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Runge-Kutta methods for ODE integration in Python

- I want to implement and illustrate the Runge-Kutta method (https://en.wikipedia.org/wiki/Runge%E2%80%93Kutta_methods) (actually, different variants), in the Python programming language (https://www.python.org/).
- The Runge-Kutta methods are a family of numerical iterative algorithms to approximate solutions of Ordinary Differential Equations (https://en.wikipedia.org/wiki/Ordinary_differential_equation). I will simply implement them, for the mathematical descriptions, I let the interested reader refer to the Wikipedia page, or any (https://en.wikipedia.org/wiki/Runge%E2%80%93Kutta_methods#References) good (https://www.directtextbook.com/isbn/9780521007948) book (https://www.decitre.fr/livres/analyse-numerique-et-equations-differentielles-9782868838919.html) or course (https://courses.maths.ox.ac.uk/node/4294) on numerical integration of ODE.
- I will start with the order 1 method, then the order 2 and the most famous order 4.
- They will be compared on different ODE.

Preliminary

In [1]:

```
import numpy as np
import matplotlib.pyplot as plt
%load_ext watermark
%watermark
```

```
2017-11-23T19:18:23+01:00

CPython 3.6.3
IPython 6.2.1

compiler   : GCC 7.2.0
system     : Linux
release    : 4.13.0-16-generic
machine    : x86_64
processor  : x86_64
CPU cores  : 4
interpreter: 64bit
```

In [2]:

```
from scipy.integrate import odeint  # for comparison
```

I will use as a first example the one included in [the scipy documentation for this `odeint` function (https://docs.scipy.org/doc/scipy/reference/generated/scipy.integrate.odeint.html)](https://docs.scipy.org/doc/scipy/reference/generated/scipy.integrate.odeint.html).

$$\theta''(t) + b\theta'(t) + c\sin(\theta(t)) = 0.$$

If $\omega(t) = \theta'(t)$, this gives

$$\begin{cases} \theta'(t) = \omega(t) \\ \omega'(t) = -b\omega(t) - c\sin(\theta(t)) \end{cases}$$

Vectorially, if $y(t) = [\theta(t), \omega(t)]$, then the equation is $y' = f(t, y)$ where $f(t, y) = [y_2(t), -by_2(t) - c\sin(y_1(t))]$.

In [3]:

```
def pend(y, t, b, c):
    return np.array([y[1], -b*y[1] - c*np.sin(y[0])])
```

We assume the values of b and c to be known, and the starting point to be also fixed:

In [44]:

```
b = 0.25
c = 5.0
y0 = np.array([np.pi - 0.1, 0.0])
```

The `odeint` function will be used to solve this ODE on the interval $t \in [0, 10]$, with 101 points.

In [5]:

```
t = np.linspace(0, 10, 101)
```

It is used like this, and our implementations will follow this signature.

In [6]:

```
sol = odeint(pend, y0, t, args=(b, c))
```

In [7]:

```
plt.plot(t, sol[:, 0], 'b', label=r'$\theta(t)$')
plt.plot(t, sol[:, 1], 'g', label=r'$\omega(t)$')
plt.legend(loc='best')
plt.xlabel('t')
plt.grid()
plt.show()
```

Out[7]:

[<matplotlib.lines.Line2D at 0x7fd32c759400>]

Out[7]:

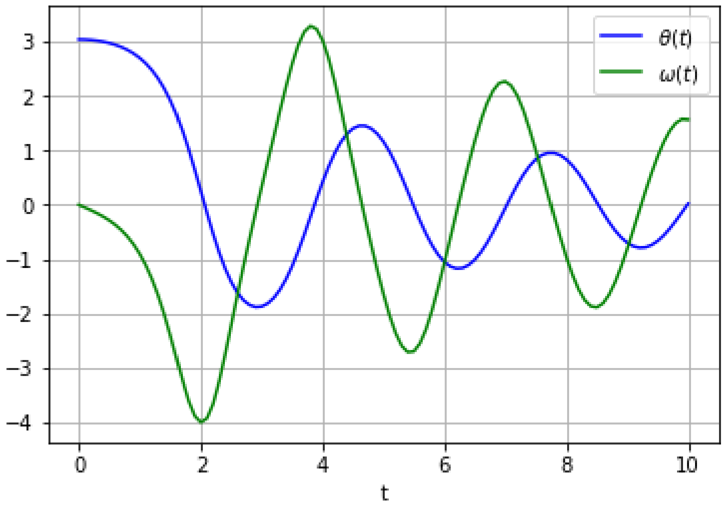
[<matplotlib.lines.Line2D at 0x7fd32c77bac8>]

Out[7]:

<matplotlib.legend.Legend at 0x7fd32c759ac8>

Out[7]:

Text(0.5,0,'t')



Runge-Kutta method of order 1, or the Euler method

The approximation is computed using this update:

$$y_{n+1} = y_n + (t_{n+1} - t_n) f(y_n, t_n).$$

The math behind this formula are the following: if g is a solution to the ODE, and so far the approximation is correct, $y_n \simeq g(t_n)$, then a small step $h = t_{n+1} - t_n$ satisfy
$g(t_n + h) \simeq g(t_n) + h g'(t_n) \simeq y_n + h f(g(t_n), t_n) + \simeq y_n + h f(y_n, t_n)$.

In [8]:

```
def rungekutta1(f, y0, t, args=()):
    n = len(t)
    y = np.zeros((n, len(y0)))
    y[0] = y0
    for i in range(n - 1):
        y[i+1] = y[i] + (t[i+1] - t[i]) * f(y[i], t[i], *args)
    return y
```

In [9]:

```
sol = rungekutta1(pend, y0, t, args=(b, c))
```

In [10]:

```
plt.plot(t, sol[:, 0], 'b', label=r'$\theta(t)$')
plt.plot(t, sol[:, 1], 'g', label=r'$\omega(t)$')
plt.legend(loc='best')
plt.xlabel('t')
plt.grid()
plt.show()
```

Out[10]:

```
[<matplotlib.lines.Line2D at 0x7fd32a6057b8>]
```

Out[10]:

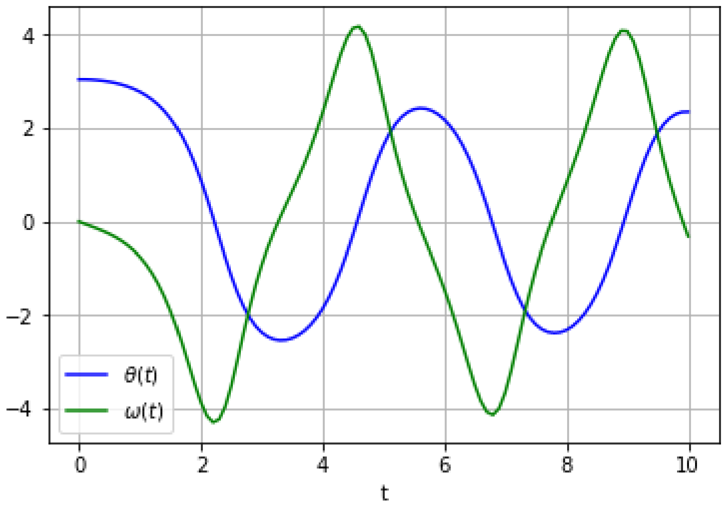
```
[<matplotlib.lines.Line2D at 0x7fd32c6ff198>]
```

Out[10]:

```
<matplotlib.legend.Legend at 0x7fd32a605e48>
```

Out[10]:

```
Text(0.5,0,'t')
```



With the same number of points, the Euler method (*i.e.* the Runge-Kutta method of order 1) is less precise than the reference `odeint` method. With more points, it can give a satisfactory approximation of the solution:

In [11]:

```
t2 = np.linspace(0, 10, 1001)
sol2 = rungekutta1(pend, y0, t2, args=(b, c))
```

In [12]:

```
t3 = np.linspace(0, 10, 10001)
sol3 = rungekutta1(pend, y0, t3, args=(b, c))
```

In [13]:

```
plt.plot(t, sol[:, 0], label=r'$\theta(t)$ with 101 points')
plt.plot(t2, sol2[:, 0], label=r'$\theta(t)$ with 1001 points')
plt.plot(t3, sol3[:, 0], label=r'$\theta(t)$ with 10001 points')
plt.legend(loc='best')
plt.xlabel('t')
plt.grid()
plt.show()
```

Out[13]:

[<matplotlib.lines.Line2D at 0x7fd32a58b470>]

Out[13]:

[<matplotlib.lines.Line2D at 0x7fd32a5b7cf8>]

Out[13]:

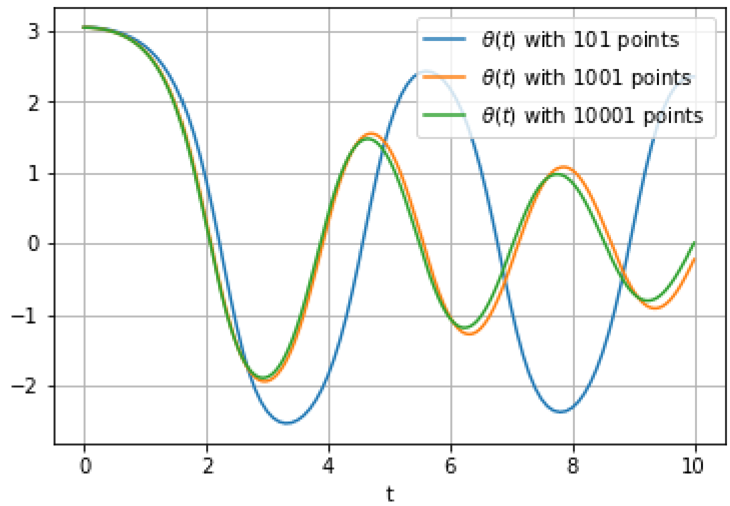
[<matplotlib.lines.Line2D at 0x7fd32a58bfd0>]

Out[13]:

<matplotlib.legend.Legend at 0x7fd32a58bf60>

Out[13]:

Text(0.5,0,'t')



Runge-Kutta method of order 2

The order 2 Runge-Method uses this update:

$$y_{n+1} = y_n + hf(t + \frac{h}{2}, y_n + \frac{h}{2} f(t, y_n)),$$

if $h = t_{n+1} - t_n$.

In [14]:

```
def rungekutta2(f, y0, t, args=()):
    n = len(t)
    y = np.zeros((n, len(y0)))
    y[0] = y0
    for i in range(n - 1):
        h = t[i+1] - t[i]
        y[i+1] = y[i] + h * f(y[i] + f(y[i], t[i], *args) * h / 2., t[i] + h / 
2., *args)
    return y
```

For our simple ODE example, this method is already quite efficient.

In [15]:

```
t4 = np.linspace(0, 10, 21)
sol4 = rungekutta2(pend, y0, t4, args=(b, c))
```

In [16]:

```
t = np.linspace(0, 10, 101)
sol = rungekutta2(pend, y0, t, args=(b, c))
```

In [17]:

```
t2 = np.linspace(0, 10, 1001)
sol2 = rungekutta2(pend, y0, t2, args=(b, c))
```

In [18]:

```
t3 = np.linspace(0, 10, 10001)
sol3 = rungekutta2(pend, y0, t3, args=(b, c))
```

In [19]:

```
plt.plot(t4, sol4[:, 0], label='with 11 points')
plt.plot(t, sol[:, 0], label='with 101 points')
plt.plot(t2, sol2[:, 0], label='with 1001 points')
plt.plot(t3, sol3[:, 0], label='with 10001 points')
plt.legend(loc='best')
plt.xlabel('t')
plt.grid()
plt.show()
```

Out[19]:

```
[<matplotlib.lines.Line2D at 0x7fd32a510b38>]
```

Out[19]:

```
[<matplotlib.lines.Line2D at 0x7fd32a530ef0>]
```

Out[19]:

```
[<matplotlib.lines.Line2D at 0x7fd32a51b208>]
```

Out[19]:

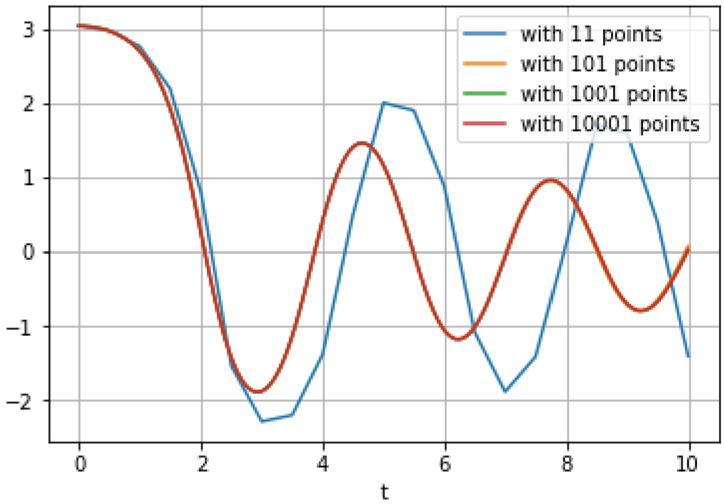
```
[<matplotlib.lines.Line2D at 0x7fd32a51b710>]
```

Out[19]:

```
<matplotlib.legend.Legend at 0x7fd32a51bb00>
```

Out[19]:

```
Text(0.5,0,'t')
```



Runge-Kutta method of order 4, *"RK4"*

The order 4 Runge-Method uses this update:

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4),$$

if $h = t_{n+1} - t_n$, and

$$\begin{cases} k_1 &= f(y_n, t_n), \\ k_2 &= f(y_n + \frac{h}{2}k_1, t_n + \frac{h}{2}), \\ k_3 &= f(y_n + \frac{h}{2}k_2, t_n + \frac{h}{2}), \\ k_4 &= f(y_n + hk_3, t_n + h). \end{cases}$$

In [20]:

```
def rungekutta4(f, y0, t, args=()):
    n = len(t)
    y = np.zeros((n, len(y0)))
    y[0] = y0
    for i in range(n - 1):
        h = t[i+1] - t[i]
        k1 = f(y[i], t[i], *args)
        k2 = f(y[i] + k1 * h / 2., t[i] + h / 2., *args)
        k3 = f(y[i] + k2 * h / 2., t[i] + h / 2., *args)
        k4 = f(y[i] + k3 * h, t[i] + h, *args)
        y[i+1] = y[i] + (h / 6.) * (k1 + 2*k2 + 2*k3 + k4)
    return y
```

For our simple ODE example, this method is even more efficient.

In [21]:

```
t4 = np.linspace(0, 10, 21)
sol4 = rungekutta4(pend, y0, t4, args=(b, c))
```

In [22]:

```
t = np.linspace(0, 10, 101)
sol = rungekutta4(pend, y0, t, args=(b, c))
```

In [23]:

```
t2 = np.linspace(0, 10, 1001)
sol2 = rungekutta4(pend, y0, t2, args=(b, c))
```

In [24]:

```
plt.plot(t4, sol4[:, 0], label='with 21 points')
plt.plot(t, sol[:, 0], label='with 101 points')
plt.plot(t2, sol2[:, 0], label='with 1001 points')
plt.legend(loc='best')
plt.xlabel('t')
plt.grid()
plt.show()
```

Out[24]:

```
[<matplotlib.lines.Line2D at 0x7fd32a483c50>]
```

Out[24]:

```
[<matplotlib.lines.Line2D at 0x7fd32a4d99e8>]
```

Out[24]:

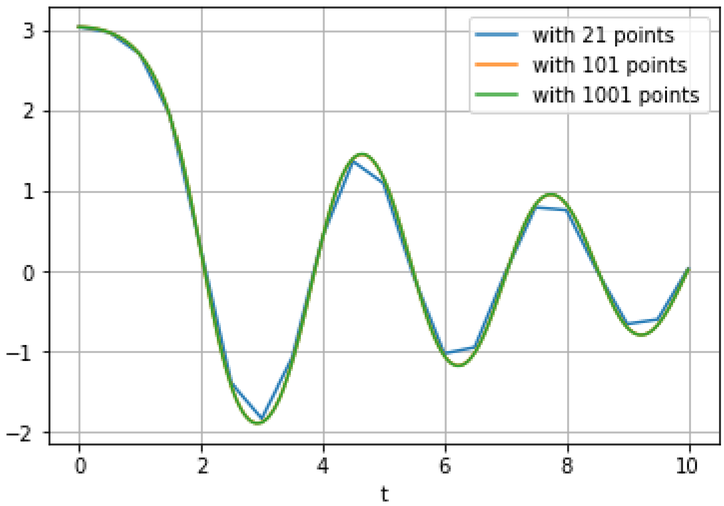
```
[<matplotlib.lines.Line2D at 0x7fd32a48d320>]
```

Out[24]:

```
<matplotlib.legend.Legend at 0x7fd32a48d748>
```

Out[24]:

```
Text(0.5,0,'t')
```



I also want to try to speed this function up by using numba (http://numba.pydata.org/).

In [45]:

```
from numba import jit
```

In [46]:

```
@jit
def rungekutta4_jit(f, y0, t, args=()):
    n = len(t)
    y = np.zeros((n, len(y0)))
    y[0] = y0
    for i in range(n - 1):
        h = t[i+1] - t[i]
        k1 = f(y[i], t[i], *args)
        k2 = f(y[i] + k1 * h / 2., t[i] + h / 2., *args)
        k3 = f(y[i] + k2 * h / 2., t[i] + h / 2., *args)
        k4 = f(y[i] + k3 * h, t[i] + h, *args)
        y[i+1] = y[i] + (h / 6.) * (k1 + 2*k2 + 2*k3 + k4)
    return y
```

Both versions compute the same thing.

In [53]:

```
t2 = np.linspace(0, 10, 1001)
sol2 = rungekutta4(pend, y0, t2, args=(b, c))
sol2_jit = rungekutta4_jit(pend, y0, t2, args=(b, c))
np.linalg.norm(sol2 - sol2_jit)
```

Out[53]:

```
0.0
```

Comparisons

In [25]:

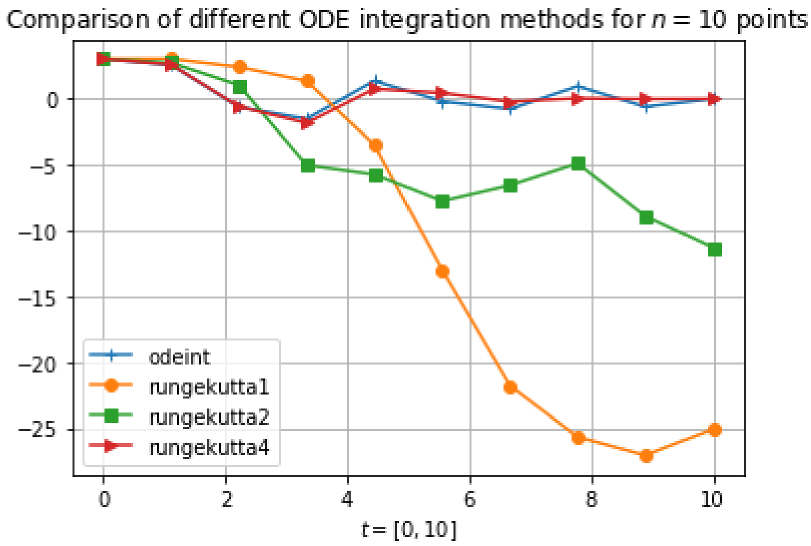
```
methods = [odeint, rungekutta1, rungekutta2, rungekutta4]
markers = ['+', 'o', 's', '>']
```

In [26]:

```
def test_1(n=101):
    t = np.linspace(0, 10, n)
    for method, m in zip(methods, markers):
        sol = method(pend, y0, t, args=(b, c))
        plt.plot(t, sol[:, 0], label=method.__name__, marker=m)
    plt.legend(loc='best')
    plt.title("Comparison of different ODE integration methods for $n={}$ point
s".format(n))
    plt.xlabel("$t = [0, 10]$")
    plt.grid()
    plt.show()
```

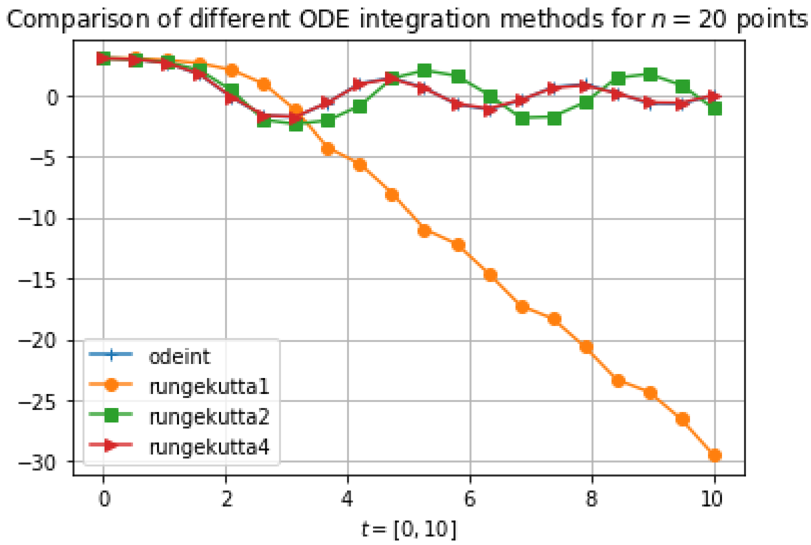
In [27]:

```
test_1(10)
```



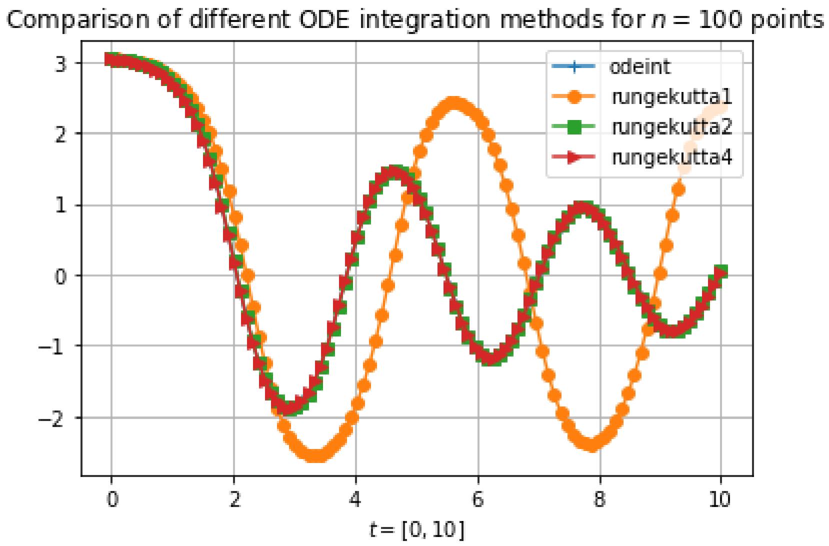
In [28]:

```
test_1(20)
```



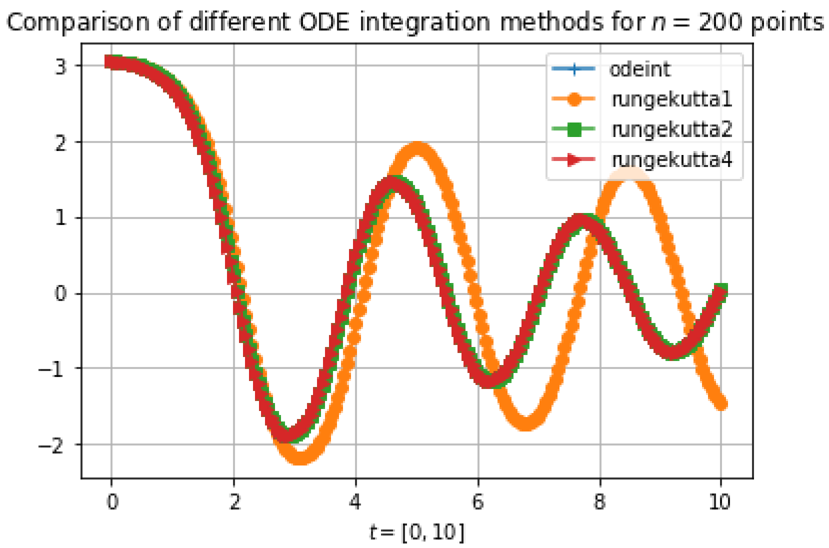
In [29]:

```
test_1(100)
```



In [30]:

```
test_1(200)
```



Comparisons on another integration problem

Consider the following ODE on $t \in [0, 1]$:

$$\begin{cases} y'''(t) = 12y(t)^{4/5} + \cos(y'(t))^3 - \sin(y''(t)) \\ y(0) = 0, y'(0) = 1, y''(0) = 0.1 \end{cases}$$

It can be written in a vectorial form like the first one:

In [31]:

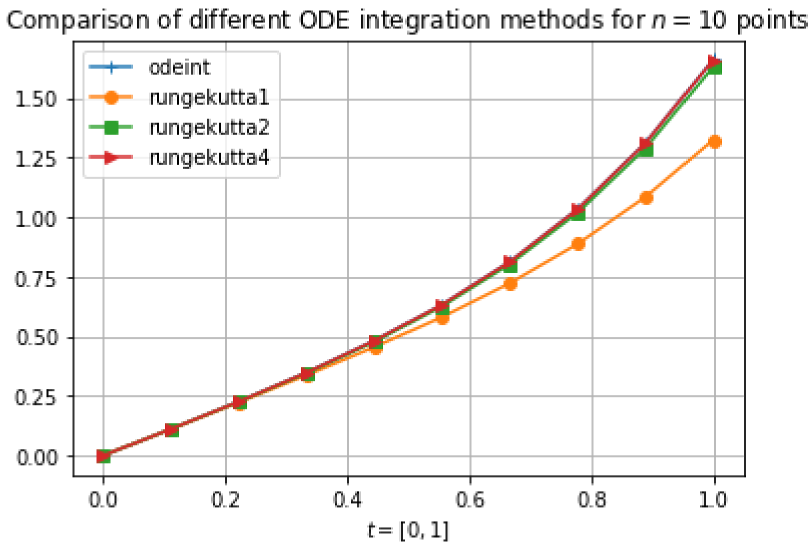
```
def f(y, t):
    return np.array([y[1], y[2], 12 * y[0] ** (4/5.) + np.cos(y[1])**3 - np.sin(
y[2])])
```

In [32]:

```
def test_2(n=101):
    t = np.linspace(0, 1, n)
    y0 = np.array([0, 1, 0.1])
    for method, m in zip(methods, markers):
        sol = method(f, y0, t)
        plt.plot(t, sol[:, 0], label=method.__name__, marker=m)
    plt.legend(loc='best')
    plt.title("Comparison of different ODE integration methods for $n={}$ point
s".format(n))
    plt.xlabel("$t = [0, 1]$")
    plt.grid()
    plt.show()
```

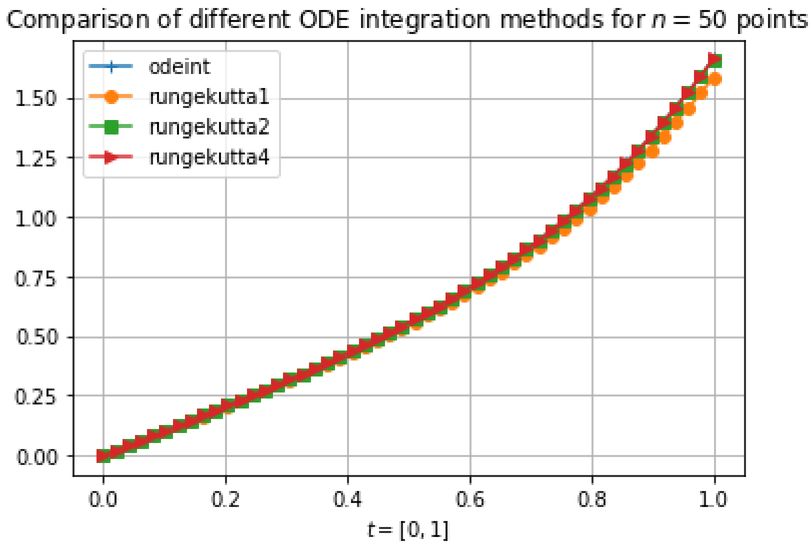
In [33]:

```
test_2(10)
```



In [34]:

```
test_2(50)
```



Consider the following ODE on $t \in [0, 3]$:

$$\begin{cases} y''''(t) = y(t)^{-5/3} \\ y(0) = 10, y'(0) = -3, y''(0) = 1, y'''(0) = 1 \end{cases}$$

It can be written in a vectorial form like the first one:

In [35]:

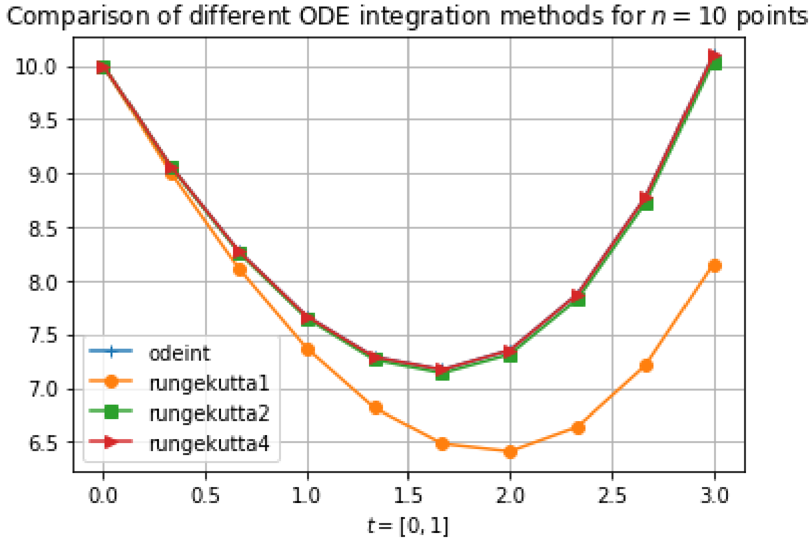
```
def f(y, t):
    return np.array([y[1], y[2], y[3], y[0]**(-5/3.)])
```

In [36]:

```
def test_3(n=101):
    t = np.linspace(0, 3, n)
    y0 = np.array([10, -3, 1, 1])
    for method, m in zip(methods, markers):
        sol = method(f, y0, t)
        plt.plot(t, sol[:, 0], label=method.__name__, marker=m)
    plt.legend(loc='best')
    plt.title("Comparison of different ODE integration methods for $n={}$ point
s".format(n))
    plt.xlabel("$t = [0, 1]$")
    plt.grid()
    plt.show()
```

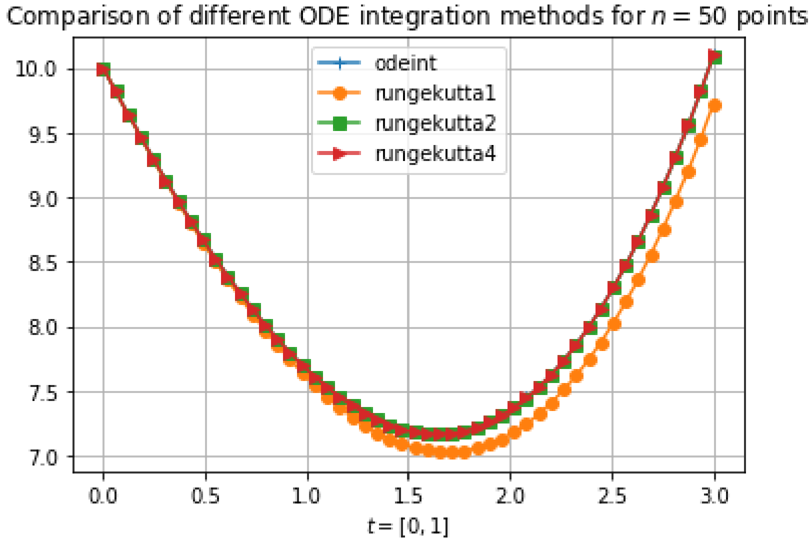
In [37]:

```
test_3(10)
```



In [38]:

```
test_3(50)
```



Our hand-written Runge-Kutta method of order 4 seems to be as efficient as the `odeint` method from `scipy`... and that's because `odeint` basically uses a Runge-Kutta method of order 4 (with smart variants).

Small benchmark

We can also compare their speed:

In [54]:

```
methods = [odeint, rungekutta1, rungekutta2, rungekutta4, rungekutta4_jit]

y0 = np.array([10, -3, 1, 1])
for n in [20, 100, 1000]:
    print("\n")
    t = np.linspace(0, 3, n)
    for method in methods:
        print("Time of solving this ODE for {} points with {} method...".format(
n, method.__name__))
        %timeit sol = method(f, y0, t)
```

```
Time of solving this ODE for 20 points with odeint method...
212 µs ± 20.5 µs per loop (mean ± std. dev. of 7 runs, 1000 loops e
ach)
Time of solving this ODE for 20 points with rungekutta1 method...
114 µs ± 5.37 µs per loop (mean ± std. dev. of 7 runs, 10000 loops
each)
Time of solving this ODE for 20 points with rungekutta2 method...
223 µs ± 12.8 µs per loop (mean ± std. dev. of 7 runs, 1000 loops e
ach)
Time of solving this ODE for 20 points with rungekutta4 method...
482 µs ± 26.2 µs per loop (mean ± std. dev. of 7 runs, 1000 loops e
ach)
Time of solving this ODE for 20 points with rungekutta4_jit metho
d...
896 µs ± 61.2 µs per loop (mean ± std. dev. of 7 runs, 1 loop each)


Time of solving this ODE for 100 points with odeint method...
222 µs ± 15 µs per loop (mean ± std. dev. of 7 runs, 1000 loops eac
h)
Time of solving this ODE for 100 points with rungekutta1 method...
548 µs ± 18.2 µs per loop (mean ± std. dev. of 7 runs, 1000 loops e
ach)
Time of solving this ODE for 100 points with rungekutta2 method...
1.16 ms ± 82.3 µs per loop (mean ± std. dev. of 7 runs, 1000 loops
each)
Time of solving this ODE for 100 points with rungekutta4 method...
2.81 ms ± 349 µs per loop (mean ± std. dev. of 7 runs, 100 loops ea
ch)
Time of solving this ODE for 100 points with rungekutta4_jit metho
d...
2.58 ms ± 140 µs per loop (mean ± std. dev. of 7 runs, 100 loops ea
ch)


Time of solving this ODE for 1000 points with odeint method...
224 µs ± 15.8 µs per loop (mean ± std. dev. of 7 runs, 1000 loops e
ach)
Time of solving this ODE for 1000 points with rungekutta1 method...
5.87 ms ± 466 µs per loop (mean ± std. dev. of 7 runs, 100 loops ea
ch)
Time of solving this ODE for 1000 points with rungekutta2 method...
11.8 ms ± 652 µs per loop (mean ± std. dev. of 7 runs, 100 loops ea
ch)
Time of solving this ODE for 1000 points with rungekutta4 method...
27.5 ms ± 1.4 ms per loop (mean ± std. dev. of 7 runs, 10 loops eac
h)
Time of solving this ODE for 1000 points with rungekutta4_jit metho
d...
29.2 ms ± 2.88 ms per loop (mean ± std. dev. of 7 runs, 10 loops ea
ch)
```

- Well, that's disappointing, the Numba Jit version was NOT faster than the manual implementation...
- The order 1 method is simpler and so faster than the order 2, which itself is simpler and faster than the order 4 method.
- And we can check that the SciPy implementation is much faster than our manual implentations!

Conclusion

> *That's it for today, folks!* See my other notebooks, available on GitHub (https://github.com/Naereen/notebooks/).