CosmoLattice

— School 2025 —

CosmoLattice School 2025 (IBS, Korea), Sept 22-26

Lecture 3: Evolution algorithms for ordinary differential equations

Part II: Runge-Kutta methods

Antonino Salvino Midiri
(University of Geneva, Switzerland)

Outline of Part II

- Runge-Kutta methods
- Symplectic vs Runge-Kutta: Hamiltonian systems
- Symplectic vs Runge-Kutta: dissipative systems

Runge-Kutta methods

We want to solve $\ddot{x}(t) \;=\; \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0),\;\; \dot{x}(t_0)$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \underline{\dot{x}(t)}]$ *NON-CONSERVATIVE SYSTEM*

Suppose we know $x(t_0),\ \dot{x}(t_0)$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \underline{\dot{x}(t)}]$ *NON-CONSERVATIVE SYSTEM*

Suppose we know $x(t_0), \ \dot{x}(t_0)$

First order Runge-Kutta (*Euler method*)

$$x(t_0 + \Delta t) = x(t_0) + \Delta t \ \dot{x}(t_0)$$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \underline{\dot{x}(t)}]$ *NON-CONSERVATIVE SYSTEM*

Suppose we know $x(t_0), \; \dot{x}(t_0)$

First order Runge-Kutta (*Euler method*)

$$x(t_0 + \Delta t) = x(t_0) + \Delta t \; \dot{x}(t_0)$$

$$\dot{x}(t_0 + \Delta t) = \dot{x}(t_0) + \Delta t \; \mathcal{F}[x(t_0), \dot{x}(t_0)]$$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \underline{\dot{x}(t)}]$ NON-CONSERVATIVE SYSTEM

Suppose we know $x(t_0), \; \dot{x}(t_0)$

First order Runge-Kutta (*Euler method*)

$$x(t_0 + \Delta t) = x(t_0) + \Delta t \; \dot{x}(t_0)$$

$$\dot{x}(t_0 + \Delta t) = \dot{x}(t_0) + \Delta t \; \mathcal{F}[x(t_0), \dot{x}(t_0)]$$

→ Equivalent to Taylor-expansion up to order $(\Delta t)^1$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0),\ \dot{x}(t_0)$

Second order Runge-Kutta (*Modified Euler*)

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0), \ \dot{x}(t_0)$

Second order Runge-Kutta (*Modified Euler*)

Intermediate step

$$x(t_1) = x(t_0) + \Delta t \, \dot{x}(t_0)$$

$$\dot{x}(t_1) = \dot{x}(t_0) + \Delta t \, \mathcal{F}[x(t_0), \dot{x}(t_0)]$$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0), \ \dot{x}(t_0)$

Intermediate step

$$x(t_1) = x(t_0) + \Delta t \, \dot{x}(t_0)$$

$$\dot{x}(t_1) = \dot{x}(t_0) + \Delta t \, \mathcal{F}[x(t_0), \dot{x}(t_0)]$$

Second order Runge-Kutta (*Modified Euler*)

$$x(t_0 + \Delta t) = x(t_0) + \Delta t \, \frac{\dot{x}(t_0) + \dot{x}(t_1)}{2}$$

$$\dot{x}(t_0 + \Delta t) = \dot{x}(t_0) + \Delta t \, \frac{\mathcal{F}[x(t_0), \dot{x}(t_0)] + \mathcal{F}[x(t_1), \dot{x}(t_1)]}{2}$$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0),\ \dot{x}(t_0)$

Intermediate step

$$x(t_1) = x(t_0) + \Delta t\, \dot{x}(t_0)$$

$$\dot{x}(t_1) = \dot{x}(t_0) + \Delta t\, \mathcal{F}[x(t_0), \dot{x}(t_0)]$$

Second order Runge-Kutta (*Modified Euler*)

$$x(t_0 + \Delta t) = x(t_0) + \Delta t \frac{\dot{x}(t_0) + \dot{x}(t_1)}{2}$$

$$\dot{x}(t_0 + \Delta t) = \dot{x}(t_0) + \Delta t \frac{\mathcal{F}[x(t_0), \dot{x}(t_0)] + \mathcal{F}[x(t_1), \dot{x}(t_1)]}{2}$$

→ Equivalent to Taylor-expansion up to order $(\Delta t)^2$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0), \ \dot{x}(t_0)$

Intermediate step

$$x(t_1) = x(t_0) + \Delta t \, \dot{x}(t_0)$$

$$\dot{x}(t_1) = \dot{x}(t_0) + \Delta t \, \mathcal{F}[x(t_0), \dot{x}(t_0)]$$

Second order Runge-Kutta (*Modified Euler*)

$$x(t_0 + \Delta t) = x(t_0) + \Delta t \, \frac{\dot{x}(t_0) + \dot{x}(t_1)}{2}$$

≡LHS ≡ RHS

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0), \; \dot{x}(t_0)$

Intermediate step

$$x(t_1) = x(t_0) + \Delta t\, \dot{x}(t_0)$$

$$\dot{x}(t_1) = \dot{x}(t_0) + \Delta t\, \mathcal{F}[x(t_0), \dot{x}(t_0)]$$

Second order Runge-Kutta (*Modified Euler*)

$$x(t_0 + \Delta t) = x(t_0) + \Delta t \frac{\dot{x}(t_0) + \dot{x}(t_1)}{2}$$

$\equiv$LHS $\equiv$ RHS

$$\text{LHS} \simeq x(t_0) + \Delta t\, \dot{x}(t_0) + \frac{1}{2}\Delta t^2\, \ddot{x}(t_0) + \mathcal{O}(\Delta t^3) = x(t_0) + \Delta t\, \dot{x}(t_0) + \frac{1}{2}\Delta t^2 \mathcal{F}[x(t_0), \dot{x}(t_0)] + \mathcal{O}(\Delta t^3)$$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0), \ \dot{x}(t_0)$

Intermediate step

$$x(t_1) = x(t_0) + \Delta t \, \dot{x}(t_0)$$

$$\dot{x}(t_1) = \dot{x}(t_0) + \Delta t \, \mathcal{F}[x(t_0), \dot{x}(t_0)]$$

Second order Runge-Kutta (*Modified Euler*)

$$x(t_0 + \Delta t) = x(t_0) + \Delta t \, \frac{\dot{x}(t_0) + \dot{x}(t_1)}{2}$$

$\equiv$LHS $\equiv$ RHS

$$\text{LHS} \simeq x(t_0) + \Delta t \, \dot{x}(t_0) + \frac{1}{2}\Delta t^2 \, \ddot{x}(t_0) + \mathcal{O}(\Delta t^3) = x(t_0) + \Delta t \, \dot{x}(t_0) + \frac{1}{2}\Delta t^2 \mathcal{F}[x(t_0), \dot{x}(t_0)] + \mathcal{O}(\Delta t^3)$$

$$\text{RHS} = x(t_0) + \Delta t \frac{\dot{x}(t_0) + \dot{x}(t_0) + \Delta t \, \mathcal{F}[x(t_0), \dot{x}(t_0)]}{2} = x(t_0) + \Delta t \, \dot{x}(t_0) + \frac{1}{2}\Delta t^2 \, \mathcal{F}[x(t_0), \dot{x}(t_0)]$$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0), \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*)

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Intermediate steps

Suppose we know $x(t_0), \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*)

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0), \dot{x}(t_0)$

Intermediate steps

$$x(t_1) = x(t_0) + \Delta t \frac{\dot{x}(t_0)}{3}$$

$$\dot{x}(t_1) = \dot{x}(t_0) + \Delta t \frac{\mathcal{F}[x(t_0), \dot{x}(t_0)]}{3}$$

Third order Runge-Kutta (*Williamson*)

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Intermediate steps

$$x(t_1) = x(t_0) + \Delta t \frac{\dot{x}(t_0)}{3}$$

$$\dot{x}(t_1) = \dot{x}(t_0) + \Delta t \frac{\mathcal{F}[x(t_0), \dot{x}(t_0)]}{3}$$

$$x(t_2) = x(t_0) + \Delta t \frac{-3\,\dot{x}(t_0) + 15\,\dot{x}(t_1)}{16}$$

$$\dot{x}(t_2) = \dot{x}(t_0) + \Delta t \frac{-3\,\mathcal{F}[x(t_0), \dot{x}(t_0)] + 15\,\mathcal{F}[x(t_1), \dot{x}(t_1)]}{16}$$

Suppose we know $x(t_0), \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*)

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0), \dot{x}(t_0)$

Intermediate steps

$$x(t_1) = x(t_0) + \Delta t \frac{\dot{x}(t_0)}{3}$$

$$\dot{x}(t_1) = \dot{x}(t_0) + \Delta t \frac{\mathcal{F}[x(t_0), \dot{x}(t_0)]}{3}$$

$$x(t_2) = x(t_0) + \Delta t \frac{-3\,\dot{x}(t_0) + 15\,\dot{x}(t_1)}{16}$$

$$\dot{x}(t_2) = \dot{x}(t_0) + \Delta t \frac{-3\,\mathcal{F}[x(t_0), \dot{x}(t_0)] + 15\,\mathcal{F}[x(t_1), \dot{x}(t_1)]}{16}$$

Third order Runge-Kutta (*Williamson*)

$$x(t_0 + \Delta t) = x(t_0) + \Delta t \frac{5\,\dot{x}(t_0) + 9\,\dot{x}(t_1) + 16\,\dot{x}(t_2)}{30}$$

$$\dot{x}(t_0 + \Delta t) = \dot{x}(t_0) + \Delta t \frac{5\,\mathcal{F}[x(t_0), \dot{x}(t_0)] + 9\,\mathcal{F}[x(t_1), \dot{x}(t_1)] + 16\,\mathcal{F}[x(t_2), \dot{x}(t_2)]}{30}$$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0), \dot{x}(t_0)$

Intermediate steps

$$x(t_1) = x(t_0) + \Delta t \frac{\dot{x}(t_0)}{3}$$

$$\dot{x}(t_1) = \dot{x}(t_0) + \Delta t \frac{\mathcal{F}[x(t_0), \dot{x}(t_0)]}{3}$$

$$x(t_2) = x(t_0) + \Delta t \frac{-3\,\dot{x}(t_0) + 15\,\dot{x}(t_1)}{16}$$

$$\dot{x}(t_2) = \dot{x}(t_0) + \Delta t \frac{-3\,\mathcal{F}[x(t_0), \dot{x}(t_0)] + 15\,\mathcal{F}[x(t_1), \dot{x}(t_1)]}{16}$$

Third order Runge-Kutta (*Williamson*)

$$x(t_0 + \Delta t) = x(t_0) + \Delta t \frac{5\,\dot{x}(t_0) + 9\,\dot{x}(t_1) + 16\,\dot{x}(t_2)}{30}$$

$$\dot{x}(t_0 + \Delta t) = \dot{x}(t_0) + \Delta t \frac{5\,\mathcal{F}[x(t_0), \dot{x}(t_0)] + 9\,\mathcal{F}[x(t_1), \dot{x}(t_1)] + 16\,\mathcal{F}[x(t_2), \dot{x}(t_2)]}{30}$$

→ Accurate at order $(\Delta t)^3$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0), \dot{x}(t_0)$

Low-storage

↓

Third order Runge-Kutta (*Williamson*)

Intermediate steps

$$x(t_1) = x(t_0) + \Delta t \frac{\dot{x}(t_0)}{3}$$

$$\dot{x}(t_1) = \dot{x}(t_0) + \Delta t \frac{\mathcal{F}[x(t_0), \dot{x}(t_0)]}{3}$$

$$x(t_2) = x(t_0) + \Delta t \frac{-3\, \dot{x}(t_0) + 15\, \dot{x}(t_1)}{16}$$

$$\dot{x}(t_2) = \dot{x}(t_0) + \Delta t \frac{-3\, \mathcal{F}[x(t_0), \dot{x}(t_0)] + 15\, \mathcal{F}[x(t_1), \dot{x}(t_1)]}{16}$$

$$x(t_0 + \Delta t) = x(t_0) + \Delta t \frac{5\, \dot{x}(t_0) + 9\, \dot{x}(t_1) + 16\, \dot{x}(t_2)}{30}$$

$$\dot{x}(t_0 + \Delta t) = \dot{x}(t_0) + \Delta t \frac{5\, \mathcal{F}[x(t_0), \dot{x}(t_0)] + 9\, \mathcal{F}[x(t_1), \dot{x}(t_1)] + 16\, \mathcal{F}[x(t_2), \dot{x}(t_2)]}{30}$$

→ Accurate at order $(\Delta t)^3$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$ Suppose we know $x(t_0),\ \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*) ⟵ Low-storage

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$ Suppose we know $x(t_0),\ \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*) ⟵ Low-storage

We only need to store one additional variable per degree of freedom (x and $\dot{x}$)

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0),\ \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*) ⟵ Low-storage

We only need to store one additional variable per degree of freedom (x and $\dot{x}$)

STEP 0

$$x^{(0)} = x(t_0)$$

$$\dot{x}^{(0)} = \dot{x}(t_0)$$

degrees of freedom

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$ Suppose we know $x(t_0),\ \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*) ⟵ Low-storage

We only need to store one additional variable per degree of freedom (x and $\dot{x}$)

STEP 0

$$x^{(0)} = x(t_0)$$

$$\dot{x}^{(0)} = \dot{x}(t_0)$$

degrees of freedom

$$\delta x^{(0)} = \Delta t\ \dot{x}^{(0)}$$

$$\delta \dot{x}^{(0)} = \Delta t\ \mathcal{F}[x^{(0)}, \dot{x}^{(0)}]$$

extra variables to store

Runge-Kutta methods

We want to solve $\ddot{x}(t) \; = \; \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0), \; \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*) ⟵ Low-storage

We only need to store one additional variable per degree of freedom (x and $\dot{x}$)

STEP 0

$$x^{(0)} = x(t_0)$$

$$\dot{x}^{(0)} = \dot{x}(t_0)$$

STEP 1

$$x^{(1)} = x^{(0)} + \frac{1}{3}\delta x^{(0)}$$

$$\dot{x}^{(1)} = \dot{x}^{(0)} + \frac{1}{3}\delta \dot{x}^{(0)}$$

$$\delta x^{(0)} = \Delta t \; \dot{x}^{(0)}$$

$$\delta \dot{x}^{(0)} = \Delta t \; \mathcal{F}[x^{(0)}, \dot{x}^{(0)}]$$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0),\ \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*) ⟵ Low-storage

We only need to store one additional variable per degree of freedom (x and $\dot{x}$)

STEP 0

$$x^{(0)} = x(t_0)$$

$$\dot{x}^{(0)} = \dot{x}(t_0)$$

$$\delta x^{(0)} = \Delta t\ \dot{x}^{(0)}$$

$$\delta \dot{x}^{(0)} = \Delta t\ \mathcal{F}[x^{(0)}, \dot{x}^{(0)}]$$

STEP 1

$$x^{(1)} = x^{(0)} + \frac{1}{3}\delta x^{(0)}$$

$$\dot{x}^{(1)} = \dot{x}^{(0)} + \frac{1}{3}\delta \dot{x}^{(0)}$$

$$\delta x^{(1)} = -\frac{5}{9}\delta x^{(0)} + \Delta t\ \dot{x}^{(1)}$$

$$\delta \dot{x}^{(1)} = -\frac{5}{9}\delta \dot{x}^{(0)} + \Delta t\ \mathcal{F}\left[x^{(1)}, \dot{x}^{(1)}\right]$$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$ Suppose we know $x(t_0),\ \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*) ⟵ Low-storage

We only need to store one additional variable per degree of freedom (x and $\dot{x}$)

STEP 0

$$x^{(0)} = x(t_0)$$

$$\dot{x}^{(0)} = \dot{x}(t_0)$$

$$\delta x^{(0)} = \Delta t\ \dot{x}^{(0)}$$

$$\delta \dot{x}^{(0)} = \Delta t\ \mathcal{F}[x^{(0)}, \dot{x}^{(0)}]$$

STEP 1

$$x^{(1)} = x^{(0)} + \frac{1}{3}\delta x^{(0)}$$

$$\dot{x}^{(1)} = \dot{x}^{(0)} + \frac{1}{3}\delta \dot{x}^{(0)}$$

$$\delta x^{(1)} = -\frac{5}{9}\delta x^{(0)} + \Delta t\ \dot{x}^{(1)}$$

$$\delta \dot{x}^{(1)} = -\frac{5}{9}\delta \dot{x}^{(0)} + \Delta t\ \mathcal{F}\left[x^{(1)}, \dot{x}^{(1)}\right]$$

STEP 2

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$ Suppose we know $x(t_0),\ \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*) ⟵ Low-storage

We only need to store one additional variable per degree of freedom (x and $\dot{x}$)

STEP 0

$$x^{(0)} = x(t_0)$$

$$\dot{x}^{(0)} = \dot{x}(t_0)$$

$$\delta x^{(0)} = \Delta t\ \dot{x}^{(0)}$$

$$\delta \dot{x}^{(0)} = \Delta t\ \mathcal{F}[x^{(0)}, \dot{x}^{(0)}]$$

STEP 1

$$x^{(1)} = x^{(0)} + \frac{1}{3}\delta x^{(0)}$$

$$\dot{x}^{(1)} = \dot{x}^{(0)} + \frac{1}{3}\delta \dot{x}^{(0)}$$

$$\delta x^{(1)} = -\frac{5}{9}\delta x^{(0)} + \Delta t\ \dot{x}^{(1)}$$

$$\delta \dot{x}^{(1)} = -\frac{5}{9}\delta \dot{x}^{(0)} + \Delta t\ \mathcal{F}\left[x^{(1)}, \dot{x}^{(1)}\right]$$

STEP 2

For this step we only need $x^{(1)}, \dot{x}^{(1)}, \delta x^{(1)}, \delta \dot{x}^{(1)}$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$ Suppose we know $x(t_0),\ \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*) ⟵ Low-storage

We only need to store one additional variable per degree of freedom (x and $\dot{x}$)

STEP 1

$$x^{(1)} = x^{(0)} + \frac{1}{3}\delta x^{(0)}$$

$$\dot{x}^{(1)} = \dot{x}^{(0)} + \frac{1}{3}\delta \dot{x}^{(0)}$$

$$\delta x^{(1)} = -\frac{5}{9}\delta x^{(0)} + \Delta t\ \dot{x}^{(1)}$$

$$\delta \dot{x}^{(1)} = -\frac{5}{9}\delta \dot{x}^{(0)} + \Delta t\ \mathcal{F}\left[x^{(1)}, \dot{x}^{(1)}\right]$$

STEP 2

$$x^{(2)} = x^{(1)} + \frac{15}{16}\delta x^{(1)}$$

$$\dot{x}^{(2)} = \dot{x}^{(1)} + \frac{15}{16}\delta \dot{x}^{(1)}$$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$ Suppose we know $x(t_0),\ \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*) ⟵ Low-storage

We only need to store one additional variable per degree of freedom (x and $\dot{x}$)

STEP 1

$$x^{(1)} = x^{(0)} + \frac{1}{3}\delta x^{(0)}$$

$$\dot{x}^{(1)} = \dot{x}^{(0)} + \frac{1}{3}\delta \dot{x}^{(0)}$$

$$\delta x^{(1)} = -\frac{5}{9}\delta x^{(0)} + \Delta t\ \dot{x}^{(1)}$$

$$\delta \dot{x}^{(1)} = -\frac{5}{9}\delta \dot{x}^{(0)} + \Delta t\ \mathcal{F}\left[x^{(1)}, \dot{x}^{(1)}\right]$$

STEP 2

$$x^{(2)} = x^{(1)} + \frac{15}{16}\delta x^{(1)}$$

$$\dot{x}^{(2)} = \dot{x}^{(1)} + \frac{15}{16}\delta \dot{x}^{(1)}$$

$$\delta x^{(2)} = -\frac{153}{128}\delta x^{(1)} + \Delta t\ \dot{x}^{(2)}$$

$$\delta \dot{x}^{(2)} = -\frac{153}{128}\delta \dot{x}^{(1)} + \Delta t\ \mathcal{F}\left[x^{(2)}, \dot{x}^{(2)}\right]$$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0),\ \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*) ⟵ Low-storage

We only need to store one additional variable per degree of freedom (x and $\dot{x}$)

STEP 1

$$x^{(1)} = x^{(0)} + \frac{1}{3}\delta x^{(0)}$$

$$\dot{x}^{(1)} = \dot{x}^{(0)} + \frac{1}{3}\delta \dot{x}^{(0)}$$

$$\delta x^{(1)} = -\frac{5}{9}\delta x^{(0)} + \Delta t\, \dot{x}^{(1)}$$

$$\delta \dot{x}^{(1)} = -\frac{5}{9}\delta \dot{x}^{(0)} + \Delta t\, \mathcal{F}\left[x^{(1)}, \dot{x}^{(1)}\right]$$

STEP 2

$$x^{(2)} = x^{(1)} + \frac{15}{16}\delta x^{(1)}$$

$$\dot{x}^{(2)} = \dot{x}^{(1)} + \frac{15}{16}\delta \dot{x}^{(1)}$$

$$\delta x^{(2)} = -\frac{153}{128}\delta x^{(1)} + \Delta t\, \dot{x}^{(2)}$$

$$\delta \dot{x}^{(2)} = -\frac{153}{128}\delta \dot{x}^{(1)} + \Delta t\, \mathcal{F}\left[x^{(2)}, \dot{x}^{(2)}\right]$$

For STEP 3 we only need
$x^{(2)}, \dot{x}^{(2)}, \delta x^{(2)}, \delta \dot{x}^{(2)}$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0),\ \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*) ⟵ Low-storage

We only need to store one additional variable per degree of freedom (x and $\dot{x}$)

STEP 2

$$x^{(2)} = x^{(1)} + \frac{15}{16}\delta x^{(1)}$$

$$\dot{x}^{(2)} = \dot{x}^{(1)} + \frac{15}{16}\delta \dot{x}^{(1)}$$

$$\delta x^{(2)} = -\frac{153}{128}\delta x^{(1)} + \Delta t\, \dot{x}^{(2)}$$

$$\delta \dot{x}^{(2)} = -\frac{153}{128}\delta \dot{x}^{(1)} + \Delta t\, \mathcal{F}\left[x^{(2)}, \dot{x}^{(2)}\right]$$

STEP 3

$$x^{(3)} = x^{(2)} + \frac{8}{15}\delta x^{(2)}$$

$$\dot{x}^{(3)} = \dot{x}^{(2)} + \frac{8}{15}\delta \dot{x}^{(2)}$$

Runge-Kutta methods

We want to solve $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

Suppose we know $x(t_0),\ \dot{x}(t_0)$

Third order Runge-Kutta (*Williamson*) ⟵ Low-storage

We only need to store one additional variable per degree of freedom (x and $\dot{x}$)

STEP 2

$$x^{(2)} = x^{(1)} + \frac{15}{16}\delta x^{(1)}$$

$$\dot{x}^{(2)} = \dot{x}^{(1)} + \frac{15}{16}\delta \dot{x}^{(1)}$$

$$\delta x^{(2)} = -\frac{153}{128}\delta x^{(1)} + \Delta t\ \dot{x}^{(2)}$$

$$\delta \dot{x}^{(2)} = -\frac{153}{128}\delta \dot{x}^{(1)} + \Delta t\ \mathcal{F}\left[x^{(2)}, \dot{x}^{(2)}\right]$$

STEP 3

$$x^{(3)} = x^{(2)} + \frac{8}{15}\delta x^{(2)} \equiv x(t_0 + \Delta t)$$

$$\dot{x}^{(3)} = \dot{x}^{(2)} + \frac{8}{15}\delta \dot{x}^{(2)} \equiv \dot{x}(t_0 + \Delta t)$$

Symplectic vs Runge-Kutta: Hamiltonian systems

- Symplectic algorithms work well at conserving energy during the evolution

Symplectic vs Runge-Kutta: Hamiltonian systems

- Symplectic algorithms work well at conserving energy during the evolution
- Among them, explicit algorithms (e. g. Leapfrog) can be used when we have a *separable* Hamiltonian system

$$\mathrm{H(p,x)} = \mathrm{T(p)} + \mathrm{V(x)} = \frac{\mathrm{p}^2}{2\mathrm{m}} + \mathrm{V(x)}$$

$$\dot{x} = \frac{p}{m}$$

$$\dot{p} = -\frac{\partial V}{\partial x} = \mathcal{F}[x(t)]$$

Symplectic vs Runge-Kutta: Hamiltonian systems

- Symplectic algorithms work well at conserving energy during the evolution
- Among them, explicit algorithms (e. g. Leapfrog) can be used when we have a *separable* Hamiltonian system

$$\mathrm{H(p,x)} = \mathrm{T(p)} + \mathrm{V(x)} = \frac{\mathrm{p}^2}{2\mathrm{m}} + \mathrm{V(x)}$$

$$\dot{x} = \frac{p}{m}$$

$$\dot{p} = -\frac{\partial V}{\partial x} = \mathcal{F}[x(t)]$$

- Explicit Runge-Kutta methods are not symplectic
- How well do they work for Hamiltonian systems?

Leapfrog vs Runge-Kutta: 1D harmonic oscillator

$$H(p, x) = T(p) + V(x) = \frac{p^2}{2m} + \frac{1}{2} k\, x^2 \longrightarrow \ddot{x} = -\omega^2\, x = \mathcal{F}[x(t)]$$

$$\omega^2 = \frac{k}{m} = 1$$

Leapfrog vs Runge-Kutta: 1D harmonic oscillator

$$\mathrm{H(p,x) = T(p) + V(x)} = \frac{\mathrm{p}^2}{2\mathrm{m}} + \frac{1}{2}\mathrm{k\,x}^2 \longrightarrow \ddot{x} = -\omega^2\, x = \mathcal{F}[x(t)]$$

$$\omega^2 = \frac{k}{m} = 1$$

Velocity-Verlet order $(\Delta t)^2$

$$\dot{x}\left(t_0 + \frac{\Delta t}{2}\right) = \dot{x}(t_0) - \frac{1}{2}\Delta t\, x(t_0)$$

$$x(t_0 + \Delta t) = x(t_0) + \Delta t\, \dot{x}(t_0 + \frac{\Delta t}{2})$$

$$\dot{x}(t_0 + \Delta t) = \dot{x}\left(t_0 + \frac{\Delta t}{2}\right) - \frac{1}{2}\Delta t\, x(t_0 + \Delta t)$$

Leapfrog vs Runge-Kutta: 1D harmonic oscillator

$$\mathrm{H(p,x) = T(p) + V(x) = \frac{p^2}{2m} + \frac{1}{2} k\, x^2} \longrightarrow \ddot{x} = -\omega^2\, x = \mathcal{F}[x(t)]$$

$$\omega^2 = \frac{k}{m} = 1$$

Velocity-Verlet order $(\Delta t)^2$ VS Runge-Kutta order $(\Delta t)^2$

$$\dot{x}\left(t_0 + \frac{\Delta t}{2}\right) = \dot{x}(t_0) - \frac{1}{2}\Delta t\; x(t_0)$$

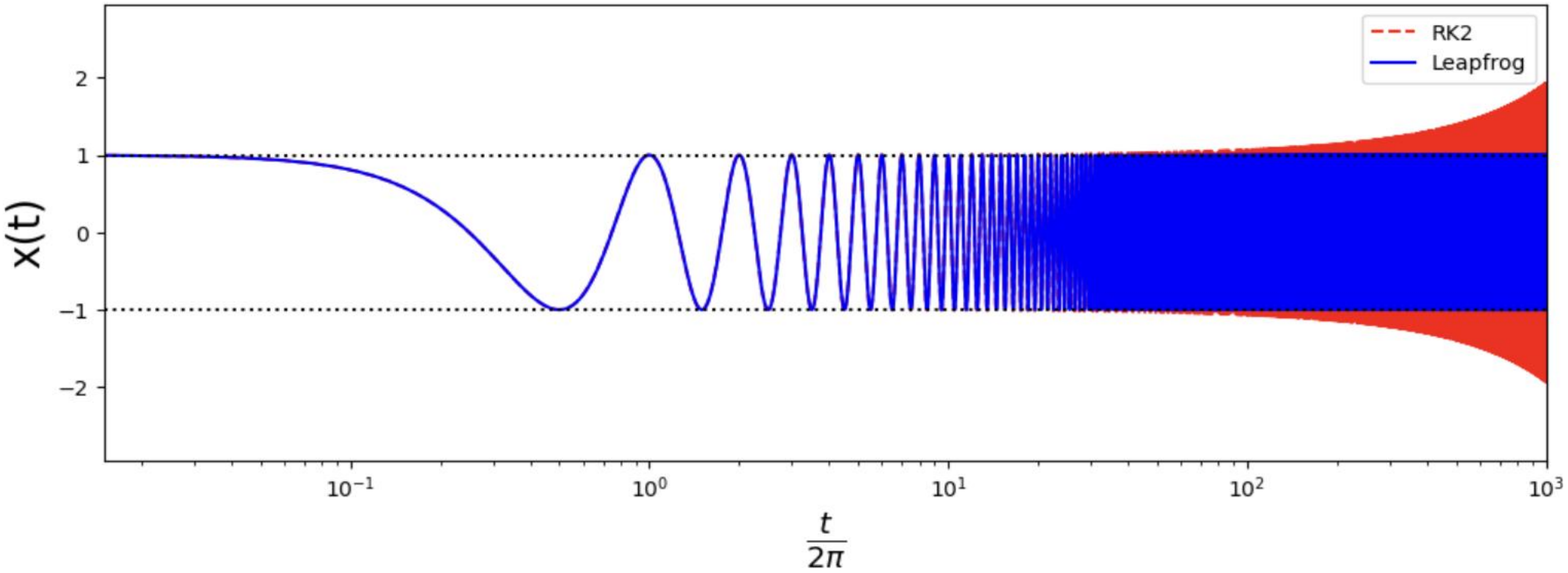
$$x(t_0 + \Delta t) = x(t_0) + \Delta t\; \dot{x}(t_0 + \frac{\Delta t}{2})$$

$$\dot{x}(t_0 + \Delta t) = \dot{x}\left(t_0 + \frac{\Delta t}{2}\right) - \frac{1}{2}\Delta t\; x(t_0 + \Delta t)$$

$$x(t_0 + \Delta t) = x(t_0) + \Delta t\; \dot{x}(t_0) - \frac{1}{2}\Delta t^2 x(t_0)$$

$$\dot{x}(t_0 + \Delta t) = \dot{x}(t_0) - \Delta t\; x(t_0) - \frac{1}{2}\Delta t^2 \dot{x}(t_0)$$

Leapfrog vs Runge-Kutta: 1D harmonic oscillator



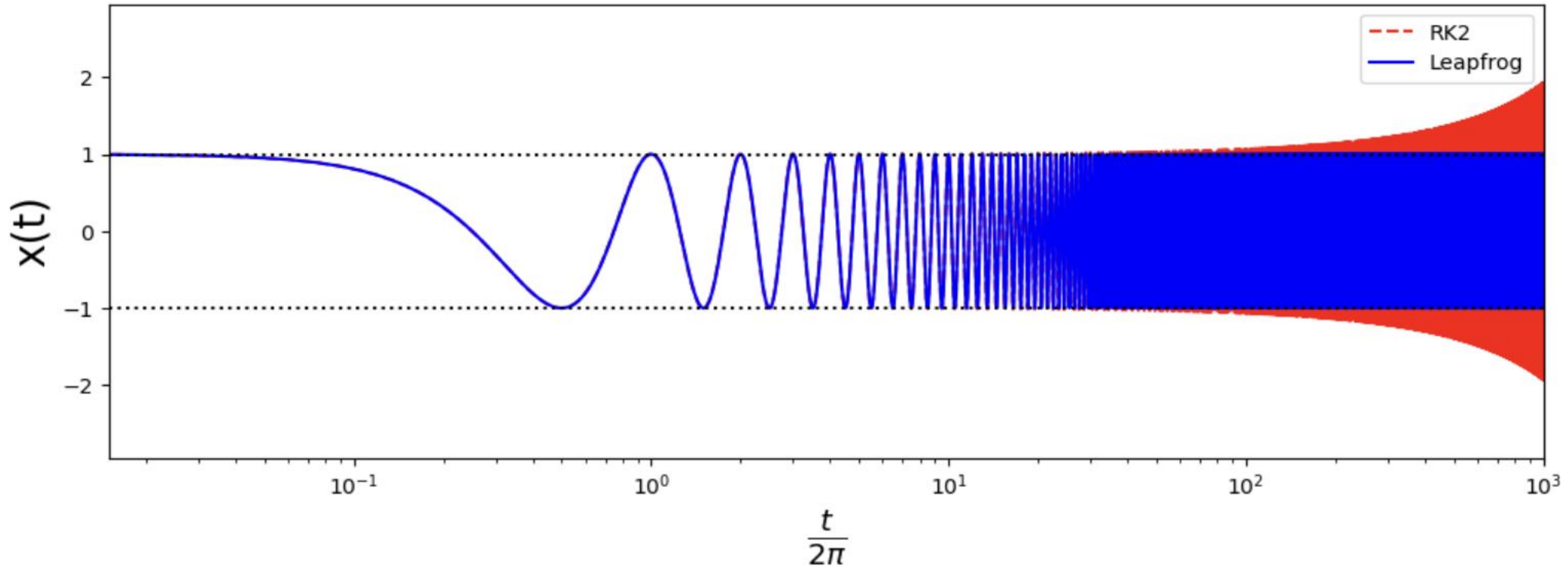
- Initial conditions

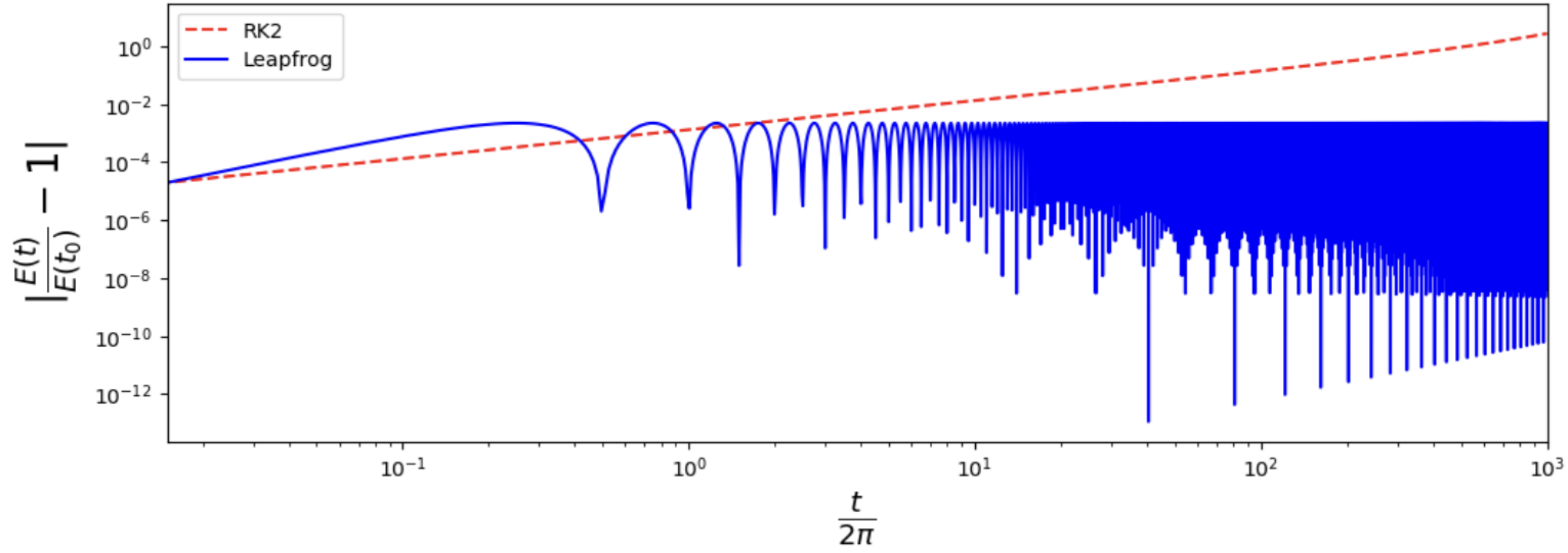
$x(t_0) = 1, \qquad \dot{x}(t_0) = 0$

- The trajectory should be bounded $|x(t)| \leq 1$

- Runge-Kutta fails before Leapfrog (same Δt)

Leapfrog vs Runge-Kutta: 1D harmonic oscillator





- Initial conditions

$$x(t_0) = 1, \qquad \dot{x}(t_0) = 0$$

- The trajectory should be bounded $|x(t)| \leq 1$

- Runge-Kutta fails before Leapfrog (same Δt)

- Energy conservation is important in the evolution of Hamiltonian systems

Symplectic vs Runge-Kutta: dissipative systems

- Symplectic algorithms work well at conserving energy during the evolution

- However, when the system is dissipative and energy is not conserved, they might become unstable (trying to force the conservation of something which should not be conserved)

- Explicit Runge-Kutta methods are a natural alternative for those systems

Symplectic vs Runge-Kutta: dissipative systems

- Symplectic algorithms work well at conserving energy during the evolution

- However, when the system is dissipative and energy is not conserved, they might become unstable (trying to force the conservation of something which should not be conserved)

- Explicit Runge-Kutta methods are a natural alternative for those systems

Example (PDE): 1D Burgers equation

$$\partial_t u\,(x,t) = -u(x,t)\,\partial_x u(x,t) + \nu\,\partial_x^2 u(x,t)$$

Viscosity (dissipation of energy)

Leapfrog vs Runge-Kutta: dissipative systems

Example (PDE): 1D Burgers equation

$$\partial_t u(x,t) = -u(x,t)\partial_x u(x,t) + \nu \partial_x^2 u(x,t) = \mathcal{F}[u(x,t)]$$

Runge-Kutta order $(\Delta t)^2$

$$u^{(0)} = u(t_0)$$

$$u^{(1)} = u(t_0) + \Delta t\, \mathcal{F}[u(t_0)]$$

$$u(t_0 + \Delta t) = u(t_0) + \Delta t \frac{\mathcal{F}[u^{(0)}] + \mathcal{F}[u^{(1)}]}{2}$$

Leapfrog vs Runge-Kutta: dissipative systems

Example (PDE): 1D Burgers equation

$$\partial_t u(x,t) = -u(x,t)\partial_x u(x,t) + \nu\, \partial_x^2 u(x,t) = \mathcal{F}[u(x,t)]$$

$$u(t_0 - \Delta t)$$

RK2 ↓

$$u(t_0)$$

Leapfrog vs Runge-Kutta: dissipative systems

Example (PDE): 1D Burgers equation

$$\partial_t u(x,t) = -u(x,t)\partial_x u(x,t) + \nu \partial_x^2 u(x,t) = \mathcal{F}[u(x,t)]$$

$$u(t_0 - \Delta t)$$

RK2

$$u(t_0)$$

RK2

$$u(t_0 + \Delta t)$$
$$= u(t_0) + \Delta t \frac{\mathcal{F}[u(t_0)] + \mathcal{F}\left[u(t_0) + \Delta t\, \mathcal{F}[u(t_0)]\right]}{2}$$

Leapfrog vs Runge-Kutta: dissipative systems

Example (PDE): 1D Burgers equation

$$\partial_t u(x,t) = -u(x,t)\partial_x u(x,t) + \nu \partial_x^2 u(x,t) = \mathcal{F}[u(x,t)]$$

$$u(t_0 - \Delta t)$$

RK2

$$u(t_0)$$

RK2

$$u(t_0 + \Delta t) = u(t_0) + \Delta t \frac{\mathcal{F}[u(t_0)] + \mathcal{F}\left[u(t_0) + \Delta t\, \mathcal{F}[u(t_0)]\right]}{2}$$

Leapfrog vs Runge-Kutta: dissipative systems

Example (PDE): 1D Burgers equation

$$\partial_t\, u\,(x,t) = -u(x,t)\partial_x\, u(x,t) + \nu\, \partial_x^2\, u(x,t) = \mathcal{F}[u(x,t)]$$

$$u(t_0 - \Delta t)$$

RK2

$$u(t_0)$$

RK2

$$u(t_0 + \Delta t)$$
$$= u(t_0) + \Delta t\, \frac{\mathcal{F}[u(t_0)] + \mathcal{F}\big[u(t_0) + \Delta t\, \mathcal{F}[u(t_0)]\big]}{2}$$

Leapfrog vs Runge-Kutta: dissipative systems

Example (PDE): 1D Burgers equation

$$\partial_t u(x,t) = -u(x,t)\partial_x u(x,t) + \nu\, \partial_x^2 u(x,t) = \mathcal{F}[u(x,t)]$$

$$u(t_0 - \Delta t)$$

RK2

$$u(t_0)$$

There is no explicit Leapfrog giving $u(t_0)$ in terms of $u(t_0 - \Delta t)$

RK2

$$u(t_0 + \Delta t)$$

$$= u(t_0) + \Delta t\, \frac{\mathcal{F}[u(t_0)] + \mathcal{F}\big[u(t_0) + \Delta t\, \mathcal{F}[u(t_0)]\big]}{2}$$

Leapfrog vs Runge-Kutta: dissipative systems

Example (PDE): 1D Burgers equation

$$\partial_t u(x,t) = -u(x,t)\partial_x u(x,t) + \nu\, \partial_x^2 u(x,t) = \mathcal{F}[u(x,t)]$$

$$u(t_0 - \Delta t)$$

RK2

$$u(t_0)$$

But there is an explicit Leapfrog giving $u(t_0 + \Delta t)$ in terms of $u(t_0)$ and $u(t_0 - \Delta t)$

RK2

$$u(t_0 + \Delta t) = u(t_0) + \Delta t \frac{\mathcal{F}[u(t_0)] + \mathcal{F}\big[u(t_0) + \Delta t\, \mathcal{F}[u(t_0)]\big]}{2}$$

Leapfrog

$$u(t_0 + \Delta t) = u(t_0 - \Delta t) + 2\,\Delta t\, \mathcal{F}[u(t_0)]$$

Leapfrog vs Runge-Kutta: dissipative systems

Example (PDE): 1D Burgers equation

$$\partial_t u\,(x,t) = -u(x,t)\partial_x\, u(x,t) + \nu\, \partial_x^2\, u(x,t) = \mathcal{F}[u(x,t)]$$

$$u(t_0 - \Delta t)$$

RK2 ↓

$$u(t_0)$$

But there is an explicit Leapfrog giving $u(t_0 + \Delta t)$ in terms of $u(t_0)$ and $u(t_0 - \Delta t)$

RK2 ↙

$$u(t_0 + \Delta t) = u(t_0) + \Delta t\, \frac{\mathcal{F}[u(t_0)] + \mathcal{F}\big[u(t_0) + \Delta t\, \mathcal{F}[u(t_0)]\big]}{2}$$

Leapfrog ↘

$$u(t_0 + \Delta t) = u(t_0 - \Delta t) + 2\,\Delta t\, \mathcal{F}[u(t_0)]$$

Leapfrog vs Runge-Kutta: dissipative systems

Example (PDE): 1D Burgers equation

$$\partial_t u(x,t) = -u(x,t)\partial_x u(x,t) + \nu\, \partial_x^2 u(x,t) = \mathcal{F}[u(x,t)]$$

$N_x = 256 \qquad L = 2\pi$

$\nu = 0.1 \qquad u(x, t_0) = \sin x$

$$E(t) = \int_0^{2\pi} \mathrm{dx}\, \frac{\mathrm{u}^2(\mathrm{x},\mathrm{t})}{2}$$

We expect energy to decay

Leapfrog vs Runge-Kutta: dissipative systems

Example (PDE): 1D Burgers equation

$$\partial_t u(x,t) = -u(x,t)\partial_x u(x,t) + \nu\, \partial_x^2 u(x,t) = \mathcal{F}[u(x,t)]$$

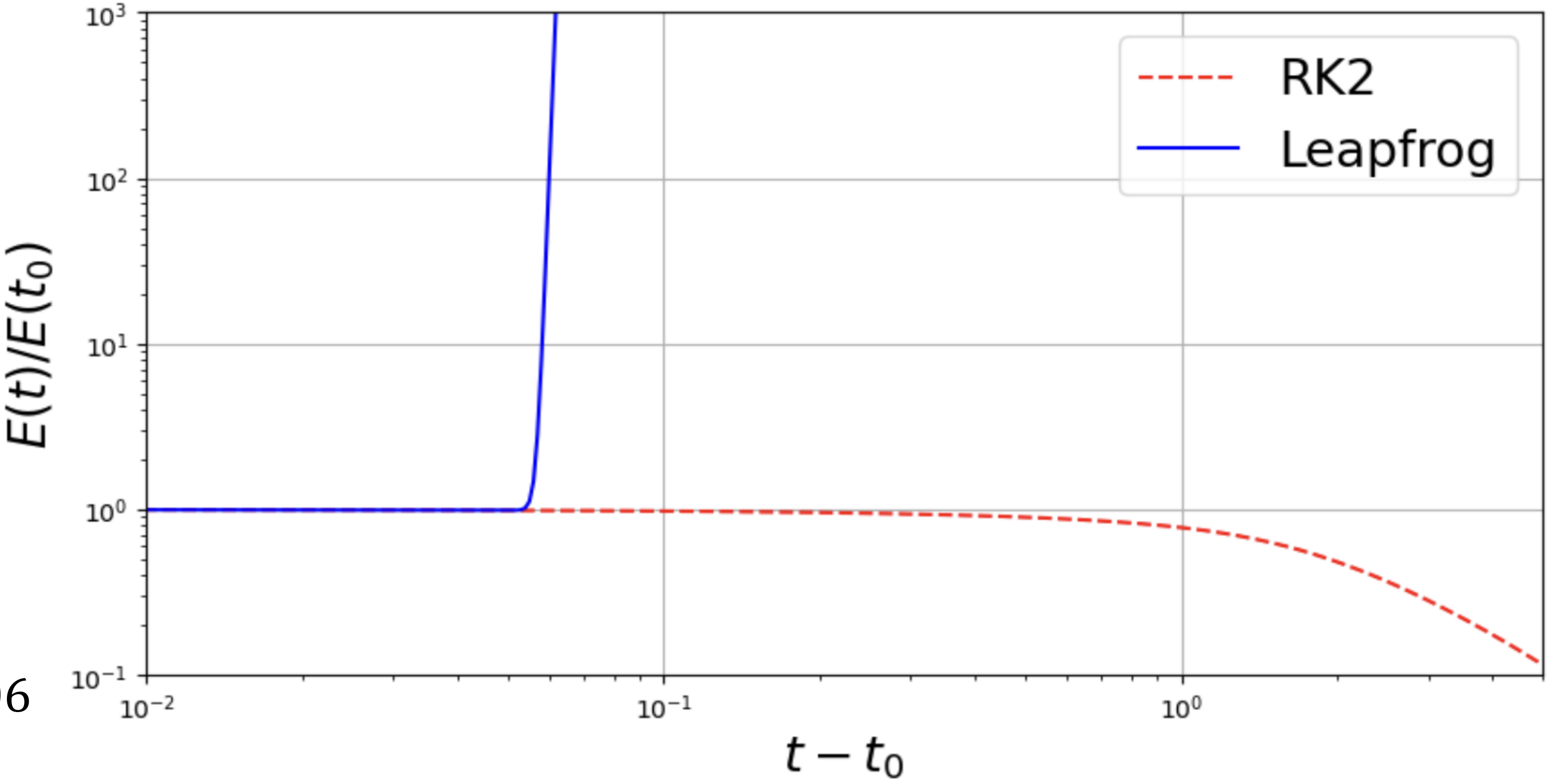
$N_x = 256 \qquad L = 2\pi$

$\nu = 0.1 \qquad u(x,t_0) = \sin x$

$$E(t) = \int_0^{2\pi} \mathrm{dx}\, \frac{\mathrm{u}^2(\mathrm{x},\mathrm{t})}{2}$$

We expect energy to decay

RK2 shows a smooth decay while Leapfrog an explosion at $t - t_0 \gtrsim 0.06$



Leapfrog vs Runge-Kutta: dissipative systems

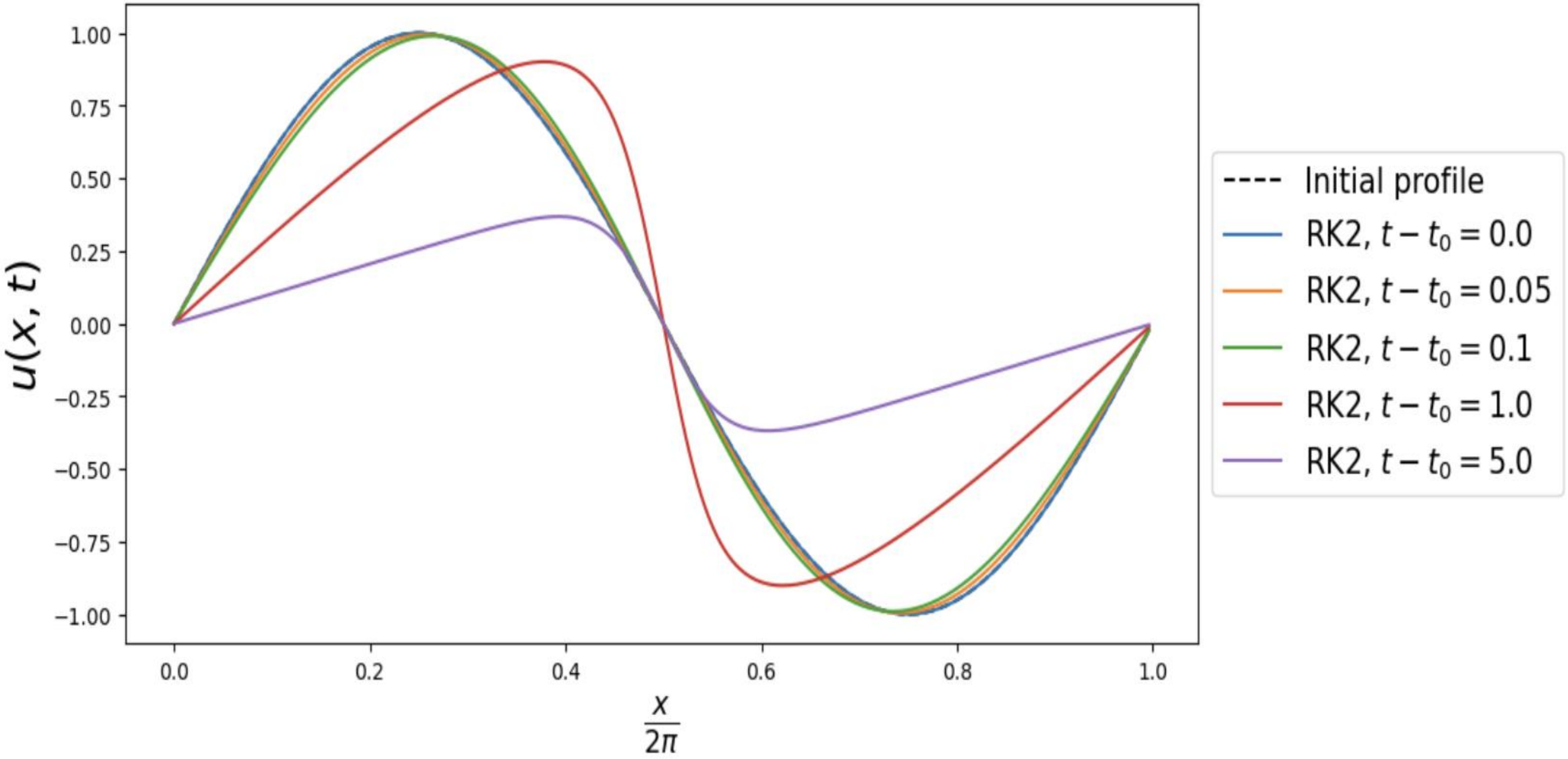
Example (PDE): 1D Burgers equation

$$\partial_t u(x,t) = -u(x,t)\partial_x u(x,t) + \nu\, \partial_x^2 u(x,t) = \mathcal{F}[u(x,t)]$$

$N_x = 256 \qquad L = 2\pi$

$\nu = 0.1 \qquad u(x, t_0) = \sin x$

Runge-Kutta reproduces the progressive damping of the profile accompanied by dissipation of energy



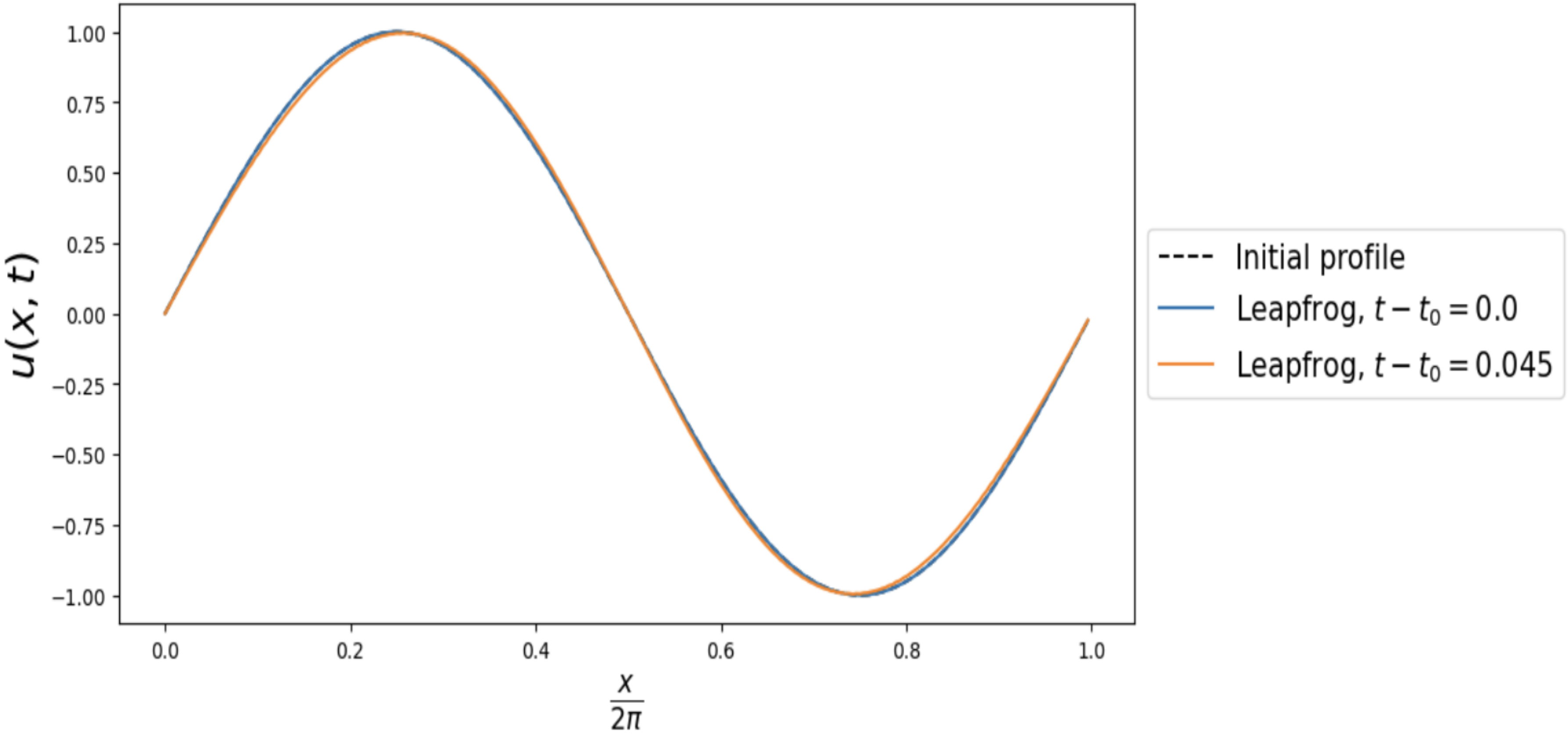
Leapfrog vs Runge-Kutta: dissipative systems

Example (PDE): 1D Burgers equation

$$\partial_t u(x,t) = -u(x,t)\partial_x u(x,t) + \nu\, \partial_x^2 u(x,t) = \mathcal{F}[u(x,t)]$$

$N_x = 256$ $\quad L = 2\pi$

$\nu = 0.1$ $\quad u(x,t_0) = \sin x$



Leapfrog vs Runge-Kutta: dissipative systems

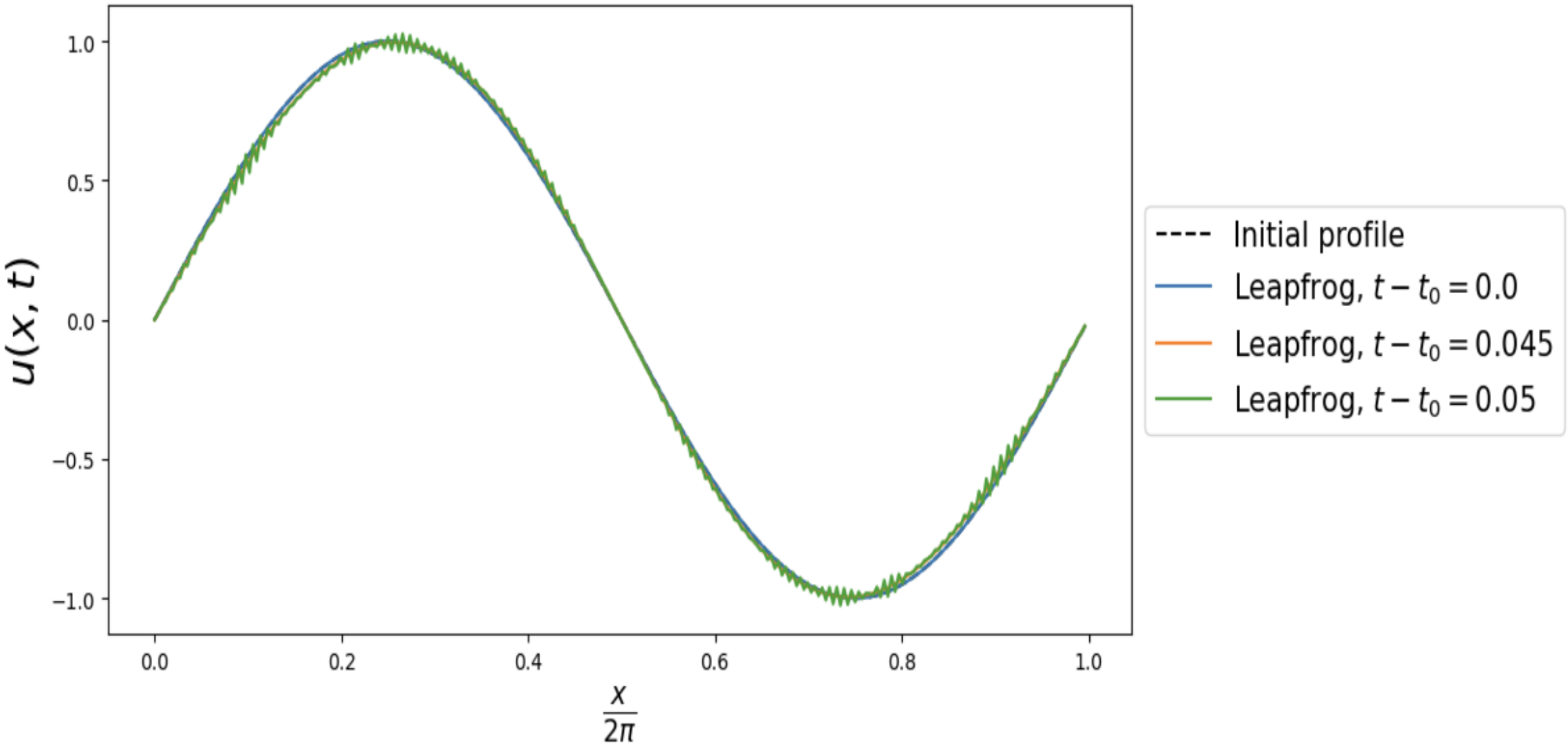
Example (PDE): 1D Burgers equation

$$\partial_t u(x,t) = -u(x,t)\partial_x u(x,t) + \nu\, \partial_x^2 u(x,t) = \mathcal{F}[u(x,t)]$$

$N_x = 256$ $\quad L = 2\pi$

$\nu = 0.1$ $\quad u(x, t_0) = \sin x$

Leapfrog generates spurious oscillations trying to force the conservation of energy which should instead be free to decay



Leapfrog vs Runge-Kutta: dissipative systems

Example (PDE): 1D Burgers equation

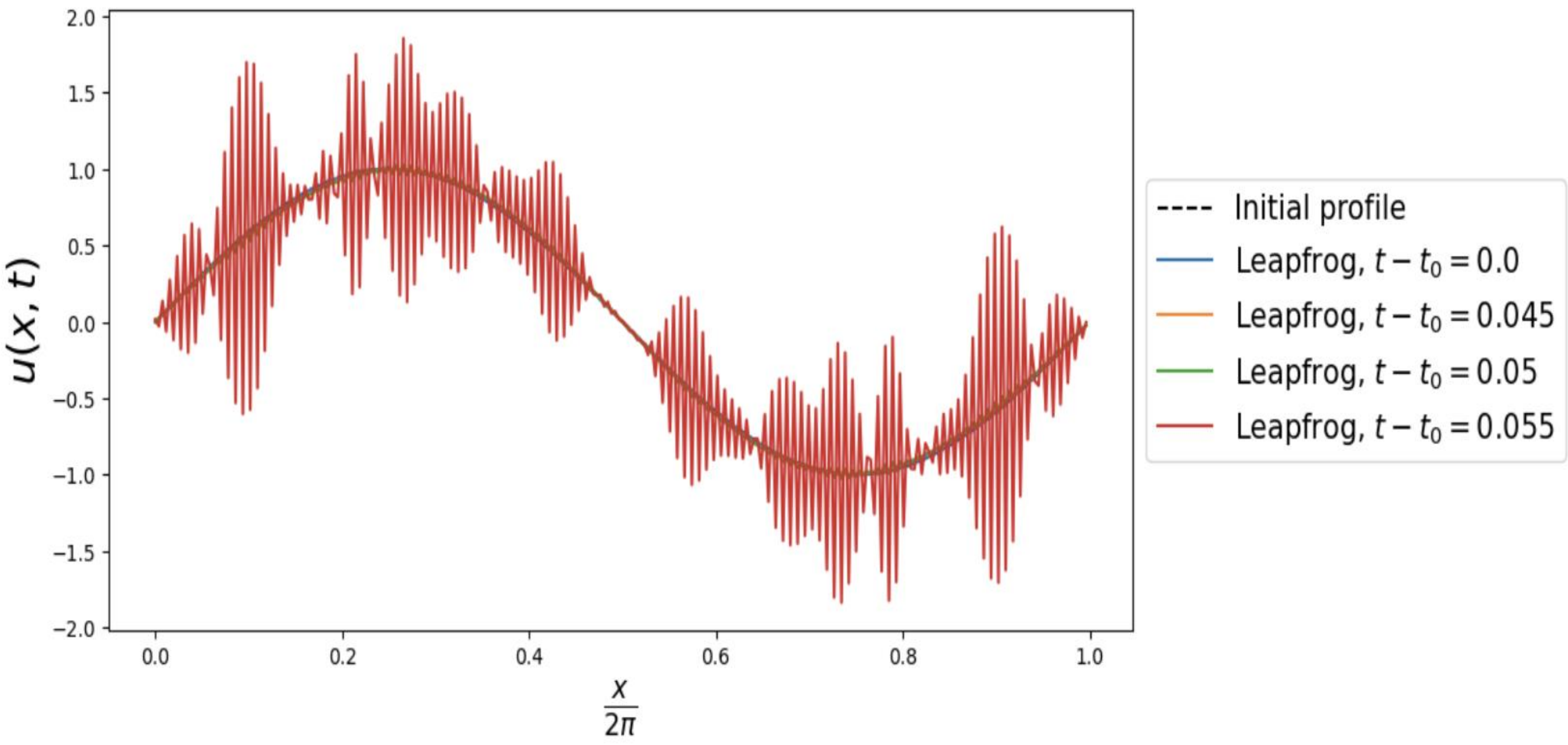
$$\partial_t u(x,t) = -u(x,t)\partial_x u(x,t) + \nu\, \partial_x^2 u(x,t) = \mathcal{F}[u(x,t)]$$

$N_x = 256$ $L = 2\pi$

$\nu = 0.1$ $u(x,t_0) = \sin x$

Leapfrog generates spurious oscillations trying to force the conservation of energy which should instead be free to decay

The spurious oscillations grow



Leapfrog vs Runge-Kutta: dissipative systems

Example (PDE): 1D Burgers equation

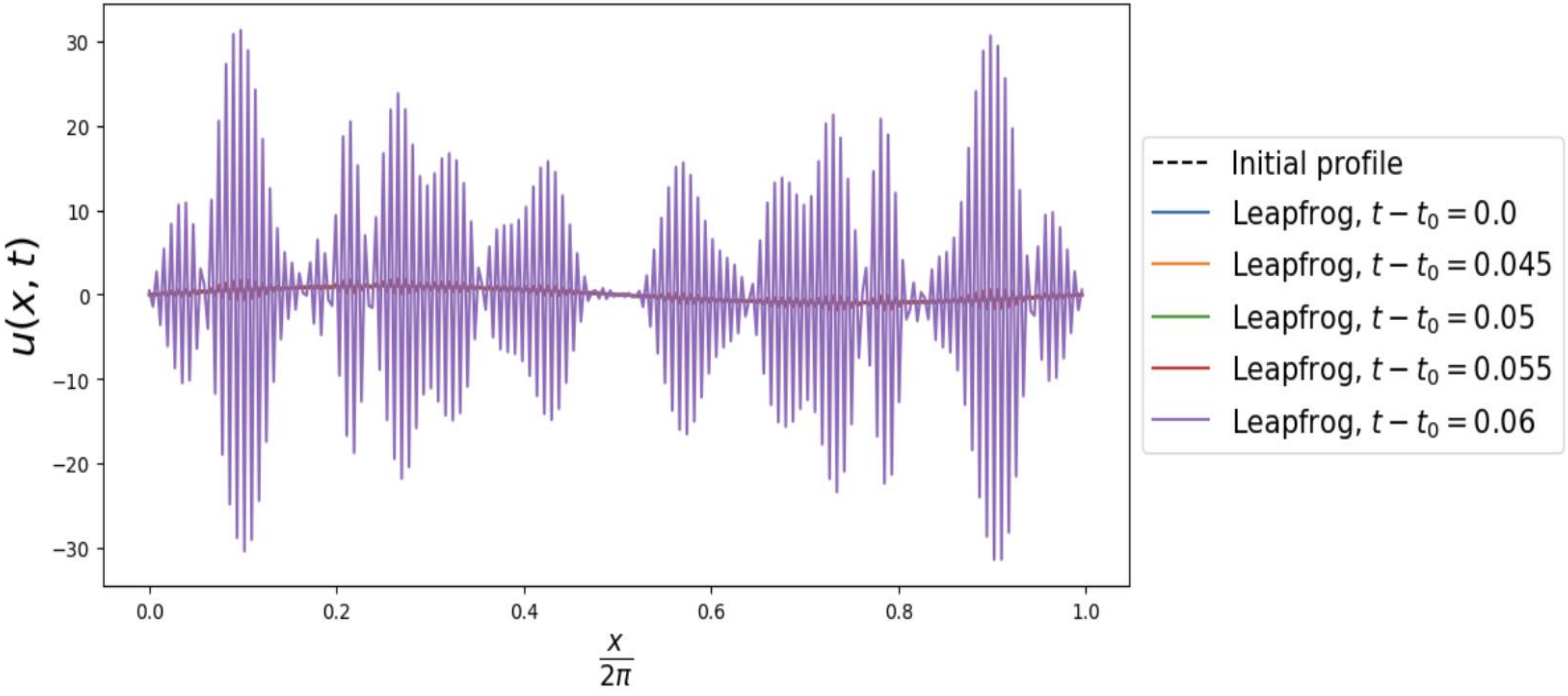
$$\partial_t u(x,t) = -u(x,t)\partial_x u(x,t) + \nu\, \partial_x^2 u(x,t) = \mathcal{F}[u(x,t)]$$

$N_x = 256 \qquad L = 2\pi$

$\nu = 0.1 \qquad u(x, t_0) = \sin x$

Leapfrog generates spurious oscillations trying to force the conservation of energy which should instead be free to decay

The spurious oscillations grow and the system becomes unstable



Conclusions

- Runge-Kutta explicit methods are a natural approach to solve equations of the form $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$ or $\dot{\mathrm{x}}(t) = \mathcal{G}[x(t)]$

- For separable Hamiltonian systems symplectic methods are more stable since they conserve energy and keep the trajectories bounded

- For dissipative systems non symplectic methods like Runge-Kutta are more stable since they do not try to force energy conservation unlike symplectic algorithms