Computational Physics (PHYS6350)

Lecture 10: Ordinary Differential Equations Part II

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

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Course materials: https://github.com/vlvovch/PHYS6350-ComputationalPhysics

Adaptive time step

For a single ODE we devised an adaptive RK4 scheme

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

Time step is adjusted as

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

Here $x_1 = RK4(RK4(x,t,h\ ),t+h,h)$ and $x_2 = RK4(x,t+2h,2h)$

How to generalize ε=|x_1-x_2| it to system of ODEs where we have a state vector **x**?

The answer depends on the physical problem at hand. One could take for example

$$\varepsilon = |\mathbf{x_1} - \mathbf{x_2}|$$

Alternatively, if the accuracy of only one variable matters (e.g. the position but not velocity), one can use just this one coordinate to define ε

The implementation of the adaptive step in systems of ODEs should thus allow for flexibility to define the accuracy

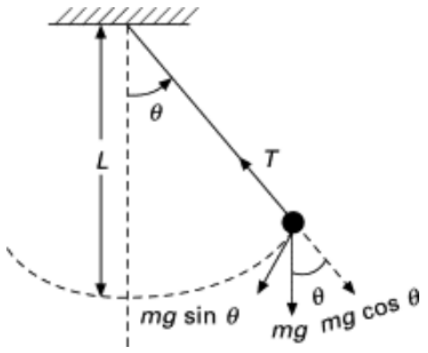
Multi-dimensional RK4 with adaptive time step

```python
def ode_rk4_adaptive_multi(f, x0, t0, h0, tmax, delta = 1.e-6, distance_definition = distance_definition_default):
    """Solve an ODE dx/dt = f(x,t) from t = t0 to t = t0 + h*steps
    using 4th order Runge-Kutta method with adaptive time step.

    Args:
          f: the function that defines the ODE.
         x0: the initial value of the dependent variable.
         t0: the initial value of the time variable.
         h0: the initial time step
       tmax: the maximum time
      delta: the desired accuracy per unit time

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

    ts = [t0]
    xs = [x0]

    h = h0
    t = t0
    i = 0
```

```python
    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)

        diffnorm = distance_definition(x1, x2)
        if diffnorm == 0.: # To avoid the division by zero
            rho = 2.**4
        else:
            rho = 30. * h * delta / diffnorm
        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
```

Adaptive time step RK4 for non-linear pendulum

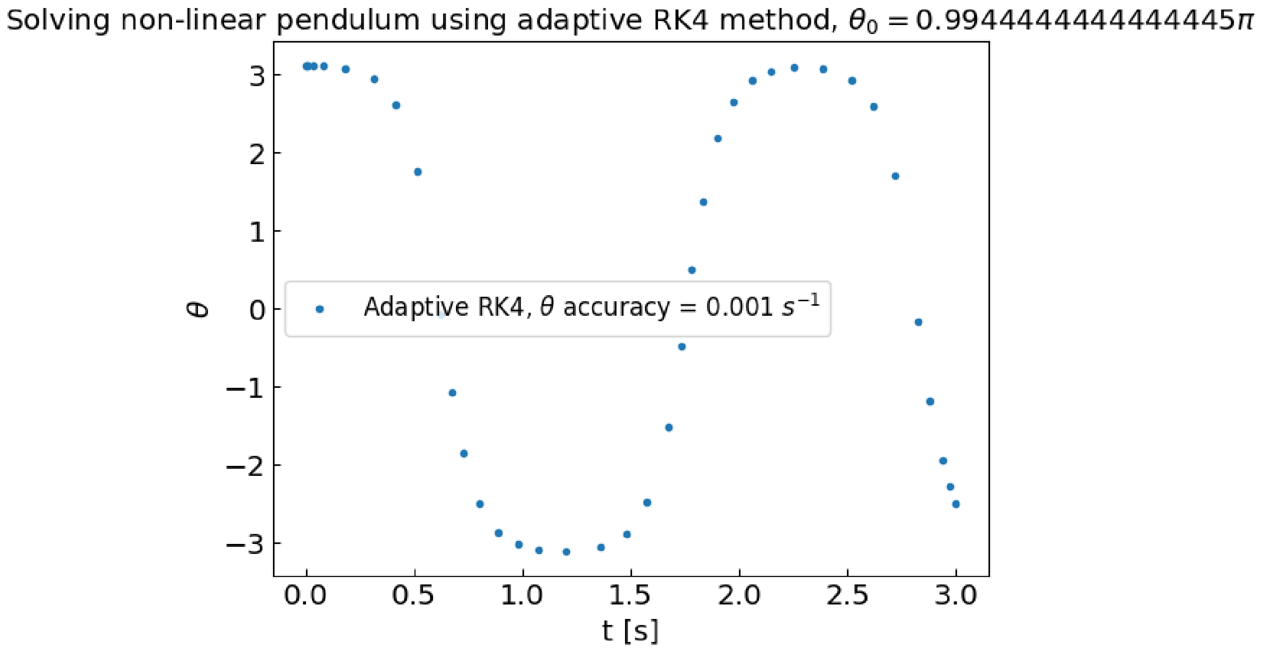
Initially at rest at angle $\theta_0 = 179° \approx 0.994\pi$ L=0.1 m, g=9.81 m/s^2

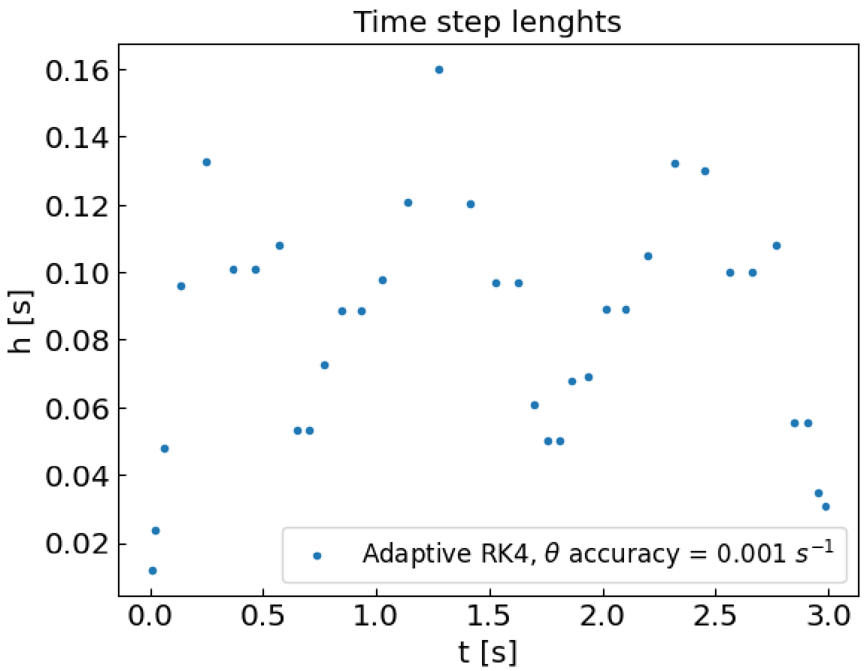


Accuracy: only the angle θ matters

```
def error_definition_pendulum(x1, x2):
    return np.abs(x1[0] - x2[0])
```

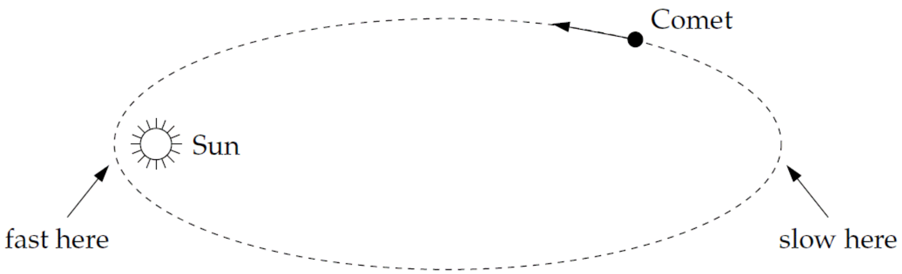
```
a = 0.
b = 3.0
N = 500
h0 = (b-a)/N
eps = 1.e-3 # accuracy in theta
sol = ode_rk4_adaptive_multi(fpendulum, x0, a, h0, b, eps, error_definition_pendulum)
```





Comet motion

Exercise 8.10 (M. Newman, *Computational Physics*)



$$m\frac{d^2\vec{r}}{dt^2} = -\left(\frac{GMm}{r^2}\right)\frac{\vec{r}}{r}$$

Angular momentum conserved, the motion is in the plane (z=0), only two equations needed

$$\frac{d^2x}{dt^2} = -GM\frac{x}{r^3}, \qquad \frac{d^2y}{dt^2} = -GM\frac{y}{r^3},$$

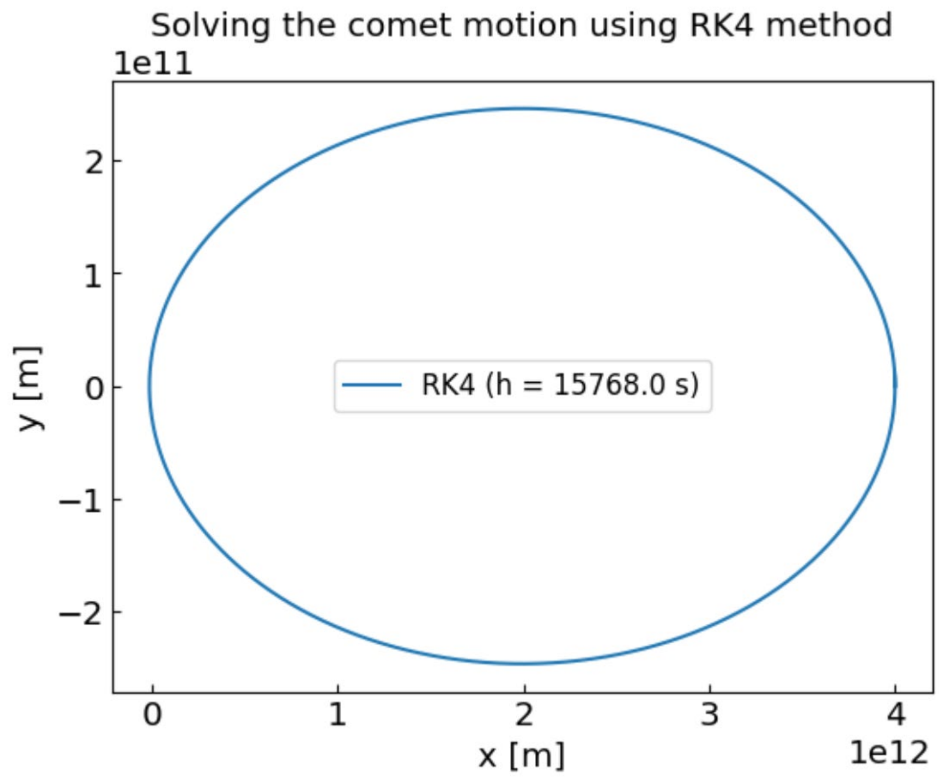
where $r = \sqrt{x^2 + y^2}$.

Initial conditions:
$x(0) = 4 \cdot 10^{12}$ m, $y(0) = 0$
$v_x(0) = 0$, $v_y(0) = 500$ m/s

```python
G = 6.67430e-11  # m^3 / kg / s^2
Msun = 1.9885e30 # kg

def fcomet(xin, t):
    x = xin[0]
    y = xin[1]
    vx = xin[2]
    vy = xin[3]
    r = np.sqrt(x*x+y*y)
    return np.array([vx,vy,-G*Msun*x/r**3,-G*Msun*y/r**3])

x0 = [4.e12,0.,0.,500.]
```

Comet motion: RK4 with fixed time step

```
a = 0.
b = 50. * 365. * 24. * 60. * 60. # 50 years
N = 100000                        # 100 thousand RK4 steps
h = (b - a) / N                   # Time step: around 1/5th of a day
sol = ode_rk4_multi(fcomet, x0, a, h, N)
```



Nice elliptic shape but are we wasting computational resources (time step very small)

Comet motion: RK4 with fixed time step

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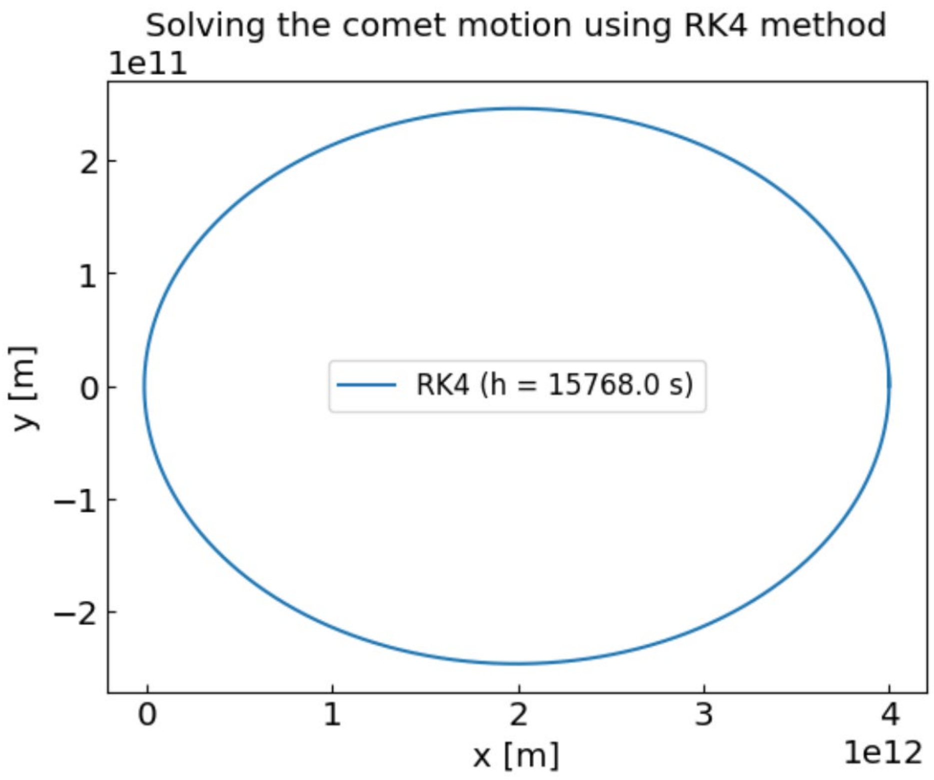
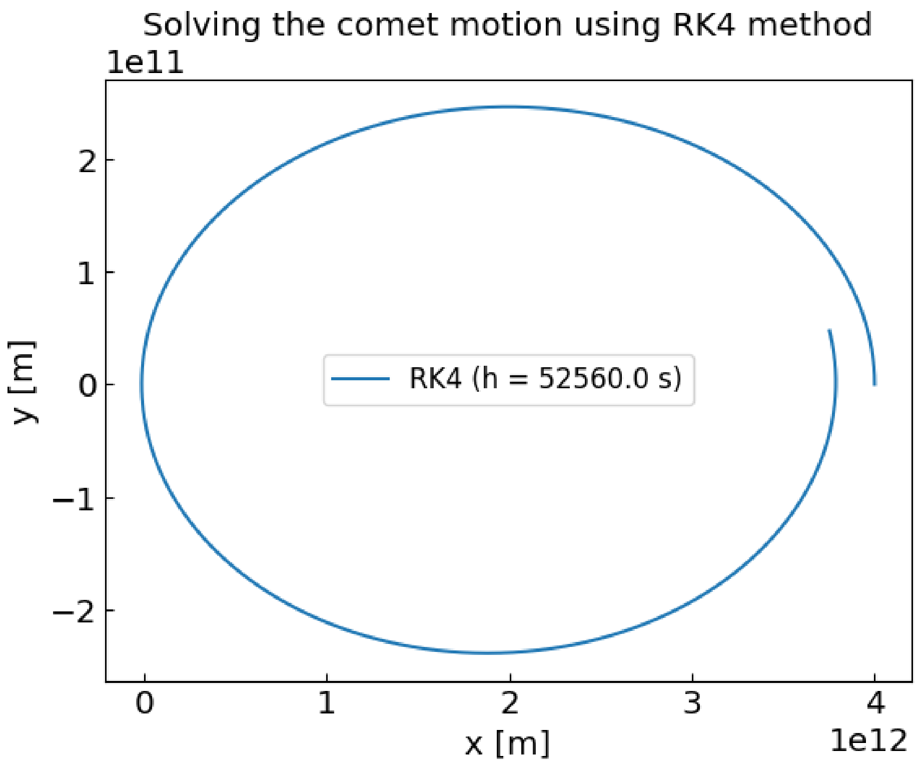
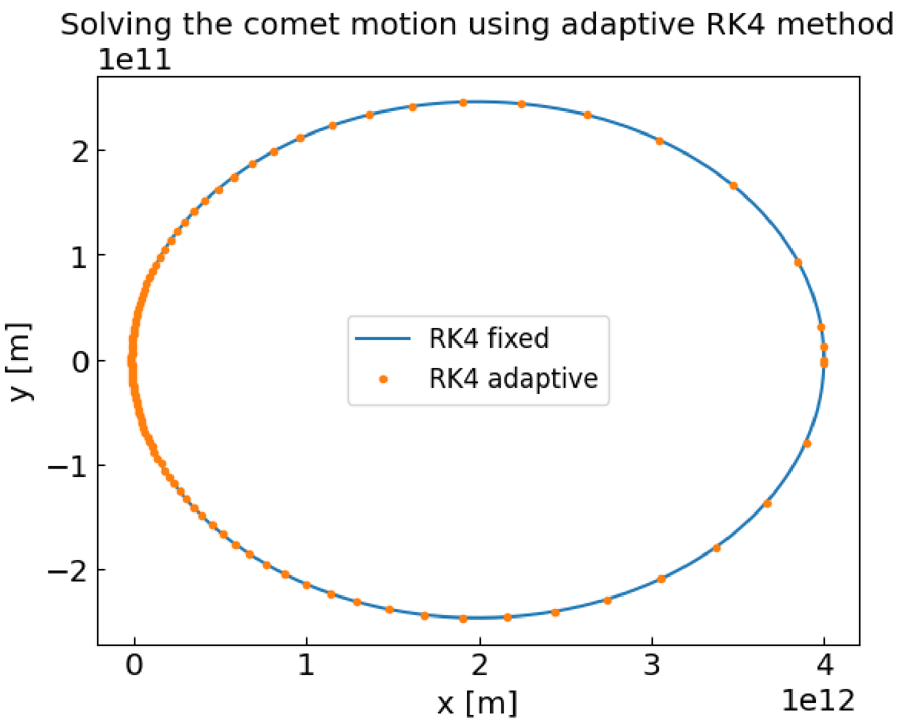


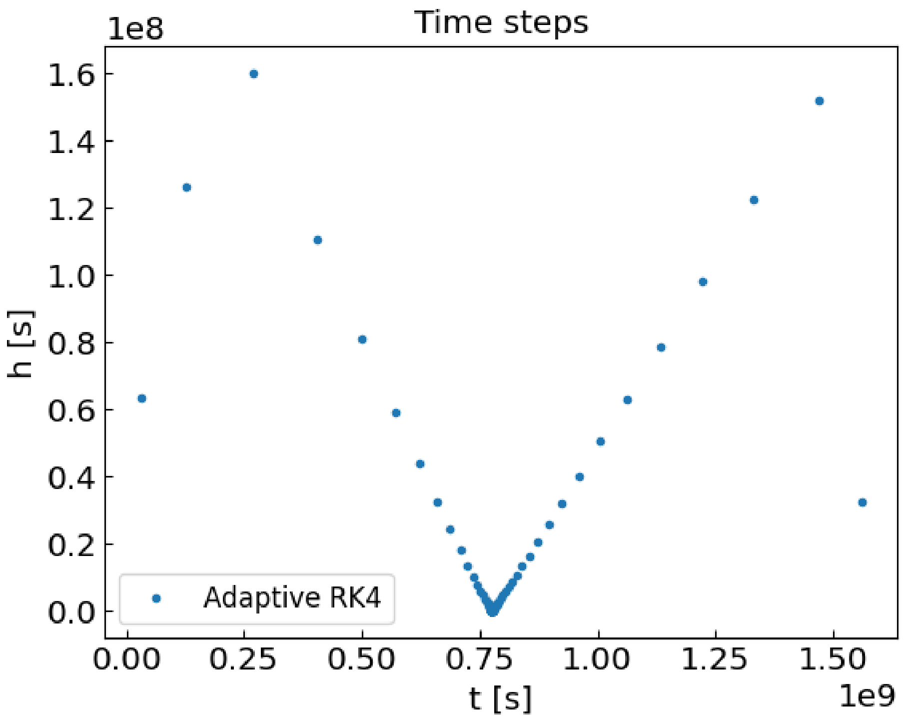


Nice elliptic shape but are we wasting computational resources (time step very small)

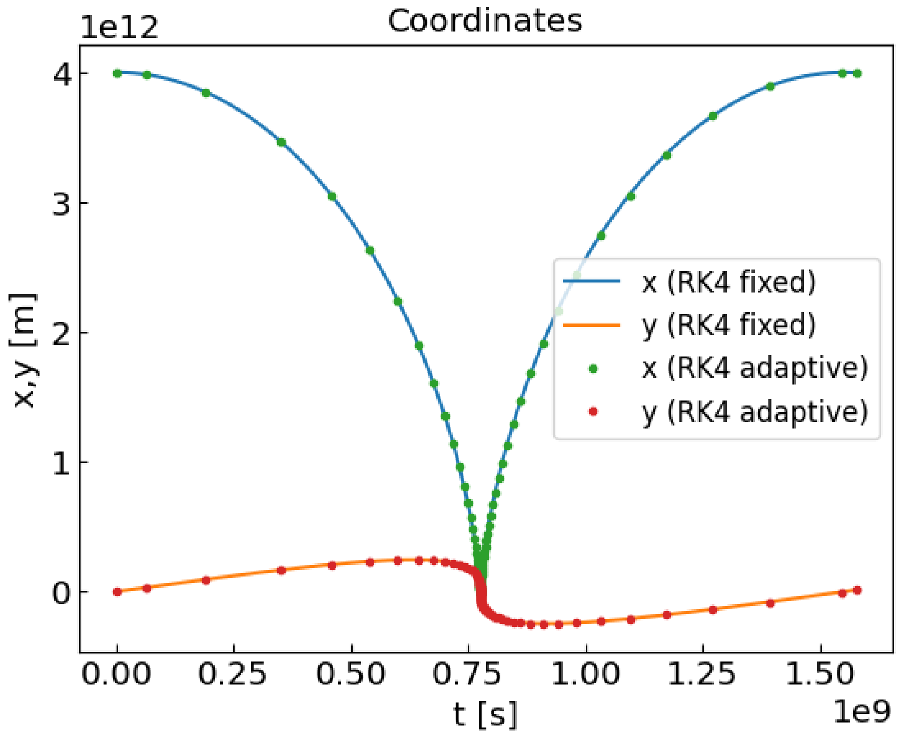
Comet motion: RK4 with adaptive time step

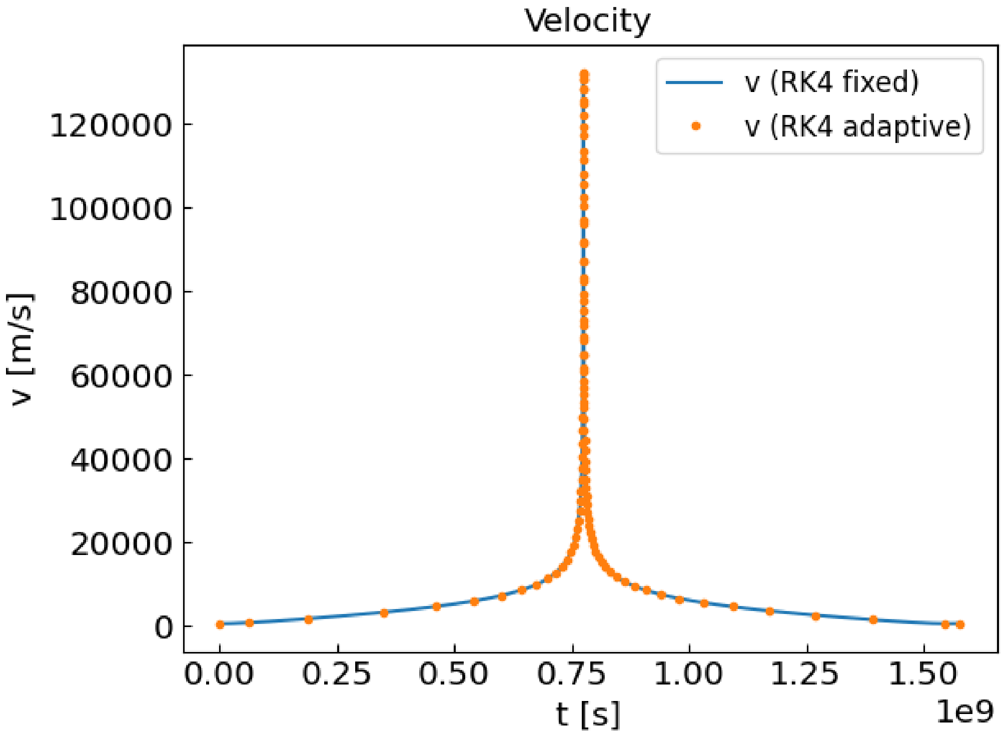
```
def error_definition_comet(x1, x2):
    return np.sqrt((x1[0]-x2[0])**2 + (x1[1]-x2[1])**2)

x0 = [4.e12,0.,0.,500.]

a = 0.
b = 50. * 365. * 24. * 60. * 60. # 50 years
h0 = 1. * 365. * 24. * 60. * 60. # Initial time step: 1 year
delta = 1000. * 1.e3 / (365. * 24. * 60. * 60.)
sol = ode_rk4_adaptive_multi(fcomet, x0, a, h0, b, delta, error_definition_comet)
```





Comet motion: RK4 with adaptive time step

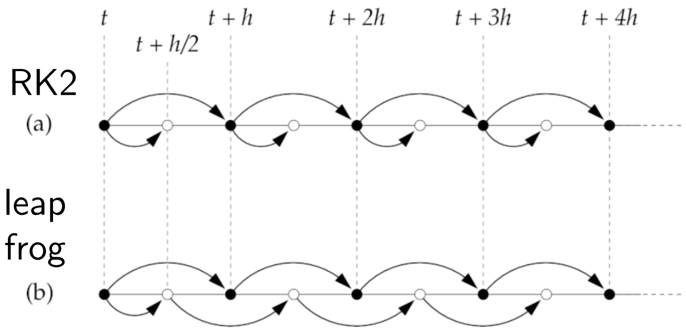




Leapfrog method

Recall the RK2 (midpoint) method

$$x(t+h) = x(t) + hf[x(t+h/2), t+h/2],$$
$$x(t+h/2) = x(t) + \frac{1}{2}hf(x,t)\,.$$



Leapfrog method: given x(t) and x(t+h/2), estimate x(t+h) and x(t+3h/2) using first equation only

$$x(t+h) = x(t) + hf[x(t+h/2), t+h/2],$$
$$x(t+3h/2) = x(t+h/2) + hf[x(t+h), t+h].$$

Leapfrog method

Euler's half-step is used in the first iteration only.

The method is **time reversible**:
By changing h->-h one recovers x(t) and x(t+h/2) from previous iteration.

Error:

- Local (per time step): O(h^3) + O(h^5) + O(h^7) + ...
- Global (N=t_{end}/h time steps): O(h^2) + O(h^3) + ...

Odd powers in the global error propagated from Euler's half-step at 1st iteration

Leapfrog method implementation

```python
def ode_leapfrog_step(f, x, x2, t, h):
    """Perform a single step h using the leapfrog method.

    Args:
     f: the function that defines the ODE.
     x: the value of x(t)
    x2: the value of x(t+h/2)
     t: the present value of the time variable.
     h: the time step

    Returns:
    xnew, xnew2: the value of the dependent variable at the steps t+h, t+3h/2
    """

    xnew = x + h * f(x2,t+h/2.)
    xnew2 = x2 + h * f(xnew, t + h)
    return xnew, xnew2
```

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

    t = np.zeros(nsteps + 1)
    x = np.zeros((len(t), len(x0)))
    x2 = np.zeros(len(x0))
    t[0] = t0
    x[0,:] = x0
    x2[:] = ode_euler_step(f, x0, t0, h/2.)
    for i in range(0, nsteps):
        t[i + 1] = t[i] + h
        x[i + 1], x2 = ode_leapfrog_step(f, x[i], x2, t[i], h)
    return t,x
```

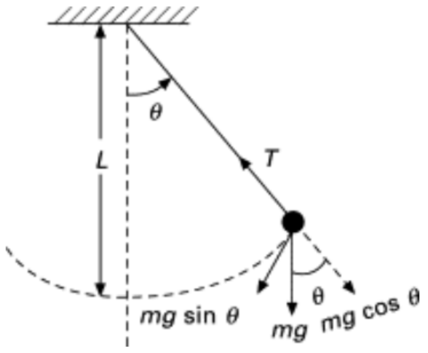
Leapfrog method and non-linear pendulum

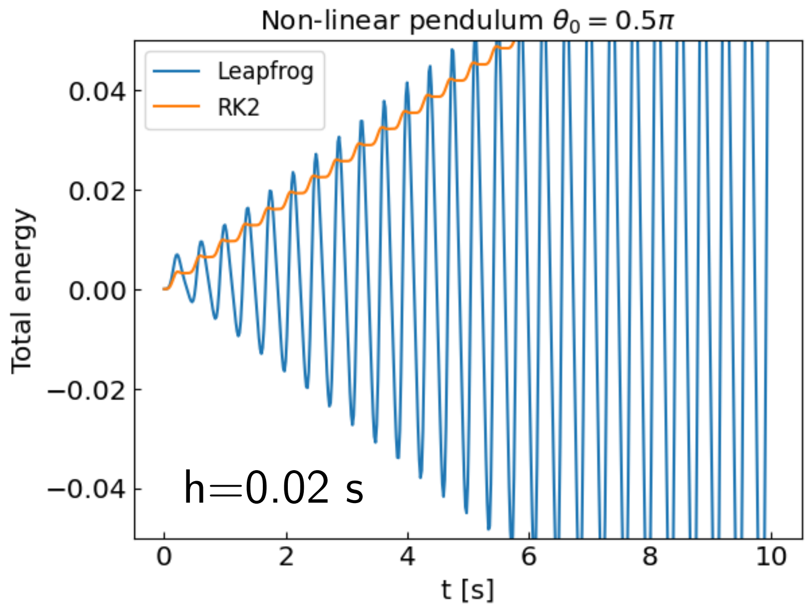
Time-reversal symmetry implies average energy conservation

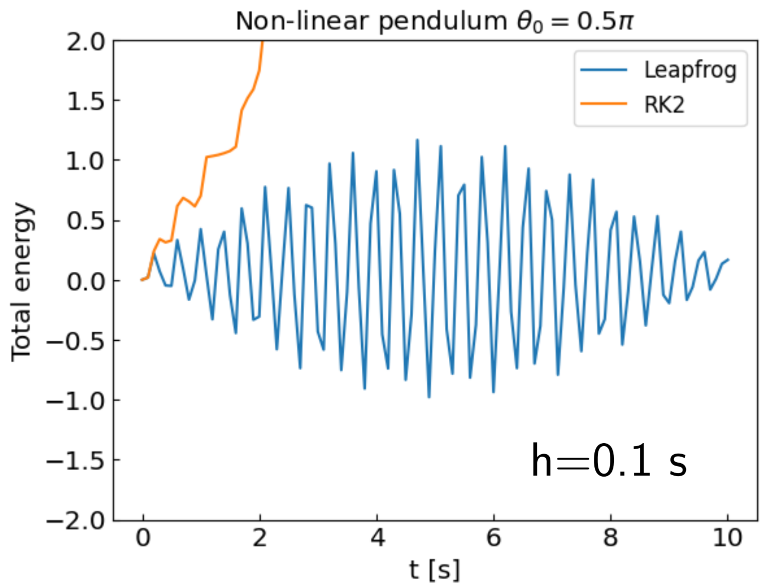
The pendulum energy is

$$E = mL^2\dot{\theta}^2/2 - mgL\cos(\theta)$$

Let us solve it with the leapfrog and RK2 methods and see how energy evolves with time







Energy is drifting in RK2 but conserved (on average) in leapfrog method

Modified midpoint method

Recall the error in the leapfrog method when integrating from t to t+H in steps of h = H/N

- Local (per time step): $O(h^3) + O(h^5) + O(h^7) + \ldots$
- Global ($N=H/h$ time steps): $O(h^2) + O(h^3) + \ldots$

Odd powers in the global error are propagated from Euler's half-step at 1st iteration $$x(t + h/2) = x(t) + \frac{1}{2} h f(x, t) \, .$$

They can be canceled out with an additional Euler half-step at the end

Let $y_n = x(t+H-h/2)$ and $x_n = x(t+H)$ be the solution estimates resulting from the leapfrog method.

$$x(t + H) = \frac{1}{2}[x_n + y_n + \frac{h}{2} f(x_n, t + H)].$$

modified midpoint method

Global error: $O(h^2) + O(h^4) + O(h^6) + \ldots$
(even powers only)

```python
def ode_MMM_multi(f, x0, t0, H, nsteps):
    """Multi-dimensional version of the modified midpoint method.
    """

    h = H / nsteps
    t = np.zeros(nsteps + 1)
    x = np.zeros((len(t), len(x0)))
    x2 = np.zeros(len(x0))
    t = t0
    x = x0
    y = ode_euler_step(f, x0, t0, h/2.)
    for i in range(0, nsteps):
        yprev = y
        x, y = ode_leapfrog_step(f, x, y, t, h)
        t = t + h

    return 0.5 * (x + yprev + 0.5 * h * f(x,t))
```

Bulirsch-Stoer method

The error in the modified midpoint method when integrating from t to t+H in steps of $h_n = H/n$ is $O(h^2) + O(h^4) + O(h^6) + \ldots$ (even powers only)

Bulirsch-Stoer method: Use the modified midpoint method with various steps *n* to cancel error terms of higher and higher order (Richardson extrapolation, similar to Romberg integration)

Let $R_{n,1}$ be an estimate of $x(t+H)$ from the n-step modified midpoint method ($h_n = H/n$)

$$x(t + H) = R_{n,1} + O(h_n^2).$$

One constructs high-order approximations $R_{n,m}$ such that

$$x(t + H) = R_{n,m} + O(h_n^{2m}),$$

Similar to Romberg integration one can derive

$$R_{n,m+1} = R_{n,m} + \frac{R_{n,m} - R_{n-1,m}}{[n/(n-1)]^{2m} - 1} \,.$$

Bulirsch-Stoer method

The method stops when the desired accuracy is achieved, $|R_{n,n}-R_{n,n-1}|<\varepsilon$

If *n* grows too large, it is better to split the (t,t+H) interval into two subintervals (t,t+H/2) & (t+H/2,t+H) and apply the method recursively to each of them

Bulirsch-Stoer method implementation

```
def bulirsch_stoer_step(f, x0, t0, H, delta = 1.e-6, distance_definition = distance_definition_default, maxsteps = 10):
    """Use Bulirsch-Stoer method to integrate for t to t+H.
    """
    n = 1
    R1 = np.empty([1,len(x0)],float)
    R1[0] = ode_MMM_multi(f, x0, t0, H, 1)
    error = 2. * H * delta
    while error > H*delta and n < maxsteps:
        n += 1
        R2 = R1
        R1 = np.empty([n,len(x0)],float)
        R1[0] = ode_MMM_multi(f, x0, t0, H, n)
        for m in range(1,n):
            epsilon = (R1[m-1]-R2[m-1])/((n/(n-1))**(2*m)-1)
            R1[m] = R1[m-1] + epsilon
        error = distance_definition(R1[n-2],R1[n-1])

    if n == maxsteps:
        # Reached maximum number of substeps in Bulirsch-Stoer method
        # reducing the time step and applying the method recursively
        sol1 = bulirsch_stoer_step(f, x0, t0, H/2., delta, distance_definition, maxsteps)
        sol2 = bulirsch_stoer_step(f, sol1[-1][1], t0 + H/2., H/2., delta, distance_definition, maxsteps)
        return sol1 + sol2

    return [[t0+H, R1[n - 1]]]
```

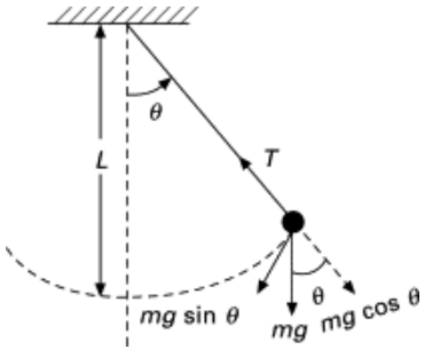
Bulirsch-Stoer method implementation

N-step Bulirsch-Stoer: apply the H step N times:

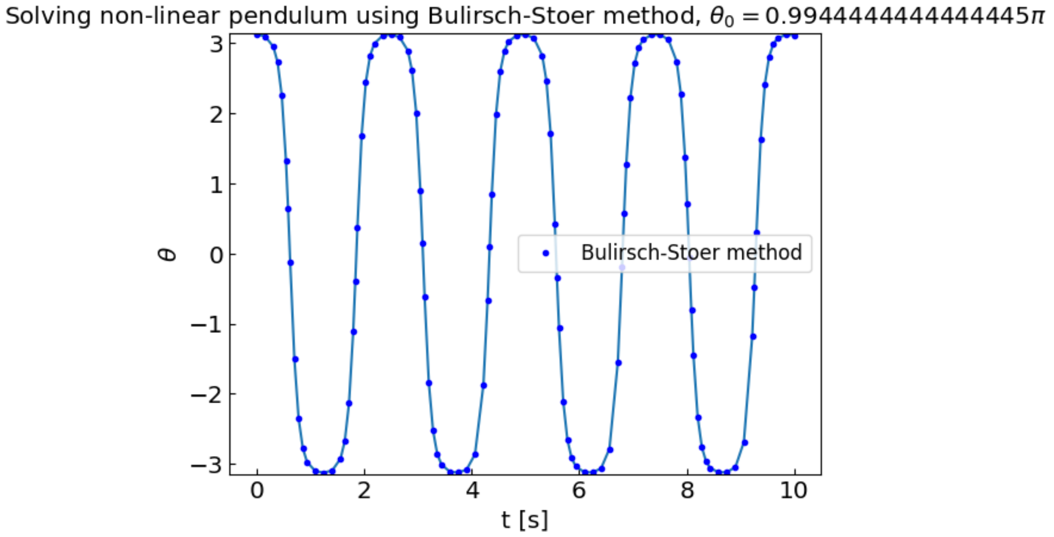
```python
def bulirsch_stoer(f, x0, t0, nsteps, tmax, delta = 1.e-6, distance_definition = distance_definition_default, maxsubstep
    """Use Bulirsch-Stoer method to integrate for t to tmax using nsteps Bulirsch-Stoer steps
    """
    H = (tmax - t0) / nsteps
    t = np.zeros(nsteps + 1)
    x = np.zeros((len(t), len(x0)))
    t = [t0]
    x = [x0]
    for i in range(0, nsteps):
        bst = bulirsch_stoer_step(f, x[-1], t[-1], H, delta, distance_definition, maxsubsteps)
        [t.append(el[0]) for el in bst]
        [x.append(el[1]) for el in bst]
    return t,x
```

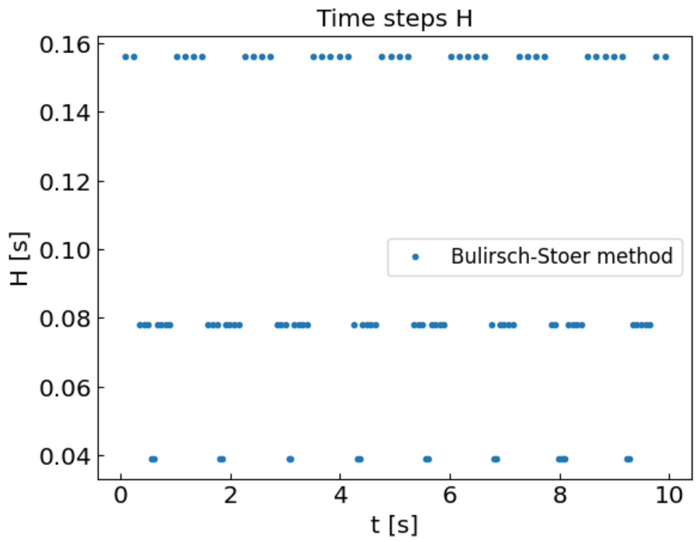
Bulirsch-Stoer method and non-linear pendulum

Apply the method to non-linear pendulum with the initial H = 10 (single step) and a maximum of 10 substeps. The method will adjust H as needed.




```
theta0 = 179. * np.pi / 180.
omega0 = 0.
x0 = np.array([theta0,omega0])
a = 0.
b = 10.0
N = 1
eps = 1.e-8
maxsubsteps = 10

sol = bulirsch_stoer(fpendulum, x0, a, N, b, eps, error_definition_pendulum, maxsubsteps)
```

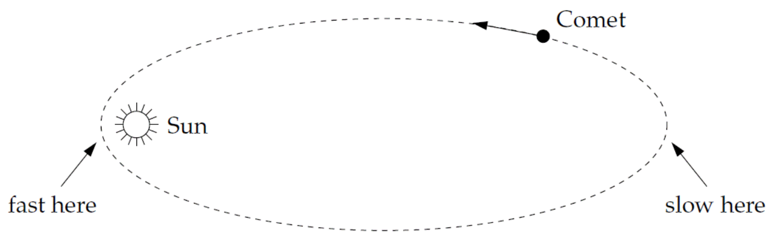


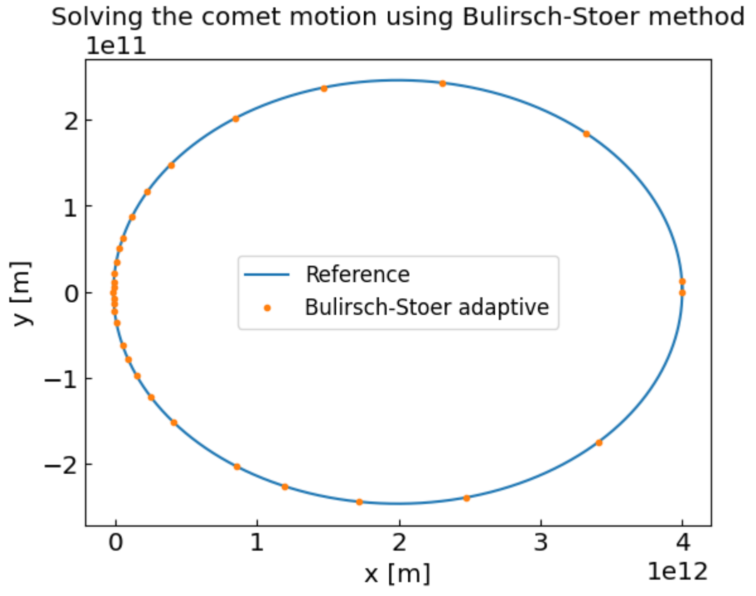


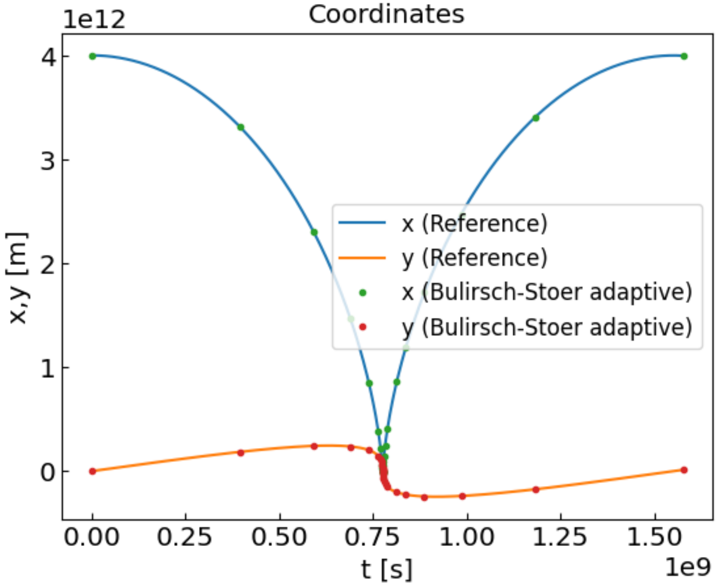
Bulirsch-Stoer method and the comet motion

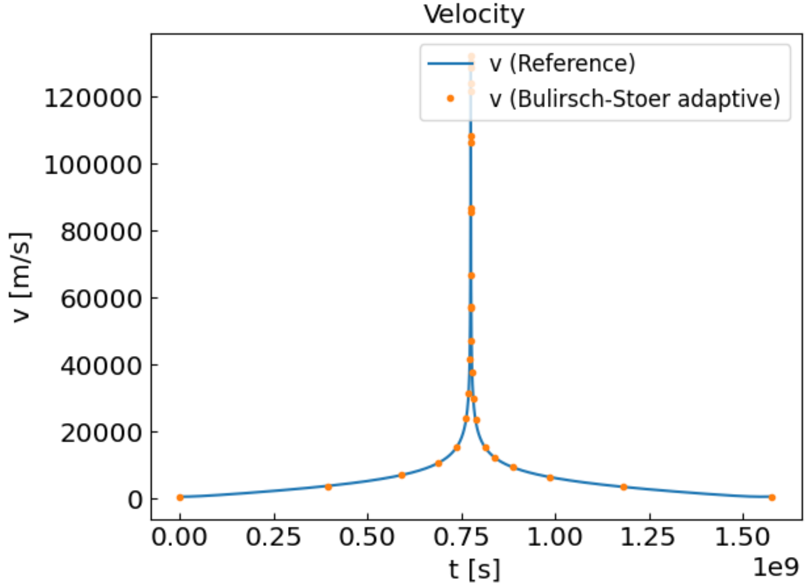
Same for the comet motion. Accuracy: 1 km per day

```
x0 = [4.e12,0.,0.,500.]
a = 0.
b = 50. * 365. * 24. * 60. * 60.
N = 1
delta = 1. * 1.e3 / (365. * 24. * 60. * 60.)
sol = bulirsch_stoer(fcomet, x0, a, N, b, delta, error_definition_comet)
```









SIR model

The SIR model is the simplest model for infection disease dynamics in the population. The population is split into susceptible (S), infected (I), and recovered/immune (R) parts.

The SIR equations read:

$$\frac{dS}{dt} = -\beta SI,$$
$$\frac{dI}{dt} = \beta SI - \gamma I,$$
$$\frac{dR}{dt} = \gamma I.$$

```
gam = 1./10.      # 10 days recovery rate
beta = 1./4.      # 4 days to infect other person
# R0 = beta/gam  # basic reproduction factor
kappa = 1. / 90. # immunity lasts for 90 days

def fSIR(xin, t):
    S = xin[0]
    I = xin[1]
    R = 1. - S - I
    return np.array([-beta * S * I, beta * I * S - gam * I])
```

Here β is the infection rate and γ is the recovery rate.

The ratio $R_0 = \beta/\gamma$ is basic reproduction number.

Given that $S + I + R = 1 = \text{const}$ at all times, one only needs to solve two ODEs, e.g. dS/dt and dI/dt.

SIR model

Solve the SIR model equations using e.g. Bulirsch-Stoer method

```
t0 = 0.
tend = 365.

I0 = 1.e-5            # Initial fraction of infected
x0 = [1. - I0, I0]    # Initial conditions

delta = 1.e-9 # The desired accuracy per day
N = 50        # Minimum number of steps
sol = bulirsch_stoer(fSIR, x0, t0, N, tend, delta)
```

SIR model

Solve the SIR model equations using e.g. Bulirsch-Stoer method

```
t0 = 0.
tend = 365.

I0 = 1.e-5           # Initial fraction of infected
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```
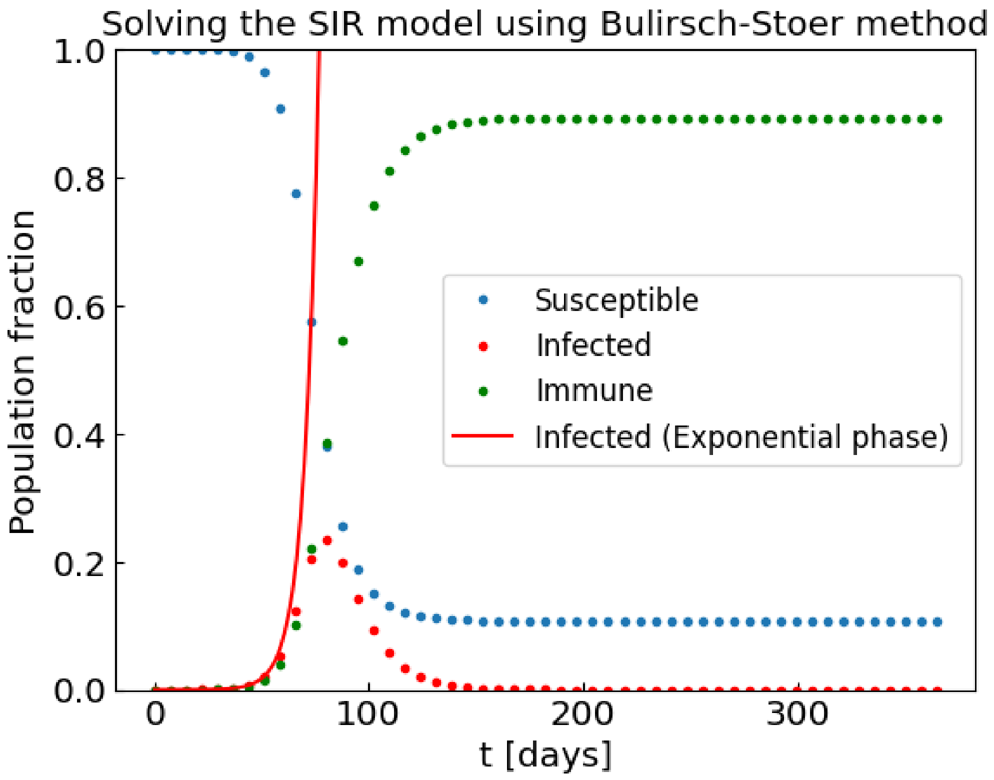



One can clearly see the initial exponential phase of the epidemic, and its end once a sufficient fraction of the population obtained immunity.

Modified SIR model

What if the immunity disappears with time?
Introduce the loss of immunity rate κ

$$\frac{dS}{dt} = -\beta SI + \kappa R,$$
$$\frac{dI}{dt} = \beta SI - \gamma I,$$
$$\frac{dR}{dt} = \gamma I - \kappa R.$$

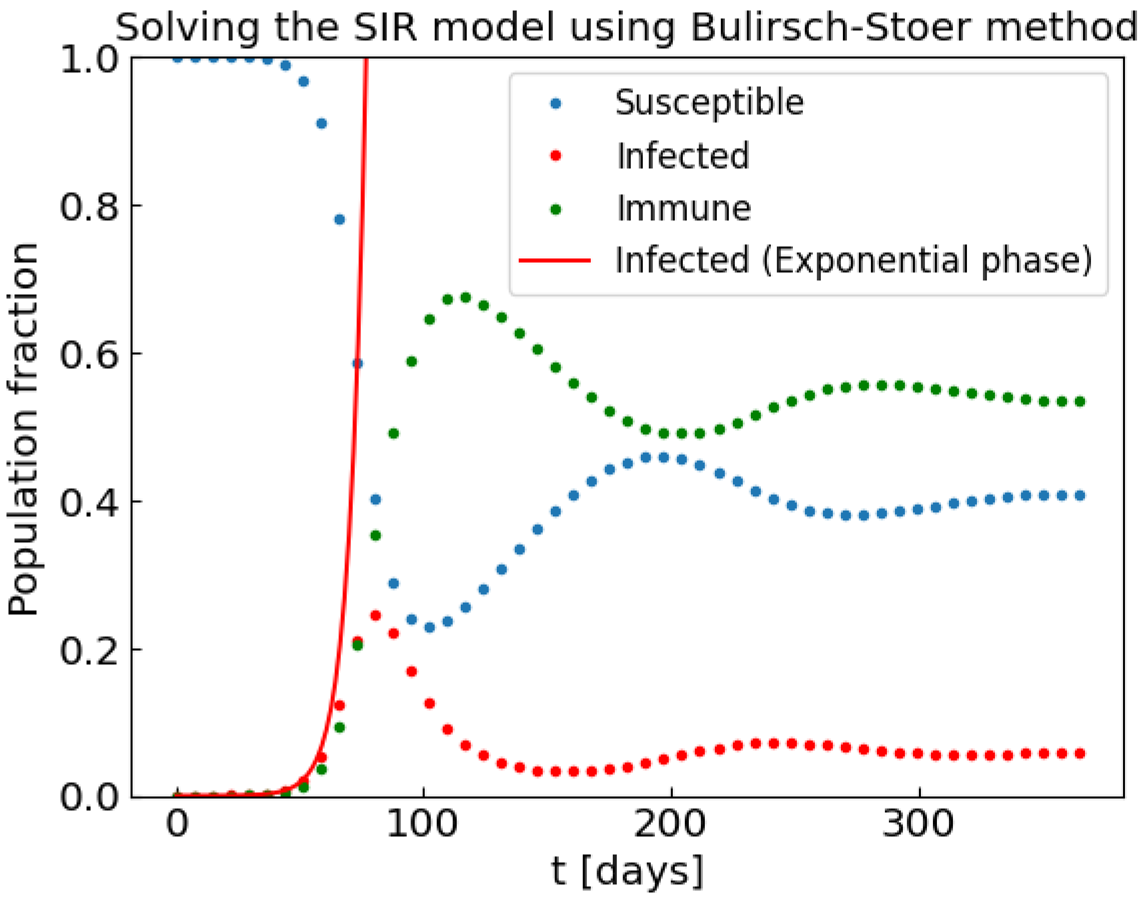
```
gam = 1./10.     # 10 days recovery rate
beta = 1./4.     # 4 days to infect other person
# R0 = beta/gam  # basic reproduction factor
kappa = 1. / 90. # immunity lasts for 90 days

def fSIR(xin, t):
    S = xin[0]
    I = xin[1]
    R = 1. - S - I
    # print(xin)
    return np.array([-beta * S * I + immu * (1. - S - I), beta * I * S - gam * I])

t0 = 0.
tend = 365.

I0 = 1.e-5
x0 = [1. - I0, I0]

delta = 1.e-9 # The desired accuracy per day
N = 50
sol = bulirsch_stoer(fSIR, x0, t0, N, tend, delta)
```

Modified SIR model

What if the immunity disappears with time?
Introduce the loss of immunity rate κ

$$\frac{dS}{dt} = -\beta SI + \kappa R,$$
$$\frac{dI}{dt} = \beta SI - \gamma I,$$
$$\frac{dR}{dt} = \gamma I - \kappa R.$$

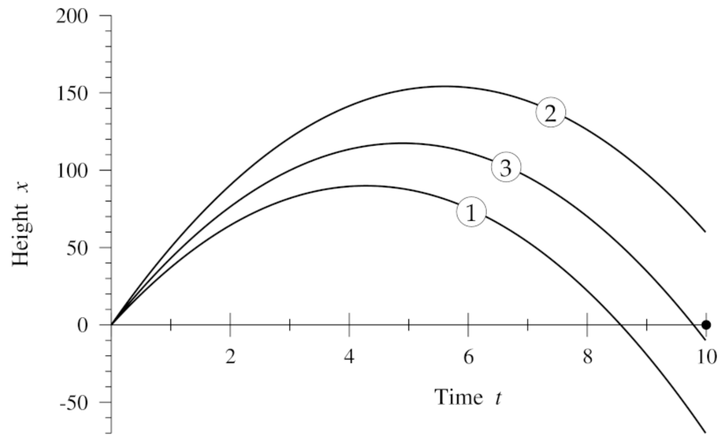
```
gam = 1./10.     # 10 days recovery rate
beta = 1./4.     # 4 days to infect other person
# R0 = beta/gam  # basic reproduction factor
kappa = 1. / 90. # immunity lasts for 90 days

def fSIR(xin, t):
    S = xin[0]
    I = xin[1]
    R = 1. - S - I
    # print(xin)
    return np.array([-beta * S * I + immu * (1. - S - I), beta * I * S - gam * I])

t0 = 0.
tend = 365.

I0 = 1.e-5
x0 = [1. - I0, I0]

delta = 1.e-9 # The desired accuracy per day
N = 50
sol = bulirsch_stoer(fSIR, x0, t0, N, tend, delta)
```



Boundary value problems and the shooting method

Sometimes we have equations, such as vertically thrown object

$$\frac{dx}{dt} = v,$$
$$\frac{dv}{dt} = -g,$$



and boundary conditions, e.g. $x(0) = 0$ and $x(10) = 0$ instead of initial conditions $v(0) = v_0$.

How to solve this problem?

In the shooting method one takes trial values of v_0 until finding the one where the solution satisfies the boundary condition $x(10) = 0$.

To find v_0 efficiently one combines numerical ODE method (e.g. RK4) with non-linear equation solver (e.g. bisection method).

Shooting method for vertically thrown object

Search for v0 using bisection method and solve the intermediate ODEs using RK4

```python
g = 9.81 # m/s^2
# ODEs
def fball(xin,t):
    x = xin[0]
    v = xin[1]
    return np.array([v,-g])

# Initial and final times
t0 = 0.
tend = 10.
# Number of RK4 steps
Nrk4 = 100
hrk4 = (tend - t0) / Nrk4

# Desired accuracy for v0
accuracy_v0 = 1.e-10 # m/s

v0min = 0.01   # m/s
v0max = 1000.0 # m/s

def fbisection(v0):
    x0 = [0., v0]
    return ode_rk4_multi(fball, x0, t0, hrk4, Nrk4)[1][-1][0]

v0sol = bisection_method(fbisection, v0min, v0max, accuracy_v0)
print("The required initial velocity is",v0sol,"m/s")
```

```
The required initial velocity is 49.0500000000017 m/s
```