Pencil Code school on early Universe physics and gravitational waves

October 2025, CERN (Switzerland)

Lecture: Numerical schemes for differential equations

Part I: timestepping

Antonino Salvino Midiri
(University of Geneva, Switzerland)

Part II: finite differences

Philippe Bourdin
(University of Graz, Austria)

Outline of Part I

- Introduction to numerical schemes for ODEs
- Symplectic methods
- Non-symplectic methods

Numerical schemes for Ordinary Differential Equations (ODEs)

How to solve numerically $\ddot{x}(t) = \mathcal{F}[x(t)]$

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$$x(t_0+\Delta t) = x(t_0) + \Delta t\, \dot{x}(t_0) + \mathcal{O}[(\Delta t)^2]$$

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How good is this algorithm?

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$\omega^2 = 1$

$m = 1$

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$$\ddot{x}(t) = -x(t)$$

$$x(t_0) = 1 \qquad\qquad x(t) = \cos t$$
$$\dot{x}(t_0) = 0 \qquad\qquad \dot{x}(t) = -\sin t$$

$\xrightarrow{\text{analytical solution}}$

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$\xrightarrow{\text{analytical solution}}$

$$x(t) = \cos t \qquad \dot{x}(t) = -\sin t$$

$\xrightarrow{\text{energy is conserved}}$

$$E(t) = \frac{1}{2} m(\dot{x}^2 + \omega^2 x^2) = \frac{1}{2}$$

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Choose $t_{fin} = 10\,T$ $\longrightarrow$ $N = \frac{t_{fin} - t_0}{\Delta t} = 10^3$ timesteps

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Compare at all timesteps

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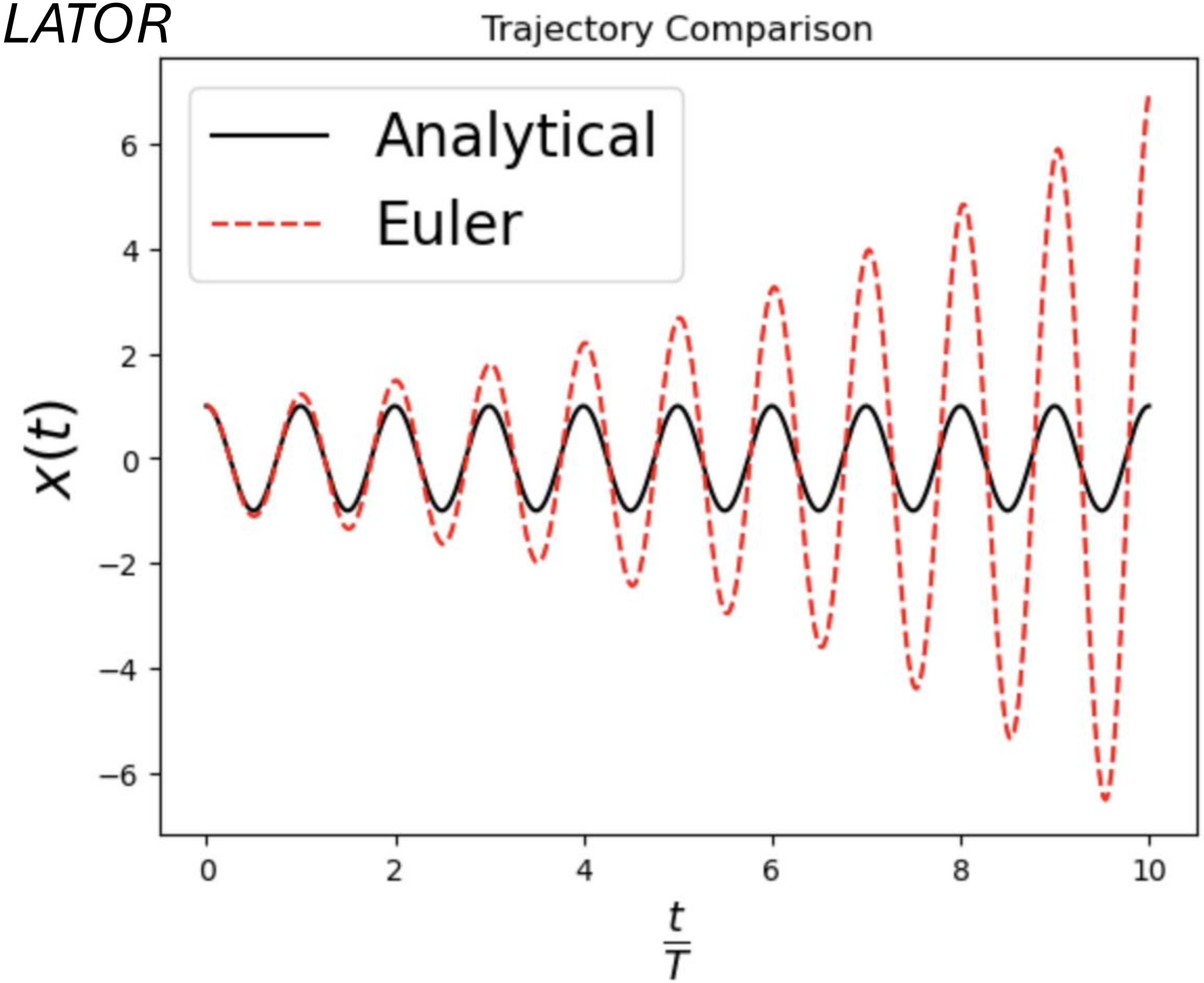

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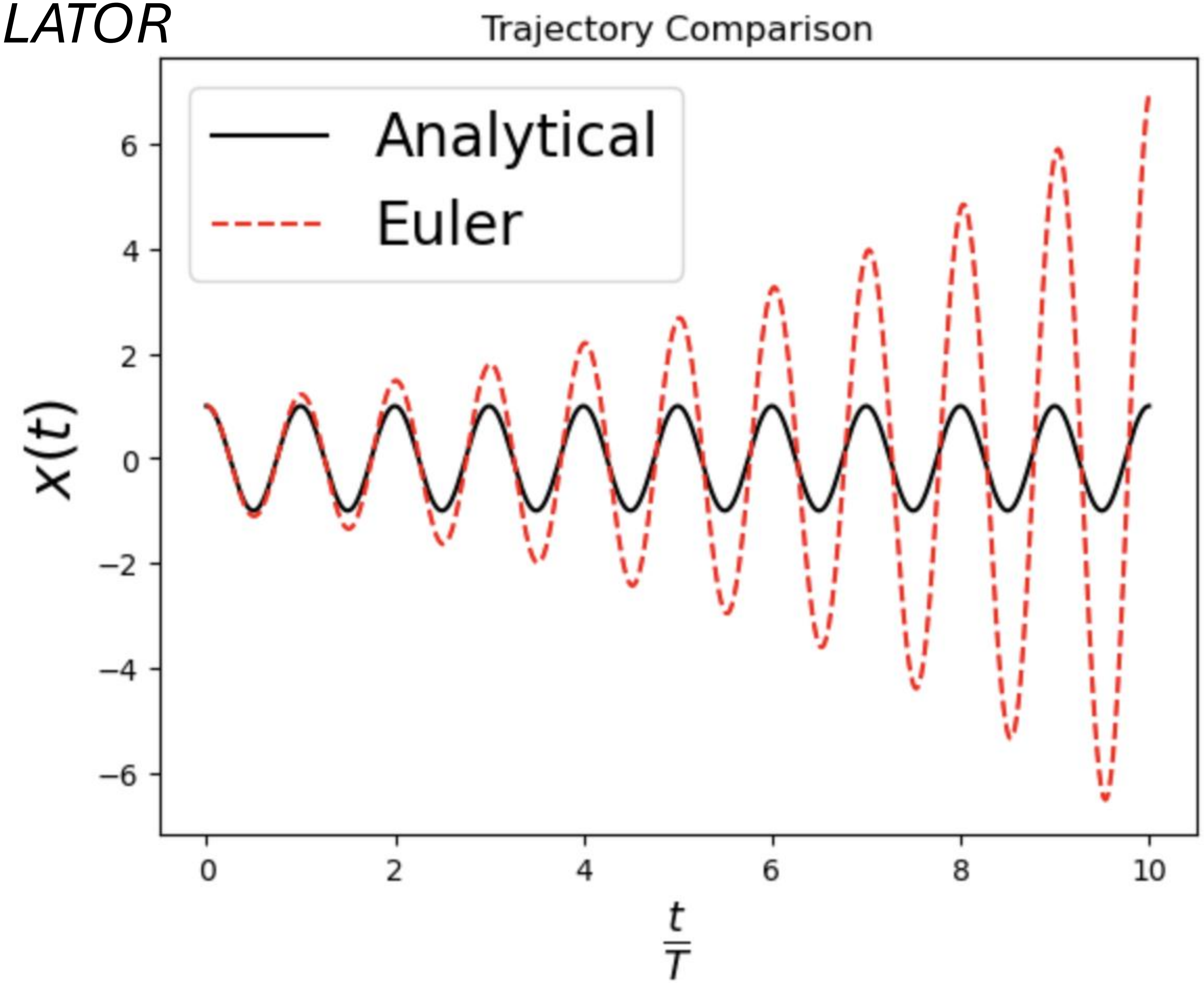

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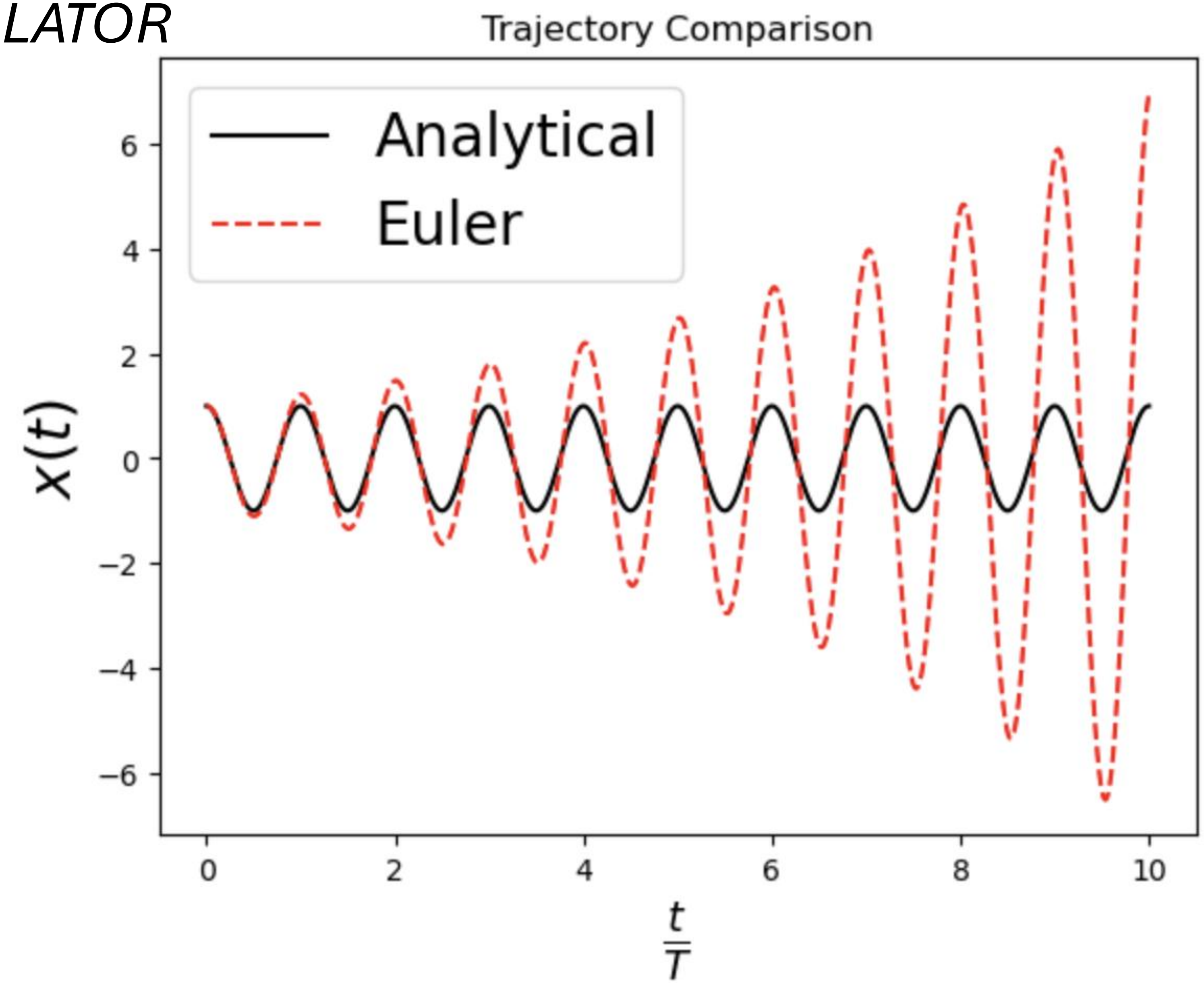

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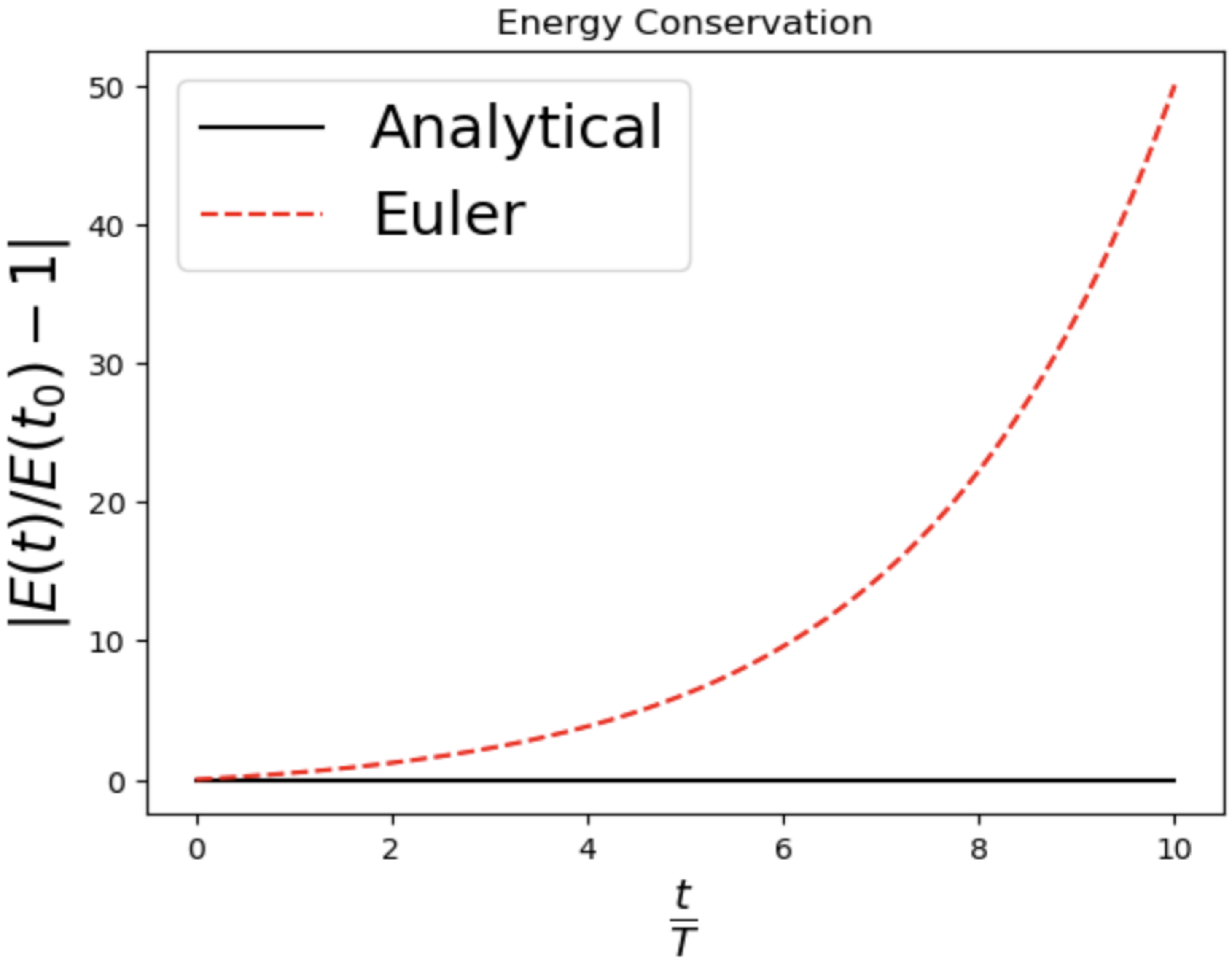

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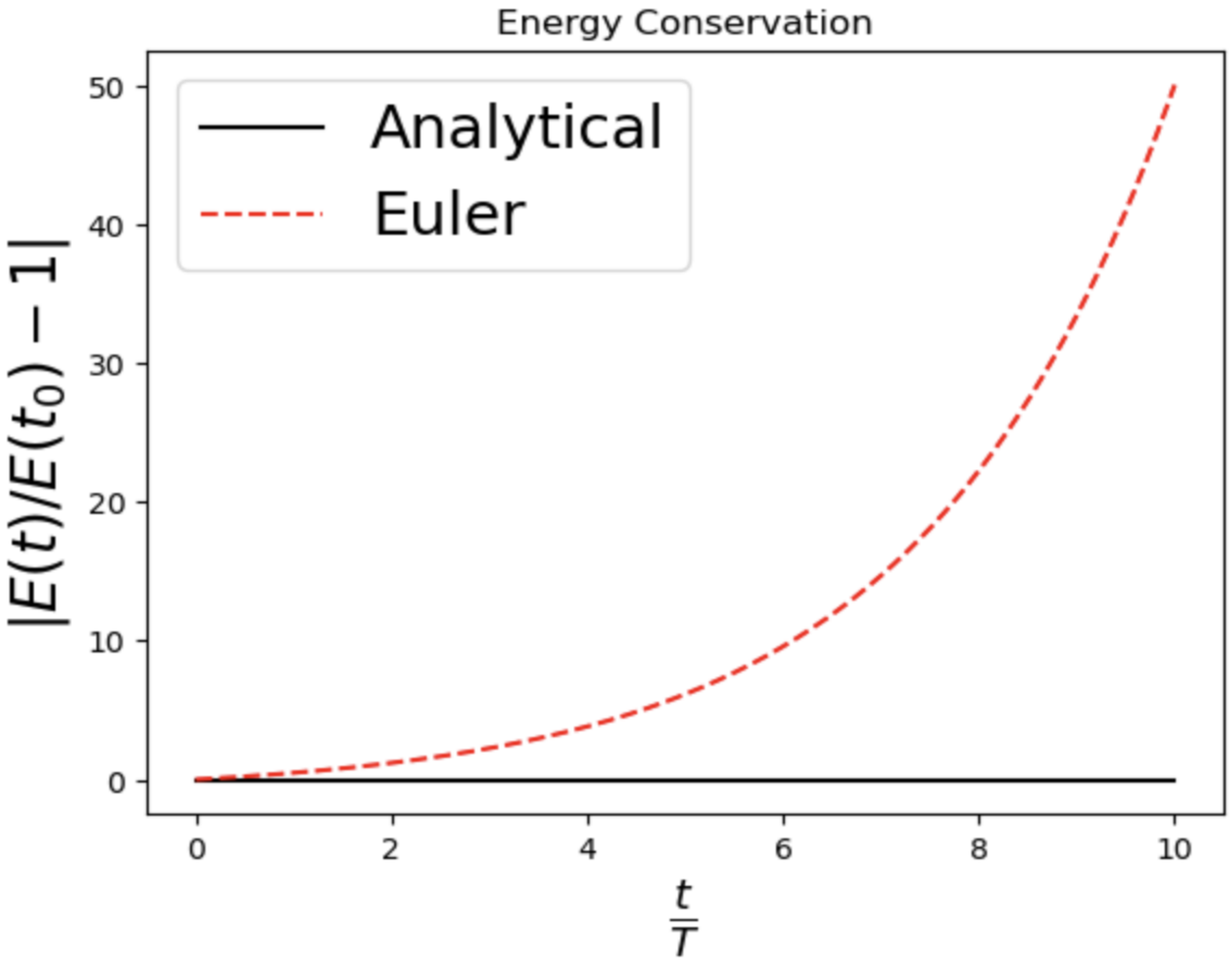

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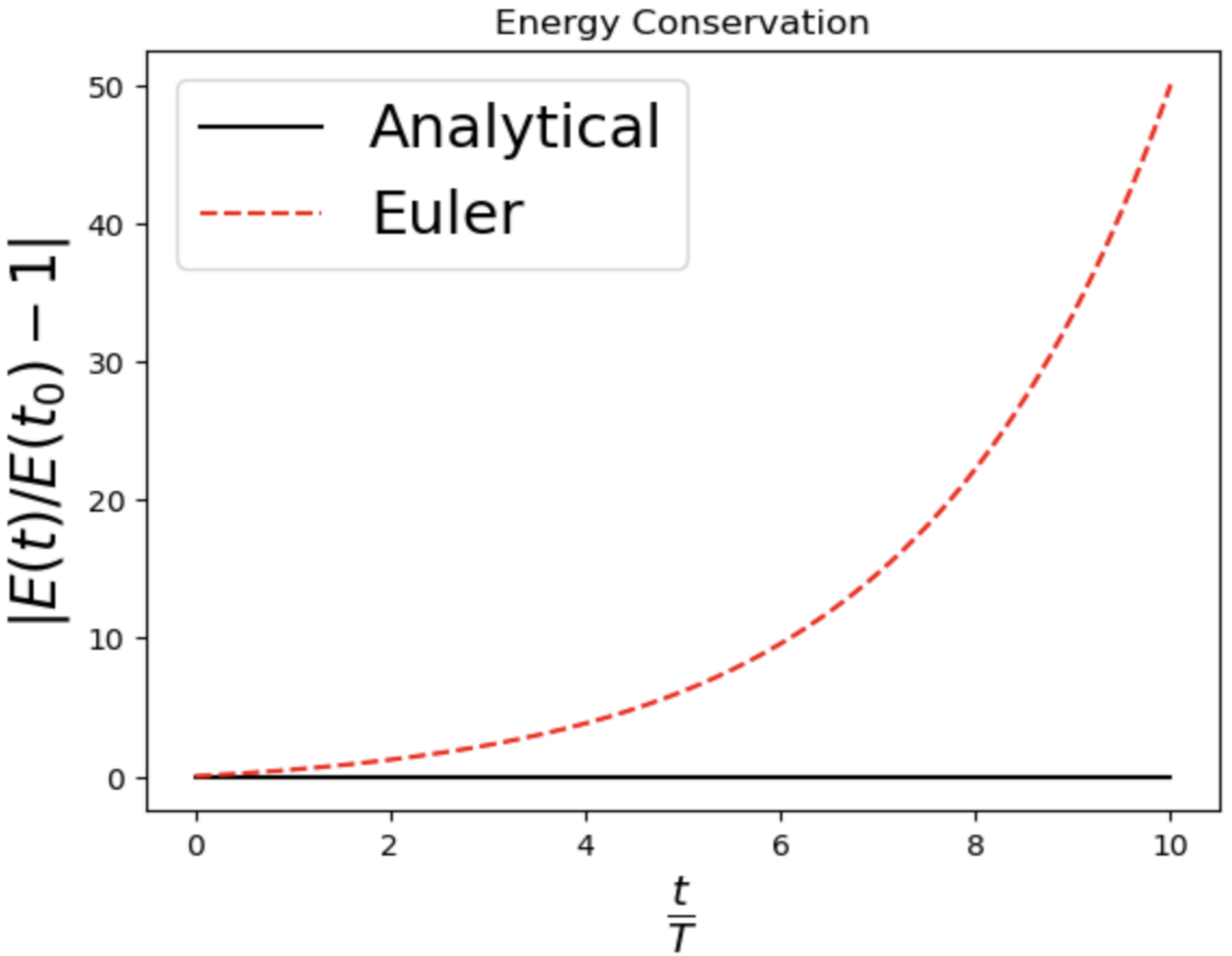
Let us look at the phase space



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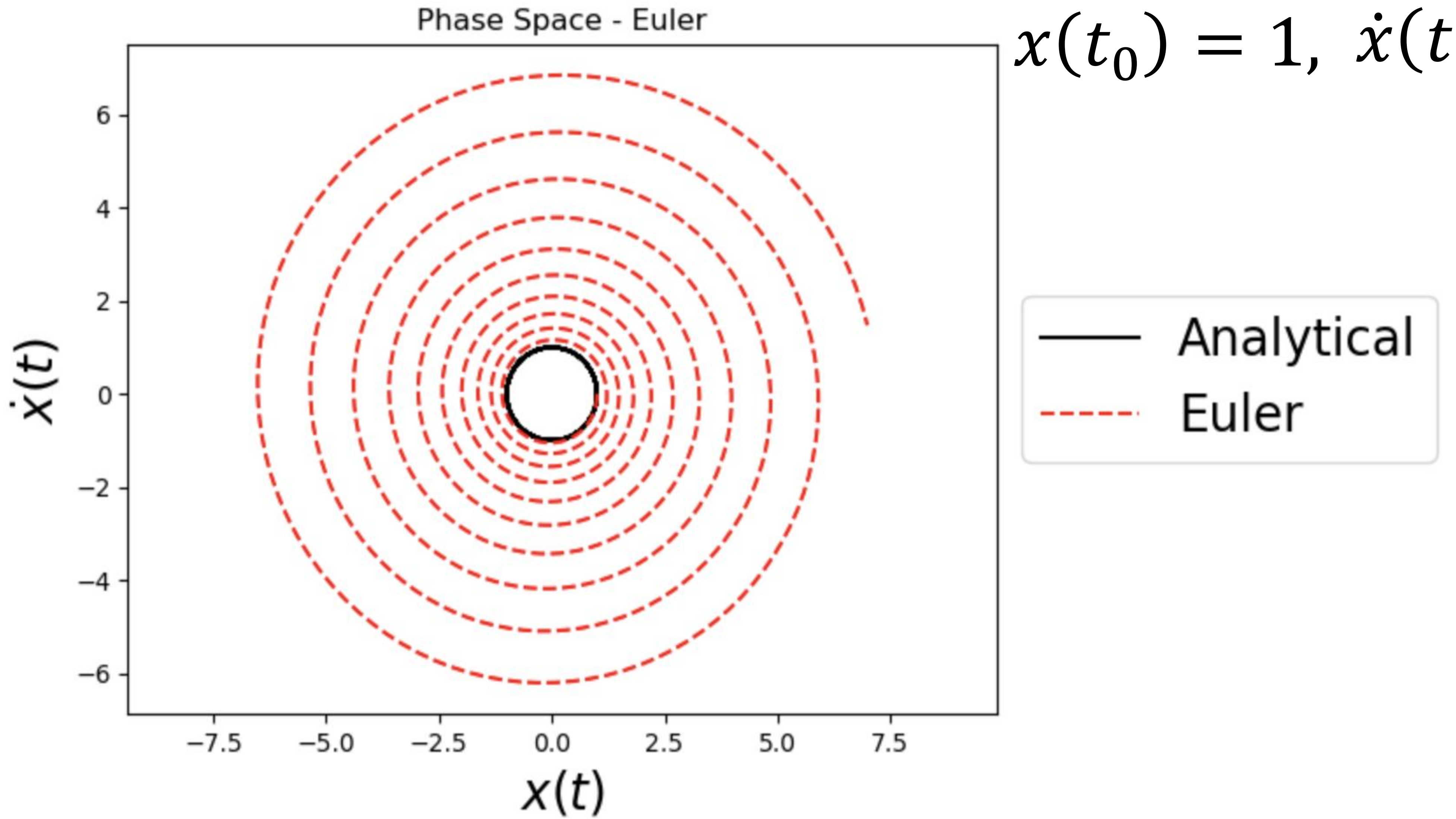

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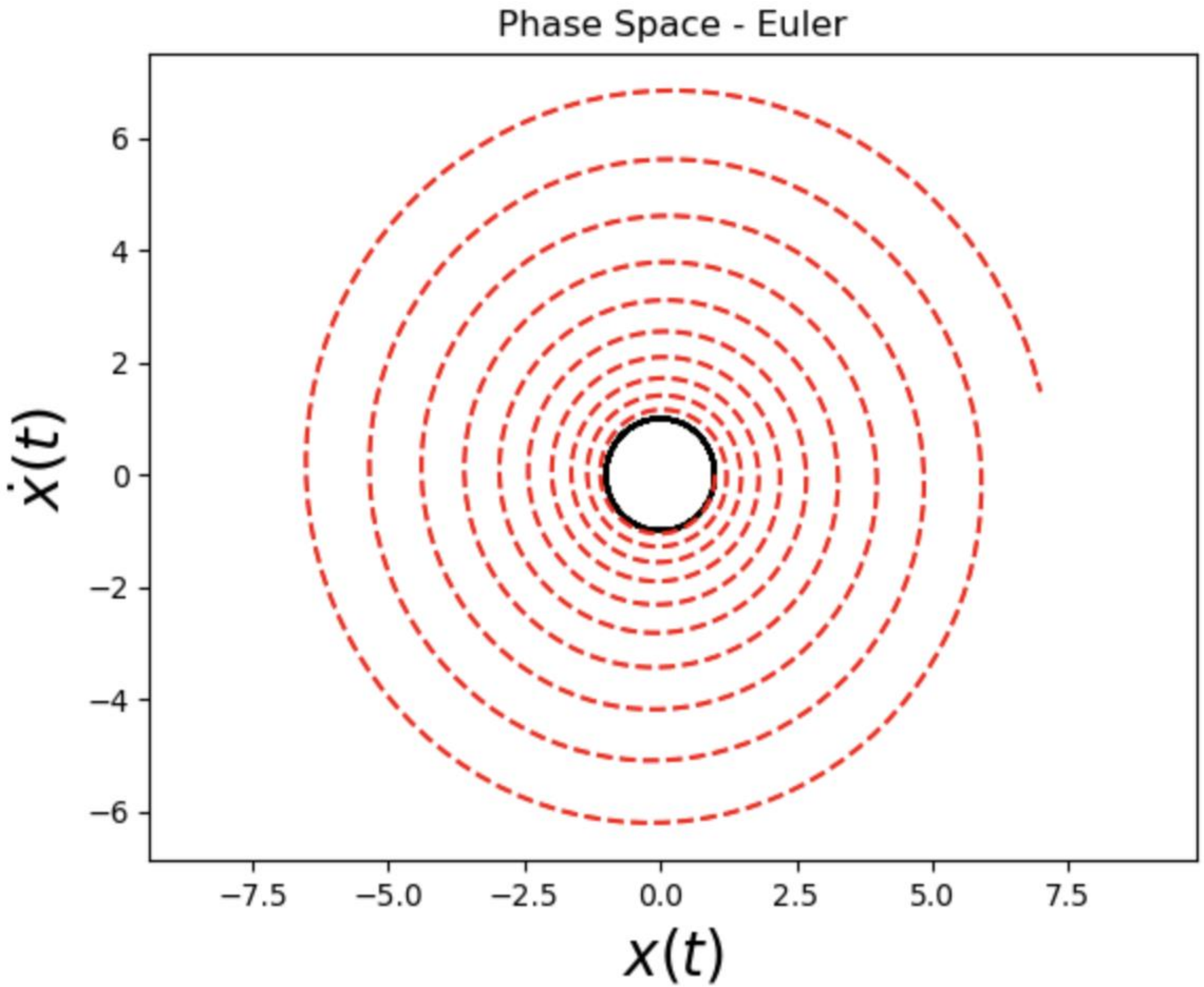

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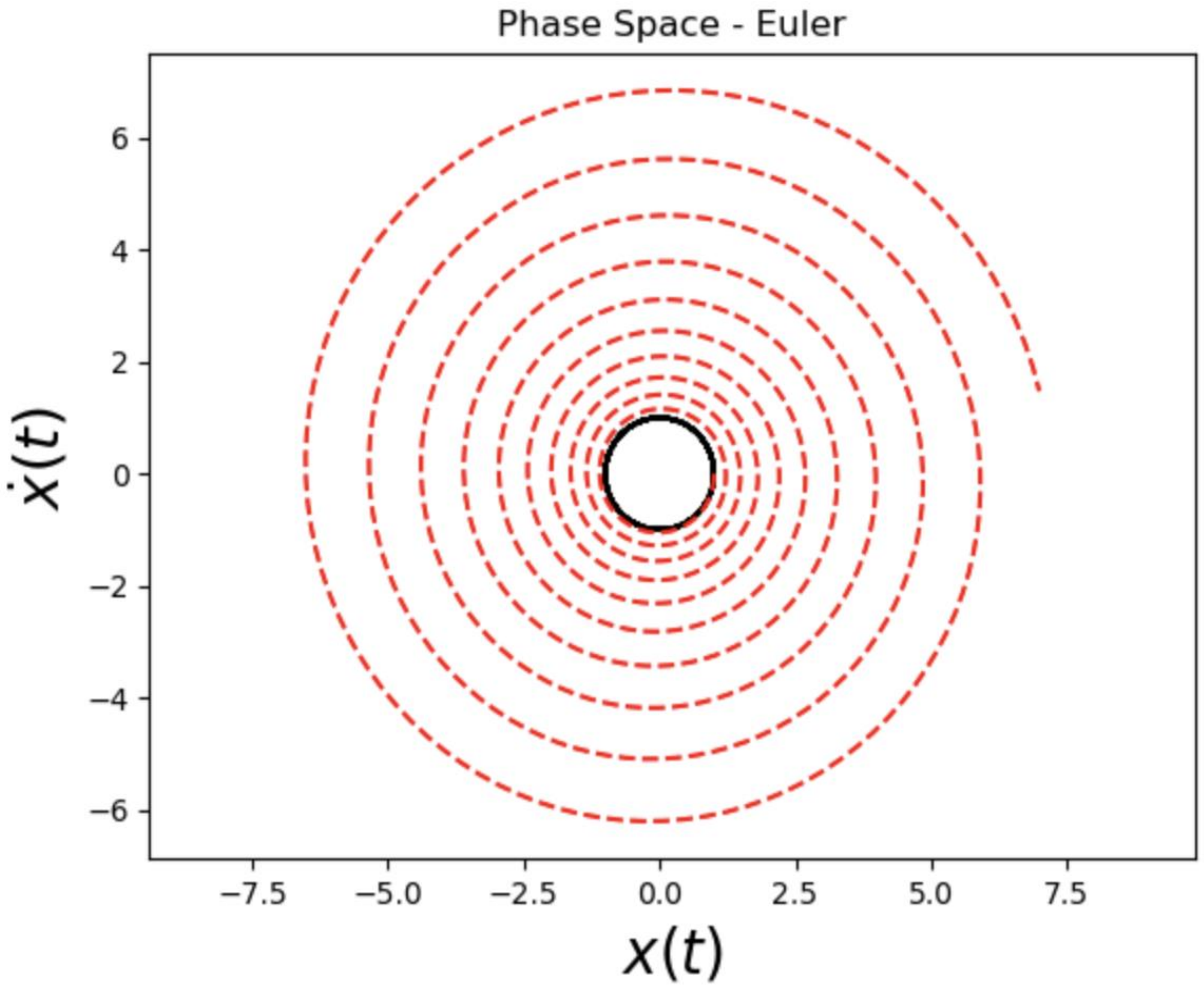

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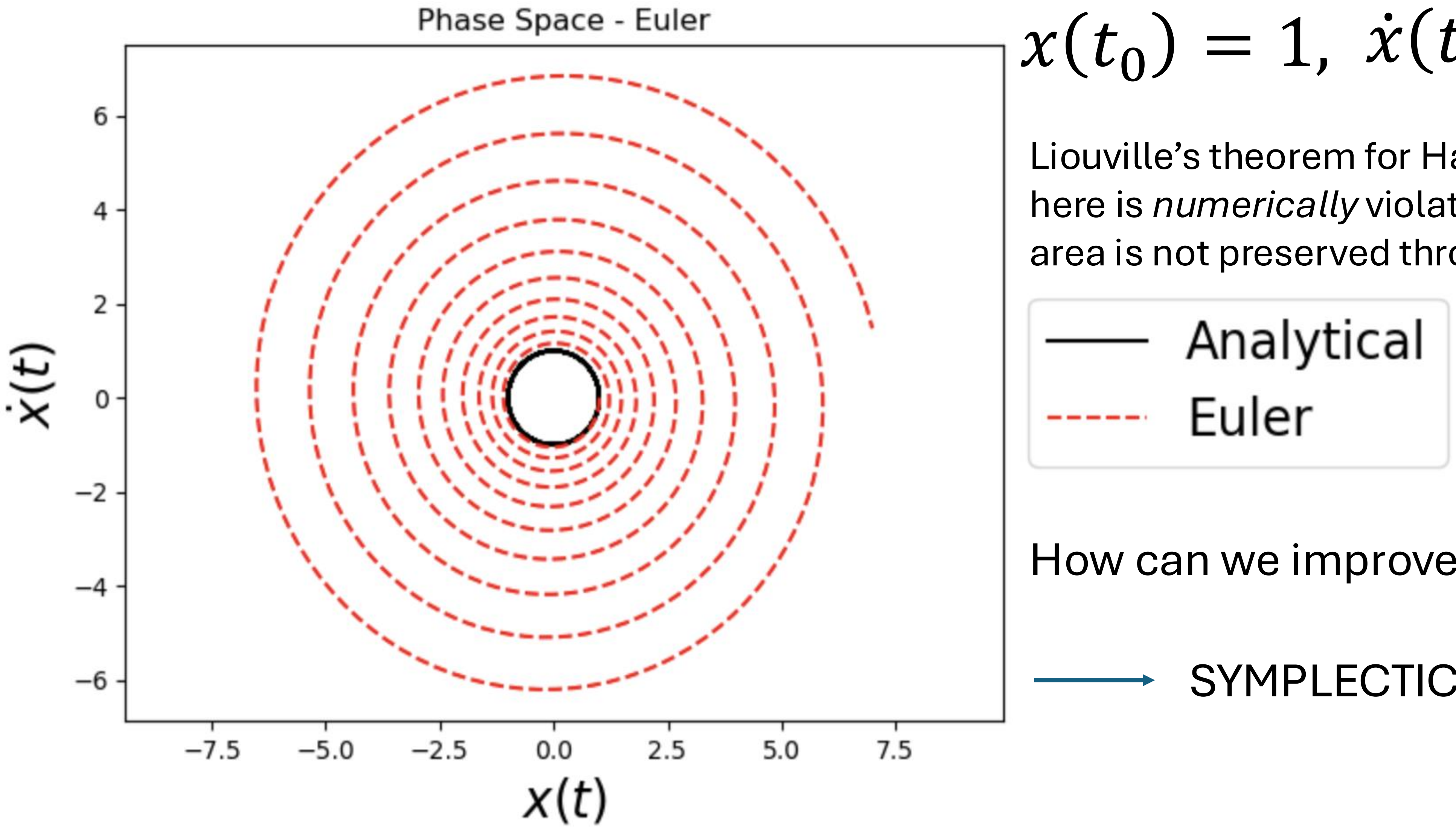

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→ SYMPLECTIC METHODS

Numerical schemes for Ordinary Differential Equations (ODEs)

Euler method does not preserve phase space area

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

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

Can we modify in order to have $\det \mathbb{J} = 1$?

$$\mathbb{J} = \begin{pmatrix} \dfrac{\partial x(t_1)}{\partial x(t_0)} & \dfrac{\partial x(t_1)}{\partial \dot{x}(t_0)} \\ \dfrac{\partial \dot{x}(t_1)}{\partial x(t_0)} & \dfrac{\partial \dot{x}(t_1)}{\partial \dot{x}(t_0)} \end{pmatrix} = \begin{pmatrix} 1 + (\Delta t)^2 \dfrac{\partial \mathcal{F}[x(t_0)]}{\partial x(t_0)} & \Delta t \\ \Delta t \dfrac{\partial \mathcal{F}[x(t_0)]}{\partial x(t_0)} & 1 \end{pmatrix}$$

$$\det \mathbb{J} = 1 + (\Delta t)^2 \frac{\partial \mathcal{F}[x(t_0)]}{\partial x(t_0)} - (\Delta t)^2 \frac{\partial \mathcal{F}[x(t_0)]}{\partial x(t_0)} = 1$$

Numerical schemes for Ordinary Differential Equations (ODEs)

SYMPLECTIC EULER

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

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→ Trajectories cannot go unbounded

→ Energy, even if not exactly conserved, is bounded

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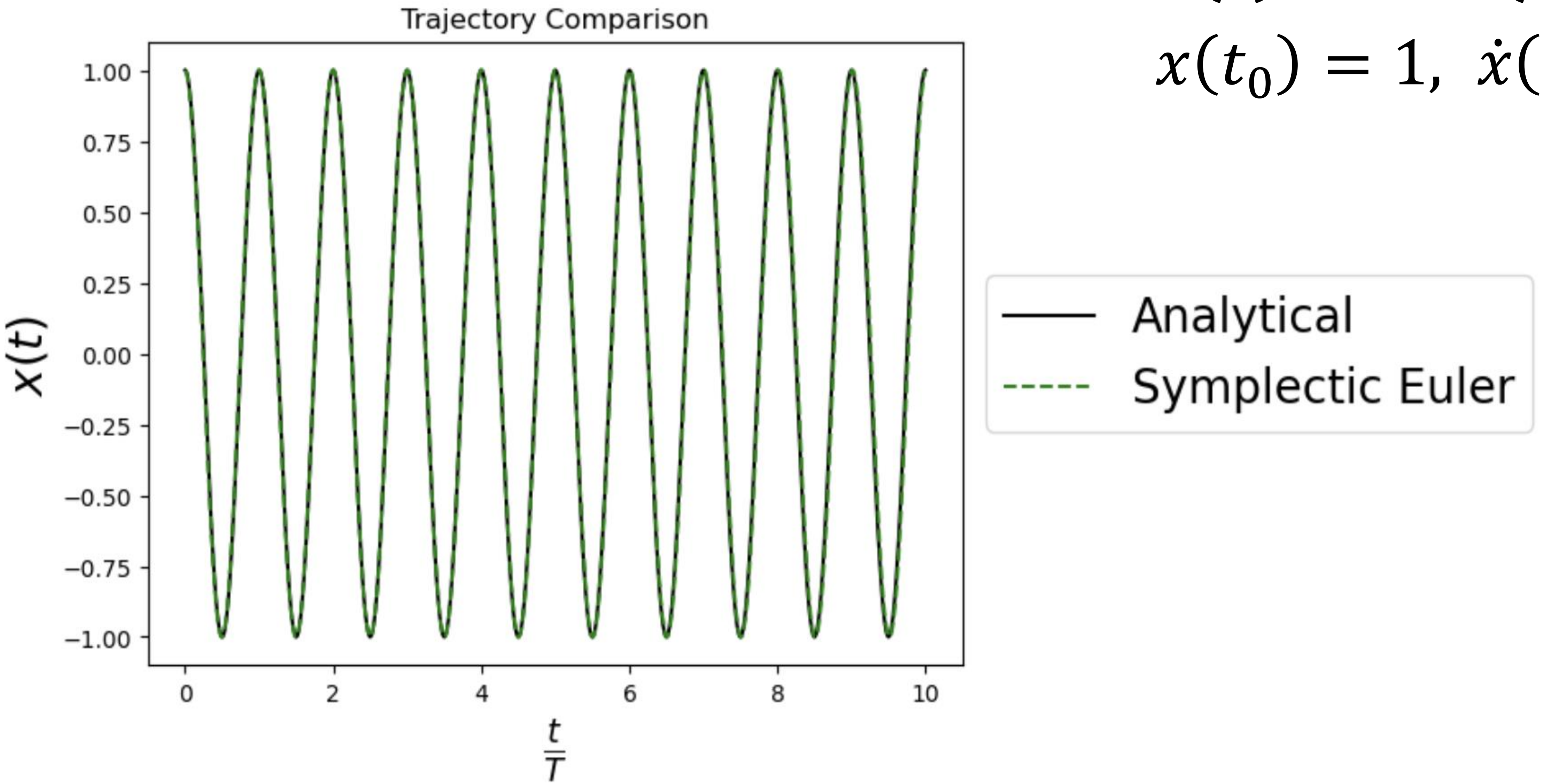
Let us apply it to the *1D HARMONIC OSCILLATOR*!

Numerical schemes for Ordinary Differential Equations (ODEs)

EXAMPLE: *1D HARMONIC OSCILLATOR*

$$\ddot{x}(t) = -x(t)$$

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



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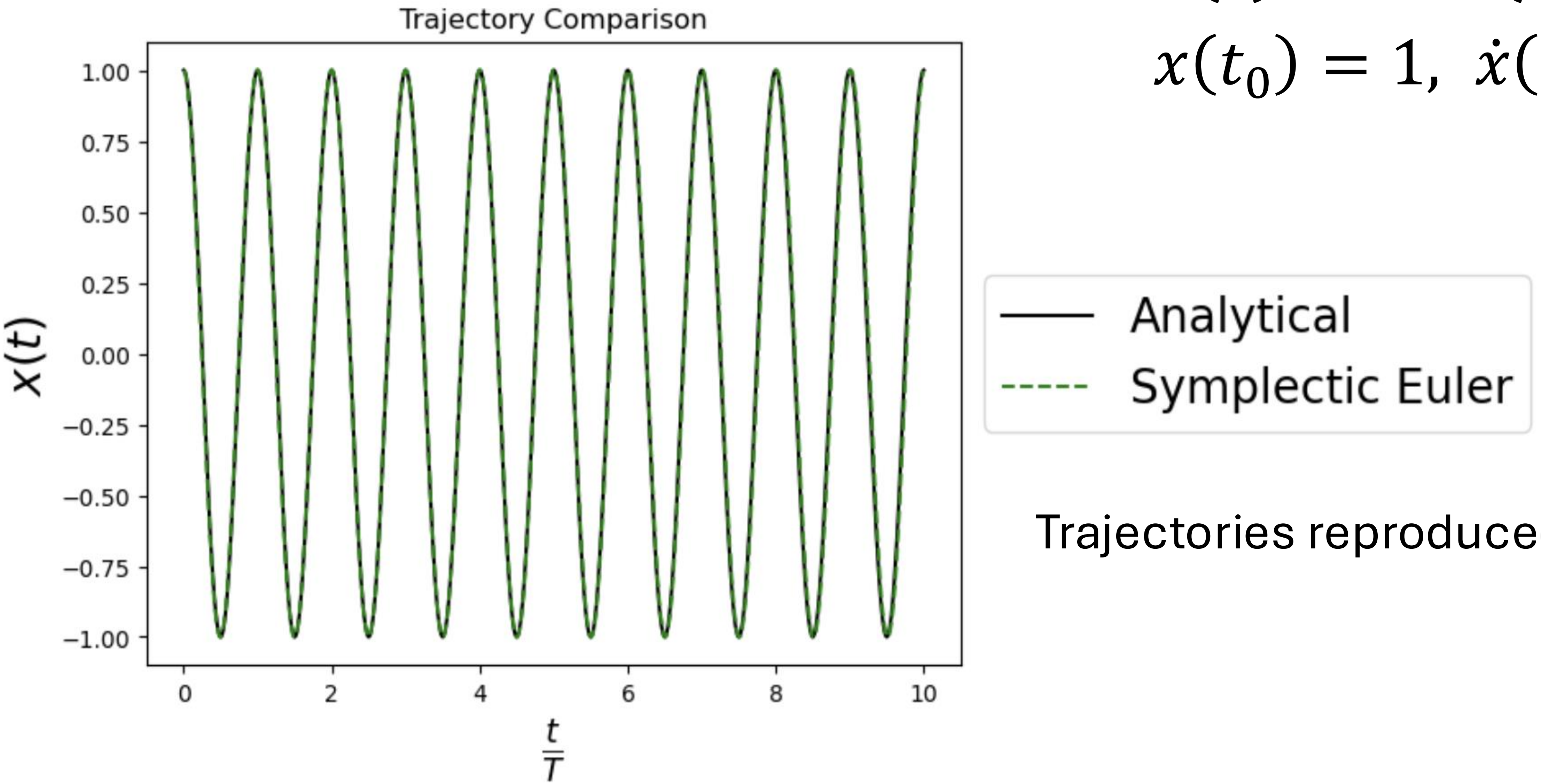

Trajectories reproduced ✓

Numerical schemes for Ordinary Differential Equations (ODEs)

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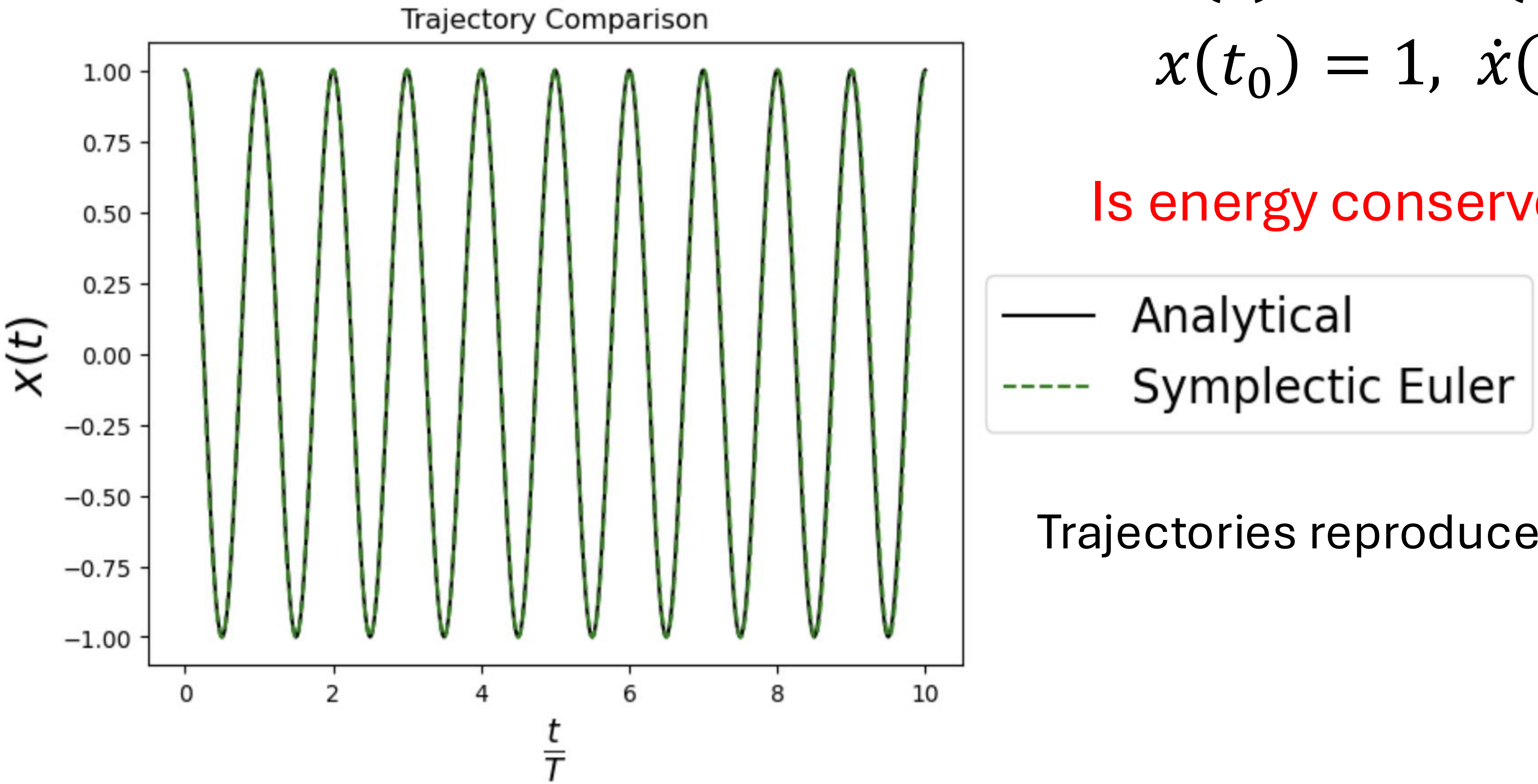

Is energy conserved?

Trajectories reproduced ✓

Numerical schemes for Ordinary Differential Equations (ODEs)

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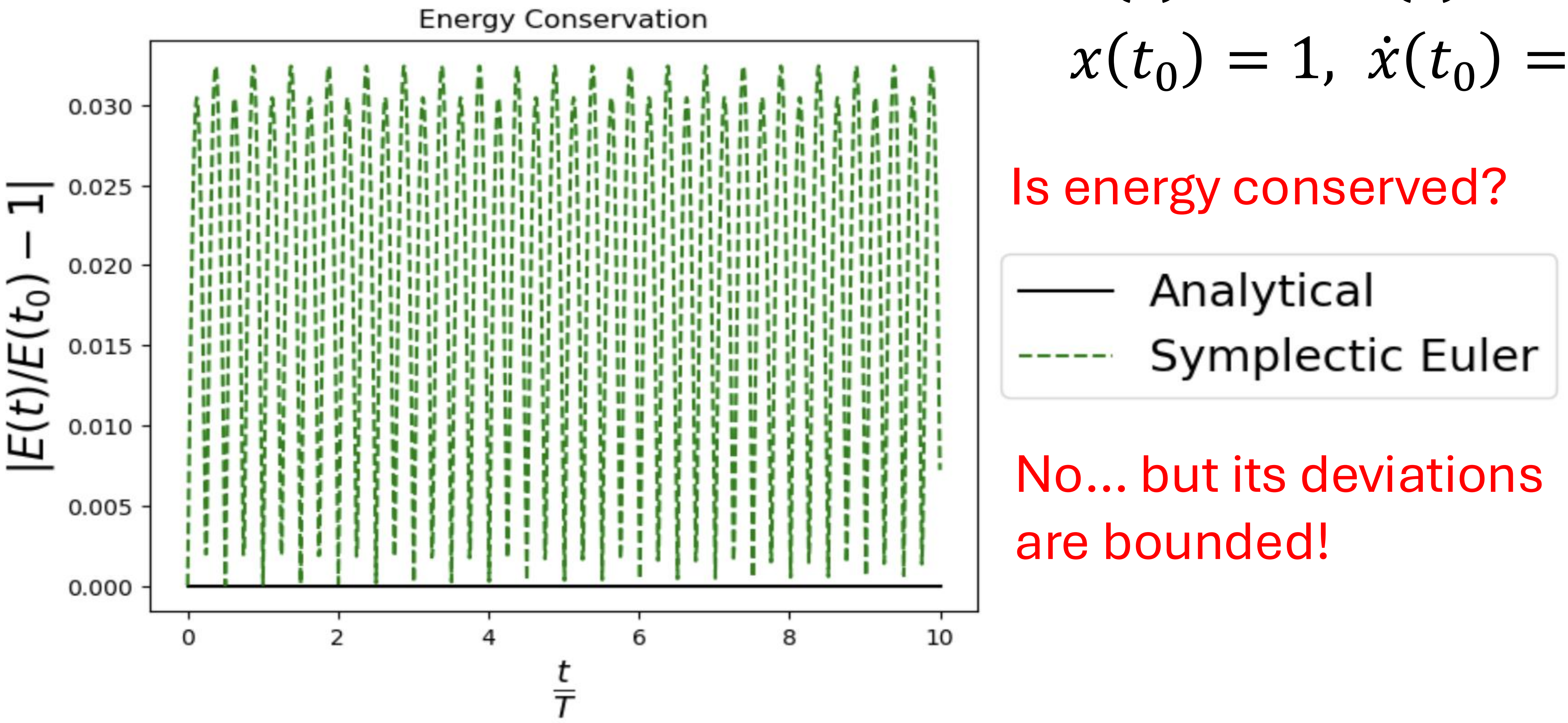

Is energy conserved?

No... but its deviations are bounded!

Numerical schemes for Ordinary Differential Equations (ODEs)

EXAMPLE: *1D HARMONIC OSCILLATOR*

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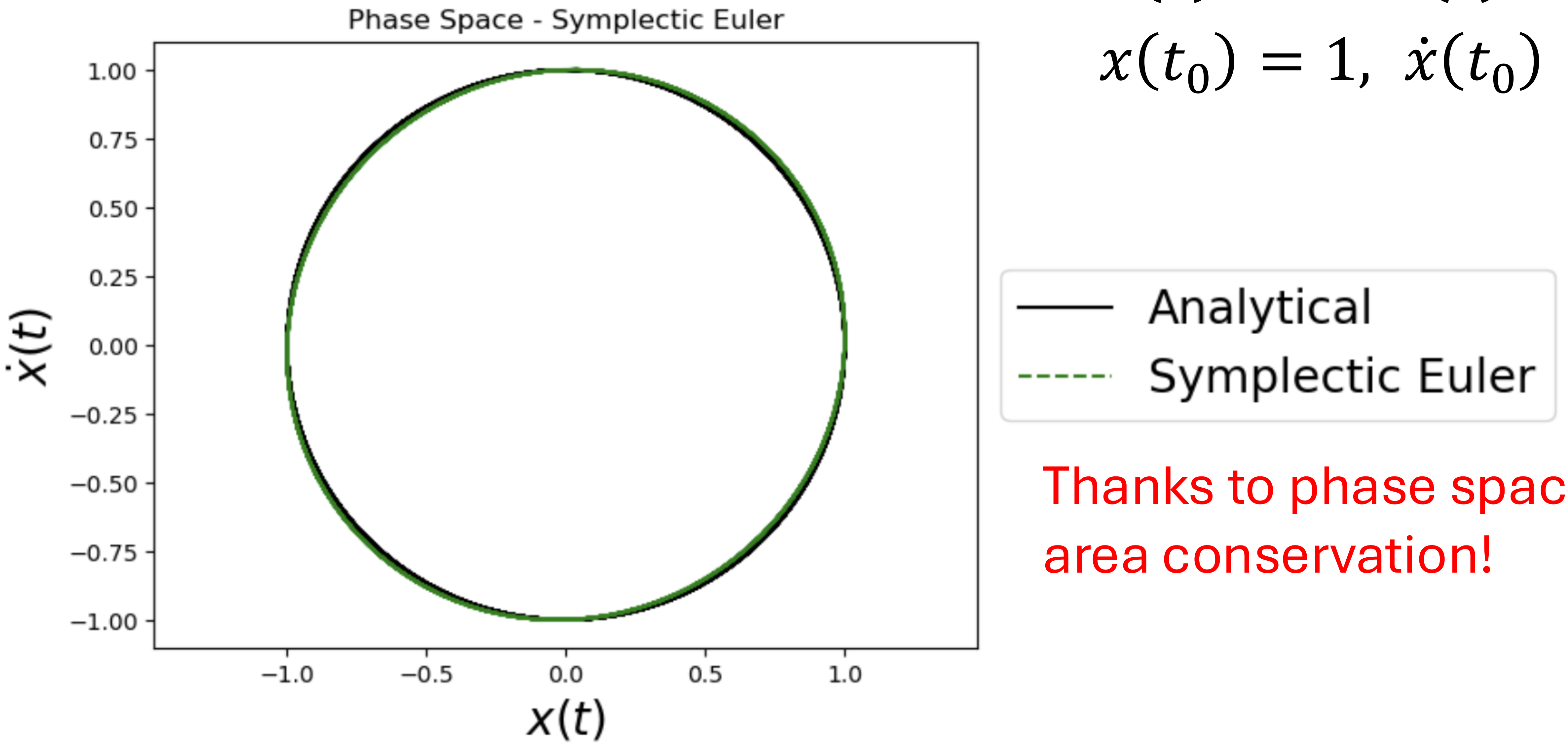

Thanks to phase space area conservation!

Symplectic methods

SYMPLECTIC EULER

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Symplectic Euler preserves phase space area $(\det \mathbb{J} = 1)$

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Consequence of the algorithmic structure but also of dealing with a CONSERVATIVE system

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$$\longrightarrow \det \mathbb{J} = 1 + \Delta t \frac{\partial \mathcal{F}}{\partial \dot{x}(t_0)} \neq 1$$

The algorithm is no longer symplectic

Symplectic methods

General property of symplectic methods

They are *simple and easy to write* for CONSERVATIVE SYSTEMS

Symplectic methods

General property of symplectic methods

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They are thus a natural choice for separable Hamiltonian systems

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

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

$$\begin{cases} \dot{x} = \dfrac{\partial H}{\partial p} = \dfrac{p}{m} \\ \ddot{x} = \dfrac{\dot{p}}{m} = -\dfrac{1}{m}\dfrac{\partial H}{\partial x} = -\dfrac{1}{m}\dfrac{\partial V}{\partial x} = \mathcal{F}[x(t)] \end{cases}$$

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... is a *first-order* method (*accurate to order Δt*)

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

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Difference between Taylor and algorithm (error) proportional to $(\Delta t)^2$!

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To reach a certain desired accuracy, one may need (depending on the problem) a very small Δt, which makes the computation longer!

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How to write a higher order symplectic method?

Symplectic methods $\ddot{x}(t) = \mathcal{F}[x(t)]$

Second order methods $\longrightarrow$ (staggered) LEAPFROG

Second order Taylor expansion gives

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

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Second order methods ⟶ (staggered) LEAPFROG

Second order Taylor expansion also for $\dot{x}\left(t_0 + \frac{\Delta t}{2}\right)$

$$x(t_0 + \Delta t) = x(t_0) + \Delta t\, \dot{x}\left(t_0 + \frac{\Delta t}{2}\right) + \mathcal{O}[(\Delta t)^3]$$

$$\dot{x}\left(t_0 + \frac{\Delta t}{2}\right) = \dot{x}\left(t_0 - \frac{\Delta t}{2}\right) + \Delta t\, \ddot{x}\left(t_0 - \frac{\Delta t}{2}\right) + \frac{1}{2}(\Delta t)^2 \dddot{x}\left(t_0 - \frac{\Delta t}{2}\right) + \mathcal{O}[(\Delta t)^3]$$

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If we compute x at integer timesteps and $\dot{x}$ at half-integer timesteps we find a simple second order symplectic method

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

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$$x(t_0) \longrightarrow x(t_0 + \Delta t)$$

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

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$x(t_0)$ $\qquad$ $x(t_0 + \Delta t)$

$\dot{x}\left(t_0 - \frac{\Delta t}{2}\right)$ $\qquad$ $\dot{x}\left(t_0 + \frac{\Delta t}{2}\right) \longrightarrow \dot{x}\left(t_0 + \frac{3\Delta t}{2}\right)$

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

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

If we compute x at integer timesteps and $\dot{x}$ at half-integer timesteps we find a simple second order symplectic method

$$x(t_0) \qquad\qquad x(t_0 + \Delta t) \longrightarrow x(t_0 + 2\,\Delta t)$$

$$\dot{x}\left(t_0 - \frac{\Delta t}{2}\right) \qquad \dot{x}\left(t_0 + \frac{\Delta t}{2}\right) \qquad \dot{x}\left(t_0 + \frac{3\Delta t}{2}\right) \qquad \ldots$$

Symplectic methods $\ddot{x}(t) = \mathcal{F}[x(t)]$

Second order methods $\longrightarrow$ (staggered) LEAPFROG

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

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

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However, measurement of several physical quantities may involve both x and $\dot{\mathrm{x}}$ at the same timestep

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If we compute x at integer timesteps and $\dot{x}$ at half-integer timesteps we find a simple second order symplectic method

However, measurement of several physical quantities may involve both x and $\dot{\mathrm{x}}$ at the same timestep

⟶ one more step needed (either advancing x or $\dot{x}$)

Symplectic methods

$$\ddot{x}(t) = \mathcal{F}[x(t)]$$

Second order methods $\longrightarrow$ (synchronized) LEAPFROG

$x(t_0),\ \dot{x}(t_0)$

Symplectic methods

$\ddot{x}(t) = \mathcal{F}[x(t)]$

Second order methods ⟶ (synchronized) LEAPFROG

$x(t_0), \dot{x}(t_0)$

Velocity Verlet (VV)

1)

2)

3)

Symplectic methods

$$\ddot{x}(t) = \mathcal{F}[x(t)]$$

Second order methods $\longrightarrow$ (synchronized) LEAPFROG

$x(t_0), \dot{x}(t_0)$

Velocity Verlet (VV)

1) Advance first the velocity by a half timestep

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

2)

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Symplectic methods

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Second order methods → (synchronized) LEAPFROG

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2) Advance the position using the velocity at half timestep

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

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Symplectic methods

$$\ddot{x}(t) = \mathcal{F}[x(t)]$$

Second order methods ⟶ (synchronized) LEAPFROG

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

3) Advance the velocity by another half timestep

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

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Second-order symplectic method → *accurate to order* $(\Delta t)^2$

Symplectic methods

$$\ddot{x}(t) = \mathcal{F}[x(t)]$$

Second order methods $\longrightarrow$ (synchronized) LEAPFROG $\quad x(t_0),\, \dot{x}(t_0)$

Position Verlet (PV)

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Symplectic methods

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$x(t_0),\ \dot{x}(t_0)$

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Symplectic methods

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Symplectic methods

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Second order methods $\longrightarrow$ (synchronized) LEAPFROG $\quad x(t_0),\ \dot{x}(t_0)$

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Second-order symplectic method → *accurate to order* $(\Delta t)^2$

Symplectic methods $\ddot{x}(t) = \mathcal{F}[x(t)]$

Higher order LEAPFROG $\longrightarrow$ YOSHIDA methods

[H. Yoshida, 1990]

Symplectic methods

$$\ddot{x}(t) = \mathcal{F}[x(t)]$$

Higher order LEAPFROG → **YOSHIDA methods**

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Instead of directly applying a synchronized leapfrog from t_0 to $t_0 + \Delta t$, we can split the timestep Δt in M sub-timesteps $\Delta t_i = \omega_i \Delta t$ $(i = 1,2,\dots,M)$ such that $\sum_{i=1}^{M} \omega_i = 1$

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Then apply Leapfrog (either VV or PV) M times in sequence (step i with timestep Δt_i)

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$$\begin{bmatrix} x(t_0) \\ \dot{x}(t_0) \end{bmatrix} \xrightarrow{\text{Leapfrog 1}} \begin{bmatrix} x(t_0 + \Delta t_1) \\ \dot{x}(t_0 + \Delta t_1) \end{bmatrix}$$

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There are specific values of M and ω_i which give accuracy to order $(\Delta t)^4$, $(\Delta t)^6$, $(\Delta t)^8$ ...

Symplectic methods

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Symplectic higher order methods require many steps but no auxiliary variables to store!

Non-symplectic methods

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

Non-symplectic methods

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

For *NON-CONSERVATIVE SYSTEMS* Liouville's theorem does not hold

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No reason to look for a symplectic method in these cases

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For *NON-CONSERVATIVE SYSTEMS* Liouville's theorem does not hold

No reason to look for a symplectic method in these cases

Runge Kutta methods are a natural choice for these systems
(easily generalized to high orders)

e. g. HYDRODYNAMICS

Non-symplectic methods

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

First order Runge-Kutta

Non-symplectic methods

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

First order Runge-Kutta (*Euler method*)

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

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

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→ Accurate to order $(\Delta t)^1$

Non-symplectic methods

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

Second order Runge-Kutta (*Modified Euler*)

Non-symplectic methods

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

Intermediate step

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

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

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Second order Runge-Kutta (*Modified Euler*)

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

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

Non-symplectic methods

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

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→ Accurate to order $(\Delta t)^2$

Non-symplectic methods

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

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Third order Runge-Kutta (*Williamson*)

Non-symplectic methods

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

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

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Third order Runge-Kutta (*Williamson*)

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

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

Non-symplectic methods

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

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Intermediate steps

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

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→ Accurate to order $(\Delta t)^3$

Non-symplectic methods

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

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Intermediate steps

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

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Non-symplectic higher order methods require auxiliary variables...

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

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→ Accurate to order $(\Delta t)^3$

Non-symplectic methods

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

given $x(t_0), \dot{x}(t_0)$

... however some schemes require only few extra variables

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 to order $(\Delta t)^3$

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Intermediate steps

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

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Low-storage

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

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→ Accurate to order $(\Delta t)^3$

Non-symplectic methods

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

Third order Runge-Kutta (*Williamson*) $\longleftarrow$ Low-storage

Non-symplectic methods

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

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

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

Non-symplectic methods

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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

$$\left.\begin{aligned} x^{(0)} &= x(t_0) \\ \dot{x}^{(0)} &= \dot{x}(t_0) \end{aligned}\right] \text{ degrees of freedom}$$

Non-symplectic methods

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

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STEP 0

$$\left.\begin{aligned} x^{(0)} &= x(t_0) \\ \dot{x}^{(0)} &= \dot{x}(t_0) \end{aligned}\right] \text{ degrees of freedom}$$

$$\left.\begin{aligned} \delta x^{(0)} &= \Delta t\, \dot{x}^{(0)} \\ \delta \dot{x}^{(0)} &= \Delta t\, \mathcal{F}[x^{(0)}, \dot{x}^{(0)}] \end{aligned}\right] \text{ extra variables to store}$$

Non-symplectic methods

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

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

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

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

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

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

Non-symplectic methods

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

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

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

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

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

STEP 1

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

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

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

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Non-symplectic methods

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

STEP 1

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STEP 2

Non-symplectic methods

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

Third order Runge-Kutta (*Williamson*) $\longleftarrow$ Low-storage

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

STEP 0

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

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

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

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

STEP 1

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

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

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STEP 2

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

Non-symplectic methods

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

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STEP 1

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

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STEP 2

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

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

Non-symplectic methods

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

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STEP 2

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

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

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

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For STEP 3 we only need

$x^{(2)}, \dot{x}^{(2)}, \delta x^{(2)}, \delta \dot{x}^{(2)}$

Non-symplectic methods

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

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STEP 3

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

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

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STEP 3

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

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

Leapfrog vs Runge Kutta

EXAMPLE: *1D DAMPED OSCILLATOR*

$$\ddot{x}(t) = -\omega^2 x(t) - 2\gamma\dot{x}(t)$$

Leapfrog vs Runge Kutta

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The system has the following analytical solution ($\gamma^2 < \omega^2$)

$$x(t) = e^{-\gamma t}\left[A\cos\sqrt{\omega^2-\gamma^2}\,t + B\sin\sqrt{\omega^2-\gamma^2}\,t\right]$$

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We can adapt a second order Velocity Verlet (VV2)...

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

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

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Leapfrog vs Runge Kutta

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... and compare it with the result given by a second order Runge-Kutta (RK2 – Modified Euler)

Leapfrog vs Runge Kutta

$$\ddot{x}(t) = -\omega^2 x(t) - 2\gamma\dot{x}(t)$$

EXAMPLE: *1D DAMPED OSCILLATOR*

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

$\omega^2 = 1, \gamma = 0.1$

Pseudoperiod $T = \frac{2\pi}{\sqrt{\omega^2 - \gamma^2}}$

$\Delta t = T/100$

Leapfrog vs Runge Kutta

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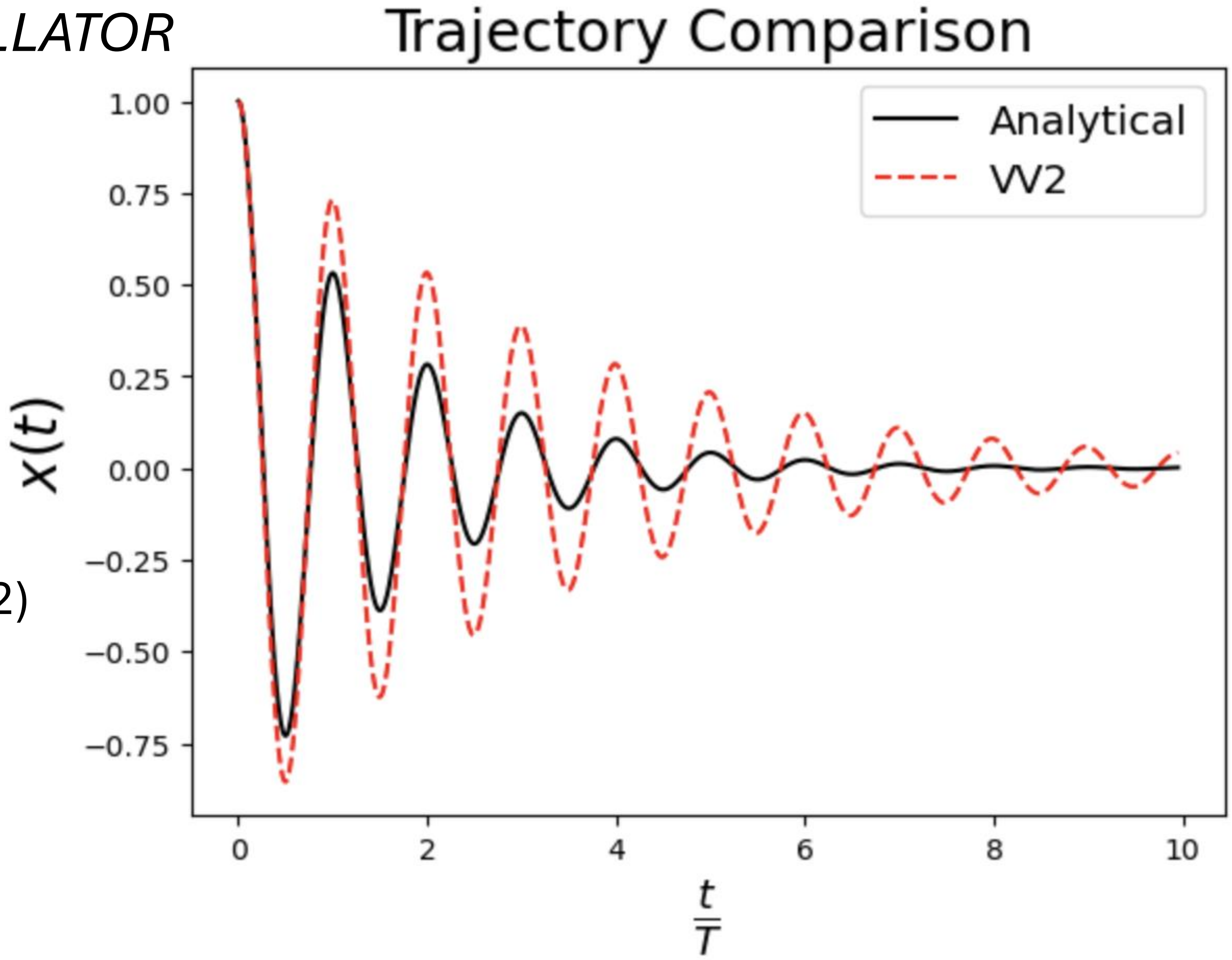
Second-order Velocity Verlet (VV2) does not reproduce correctly the analytical solution



Leapfrog vs Runge Kutta

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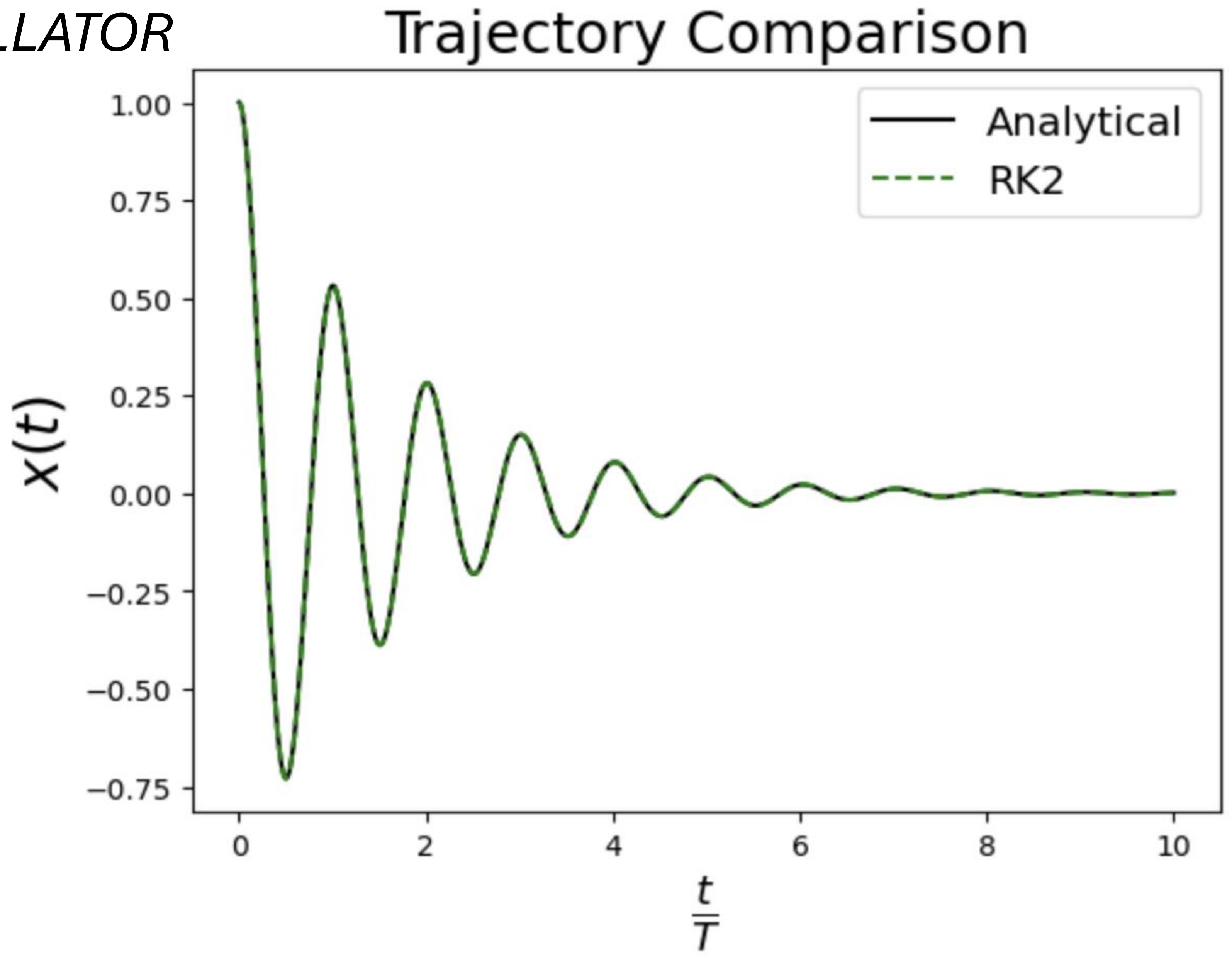
$\Delta t = T/100$

Second-order Runge-Kutta (RK2) follows correctly the damping of the analytical solution



Numerical schemes for Partial Differential Equations (PDEs)

How to deal with PDEs? $\ddot{f}(x,t) = \mathcal{F}\left[f(x,t), \dot{f}(x,t), \partial_x f(x,t), \ldots\right]$

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We have shown timestepping schemes for the case

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However, once all derivative operators are discretized
(i.e. written as a linear superposition of field values at difference lattice points),
PDEs become ODEs *in the lattice*

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However, once all derivative operators are discretized
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PDEs become ODEs *in the lattice*

How to discretize derivative operators? $\longrightarrow$ see Part II

Conclusions of part I

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- Symplectic methods are a natural approach for conservative systems $\ddot{x}(t) = \mathcal{F}[x(t)]$

- Runge-Kutta methods are a natural approach for non-conservative systems $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

- What is the best algorithm depends on the physical problem!

Conclusions of part I

- Symplectic methods are a natural approach for conservative systems $\ddot{x}(t) = \mathcal{F}[x(t)]$

- Runge-Kutta methods are a natural approach for non-conservative systems $\ddot{x}(t) = \mathcal{F}[x(t), \dot{x}(t)]$

- What is the best algorithm depends on the physical problem!

THANKS FOR YOUR ATTENTION!