# Study guide: Scientific software engineering with a simple ODE model as example

**Hans Petter Langtangen**[1,2]

[1]Center for Biomedical Computing, Simula Research Laboratory
[2]Department of Informatics, University of Oslo

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## Creating user interfaces

- Never edit the program to change input!
- Set input data on the command line or in a graphical user interface
- How is explained next

### Accessing command-line arguments

- All command-line arguments are available in `sys.argv`
- `sys.argv[0]` is the program
- `sys.argv[1:]` holds the command-line arguments
- Method 1: fixed sequence of parameters on the command line
- Method 2: `--option value` pairs on the command line (with default values)

```
Terminal> python myprog.py 1.5 2 0.5 0.8 0.4
Terminal> python myprog.py --I 1.5 --a 2 --dt 0.8 0.4
```

## Reading a sequence of command-line arguments

The program decay_plot.py needs this input:

- $I$
- $a$
- $T$
- an option to turn the plot on or off (`makeplot`)
- a list of $\Delta t$ values

Give these on the command line in correct sequence

```
Terminal> python decay_cml.py 1.5 2 0.5 0.8 0.4
```

## Implementation

```
import sys

def read_command_line():
    if len(sys.argv) < 6:
        print 'Usage: %s I a T on/off dt1 dt2 dt3 ...' % \
              sys.argv[0]; sys.exit(1)  # abort

    I = float(sys.argv[1])
    a = float(sys.argv[2])
    T = float(sys.argv[3])
    makeplot = sys.argv[4] in ('on', 'True')
    dt_values = [float(arg) for arg in sys.argv[5:]]

    return I, a, T, makeplot, dt_values
```

Note:

- `sys.argv[i]` is *always a string*
- Must explicitly convert to (e.g.) `float` for computations
- List comprehensions make lists: `[expression for e in somelist]`

Complete program: decay_cml.py.

## Working with an argument parser

Set option-value pairs on the command line if the default value is not suitable:

```
Terminal> python decay_argparse.py --I 1.5 --a 2 --dt 0.8 0.4
```

Code:

```python
def define_command_line_options():
    import argparse
    parser = argparse.ArgumentParser()
    parser.add_argument('--I', '--initial_condition', type=float,
                        default=1.0, help='initial condition,
                            u(0)',
                        metavar='I')
    parser.add_argument('--a', type=float,
                        default=1.0, help='coefficient in ODE',
                        metavar='a')
    parser.add_argument('--T', '--stop_time', type=float,
                        default=1.0, help='end time of
                            simulation',
                        metavar='T')
    parser.add_argument('--makeplot', action='store_true',
                        help='display plot or not')
    parser.add_argument('--dt', '--time_step_values', type=float,
                        default=[1.0], help='time step values',
                        metavar='dt', nargs='+',
                            dest='dt_values')
    return parser
```

(`metavar` is the symbol used in help output)

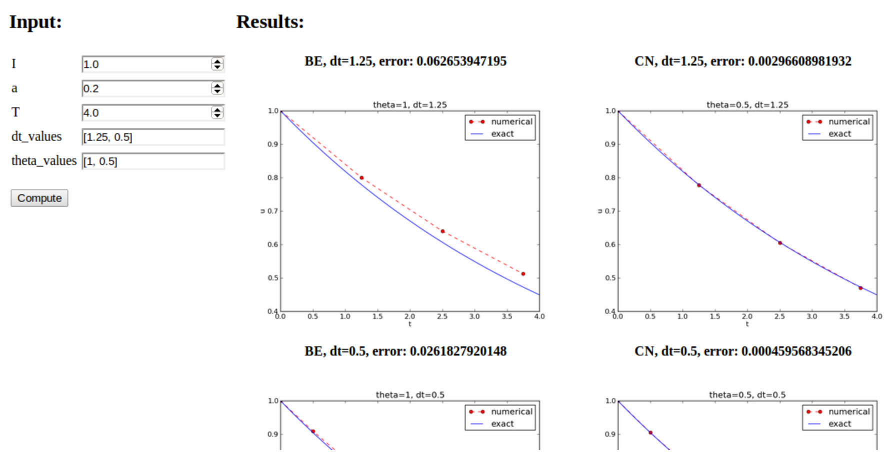
## Reading option-values pairs

`argparse.ArgumentParser` parses the command-line arguments:

```python
def read_command_line():
    parser = define_command_line_options()
    args = parser.parse_args()
    print 'I={}, a={}, T={}, makeplot={}, dt_values={}'.format(
        args.I, args.a, args.T, args.makeplot, args.dt_values)
    return args.I, args.a, args.T, args.makeplot, args.dt_values
```

Complete program: `decay_argparse.py`.

## A graphical user interface




Normally very much programming required - and much competence on graphical user interfaces.

Here: use a tool to automatically create it in a few minutes (!)

## The Parampool package

- Parampool is a package for handling a large pool of input parameters in simulation programs
- Parampool can automatically create a sophisticated web-based graphical user interface (GUI) to set parameters and view solutions

**Remark.** The forthcoming material aims at those with particular interest in equipping their programs with a GUI - others can safely skip it.

## Making a compute function

- Key concept: a *compute function* that takes all input data as arguments and returning HTML code for viewing the results (e.g., plots and numbers)
- What we have: `decay_plot.py`
- `main` function carries out simulations and plotting for a series of $\Delta t$ values
- Goal: steer and view these experiments from a web GUI
- What to do:
  - create a compute function
  - call `parampool` functionality

The compute function `main_GUI`:

```
def main_GUI(I=1.0, a=.2, T=4.0,
         dt_values=[1.25, 0.75, 0.5, 0.1],
         theta_values=[0, 0.5, 1]):
```

## The hard part of the compute function: the HTML code

- The results are to be displayed in a web page
- Only you know what to display in your problem
- Therefore, you need to specify the HTML code

Suppose `explore` solves the problem, makes a plot, computes the error *and* returns appropriate HTML code with the plot. Embed error and plots in a table:

```
def main_GUI(I=1.0, a=.2, T=4.0,
         dt_values=[1.25, 0.75, 0.5, 0.1],
         theta_values=[0, 0.5, 1]):
    # Build HTML code for web page. Arrange plots in columns
    # corresponding to the theta values, with dt down the rows
    theta2name = {0: 'FE', 1: 'BE', 0.5: 'CN'}
    html_text = '<table>\n'
    for dt in dt_values:
        html_text += '<tr>\n'
        for theta in theta_values:
            E, html = explore(I, a, T, dt, theta, makeplot=True)
            html_text += """
<td>
<center><b>%s, dt=%g, error: %s</b></center><br>
%s
</td>
""" % (theta2name[theta], dt, E, html)
        html_text += '</tr>\n'
    html_text += '</table>\n'
    return html_text
```

## How to embed a PNG plot in HTML code

In `explore`:

```
import matplotlib.pyplot as plt
...
# plot
plt.plot(t, u, r-')
plt.xlabel('t')
plt.ylabel('u')
...
from parampool.utils import save_png_to_str
html_text = save_png_to_str(plt, plotwidth=400)
```

If you know HTML, you can return more sophisticated layout etc.

## Generating the user interface

Make a file `decay_GUI_generate.py`:

```
from parampool.generator.flask import generate
from decay_GUI import main
generate(main,
         output_controller='decay_GUI_controller.py',
         output_template='decay_GUI_view.py',
         output_model='decay_GUI_model.py')
```

Running `decay_GUI_generate.py` results in

1. `decay_GUI_model.py` defines HTML widgets to be used to set input data in the web interface,
2. `templates/decay_GUI_views.py` defines the layout of the web page,
3. `decay_GUI_controller.py` runs the web application.

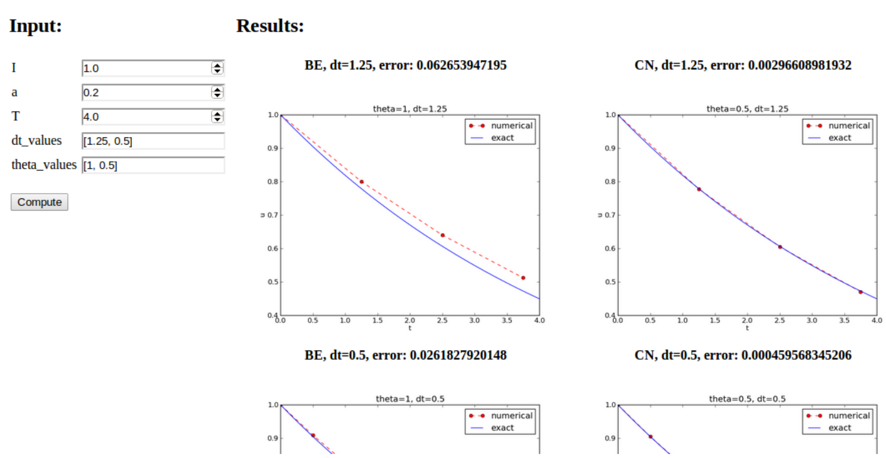
Good news: we only need to run `decay_GUI_controller.py` and there is no need to look into any of these files!

## Running the web application

Start the GUI

```
Terminal> python decay_GUI_controller.py
```

Open a web browser at `127.0.0.1:5000`




## More advanced use

- The compute function can have arguments of type float, int, string, list, dict, numpy array, filename (file upload)

- Alternative: specify a hierarchy of input parameters with name, default value, data type, widget type, unit (m, kg, s), validity check
- The generated web GUI can have user accounts with login and storage of results in a database

# Computing convergence rates

Frequent assumption on the relation between the numerical error $E$ and some discretization parameter $\Delta t$:

$$E = C\Delta t^r, \tag{1}$$

- Unknown: $C$ and $r$.
- Goal: estimate $r$ (and $C$) from numerical experiments

## Estimating the convergence rate $r$

Perform numerical experiments: $(\Delta t_i, E_i)$, $i = 0, \ldots, m-1$. Two methods for finding $r$ (and $C$):

1. Take the logarithm of (**??**), $\ln E = r \ln \Delta t + \ln C$, and fit a straight line to the data points $(\Delta t_i, E_i)$, $i = 0, \ldots, m-1$.
2. Consider two consecutive experiments, $(\Delta t_i, E_i)$ and $(\Delta t_{i-1}, E_{i-1})$. Dividing the equation $E_{i-1} = C\Delta t_{i-1}^r$ by $E_i = C\Delta t_i^r$ and solving for $r$ yields

$$r_{i-1} = \frac{\ln(E_{i-1}/E_i)}{\ln(\Delta t_{i-1}/\Delta t_i)} \tag{2}$$

for $i = 1, = \ldots, m-1$.

Method 2 is best.

## Implementation

Compute $r_0, r_1, \ldots, r_{m-2}$:

```
from math import log

def main():
    I, a, T, makeplot, dt_values = read_command_line()
    r = {}  # estimated convergence rates
    for theta in 0, 0.5, 1:
        E_values = []
        for dt in dt_values:
            E = explore(I, a, T, dt, theta, makeplot=False)
            E_values.append(E)
```

```
        # Compute convergence rates
        m = len(dt_values)
        r[theta] = [log(E_values[i-1]/E_values[i])/
                    log(dt_values[i-1]/dt_values[i])
                    for i in range(1, m, 1)]

    for theta in r:
        print '\nPairwise convergence rates for theta=%g:' %
            theta
        print ' '.join(['%.2f' % r_ for r_ in r[theta]])
    return r
```

Complete program: `decay_convrate.py`.

## Execution

```
Terminal> python decay_convrate.py --dt 0.5 0.25 0.1 0.05 0.025 0.01
...
Pairwise convergence rates for theta=0:
1.33 1.15 1.07 1.03 1.02

Pairwise convergence rates for theta=0.5:
2.14 2.07 2.03 2.01 2.01

Pairwise convergence rates for theta=1:
0.98 0.99 0.99 1.00 1.00
```

**Strong verification method.** Verify that $r$ has the expected value!

## Debugging via convergence rates

Potential bug: missing `a` in the denominator,

```
u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt)*u[n]
```

Running `decay_convrate.py` gives same rates.

Why? The value of $a$... ($a = 1$)

0 and 1 are *bad values* in tests!

Better:

```
Terminal> python decay_convrate.py --a 2.1 --I 0.1  \
          --dt 0.5 0.25 0.1 0.05 0.025 0.01
...
Pairwise convergence rates for theta=0:
1.49 1.18 1.07 1.04 1.02

Pairwise convergence rates for theta=0.5:
-1.42 -0.22 -0.07 -0.03 -0.01

Pairwise convergence rates for theta=1:
0.21 0.12 0.06 0.03 0.01
```

Forward Euler works...because $\theta = 0$ hides the bug.

This bug gives $r \approx 0$:

```
u[n+1] = ((1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
```

## Software engineering

Goal: make more professional numerical software.

Topics:

- How to make modules (reusable libraries)
- Testing frameworks (doctest, nose, unittest)
- Implementation with classes

### Making a module

- Previous programs: much repetitive code (esp. `solver`)
- DRY (Don't Repeat Yourself) principle: no copies of code
- A change needs to be done in one *and only one* place
- Module = just a file with functions (reused through `import`)
- Let's make a module by putting these functions in a file:
  - `solver`
  - `verify_three_steps`
  - `verify_discrete_solution`
  - `explore`
  - `define_command_line_options`
  - `read_command_line`
  - `main` (with convergence rates)
  - `verify_convergence_rate`

Module name: `decay_mod`, filename: `decay_mod.py`.

### Sketch of the module

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

def solver(I, a, T, dt, theta):
    ...

def verify_three_steps():
    ...

def verify_exact_discrete_solution():
    ...
```

```python
def u_exact(t, I, a):
    ...

def explore(I, a, T, dt, theta=0.5, makeplot=True):
    ...

def define_command_line_options():
    ...

def read_command_line(use_argparse=True):
    ...

def main():
    ...
```

That is! It's a module `decay_mod` in file `decay_mod.py`.

Usage in some other program:

```python
from decay_mod import solver
u, t = solver(I=1.0, a=3.0, T=3, dt=0.01, theta=0.5)
```

## Test block

At the end of a module it is common to include a *test block*:

```python
if __name__ == '__main__':
    main()
```

Note:

- If `decay_mod` is imported, `__name__` is `decay_mod`.
- If `decay_mod.py` is run, `__name__` is `__main__`.
- Use test block for testing, demo, user interface, ...

## Extended test block

```python
if __name__ == '__main__':
    if 'verify' in sys.argv:
        if verify_three_steps() and verify_discrete_solution():
            pass # ok
        else:
            print 'Bug in the implementation!'
    elif 'verify_rates' in sys.argv:
        sys.argv.remove('verify_rates')
        if not '--dt' in sys.argv:
            print 'Must assign several dt values'
            sys.exit(1)  # abort
        if verify_convergence_rate():
            pass
        else:
            print 'Bug in the implementation!'
```

```
    else:
        # Perform simulations
        main()
```

### Prefixing imported functions by the module name

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

This imports a large number of names (`sin`, `exp`, `linspace`, `plot`, ...).
Confusion: is a function from `numpy`? Or `matplotlib.pyplot`?
Alternative (recommended) import:

```
import numpy
import matplotlib.pyplot
```

Now we need to prefix functions with module name:

```
t = numpy.linspace(0, T, Nt+1)
u_e = I*numpy.exp(-a*t)
matplotlib.pyplot.plot(t, u_e)
```

Common standard:

```
import numpy as np
import matplotlib.pyplot as plt

t = np.linspace(0, T, Nt+1)
u_e = I*np.exp(-a*t)
plt.plot(t, u_e)
```

### Downside of module prefix notation

A math line like $e^{-at}\sin(2\pi t)$ gets cluttered with module names,

```
numpy.exp(-a*t)*numpy.sin(2(numpy.pi*t)
# or
np.exp(-a*t)*np.sin(2*np.pi*t)
```

Solution (much used in this course): do two imports

```
import numpy as np
from numpy import exp, sin, pi
...
t = np.linspace(0, T, Nt+1)
u_e = exp(-a*t)*sin(2*pi*t)
```

### Doctests

Doc strings can be equipped with interactive Python sessions for demonstrating usage and *automatic testing* of functions.

```python
def solver(I, a, T, dt, theta):
    """
    Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt.


    >>> u, t = solver(I=0.8, a=1.2, T=4, dt=0.5, theta=0.5)
    >>> for t_n, u_n in zip(t, u):
    ...     print 't=%.1f, u=%.14f' % (t_n, u_n)
    t=0.0, u=0.80000000000000
    t=0.5, u=0.43076923076923
    t=1.0, u=0.23195266272189
    t=1.5, u=0.12489758761948
    t=2.0, u=0.06725254717972
    t=2.5, u=0.03621291001985
    t=3.0, u=0.01949925924146
    t=3.5, u=0.01049960113002
    t=4.0, u=0.00565363137770
    """
    ...
```

## Running doctests

Automatic check that the code reproduces the doctest output:

```
Terminal> python -m doctest decay_mod_doctest.py
```

Report in case of failure:

```
Terminal> python -m doctest decay_mod_doctest.py
********************************************************
File "decay_mod_doctest.py", line 12, in decay_mod_doctest....
Failed example:
    for t_n, u_n in zip(t, u):
        print 't=%.1f, u=%.14f' % (t_n, u_n)
Expected:
    t=0.0, u=0.80000000000000
    t=0.5, u=0.43076923076923
    t=1.0, u=0.23195266272189
    t=1.5, u=0.12489758761948
    t=2.0, u=0.06725254717972
Got:
    t=0.0, u=0.80000000000000
    t=0.5, u=0.43076923076923
    t=1.0, u=0.23195266272189
    t=1.5, u=0.12489758761948
    t=2.0, u=0.06725254718756
********************************************************
1 items had failures:
   1 of   2 in decay_mod_doctest.solver
***Test Failed*** 1 failures.
```

**Floats are difficult to compare.** Limit the number of digits in the output in doctests! Otherwise, round-off errors on a different machine may ruin the test.

Complete program: decay_mod_doctest.py.

## Unit testing with nose

- Nose is a very user-friendly testing framework
- Based on *unit testing*
- Identify (small) units of code and test each unit
- Nose automates running all tests
- Good habit: run all tests after (small) edits of a code
- Even better habit: write tests *before* the code (!)
- Remark: unit testing in scientific computing is not yet well established

## Basic use of nose

1. Implement tests in *test functions* with names starting with `test_`.
2. Test functions cannot have arguments.
3. Test functions perform assertions on computed results using `assert` functions from the `nose.tools` module.
4. Test functions can be in the source code files or be collected in separate files `test*.py`.

## Example on a nose test in the source code

Very simple module `mymod` (in file `mymod.py`):

```
def double(n):
    return 2*n
```

Write test function in `mymod.py`:

```
def double(n):
    return 2*n

import nose.tools as nt

def test_double():
    result = double(4)
    nt.assert_equal(result, 8)
```

Running

```
Terminal> nosetests -s mymod
```

makes the `nose` tool run all `test_*()` functions in `mymod.py`.

## Example on a nose test in a separate file

Write the test in a separate file, say `test_mymod.py`:

```
import nose.tools as nt
import mymod

def test_double():
    result = mymod.double(4)
    nt.assert_equal(result, 8)
```

Running

```
Terminal> nosetests -s
```

makes the `nose` tool run all `test_*()` functions in all files `test*.py` in the current directory and in all subdirectories (recursevely) with names `tests` or `*_tests`.

**Tip.** Start with test functions in the source code file. When the file contains many tests, or when you have many source code files, move tests to separate files.

## The habit of writing nose tests

- Put `test_*()` functions in the module
- When you get many `test_*()` functions, collect them in `tests/test*.py`

## Purpose of a test function: raise AssertionError if failure

Alternative ways of raising AssertionError if `result` is not 8:

```
import nose.tools as nt

def test_double():
    result = ...

    nt.assert_equal(result, 8)     # alternative 1

    assert result == 8             # alternative 2

    if result != 8:                # alternative 3
        raise AssertionError()
```

## Advantages of nose

- Easier to use than other test frameworks
- Tests are written and collected in a *compact* and structured way

- Large collections of tests, scattered throughout a directory tree can be executed with one command (`nosetests -s`)
- Nose is a much-adopted standard

## Demonstrating nose (ideas)

Aim: test function `solver` for $u' = -au$, $u(0) = I$.

We design three unit tests:

1. A comparison between the computed $u^n$ values and the exact discrete solution
2. A comparison between the computed $u^n$ values and precomputed verified reference values
3. A comparison between observed and expected convergence rates

These tests follow very closely the previous `verify*` functions.

## Demonstrating nose (code)

```
import nose.tools as nt
import decay_mod_unittest as decay_mod
import numpy as np

def exact_discrete_solution(n, I, a, theta, dt):
    """Return exact discrete solution of the theta scheme."""
    dt = float(dt)  # avoid integer division
    factor = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)
    return I*factor**n

def test_exact_discrete_solution():
    """
    Compare result from solver against
    formula for the discrete solution.
    """
    theta = 0.8; a = 2; I = 0.1; dt = 0.8
    N = int(8/dt)  # no of steps
    u, t = decay_mod.solver(I=I, a=a, T=N*dt, dt=dt, theta=theta)
    u_de = np.array([exact_discrete_solution(n, I, a, theta, dt)
                     for n in range(N+1)])
    diff = np.abs(u_de - u).max()
    nt.assert_almost_equal(diff, 0, delta=1E-14)
```

## Floats as test results require careful comparison

- Round-off errors make exact comparison of floats unreliable
- `nt.assert_almost_equal`: compare two floats to some digits or precision

```
def test_solver():
    """
    Compare result from solver against
    precomputed arrays for theta=0, 0.5, 1.
    """
    I=0.8; a=1.2; T=4; dt=0.5  # fixed parameters
    precomputed = {
        't': np.array([ 0. ,  0.5,  1. ,  1.5,  2. ,  2.5,
                        3. ,  3.5,  4. ]),
        0.5: np.array(
            [ 0.8       ,  0.43076923,  0.23195266, 0.12489759,
              0.06725255,  0.03621291,  0.01949926, 0.0104996 ,
              0.00565363]),
        0: ...,
        1: ...
        }
    for theta in 0, 0.5, 1:
        u, t = decay_mod.solver(I, a, T, dt, theta=theta)
        diff = np.abs(u - precomputed[theta]).max()
        # Precomputed numbers are known to 8 decimal places
        nt.assert_almost_equal(diff, 0, places=8,
                               msg='theta=%s' % theta)
```

## Test of wrong use

- Find input data that may cause trouble and test such cases
- Here: the formula for $u^{n+1}$ may involve integer division

Example:

```
theta = 1; a = 1; I = 1; dt = 2
```

may lead to integer division:

```
(1 - (1-theta)*a*dt)  # becomes 1
(1 + theta*dt*a)      # becomes 2
(1 - (1-theta)*a*dt)/(1 + theta*dt*a)  # becomes 0 (!)
```

Test that `solver` does not suffer from such integer division:

```
def test_potential_integer_division():
    """Choose variables that can trigger integer division."""
    theta = 1; a = 1; I = 1; dt = 2
    N = 4
    u, t = decay_mod.solver(I=I, a=a, T=N*dt, dt=dt, theta=theta)
    u_de = np.array([exact_discrete_solution(n, I, a, theta, dt)
                     for n in range(N+1)])
    diff = np.abs(u_de - u).max()
    nt.assert_almost_equal(diff, 0, delta=1E-14)
```

## Test of convergence rates

Convergence rate tests are very common for differential equation solvers.

```
def test_convergence_rates():
    """Compare empirical convergence rates to exact ones."""
    # Set command-line arguments directly in sys.argv
    import sys
    sys.argv[1:] = '--I 0.8 --a 2.1 --T 5 '\
                   '--dt 0.4 0.2 0.1 0.05 0.025'.split()
    r = decay_mod.main()
    for theta in r:
        nt.assert_true(r[theta])  # check for non-empty list

    expected_rates = {0: 1, 1: 1, 0.5: 2}
    for theta in r:
        r_final = r[theta][-1]
        # Compare to 1 decimal place
        nt.assert_almost_equal(expected_rates[theta], r_final,
                               places=1, msg='theta=%s' % theta)
```

Complete program: `test_decay_nose.py`.

## Classical unit testing with unittest

- `unittest` is a Python module mimicing the classical JUnit class-based unit testing framework from Java
- This is how unit testing is normally done
- Requires knowledge of object-oriented programming

**Remark.** You will probably not use it, but you're not educated unless you know what unit testing with classes is.

## Basic use of unittest

Write file `test_mymod.py`:

```
import unittest
import mymod

class TestMyCode(unittest.TestCase):
    def test_double(self):
        result = mymod.double(4)
        self.assertEqual(result, 8)

if __name__ == '__main__':
    unittest.main()
```

## Demonstration of unittest

```
import unittest
import decay_mod_unittest as decay
import numpy as np
```

```python
def exact_discrete_solution(n, I, a, theta, dt):
    factor = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)
    return I*factor**n

class TestDecay(unittest.TestCase):

    def test_exact_discrete_solution(self):
        ...
        diff = np.abs(u_de - u).max()
        self.assertAlmostEqual(diff, 0, delta=1E-14)

    def test_solver(self):
        ...
        for theta in 0, 0.5, 1:
            ...
            self.assertAlmostEqual(diff, 0, places=8,
                                   msg='theta=%s' % theta)

    def test_potential_integer_division():
        ...
        self.assertAlmostEqual(diff, 0, delta=1E-14)

    def test_convergence_rates(self):
        ...
        for theta in r:
            ...
            self.assertAlmostEqual(...)

if __name__ == '__main__':
    unittest.main()
```

Complete program: `test_decay_unittest.py`.

# Implementing simple problem and solver classes

- So far: programs are built of Python functions
- New focus: alternative implementations using classes
- Class-based implementations are very popular, especially in business/adm applications
- Class-based implementations scales better to large and complex scientific applications

## What to learn

Tasks:

- Explain basic use of classes to build a differential equation solver

* Introduce concepts that make such programs easily scale to more complex applications
* Demonstrate the advantage of using classes

Ideas:

* Classes for Problem, Solver, and Visualizer
* Problem: all the physics information about the problem
* Solver: all the numerics information + numerical computations
* Visualizer: plot the solution and other quantities

## The problem class

* Model problem: $u' = -au$, $u(0) = I$, for $t \in (0, T]$.
* Class `Problem` stores the physical parameters $a$, $I$, $T$
* May also offer other data, e.g., $u_{\mathrm{e}}(t) = Ie^{-at}$

Implementation:

```
from numpy import exp

class Problem:
    def __init__(self, I=1, a=1, T=10):
        self.T, self.I, self.a = I, float(a), T

    def u_exact(self, t):
        I, a = self.I, self.a     # extract local variables
        return I*exp(-a*t)
```

Basic usage:

```
problem = Problem(T=5)
problem.T = 8
problem.dt = 1.5
```

## Improved problem class

More flexible input from the command line:

```
class Problem:
    def __init__(self, I=1, a=1, T=10):
        self.T, self.I, self.a = I, float(a), T

    def define_command_line_options(self, parser=None):
        if parser is None:
            import argparse
            parser = argparse.ArgumentParser()
```

```
        parser.add_argument(
            '--I', '--initial_condition', type=float,
            default=self.I, help='initial condition, u(0)',
            metavar='I')
        parser.add_argument(
            '--a', type=float, default=self.a,
            help='coefficient in ODE', metavar='a')
        parser.add_argument(
            '--T', '--stop_time', type=float, default=self.T,
            help='end time of simulation', metavar='T')
        return parser

    def init_from_command_line(self, args):
        self.I, self.a, self.T = args.I, args.a, args.T

    def exact_solution(self, t):
        I, a = self.I, self.a
        return I*exp(-a*t)
```

- Can utilize user's `ArgumentParser`, or make one
- `None` is used to indicate a non-initialized variable

## The solver class

- Store numerical data $\Delta t$, $\theta$
- Compute solution and quantities derived from the solution

Implementation:

```
class Solver:
    def __init__(self, problem, dt=0.1, theta=0.5):
        self.problem = problem
        self.dt, self.theta = float(dt), theta

    def define_command_line_options(self, parser):
        parser.add_argument(
            '--dt', '--time_step_value', type=float,
            default=0.5, help='time step value', metavar='dt')
        parser.add_argument(
            '--theta', type=float, default=0.5,
            help='time discretization parameter', metavar='dt')
        return parser

    def init_from_command_line(self, args):
        self.dt, self.theta = args.dt, args.theta

    def solve(self):
        from decay_mod import solver
        self.u, self.t = solver(
            self.problem.I, self.problem.a, self.problem.T,
            self.dt, self.theta)
```

Note: reuse of the numerical algorithm from the `decay_mod` module (i.e., the class is a wrapper of the procedural implementation).

## The visualizer class

```
class Visualizer:
    def __init__(self, problem, solver):
        self.problem, self.solver = problem, solver

    def plot(self, include_exact=True, plt=None):
        """
        Add solver.u curve to the plotting object plt,
        and include the exact solution if include_exact is True.
        This plot function can be called several times (if
        the solver object has computed new solutions).
        """
        if plt is None:
            import scitools.std  as plt # can use matplotlib as
                well

        plt.plot(self.solver.t, self.solver.u, '--o')
        plt.hold('on')
        theta2name = {0: 'FE', 1: 'BE', 0.5: 'CN'}
        name = theta2name.get(self.solver.theta, '')
        legends = ['numerical %s' % name]
        if include_exact:
            t_e = linspace(0, self.problem.T, 1001)
            u_e = self.problem.exact_solution(t_e)
            plt.plot(t_e, u_e, 'b-')
            legends.append('exact')
        plt.legend(legends)
        plt.xlabel('t')
        plt.ylabel('u')
        plt.title('theta=%g, dt=%g' %
                  (self.solver.theta, self.solver.dt))
        plt.savefig('%s_%g.png' % (name, self.solver.dt))
        return plt
```

Remark: The `plt` object in `plot` adds a new curve to a plot, which enables comparing different solutions from different runs of `Solver.solve`

## Combing the classes

Let `Problem`, `Solver`, and `Visualizer` play together:

```
def main():
    problem = Problem()
    solver = Solver(problem)
    viz = Visualizer(problem, solver)

    # Read input from the command line
    parser = problem.define_command_line_options()
    parser = solver. define_command_line_options(parser)
    args = parser.parse_args()
    problem.init_from_command_line(args)
    solver. init_from_command_line(args)

    # Solve and plot
    solver.solve()
    import matplotlib.pyplot as plt
```

```
    #import scitools.std as plt
    plt = viz.plot(plt=plt)
    E = solver.error()
    if E is not None:
        print 'Error: %.4E' % E
    plt.show()
```

Complete program: decay_class.py.

# Implementing more advanced problem and solver classes

- The previous `Problem` and `Solver` classes soon contain much repetitive code when the number of parameters increases
- Much of such code can be parameterized and be made more compact
- Idea: collect all parameters in a dictionary `self.prms`, with two associated dictionaries `self.types` and `self.help` for holding associated object types and help strings
- Collect common code in class `Parameters`
- Let `Problem`, `Solver`, and maybe `Visualizer` be subclasses of class `Parameters`, basically defining `self.prms`, `self.types`, `self.help`

## A generic class for parameters

```
class Parameters:
    def set(self, **parameters):
        for name in parameters:
            self.prms[name] = parameters[name]

    def get(self, name):
        return self.prms[name]

    def define_command_line_options(self, parser=None):
        if parser is None:
            import argparse
            parser = argparse.ArgumentParser()

        for name in self.prms:
            tp = self.types[name] if name in self.types else str
            help = self.help[name] if name in self.help else None
            parser.add_argument(
                '--' + name, default=self.get(name),
                    metavar=name,
                type=tp, help=help)

        return parser
```

```
    def init_from_command_line(self, args):
        for name in self.prms:
            self.prms[name] = getattr(args, name)
```

Slightly more advanced version in `class_decay_verf1.py`.

## The problem class

```
class Problem(Parameters):
    """
    Physical parameters for the problem u'=-a*u, u(0)=I,
    with t in [0,T].
    """
    def __init__(self):
        self.prms = dict(I=1, a=1, T=10)
        self.types = dict(I=float, a=float, T=float)
        self.help = dict(I='initial condition, u(0)',
                         a='coefficient in ODE',
                         T='end time of simulation')

    def exact_solution(self, t):
        I, a = self.get('I'), self.get('a')
        return I*np.exp(-a*t)
```

## The solver class

```
class Solver(Parameters):
    def __init__(self, problem):
        self.problem = problem
        self.prms = dict(dt=0.5, theta=0.5)
        self.types = dict(dt=float, theta=float)
        self.help = dict(dt='time step value',
                         theta='time discretization parameter')

    def solve(self):
        from decay_mod import solver
        self.u, self.t = solver(
            self.problem.get('I'),
            self.problem.get('a'),
            self.problem.get('T'),
            self.get('dt'),
            self.get('theta'))

    def error(self):
        try:
            u_e = self.problem.exact_solution(self.t)
            e = u_e - self.u
            E = np.sqrt(self.get('dt')*np.sum(e**2))
        except AttributeError:
            E = None
        return E
```

### The visualizer class

- No parameters needed (for this simple problem), no need to inherit class `Parameters`
- Same code as previously shown class `Visualizer`
- Same code as previously shown for combining `Problem`, `Solver`, and `Visualizer`

## Performing scientific experiments

Goal: explore the behavior of a numerical method for a differential equation and show how scientific experiments can be set up and reported.

Tasks:

- Write scripts to automate experiments
- Generate scientific reports from scripts

Tools to learn:

- `os.system` for running other programs
- `subprocess` for running other programs and extracting the output
- List comprehensions
- Formats for scientific reports: HTML w/MathJax, LaTeX, Sphinx, DocOnce

### Model problem and numerical solution method

Problem:

$$u'(t) = -au(t), \quad u(0) = I,\ 0 < t \leq T, \tag{3}$$

Solution method ($\theta$-rule):

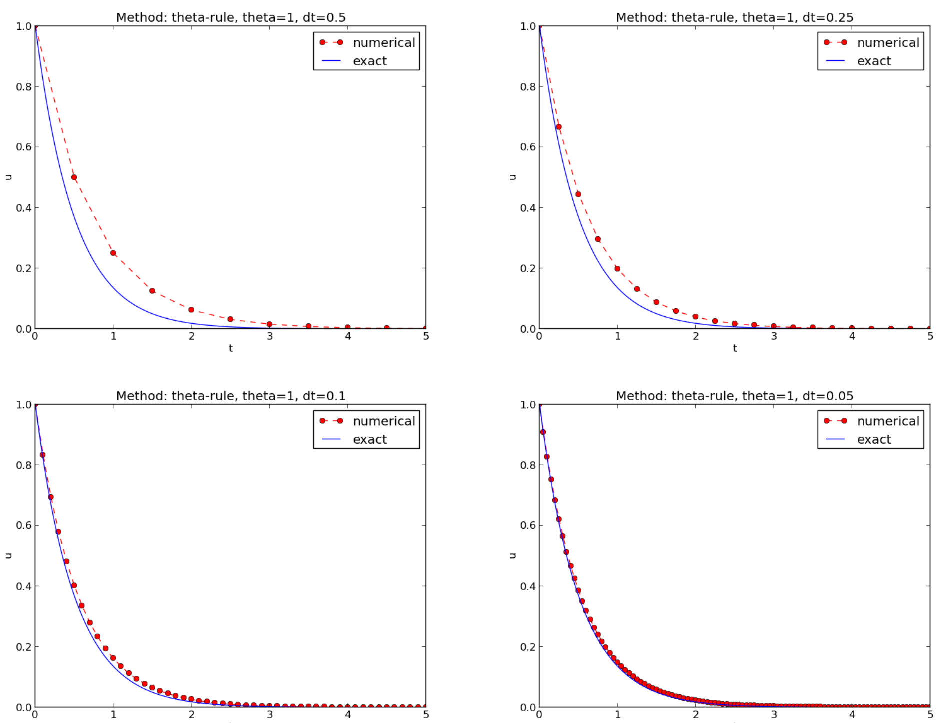
$$u^{n+1} = \frac{1 - (1-\theta)a\Delta t}{1 + \theta a\Delta t}u^n, \quad u^0 = I\,.$$

## Plan for the experiments

- Plot $u^n$ against $u_e = Ie^{-at}$ for various choices of the parameters $I$, $a$, $\Delta t$, and $\theta$
- How does the discrete solution compare with the exact solution when $\Delta t$ is varied and $\theta = 0, 0.5, 1$?
- Use the `decay_mod.py` module (little modification of the plotting, see `experiments/decay_mod.py`)
- Make separate program for running (automating) the experiments (*script*)

  1. `python decay_mod.py --I 1 --a 2 --makeplot --T 5 --dt 0.5 0.25 0.1 0.05`
  2. Combine generated figures `FE_*.png`, `BE_*.png`, and `CN_*.png` to new figures with multiple plots
  3. Run script as `python decay_exper0.py 0.5 0.25 0.1 0.05` ($\Delta t$ values on the command line)

## Typical plot summarizing the results



### Script code

Typical *script* (small administering program) for running the experiments:

```
import os, sys

def run_experiments(I=1, a=2, T=5):
    # The command line must contain dt values
    if len(sys.argv) > 1:
        dt_values = [float(arg) for arg in sys.argv[1:]]
    else:
        print 'Usage: %s dt1 dt2 dt3 ...' %  sys.argv[0]
        sys.exit(1)  # abort

    # Run module file as a stand-alone application
    cmd = 'python decay_mod.py --I %g --a %g --makeplot --T %g'
        % \
          (I, a, T)
    dt_values_str = ' '.join([str(v) for v in dt_values])
    cmd += ' --dt %s' % dt_values_str
    print cmd
    failure = os.system(cmd)
    if failure:
        print 'Command failed:', cmd; sys.exit(1)

    # Combine images into rows with 2 plots in each row
    image_commands = []
    for method in 'BE', 'CN', 'FE':
        pdf_files = ' '.join(['%s_%g.pdf' % (method, dt)
                              for dt in dt_values])
        png_files = ' '.join(['%s_%g.png' % (method, dt)
                              for dt in dt_values])
        image_commands.append(
            'montage -background white -geometry 100%' +
            ' -tile 2x %s %s.png' % (png_files, method))
        image_commands.append(
            'convert -trim %s.png %s.png' % (method, method))
        image_commands.append(
            'convert %s.png -transparent white %s.png' %
            (method, method))
        image_commands.append(
            'pdftk %s output tmp.pdf' % pdf_files)
        num_rows = int(round(len(dt_values)/2.0))
        image_commands.append(
            'pdfnup --nup 2x%d tmp.pdf' % num_rows)
        image_commands.append(
            'pdfcrop tmp-nup.pdf %s.pdf' % method)

    for cmd in image_commands:
        print cmd
        failure = os.system(cmd)
        if failure:
            print 'Command failed:', cmd; sys.exit(1)

    # Remove the files generated above and by decay_mod.py
    from glob import glob
    filenames = glob('*_*.png') + glob('*_*.pdf') + \
                glob('*_*.eps') + glob('tmp*.pdf')
```

```
    for filename in filenames:
        os.remove(filename)

if __name__ == '__main__':
    run_experiments()
```

Complete program: experiments/decay_exper0.py.

### Comments to the code

Many useful constructs in the previous script:

- [float(arg) for arg in sys.argv[1:]] builds a list of real numbers from all the command-line arguments
- failure = os.system(cmd) runs an operating system command (e.g., another program)
- sys.exit(1) aborts the program
- ['%s_%s.png' % (method, dt) for dt in dt_values] builds a list of filenames from a list of numbers (dt_values)
- All montage commands for creating composite figures are stored in a list and thereafter executed in a loop
- glob.glob('*_*.png') returns a list of the names of all files in the current folder where the filename matches the *Unix wildcard notation* *_*.png (meaning "any text, underscore, any text, and then '.png'")
- os.remove(filename) removes the file with name filename

### Interpreting output from other programs

In decay_exper0.py we run a program (os.system) and want to grab the output, e.g.,

```
Terminal> python decay_plot_mpl.py
0.0   0.40:    2.105E-01
0.0   0.04:    1.449E-02
0.5   0.40:    3.362E-02
0.5   0.04:    1.887E-04
1.0   0.40:    1.030E-01
1.0   0.04:    1.382E-02
```

Tasks:

- read the output from the decay_mod.py program
- interpret this output and store the $E$ values in arrays for each $\theta$ value
- plot $E$ versus $\Delta t$, for each $\theta$, in a log-log plot

## Code for grabbing output from another program

Use the `subprocess` module to grab output:

```
    from subprocess import Popen, PIPE, STDOUT
    p = Popen(cmd, shell=True, stdout=PIPE, stderr=STDOUT)
    output, dummy = p.communicate()
    failure = p.returncode
    if failure:
        print 'Command failed:', cmd; sys.exit(1)
```

## Code for interpreting the grabbed output

- Run through the `output` string, line by line
- If the current line prints $\theta$, $\Delta t$, and $E$, split the line into these three pieces and store the data
- Store data in a dictionary `errors` with keys `dt` and the three $\theta$ values

```
errors = {'dt': dt_values, 1: [], 0: [], 0.5: []}
for line in output.splitlines():
    words = line.split()
    if words[0] in ('0.0', '0.5', '1.0'):  # line with E?
        # typical line: 0.0   1.25:    7.463E+00
        theta = float(words[0])
        E = float(words[2])
        errors[theta].append(E)
```

Next: plot $E$ versus $\Delta t$ for $\theta = 0, 0.5, 1$
Complete program: `experiments/decay_exper1.py`. Fine recipe for

- how to run other programs
- how to extract and interpret output from other programs
- how to automate many manual steps in creating simulations and figures

## Making a report

- Scientific investigations are best documented in a report!
- A sample report
- How can we write such a report?
- First problem: what format should I write in?
- Plain HTML, generated by `decay_exper1_html.py`
- HTML with MathJax, generated by `decay_exper1_mathjax.py`
- LaTeX PDF, based on LaTeX source

- Sphinx HTML, based on reStructuredText
- Markdown, MediaWiki, ...
- DocOnce can generate LaTeX, HTML w/MathJax, Sphinx, Markdown, MediaWiki, ... (DocOnce source for the examples above, and Python program for generating the DocOnce source)
- Examples on different report formats

## Publishing a complete project

- Make folder (directory) tree
- Keep track of all files via a *version control system* (Mercurial, Git, ...)
- Publish as private or public repository
- Utilize Bitbucket, Googlecode, GitHub, or similar
- See the intro to such tools

# Index