

Computational Physics



Lecture-24

M. Reza Mozaffari

Physics Group, University of Qom

Contents

- Basis Concepts
- Numerical Differentiation
- Numerical Integration
- Numerical Finding Root
- Classical Scattering
- Solving Linear Systems
- Transmission of Rectangular Barriers
- Approximation of a Function
- Ordinary Differential Equation (Initial Value Problem)

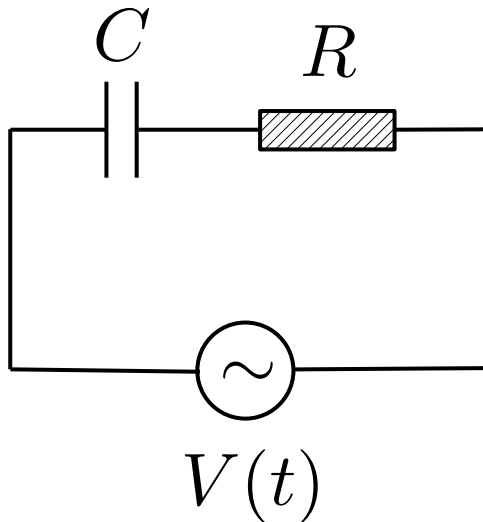
Ordinary Differential Equation

- Initial Value Problem

First Order ODE

$$\frac{q}{C} + R \frac{dq}{dt} = V(t)$$

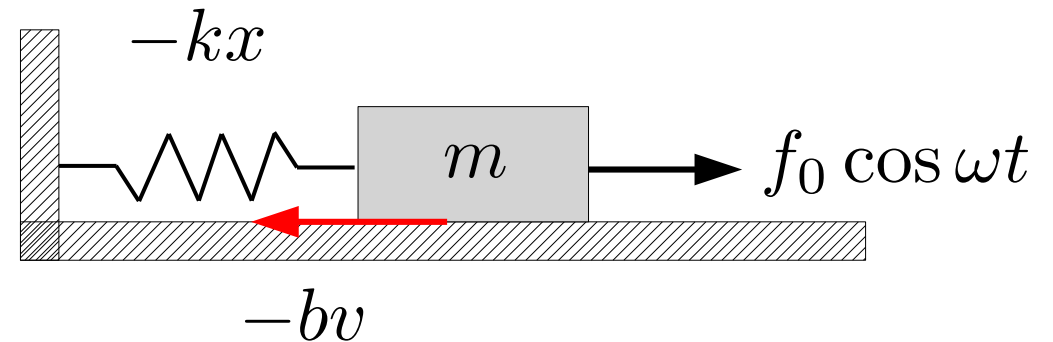
$$q(t = t_0) = q_0$$



Second Order ODE

$$m \frac{d^2 x}{dt^2} = -kx - bv + f_0 \cos \omega t$$
$$x(t = t_0) = x_0, \quad v(t = t_0) = v_0$$

$$v = \frac{dx}{dt}$$



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

$$\ddot{y} = f(\dot{y}, y, t), \quad \dot{y}(t = t_0) = \dot{y}_0, \quad y(t = t_0) = y_0$$

$$\dot{y} = v$$

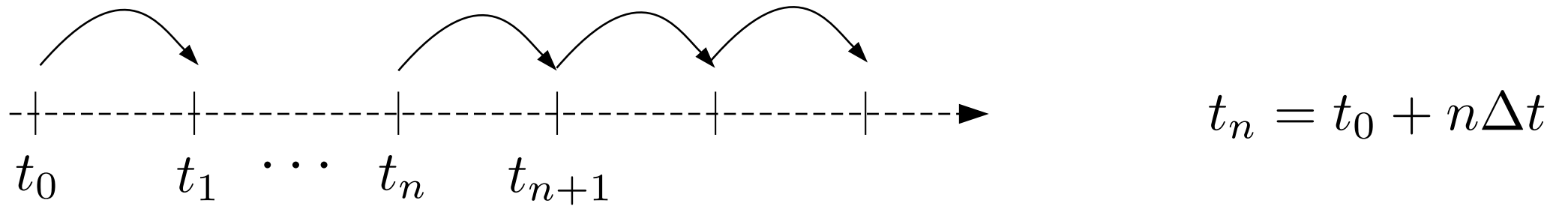
$$\begin{aligned} \frac{dv}{dt} &= f(v, y, t), & \frac{dy}{dt} &= v \\ v(t = t_0) &= v_0, & y(t = t_0) &= y_0 \end{aligned}$$

$$\begin{cases} \frac{dv}{dt} = f(v, y, t) \\ \frac{dy}{dt} = g(v, y, t) = v \end{cases} \quad \begin{cases} v(t = t_0) = v_0 \\ y(t = t_0) = y_0 \end{cases}$$

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

- Euler Method (Explicit Method)

$$\frac{dv}{dt} = f(v, y, t), \quad \frac{dy}{dt} = g(v, y, t) = v, \quad v(t = t_0) = v_0, \quad y(t = t_0) = y_0$$



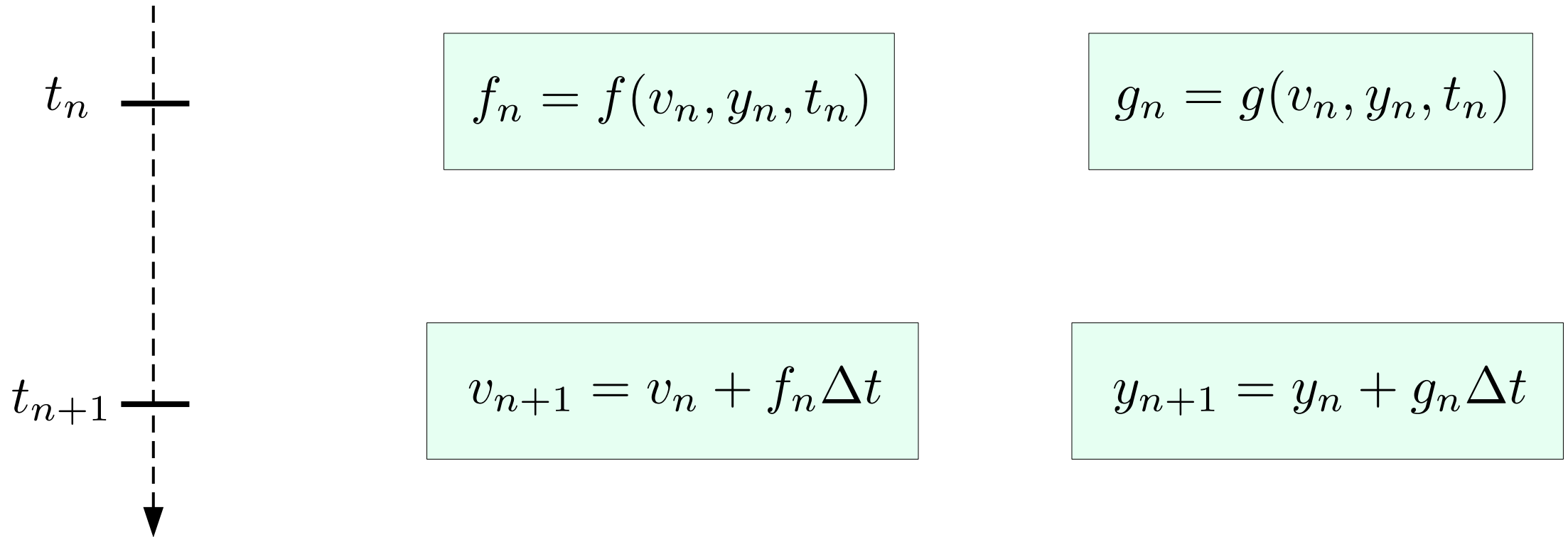
$$\begin{cases} v_{n+1} = v_n + f_n \Delta t + O(\Delta t^2), & f_n = f(v_n, y_n, t_n) \\ y_{n+1} = y_n + g_n \Delta t + O(\Delta t^2), & g_n = g(v_n, y_n, t_n) \end{cases}$$

• Ordinary Differential Equation (Initial Value Problem)

• Euler Method (Explicit Method)

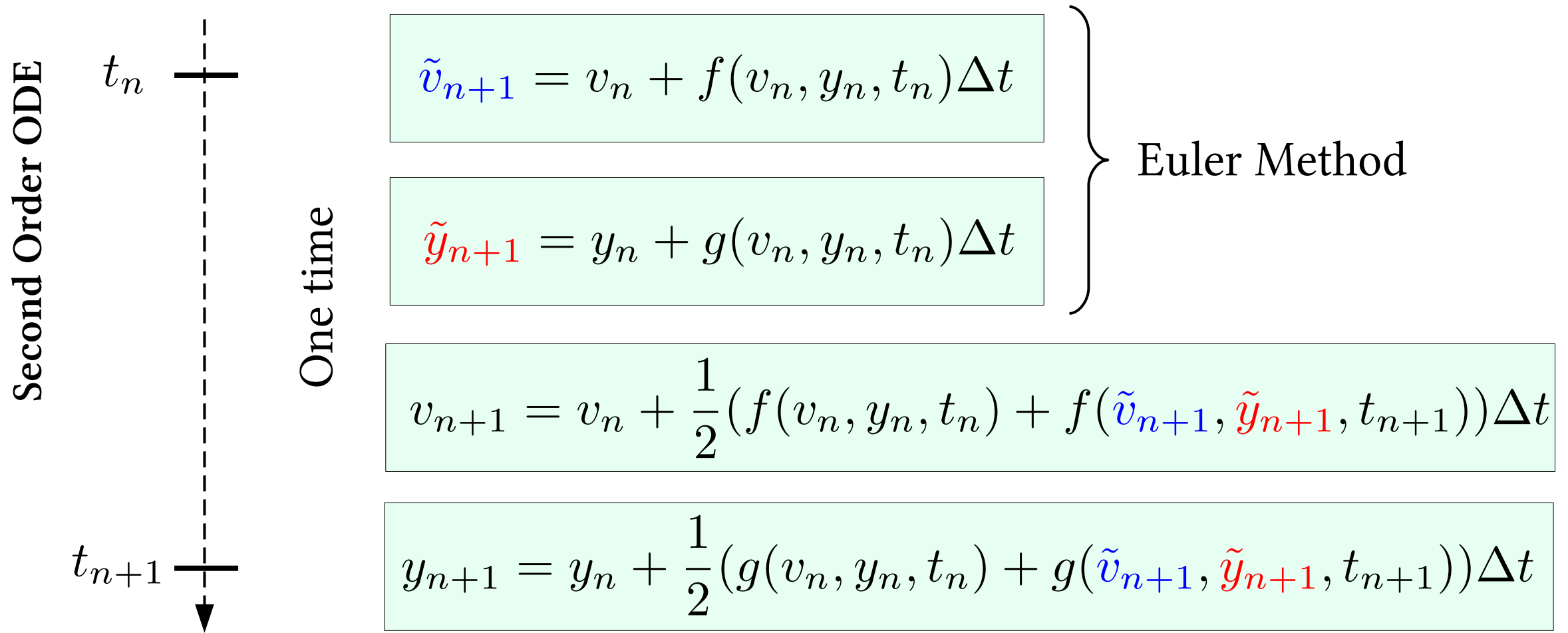
$$\frac{dv}{dt} = f(v, y, t), \quad \frac{dy}{dt} = g(v, y, t) = v, \quad v(t = t_0) = v_0, \quad y(t = t_0) = y_0$$

Second Order ODE



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

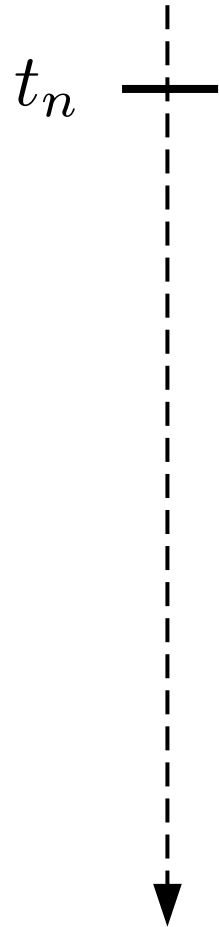
- Picard Method (Implicit Methods)



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

- Predictor–corrector methods (Implicit Methods)

Second Order ODE



Two times

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

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

} Euler Method

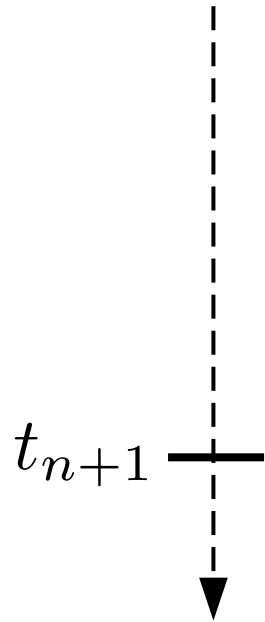
$$\hat{v}_{n+1} = v_n + \frac{1}{2} (f(v_n, y_n, t_n) + f(\tilde{v}_{n+1}, \tilde{y}_{n+1}, t_{n+1})) \Delta t$$

$$\hat{y}_{n+1} = y_n + \frac{1}{2} (g(v_n, y_n, t_n) + g(\tilde{v}_{n+1}, \tilde{y}_{n+1}, t_{n+1})) \Delta t$$

- **Ordinary Differential Equation** (Initial Value Problem)
- Predictor–corrector methods (Implicit Methods)

Second Order ODE

Two times



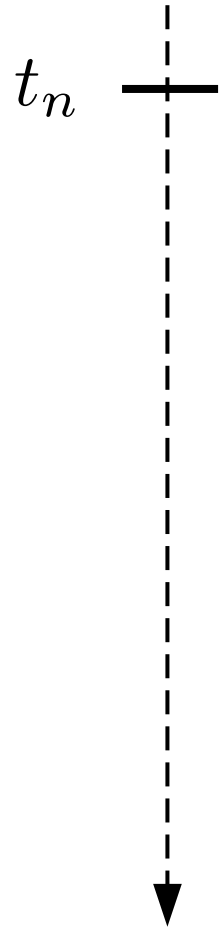
$$v_{n+1} = v_n + \frac{1}{2} (f(v_n, y_n, t_n) + f(\hat{v}_{n+1}, \hat{y}_{n+1}, t_{n+1})) \Delta t$$

$$y_{n+1} = y_n + \frac{1}{2} (g(v_n, y_n, t_n) + g(\hat{v}_{n+1}, \hat{y}_{n+1}, t_{n+1})) \Delta t$$

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

- Predictor–corrector methods (Implicit Methods)

Second Order ODE



Three times

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

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

} Euler Method

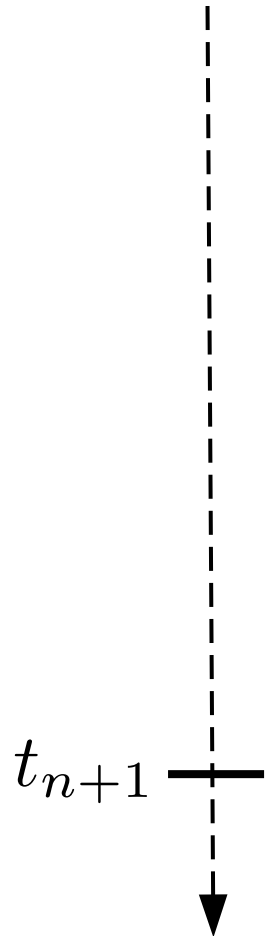
$$\hat{v}_{n+1} = v_n + \frac{1}{2} (f(v_n, y_n, t_n) + f(\tilde{v}_{n+1}, \tilde{y}_{n+1}, t_{n+1})) \Delta t$$

$$\hat{y}_{n+1} = y_n + \frac{1}{2} (g(v_n, y_n, t_n) + g(\tilde{v}_{n+1}, \tilde{y}_{n+1}, t_{n+1})) \Delta t$$

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

- Predictor–corrector methods (Implicit Methods)

Second Order ODE



Three times

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

$$\bar{y}_{n+1} = y_n + \frac{1}{2} (g(v_n, y_n, t_n) + g(\hat{v}_{n+1}, \hat{y}_{n+1}, t_{n+1})) \Delta t$$

$$v_{n+1} = v_n + \frac{1}{2} (f(v_n, y_n, t_n) + f(\bar{v}_{n+1}, \bar{y}_{n+1}, t_{n+1})) \Delta t$$

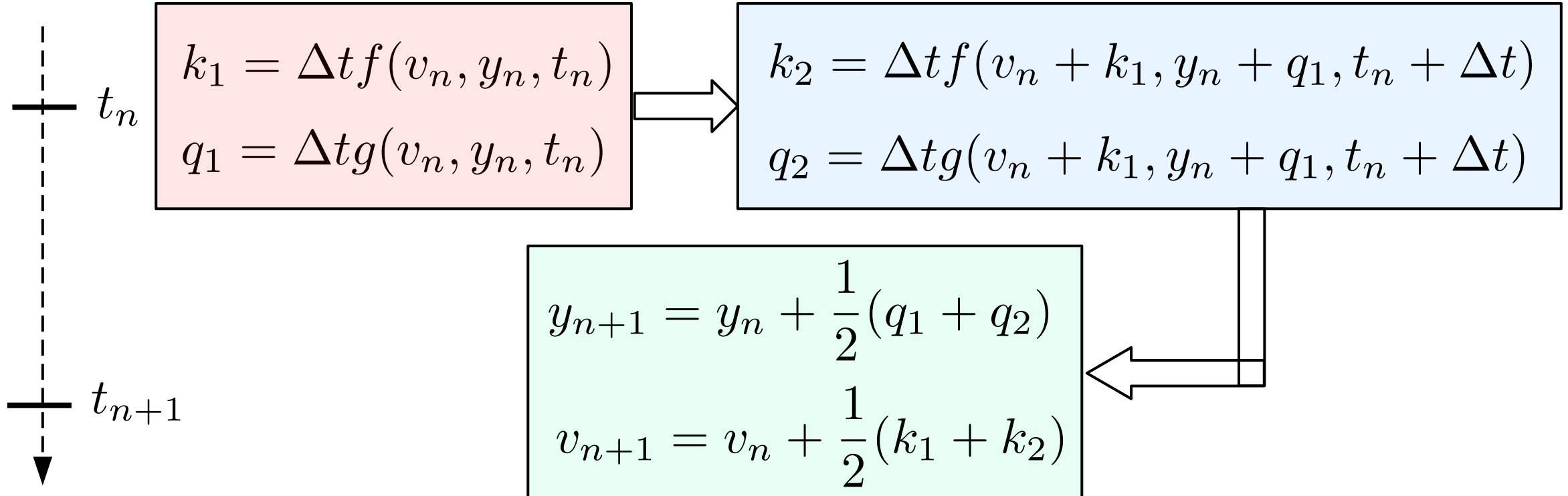
$$y_{n+1} = y_n + \frac{1}{2} (g(v_n, y_n, t_n) + g(\bar{v}_{n+1}, \bar{y}_{n+1}, t_{n+1})) \Delta t$$

• Ordinary Differential Equation (Initial Value Problem)

- Runge-Kutta Methods (Implicit Methods)

$$\frac{dv}{dt} = f(v, y, t), \quad \frac{dy}{dt} = g(v, y, t) = v, \quad v(t = t_0) = v_0, \quad y(t = t_0) = y_0$$

Second Order ODE

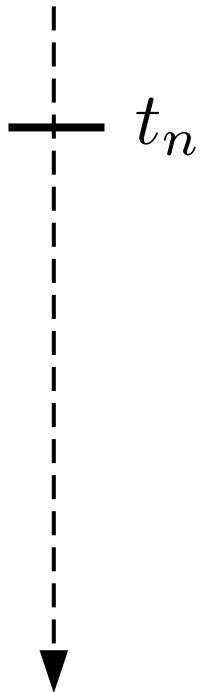


• Ordinary Differential Equation (Initial Value Problem)

- Runge-Kutta Methods (Implicit Methods)

$$\frac{dv}{dt} = f(v, y, t), \quad \frac{dy}{dt} = g(v, y, t) = v, \quad v(t = t_0) = v_0, \quad y(t = t_0) = y_0$$

Second Order ODE



$$k_1 = \Delta t f(v_n, y_n, t_n)$$
$$q_1 = \Delta t g(v_n, y_n, t_n)$$



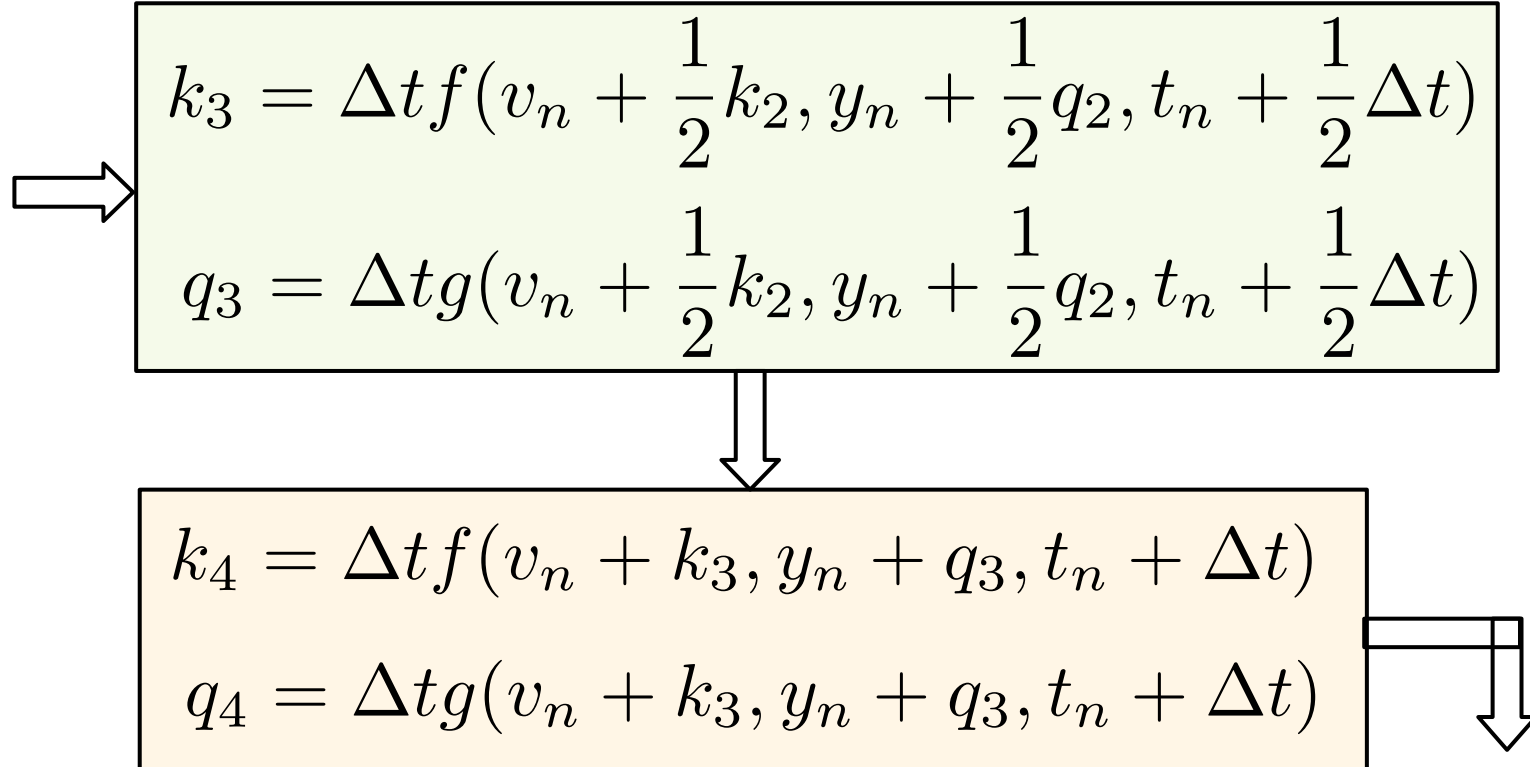
$$k_2 = \Delta t f\left(v_n + \frac{1}{2}k_1, y_n + \frac{1}{2}q_1, t_n + \frac{1}{2}\Delta t\right)$$
$$q_2 = \Delta t g\left(v_n + \frac{1}{2}k_1, y_n + \frac{1}{2}q_1, t_n + \frac{1}{2}\Delta t\right)$$

• Ordinary Differential Equation (Initial Value Problem)

- Runge-Kutta Methods (Implicit Methods)

$$\frac{dv}{dt} = f(v, y, t), \quad \frac{dy}{dt} = g(v, y, t) = v, \quad v(t = t_0) = v_0, \quad y(t = t_0) = y_0$$

Second Order ODE

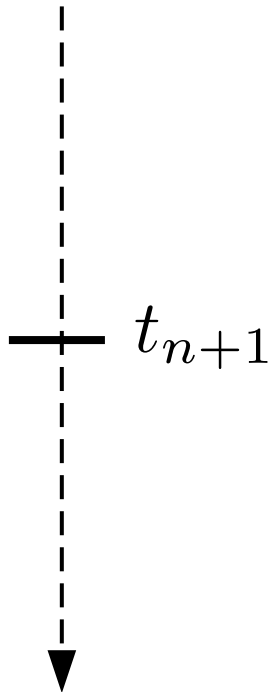


• Ordinary Differential Equation (Initial Value Problem)

- Runge-Kutta Methods (Implicit Methods)

$$\frac{dv}{dt} = f(v, y, t), \quad \frac{dy}{dt} = g(v, y, t) = v, \quad v(t = t_0) = v_0, \quad y(t = t_0) = y_0$$

Second Order ODE



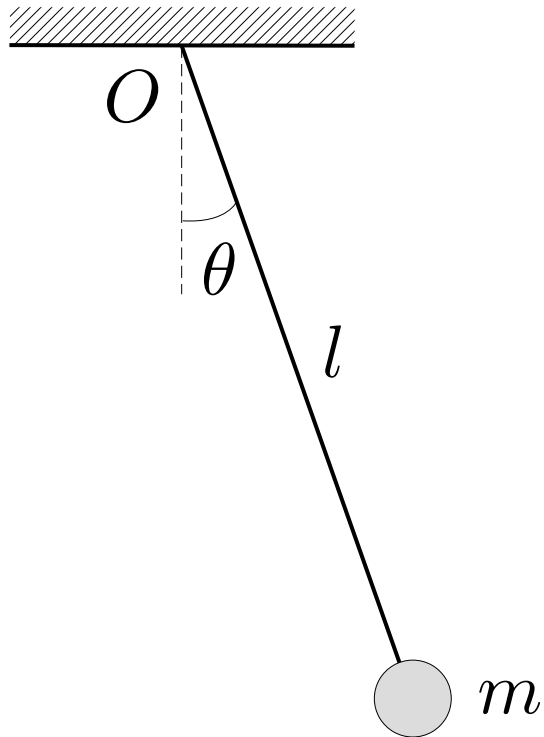
$$y_{n+1} = y_n + \frac{1}{6}(q_1 + 2q_2 + 2q_3 + q_4)$$

$$v_{n+1} = v_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

• Ordinary Differential Equation (Initial Value Problem)

• Driven Pendulum

$$\tau = I_O \ddot{\theta}$$



$$ml^2 \ddot{\theta} = -mgl \sin \theta - b \dot{\theta} + \tau_0 \cos \omega_d t$$

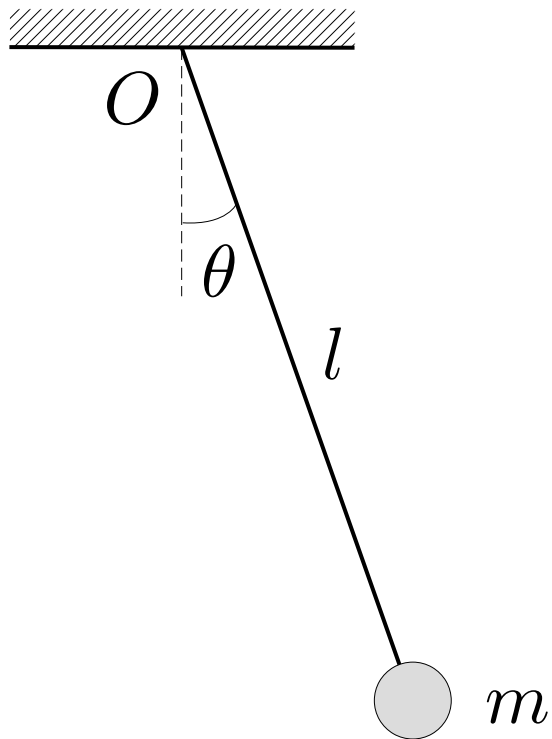
$$\frac{ml^2}{ml^2} \ddot{\theta} = -\frac{mgl}{ml^2} \sin \theta - \frac{b}{ml^2} \dot{\theta} + \frac{\tau_0}{ml^2} \cos \omega_d t$$

$$\ddot{\theta} = -\frac{g}{l} \sin \theta - \frac{b}{ml^2} \dot{\theta} + \frac{\tau_0}{ml^2} \cos \omega_d t$$

$$\omega_0 = \sqrt{\frac{g}{l}}$$

• Ordinary Differential Equation (Initial Value Problem)

• Driven Pendulum



$$\ddot{\theta} = -\omega_0^2 \sin \theta - \frac{b}{ml^2} \dot{\theta} + \frac{\tau_0}{ml^2} \cos \omega_d t$$

$$\begin{cases} \dot{\omega} = f(\omega, \theta, t) = -\omega_0^2 \sin \theta - \frac{b}{ml^2} \omega + \frac{\tau_0}{ml^2} \cos \omega_d t \\ \dot{\theta} = g(\omega, \theta, t) = \omega \end{cases}$$

ω_0	$\frac{b}{ml^2}$	ω_d
1	1/2	2/3

$$\begin{cases} \frac{\tau_0}{ml^2} = 0.9 \\ \frac{\tau_0}{ml^2} = 1.15 \end{cases}$$

• Ordinary Differential Equation (Initial Value Problem)

• Driven Pendulum

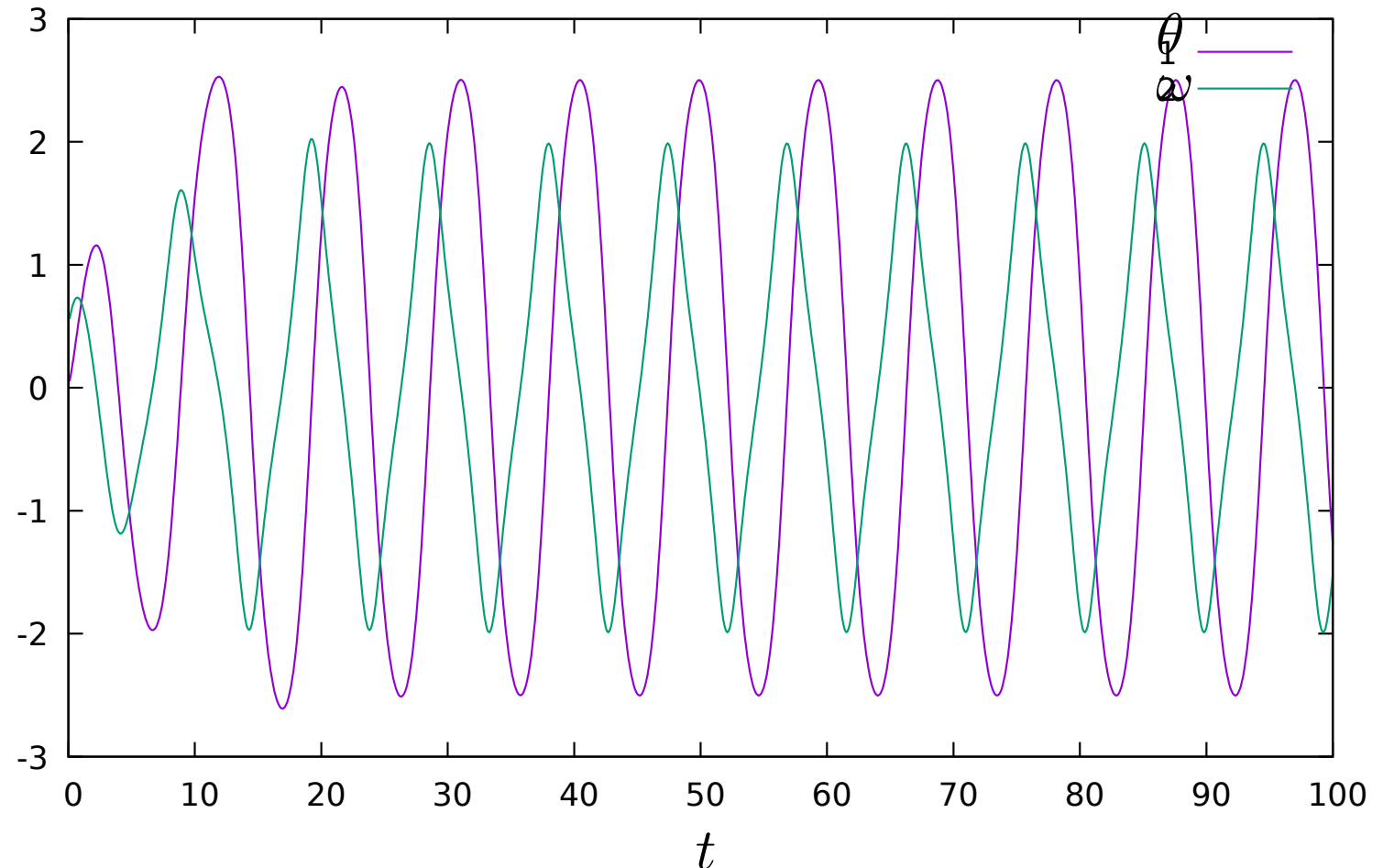
ω_0	$\frac{b}{ml^2}$	ω_d
1	1/2	2/3

$$\frac{\tau_0}{ml^2} = 0.9$$

$$\theta(t = 0) = 0$$

$$\omega(t = 0) = 0.5$$

$$\Delta t = 0.1$$



• Ordinary Differential Equation (Initial Value Problem)

• Driven Pendulum

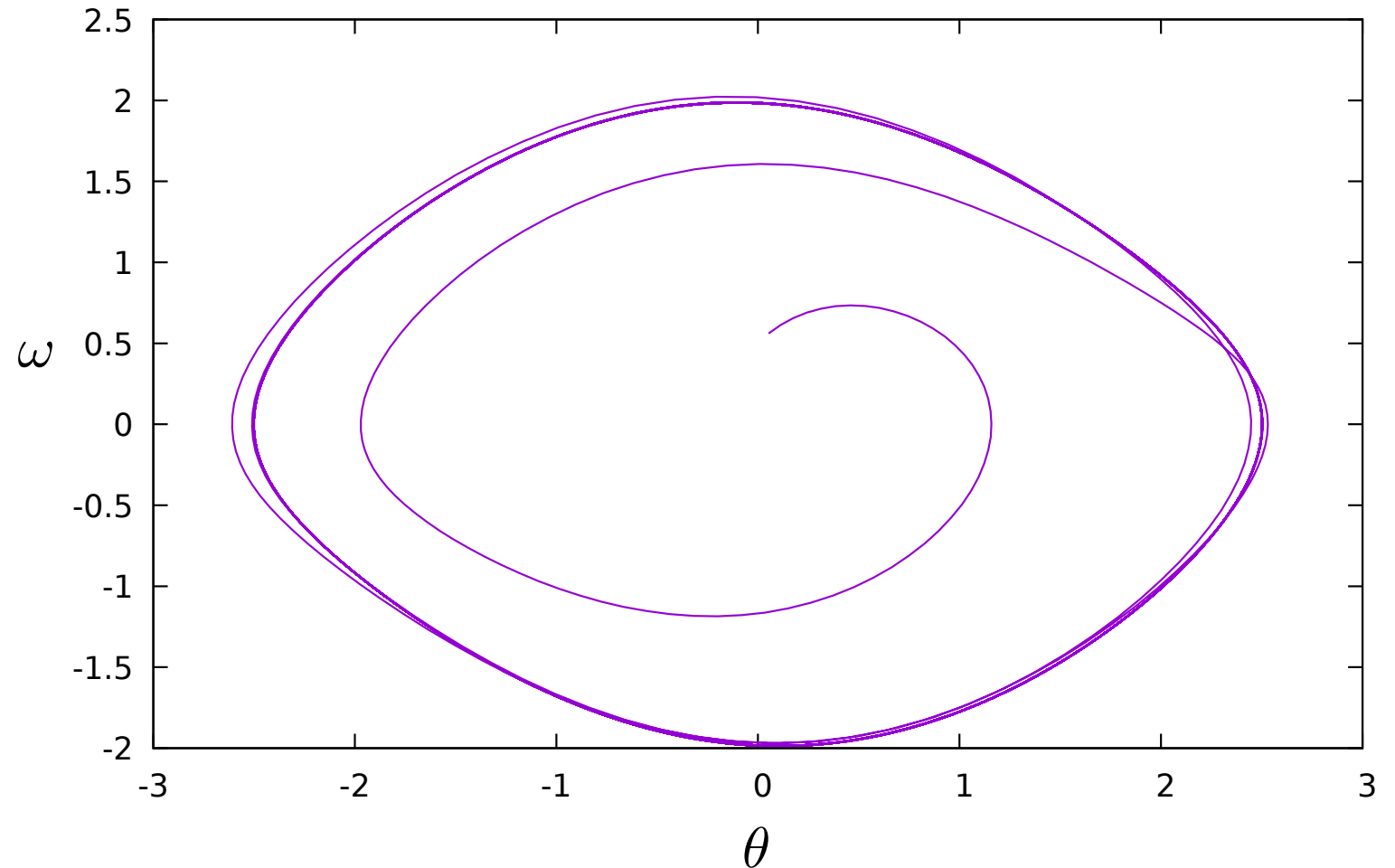
ω_0	$\frac{b}{ml^2}$	ω_d
1	1/2	2/3

$$\frac{\tau_0}{ml^2} = 0.9$$

$$\theta(t = 0) = 0$$

$$\omega(t = 0) = 0.5$$

$$\Delta t = 0.1$$



• Ordinary Differential Equation (Initial Value Problem)

• Driven Pendulum

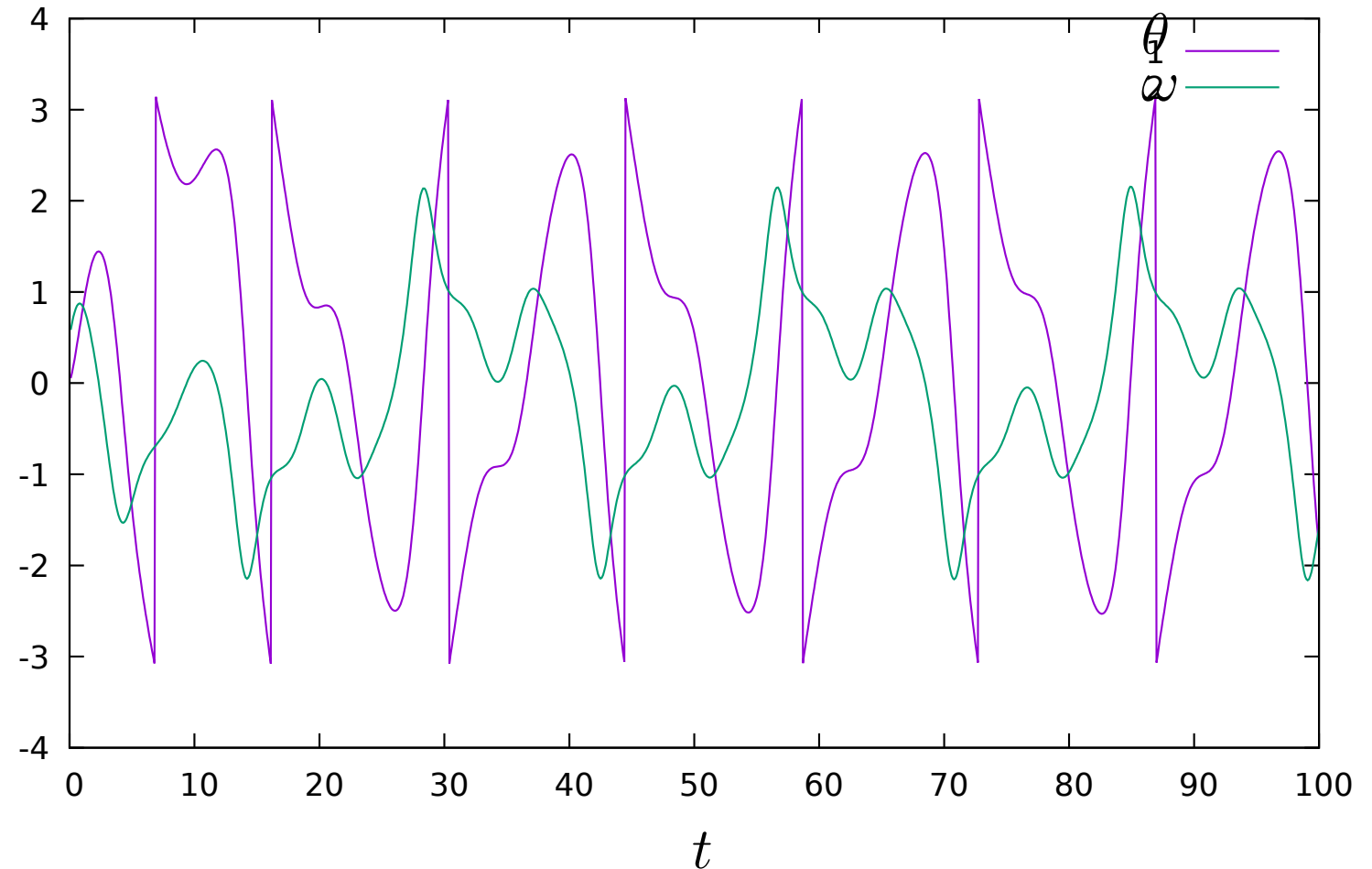
ω_0	$\frac{b}{ml^2}$	ω_d
1	1/2	2/3

$$\frac{\tau_0}{ml^2} = 1.15$$

$$\theta(t = 0) = 0$$

$$\omega(t = 0) = 0.5$$

$$\Delta t = 0.1$$



• Ordinary Differential Equation (Initial Value Problem)

• Driven Pendulum

ω_0	$\frac{b}{ml^2}$	ω_d
1	1/2	2/3

$$\frac{\tau_0}{ml^2} = 1.15$$

$$\Delta t = 0.1$$

$$\theta(t = 0) = 0$$

$$\omega(t = 0) = 0.5$$

