Kai-Feng Chen National Taiwan University

PROGRAMMING & NUMERICAL ANALYSIS

Lecture 11: Solving Differential Equations

WORK OF "PHYSICISTS"

- Solving the differential equations is probably one of your most "ordinary" work when you study the classical mechanics?
- Many differential equations in nature cannot be solved analytically easily; however, in many of the cases, a numeric approximation to the solution is often good enough to solve the problem. You will see several examples today.
- In this lecture we will discuss the numerical methods for finding numerical approximations to the solutions of ordinary differential equations, as well as how to demonstrate the "motions" with an animation in matplotlib.

WORK OF "PHYSICISTS" (II)

■ Let's get back to our "lovely" **F=ma** equations!



THE BASIS: A BRAINLESS EXAMPLE



■ Let's try to solve such a (mostly) trivial differential equation:

 $\frac{dy}{dt} = f(y, t) = y$ with the initial condition: $\mathbf{t} = \mathbf{0}, \mathbf{y} = \mathbf{1}$

You should know the obvious solution is $-y = \exp(t)$

 $\frac{dy}{dt} = f(y,t)$ Actually, this is the **general form** of any first-order ordinary differential equation. In general, it can be very complicated, but it's still a 1st order ODE, e.g.

 $\frac{dy}{dt} = f(y,t) = y^3 \cdot t^2 + \sin(t+y) + \sqrt{t+y}$

THE NUMERICAL SOLUTION

Here are the minimal algorithm — integrate the differential equation by one step in t:

$$\frac{dy}{dt} = f(y, t)$$

$$\frac{y(t_{n+1}) - y(t_n)}{h} = f(y, t_n) \quad \forall y_{n+1} \approx y_n + h \cdot f(y_n, t_n)$$

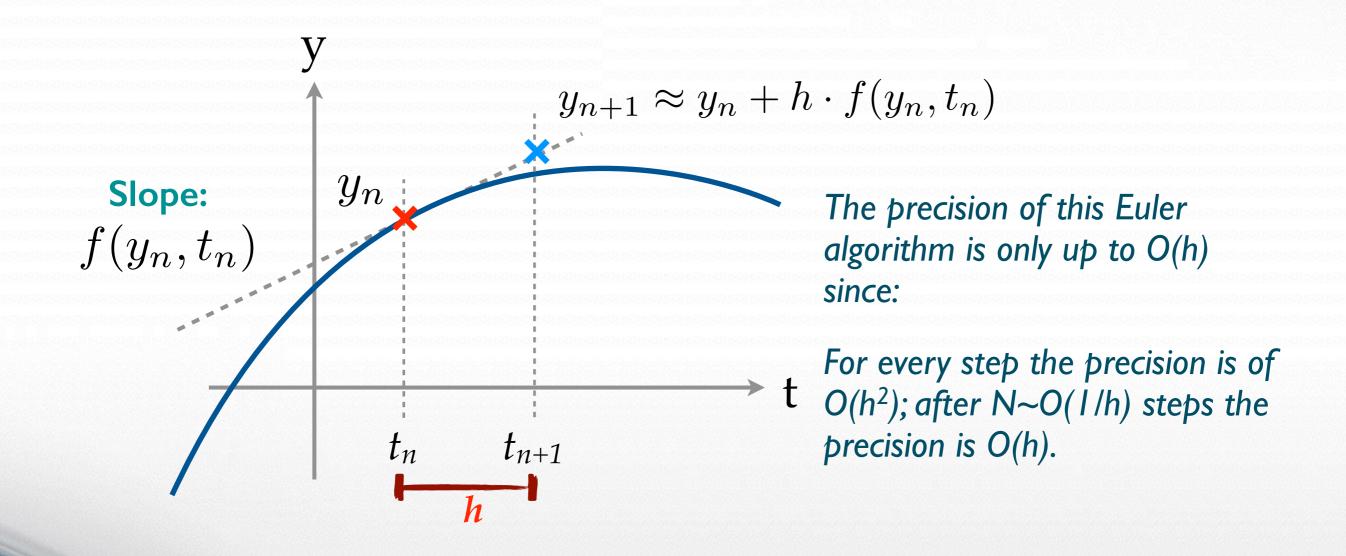
$$next step \quad for our trivial example: \quad \frac{dy}{dt} = y \quad \forall y_{n+1} \approx y_n + h \cdot y_n$$

This is the classical **Euler algorithm (method)**

EULER ALGORITHM



A more graphical explanation is as like this:



EULER ALGORITHM (II)

■ Let's prepare a simple code to see how it works:

```
import math
def f(t,y): return y
t, y = 0, 1 \in \text{Initial conditions} (t = 0, y = 1)
h = 0.001 \iff stepping in t
while t<1.:
    k1 = f(t, y) \leftarrow the given f(y,t) function
    y += h*k1
    t += h
y exact = math.exp(t)
print 'Euler method: %.16f, exact: %.16f, diff: %.16f' % \
(y,y_exact,abs(y-y_exact))
                                                         III-example-01.py
Euler method: 2.7169239322358960,
               2.7182818284590469,
exact:
               0.0013578962231509 \Leftarrow Indeed the precision is of O(h)
diff:
```

SECOND ORDER RUNGE-KUTTA METHOD

- Surely one can introduce a similar trick of error reduction we have played though out the latter half of the semester.
- Here comes the Runge-Kutta algorithm for integrating differential equations, which is based on a formal integration:

Expand f(t,y) in a Taylor series around $(t,y) = (t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}})$

$$f(t,y) = f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}) + (t - t_{n+\frac{1}{2}}) \cdot \frac{df}{dt}(t_{n+\frac{1}{2}}) + O(h^2)$$

Something smells familiar?

SECOND ORDER RUNGE-KUTTA METHOD (II)

$$f(t,y) = f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}) + (t - t_{n+\frac{1}{2}}) \cdot \left| \frac{df}{dt}(t_{n+\frac{1}{2}}) + O(h^2) \right|$$

Insert the expansion into the integration:

It's just a number (slope)!

$$\int_{t_n}^{t_{n+1}} f(t,y)dt = \int_{t_n}^{t_{n+1}} f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}})dt + \int_{t_n}^{t_{n+1}} (t - t_{n+\frac{1}{2}}) \cdot \frac{df}{dt}(t_{n+\frac{1}{2}}) dt + \dots$$

Linear (first order) term must be cancelled

Insert the integral back:

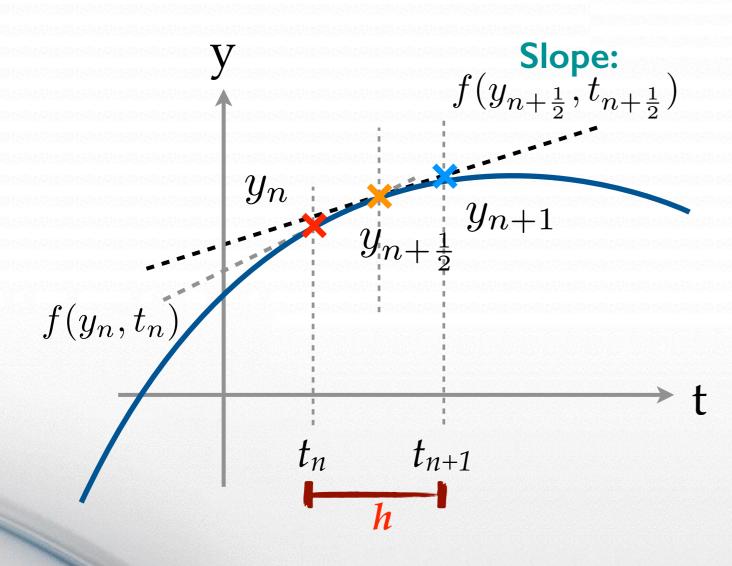
$$\int_{t_n}^{t_{n+1}} f(t,y)dt \approx h \cdot f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}})$$

$$y_{n+1} \approx y_n + h \cdot f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}) + O(h^3)$$

If one knows the solution half-step in the future — the $O(h^2)$ term can be cancelled. BUT HOW?

SECOND ORDER RUNGE-KUTTA METHOD (III)

The trick: use the Euler's method to solve half-step first, starting from the given initial conditions:



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

$$t_{n+\frac{1}{2}} = t + \frac{h}{2}$$

$$y_{n+1} \approx y_n + h \cdot f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}})$$

Explicit formulae

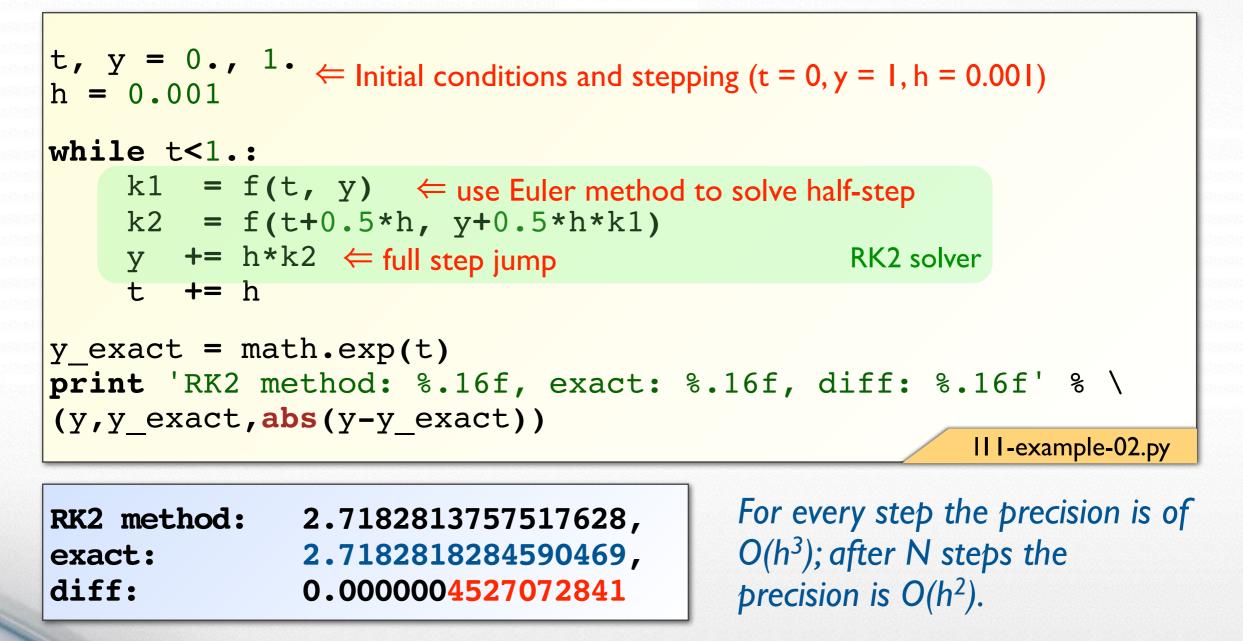
$$k_1 = f(t_n, y_n)$$

$$k_2 = f(t_n + \frac{h}{2}, y_n + \frac{h}{2} \cdot k_1)$$

$$y_{n+1} \approx y_n + h \cdot k_2 + O(h^3)$$

IMPLEMENTATION OF "RK2"

The coding is actually extremely simple:



FOURTH ORDER **RUNGE-KUTTA**

The 4th order Runge-Kutta method provides an excellent balance of power, precision, and programming simplicity. Using a similar idea of the 2nd order version, one could have these formulae:

$$k_{1} = f(t_{n}, y_{n})$$

$$k_{2} = f(t_{n} + \frac{h}{2}, y_{n} + \frac{h}{2} \cdot k_{1})$$

$$k_{3} = f(t_{n} + \frac{h}{2}, y_{n} + \frac{h}{2} \cdot k_{2})$$

$$k_{4} = f(t_{n} + h, y_{n} + h \cdot k_{3})$$

$$y_{n+1} \approx y_{n} + \frac{h}{c} \cdot (k_{1} + 2k_{2} + 2k_{3})$$

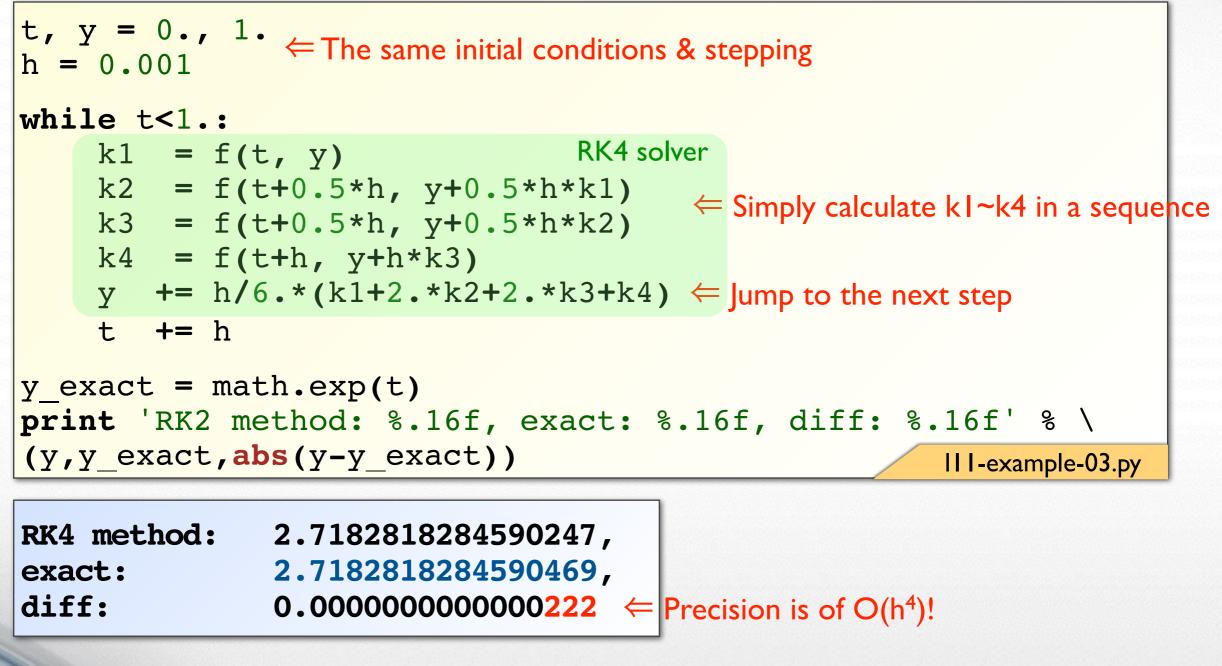
Basically the 4th order Runge-Kutta has a precision of $O(h^5)$ at each step, an over all **O(h⁴)** precision.

Actually, the RK4 is a variation of Simpson's method...

 $_{3} + k_{4}) + O(h^{5})$ 0

IMPLEMENTATION OF "RK4"

The RK4 routine is not too different from the previous RK2 code!



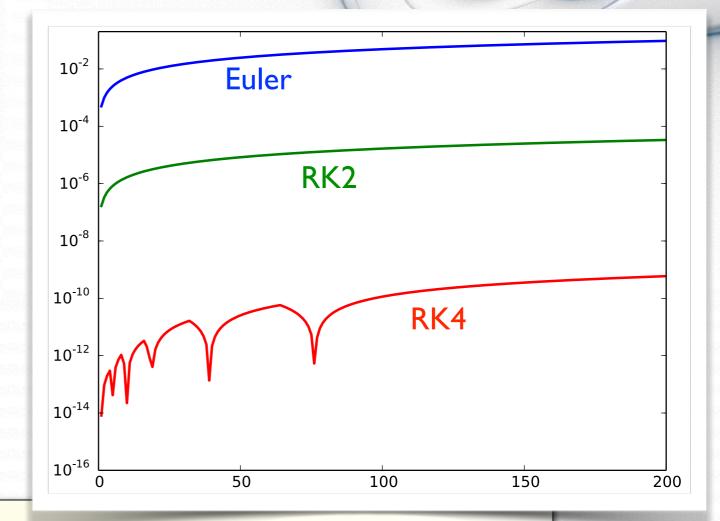
PRECISION EVOLUTION

- Let's write a small
 code to demonstrate
 the "precision" of the
 solution as it evolves.
- You should be able to see the "accumulation" of numerical errors.

vt = np.zeros(200) \leftarrow NumPy arrays for vy = np.zeros((4,200))storing the output t = 0.y1 = y2 = y4 = 1. h = 0.001Only keep the result for idx in range(200): for step in range(1000): k1 = f(t, y1) Euler method y1 += h*k1 k1 = f(t, y2)RK2 k2 = f(t+0.5*h, y2+0.5*h*k1)y2 += h*k2 k1 = f(t, y4)RK4 k2 = f(t+0.5*h, y4+0.5*h*k1) $k_3 = f(t+0.5*h, y_4+0.5*h*k_2)$ k4 = f(t+h, y4+h*k3)y4 += h/6.*(k1+2.*k2+2.*k3+k4)t += h vt[idx] = t vy[0,idx] = np.exp(t)vy[1, idx] = y1 $vy[2,idx] = y2 \iff$ Store the results vy[3,idx] = y4partial III-example-04.py

PRECISION EVOLUTION (II)

- Just make a simple plot.
- The initial uncertainties are of O(h), O(h²), and O(h⁴).
- After 200,000 steps or more, the accumulated errors can be large.



plt.plot(vt, abs(vy[1]-vy[0])/vy[0], lw=2, c='Blue')
plt.plot(vt, abs(vy[2]-vy[0])/vy[0], lw=2, c='Green')
plt.plot(vt, abs(vy[3]-vy[0])/vy[0], lw=2, c='Red')
plt.yscale('log')
plt.ylim(1E-16,0.2)
plt.xlim(0.,200.)
plt.show()
partial III-example-04.py

INTERMISSION



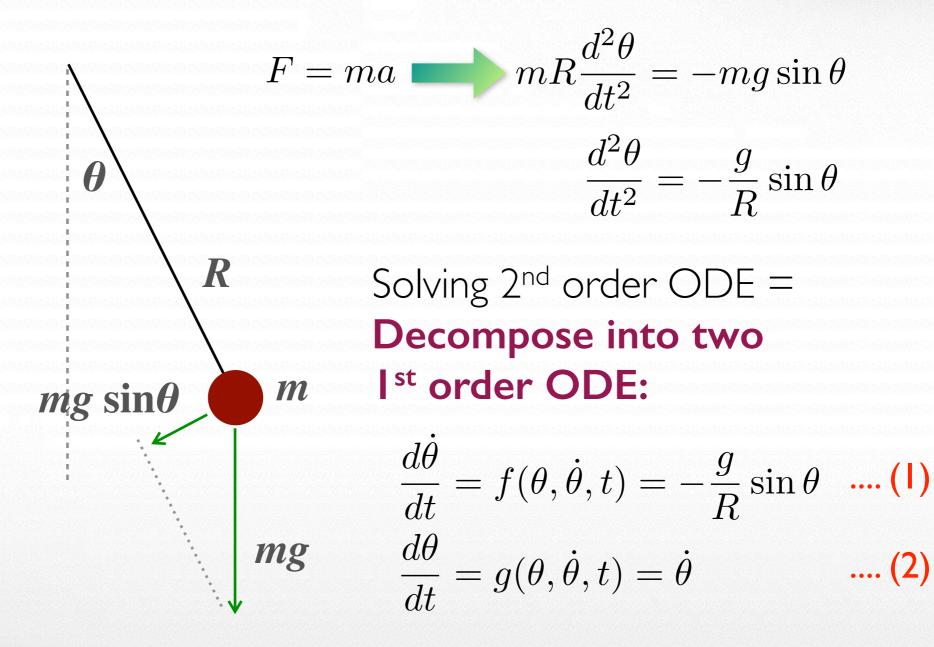
It could be interesting to solve some other trivial differential equations with the methods introduced above, for example:

$$\frac{dy}{dt} = -y$$
$$\frac{dy}{dt} = \cos(t)$$

Try to modify the previous example code (l11-example-04.py) and see how the error accumulated along with steps for a different differential equation.



A LITTLE BIT OF PHYSICS: SIMPLE PENDULUM



A LITTLE BIT OF PHYSICS: SIMPLE PENDULUM (II)

m = 1 kgR = 1 m $\theta = 0.9999 \,\pi$

 $g = 9.8 \text{m/s}^2$

With a trial Initial condition at $\mathbf{t} = \mathbf{0}$:

 $\theta = 0.9999\pi \approx 3.141278...$ $\dot{\theta} = 0$

Almost at the largest possible angle (No small angle approximation! Not a "simple" pendulum) Standstill at the beginning.

In principle it should stand for a moment, and start to falling down...

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SOLVE FOR 2 ODE'S TOGETHER

```
m, g, R = 1., 9.8, 1.
t, h = 0.001 \Leftarrow Initial condition t = 0 sec, stepping = 0.001 sec.
y = np.array([np.pi*0.9999,0.]) \leftarrow Initial \theta and \theta'
def f(t,y):
    theta = y[0] \Leftarrow input array contains \theta and \theta'
    thetap = y[1]
    thetapp = -g/R*np.sin(theta) \leftarrow output array contains \theta' and \theta''
    return np.array([thetap,thetapp])
while t<8.:
    k1 = f(t, y)
         y += h*k1 \leftarrow Euler method
         t += h
    theta = y[0]
    thetap = y[1]
    print 'At %.2f sec : (%+14.10f, %+14.10f)' % (t, theta, thetap)
                                                          III-example-05.py
```

SOLVE FOR 2 ODE'S TOGETHER (II)

- The terminal output:
- Works, but not so straight forward...

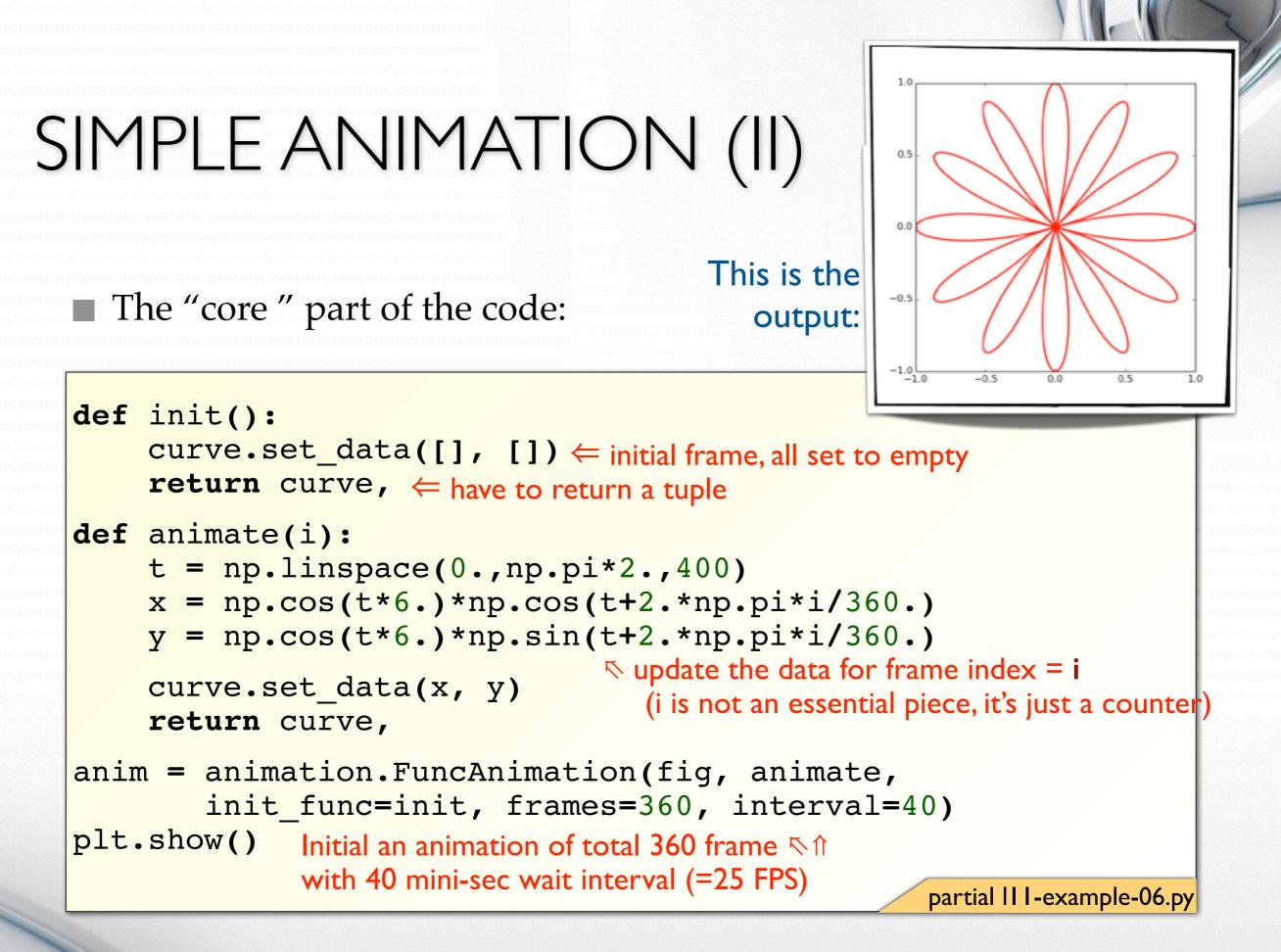
Let's introduce some **animations** to demonstrate the motion!

).53).53).	50(59)	life on mon Climan mon			$\theta\downarrow$	$\theta\downarrow$
At	0.10	sec	:	(+3.1412631358,	-0.0003127772)
	0.20			•	+3.1412152508,	-0.0006561363)
	0.30			•	+3.1411301423,	-0.0010639557)
At	0.40	sec	:	Ì	+3.1409994419,	-0.0015764466)
At	0.50	sec	:	(+3.1408102869,	-0.0022441174)
 At	1.00	sec	:	(+3.1380085436,	-0.0111772696)
At	1.50	sec	:	(+3.1245199136,	-0.0534365650)
At	2.00	sec	:	(+3.0601357015,	-0.2549284063)
At	2.50	sec	:	(+2.7540224966,	-1.2057243644)
At	3.00	sec	:	(+1.4037054845,	-4.7826081916)
At	4.00	sec	:	(-2.7787118486,	-1.1997994809)
At	5.00	sec	:	(-3.3781806892, ℕ wait, θ<	-

SIMPLE ANIMATION



- It is easy to create animations with matplotlib. It is useful to demonstrate some of the results that suppose to "move" as a function of time!
- Here are a very simple example code to show how it works!



SOLVING ODE X ANIMATION



"Merge" two previous codes as following:

```
fig = plt.figure(figsize=(6,6), dpi=80)
ax = plt.axes(xlim=(-1.2,+1.2), ylim=(-1.2,+1.2))
stick, = ax.plot([], [], lw=2, color='black')
ball, = ax.plot([], [], 'ro', ms=10)
text = ax.text(0.,1.1,'', fontsize = 16, color='black',
          ha='center', va='center')
                                               \bigtriangledown initial empty objects:
m, q, R = 1., 9.8, 1.
t, h = 0., 0.001
y = np.array([np.pi*0.9999,0.]) \leftarrow Initial \theta and \theta'
def f(t,y):
                          \leftarrow function for calculating \theta' and \theta"
    theta = y[0]
    thetap = y[1]
    thetapp = -g/R*np.sin(theta)
    return np.array([thetap,thetapp])
                                                      partial II I-example-05a.py
```

SOLVING ODE X ANIMATION (II)

Core animation + solving ODE:

```
-0.5
def animate(i):
    global t, y \leftarrow force t and y to be global variables
                                                     -1.0
     for step in range(40):
                                                        -1.0
                                                            -0.5
                                                                0.0
                                                                    0.5
                                                                        1.0
         k1 = f(t, y) \Leftarrow solve 40 steps
         y += h*k1 (0.04 sec per frame)
         t += h
    theta = y[0]
    thetap = y[1]
    bx = np.sin(theta)
    by = -np.cos(theta)
    ball.set data(bx, by)
                                             \Leftarrow plot the "ball" and "stick"
    stick.set data([0.,bx], [0.,by])
    E = m*g*by + 0.5*m*(R*thetap)**2
                                             \Leftarrow show the total energy
    text.set(text='E = %.16f' % E)
    return stick, ball, text
anim = animation.FuncAnimation(fig, animate, init func=init,
        frames=10, interval=40)
                                                         partial II I-example-05a.py
```

1

1.0

0.5

0.0

"text"

E = 9.7999995163882581

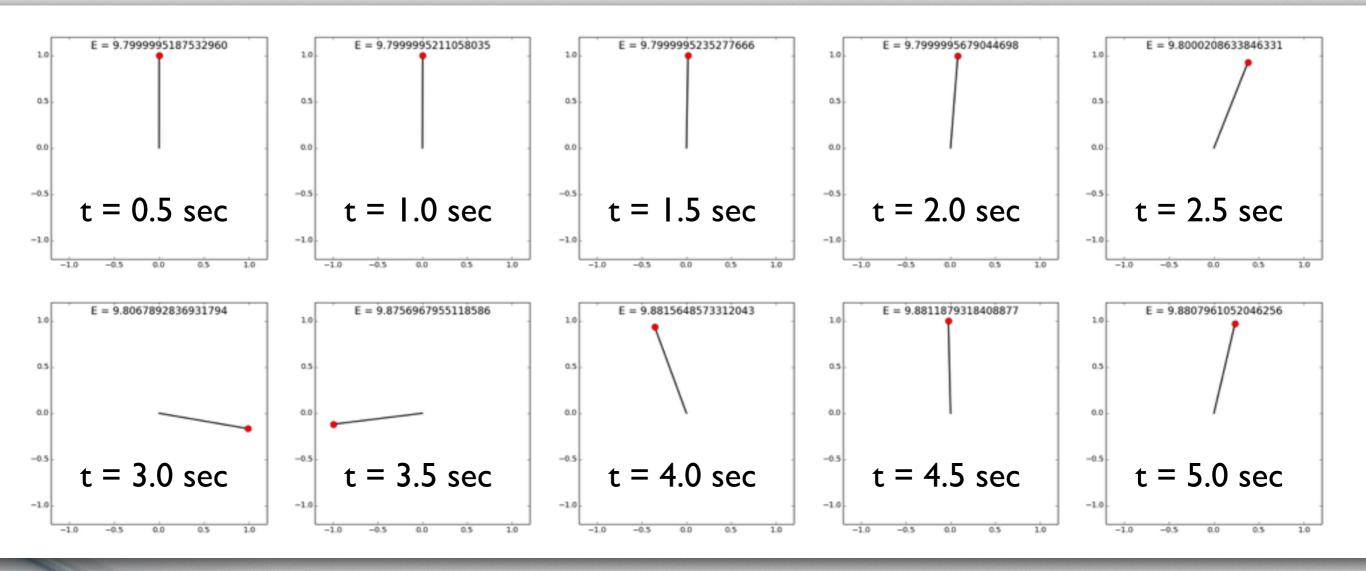
′**∿"ball**"

∕="stick"

DEMO TIME!

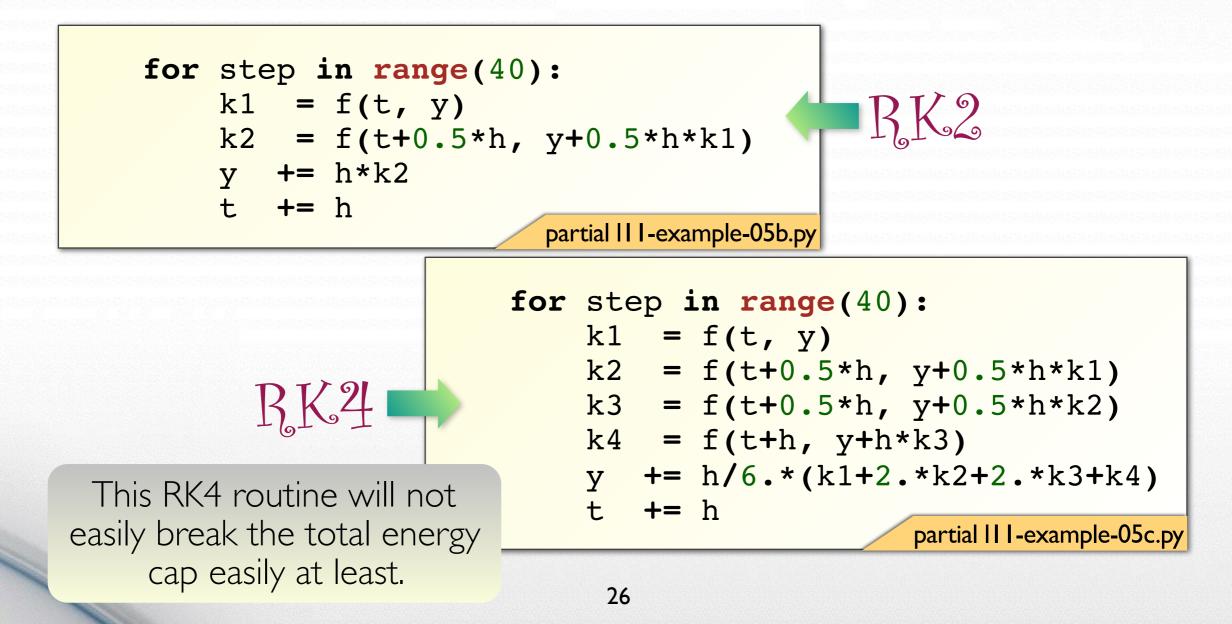


It moves! But you will find the solver does not work too good almost immediately; the energy is not even conserved!



THAT'S WHY WE NEED A BETTER ODE SOLVER...

One can simply replace the core part of the code to "upgrade" the ODE solutions.



USING THE ODE SOLVER // FROM SCIPY

The ODE solver under SciPy is also available in scipy.integrate module, together with the numerical integration tools:

S Sc	iPy.org		
1999 (1999 (1999 (1999 (1999 (1999 (1999 (1999 (1999 (1999 (1999 (1999 (1999 (1999 (1999 (1999 (1999 (1999 (199	SciPy v0.14.0 Reference Guide		
Integrators of ODE systems			
odeint(func, y0, t[, args, Dfun, col_deriv,]) ode(f[, jac]) complex_ode(f[, jac])	Integrate a system of ordinary differential equations. A generic interface class to numeric integrators. A wrapper of ode for complex systems.		

http://docs.scipy.org/doc/scipy/reference/integrate.html#module-scipy.integrate

USING THE ODE SOLVER FROM SCIPY (II)

```
import numpy as np
from scipy.integrate import ode import the module
m, g, R = 1., 9.8, 1.
t, y = 0., np.array([np.pi*0.9999,0.]) /= now t and y are
                                          just initial conditions
def f(t,y):
    theta = y[0]
thetap = y[1] \Leftarrow exactly the same f(x,y)
    thetapp = -q/R*np.sin(theta)
    return np.array([thetap,thetapp])
intr = ode(f).set_integrator('dop853') \equiv initialize the ode class
intr.set initial value(y, t)
                                           with 'dop853' integrator
while intr.t<8.:
    theta = intr.y[0]
    thetap = intr.y[1]
    print 'At %.2f sec : (%+14.10f, %+14.10f)' \
     % (intr.t, theta, thetap)
                                                 III-example-07.py
```

USING THE ODE SOLVER FROM SCIPY (III)

20,220,22) 다리(다리) 다리(), : : : : : : : : : : : : : : : : : : :	119.13	(), (2), (3), (3), (3), (3), (3), (3), (3), (3		
At	0.10	sec	:	(+3.1412629744,	-0.0003129294)
At	0.20	sec	:	(+3.1412148812,	-0.0006567772)
At	0.30	sec	:	(+3.1411294629,	-0.0010655165)
At	0.40	sec	:	(+3.1409982801,	-0.0015795319)
At	0.50	sec	•	(+3.1408083714,	-0.0022496097)
At	1.00	sec	:	(+3.1379909749,	-0.0112320574)
At	1.50	sec	:	(+3.1243942321,	-0.0538299284)
At	2.00	sec	:	(+3.0593354818,	-0.2574312087)
At	2.50	sec	:	(+2.7492944690,	-1.2202273084)
At	3.00	sec	:	(+1.3819060253,	-4.8249634626)
At	4.00	sec	:	(-2.7713127817,	-1.1525482114)
At	5.00	sec	:	(-3.1253649922,	-0.0507902190)

- It's simply working smoothly.
- There are few more different integrator available in the scipy ode class, e.g.
 "vode", "zvode", etc.
- Please read the manual for details.

USING THE ODE SOLVER FROM SCIPY (IV)

It's also pretty easy to merge the ODE solver with animation.

Initial the integrator

Replace the for-loop with a single commend

```
m, g, R = 1., 9.8, 1.
t = 0.
y = np.array([np.pi*0.9999,0.])
def f(t,y):
    theta = y[0]
    thetap = y[1]
    thetapp = -g/R*np.sin(theta)
    return np.array([thetap,thetapp])
intr = ode(f).set_integrator('dop853')
intr.set initial value(y, t)
def animate(i):
  > intr.integrate(intr.t+0.040)
    theta = intr.y[0]
    thetap = intr.y[1]
                           partial II I-example-07a.py
```

INTERMISSION



- What will happen if you given a critical initial condition to the preview simple pendulum example, e.g. $\theta = \pi$
- It could be fun if you can try to record the angle versus time (this can be done by a small modification to l11-example-07.py), and make a plot. If you set the initial condition to a small angle (when the small angle approximation still works), will you see if your solution close to a sine/cosine function?

 $\dot{\theta} = 0$



FEW MORE EXAMPLES FOR YOUR AMUSEMENT

Replace the "stick" with a spring:

$$f = -k(R - R_0)$$

$$R_0 = 0.5m$$

$$k = 100 \text{ N/m}$$

$$f = -k(R - R_0)$$

$$R = \sqrt{x^2 + y^2}$$

$$f_x = f \cdot \frac{x}{R}\hat{i}$$

$$f_y = f \cdot \frac{y}{R}\hat{j}$$
Coordinate (x,y) is used
instead of (R,0) here.
Need to solve 4 equations
(x,y,v_x,v_y) simultaneously

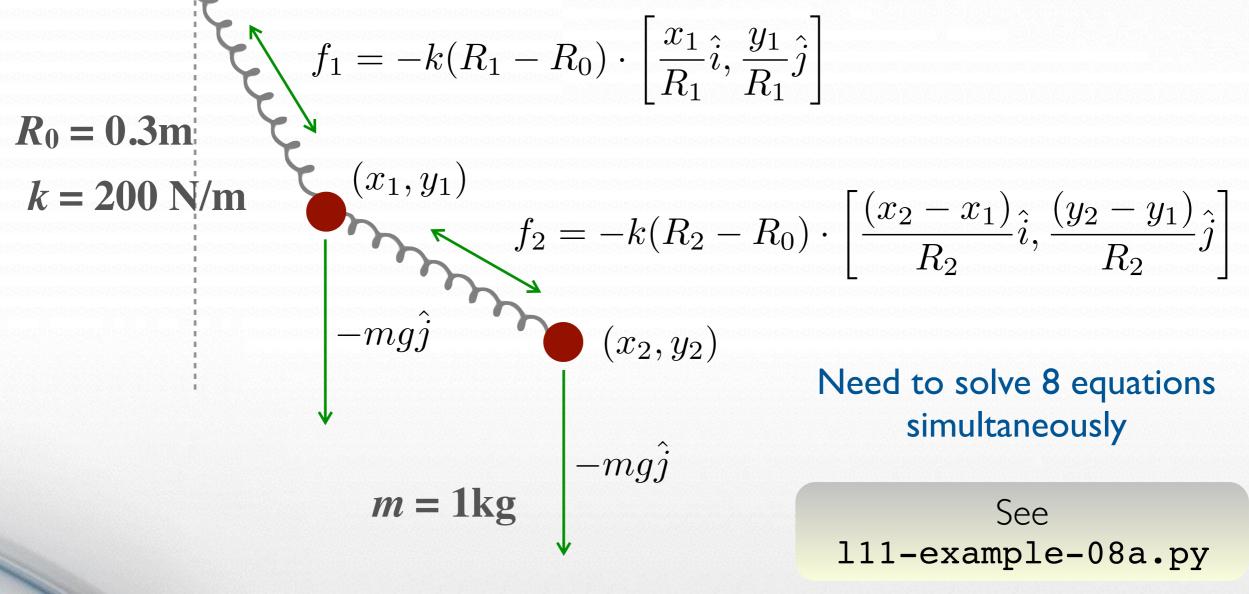
$$g = 9.8m/s^2$$

$$See$$
111-example-08.py



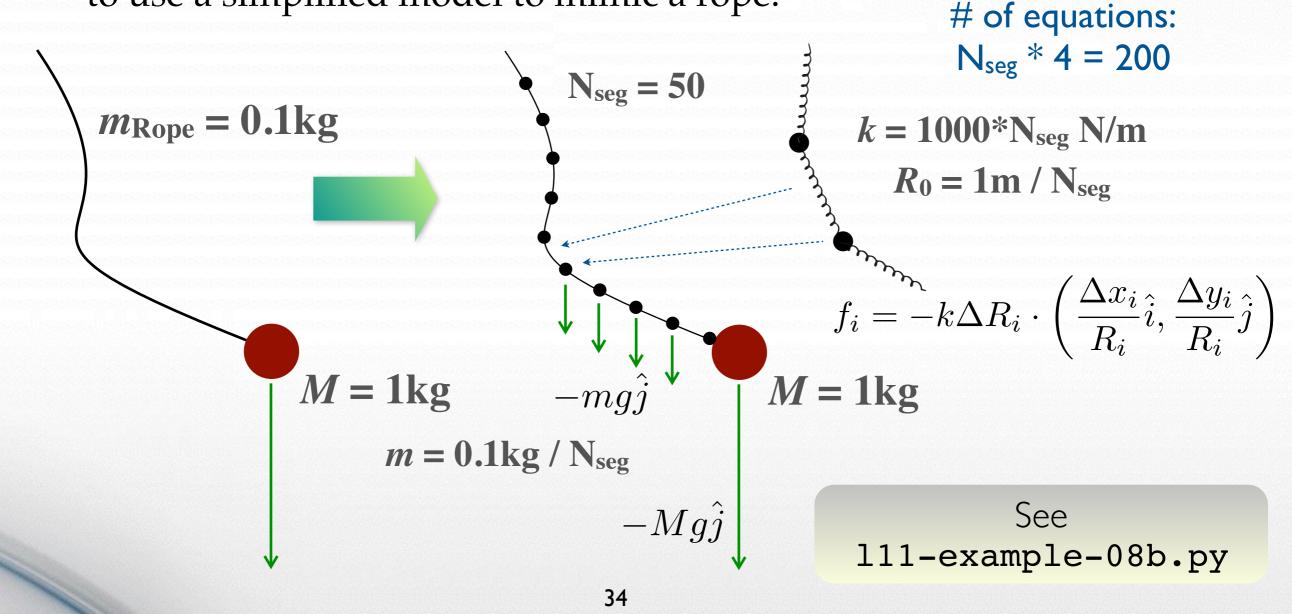
ONE IS COOL, TWO ARE CHAOTIC?

A joint two-spring-ball system:



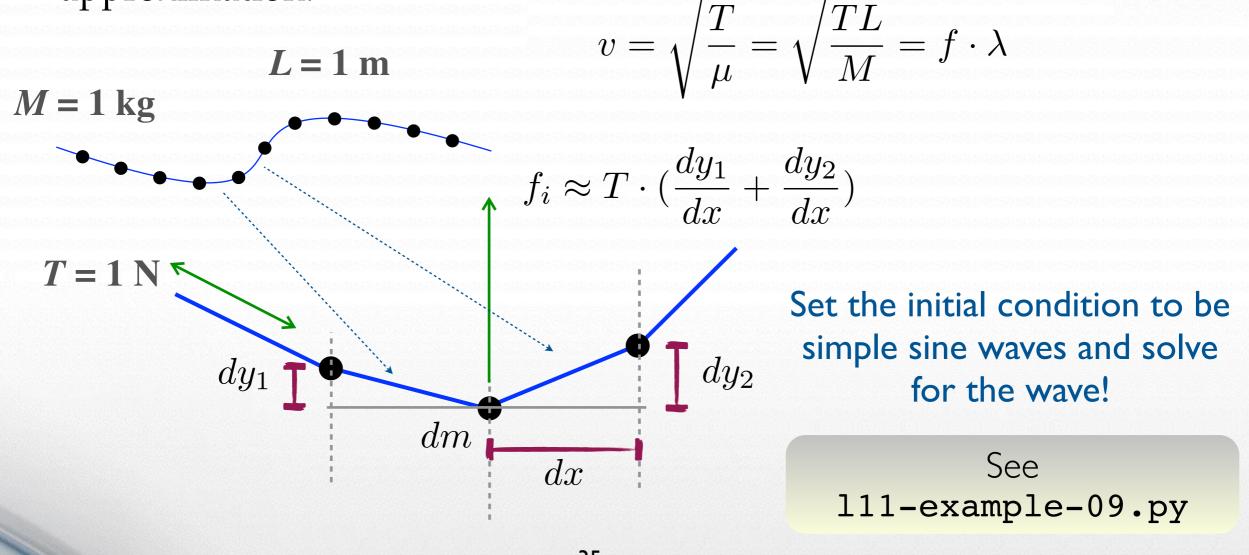
A CHAIN OF SPRING-BALL = A ROPE?

If we replace the "stick" with a rope, is it possible? Surely we need to use a simplified model to mimic a rope.



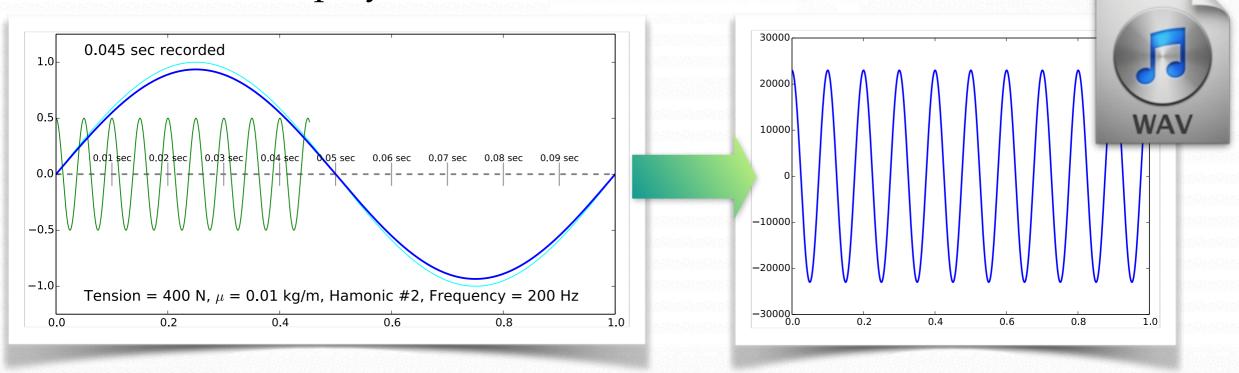
WAVE ON A STRING

- Actually one can use a similar way to model a string construct a N segment (massive) string and solve it with small angle approximation.



WAVE ON A STRING (II)

It is also fun to record the vibration of the string, convert it to a wave file and play it out!



For the case of T = 400 N, μ = 0.01 kg/m, λ = 1m, we are expecting to hear a 200 Hz sound!

See 111-example-09a.py

COMMENTS



- We have demonstrated several interesting examples, surely you are encouraged to modify the code and test some different physics parameters, or different initial conditions.
- Basically all of those tasks can be easily done with the given ODE solver. In any case these are examples are VERY PHYSICS!
- Then you may want to ask how about PDEs? The general idea of PDE solving is similar but require some different implementations. There is no PDE solver available in SciPy yet. If you want, you can try the following packages:
 - FiPy <u>http://www.ctcms.nist.gov/fipy/</u>
 - SfePy http://sfepy.org/doc-devel/index.html



HANDS-ON SESSION

Practice 1:

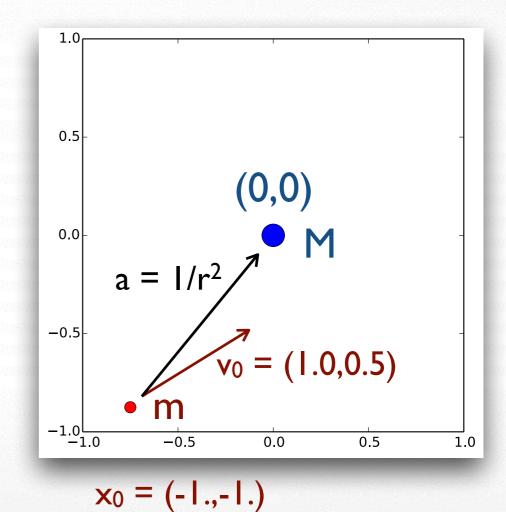
Add some simple gravity to the system: there is a red star shooting toward the earth. Assuming the only acceleration between the earth and the red star is contributed by the gravitational force:

$$F = \frac{GMm}{r^2}$$

with $G \times M = 1$. Thus:

$$a = \frac{dv}{dt} = F/m = \frac{1}{r^2}$$

implement the code and produce the animation.



HANDS-ON SESSION



Practice 2:

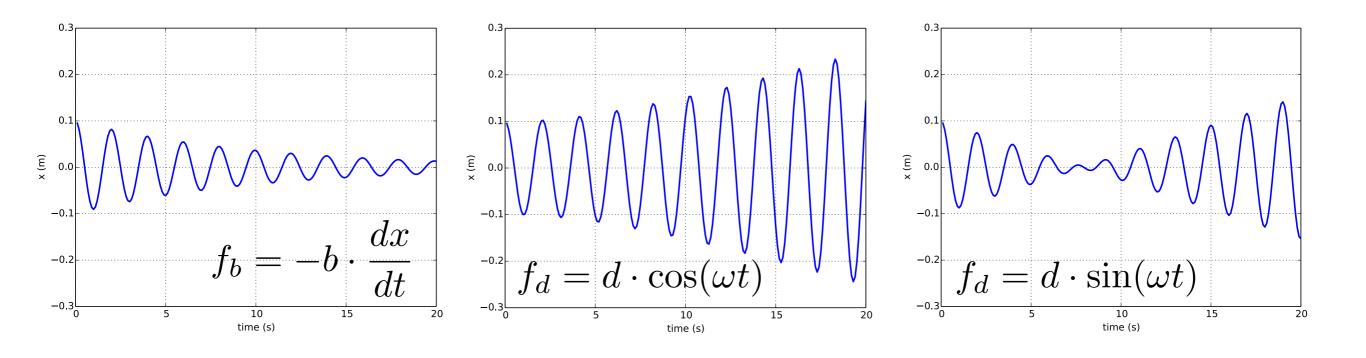
damped or driven oscillators – please solve the following system with the extra (damping/driving) force and the given physics parameters.

Initial condition: $\mathbf{t} = \mathbf{0} \sec, \mathbf{x} = +\mathbf{0.1} \mathbf{m}$ $\mathbf{k} = 10 \,\mathrm{N/m}$ $\mathbf{m} = 1 \,\mathrm{kg}$ $f_b = -b \cdot \frac{dx}{dt}$ $b = 0.2 \,\mathrm{Ns/m}$ $f_d = d \cdot \cos(\omega t)$ $d = 0.08 \,\mathrm{N}$ $\omega = \pi \,\mathrm{rad/s}$ $f_d = d \cdot \sin(\omega t)$

HANDS-ON SESSION



Please start with the given template on CEIBA. It can produce the following plots if you solve them correctly.



You may also play around with some what different physics parameters as well as the initial conditions.