A worked example on scientific computing with Python

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Contents

This worked example

- fetches a data file from a web site,
- applies that file as input data for a differential equation modeling a vibrating mechanical system,
- solves the equation by a finite difference method,
- visualizes various properties of the solution and the input data.

The following programming topics are illustrated

- basic Python constructs: variables, loops, if-tests, arrays, functions
- flexible storage of objects in lists
- storage of objects in files (persistence)
- downloading files from the web
- user input via the command line
- signal processing and FFT
- curve plotting of data
- testing
- modules

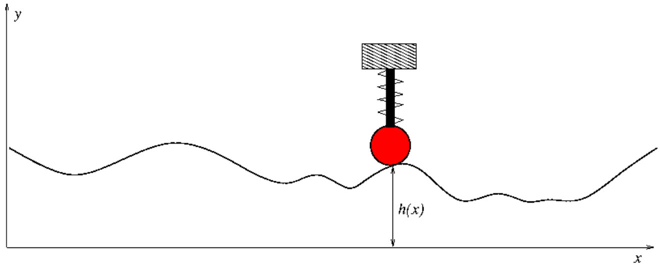
All files can be forked at `https://github.com/hplgit/bumpy`

Scientific application

Physical problem and mathematical model

$$mu'' + f(u') + s(u) = F(t), \quad u(0) = I, \; u'(0) = V \qquad (1)$$

- Input: mass m, friction force $f(u')$, spring $s(u)$, external forcing $F(t)$, I, V
- Output: vertical displacement $u(t)$



Relatively stiff spring $k = 5$

Go to movie on github.com

Softer spring $k = 1$

Go to movie on github.com

Numerical model

- Finite difference method
- Centered differences
- u^n: approximation to exact u at $t = t_n = n\Delta t$
- First: linear damping $f(u') = bu'$

$$u^{n+1} = \left(2mu^n + (\frac{b}{2}\Delta t - m)u^{n-1} + \Delta t^2(F^n - s(u^n))\right)(m + \frac{b}{2}\Delta t)^{-1}$$

A special formula must be applied for $n = 0$:

$$u^1 = u^0 + \Delta t\, V + \frac{\Delta t^2}{2m}(-bV - s(u^0) + F^0)$$

Extension to quadratic damping: $f(u') = b|u'|u'$

Linearization via geometric mean:

$$f(u'(t_n)) = |u'|u'|^n \approx |u'|^{n-\frac{1}{2}}(u')^{n+\frac{1}{2}}$$

$$\begin{aligned} u^{n+1} = &\left(m + b|u^n - u^{n-1}|\right)^{-1} \times \\ &\left(2mu^n - mu^{n-1} + bu^n|u^n - u^{n-1}| + \Delta t^2(F^n - s(u^n))\right) \end{aligned}$$

(and again a special formula for u^1)

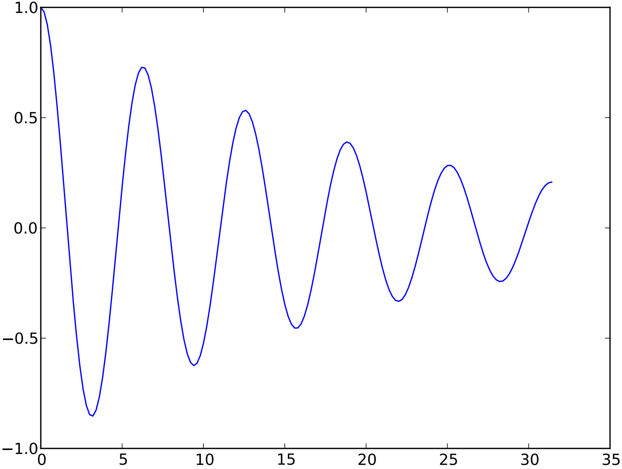
Simple implementation

```python
from numpy import *

def solver_linear_damping(I, V, m, b, s, F, t):
    N = t.size - 1              # No of time intervals
    dt = t[1] - t[0]            # Time step
    u = zeros(N+1)              # Result array
    u[0] = I
    u[1] = u[0] + dt*V + dt**2/(2*m)*(-b*V - s(u[0]) + F[0])

    for n in range(1,N):
        u[n+1] = 1./(m + b*dt/2)*(2*m*u[n] + \
                 (b*dt/2 - m)*u[n-1] + dt**2*(F[n] - s(u[n])))
    return u
```

Using the solver function to solve a problem

```
from solver import solver_linear_damping
from numpy import *

def s(u):
    return 2*u

T = 10*pi       # simulate for t in [0,T]
dt = 0.2
N = int(round(T/dt))
t = linspace(0, T, N+1)
F = zeros(t.size)
I = 1; V = 0
m = 2; b = 0.2
u = solver_linear_damping(I, V, m, b, s, F, t)

from matplotlib.pyplot import *
plot(t, u)
savefig('tmp.pdf')    # save plot to PDF file
savefig('tmp.png')    # save plot to PNG file
show()
```

The resulting plot



More advanced implementation

Improvements:

- Treat linear *and* quadratic damping
- Allow $F(t)$ to be either a function or an array of measurements
- Use doc strings for documentation
- Report errors through raising exceptions
- Watch out for integer division

```
>>> 2/3
0
>>> 2.0/3
0.66666666666666663
>>> 2/3.0
0.66666666666666663
```

At least one of the operands in division must be `float` to get correct real division!

The code (part I)

```
def solver(I, V, m, b, s, F, t, damping='linear'):
    """
    Solve m*u'' + f(u') + s(u) = F for time points in t.
    u(0)=I and u'(0)=V,
    by a central finite difference method with time step dt.
    If damping is 'linear', f(u')=b*u, while if damping is
    'quadratic', we have f(u')=b*u'*abs(u').
    s(u) is a Python function, while F may be a function
    or an array (then F[i] corresponds to F at t[i]).
    """
    N = t.size - 1              # No of time intervals
    dt = t[1] - t[0]            # Time step
    u = np.zeros(N+1)           # Result array
    b = float(b); m = float(m)  # Avoid integer division

    # Convert F to array
    if callable(F):
        F = F(t)
    elif isinstance(F, (list,tuple,np.ndarray)):
        F = np.asarray(F)
    else:
        raise TypeError(
            'F must be function or array, not %s' % type(F))
```

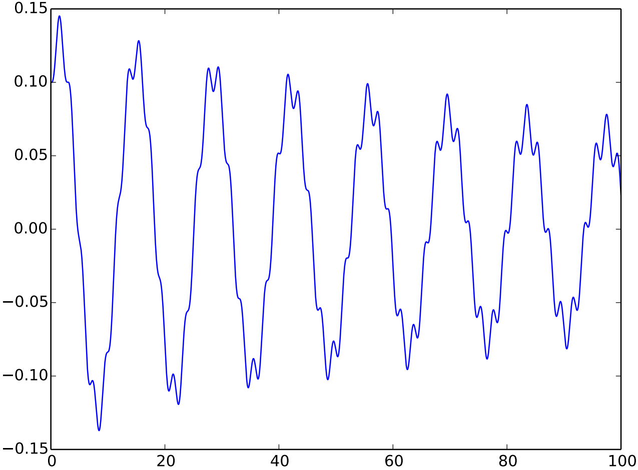
The code (part II)

```
def solver(I, V, m, b, s, F, t, damping='linear'):
    ...
    u[0] = I
    if damping == 'linear':
        u[1] = u[0] + dt*V + dt**2/(2*m)*(-b*V - s(u[0]) + F[0])
    elif damping == 'quadratic':
        u[1] = u[0] + dt*V + \
               dt**2/(2*m)*(-b*V*abs(V) - s(u[0]) + F[0])
    else:
        raise ValueError('Wrong value: damping="%s"' % damping)

    for n in range(1,N):
        if damping == 'linear':
            u[n+1] = (2*m*u[n] + (b*dt/2 - m)*u[n-1] +
                      dt**2*(F[n] - s(u[n])))/(m + b*dt/2)
        elif damping == 'quadratic':
            u[n+1] = (2*m*u[n] - m*u[n-1] + b*u[n]*abs(u[n] - u[n-1])
                      - dt**2*(s(u[n]) - F[n]))/\
                      (m + b*abs(u[n] - u[n-1]))
    return u, t
```

Using the solver function to solve a problem

```python
import numpy as np
from numpy import sin, pi  # for nice math
from solver import solver

def F(t):
    # Sinusoidal bumpy road
    return A*sin(pi*t)

def s(u):
    return k*(0.2*u + 1.5*u**3)

A = 0.25
k = 2
t = np.linspace(0, 100, 10001)
u, t = solver(I=0.1, V=0, m=2, b=0.5, s=s, F=F, t=t,
              damping='quadratic')

# Show u(t) as a curve plot
import matplotlib.pyplot as plt
plt.plot(t, u)
plt.show()
```

The resulting plot



Local vs global variables

```python
def f(u):
    return k*u
```

Here,

- `u` is a *local variable*, which is accessible just inside in the function
- `k` is a *global variable*, which must be initialized outside the function prior to calling `f`

Advanced programming of functions with parameters

- $f(u) = ku$ needs parameter k
- Implement f as a class with k as attribute and `__call__` for evaluating `f(u)`

```python
class Spring:
    def __init__(self, k):
        self.k = k

    def __call__(self, u):
        return self.k*u

f = Spring(k)

# f looks like a function: can call f(0.2)
```

The excitation force

- A bumpy road gives an excitation $F(t)$
- File bumpy.dat.gz contains various road profiles $h(x)$
- http://hplbit.bitbucket.org/data/bumpy/bumpy.dat.gz

Download road profile data $h(x)$ from the Internet:

```
filename = 'bumpy.dat.gz'
url = 'http://hplbit.bitbucket.org/data/bumpy/bumpy.dat.gz'
import urllib
urllib.urlretrieve(url, filename)
h_data = np.loadtxt(filename)     # read numpy array from file

x = h_data[0,:]                   # 1st column: x coordinates
h_data = h_data[1:,:]             # other columns: h shapes
```

The very basics of two-dimensional arrays

0	0.2	0.25	0.15
-0.1	0.15	0.2	0.15

```
>>> import numpy as np
>>> h_data = np.array([[0, 0.2, 0.25, 0.15],
                       [-0.1, 0.15, 0.2, 0.15]])
>>> h_data.shape  # size of each dimension
(2, 4)
>>> h_data[0,:]
array([ 0.  ,  0.2 ,  0.25,  0.15])
>>> h_data[:,0]
array([ 0. , -0.1])
>>> profile1 = h_data[1,:]
>>> profile1
array([-0.1 ,  0.15,  0.2 ,  0.15])
>>> h_data[1,1:3]                    # elements [1,1] [1,2]
array([ 0.15,  0.2 ])
```

Computing the force from the road profile

$$F(t) \sim \frac{d^2}{dt^2} h(x), \quad v = xt, \quad \Rightarrow \quad F(t) \sim v^2 h''(x)$$

```python
def acceleration(h, x, v):
    """Compute 2nd-order derivative of h."""
    # Method: standard finite difference aproximation
    d2h = np.zeros(h.size)
    dx = x[1] - x[0]
    for i in range(1, h.size-1, 1):
        d2h[i] = (h[i-1] - 2*h[i] + h[i+1])/dx**2
    # Extraplolate end values from first interior value
    d2h[0] = d2h[1]
    d2h[-1] = d2h[-2]
    a = d2h*v**2
    return a
```

Vectorized version of the previous function

```
def acceleration_vectorized(h, x, v):
    """Compute 2nd-order derivative of h. Vectorized version."""
    d2h = np.zeros(h.size)
    dx = x[1] - x[0]
    d2h[1:-1] = (h[:-2] - 2*h[1:-1] + h[2:])/dx**2
    # Extraplolate end values from first interior value
    d2h[0] = d2h[1]
    d2h[-1] = d2h[-2]
    a = d2h*v**2
    return a
```

Performing the simulation of vibrations

Use a list data to hold all input and output data

```
data = [x, t]
for i in range(h_data.shape[0]):
    h = h_data[i,:]            # extract a column
    a = acceleration(h, x, v)
    u = solver(t=t, I=0, m=m, b=b, f=f, F=-m*a)
    data.append([h, a, u])
```

Parameters for bicycle conditions: $m = 60$ kg, $v = 5$ m/s, $k = 60$ N/m, $b = 80$ Ns/m

A high-level solve function (part I)

```python
def solve(url=None, m=60, b=80, k=60, v=5):
    """
    Solve model for verticle vehicle vibrations.

    =========   ==============================================
    variable    description
    =========   ==============================================
    url         either URL of file with excitation force data,
                or name of a local file
    m           mass of system
    b           friction parameter
    k           spring parameter
    v           (constant) velocity of vehicle
    Return      data (list) holding input and output data
                [x, t, [h,a,u], [h,a,u], ...]
    =========   ==============================================
    """
    # Download file (if url is not the name of a local file)
    if url.startswith('http://') or url.startswith('file://'):
        import urllib
        filename = os.path.basename(url)  # strip off path
        urllib.urlretrieve(url, filename)
    else:
        # Check if url is the name of a local file
        if not os.path.isfile(url):
            print url, 'must be a URL or a filename'; sys.exit(1)
```

A high-level solve function (part II)

```python
def solve(url=None, m=60, b=80, k=60, v=5):
    ...
    h_data = np.loadtxt(filename)  # read numpy array from file

    x = h_data[0,:]                # 1st column: x coordinates
    h_data = h_data[1:,:]          # other columns: h shapes

    t = x/v                        # time corresponding to x
    dt = t[1] - t[0]

    def f(u):
        return k*u

    data = [x, t]        # key input and output data (arrays)
    for i in range(h_data.shape[0]):
        h = h_data[i,:]            # extract a column
        a = acceleration(h, x, v)

        u = solver(t=t, I=0.2, m=m, b=b, f=f, F=-m*a)
        data.append([h, a, u])
    return data
```

Computing an expression for the noise level of the vibrations

$$\mathrm{RMS} = \sqrt{\int_0^T u^2 dt} \approx \sqrt{\frac{1}{N+1}\sum_{i=0}^{N}(u^n)^2}$$

```python
def rms(data):
    u_rms = np.zeros(t.size)  # for accumulating the rms value
    for h, a, u in data[2:]:  # loop over results
        u_rms += u**2
    u_rms = np.sqrt(u_rms/u_rms.size)
    data.append(u_rms)
    return data
```

Pickling: storing Python objects in files

After calling

```
road_url = 'http://hplbit.bitbucket.org/data/bumpy/bumpy.dat.gz'
data = solve(url=road_url,
             m=60, b=200, k=60, v=6)
data = rms(data)
```

the data array contains single arrays and triplets of arrays,

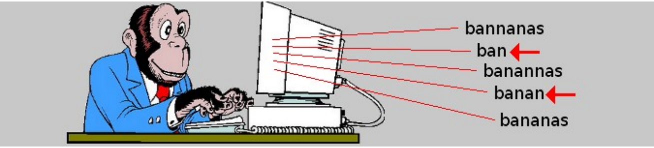
```
[x, t, [h,a,u], [h,a,u], ..., [h,a,u], u_rms]
```

This list, or any Python object, can be stored on file for later retrieval of the results, using *pickling*:

```
import cPickle
outfile = open('bumpy.res', 'w')
cPickle.dump(data, outfile)
outfile.close()
```

See `bumpy.py`.

User input



Positional command-line arguments

Suppose b is given on the command line:

```
Terminal> python bumpy.py 10
```

Code:

```
try:
    b = float(sys.argv[1])
except IndexError:
    b = 80  # default
```

Note: 1st command-line argument in `sys.argv[1]`, but that is a string

Option-value pairs on the command line

Now we want to use option-value pairs on the command line:

```
Terminal> python bumpy.py --m 40 --b 280
```

Note:

- All parameters have default values
- The default value can be overridden on the command line with `--option value`
- We use the `argparse` module for defining, reading, and accessing option-value pairs

Example on using argparse

```
def command_line_options():
    import argparse
    parser = argparse.ArgumentParser()
    parser.add_argument('--m', '--mass', type=float,
                        default=60, help='mass of vehicle')
    parser.add_argument('--k', '--spring', type=float,
                        default=60, help='spring parameter')
    parser.add_argument('--b', '--damping', type=float,
                        default=80, help='damping parameter')
    parser.add_argument('--v', '--velocity', type=float,
                        default=5, help='velocity of vehicle')
    url = 'http://hplbit.bitbucket.org/data/bumpy/bumpy.dat.gz'
    parser.add_argument('--roadfile', type=str,
              default=url, help='filename/URL with road data')
    args = parser.parse_args()
    # Extract input parameters
    m = args.m; k = args.k; b = args.b; v = args.v
    url = args.roadfile
    return url, m, b, k, v
```

Visual exploration

Plot

- the root mean square value of $u(t)$, to see the typical amplitudes
- the spectrum of $u(t)$, for $t > t_s$ (using FFT) to see which frequencies that dominate in the signal
- for each road shape, a plot of $h(x)$, $a(t)$, and $u(t)$, for $t \geq t_s$

Code (part I)

For convenience:

```python
from numpy import *
from matplotlib.pyplot import *
```

Loading results from file:

```python
import cPickle
outfile = open('bumpy.res', 'r')
data = cPickle.load(outfile)
outfile.close()

x, t = data[0:2]
u_rms = data[-1]
```

Recall list data:

```
[x, t, [h,a,u], [h,a,u], ..., [h,a,u], u_rms]
```

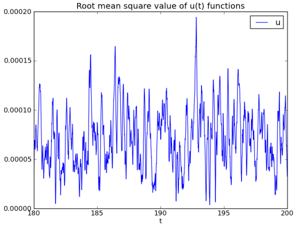
Code (part II)

Display only the last portion of time series:

```
indices = t >= t_s    # True/False boolean array
t = t[indices]        # fetch the part of t for which t > t_s
x = x[indices]        # fetch the part of x for which t > t_s
```

Plotting the root mean square value array `u_rms` for `t >= t_s` is now done by

```
figure()
u_rms = u_rms[indices]
plot(t, u_rms)
legend(['u'])
xlabel('t')
title('Root mean square value of u(t) functions')
show()
```

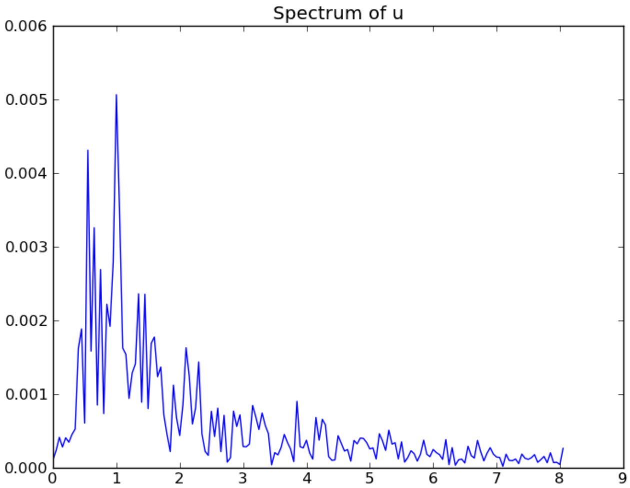


Code (part III)

The spectrum of a discrete function $u(t)$:

```
def frequency_analysis(u, t):
    A = fft(u)
    A = 2*A
    dt = t[1] - t[0]
    N = t.size
    freq = arange(N/2, dtype=float)/N/dt
    A = abs(A[0:freq.size])/N
    # Remove small high frequency part
    tol = 0.05*A.max()
    for i in xrange(len(A)-1, 0, -1):
        if A[i] > tol:
            break
    return freq[:i+1], A[:i+1]

figure()
u = data[3][2][indices]  # 2nd realization of u
f, A = frequency_analysis(u, t)
plot(f, A)
title('Spectrum of u')
show()
```

Plot of the spectrum

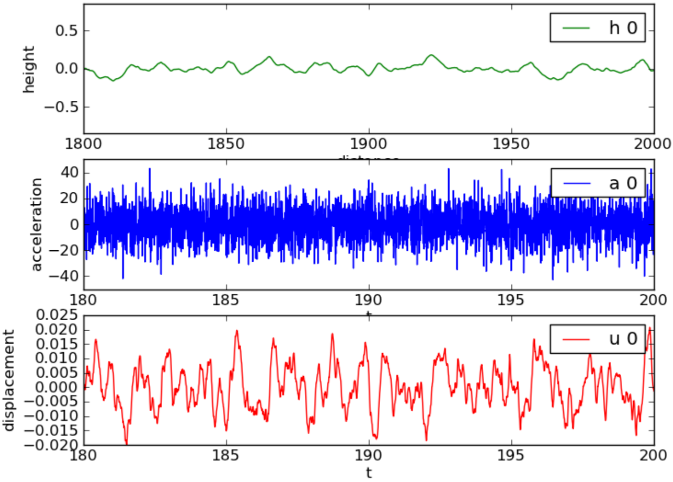


Code (part IV)

Run through all the 3-lists [h, a, u] and plot these arrays:

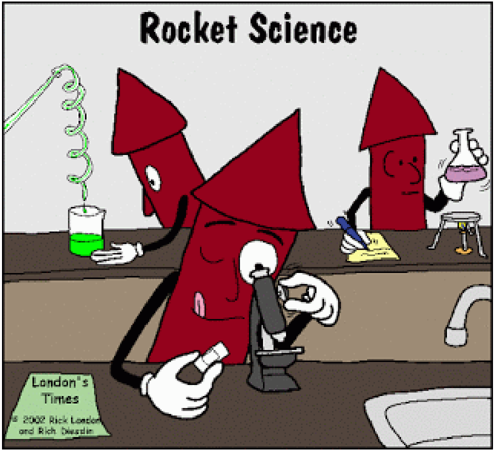
```
case_counter = 0
for h, a, u in data[2:-1]:
    h = h[indices]
    a = a[indices]
    u = u[indices]

    figure()
    subplot(3, 1, 1)
    plot(x, h, 'g-')
    legend(['h %d' % case_counter])
    hmax = (abs(h.max()) + abs(h.min()))/2
    axis([x[0], x[-1], -hmax*5, hmax*5])
    xlabel('distance'); ylabel('height')

    subplot(3, 1, 2)
    plot(t, a)
    legend(['a %d' % case_counter])
    xlabel('t'); ylabel('acceleration')

    subplot(3, 1, 3)
    plot(t, u, 'r-')
    legend(['u %d' % case_counter])
    xlabel('t'); ylabel('displacement')
    savefig('tmp%d.png' % case_counter)
    case_counter += 1
```

Plot



See `explore.py`

Advanced topics



Symbolic computing via SymPy

```
>>> import sympy as sp
>>> x, a = sp.symbols('x a')        # Define mathematical symbols
>>> Q = a*x**2 - 1                  # Quadratic function
>>> dQdx = sp.diff(Q, x)            # Differentiate wrt x
>>> dQdx
2*a*x
>>> Q2 = sp.integrate(dQdx, x)      # Integrate (no constant)
>>> Q2
a*x**2
>>> Q2 = sp.integrate(Q, (x, 0, a)) # Definite integral
>>> Q2
a**4/3 - a
>>> roots = sp.solve(Q, x)          # Solve Q = 0 wrt x
>>> roots
[-sqrt(1/a), sqrt(1/a)]
```

Go seamlessly from symbolic expression to Python function

Convert a SymPy expression `Q` into a Python function `Q(x, a)`:

```
>>> Q = sp.lambdify([x, a], Q)        # Turn Q into Py func.
>>> Q(x=2, a=3)                       # 3*2**2 - 1 = 11
11
```

This `Q(x, a)` function can be used for numerical computing

Testing via test functions and test frameworks

Modern test frameworks:

- nose
- pytest

Recommendation: use pytest, stay away from `unittest`

Example on a test function

```python
def halve(x):
    """Return half of x."""
    return x/2.0

def test_halve():
    x = 4
    expected = 2
    computed = halve(x)
    # Compare real numbers using tolerance
    tol = 1E-14
    diff = abs(computed - expected)
    assert diff < tol
```

Note:

- Name starts with `test_*`
- No arguments
- Must have `assert` on a boolean expression for passed test

Test function for the numerical solver (part I)

```
def lhs_eq(t, m, b, s, u, damping='linear'):
    """Return lhs of differential equation as sympy expression."""
    v = sm.diff(u, t)
    d = b*v if damping == 'linear' else b*v*sm.Abs(v)
    return m*sm.diff(u, t, t) + d + s(u)

def test_solver():
    """Verify linear/quadratic solution."""
    # Set input data for the test
    I = 1.2; V = 3; m = 2; b = 0.9; k = 4
    s = lambda u: k*u
    T = 2
    dt = 0.2
    N = int(round(T/dt))
    time_points = np.linspace(0, T, N+1)

    # Test linear damping
    t = sm.Symbol('t')
    q = 2  # arbitrary constant
    u_exact = I + V*t + q*t**2   # sympy expression
    F_term = lhs_eq(t, m, b, s, u_exact, 'linear')
    print 'Fitted source term, linear case:', F_term
    F = sm.lambdify([t], F_term)
    u, t_ = solver(I, V, m, b, s, F, time_points, 'linear')
    u_e = sm.lambdify([t], u_exact, modules='numpy')
    error = abs(u_e(t_) - u).max()
    tol = 1E-13
    assert error < tol
```

Test function for the numerical solver (part II)

```
def test_solver():
    ...
    # Test quadratic damping: u_exact must be linear
    u_exact = I + V*t
    F_term = lhs_eq(t, m, b, s, u_exact, 'quadratic')
    print 'Fitted source term, quadratic case:', F_term
    F = sm.lambdify([t], F_term)
    u, t_ = solver(I, V, m, b, s, F, time_points, 'quadratic')
    u_e = sm.lambdify([t], u_exact, modules='numpy')
    error = abs(u_e(t_) - u).max()
    assert error < tol
```

Using a test framework

Examine all subdirectories `test*` for `test_*.py` files:

```
Terminal> py.test -s
====================== test session starts =======================
...
collected 3 items

tests/test_bumpy.py .
Fitted source term, linear case: 8*t**2 + 15.6*t + 15.5
Fitted source term, quadratic case: 12*t + 12.9
testing solver
testing solver_linear_damping_wrapper

==================== 3 passed in 0.40 seconds ====================
```

Test a single file:

```
Terminal> py.test -s tests/test_bumpy.py
...
```

Modules

- Put functions in a file - that is a module
- Move main program to a function
- Use a test block for executable code (call to main function)

```
if __name__ == '__main__':
    <statements in the main program>
```

Example on a module file

```
import module1
from module2 import somefunc1, somefunc2

def myfunc1(...):
    ...

def myfunc2(...):
    ...

if __name__ == '__main__':
    <statements in the main program>
```

What gets imported?

Import everything from the previous module:

```
from mymod import *
```

This imports

- `module1`, `somefunc1`, `somefunc2` (global names in `mymod`)
- `myfunc1`, `myfunc2` (global functions in `mymod`)