Computational Physics (PHYS6350)

Lecture 11: Ordinary Differential Equations

$$\frac{dx}{dt} = f(x,t),$$

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Course materials: https://github.com/vlvovch/PHYS6350-ComputationalPhysics
Online textbook: https://vovchenko.net/computational-physics/

Ordinary Differential Equations (ODE)

First-order ordinary differential equation (ODE) is an equation of the form

$$\frac{dx}{dt} = f(x, t),$$

with initial condition

$$x(t = 0) = x_0$$

This determines the x(t) dependence at t>0.

In many physical applications t plays the role of the time variable (classical mechanics problems), although this is not always the case.

References: Chapter 8 of *Computational Physics* by Mark Newman

When we need numerical methods for ODEs

The solution to an ODE

$$\frac{dx}{dt} = f(x, t), \qquad\qquad x(t = 0) = x_0$$

can formally be written as

$$x(t) = x_0 + \int_0^t f[x(t'), t'])dt'$$

If f does not depend on x, the solution can be obtained through (numerical) integration

In some other cases the solution can be obtained through the separation of variables, e.g.

$$\frac{dx}{dt} = \frac{2x}{t}$$

In all other cases, the solution has to be obtained numerically.

Numerical methods for ODEs

Typically obtain the solution by taking small steps from $x(t)$ to $x(t+h)$

Characteristics:

- Explicit or implicit
  - Explicit methods: use $x(t)$ to calculate $x(t+h)$ directly
  - Implicit methods: have to solve a (non-linear) equation for $x(t+h)$

- Accuracy
  - Truncation error at each step is of order $O(h^n)$
  - Some schemes are explicitly time-reversal and/or conserve energy
  - Adaptive methods adjust the step size h to control the error to the desired accuracy

- Stability
  - Whether the accumulated error is bounded (that's where implicit methods shine)

- Consistency
  - Consistent methods reproduce the exact solution in the limit $h \to 0$

Euler's method

$$\frac{dx}{dt} = f(x,t),$$

Let us apply the Taylor expansion to express *x(t+h)* in terms of *x(t)*:

$$x(t+h) = x(t) + h\,\frac{dx}{dt} + O(h^2)\ .$$

Given that dx/dt = f(x,t) and neglecting the high-order terms in *h* we have

$$x(t+h) \approx x(t) + h\,f[x(t),t] \qquad \textit{Euler method}$$

We can iteratively apply this relation starting from t = 0 to evaluate x(t) at t > 0.

This is the essence of **Euler's method** – the simplest method for solving ODEs numerically.

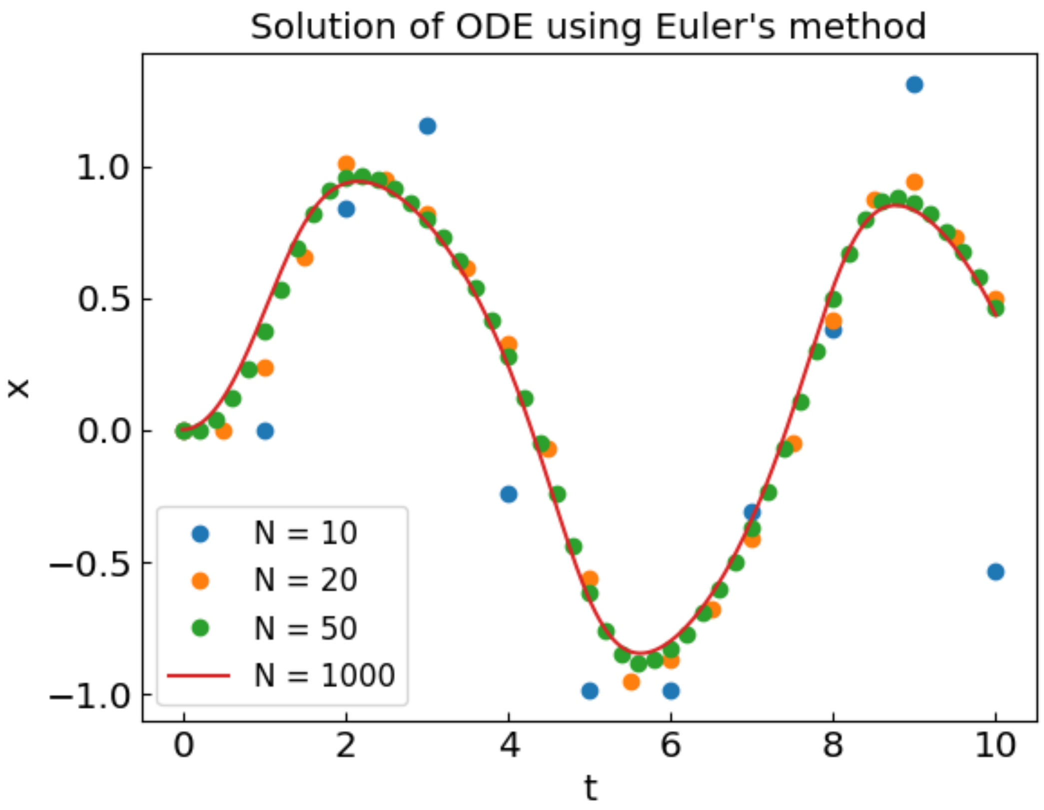
Error:

- Local (per time step): $O(h^2)$
- Global ($N = t_{end}/h$ time steps): $O(h)$

Euler's method

```python
import numpy as np

def ode_euler_step(f, x, t, h):
    """Perform a single step h using Euler's scheme.

    Args:
    f: the function that defines the ODE.
    x: the value of the dependent variable at the present step.
    t: the present value of the time variable.
    h: the time step

    Returns:
    xnew: the value of the dependent variable at the step t+h
    """
    return x + h * f(x,t)

def ode_euler(f, x0, t0, h, nsteps):
    """Solve an ODE dx/dt = f(x,t) from t = t0 to t = t0 + h*steps using Euler's method.

    Args:
          f: the function that defines the ODE.
         x0: the initial value of the dependent variable.
         t0: the initial value of the time variable.
          h: the time step
     nsteps: the total number of Euler steps

    Returns:
    t,x: the pair of arrays corresponding to the time and dependent variables
    """

    t = np.zeros(nsteps + 1)
    x = np.zeros(nsteps + 1)
    x[0] = x0
    t[0] = t0
    for i in range(0, nsteps):
        t[i + 1] = t[i] + h
        x[i + 1] = ode_euler_step(f, x[i], t[i], h)
    return t,x
```

$$\frac{dx}{dt} = -x^3 + \sin t, \qquad x(t=0) = 0.$$



Midpoint method (2nd order Runge-Kutta)

Euler's method essentially corresponds to approximating the derivative dx/dt with a *forward difference*

$$\frac{dx}{dt} = f(x,t) \approx \frac{x(t+h) - x(t)}{h} + \mathcal{O}(h).$$

Recall that central (midpoint) difference gives better accuracy

$$f(x, t+h/2) \approx \frac{x(t+h) - x(t)}{h} + \mathcal{O}(h^2).$$

therefore

$$x(t+h) = x(t) + hf[x(t+h/2), t+h/2)] + \mathcal{O}(h^3)$$

How to calculate *x(t+h/2)* entering the r.h.s? Use Euler's method $x(t+h/2) = x(t) + \frac{1}{2}hf(x,t) + \mathcal{O}(h^2)$

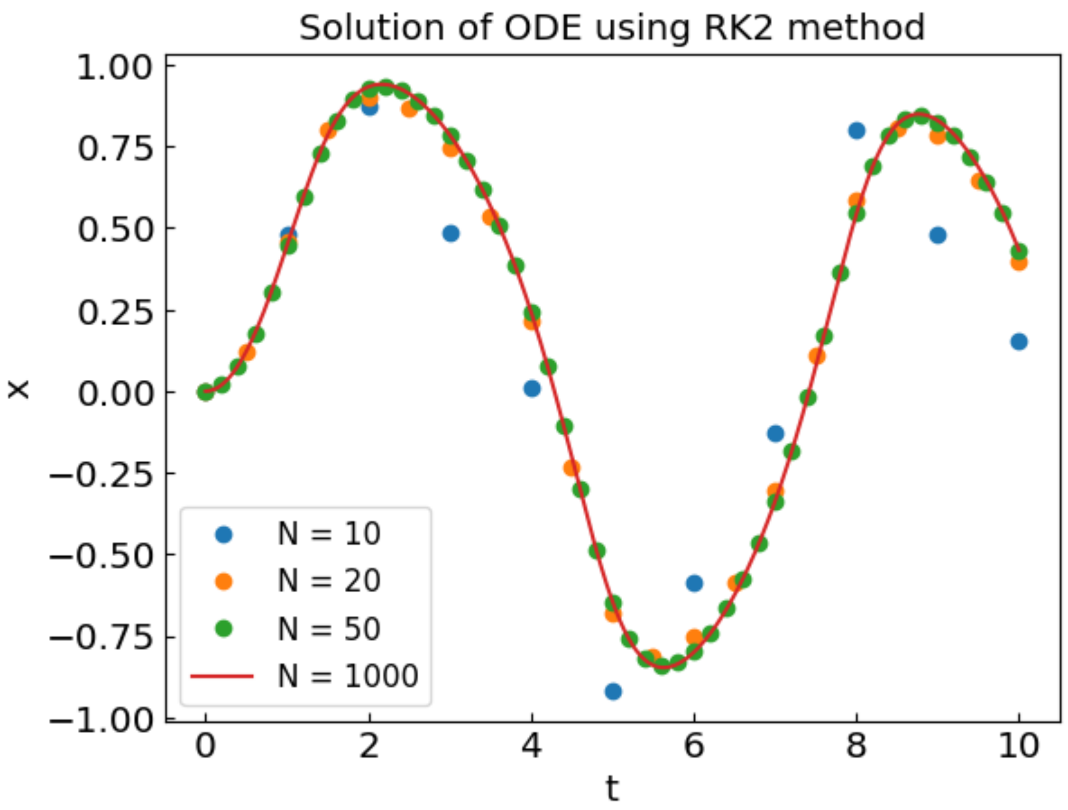
Therefore, $x(t+h) = x(t) + hf\left[x(t) + \frac{1}{2}hf(x,t), t + \frac{1}{2}h\right] + \mathcal{O}(h^3)$, which can be written in two steps

$$\begin{aligned} k_1 &= h\,f(x,t), && \textit{trial step} \\ k_2 &= h\,f(x + k_1/2, t + h/2), && \textit{real step} \\ x(t+h) &= x(t) + k_2\ . \end{aligned}$$

Midpoint method (2^{nd} order Runge-Kutta)

```python
def ode_rk2_step(f, x, t, h):
    """Perform a single step h using 2nd order Runge-Kutta scheme.

    Args:
    f: the function that defines the ODE.
    x: the value of the dependent variable at the present step.
    t: the present value of the time variable.
    h: the time step

    Returns:
    xnew: the value of the dependent variable at the step t+h
    """
    k1 = h * f(x,t)
    k2 = h * f(x + k1/2., t + h /2.)
    return x + k2

def ode_rk2(f, x0, t0, h, nsteps):
    """Solve an ODE dx/dt = f(x,t) from t = t0 to t = t0 + h*steps using Euler's method.

    Args:
          f: the function that defines the ODE.
         x0: the initial value of the dependent variable.
         t0: the initial value of the time variable.
          h: the time step
     nsteps: the total number of Euler steps

    Returns:
    t,x: the pair of arrays corresponding to the time and dependent variables
    """

    t = np.zeros(nsteps + 1)
    x = np.zeros(nsteps + 1)
    x[0] = x0
    t[0] = t0
    for i in range(0, nsteps):
        t[i + 1] = t[i] + h
        x[i + 1] = ode_rk2_step(f, x[i], t[i], h)
    return t,x
```

$$\frac{dx}{dt} = -x^3 + \sin t, \qquad x(t=0) = 0.$$



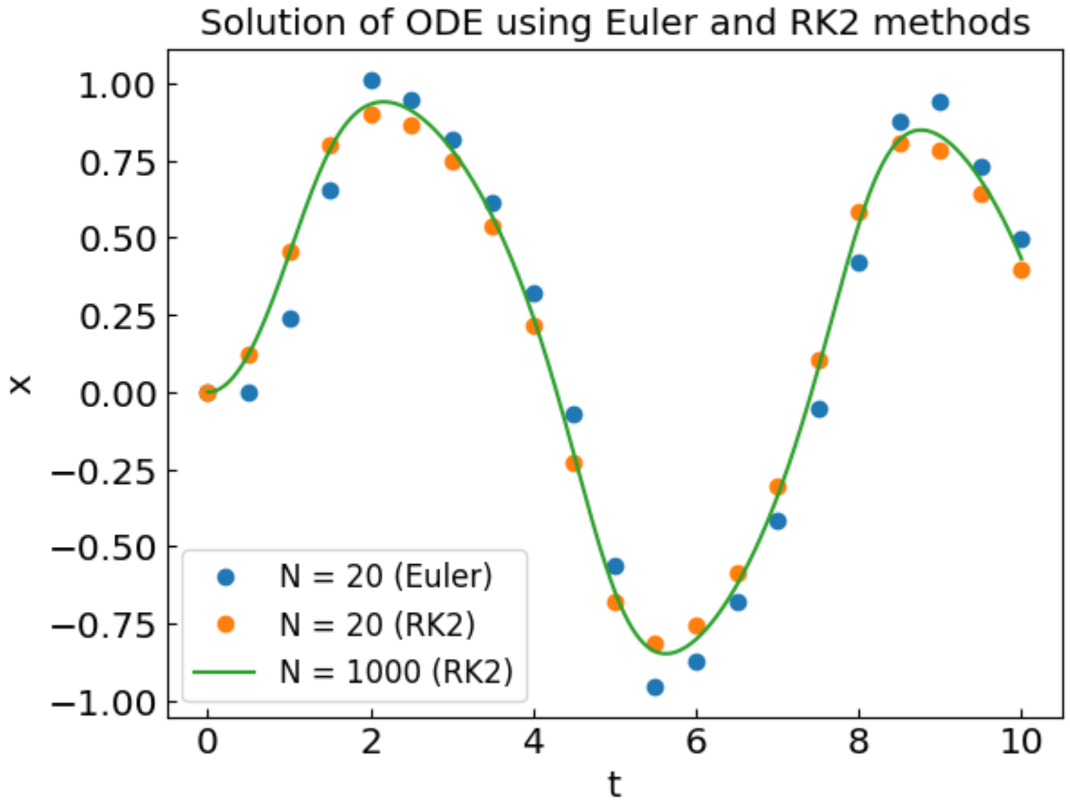
Error:

- Local (per time step): $O(h^3)$
- Global ($N = t_{end}/h$ time steps): $O(h^2)$

Midpoint method (2^{nd} order Runge-Kutta)

```python
def ode_rk2_step(f, x, t, h):
    """Perform a single step h using 2nd order Runge-Kutta scheme.

    Args:
    f: the function that defines the ODE.
    x: the value of the dependent variable at the present step.
    t: the present value of the time variable.
    h: the time step

    Returns:
    xnew: the value of the dependent variable at the step t+h
    """
    k1 = h * f(x,t)
    k2 = h * f(x + k1/2., t + h /2.)
    return x + k2

def ode_rk2(f, x0, t0, h, nsteps):
    """Solve an ODE dx/dt = f(x,t) from t = t0 to t = t0 + h*steps using Euler's method.

    Args:
          f: the function that defines the ODE.
         x0: the initial value of the dependent variable.
         t0: the initial value of the time variable.
          h: the time step
     nsteps: the total number of Euler steps

    Returns:
    t,x: the pair of arrays corresponding to the time and dependent variables
    """

    t = np.zeros(nsteps + 1)
    x = np.zeros(nsteps + 1)
    x[0] = x0
    t[0] = t0
    for i in range(0, nsteps):
        t[i + 1] = t[i] + h
        x[i + 1] = ode_rk2_step(f, x[i], t[i], h)
    return t,x
```

$$\frac{dx}{dt} = -x^3 + \sin t, \qquad x(t=0) = 0.$$



Error:

- Local (per time step): $O(h^3)$
- Global ($N = t_{end}/h$ time step): $O(h^2)$

Classical 4th order Runge-Kutta method

The above logic can be generalized to cancel high-order error terms in various powers in h, requiring more and more evaluations of function $f(x,t)$ at intermediate steps.

The classical 4th-order Runge-Kutta method is often considered a sweet spot.

It corresponds to the following scheme:

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

Error:

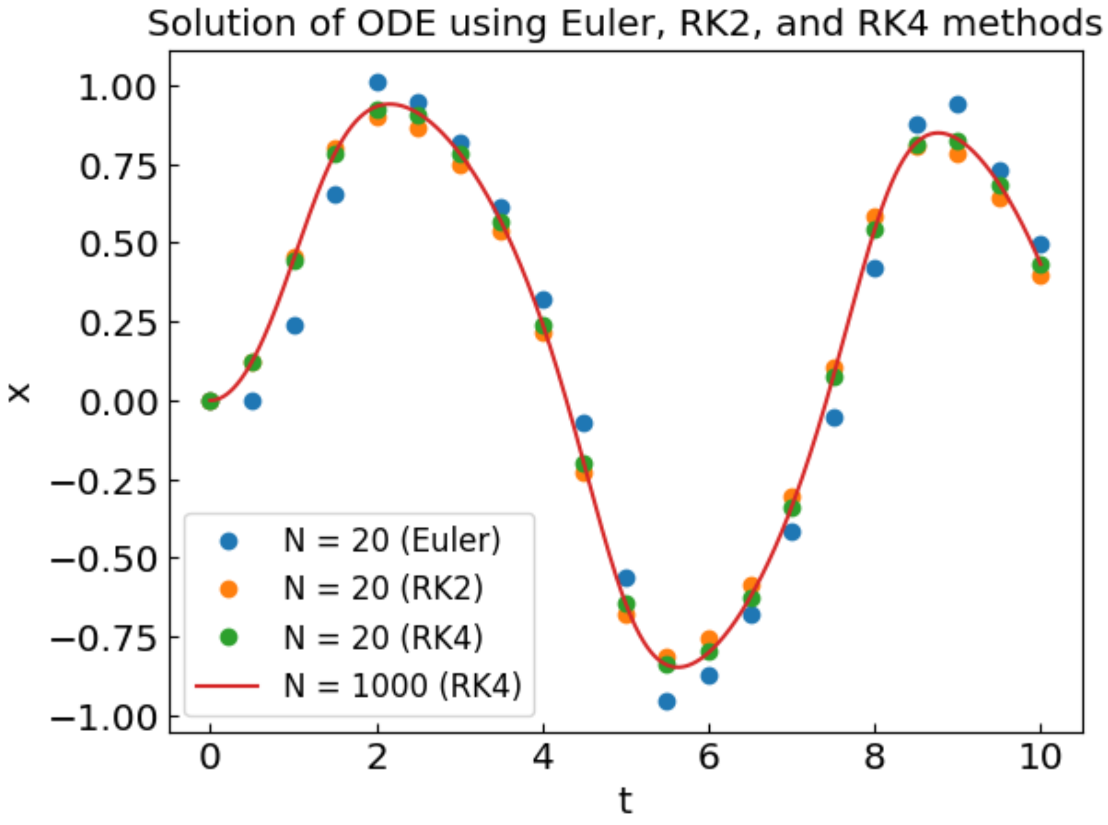
- Local (per time step): $O(h^5)$
- Global ($N=t_{end}/h$ time steps): $O(h^4)$

The classical 4th-order Runge-Kutta method is a good first choice for solving physics ODEs.

Classical 4th order Runge-Kutta method

```python
def ode_rk4_step(f, x, t, h):
    """Perform a single step h using 4th order Runge-Kutta method.

    Args:
    f: the function that defines the ODE.
    x: the value of the dependent variable at the present step.
    t: the present value of the time variable.
    h: the time step

    Returns:
    xnew: the value of the dependent variable at the step t+h
    """
    k1 = h * f(x,t)
    k2 = h * f(x + k1/2., t + h /2.)
    k3 = h * f(x + k2/2., t + h /2.)
    k4 = h * f(x + k3, t + h)
    return x + (k1 + 2. * k2 + 2. * k3 + k4) / 6.

def ode_rk4(f, x0, t0, h, nsteps):
    """Solve an ODE dx/dt = f(x,t) from t = t0 to t = t0 + h*steps using 4th order Runge-Kutta method.

    Args:
          f: the function that defines the ODE.
         x0: the initial value of the dependent variable.
         t0: the initial value of the time variable.
          h: the time step
     nsteps: the total number of Euler steps

    Returns:
    t,x: the pair of arrays corresponding to the time and dependent variables
    """

    t = np.zeros(nsteps + 1)
    x = np.zeros(nsteps + 1)
    x[0] = x0
    t[0] = t0
    for i in range(0, nsteps):
        t[i + 1] = t[i] + h
        x[i + 1] = ode_rk4_step(f, x[i], t[i], h)
    return t,x
```

$$\frac{dx}{dt} = -x^3 + \sin t, \qquad x(t=0) = 0.$$



Adaptive time step

$$\frac{dx}{dt} = f(x, t)$$

The choice of the time step is important to reach the desired accuracy/performance.

- h too large: the desired accuracy not reached
- h too small: we waste computing resources on unnecessary iterations
- Local truncation error itself is a function of time depending on the behavior of f(x,t)

Adaptive time step: make a local error estimate and adjust h to correspond to the desired accuracy

Ways to estimate the error:

- Make two small steps (h) to compute x(t+2h) and compare to the one from a single double step *2h*

- Use two methods of a different order and compare their results (e.g. [Runge-Kutta-Fehlberg method]() RKF45)

Adaptive time step in RK4 using double step

Recall that the error for one RK4 time step h is of order ch^5.
Let us take two RK4 steps h to approximate $x(t+2h) \approx x_1$. Then,

$$x(t+2h) \approx x_1 + 2ch^5$$

Now take single RK4 step $x(t+2h) \approx x_2$ of length $2h$

$$x(t+2h) \approx x_2 + 32ch^5$$

The local error estimate for a single RK4 time step h is then

$$\epsilon_{\mathrm{RK4}} = |ch^5| = \frac{|x_1 - x_2|}{30}.$$

If the desired accuracy per unit time is δ, the desired accuracy per time step h' is

$$h'\delta = ch'^5$$

so the time step should be adjusted from h to h' as

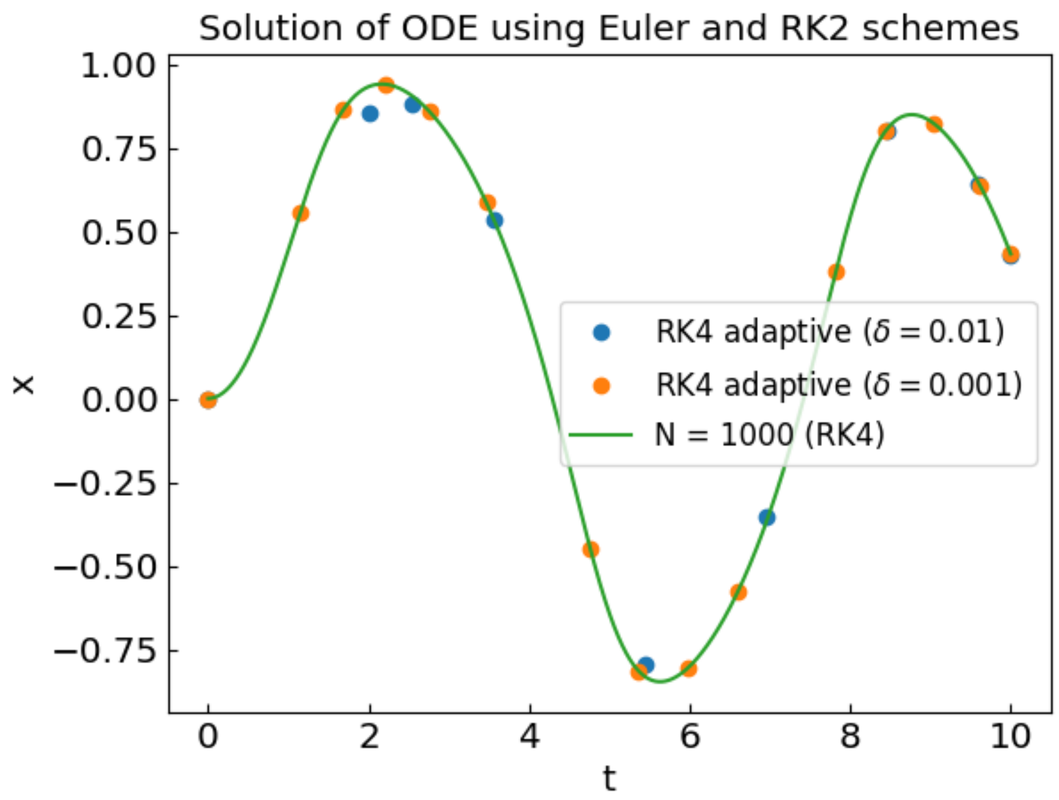
$$h' = h\left(\frac{30h\delta}{|x_1 - x_2|}\right)^{1/4} .$$

- $h' > h$: our step size is too small, move on to x(t+2h) and increase the step size to h'
- $h' < h$: our step size is too large, decrease step size to h' and try the current step again

RK4 method with adaptive step size

```python
def ode_rk4_adaptive(f, x0, t0, h0, tmax, delta = 1.e-6):

    ts = [t0]
    xs = [x0]
    h = h0
    t = t0
    i = 0
    while (t < tmax):
        if (t + h >= tmax):
            ts.append(tmax)
            h = tmax - t
            xs.append(ode_rk4_step(f, xs[i], ts[i], h))
            t = tmax
            break

        x1 = ode_rk4_step(f, xs[i], ts[i], h)
        x1 = ode_rk4_step(f, x1, ts[i] + h, h)
        x2 = ode_rk4_step(f, xs[i], ts[i], 2*h)

        rho = 30. * h * delta / np.abs(x1 - x2)
        if rho < 1.:
            h *= rho**(1/4.)
        else:
            if (t + 2.*h) < tmax:
                xs.append(x1)
                ts.append(t + 2*h)
                t += 2*h
            else:
                xs.append(ode_rk4_step(f, xs[i], ts[i], h))
                ts.append(t + h)
                t += h
            i += 1
            h = min(2.*h, h * rho**(1/4.))

    return ts,xs
```

$$\frac{dx}{dt} = -x^3 + \sin t, \qquad x(t=0) = 0.$$



Step size tends to decrease when dx/dt (the r.h.s) is large

Stability, stiff equations, and implicit methods

Consider the following ODE

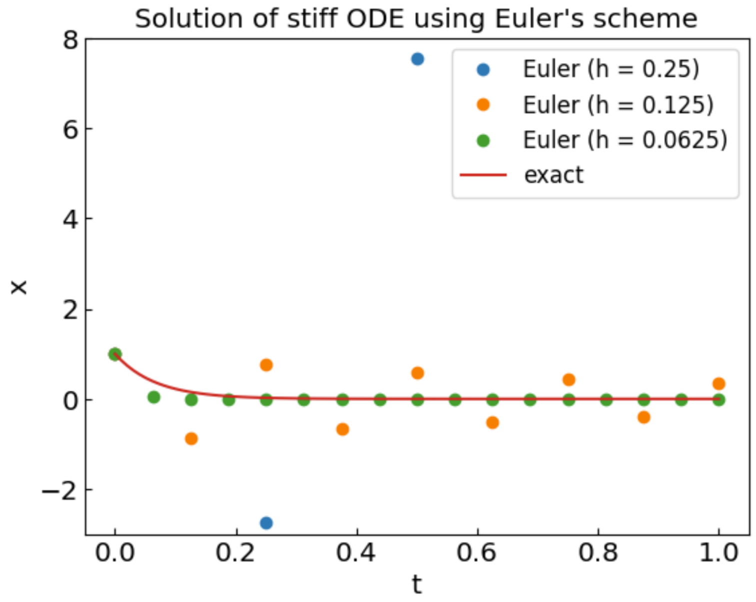
$$\frac{dx}{dt} = -15x, \qquad \textit{stiff equation}$$

with the initial condition $x(t{=}0) = 1$.

The exact solution is of course $x(t) = e^{-15t}$ and goes to zero at large times.

Let us apply Euler's method
with h=1/4, 1/8, 1/16

Divergence for h=1/4!



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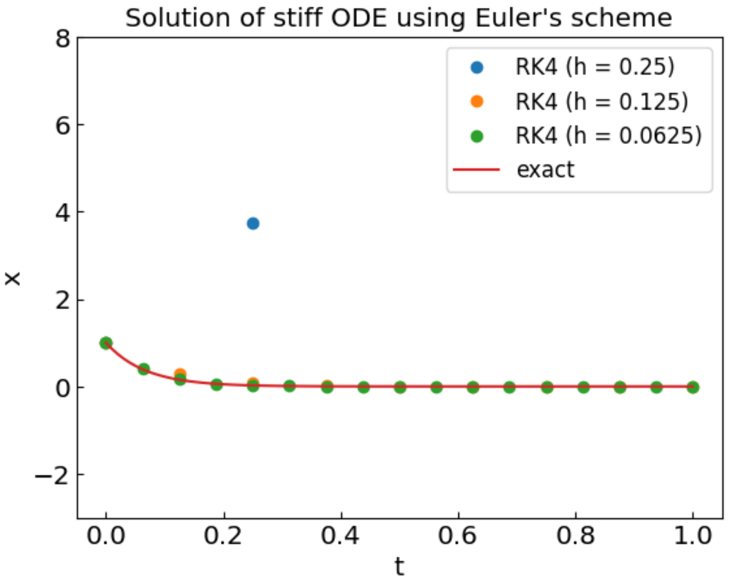
Divergence for h=1/4!

RK4: better but still diverges for h=1/4



Euler methods and stiff equations

Recall that in Euler's method x(t+h) = x(t) + h f(x,t)

For $\frac{dx}{dt} = -15x$, we have $x_{n+1} = x_n - 15hx_n = (1-15h)x_n = (1-15h)^n x_0, \qquad x_n \equiv x(t+nh)$

If $|1-15h| > 1$, i.e. $h > 2/15$, the Euler method diverges!

Solution: *implicit methods*

Implicit Euler method: $\mathbf{x(t+h)} = x(t) + hf[\mathbf{x(t+h)}, t+h]$

Our stiff equation: $x_{n+1} = x_n - 15hx_{n+1}$ thus $x_{n+1} = \frac{x_n}{1+15h} = \frac{x_0}{(1+15h)^n} \xrightarrow{n\to\infty} 0$ for all $h > 0$.

- Implicit methods are ***more stable*** than explicit methods
- But require solving non-linear equation for *x(t+h)* at each step
- *Semi-implicit methods:* use one iteration of Newton's method to solve for *x(t+h)*

Other implicit methods: trapezoidal rule, family of implicit Runge-Kutta methods

Systems of Ordinary Differential Equations

System of N first-order ODE

$$\begin{aligned}
\frac{dx_1}{dt} &= f_1(x_1, \dots, x_N, t), \\
\frac{dx_2}{dt} &= f_2(x_1, \dots, x_N, t), \\
&\dots \\
\frac{dx_N}{dt} &= f_N(x_1, \dots, x_N, t).
\end{aligned}$$

Vector notation:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t).$$

- all the methods we covered have the same structure when applied for systems of ODEs
- simply apply component by component

Systems of Ordinary Differential Equations

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t).$$

- Euler method

$$\mathbf{x}(t+h) = \mathbf{x}(t) + h\mathbf{f}[\mathbf{x}(t), t]$$

- RK2

$$\boldsymbol{k_1} = h\,\mathbf{f}[\mathbf{x}(t), t]$$
$$\boldsymbol{k_2} = h\,\mathbf{f}[\mathbf{x}(t) + \mathbf{k}_1/2, t + h/2]$$
$$\mathbf{x}(t+h) = \mathbf{x}(t) + \mathbf{k}_2$$

- RK4

$$\boldsymbol{k_1} = h\,\mathbf{f}[\mathbf{x}(t), t]$$
$$\boldsymbol{k_2} = h\,\mathbf{f}[\mathbf{x}(t) + \mathbf{k}_1/2, t + h/2]$$
$$\boldsymbol{k_3} = h\,\mathbf{f}[\mathbf{x}(t) + \mathbf{k}_2/2, t + h/2]$$
$$\boldsymbol{k_4} = h\,\mathbf{f}[\mathbf{x}(t) + \mathbf{k}_3, t + h]$$
$$\mathbf{x}(t+h) = \mathbf{x}(t) + \frac{1}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)$$

Systems of Ordinary Differential Equations

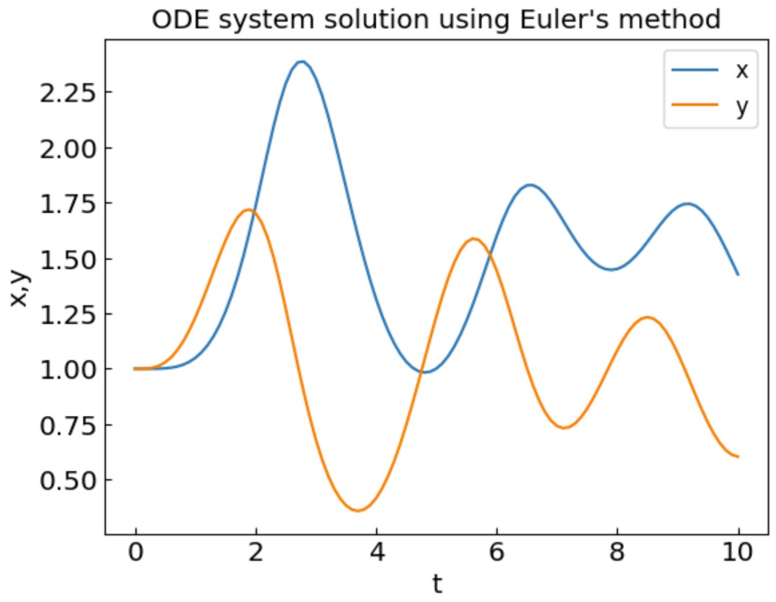
```python
def ode_euler_multi(f, x0, t0, h, nsteps):
    """Multi-dimensional version of the Euler method.
    """

    t = np.zeros(nsteps + 1)
    x = np.zeros((len(t), len(x0)))
    t[0] = t0
    x[0,:] = x0
    for i in range(0, nsteps):
        t[i + 1] = t[i] + h
        x[i + 1,:] = ode_euler_step(f, x[i], t[i], h)
    return t,x
```

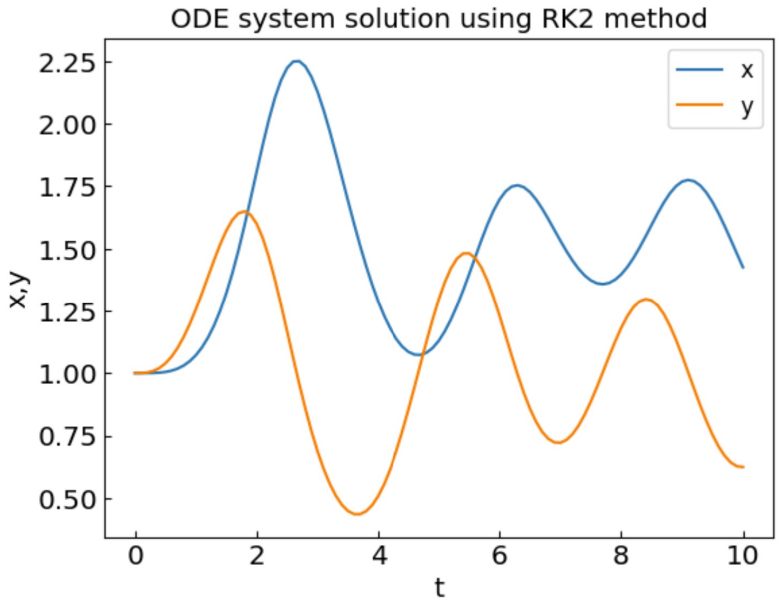
```python
def ode_rk2_multi(f, x0, t0, h, nsteps):
    """Multi-dimensional version of the RK2 method.
    """

    t = np.zeros(nsteps + 1)
    x = np.zeros((len(t), len(x0)))
    t[0] = t0
    x[0,:] = x0
    for i in range(0, nsteps):
        t[i + 1] = t[i] + h
        x[i + 1] = ode_rk2_step(f, x[i], t[i], h)
    return t,x
```

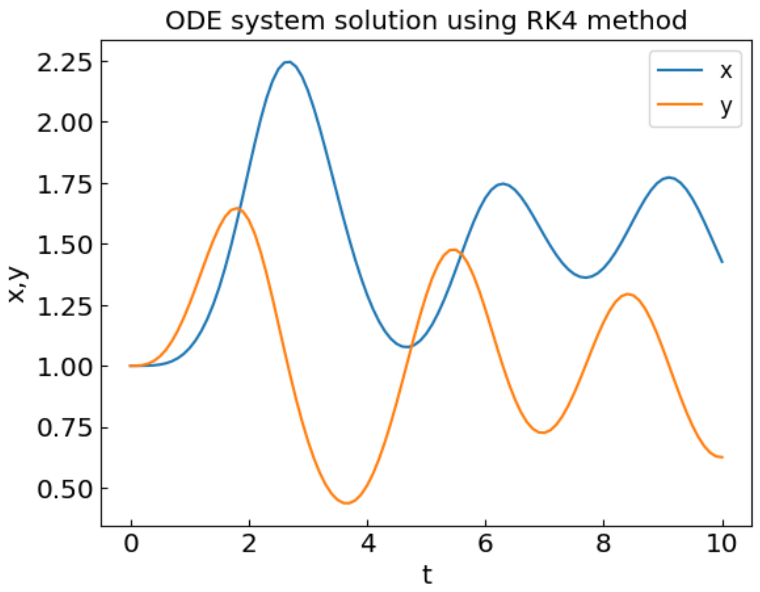
```python
def ode_rk4_multi(f, x0, t0, h, nsteps):
    """Multi-dimensional version of the RK4 method.
    """

    t = np.zeros(nsteps + 1)
    x = np.zeros((len(t), len(x0)))
    t[0] = t0
    x[0,:] = x0
    for i in range(0, nsteps):
        t[i + 1] = t[i] + h
        x[i + 1] = ode_rk4_step(f, x[i], t[i], h)
    return t,x
```

Systems of Ordinary Differential Equations: Example

$$\frac{dx}{dt} = xy - x,$$
$$\frac{dy}{dt} = y - xy + (\sin t)^2$$







Systems of 2nd-order ODEs

Newton/Lagrange equations of motion are 2nd order systems of ODE $m_i \frac{d^2 x_i}{dt^2} = F_i(\{x_j\}, \{dx_j/dt\}, t)$

A system of N second-order ODEs

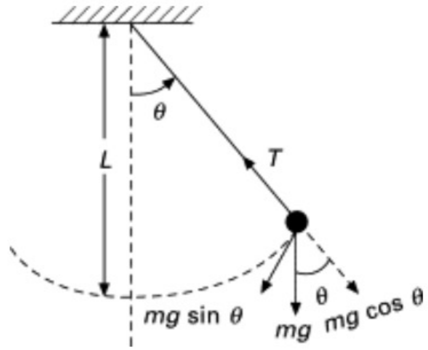
$$\frac{d^2\mathbf{x}}{dt^2} = \mathbf{f}(\mathbf{x}, d\mathbf{x}/dt, t),$$

can be written as a system of *2N* first-order ODEs by denoting $\frac{d\mathbf{x}}{dt} = \mathbf{v}$

$$\frac{d\mathbf{x}}{dt} = \mathbf{v},$$
$$\frac{d\mathbf{v}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{v}, t),$$

and can be solved for $\mathbf{x}(t)$ and $\mathbf{v}(t)$ using standard methods

Example: Simple pendulum



The equation of motion for a simple pendulum reads

$$mL\frac{d^2\theta}{dt^2} = -mg\sin\theta.$$

denote $\frac{d\theta}{dt} = \omega$ and write a system of two first-order ODE

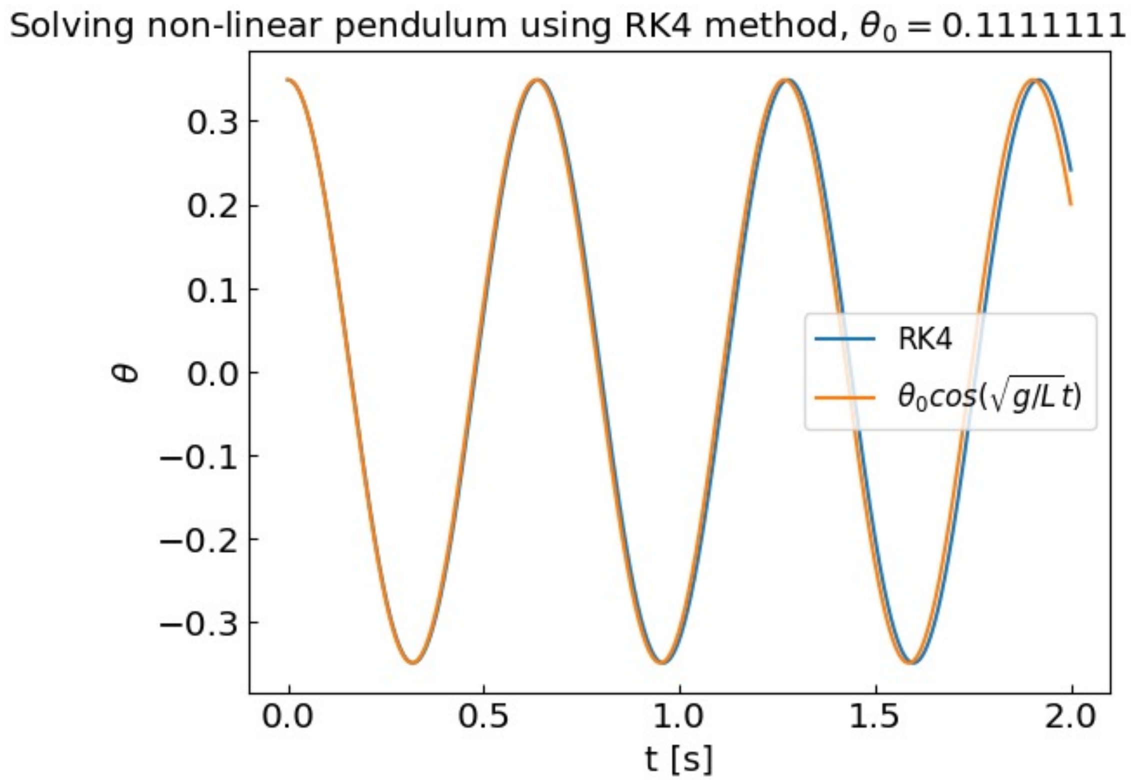
$$\frac{d\theta}{dt} = \omega,$$
$$\frac{d\omega}{dt} = -\frac{g}{L}\sin\theta\,,$$

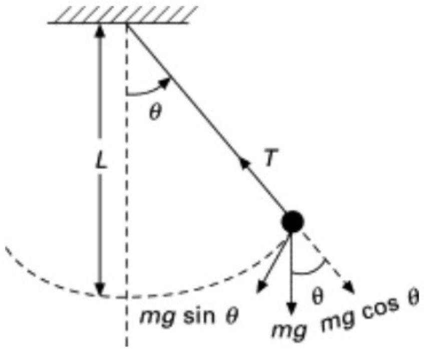
For small angles $\sin\theta \approx \theta$, an analytic solution exists

$$\theta(t) \approx \theta_0 \cos\left(\sqrt{\frac{g}{L}}t + \phi\right)$$

Example: Simple pendulum

Initially at rest at angle $\theta_0 = 20° \approx 0.111\pi$ L=0.1 m, g=9.81 m/s^2

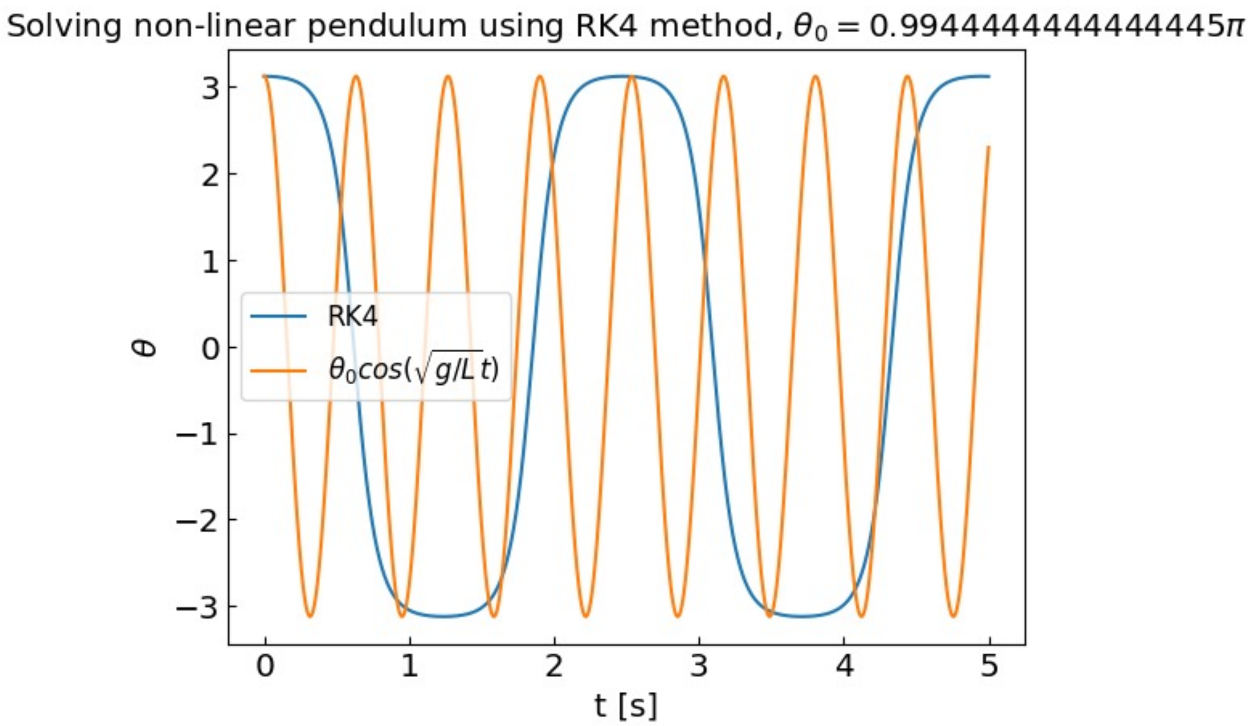


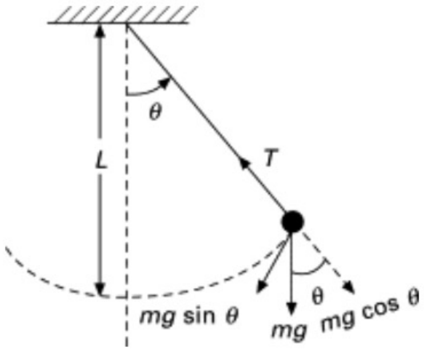


Linear regime at small angles

Example: Simple pendulum

Initially at rest at angle $\theta_0 = 179° \approx 0.994\pi$ L=0.1 m, g=9.81 m/s^2





Non-linear regime at large angles, approximate analytic solution fails