Numerical Integration

Differential equations describe the relation between an unknown function and its derivatives. To solve a differential equation is to find a function that satisfies the relation, typically while satisfying some additional conditions as well. In this course we will be concerned primarily with a particular class of problems, called initial value problems. In a canonical initial value problem, the behavior of the system is described by an ordinary differential equation (ODE) of the form

$$\dot{\mathbf{x}} = f(\mathbf{x}, t)$$

where f is a known function $\mathbf{x}$ is the state of the system, and $\dot{\mathbf{x}}$ is $\mathbf{x}$'s time derivative. Typically, $\mathbf{x}$ and $\dot{\mathbf{x}}$ are vectors. As the name suggests, in an initial value problem we are given $\mathbf{x}(t_0) = \mathbf{x_0}$ at some starting time t_0, and wish to follow $\mathbf{x}$ over time thereafter.

In [2]:

```
# python packages and configurations
# %matplotlib nbagg
%matplotlib inline
from random import uniform
import numpy as np
import sympy as sp
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from matplotlib import animation
# plt.style.use('grayscale')
from scipy.integrate import odeint
from IPython.display import HTML, Video, Image

# utility function
def visualize(t, y, u, analytical_solution):
    t = np.array(t)
    y = np.array(y)
    u = np.array(u)
    fig = plt.figure(figsize=(12, 6))
    ax = fig.subplots(1, 2)
    ax[0].plot(t, analytical_solution(t).real, label='analytical')
    ax[0].plot(t, y, 'x', label='numerical')
    ax[0].set_xlabel('$t (s)$')
    ax[0].set_ylabel('$y (m)$')
    ax[0].set_title('Solution')
    ax[0].legend()
    ax[1].quiver(y[:-1], u[:-1], y[1:] - y[:-1], u[1:] - u[:-1],
                 scale_units='xy', angles='xy', scale=1)
    ax[1].set_xlabel('$y (m)$')
    ax[1].set_ylabel('$u (m / s)$')
    ax[1].set_title('State-space')
```

Analytical Solution

Let us examine the following second-order ODE that represents a mass-spring-damper system:

$$my'' + dy' + ky = 0, \;\; y(t_0) = y_0, y'(t_0) = u_0$$

where m, d and k are the mass, spring constant and damping coefficient, respectively. The analytical solution of this equation is of the following form:

$$y(t) = Ae^{r_1 t} + Be^{r_2 t}$$

where r_1 and r_2 are the roots of the homogeneous equation. Constants A and B are determined such as that the above equation satisfies the initial conditions.

In [6]:

```
# model parameters and initial conditions
m = 1.0   # mass
k = 5.0   # spring constant
d = 0.0   # damping coefficient
y0 = -5.0 # initial position
u0 = 0.0  # initial velocity

# find the roots of the homogeneous equation
def calc_analytical_solution():
    roots = sp.solve('m * y**2 + d * y + k', 'y')

    # find the constants of the analytical solution
    constants = sp.solve(['A + B - y0', 'r1 * A + r2 * B - u0'], 'A', 'B')

    # substitute the parameters
    parameters = {'m': m, 'd': d, 'k': k}
    r1 = roots[0].subs(parameters)
    r2 = roots[1].subs(parameters)
    parameters['r1'] = r1
    parameters['r2'] = r2
    parameters['y0'] = y0
    parameters['u0'] = u0
    A = constants[sp.symbols('A')].subs(parameters)
    B = constants[sp.symbols('B')].subs(parameters)

    # calculate the analytical solution as a function of time
    t = sp.symbols('t')
    analytical_solution = sp.lambdify(t, A * sp.exp(r1 * t) + B * sp.exp(r2 * t))
    return analytical_solution
```

Explicit Euler

The simplest numerical method is called explicit Euler. This method computes the next value of the solution $x(t + dt)$ by taking a step in the derivative direction

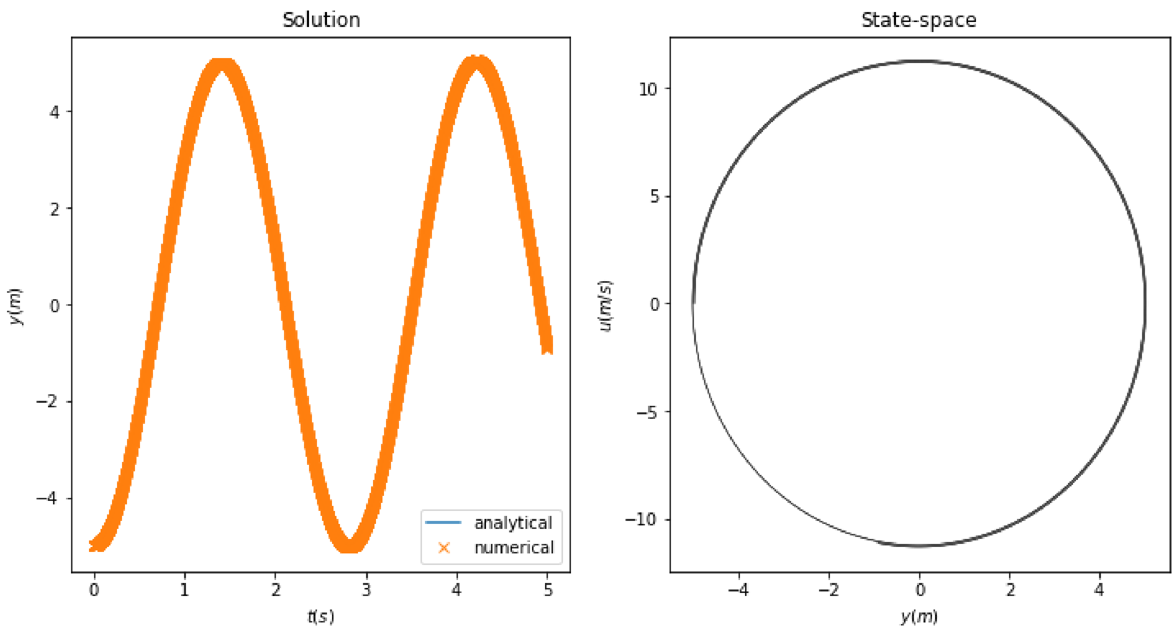
$$x(t_0 + dt) = x(t_0) + x'(t_0)dt + O(dt^2)$$

where $x'(t_0)$ is the first derivative valuated at t_0 and dt is the step size. This is a first-order approximation of the Taylor series. To solve a second order differential equation, one can apply the Euler method twice. Assuming that $u(t) = y'(t)$ and $a(t) = y''(t)$ then the problem is expressed as follows:

$$\begin{aligned} a(t_0) &= -\frac{k}{m}y(t_0) - \frac{d}{m}u(t_0) \\ u(t_0 + dt) &= u(t_0) + a(t_0)dt \\ y(t_0 + dt) &= y(t_0) + u(t_0)dt. \end{aligned}$$

In [10]:

```
# integration parameters
end_time = 5
dt = 0.01

# solution vectors
t = [0.0]
y = [y0]
u = [u0]

# numerical integration
while t[-1] < end_time:
    t0 = t[-1]
    y_t0 = y[-1]
    u_t0 = u[-1]

    #TASK calculate a, u and y
    a_t0 = -(k/m)*y_t0-(d/m)*u_t0
    u_t0_dt = u_t0+a_t0*dt
    y_t0_dt =y_t0 + u_t0*dt

    u.append(u_t0_dt)
    y.append(y_t0_dt)
    t.append(t0 + dt)
# visualization
visualize(t, y, u, calc_analytical_solution())
```



1. Calculate a_t0, u_t0_dt, y_t0_dt.
2. Experiment with different spring parameters and/or initial conditions.
3. Explain the meaning of the state-space plot (right subfigure). What should be the expected state-space plot (hint: change visualize function)?
4. Why does the numerical solution diverges from the true solution (hint: Taylor expansion)?
5. What can you do to better approximate the actual solution with this method?

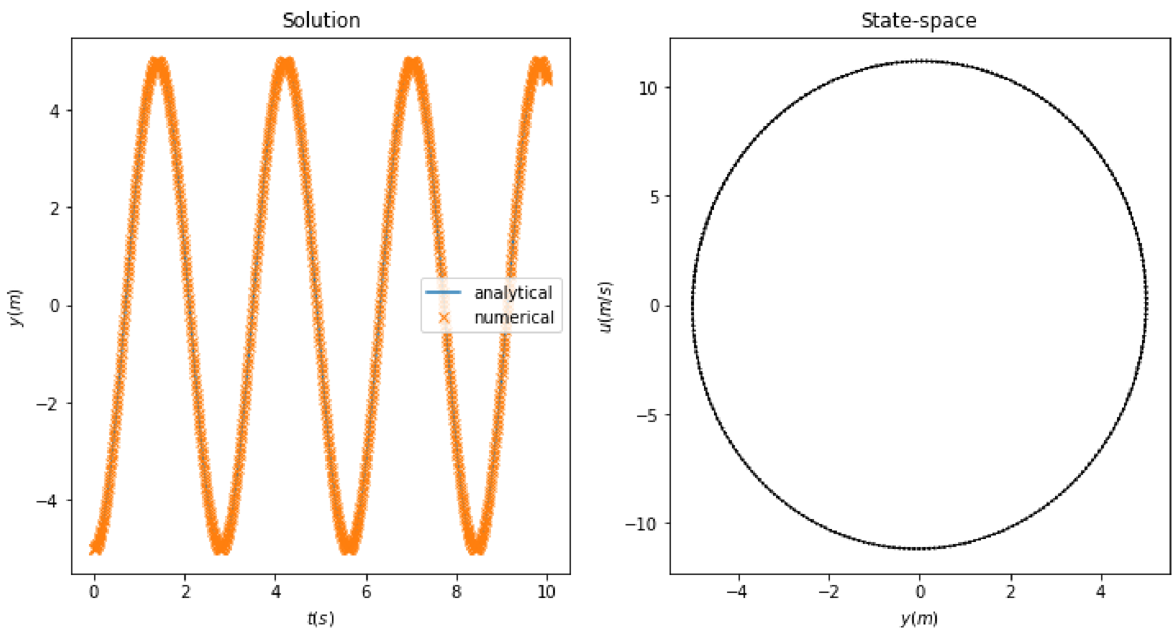
Semi-implicit Euler

The difference with the standard Euler method is that the semi-implicit Euler method uses $u(t_0 + dt)$ in the equation for $y(t_0 + dt)$, while the Euler method uses $u(t_0)$

$$a(t_0) = -\frac{k}{m}y(t_0) - \frac{d}{m}u(t_0)$$
$$u(t_0 + dt) = u(t_0) + a(t_0)dt$$
$$y(t_0 + dt) = x(t_0) + u(t_0 + dt)dt.$$

In [15]:

```
# integration parameters
end_time = 10
dt = 0.01

# solution vectors
t = [0]
y = [y0]
u = [u0]

# numerical integration
while t[-1] < end_time:
    t0 = t[-1]
    y_t0 = y[-1]
    u_t0 = u[-1]

    #TASK calculate a, u and y
    a_t0 = -(k/m)*y_t0-(d/m)*u_t0
    u_t0_dt = u_t0+a_t0*dt
    y_t0_dt = y_t0 + u_t0_dt*dt

    y.append(y_t0_dt)
    u.append(u_t0_dt)
    t.append(t0 + dt)

# visualization
visualize(t, y, u, calc_analytical_solution())
```



1. Is this method stable and when?
2. What about the accuracy of the obtained solution?

The Midpoint Method and the Runge-Kutta method of Order 4

If we were able to evaluate $\ddot{\mathbf{x}}$ as well as $\dot{\mathbf{x}}$, we could acheive $O(dt^3)$ accuracy instead of $O(dt^2)$ simply by retaining one additional term in the truncated Taylor series:

$$\mathbf{x}(t_0 + dt) = \mathbf{x}(t_0) + \dot{\mathbf{x}}(t_0)dt + \ddot{\mathbf{x}}(t_0)\frac{dt^2}{2} + O(dt^3). \qquad (1)$$

Recall that the time derivative $\dot{\mathbf{x}}$ is given by a function $f(\mathbf{x}(t), t)$. For simplicity in what follows, we will assume that the derivative function f does depends on time only indirectly through $\mathbf{x}$, so that $\dot{\mathbf{x}} = f(\mathbf{x}(t))$. The chain rule then gives

$$\ddot{\mathbf{x}} = \frac{df}{d\mathbf{x}}\dot{\mathbf{x}} = f' f.$$

To avoid having to evaluate f', which would often be complicated and expensive, we can approximate the second-order term just in terms of f, and substitute the approximation into Eq. (1), leaving us with $O(dt^3)$ error. To do this, we perform another Taylor expansion, this time of the function of f

$$f(\mathbf{x}_0 + \Delta\mathbf{x}) = f(\mathbf{x}_0) + f'(\mathbf{x}_0)\Delta\mathbf{x} + O(\Delta\mathbf{x}^2).$$

We first induce $\ddot{\mathbf{x}}$ into this expression by choosing

$$\Delta\mathbf{x} = f(\mathbf{x}_0)\frac{dt}{2}$$

so that

$$f(\mathbf{x}_0 + f(\mathbf{x}_0)\frac{dt}{2}) = f(\mathbf{x}_0) + f'(\mathbf{x}_0)f(\mathbf{x}_0)\frac{dt}{2} + O(dt^2) = f(\mathbf{x}_0) + \ddot{\mathbf{x}}(t_0)\frac{dt}{2} + O(dt^2)$$

where $\mathbf{x}_0 = \mathbf{x}(t_0)$. We can now multiply both sides by dt (turning the $O(dt^2)$ term into $O(dt^3)$) and rearrange, yielding

$$\ddot{\mathbf{x}}(t_0)\frac{dt^2}{2} + O(dt^3) = (f(\mathbf{x}_0 + f(\mathbf{x}_0)\frac{dt}{2}) - f(\mathbf{x}_0))dt$$

Substituting the right hand side into Eq. (1) gives the update formula

$$\mathbf{x}(t_0 + dt) = \mathbf{x}(t_0) + f(\mathbf{x}_0 + f(\mathbf{x}_0)\frac{dt}{2})dt$$

This formula first evaluates an Euler step, then performs a second derivative evaluation at the midpoint of the step, using the midpoint evaluation to update $\mathbf{x}$. Hence the name midpoint method. The midpoint method is correct to within $O(dt^3)$, but requires two evaluations of f.

We don't have to stop with an error of $O(dt^3)$. By evaluating f a few more times, we can eliminate higher and higher orders of derivatives. The most popular procedure for doing this is a method called Runge-Kutta of order 4 and has an error per step of $O(dt^4)$ (the midpoint method could be called Runge-Kutta of order 2). We won't derive the fourth order Runge-Kutta method, but the formula for computing $\mathbf{x}(t_0 + dt)$ is listed below:

$$\begin{aligned}
k_1 &= f(\mathbf{x}_0, t_0)dt \\
k_2 &= f(\mathbf{x}_0 + \frac{k_1}{2}, t_0 + \frac{dt}{2})dt \\
k_3 &= f(\mathbf{x}_0 + \frac{k_2}{2}, t_0 + \frac{dt}{2})dt \\
k_4 &= f(\mathbf{x}_0 + k_3, t_0 + dt)dt \\
\mathbf{x}(t_0 + dt) &= \mathbf{x}_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4).
\end{aligned}$$

In order to express the second-order ODE into a cannonical first-order form

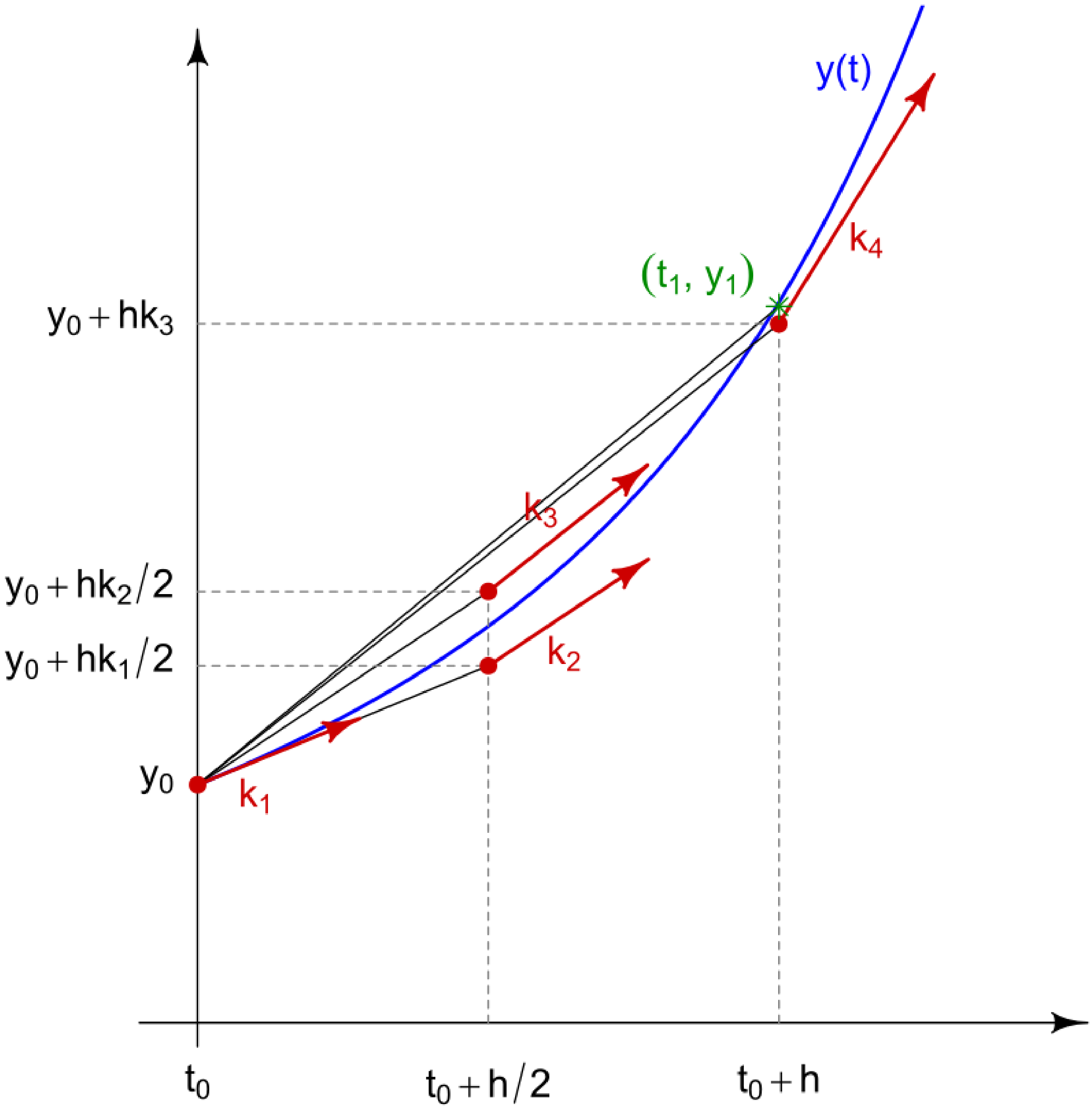
$$\dot{\mathbf{x}} = f(\mathbf{x}, t)$$

one can use the following transformation $x_1 = y, x_2 = y'$, $x_1' = x_2$ and $x_2' = y''$. Therefore, the transformed system of equations becomes:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} y \\ u \end{bmatrix}$$

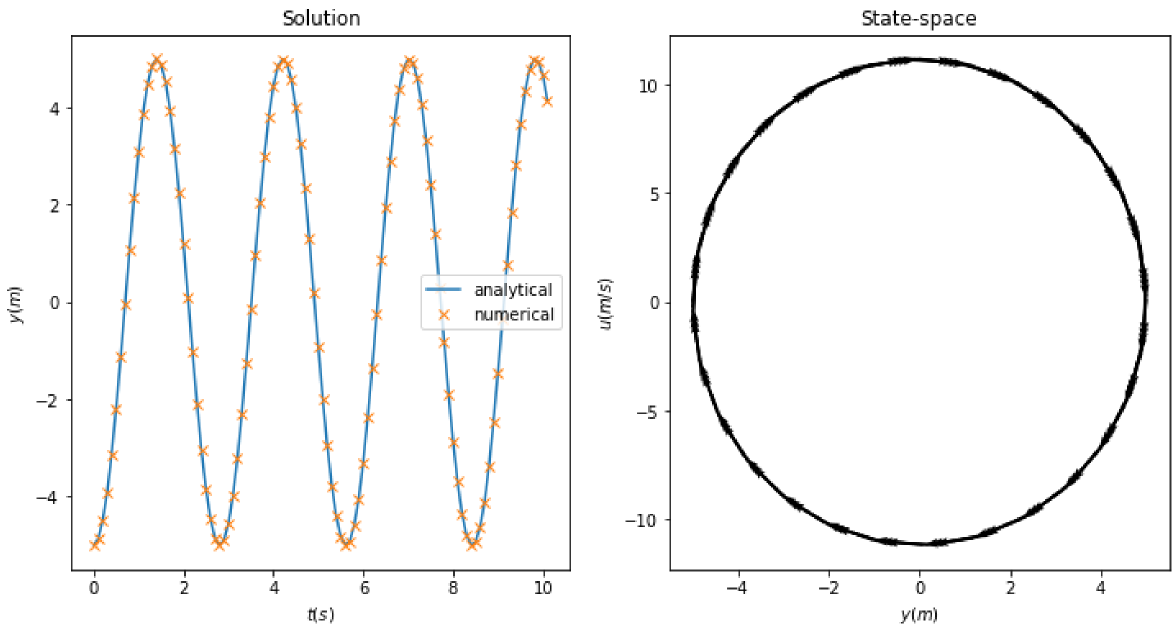
$$\dot{\mathbf{x}} = \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} u \\ a \end{bmatrix} = \begin{bmatrix} x_2 \\ -\frac{k}{m}x_1 - \frac{d}{m}x_2 \end{bmatrix} = f(\mathbf{x}, t).$$

A more visual presentation of the k variables and what they mean is shown here


y(t)
k4
(t1, y1)
y0 + hk3
k3
y0 + hk2/2
y0 + hk1/2
k2
y0
k1
t0
t0 + h/2
t0 + h

In [17]:

```
# integration parameters
end_time = 10
dt = 0.1

# solution vectors
t = [0]
x = [[y0, u0]]

# first-order derivative function
def f(x, t):
    return np.array([x[1], -k / m * x[0] - d / m * x[1]])

# numerical integration
while t[-1] < end_time:
    t0 = t[-1]
    x_t0 = np.array(x[-1])

    #Calculate k1, k2, k3, k4 and finally x_t0_dt
    k1 = f(x_t0,t0)*dt
    k2 = f(x_t0+k1/2,t0+dt/2)*dt
    k3 = f(x_t0+k2/2,t0+dt/2)*dt
    k4 = f(x_t0+k3,t0+dt)*dt
    x_t0_dt = x_t0+(1/6)*(k1+2*k2+2*k3+k4)


    x.append(x_t0_dt)
    t.append(t0 + dt)

# visualization
x = np.array(x)
visualize(t, x[:, 0], x[:, 1], calc_analytical_solution())
```



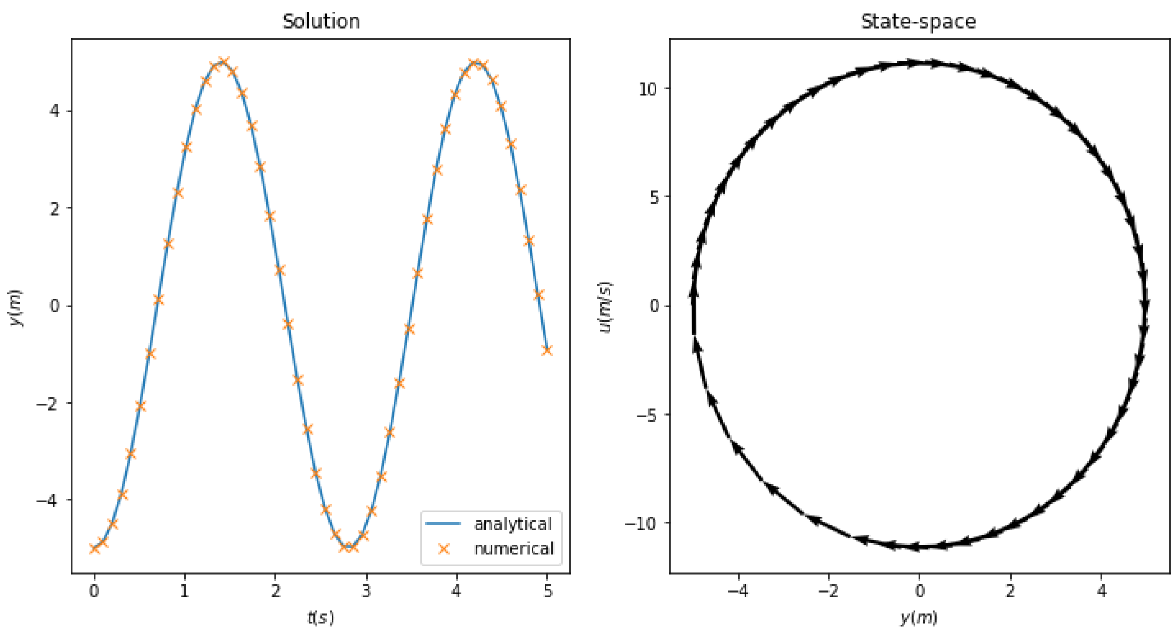
1. What is the error of this method?
2. Do you expect the solution to diverge?

Adaptive Time Stepping

Whatever the underlying method, a major problem lies in determing a good stepsize. Ideally, we want to choose h as large as possible—but not so large as to give us an unreasonable amount of error, or worse still, to induce instability. If we choose a fixed stepsize, we can only proceed as fast as the “worst” sections of x(t) will allow.

In [18]:

```
# integration parameters
end_time = 5
t = np.linspace(0, end_time, end_time * 10)

x0 = [y0, u0]

# first-order derivative function
def f(x, t):
    return [x[1], -k / m * x[0] - d / m * x[1]]

# numerical integration
[x, infodict] = odeint(f, x0, t, full_output=True)

# visualization
visualize(t, x[:, 0], x[:, 1], calc_analytical_solution())
#print(len(infodict['tcur']))
#print(len(t))
```



1. Change the density of the time points in np.linspace. What do you observe?
2. Do you expect the solution to diverge?
3. Which algorithms are supported by odeint?

Cloth Simulation

In [19]:

```
# topology
W = 1.0  # grid width
H = 1.0  # grid heigh
particles_x = 11  # number of particles on x-axis
particles_y = 11  # number of particles on y-axis
# l is the spring rest lenght (x-axis, y-axis, xy: diagonal)
# type-1 (+-1, +-1) or type-2 (+-2, +-2) refers to the connectivity
lx_type1 = W / (particles_x - 1)
ly_type1 = H / (particles_y - 1)
lxy_type1 = np.sqrt(lx_type1 ** 2 + ly_type1 ** 2)
lx_type2 = 2 * lx_type1
ly_type2 = 2 * ly_type1
lxy_type2 = 2 * lxy_type1
indices = [(i, j) for i in range(0, particles_y) for j in range(0, particles_x)]

def cartesian_product(arrays, out=None):
    arrays = [np.asarray(x) for x in arrays]
    dtype = arrays[0].dtype

    n = np.prod([x.size for x in arrays])
    if out is None:
        out = np.zeros([n, len(arrays)], dtype=dtype)

    m = int(n / arrays[0].size)
    out[:, 0] = np.repeat(arrays[0], m)
    if arrays[1:]:
        cartesian_product(arrays[1:], out=out[0:m, 1:])
        for j in range(1, arrays[0].size):
            out[j * m:(j + 1) * m, 1:] = out[0:m, 1:]

    return out

def is_valid_coordinate(i, j):
    if i < 0 or i >= particles_y or j < 0 or j >= particles_x:
        return False
    else:
        return True

def append_connectivity_if_valid(i, j, i_inc, j_inc, connectivity):
    if is_valid_coordinate(i + i_inc, j + j_inc):
        connectivity[i, j].append((i + i_inc, j + j_inc))

def generate_connectivity(indices, combinations):
    permutations = tuple(map(tuple, cartesian_product(combinations)))
    permutations = list(set(permutations))  # to remove duplicate combinations
    permutations.remove((0, 0))  # to remove identity
    connectivity = {}
    for i, j in indices:
        connectivity[i, j] = []
        for i_inc, j_inc in permutations:
            append_connectivity_if_valid(i, j, i_inc, j_inc, connectivity)

    return connectivity

# define type-1 and type-2 connectivity
type1_connectivity = generate_connectivity(indices, ([1, 0, -1], [1, 0, -1]))
type2_connectivity = generate_connectivity(indices, ([2, 0, -2], [2, 0, -2]))
```

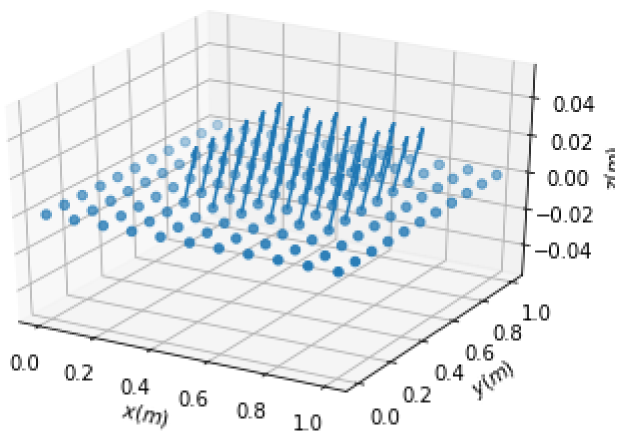
In [20]:

```
# initial state variables
u0 = uniform(5, 10)
print(u0)
X0 = np.zeros((particles_y, particles_x, 3))
U0 = np.zeros((particles_y, particles_x, 3))

# initialize particle state (position and velocity)
for i, j in indices:
    X0[i, j, :] = np.array([i * H / (particles_y - 1),
                            j * W / (particles_x - 1), 0])

    # particles that have initial velocity
    if j > 2 and j < particles_x - 2 and i > 2 and i < particles_y - 2:
        U0[i, j, :] = np.array([u0, u0, u0])

    # make sure that upper part particles have zero initial velocity
    # since they are assumed fixed
    for i in range(0, particles_y):
        U0[i, particles_x - 1, :] = np.array([0, 0, 0])

# visualize initial conditions
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
ax.set_xlabel('$x (m)$')
ax.set_ylabel('$y (m)$')
ax.set_zlabel('$z (m)$')
ax.scatter(X0[:, :, 0], X0[:, :, 1], X0[:, :, 2])
ax.quiver(X0[:, :, 0], X0[:, :, 1], X0[:, :, 2],
          U0[:, :, 0], U0[:, :, 1], U0[:, :, 2],
          length=0.05, normalize=True)
```

```
7.7865374242301755
```

Out[20]:

```
<mpl_toolkits.mplot3d.art3d.Line3DCollection at 0x26d3defa688>
```



In [21]:

```
total_cloth_mass = 3.0
m = total_cloth_mass / (particles_x * particles_y)  # particle mass
k = 10.0
d = 0.05
g = 9.8
def calc_total_force(i, j, X_n, U_n):
    f_ij = np.array([0 ,0, 0])

    # type-1 internal forces
    for i_n, j_n in type1_connectivity[i, j]:
        x_ij = X_n[i_n, j_n, :] - X_n[i, j, :]
        x_ij_mag = np.linalg.norm(x_ij)

        #calculate resting length
        l = 0
        if np.abs(i - i_n) > 0 and np.abs(j - j_n) > 0:
            l = lxy_type1
        elif np.abs(i - i_n) > 0 and not np.abs(j - j_n) > 0:
            l = ly_type1
        else:
            l = lx_type1

        # spring force only during elongation
        if x_ij_mag - l >= 0:
            f_ij = f_ij + k * (x_ij_mag - l) * x_ij / x_ij_mag

        # damping force
        f_ij = f_ij - d * (U_n[i, j, :] - U_n[i_n, j_n, :])

    # other types of internal forces can be implemented for type-2
    for i_n, j_n in type2_connectivity[i, j]:
        x_ij = X_n[i_n, j_n, :] - X_n[i, j, :]
        x_ij_mag = np.linalg.norm(x_ij)
        l = 0
        if np.abs(i - i_n) > 0 and np.abs(j - j_n) > 0:
            l = lxy_type2
        elif np.abs(i - i_n) > 0 and not np.abs(j - j_n) > 0:
            l = ly_type2
        else:
            l = lx_type2

        # spring force only during elongation
        if x_ij_mag - l >= 0:
            f_ij = f_ij + k * (x_ij_mag - l) * x_ij / x_ij_mag

        # damping force
        f_ij = f_ij - d * (U_n[i, j, :] - U_n[i_n, j_n, :])

    return f_ij


def calc_acceleration(X_t0, U_t0):
    A_t0 = np.zeros((particles_y, particles_x, 3))
    for i, j in indices:
        A_t0[i, j, :] = 1.0 / m * calc_total_force(i, j, X_t0, U_t0) \
                        + np.array([0, -g, 0])

    # upper part particles are fixed, therefore ensure zeor acceleration
    for i in range(0, particles_y):
```

```
        A_t0[i, particles_x - 1, :] = np.array([0, 0, 0])

    return A_t0
```

In [22]:

```
# integration parameters
end_time = 10
dt = 0.01

# solution vectors
t = [0]
X = [X0]
U = [U0]

# numerical integration (Semi-implicit Euler)
while t[-1] < end_time:
    t_0 = t[-1]
    X_t0 = X[-1]
    U_t0 = U[-1]
    A_t0 = calc_acceleration(X_t0, U_t0)
    U_t0_dt = U_t0 + A_t0 * dt
    X_t0_dt = X_t0 + U_t0_dt * dt
    t.append(t_0 + dt)
    X.append(X_t0_dt)
    U.append(U_t0_dt)
```

In [23]:

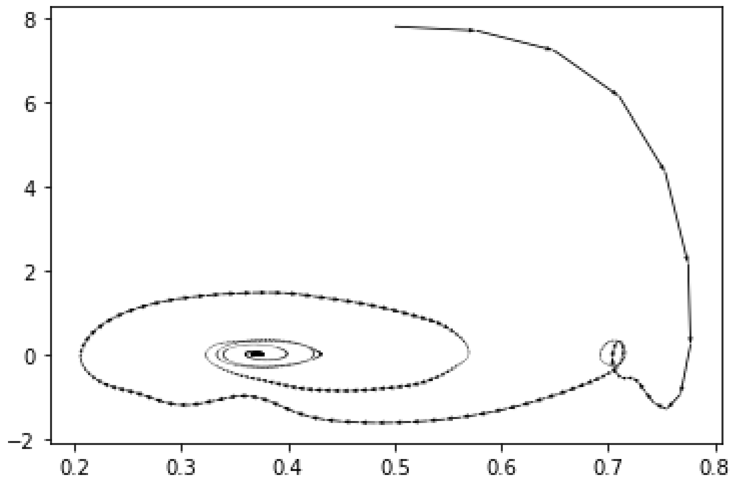
```
# initialize graph
if False:
    fig = plt.figure()
    ax = fig.add_subplot(111, projection='3d')
    title = ax.set_title('')
    ax.set_xlabel('$x (m)$')
    ax.set_ylabel('$y (m)$')
    ax.set_zlabel('$z (m)$')
    ax.set_xlim([-0.5, W + 0.5])
    ax.set_ylim([-0.5, W + 0.5])
    ax.set_zlim([-0.5, 0.5])
    graph, = ax.plot([], [], [], linestyle='', marker='o')

    # animation update function
    def update_graph(i):
        graph.set_data(X[i][:, :, 0].reshape(-1), X[i][:, :, 1].reshape(-1))
        graph.set_3d_properties(X[i][:, :, 2].reshape(-1))
        title.set_text('time={:.2f}'.format(t[i]))
        return graph, title,

    # create animation; blit=True means only re-draw the parts that have changed
    anim = animation.FuncAnimation(fig, update_graph,
                                   frames=len(X), interval=30, blit=True)
    anim.save('simulation.mp4', writer="ffmpeg")
    plt.close()
    # HTML(anim.to_html5_video())
    Video("simulation.mp4")
```

In [24]:

```
# select particle and coordinate variable
particle_i = 5
particle_j = 5
axis = 1  # 0, 1, 2 for x, y, z
X_p = np.array(X)[:, particle_i, particle_j, axis]
U_p = np.array(U)[:, particle_i, particle_j, axis]

# create state-space diagram
fig, ax = plt.subplots()
ax.quiver(X_p[:-1], U_p[:-1],
          X_p[1:] - X_p[:-1],
          U_p[1:] - U_p[:-1],
          scale_units='xy', angles='xy', scale=1)
```

Out[24]:

```
<matplotlib.quiver.Quiver at 0x26d3df997c8>
```



In [25]:

```
import sys
import time

sys.path.append('pythonGL/')
import opengl
import pygame


opengl.init()
for i in range(0, len(X[:])):
    (verts,norms, uvs) = opengl.create_list_of_vertices(X[i])
    opengl.draw(verts, norms, uvs)
    for event in pygame.event.get():
            if event.type == pygame.QUIT:
                opengl.closeAll()
    time.sleep(1*dt)
```

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pygame 1.9.6
Hello from the pygame community. https://www.pygame.org/contribute.html (htt
ps://www.pygame.org/contribute.html)
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In [ ]:

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