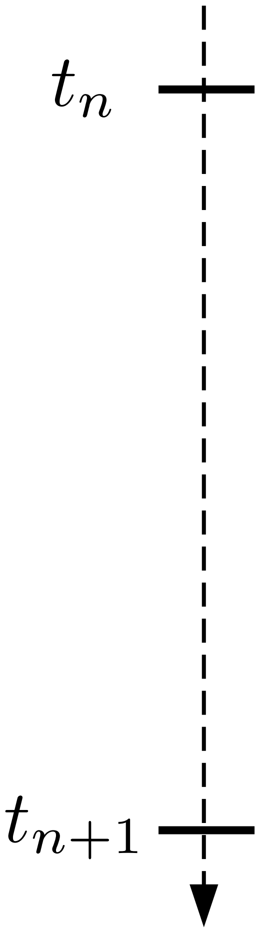
$$f_n = f(y_n, t_n), \quad f_{n+1} = f(y_{n+1}, t_{n+1})$$



• **Ordinary Differential Equation** (Initial Value Problem)

• Picard Method (Implicit Method)

First Order ODE



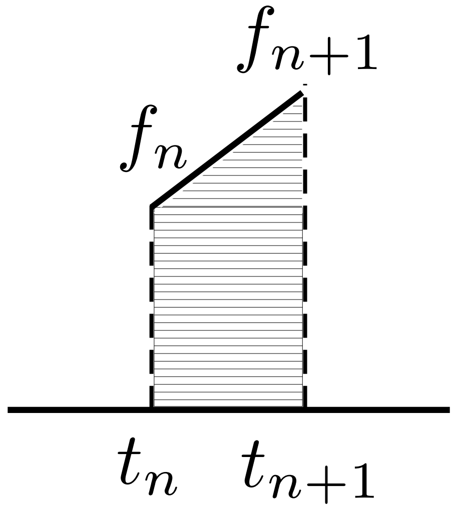
Euler Method

$$f_n = f(y_n, t_n)$$

$$\tilde{y}_{n+1} = y_n + f_n \Delta t$$

$$f_{n+1} = f(\tilde{y}_{n+1}, t_{n+1})$$

$$y_{n+1} = y_n + \frac{1}{2}(f_n + f_{n+1})\Delta t$$



• **Ordinary Differential Equation** (Initial Value Problem)

• Stability of Picard Method (Implicit Method)

First Order ODE

$$y_{n+1} = y_n + \Delta t \frac{1}{2}(f_n + f_{n+1})$$

$$y_{n+1} \to y_{n+1} + \delta y_{n+1}$$

$$y_n \to y_n + \delta y_n$$

$$\underbrace{y_{n+1} + \delta y_{n+1}}_{y_{n+1}} = \underbrace{y_n + \delta y_n}_{y_n} + \Delta t \frac{1}{2}(f(\underbrace{y_n + \delta y_n}_{y_n}, t_n) + f(\underbrace{y_{n+1} + \delta y_{n+1}}_{y_{n+1}}, t_{n+1}))$$

• **Ordinary Differential Equation** (Initial Value Problem)

- Stability of Picard Method (Implicit Method)

First Order ODE

$$y_{n+1} = y_n + \Delta t \frac{1}{2}(f_n + f_{n+1})$$

$$y_{n+1} + \delta y_{n+1} = y_n + \delta y_n$$

$$+\Delta t \frac{1}{2}\left(\boxed{f(y_n + \delta y_n, t_n)} + \boxed{f(y_{n+1} + \delta y_{n+1}, t_{n+1})}\right)$$

$$f(y_n + \delta y_n, t_n) = f(y_n, t_n) + \left(\frac{\partial f}{\partial y}\right)_n \delta y_n + O(\delta y_n^2)$$

$$f(y_{n+1} + \delta y_{n+1}, t_{n+1}) = f(y_{n+1}, t_{n+1}) + \left(\frac{\partial f}{\partial y}\right)_{n+1} \delta y_{n+1} + O(\delta y_{n+1}^2)$$

• **Ordinary Differential Equation** (Initial Value Problem)

- Stability of Picard Method (Implicit Method)

First Order ODE

$$y_{n+1} = y_n + \Delta t \frac{1}{2}(f_n + f_{n+1})$$

$$y_{n+1} + \delta y_{n+1} = y_n + \delta y_n$$

$$+\Delta t \frac{1}{2}\left[f(y_n, t_n) + \left(\frac{\partial f}{\partial y}\right)_n \delta y_n \right.$$

$$\left. + f(y_{n+1}, t_{n+1}) + \left(\frac{\partial f}{\partial y}\right)_{n+1} \delta y_{n+1}\right]$$

• Ordinary Differential Equation (Initial Value Problem)

• Stability of Picard Method (Implicit Method)

First Order ODE

$$y_{n+1} = y_n + \Delta t \frac{1}{2}(f_n + f_{n+1})$$

$$\cancel{y_{n+1}} + \left[1 - \frac{1}{2}\Delta t \left(\frac{\partial f}{\partial y}\right)_{n+1}\right] \delta y_{n+1} = y_n + \cancel{\Delta t \frac{1}{2}(f_n + f_{n+1})}$$

$$+ \left[1 + \frac{1}{2}\Delta t \left(\frac{\partial f}{\partial y}\right)_{n}\right] \delta y_n$$

$$\left[1 - \frac{1}{2}\Delta t \left(\frac{\partial f}{\partial y}\right)_{n+1}\right] \delta y_{n+1} = \left[1 + \frac{1}{2}\Delta t \left(\frac{\partial f}{\partial y}\right)_{n}\right] \delta y_n$$

• **Ordinary Differential Equation** (Initial Value Problem)

• Stability of Picard Method (Implicit Method)

First Order ODE

$$y_{n+1} = y_n + \Delta t \frac{1}{2}(f_n + f_{n+1})$$

$$\left[1 - \frac{1}{2}\Delta t \left(\frac{\partial f}{\partial y}\right)_{n+1}\right] \delta y_{n+1} = \left[1 + \frac{1}{2}\Delta t \left(\frac{\partial f}{\partial y}\right)_{n}\right] \delta y_n$$

$$\frac{\delta y_{n+1}}{\delta y_n} = \frac{1 + \frac{1}{2}\Delta t \left(\frac{\partial f}{\partial y}\right)_n}{1 - \frac{1}{2}\Delta t \left(\frac{\partial f}{\partial y}\right)_{n+1}}, \quad \left|\frac{\delta y_{n+1}}{\delta y_n}\right| \leq 1$$

• Ordinary Differential Equation (Initial Value Problem)

• Stability of Picard Method (Implicit Method)

First Order ODE

$$y_{n+1} = y_n + \Delta t \frac{1}{2}(f_n + f_{n+1})$$

$$\left| \frac{1 + \frac{1}{2}\Delta t \left(\frac{\partial f}{\partial y}\right)_n}{1 - \frac{1}{2}\Delta t \left(\frac{\partial f}{\partial y}\right)_{n+1}} \right| \leq 1$$

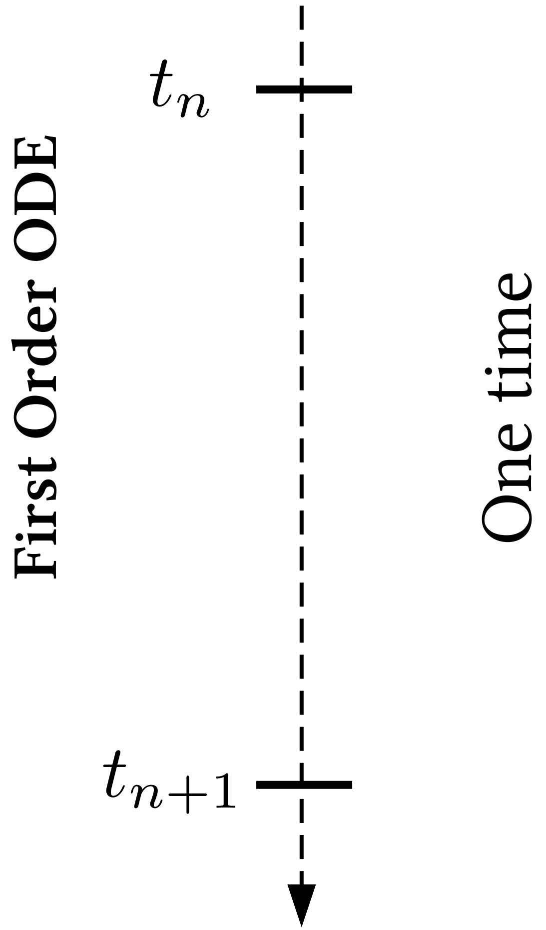
Stability Condition

Example: $y' = -ky, \quad y(0) = y_0, \quad k > 0$

$$\left| \frac{1 - \frac{1}{2}k\Delta t}{1 + \frac{1}{2}k\Delta t} \right| \leq 1$$

• **Ordinary Differential Equation** (Initial Value Problem)

• Predictor–corrector methods (Implicit Method)

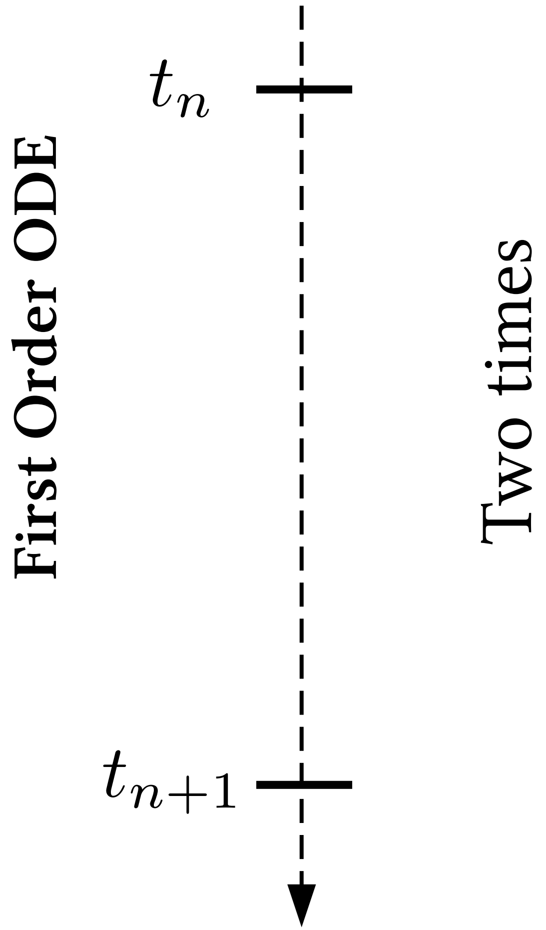


$$\tilde{y}_{n+1} = y_n + f(y_n, t_n)\Delta t$$

$$y_{n+1} = y_n + \frac{1}{2}[f(y_n, t_n) + f(\tilde{y}_{n+1}, t_{n+1})]\Delta t$$

• **Ordinary Differential Equation** (Initial Value Problem)

• Predictor–corrector methods (Implicit Method)



$$\tilde{y}_{n+1} = y_n + f(y_n, t_n)\Delta t$$

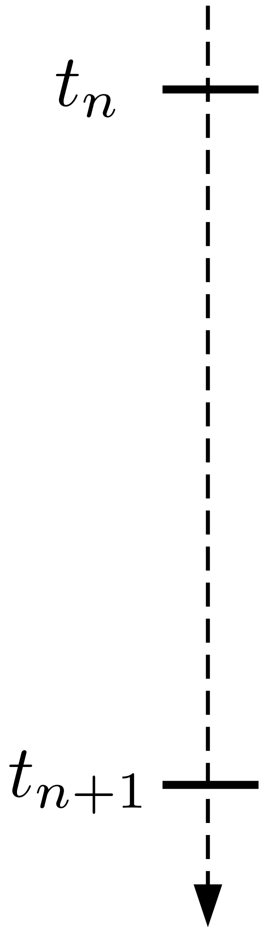
$$\hat{y}_{n+1} = y_n + \frac{1}{2}[f(y_n, t_n) + f(\tilde{y}_{n+1}, t_{n+1})]\Delta t$$

$$y_{n+1} = y_n + \frac{1}{2}[f(y_n, t_n) + f(\hat{y}_{n+1}, t_{n+1}]\Delta t$$

• **Ordinary Differential Equation** (Initial Value Problem)

• Predictor–corrector methods (Implicit Method)

First Order ODE



Three times

$$\tilde{y}_{n+1} = y_n + f(y_n, t_n)\Delta t$$

$$\hat{y}_{n+1} = y_n + \frac{1}{2}[f(y_n, t_n) + f(\tilde{y}_{n+1}, t_{n+1})]\Delta t$$

$$\bar{y}_{n+1} = y_n + \frac{1}{2}[f(y_n, t_n) + f(\hat{y}_{n+1}, t_{n+1})]\Delta t$$

$$y_{n+1} = y_n + \frac{1}{2}[f(y_n, t_n) + f(\bar{y}_{n+1}, t_{n+1})]\Delta t$$

• **Ordinary Differential Equation** (Initial Value Problem)

- Leap-Frog Method (Explicit Method)

First Order ODE

$$\dot{y} = f(y,t), \quad y(t=t_0) = y_0$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(y,t)$$

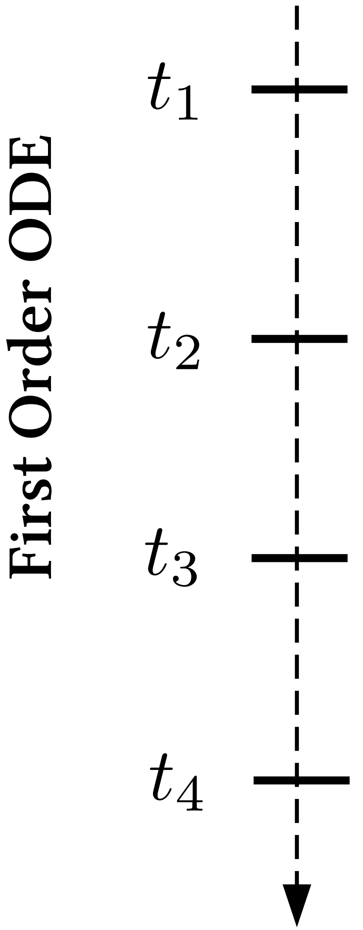
Central Difference Formula: $$\left(\frac{\mathrm{d}y}{\mathrm{d}t}\right)_n = \frac{y_{n+1} - y_{n-1}}{2\Delta t} + O(\Delta t^2)$$

$$\frac{y_{n+1} - y_{n-1}}{2\Delta t} + O(\Delta t^2) = f(y_n, t_n)$$

$$\boxed{y_{n+1} = y_{n-1} + 2\Delta t f(y_n, t_n)}, \text{ need to } y_n \text{ and } y_{n-1}$$

• Ordinary Differential Equation (Initial Value Problem)

• Leap-Frog Method (Explicit Method)



$$y_1 = y_0 + \Delta t f(y_0, t_0)$$ Euler Method

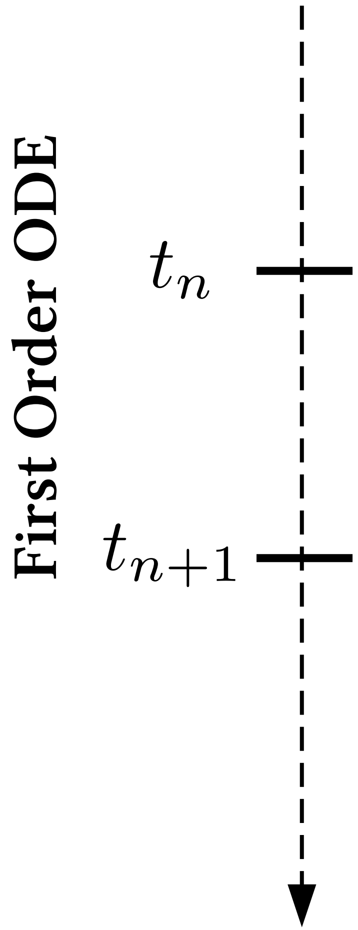
$$y_2 = y_0 + 2\Delta t f(y_1, t_1)$$ Leap-Frog Method

$$y_3 = y_1 + 2\Delta t f(y_2, t_2)$$ Leap-Frog Method

$$y_4 = y_2 + 2\Delta t f(y_3, t_3)$$ Leap-Frog Method

• Ordinary Differential Equation (Initial Value Problem)

• Leap-Frog Method (Explicit Method)



$$y_n = y_{n-2} + 2\Delta t f(y_{n-1}, t_{n-1})$$

Leap-Frog Method

$$y_{n+1} = y_{n-1} + 2\Delta t f(y_n, t_n)$$

Leap-Frog Method

• Ordinary Differential Equation (Initial Value Problem)

• Stability of Leap-Frog Method (Explicit Method)

First Order ODE

$$y_{n+1} = y_{n-1} + 2\Delta t f(y_n, t_n)$$

$$y_{n+1} \to y_{n+1} + \delta y_{n+1}$$

$$y_n \to y_n + \delta y_n$$

$$y_{n-1} \to y_{n-1} + \delta y_{n-1}$$

$$\underbrace{y_{n+1} + \delta y_{n+1}}_{y_{n+1}} = \underbrace{y_{n-1} + \delta y_{n-1}}_{y_{n-1}} + 2\Delta t f(\underbrace{y_n + \delta y_n}_{y_n}, t_n)$$

• Ordinary Differential Equation (Initial Value Problem)

• Stability of Leap-Frog Method (Explicit Method)

First Order ODE

$$y_{n+1} = y_{n-1} + 2\Delta t f(y_n, t_n)$$

$$y_{n+1} + \delta y_{n+1} = y_{n-1} + \delta y_{n-1} + 2\Delta t f(y_n + \delta y_n, t_n)$$

$$f(y_n + \delta y_n, t_n) = f(y_n, t_n) + \left(\frac{\partial f}{\partial y}\right)_n \delta y_n + O(\delta y_n^2)$$

$$y_{n+1} + \delta y_{n+1} = y_{n-1} + \delta y_{n-1} + 2\Delta t f(y_n, t_n) + 2\Delta t \left(\frac{\partial f}{\partial y}\right)_n \delta y_n$$

$$y_{n+1} + \delta y_{n+1} = \boxed{y_{n-1} + 2\Delta t f(y_n, t_n)} + \delta y_{n-1} + 2\Delta t \left(\frac{\partial f}{\partial y}\right)_n \delta y_n$$

• **Ordinary Differential Equation** (Initial Value Problem)

• Stability of Leap-Frog Method (Explicit Method)

$$y_{n+1} = y_{n-1} + 2\Delta t f(y_n, t_n)$$

First Order ODE

$$y_{n+1} + \delta y_{n+1} = \boxed{y_{n-1} + 2\Delta t f(y_n, t_n)} + \delta y_{n-1} + 2\Delta t \left(\frac{\partial f}{\partial y}\right)_n \delta y_n$$

$$\cancel{y_{n+1}} + \delta y_{n+1} = \cancel{y_{n+1}} + \delta y_{n-1} + 2\Delta t \left(\frac{\partial f}{\partial y}\right)_n \delta y_n$$

$$\delta y_{n+1} = \delta y_{n-1} + 2\Delta t \left(\frac{\partial f}{\partial y}\right)_n \delta y_n$$

let's set $\delta y_{n+1} = g\delta y_n, \quad \delta y_n = g\delta y_{n-1} \Rightarrow \delta y_{n+1} = g^2 \delta y_{n-1}$

• **Ordinary Differential Equation** (Initial Value Problem)

- Stability of Leap-Frog Method (Explicit Method)

First Order ODE

$$y_{n+1} = y_{n-1} + 2\Delta t f(y_n, t_n)$$

$$\delta y_{n+1} = \delta y_{n-1} + 2\Delta t \left(\frac{\partial f}{\partial y}\right)_n \delta y_n$$

$$\delta y_{n+1} = g\delta y_n, \quad \delta y_n = g\delta y_{n-1} \Rightarrow \delta y_{n+1} = g^2 \delta y_{n-1}$$

$$g^2 \delta y_{n-1} = \delta y_{n-1} + 2\Delta t \left(\frac{\partial f}{\partial y}\right)_n g\delta y_{n-1}$$

$$g^2 - 2\Delta t \left(\frac{\partial f}{\partial y}\right)_n g - 1 = 0$$

• Ordinary Differential Equation (Initial Value Problem)

• Stability of Leap-Frog Method (Explicit Method)

First Order ODE

$$y_{n+1} = y_{n-1} + 2\Delta t f(y_n, t_n)$$

$$g^2 - 2\Delta t\left(\frac{\partial f}{\partial y}\right) g - 1 = 0$$

$$g_{\pm} = \Delta t\left(\frac{\partial f}{\partial y}\right) \pm \sqrt{\Delta t^2\left(\frac{\partial f}{\partial y}\right)^2 + 1}$$

$$g_+ g_- = -1 \Rightarrow g_+ = -\frac{1}{g_-} \Rightarrow |g_+| = \frac{1}{|g_-|}$$

One of the solutions will have a magnitude greater than 1, making the leap-frog method unstable.

• Ordinary Differential Equation (Initial Value Problem)

• Stability of Leap-Frog Method (Explicit Method)

First Order ODE

$$y_{n+1} = y_{n-1} + 2\Delta t f(y_n, t_n)$$

$$g_{\pm} = \Delta t \left(\frac{\partial f}{\partial y}\right) \pm \sqrt{\Delta t^2 \left(\frac{\partial f}{\partial y}\right)^2 + 1}$$

But, if $\partial f / \partial y$ **is purely imaginary, i.e.** $\frac{\partial f}{\partial y} = ik$

$$g_{\pm} = ik\Delta t \pm \sqrt{1 - k^2 \Delta t^2}$$

$$1 - k^2 \Delta t^2 \geq 0 \Rightarrow \Delta t \leq \frac{1}{|k|}$$