Supporting textbook chapters for week 6: Chapters 8.1, 8.2, 8.5.1 to 8.5.3 Lecture 6, topics:

- Euler method
- Runge-Kutta methods
- Leapfrog and Verlet Methods --- energy conservation

Consider ODE(s) with some initial condition(s):

- 1D: $\frac{\mathrm{d}x}{\mathrm{d}t} = f(x,t) \quad \text{with} \quad x(t=0) = x_0.$
- *n*D: $\frac{\mathrm{d}x_i}{\mathrm{d}t} = f_i(x_1, \ldots, x_n, t) \quad \text{with} \quad x_i(t=0) = x_{i0}.$
- higher order, e.g.:

$$\frac{\mathrm{d}^3 x}{\mathrm{d}t^3} = f(x,t) \quad \Leftrightarrow \quad \frac{\mathrm{d}x}{\mathrm{d}t} = v, \ \frac{\mathrm{d}v}{\mathrm{d}t} = a, \ \frac{\mathrm{d}a}{\mathrm{d}t} = f.$$

These equations can be impossible to solve anaytically, but easy to solve on a computer.

SciPy's canned routines

- Python has built-in ODE solvers called `odeint` (older) and `solve_ivp` (preferred) located in the `scipy.integrate` module. (*Aside: This module also contains a bunch of integration functions that can do Gaussian quadrature, Simpson's rule etc.*).
- See http://docs.scipy.org/doc/scipy/reference/tutorial/integrate.html (http://docs.scipy.org/doc/scipy/reference/tutorial/integrate.html)
- `odeint` uses the LSODA algorithm. Very powerful but lots of automatic knobs make it difficult to track what is actually going on (error estimate?).
- `solve_ivp` allows more user control. Still, useful to know how these methods work under the hood to really know how to use canned routines.
- If that doesn't matter to your specific application, then just use `odeint` or `solve_ivp` . However, if it does matter, then you can write your own ODE solver with the method that you want.

Euler method

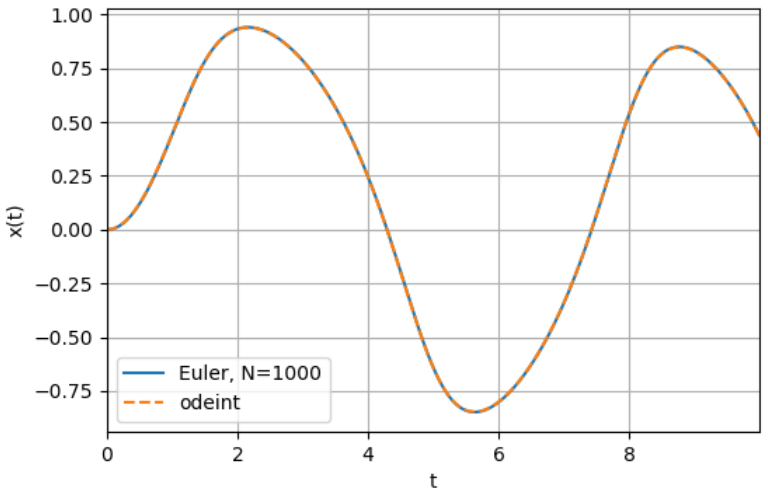
Let's solve for

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -x^3(t) + \sin(t)$$

In [2]:
```
# load euler-odeint.py  modified from Newman
import numpy as np
import matplotlib.pyplot as plt
from scipy.integrate import odeint

def f(x,t):
    return -x**3 + np.sin(t)

a = 0.0           # Start of the interval
b = 10.0          # End of the interval
N = 1000            # Number of steps
h = (b-a)/N       # Size of a single step
x = 0.0           # Initial condition

tpoints = np.arange(a,b,h)
xpoints = []
for t in tpoints:
    xpoints.append(x)
    x += h*f(x,t)

#also solve by odeint
x_new = odeint(func=f, y0=0, t=tpoints)
```

In [3]:
```
plt.figure(dpi=100)
plt.plot(tpoints, xpoints, label='Euler, N={:d}'.format(N))
plt.xlabel("t")
plt.ylabel("x(t)")
plt.plot(tpoints, x_new, '--', label='odeint')
plt.autoscale(enable=True, axis='x', tight=True)
plt.grid()
plt.legend()
```

Out[3]: <matplotlib.legend.Legend at 0x7f1bb71126a0>



- The Euler method has error $O(h^2)$ at each step (error $= O(h^2)$),
- integrating across the whole interval: global error is $O(h)$ (see eqn 8.8, p. 331):

$$\text{Taylor expansion} \Rightarrow x(t+h) = x(t) + h\frac{dx}{dt} + \overbrace{\frac{h^2}{2}\frac{\mathrm{d}^2x}{\mathrm{d}t^2}}^{\epsilon} + O(h^3)$$

$$\sum \epsilon = \sum_{k=0}^{N-1} \frac{h^2}{2}\frac{\mathrm{d}^2x}{\mathrm{d}t^2}\bigg|_{x_k,t_k} = \frac{h}{2}\sum_{k=0}^{N-1} h\frac{df}{dt}\bigg|_{x_k,t_k}$$

$$\approx \frac{h}{2}\int_a^b \frac{\mathrm{d}f}{\mathrm{d}t}\mathrm{d}t = \frac{h}{2}[f_b - f_a]$$

- For some applications, this is good enough. But for others, we need to do better!

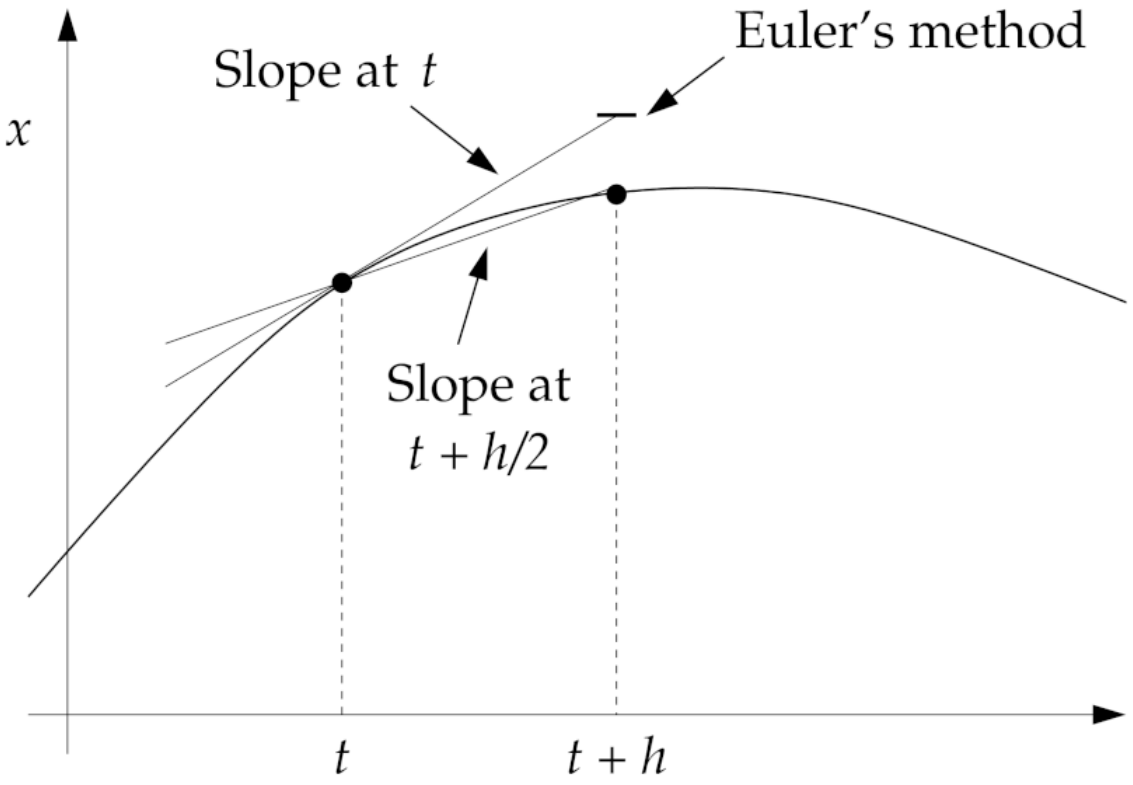
2nd-order Runge-Kutta (RK2) method

- Use the middle point $t + h/2$ and evaluate with Euler's method,

$$x\left(t + \frac{h}{2}\right) \approx x(t) + \frac{h}{2}f[x(t), t]$$

- Slope at $t + \frac{h}{2} \approx f\left[x(t) + \frac{h}{2}f\left[x(t), t\right], t + \frac{h}{2}\right]$

$$\Rightarrow \boxed{x(t+h) = x(t) + hf\left[x(t) + \frac{h}{2}f[x(t), t], t + \frac{h}{2}\right]}$$



RK2 usually coded by defining intermediate quantities:

- $k_1 = hf(x,t)$ as preliminary step before $x(t+h/2)$,
- $k_2 = hf\left(x + \frac{k_1}{2}, t + \frac{h}{2}\right)$,
- $x(t+h) = x(t) + k_2$.

RK2: $O(h^3)$ step-by-step error, usually $O(h^2)$ global error.

Coding Euler:

In [ ]:
```
for t in tpoints:
    x += h*f(x, t)
```

Coding RK2:

In [ ]:
```
for t in tpoints:
    k1 = h*f(x, t)
    k2 = h*f(x + 0.5*k1, t+0.5*h)
    x += k2
```

4th-order Runge-Kutta method (RK4)

- Various Taylor expansions at various points in the interval ⇒ higher-order RK's.
- RK4 is reasonable to code yourself. Higher-order methods ⇒ use canned routines.
- End result, after tedious algebra:
  1. $k_1 = hf(x,t)$,
  2. $k_2 = hf\left(x + \frac{k_1}{2}, t + \frac{h}{2}\right)$,
  3. $k_3 = hf\left(x + \frac{k_2}{2}, t + \frac{h}{2}\right)$,
  4. $k_4 = hf\left(x + k_3, t + h\right)$,
  5. $x(t+h) = x(t) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$.

Coding RK4:

In [ ]:
```
for t in tpoints:
    k1 = h*f(x, t)
    k2 = h*f(x+0.5*k1, t+0.5*h)
    k3 = h*f(x+0.5*k2, t+0.5*h)
    k4 = h*f(x+k3, t+h)
    x += (k1 + 2*k2 + 2*k3 + k4)/6
```

- RK4 carries $O(h^4)$ error globally
- Many small things to keep track of: easy to introduce a coding error!

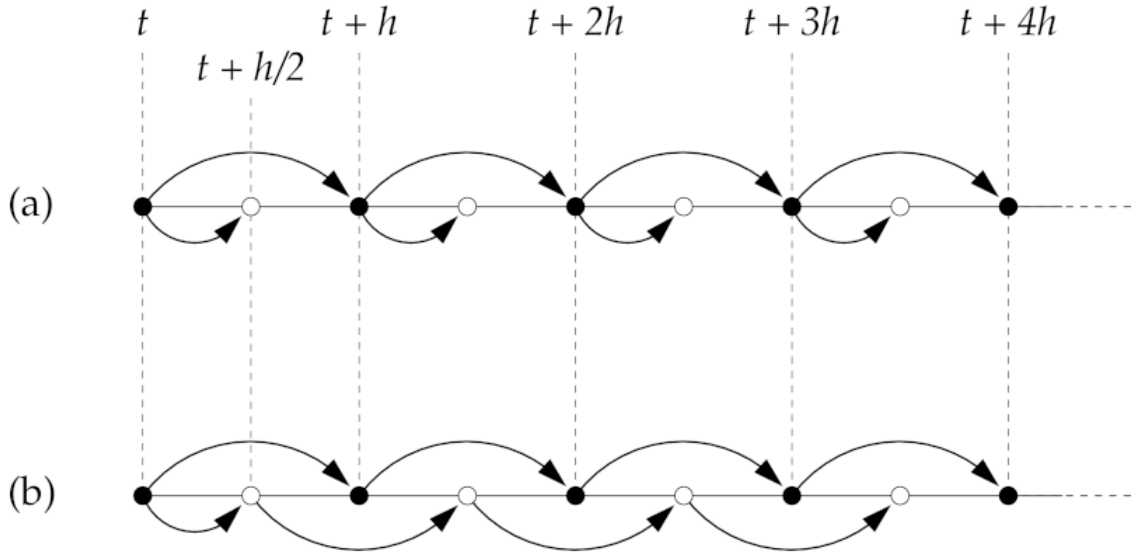
Leapfrog methods

- RK2: Use mid-point location to jump to $t + h$

$$x(t+h) = x(t) + hf\left[x + \frac{h}{2}f(x,t), t + \frac{h}{2}\right]$$

- Leapfrog: use each point as a mid-point.

$$x(t+h) = x(t) + hf\left[x + \frac{h}{2}f(x,t), t + \frac{h}{2}\right],$$
$$x\left(t + \frac{3}{2}h\right) = x\left(t + \frac{h}{2}\right) + hf[x(t+h), t+h].$$



- Also $O(h^2)$ global error, and not RK4-able (not trivially at least, cf. Yoshida algorithms).
- So, why is it useful?

- It is **time-reversible**!
- Noether's Theorem: If a system has a continuous symmetry property, then there are corresponding quantities whose values are conserved in time.
- Invariance in time of the laws of Physics ⇒ conservation of energy.

Leapfrog timestepping is reversible!

Forward leapfrog:

$$x(t+h) = x(t) + hf\left(x\left(t + \frac{h}{2}\right), t + \frac{h}{2}\right),$$
$$x\left(t + \frac{3}{2}h\right) = x\left(t + \frac{h}{2}\right) + hf(x(t+h), t+h).$$

Backward Leapfrog: $h \to -h$

$$x(t-h) = x(t) - hf\left(x\left(t - \frac{h}{2}\right), t - \frac{h}{2}\right),$$
$$x\left(t - \frac{3}{2}h\right) = x\left(t - \frac{h}{2}\right) - hf(x(t-h), t-h).$$

Leapfrog timestepping is reversible!

Forward leapfrog:

$$x(t+h) = x(t) + hf\left(x\left(t+\frac{h}{2}\right), t+\frac{h}{2}\right),$$
$$x\left(t+\frac{3}{2}h\right) = x\left(t+\frac{h}{2}\right) + hf(x(t+h), t+h).$$

Shift in time: $t \to t + 3h/2$

$$x\left(t+\frac{h}{2}\right) = x\left(t+\frac{3}{2}h\right) - hf\left(x\left(t+h\right), t+h\right),$$
$$x\left(t\right) = x\left(t+h\right) - hf\left(x\left(t+\frac{h}{2}\right), t+\frac{h}{2}\right).$$

Doesn't work with RK2

Forward RK2:

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

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

Backward RK2: $h \to -h$

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

$x(t-h) = x(t) - hf\left(x\left(t-\frac{h}{2}\right), t-\frac{h}{2}\right)$

Doesn't work with RK2

Forward RK2:

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

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

Shift in time: $t \to t + h$

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

$x\left(t\right) = x\left(t+h\right) - hf\left(x\left(t+\frac{h}{2}\right), t+\frac{h}{2}\right)$

Doesn't work with RK2

- Everything "resets" at $t + h$, so the info at the mid-point is lost and the reverse path is not a "retracing of the steps".
- Graphically, reverse is not like drawing the arrows in reverse

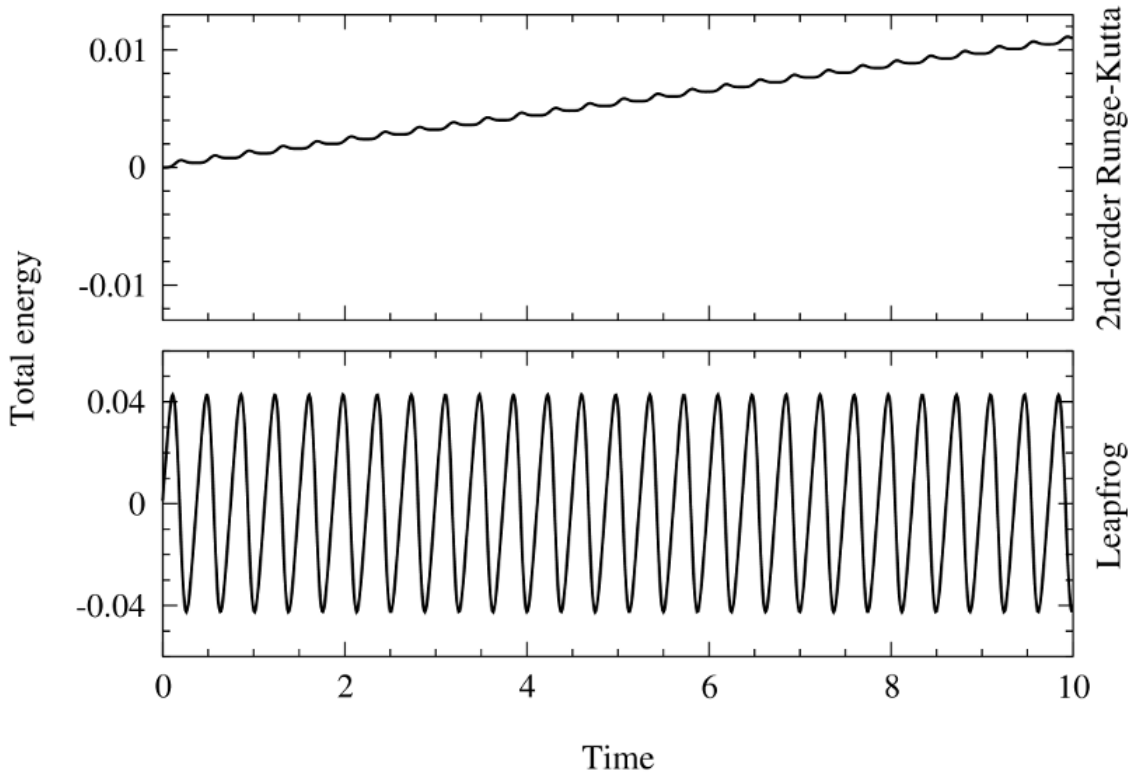
Example: Energy of a nonlinear pendulum

Solving

$$\frac{\mathrm{d}^2\theta}{\mathrm{d}t^2} = -\sin\theta$$

(angular frequency = 1 rad/s)

Try RK2 vs Leapfrog: with RK2 we see energy drift over time. RK4 would be more precise, so energy drift would be less significant, but still there.



Leapfrog to Verlet

- Leapfrog extension to two (or n) coupled ODEs: cf. §§ 8.2, 8.3 in textbook.
- Verlet is for the special case of two coupled ODEs, with LHS and RHS having separated variables. Like for Newton's 2nd law for conservative forces:

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = \frac{F(x)}{m} \quad \Rightarrow \quad \frac{\mathrm{d}x}{\mathrm{d}t} = v \quad \text{and} \quad \frac{\mathrm{d}v}{\mathrm{d}t} = \frac{F(x)}{m}.$$

1st ODE: x on LHS, v on RHS; 2nd ODE: v on LHS, x on RHS.

- Verlet method:

$$x(t+h) = x(t) + hv\left(t + \frac{h}{2}\right),$$
$$v\left(t + \frac{3}{2}h\right) = v\left(t + \frac{h}{2}\right) + h\frac{F(x(t+h))}{m}.$$

- Verlet is a 2-variable leapfrog method at 1/2 the cost.
- It conserves energy too.
- If diagnostics (like energy) are needed at specific time steps, we need to recompute the half-step quantities.

Pros and Cons of each method

RK2:

- ⊕ Easily extended to RK4
- ⊕ Possible to use adaptive time step (see next week)
- ⊖ not time-reversible
- ⊖ not great accuracy

RK4:

- ⊕ accuracy
- ⊕ Possible to use adaptive time step (see next week)
- ⊖ not time-reversible

Leapfrog:

- ⊕ time-reversible
- ⊕ basis for higher-order methods (Bulirsch-Stoer, see next week)
- ⊖ not great accuracy
- ⊖ time step has to be constant.

Let's return to our example of solving

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -x^3(t) + \sin(t)$$

In [5]:
```
# load euler-odeint.py  modified from Newman
import numpy as np
import matplotlib.pyplot as plt
from scipy.integrate import odeint

def f(x,t):
    return -x**3 + np.sin(t)

a = 0.0           # Start of the interval
b = 10.0          # End of the interval
N = 12            # Number of steps
h = (b-a)/N       # Size of a single step
xE = 0.0           # Initial condition for Euler

tpoints = np.arange(a,b,h)
```

In [6]:
```
x2 = 0.  # Initial condition for RK2
x4 = 0.  # Initial condition for RK4
xEpoints = [] # results for Euler
x2points = [] # for RK2
x4points = [] # for RK4
for t in tpoints:
    xEpoints.append(xE) #Euler
    xE += h*f(xE, t)

    x2points.append(x2) #RK2
    k1 = h*f(x2, t)
    k2 = h*f(x2 + 0.5*k1, t+0.5*h)
    x2 += k2

    x4points.append(x4) #RK4
    k2 = h*f(x4+0.5*k1, t+0.5*h)
    k3 = h*f(x4+0.5*k2, t+0.5*h)
    k4 = h*f(x4+k3, t+h)
    x4 += (k1 + 2*k2 + 2*k3 + k4)/6

#also solve by odeint
x_new = odeint(func=f, y0=0, t=tpoints)
```

In [8]:
```
plt.figure(dpi=100)
plt.plot(tpoints, xEpoints, label='Euler, N={:d}'.format(N))
plt.plot(tpoints, np.array(x2points), label='RK2, N={:d}'.format(N))
plt.plot(tpoints, np.array(x4points), label='RK4, N={:d}'.format(N))
plt.xlabel("t")
plt.ylabel("x(t)")
plt.plot(tpoints, x_new, '--', label='odeint')
plt.autoscale(enable=True, axis='x', tight=True)
plt.grid()
plt.legend()
```

Out[8]: <matplotlib.legend.Legend at 0x7f1bb6fad6a0>