

Numerical Methods for Astrophysics:

ORDINARY DIFFERENTIAL EQUATIONS (ODEs)

Part 1

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Ordinary Differential Equations (ODEs). Concept

ODEs ARE UBIQUITOUS IN ASTROPHYSICS

Examples:

- equation of motion of a particle subject to Newton's gravitational force

$$\frac{d^2 \mathbf{x}_i}{dt^2} = -G \sum_{j=1, j \neq i}^N m_j \frac{\mathbf{x}_i - \mathbf{x}_j}{|\mathbf{x}_i - \mathbf{x}_j|^3}$$

- equation of hydrostatic equilibrium of a star interior

$$\frac{dP}{dr} = -G \frac{M \rho}{r^2}$$

ODEs. Euler Method

General form of an ODE in 1 variable: $\frac{dx}{dt} = f(x, t)$

For simplicity, let's assume t is time

Simplest way to proceed: TAYLOR EXPANSION

$$x(t + h) = x(t) + \frac{dx}{dt} h + \frac{1}{2} \frac{d^2x}{dt^2} h^2 + \dots$$

or with different notation

$$x(t + h) = x(t) + h f(x, t) + \mathcal{O}(h^2)$$

If we neglect higher order terms we can calculate $x(t+h)$ as

$$x(t + h) = x(t) + h f(x, t)$$

**equation of the
Euler scheme**

if we know the value of x at time t , then we can derive the value of x at time $(t+h)$

This approximation is “good” if h is small

ODEs. Euler Method

Equation of the Euler's method: $x(t + h) = x(t) + h f(x, t)$

To integrate the ODE between $t = t_0$ and $t = t_f$

I need to choose a $h \ll (t_f - t_0)$

and then to repeat Euler's equation for N steps with

$$N = (t_f - t_0) / h$$

Euler equation is 1st order method → errors scale as h^2

→ we can reduce the error by reducing h

but if we reduce h the computing time increases

We will see other methods that have a smaller error
for the same (or similar) computing time

ODEs. Runge-Kutta family

Family of algorithms that solve ODEs via Taylor's expansion

First order: Euler method or first-order Runge-Kutta method

Second order: midpoint or second-order Runge-Kutta method

Fourth order: fourth-order Runge-Kutta method

etcetc

ODEs. Midpoint or second-order Runge-Kutta method

Evaluate the slope dx/dt of $x(t)$

not at the end of the interval h , but at the midpoint of the interval $h/2$

Mathematically, corresponds to a Taylor expansion around $t+h/2$ instead that around t

$$x(t+h) = x\left(t + \frac{1}{2}h\right) + \frac{1}{2}h \left(\frac{dx}{dt}\right)_{t+\frac{1}{2}h} + \frac{1}{8}h^2 \left(\frac{d^2x}{dt^2}\right)_{t+\frac{1}{2}h} + \mathcal{O}(h^3)$$

$$x(t) = x\left(t + \frac{1}{2}h\right) - \frac{1}{2}h \left(\frac{dx}{dt}\right)_{t+\frac{1}{2}h} + \frac{1}{8}h^2 \left(\frac{d^2x}{dt^2}\right)_{t+\frac{1}{2}h} + \mathcal{O}(h^3)$$

Subtracting the second expression from the first, we get

$$\begin{aligned} x(t+h) &= x(t) + h \left(\frac{dx}{dt}\right)_{t+\frac{1}{2}h} + \mathcal{O}(h^3) \\ &= x(t) + h f\left(x\left(t + \frac{1}{2}h\right), t + \frac{1}{2}h\right) + \mathcal{O}(h^3) \end{aligned}$$

The error scales as $h^3 \rightarrow$ is a second-order scheme

BUT THERE IS A PROBLEM HERE

ODEs. Midpoint or second-order Runge-Kutta method

PROBLEM:

$$x(t+h) = x(t) + h \left(\frac{dx}{dt} \right)_{t+\frac{1}{2}h} + \mathcal{O}(h^3)$$
$$= x(t) + h f \left(x \left(t + \frac{1}{2}h \right), t + \frac{1}{2}h \right) + \mathcal{O}(h^3)$$

This eq. **requires that we know $x(t+h/2)$ which we still do not know**

IMPLICIT SCHEME: method that depends on quantities that we still need to calculate (because they refer to the next step)

vs EXPLICIT SCHEME: method depending only on quantities that we already know (because they refer to current step)

ODEs. Midpoint or second-order Runge-Kutta method

PROBLEM:

$$x(t+h) = x(t) + h \left(\frac{dx}{dt} \right)_{t+\frac{1}{2}h} + \mathcal{O}(h^3)$$
$$= x(t) + h f \left(x \left(t + \frac{1}{2}h \right), t + \frac{1}{2}h \right) + \mathcal{O}(h^3)$$

This eq. **requires that we know $x(t+h/2)$ which we still do not know**

We get around this problem by approximating $x(t+h/2)$

with the Euler method $x \left(t + \frac{h}{2} \right) = x(t) + \frac{h}{2} f(x(t), t)$ **where** $f(x(t), t) = \frac{dx}{dt}$

and then substituting into the above equation:

$$k_1 = \frac{h}{2} f(x(t), t)$$
$$k_2 = h f \left(x(t) + k_1, t + \frac{h}{2} \right)$$
$$x(t+h) = x(t) + k_2$$

equation of the midpoint scheme

which is the practical implementation of the midpoint scheme

ODEs. Fourth-order Runge-Kutta method

We can use the same approach to go to higher order i.e.

- * by using Taylor expansion
- * by evaluating the ODE in several intermediate time steps

With calculations, we derive the fourth-order Runge-Kutta as

$$\begin{aligned}k_1 &= \frac{1}{2} h f(x, t) \\k_2 &= \frac{1}{2} h f\left(x + k_1, t + \frac{1}{2}h\right) \\k_3 &= h f\left(x + k_2, t + \frac{1}{2}h\right) \\k_4 &= h f(x + k_3, t + h) \\x(t + h) &= x(t) + \frac{1}{6} (2 k_1 + 4 k_2 + 2 k_3 + k_4)\end{aligned}$$

- * Errors scale as h^5
- * Fourth-order Runge-Kutta (RK4) is considered the best match between accuracy and not-too-complicated programming

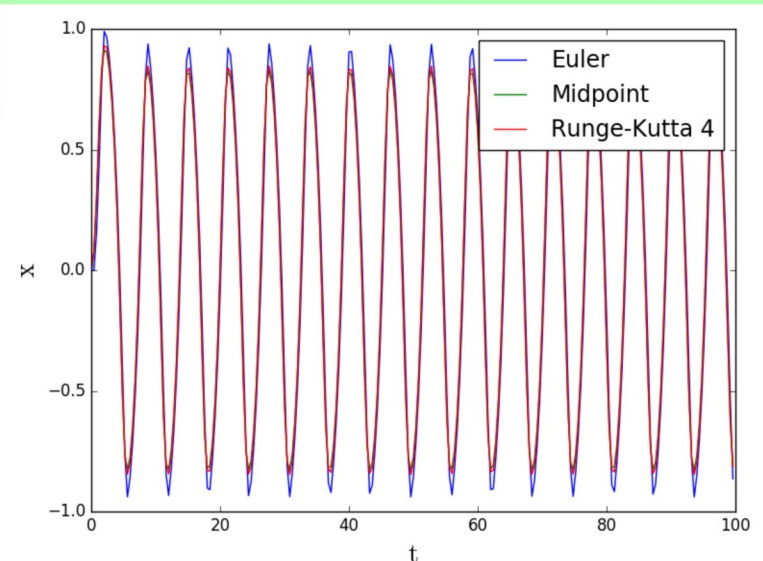
ODEs. EXERCISE on Euler, Midpoint, Runge-Kutta 4

EXERCISE:

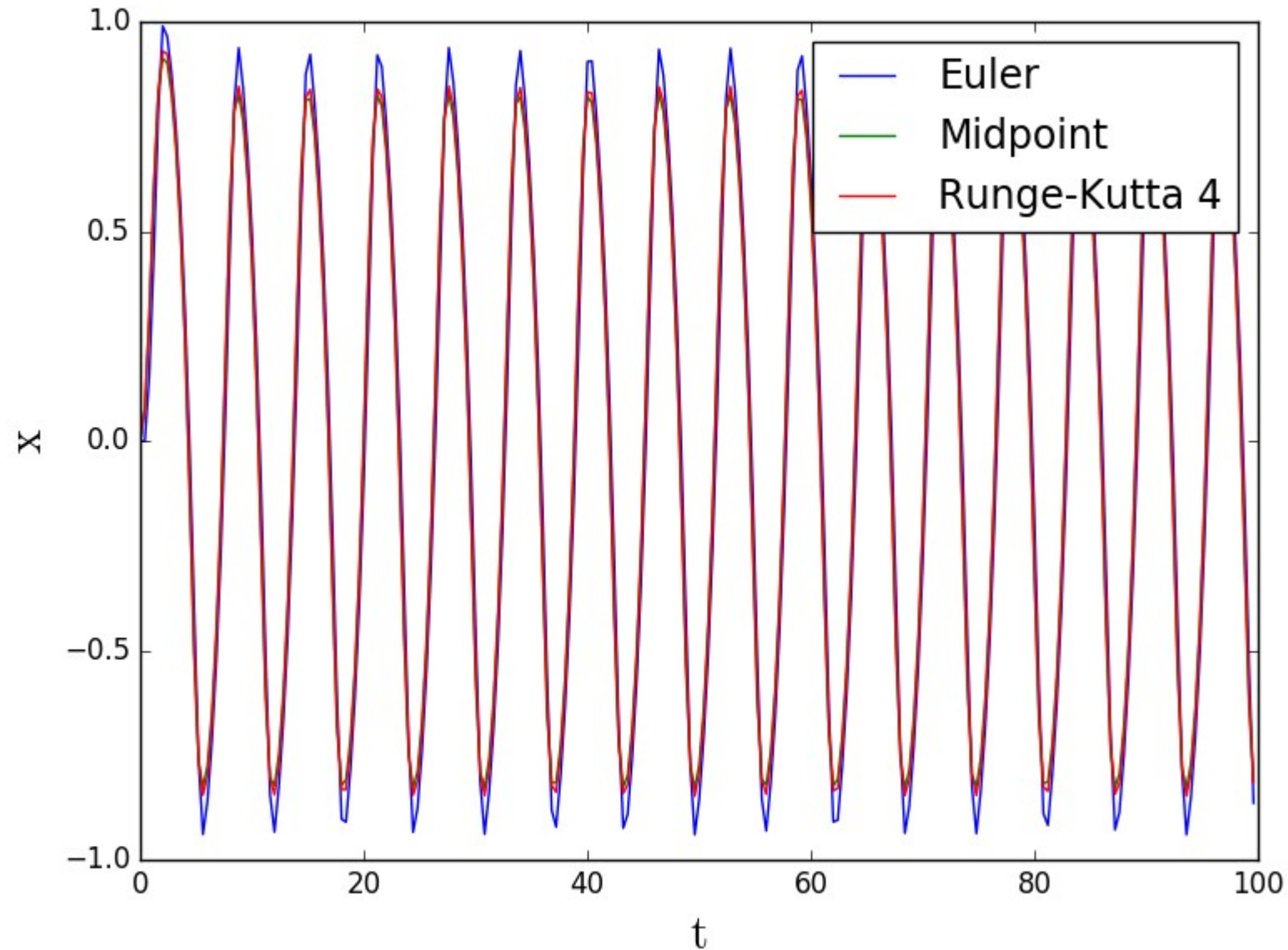
Write a python script to implement the Euler's method, the midpoint method and the fourth-order Runge-Kutta method. Use this script to integrate the following differential equation:

$$\frac{dx}{dt} = -x^3 + \sin t \quad (146)$$

Compare the results. For a choice of initial time $t_0 = 0.0$, final time $t_{\text{fin}} = 100$, initial position $x(t_0) = 0.0$ and step-size $h = 0.4$, you should obtain something similar to Figure 41.



ODEs. EXERCISE on Euler, Midpoint, Runge-Kutta 4



ODEs. Systems of ordinary differential equations

Same approach as we have seen in the previous sections, provided that the derivatives are with respect to a single variable

$$\frac{dx}{dt} = f_1(x, y, t)$$
$$\frac{dy}{dt} = f_2(x, y, t)$$

They must be integrated in the same timestep, simultaneously, to avoid mismatch between x and y

In contrast, partial differential equations require a different treatment

$$\frac{\partial x}{\partial t} + \frac{\partial x}{\partial s} = f_1(x, y, t, s)$$
$$\frac{\partial y}{\partial t} + \frac{\partial y}{\partial s} = f_2(x, y, t, s),$$

ODEs. Second-order and higher-order ODEs

Solving second-order (or higher-order) ODEs with one variable is trivial once we know how to solve first-order ODEs.

$$\frac{d^2x}{dt^2} = f\left(x, \frac{dx}{dt}, t\right)$$

Can be rewritten as a **SYSTEM** of **TWO FIRST-ORDER ODES**

$$\begin{cases} \frac{dx}{dt} = y \\ \frac{dy}{dt} = f(x, y, t) \end{cases}$$

Solve this system using the algorithms we learnt for first-order ODEs.

To solve higher ODEs, we repeat this trick till we have a system of first-order ODEs only.

ODEs. Second-order and higher-order ODEs

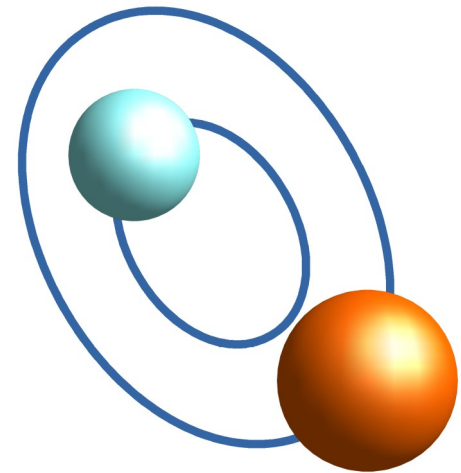
CLASSICAL EXAMPLE of 2nd order ODE for astrophysicists:

equation of motion of a star in a binary system

$$\frac{d^2 \vec{x}_i}{dt^2} = -G m_j \frac{\vec{x}_i - \vec{x}_j}{|\vec{x}_i - \vec{x}_j|^3}$$

can be rewritten as

$$\left\{ \begin{array}{l} \frac{d\vec{x}_i}{dt} = \vec{v}_i \\ \frac{d\vec{v}_i}{dt} = -G m_j \frac{\vec{x}_i - \vec{x}_j}{|\vec{x}_i - \vec{x}_j|^3} \end{array} \right.$$



ODEs. Astrophysical N-body problem

Integration of the equations of motion for N –bodies subject to Newton's gravity force (1687)

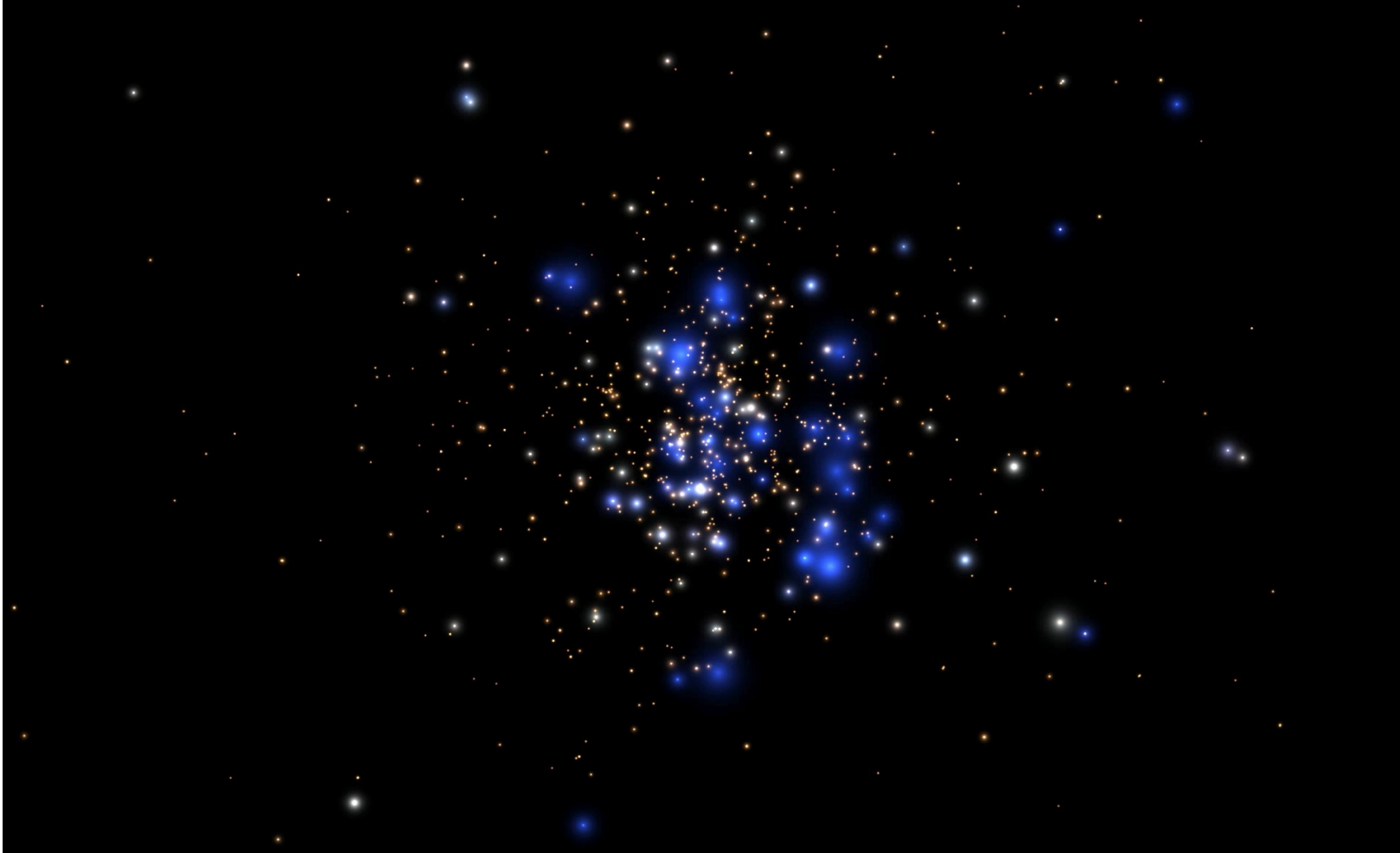
$$\frac{d^2 \mathbf{x}_i}{dt^2} = -G \sum_{j=1, j \neq i}^N m_j \frac{\mathbf{x}_i - \mathbf{x}_j}{|\mathbf{x}_i - \mathbf{x}_j|^3}$$

can be split into a system of 2 first-order ODEs

$$\left\{ \begin{array}{l} \frac{d\mathbf{v}_i}{dt} = -G \sum_{j=1, j \neq i}^N m_j \frac{\mathbf{x}_i - \mathbf{x}_j}{|\mathbf{x}_i - \mathbf{x}_j|^3}, \\ \frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i \end{array} \right.$$

ODEs. Astrophysical N-body problem

It is the first thing you need to solve to simulate a star cluster



The second thing you need is stellar evolution

ODEs. Astrophysical N-body problem

- This eq. can be solved analytically for $N = 2$ (Bernoulli solution, 1710).
- In 1885, a challenge was proposed, to be answered before January 21st 1889, in honour of the 60th birthday of King Oscar II of Sweden and Norway:

“Given a system of arbitrarily many mass points that attract each according to Newton’s law, under the assumption that no two points ever collide, try to find a representation of the coordinates of each point as a series in a variable that is some known function of time and for all of whose values the series converges uniformly.”

Nobody found the solution, although many participated (including Henry Poincaré).

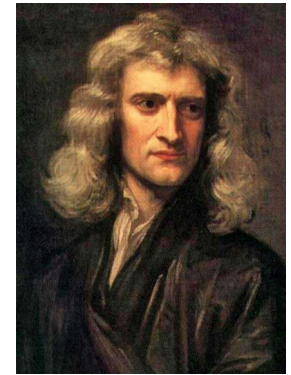
- **1991: the mathematician Qiudong Wang found the first convergent power series solution for a generic number of bodies.**

However, the solution by Q. Wang is too difficult to implement and slow to convergence.

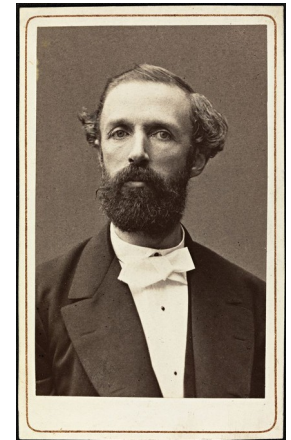
Thus, everybody solves Newton’s equation numerically for $N \geq 3$.



Bernoulli



Newton



*Oscar II
of Sweden*



Q. Wang

ODEs. Astrophysical N-body problem

Newton's equation can be solved with Runge-Kutta methods.
For example, the Euler scheme:

$$x(t + h) = x(t) + h f(x, t)$$



$$\vec{a}_i(t) = -G \sum_{j=1, j \neq i}^N m_j \frac{\vec{x}_i(t) - \vec{x}_j(t)}{|\vec{x}_i(t) - \vec{x}_j(t)|^3}$$

$$\vec{x}_i(t + h) = \vec{x}_i(t) + \vec{v}_i(t) h$$

$$\vec{v}_i(t + h) = \vec{v}_i(t) + \vec{a}_i(t) h$$

ODEs. EXERCISE on binary star with Euler

Newton's equation can be solved with Runge-Kutta methods.
For example, the Euler scheme:

EXERCISE:

Write a new script to implement Euler's method to evolve a system of two points in two dimensions (xy plane), subject to gravity forces, with the following initial conditions. Initial positions of particles 1 and 2 (in the plane xy): $\mathbf{x} = (1.0, -1.0)$, $\mathbf{y} = (1.0, -1.0)$.

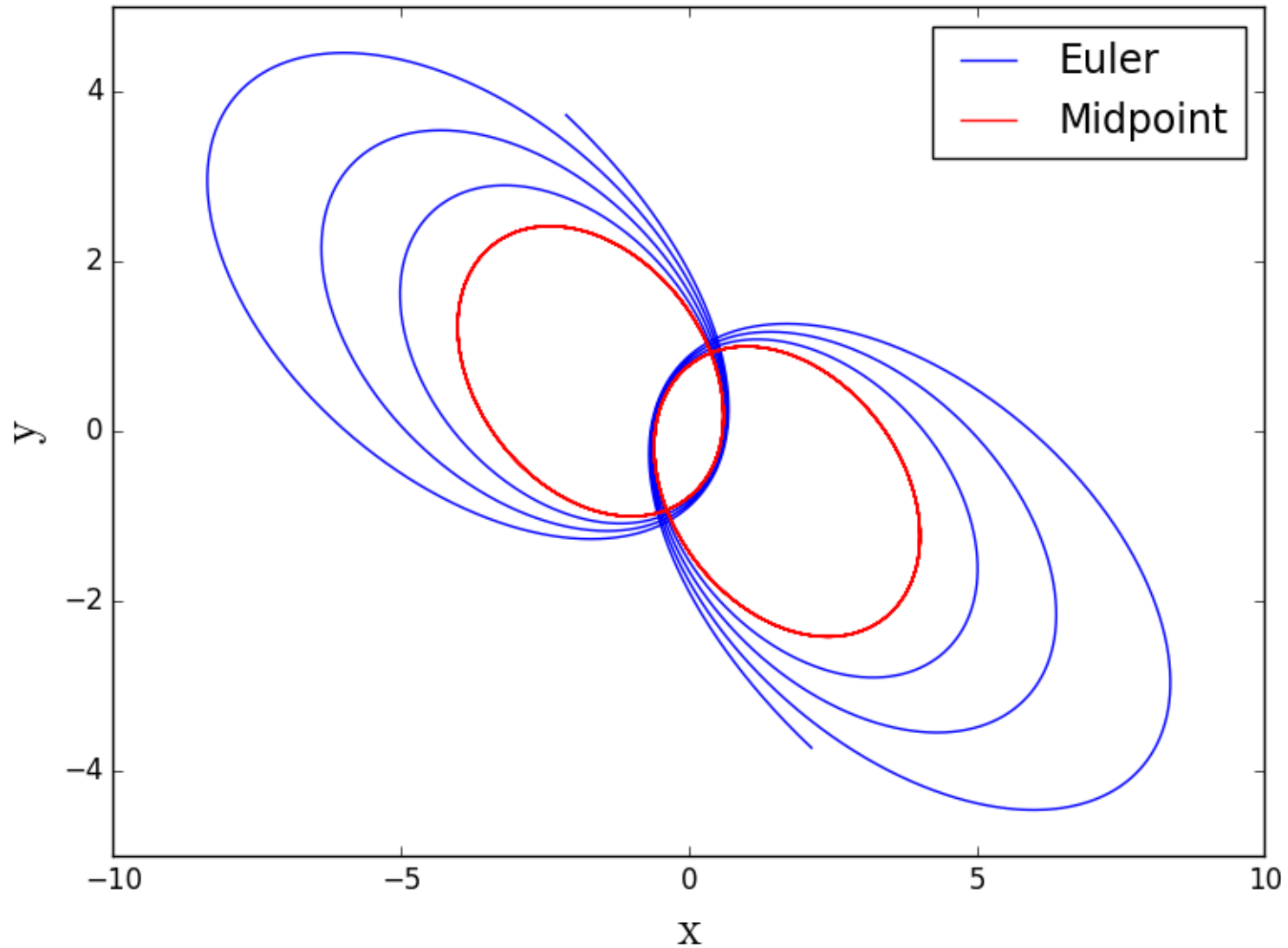
Initial velocities of particles 1 and 2 (in the plane xy): $\mathbf{v}_x = (-0.5, 0.5)$, $\mathbf{v}_y = (0.0, 0.0)$.

Let us assume that the masses are $m_1 = m_2 = 1$, and the gravity constant in our units is $G = 1$.

Let us assume $t_0 = 0$, $t_{\text{fin}} = 300$ and $h = 0.01$. The result should look like the blue line in Figure 42.

ODEs. EXERCISE on binary star with Euler

Result of previous exercise is the blue line:



ODEs. Midpoint & the astrophysical N-body problem

General expression of the midpoint scheme

$$k_1 = \frac{h}{2} f(x(t), t)$$
$$k_2 = h f\left(x(t) + k_1, t + \frac{h}{2}\right)$$
$$x(t+h) = x(t) + k_2$$

How does it look like when applied to the astrophysical N-body problem?

$$k_1 = \frac{h}{2} f(x(t), t)$$

$$k_{1,x} = \frac{h}{2} \frac{dx_i(t)}{dt}$$
$$k_{1,v} = \frac{h}{2} \frac{dv_i(x_i(t), t)}{dt}$$

$$k_2 = h f\left(x(t) + k_1, t + \frac{h}{2}\right)$$

$$k_{2,x} = h \frac{d(x_i(t) + k_{1,x}, t + h/2)}{dt}$$
$$k_{2,v} = h \frac{d(v_i(t) + k_{1,v}, t + h/2)}{dt}$$

$$x(t+h) = x(t) + k_2$$

$$x_i(t+h) = x_i(t) + k_{2,x}$$
$$v_i(t+h) = v_i(t) + k_{2,v}$$

ODEs. Midpoint & the astrophysical N-body problem

$$k_{1,x} = \frac{h}{2} \frac{dx_i(t)}{dt}$$
$$k_{1,v} = \frac{h}{2} \frac{dv_i(x_i(t), t)}{dt}$$

$$k_{1,x} = \frac{h}{2} v_i(t)$$
$$k_{1,v} = \frac{h}{2} a_i(t)$$

$$k_{2,x} = h \frac{d(x_i(t) + k_{1,x}, t + h/2)}{dt}$$
$$k_{2,v} = h \frac{d(v_i(t) + k_{1,v}, t + h/2)}{dt}$$

$$k_{2,x} = h \frac{d}{dt} \left(x_i(t) + \underbrace{\frac{h}{2} v_i(t)}_{k_{1,x} = \frac{h}{2} v_i(t)} \right) = h \left(v_i(t) + \frac{h}{2} a_i(t) \right)$$
$$k_{2,v} = h \frac{d}{dt} \left(v_i(t) + \frac{h}{2} a_i(t) \right)$$

$$x_i(t + h) = x_i(t) + k_{2,x}$$
$$v_i(t + h) = v_i(t) + k_{2,v}$$

ODEs. Midpoint & the astrophysical N-body problem

$$k_{1,x} = \frac{h}{2} v_i(t)$$
$$k_{1,v} = \frac{h}{2} a_i(t)$$

$$k_{2,x} = h \left(v_i(t) + \frac{h}{2} a_i(t) \right)$$
$$k_{2,v} = h \frac{d}{dt} \left(v_i(t) + \frac{h}{2} a_i(t) \right)$$

$$x_i(t+h) = x_i(t) + k_{2,x}$$
$$v_i(t+h) = v_i(t) + k_{2,v}$$

ODEs. Midpoint & the astrophysical N-body problem

$$k_{1,x} = \frac{h}{2} v_i(t)$$
$$k_{1,v} = \frac{h}{2} a_i(t)$$

Remember that the acceleration in Newton eqs depends only on positions (a does not depend on v)

$$k_{2,x} = h \left(v_i(t) + \frac{h}{2} a_i(t) \right)$$
$$k_{2,v} = h \frac{d}{dt} \left(v_i(t) + \frac{h}{2} a_i(t) \right)$$

$$k_{2,v} = h \frac{d^2 x}{dt^2} \Big|_{t+\frac{h}{2}} = h a_i(x_i(t + h/2), t + h/2)$$

Writing Euler explicitly

$$x_i(t + h) = x_i(t) + k_{2,x}$$
$$v_i(t + h) = v_i(t) + k_{2,v}$$

$$k_{2,v} = h a_i(x_i(t) + h/2 v_i(t))$$

ODEs. Midpoint & the astrophysical N-body problem

$$k_{1,x} = \frac{h}{2} v_i(t)$$
$$k_{1,v} = \frac{h}{2} a_i(t)$$

$$k_{2,x} = h \left(v_i(t) + \frac{h}{2} a_i(t) \right)$$
$$k_{2,v} = h a_i(x_i(t) + h/2 v_i(t))$$

$$k_{2,x} = h (v_i(t) + k_{1,v})$$

$$k_{2,v} = h a_i(x_i(t) + k_{1,x})$$

$$x_i(t+h) = x_i(t) + k_{2,x}$$
$$v_i(t+h) = v_i(t) + k_{2,v}$$

ODEs. Midpoint & the astrophysical N-body problem

$$k_{1,x} = \frac{h}{2} v_i(t)$$
$$k_{1,v} = \frac{h}{2} a_i(t)$$

$$k_{2,x} = h [v_i(t) + k_{1,v}]$$
$$k_{2,v} = h a_i(x_i(t) + k_{1,x})$$

$$x_i(t + h) = x_i(t) + k_{2,x}$$
$$v_i(t + h) = v_i(t) + k_{2,v}$$

**This is the most elegant form
of the midpoint scheme
for the N-body problem**

ODEs. Midpoint & the astrophysical N-body problem

In practice,

$$k_{1,x} = \frac{h}{2} v_i(t)$$
$$k_{1,v} = \frac{h}{2} a_i(t)$$

$$a_i(t) = -G \sum_{j=1, j \neq i}^n \frac{m_j (x_i(t) - x_j(t))}{|x_i(t) - x_j(t)|^3}$$

$$k_{1,x} = \frac{h}{2} v_i(t)$$
$$k_{1,v} = \frac{h}{2} a_i(t)$$

$$k_{2,x} = h [v_i(t) + k_{1,v}]$$
$$k_{2,v} = h a_i(x_i(t) + k_{1,x})$$

$$x_i(t + h/2) = x_i(t) + k_{1,x}$$
$$a_i(t + h/2) = -G \sum_{j=1, j \neq i}^n \frac{m_j (x_i(t + h/2) - x_j(t + h/2))}{|x_i(t + h/2) - x_j(t + h/2)|^3}$$

$$k_{2,x} = h (v_i(t) + k_{1,v})$$
$$k_{2,v} = h a_i(t + h/2)$$

$$x_i(t + h) = x_i(t) + k_{2,x}$$
$$v_i(t + h) = v_i(t) + k_{2,v}$$

$$x_i(t + h) = x_i(t) + k_{2,x}$$
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ODEs. EXERCISE on binary star with midpoint/ RK 4

EXERCISE:

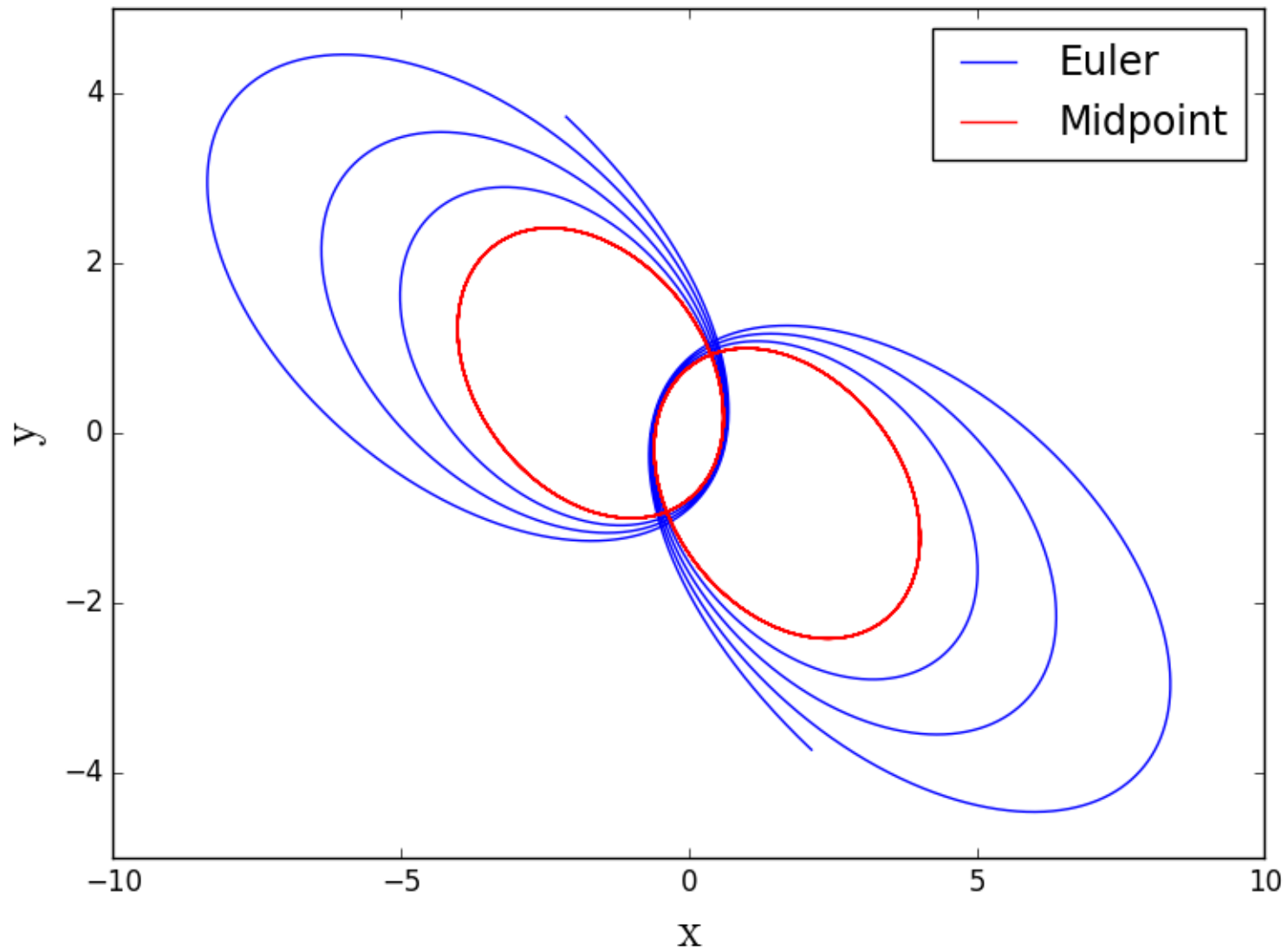
Write a new script to implement the Midpoint method and/or the Runge-Kutta 4th order method to evolve a system of two points in two dimensions (xy plane) described in the previous exercise.

Let us assume $t_0 = 0$, $t_{\text{fin}} = 300$ and $h = 0.01$. The result should look like the red line in Figure 42 (Midpoint and Runge-Kutta 4th order cannot be distinguished by eye in this case).

ODEs. EXERCISE on binary star with midpoint/ RK 4

Result of Euler is the blue line

Result of Midpoint is the red line



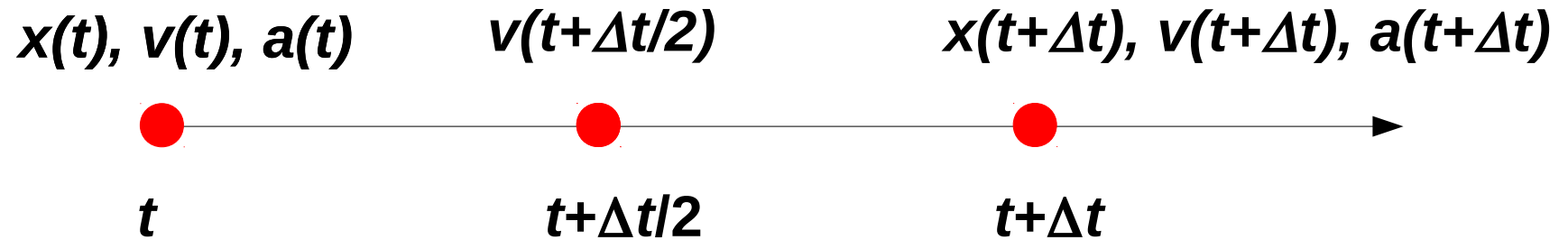
ODEs. Leapfrog scheme

- a particular version of the midpoint method
- leapfrog play (Italian: la cavallina)
- similar to Euler's method but evaluated in between a time-step



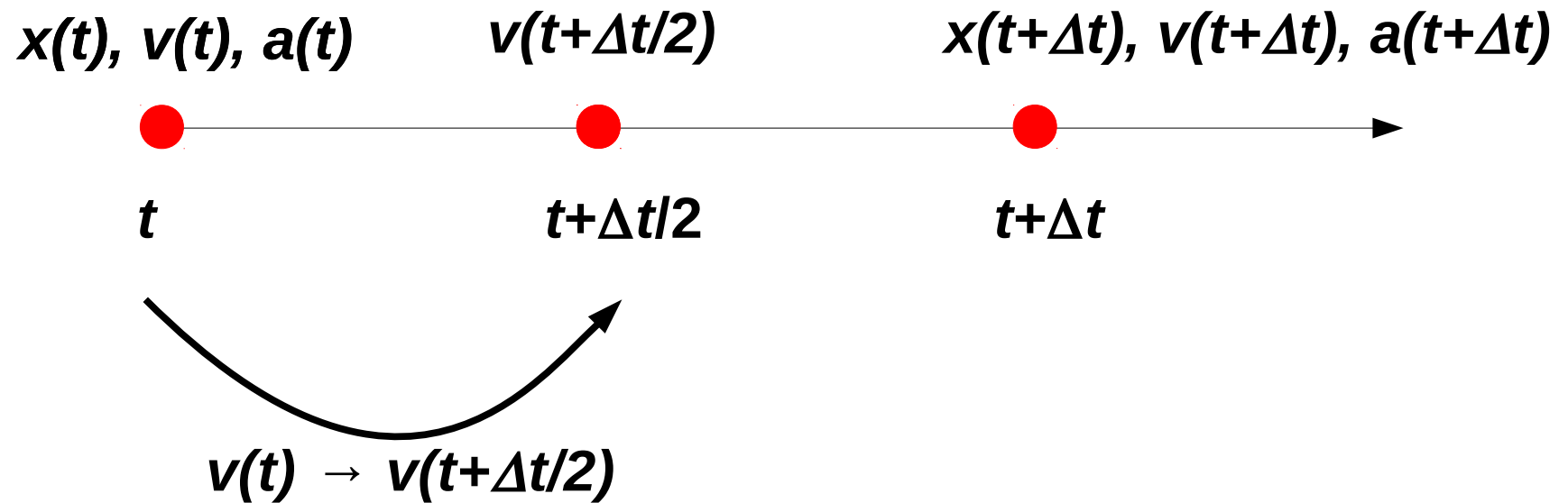
ODEs. Leapfrog scheme

Most common version of leapfrog scheme is
Kick – Drift – Kick (KDK) algorithm



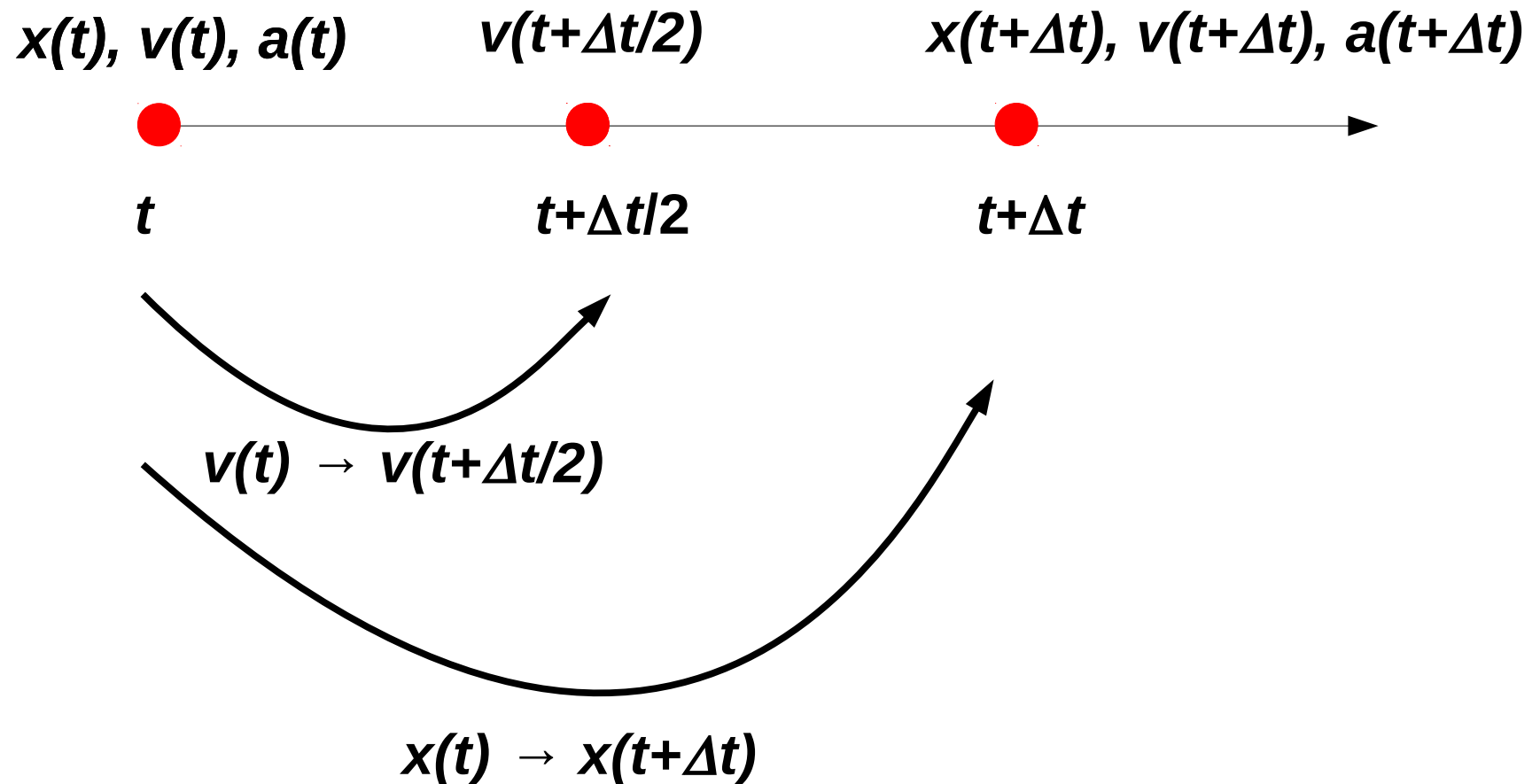
ODEs. Leapfrog scheme

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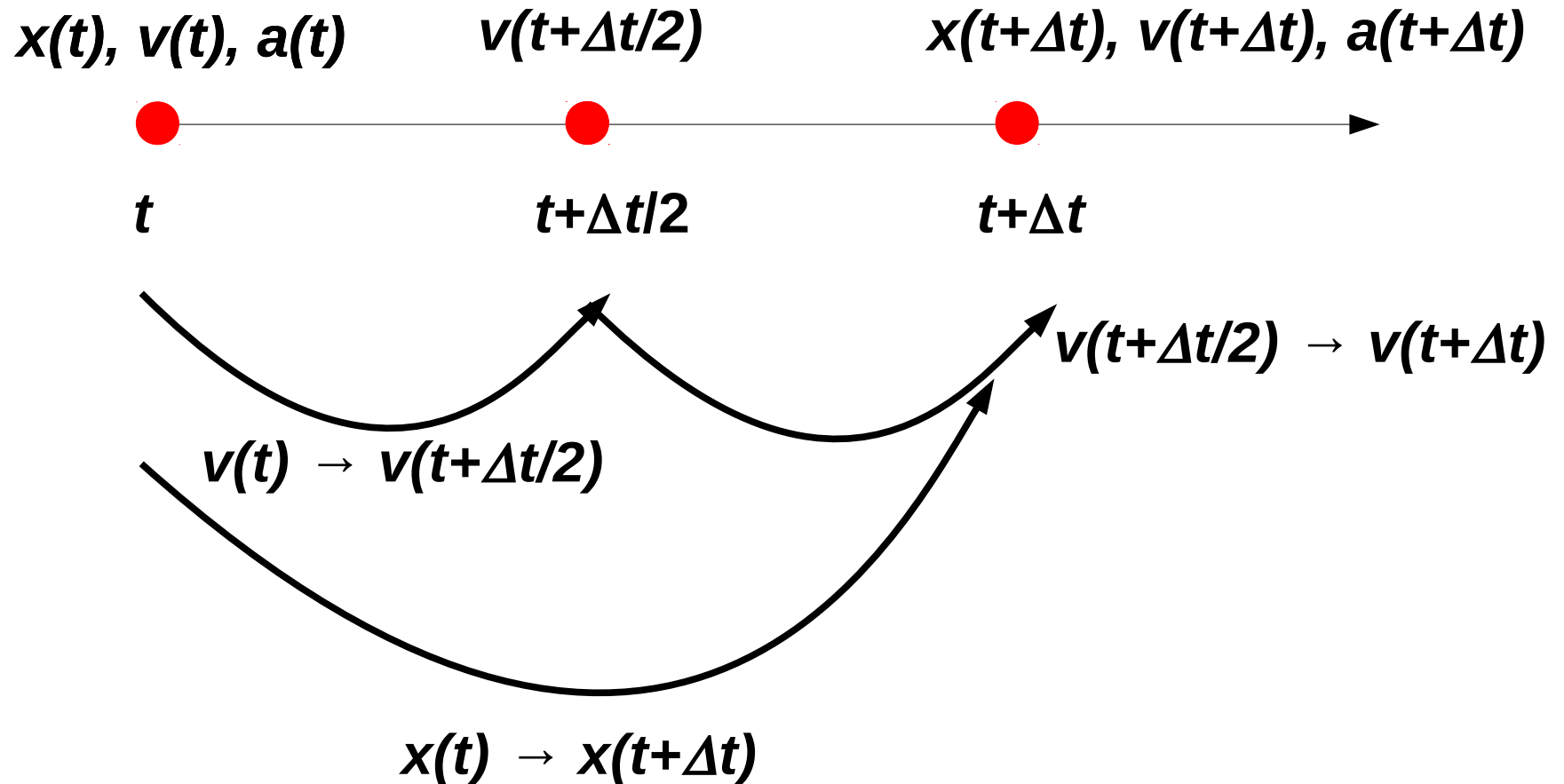
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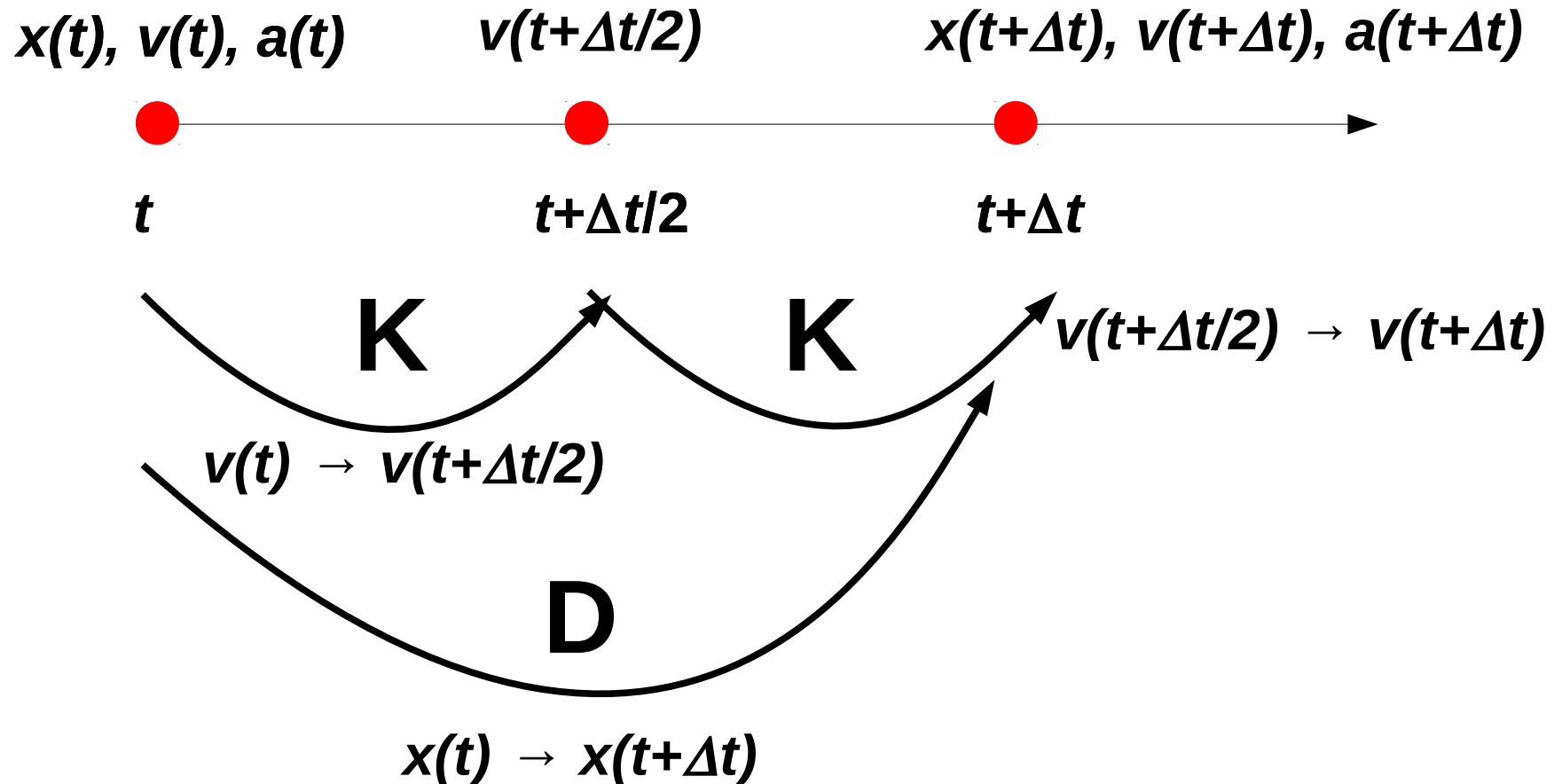
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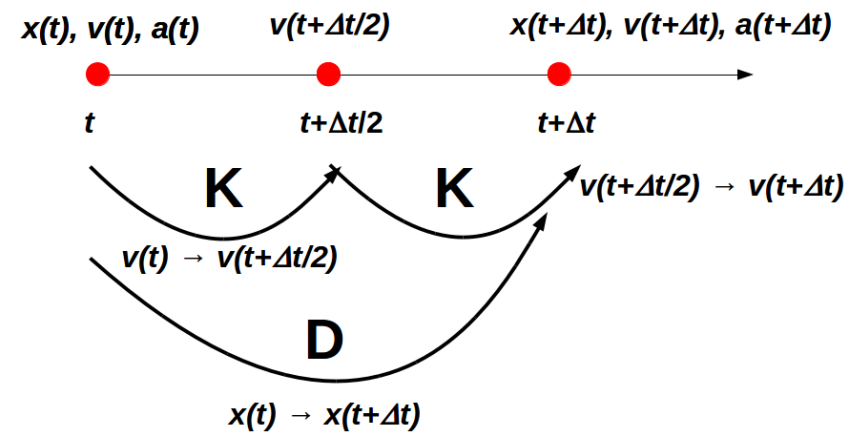
ODEs. Leapfrog scheme

Most common version of leapfrog scheme is
Kick – Drift – Kick (KDK) algorithm



Kick + Drift + Kick (KDK) scheme

ODEs. Leapfrog scheme



Kick + Drift + Kick (KDK) scheme

Mathematically

$$\vec{a}_i(t) = -G \sum_{j=1, j \neq i}^N m_j \frac{\vec{x}_i(t) - \vec{x}_j(t)}{|\vec{x}_i(t) - \vec{x}_j(t)|^3},$$

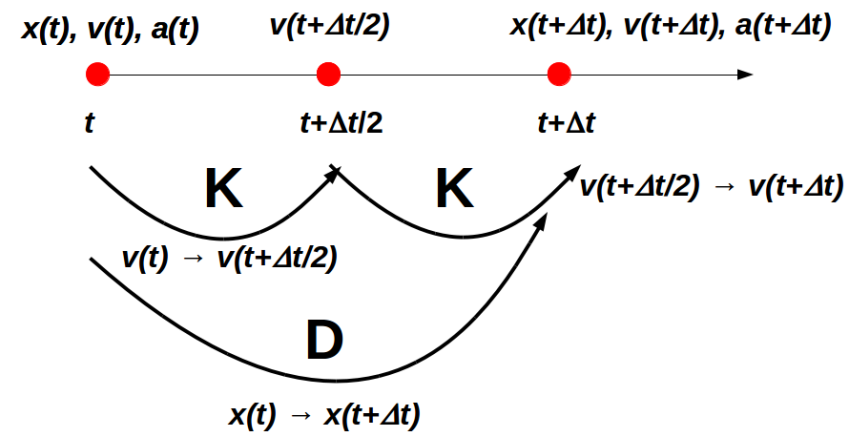
$$\vec{v}_i\left(t + \frac{h}{2}\right) = \vec{v}_i(t) + \frac{h}{2} \vec{a}_i(t)$$

$$\vec{x}_i(t + h) = \vec{x}_i(t) + h \vec{v}_i\left(t + \frac{h}{2}\right)$$

$$\vec{a}_i(t + h) = -G \sum_{j=1, j \neq i}^N m_j \frac{\vec{x}_i(t + h) - \vec{x}_j(t + h)}{|\vec{x}_i(t + h) - \vec{x}_j(t + h)|^3},$$

$$\vec{v}_i(t + h) = \vec{v}_i\left(t + \frac{h}{2}\right) + \frac{h}{2} \vec{a}_i(t + h)$$

ODEs. Leapfrog scheme



Kick + Drift + Kick (KDK) scheme

In more compact form:

$$\vec{a}_i(t) = -G \sum_{j=1, j \neq i}^N m_j \frac{\vec{x}_i(t) - \vec{x}_j(t)}{|\vec{x}_i(t) - \vec{x}_j(t)|^3},$$

$$\vec{x}_i(t+h) = \vec{x}_i(t) + h \vec{v}_i(t) + \frac{h^2}{2} \vec{a}_i(t)$$

$$\vec{a}_i(t+h) = -G \sum_{j=1, j \neq i}^N m_j \frac{\vec{x}_i(t+h) - \vec{x}_j(t+h)}{|\vec{x}_i(t+h) - \vec{x}_j(t+h)|^3},$$

$$\vec{v}_i(t+h) = \vec{v}_i(t) + \frac{h}{2} [\vec{a}_i(t) + \vec{a}_i(t+h)]$$

ODEs. Leapfrog scheme

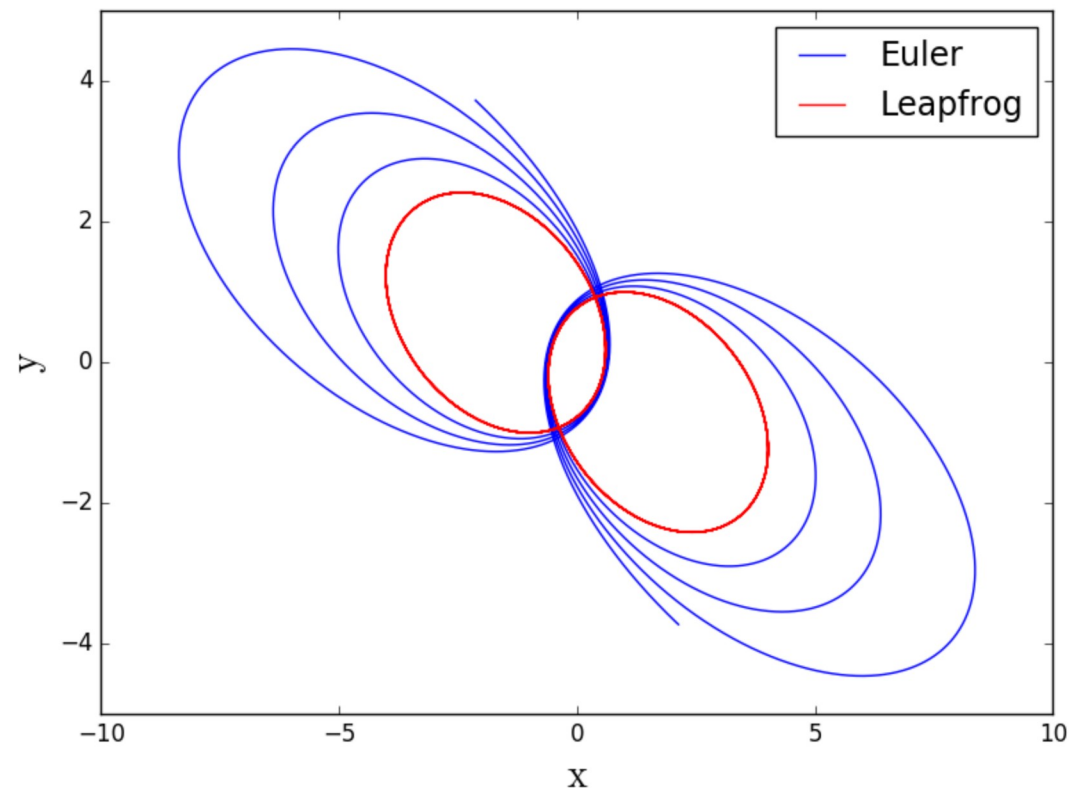
- second-order scheme (barely)
- surprisingly accurate
- alternative version: drift-kick-drift (DKD) leapfrog scheme, in which position is evaluated at the midpoint ($t+h/2$), then velocity is advanced to the end and finally position is recalculated to the end of the step. You can try to derive this one by yourself
- **(unlike Runge-Kutta) leapfrog is time-reversal symmetric**
→ **the error on energy conservation does not grow with time**

NOTE: A nice way to estimate how well an integrator of celestial dynamics works is to calculate the conservation of total energy and total angular momentum as a function of time during the integration

ODEs. Exercise on binary star with leapfrog

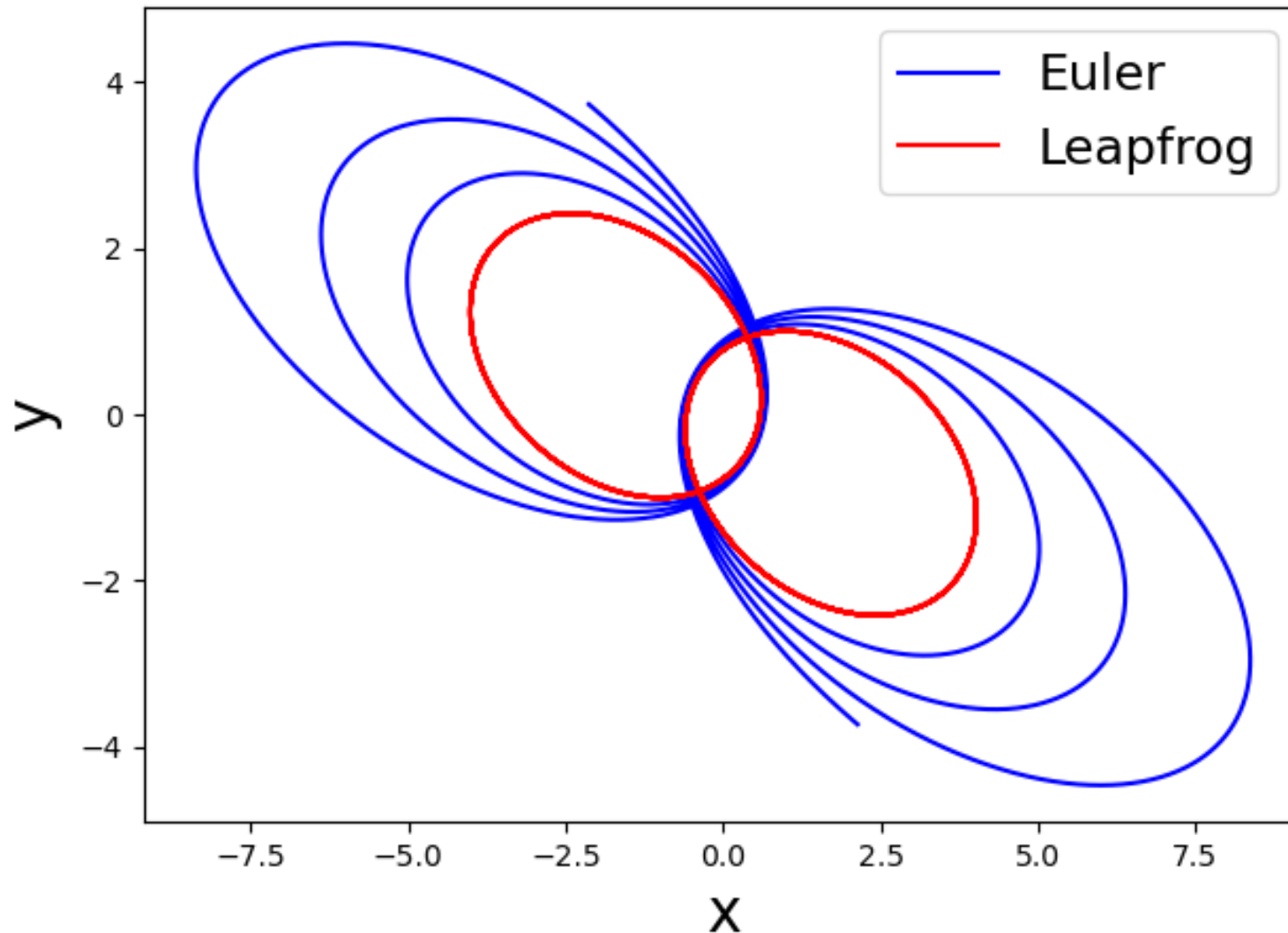
EXERCISE:

Write a code to implement the leapfrog scheme. Integrate the binary star in the previous exercises with the leapfrog scheme. Compare Euler's method with the leapfrog scheme. Choose $t_0 = 0$, $t_{\text{fin}} = 300$ and $h = 0.01$. The result should look like Figure 44. Leapfrog is much better, isn't it?



ODEs. Exercise on binary star with leapfrog

Euler versus Leapfrog



Same initial conditions: integration of a Keplerian binary

ODEs. Euler vs Leapfrog: a simple test

Energy of an N-body system

$$E = \sum_{i=1}^N \frac{1}{2} m_i v_i^2 - G \sum_{i=1}^N \sum_{j>i}^N \frac{m_i m_j}{|r_i - r_j|}$$

For a binary star, energy in the center of mass of the system

$$E = \frac{1}{2} \frac{m_1 m_2}{(m_1 + m_2)} |v_1 - v_2|^2 - G \frac{m_1 m_2}{|r_1 - r_2|}$$

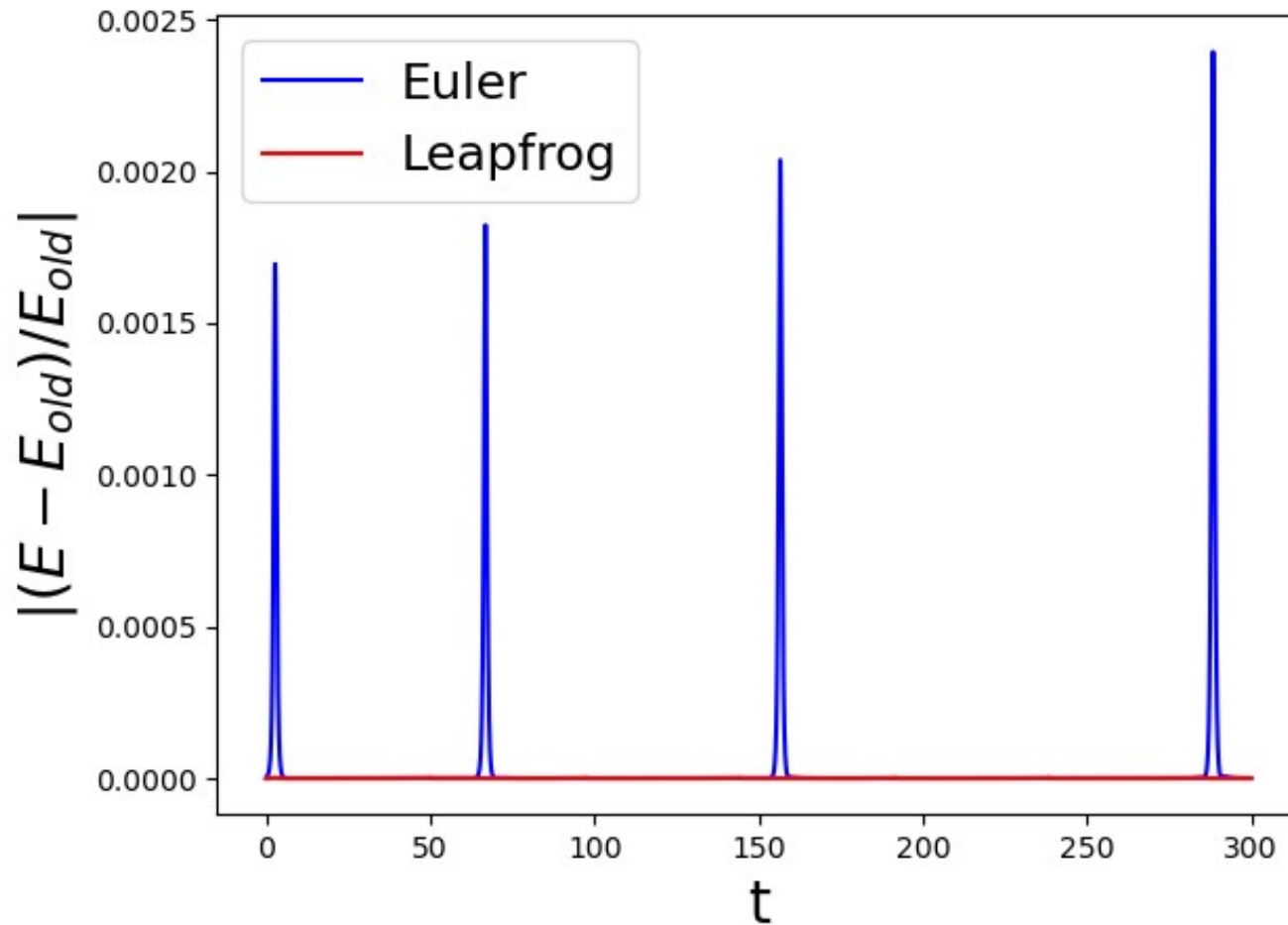
Modulus of angular momentum

$$L = \sum_{i=1}^N |m_i v_i \times r_i|$$

If energy and angular momentum are supposed to be conserved in the system we simulate, the level of energy / angular momentum conservation between previous and next step is a good indicator of the accuracy of the integrator

ODEs. Euler vs Leapfrog: a simple test

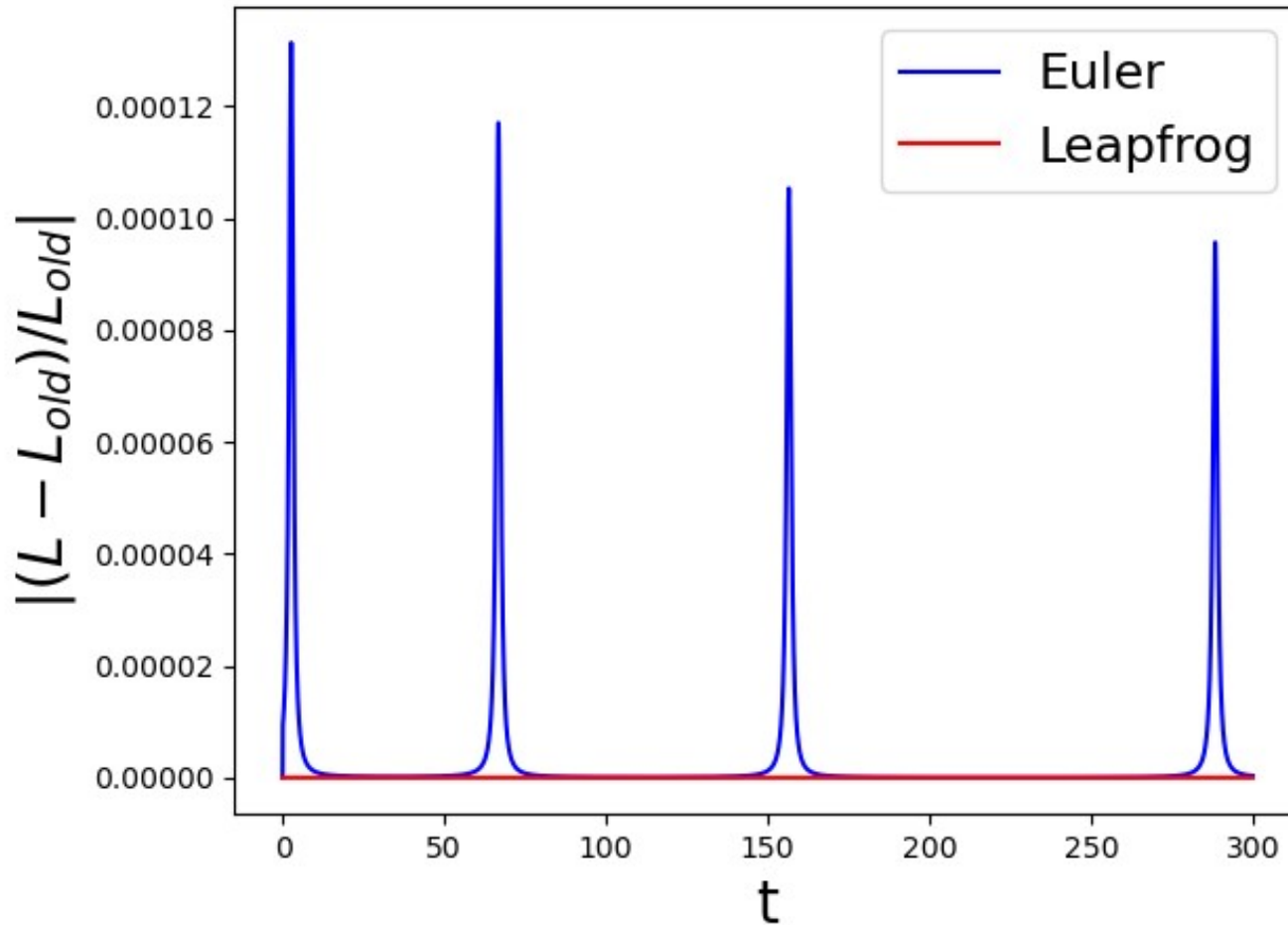
Energy conservation test



Leapfrog $\Delta E / E \sim 2.1e-06$ Euler $\Delta E / E = 0.0024$

ODEs. Euler vs Leapfrog: a simple test

Angular momentum conservation test



Leapfrog $\Delta L / L \sim 5.6e-16$ Euler $\Delta L / L = 0.00013$