INF5620 Lectures: Exponential Decay ODEs

Hans Petter Langtangen[1,2]

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

Aug 11, 2013

Contents

1 INF5620 in a nutshell

- Numerical methods for partial differential equations (PDEs)
- How to we solve a PDE in practice and produce numbers?
- How to we trust the answer?

After the course.
You see a PDE and can't wait to program a method and visualize a solution! Somebody asks if the solution is right and you can give convincing answer.

1.1 The new official six-point course description

After having completed INF5620 you

- can derive methods and implement them to solve frequently arising partial differential equations (PDEs) from physics and mechanics.
- have a good understanding of finite difference and finite element methods and how they are applied in linear and nonlinear PDE problems.
- can identify numerical artifacts and perform mathematical analysis to understand and cure non-physical effects.
- can apply sophisticated programming techniques in Python, combined with Cython, C, C++, and Fortran code, to create modern, flexible simulation programs.
- can construct verification tests and automate them.
- have experience with project hosting sites (Bitbucket, GitHub), version control systems (Git), report writing (LaTeX), and Python scripting for performing reproducible computational science.

1.2 More specific description of the contents; part 1

- Finite difference methods
  - ODEs
  - the wave equation $u_{tt} = u_{xx}$ in 1D, 2D, 3D
  - the diffusion equation $u_t = u_{xx}$ in 1D, 2D, 3D
  - write your own software from scratch

    - understand how the methods work and why they fail

- Finite element methods for
    - stationary diffusion equations $u_{xx} = f$ in 1D
    - time-dependent diffusion and wave equations in 1D
    - PDEs in 2D and 3D by use of the FEniCS software
    - perform hand-calculations, write your own software (1D)
    - understand how the methods work and why they fail

1.3 More specific description of the contents; part 2

- Nonlinear PDEs
    - Newton and Picard iteration methods, finite differences and elements
- More advanced PDEs for fluid flow and elasticity
- Parallel computing

1.4 The exam

- Oral exam
- 6 problems (topics) are announced two weeks before the exam
- Work out a 20 min presentations (talks) for each problem
- At the exam: throw a die to pick your problem to be presented
- Aids: plots, computer programs
- Why? Very effective way of learning
- Sure? Excellent results over 15 years
- When? Late december

1.5 Assumed/ideal background

- INF1100: Python programming, solution of ODEs
- Some experience with finite difference methods
- Some analytical and numerical knowledge of PDEs
- Much experience with calculus and linear algebra
- Much experience with programming of mathematical problems
- Experience with mathematical modeling with PDEs (from physics, mechanics, geophysics, or ...)

1.6 Start-up example for the course

What if you don't have this ideal background?

- Students come to this course with very different backgrounds
- First task: summarize assumed background knowledge by going through a simple example
- Also:
  - Add some fundamental material on software implementation and software testing
  - Add material on analyzing numerical methods to understand why they can fail
  - Apply the numerical methods to real-world problems

1.7 Start-up example

ODE problem.

$$u' = -au, \quad u(0) = I,\ t \in (0, T],$$

where $a > 0$ is a constant.

Everything we do is motivated by what we need as building blocks for solving PDEs.

1.8 What to learn in the start-up example; standard topics

- How to think when constructing finite difference methods, with special focus on the Forward Euler, Backward Euler, and Crank-Nicolson (midpoint) schemes
- How to formulate a computational algorithm and translate it into Python code
- How to make curve plots of the solutions
- How to compute numerical errors
- How to compute convergence rates

1.9 What to learn in the start-up example; programming topics

- How to verify an implementation and automate verification through nose tests in Python
- How to structure code in terms of functions, classes, and modules
- How to work with Python concepts such as arrays, lists, dictionaries, lambda functions, functions in functions (closures), doctests, unit tests, command-line interfaces, graphical user interfaces
- How to perform array computing and understand the difference from scalar computing
- How to conduct and automate large-scale numerical experiments
- How to generate scientific reports

1.10 What to learn in the start-up example; mathematical analysis

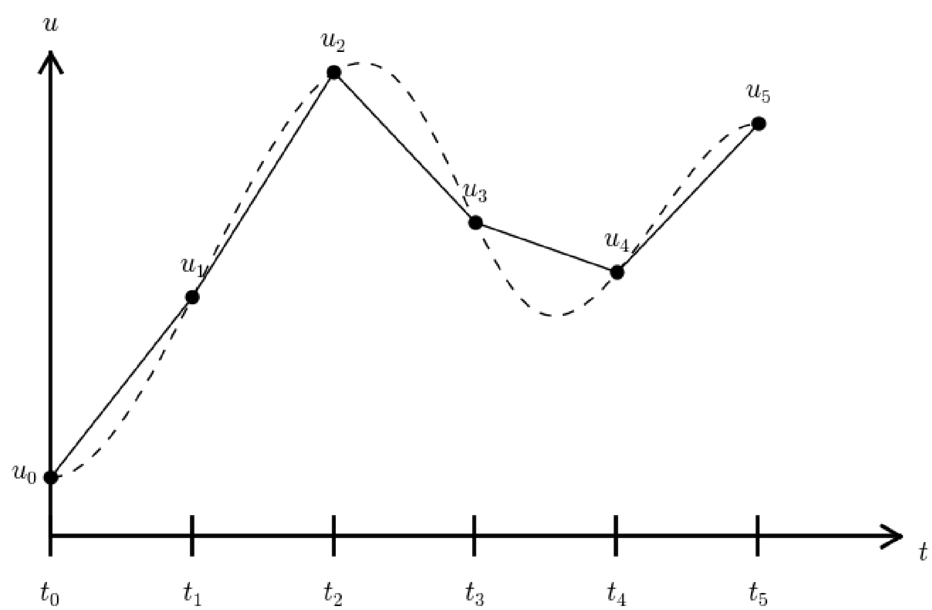
- How to uncover numerical artifacts in the computed solution
- How to analyze the numerical schemes mathematically to understand why artifacts occur
- How to derive mathematical expressions for various measures of the error in numerical methods, frequently by using the `sympy` software for symbolic computation
- Introduce concepts such as finite difference operators, mesh (grid), mesh functions, stability, truncation error, consistency, and convergence

1.11 What to learn in the start-up example; generalizations

- Generalize the example to $u'(t) = -a(t)u(t) + b(t)$
- Present additional methods for the general nonlinear ODE $u' = f(u,t)$, which is either a scalar ODE or a system of ODEs
- How to access professional packages for solving ODEs
- How our model equations like $u' = -au$ arises in a wide range of phenomena in physics, biology, and finance

2 Finite difference methods

- The finite difference method is the simplest method for solving differential equations
- Fast to learn, derive, and implement
- A very useful tool to know, even if you aim at using the finite element or the finite volume method



2.1 Topics in the first intro to the finite difference method

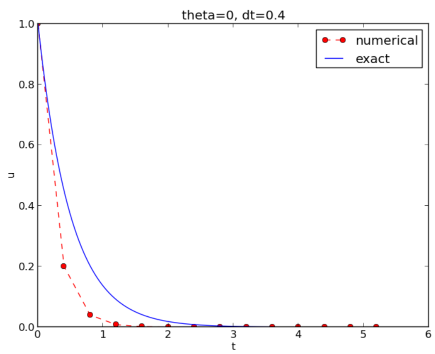
- How to derive a finite difference discretization of an ODE
- Key concepts: mesh, mesh function, finite difference approximations
- The Forward Euler, Backward Euler, and Crank-Nicolson methods
- Finite difference operator notation
- How to derive an algorithm and implement it in Python
- How to test the implementation

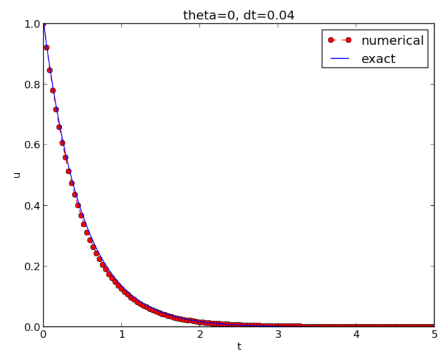
2.2 A basic model for exponential decay

The world's simplest (?) ODE:

$$u'(t) = -au(t), \quad u(0) = I,\ t \in (0, T]\,.$$

Observation.
We can learn a lot about numerical methods, computer implementation, program testing, and real applications of these tools by using this very simple ODE as example. The teaching principle is to keep the math as simple as possible while learning computer tools.





2.3 Applications

- Growth and decay of populations (cells, animals, human)
- Growth and decay of a fortune
- Radioactive decay
- Cooling/heating of an object
- Pressure variation in the atmosphere
- Vertical motion of a body in water/air
- Time-discretization of diffusion PDEs by Fourier techniques

2.4 Continuous problem

$$u' = -au,\ t \in (0, T], \quad u(0) = I\,. \tag{1}$$

Solution of the continuous problem ("continuous solution"):

$$u(t) = Ie^{-at}\,.$$

(special case that we can derive a formula for the discrete solution)

2.5 Discrete problem

$u^n \approx u(t_n)$ - u is found at discrete time points $t_1, t_2, t_3, \ldots$

$$u^{n+1} = Au^n \,.$$

A depends on the type of finite difference method.

Solution of the discrete problem ("discrete solution"):

$$u^{n+1} = IA^n \,.$$

(special case that we can derive a formula for the discrete solution)

2.6 The steps in the finite difference method

Solving a differential equation by a finite difference method consists of four steps:

1. discretizing the domain,
2. fulfilling the equation at discrete time points,
3. replacing derivatives by finite differences,
4. formulating a recursive algorithm.

2.7 Step 1: Discretizing the domain

The time domain $[0, T]$ is represented by a *mesh*: a finite number of $N_t + 1$ points

$$0 = t_0 < t_1 < t_2 < \cdots < t_{N_t-1} < t_{N_t} = T \,.$$

- We seek the solution u at the mesh points: $u(t_n)$, $n = 1, 2, \ldots, N_t$.
- Note: u^0 is known as I.
- Notational short-form for the numerical approximation to $u(t_n)$: u^n
- In the differential equation: u is the exact solution
- In the numerical method and implementation: u^n is the numerical approximation, $u_{\mathrm{e}}(t)$ is the exact solution

2.8 Step 1: Discretizing the domain

u^n is a mesh function, defined at the mesh points t_n, $n = 0, \ldots, N_t$ only.

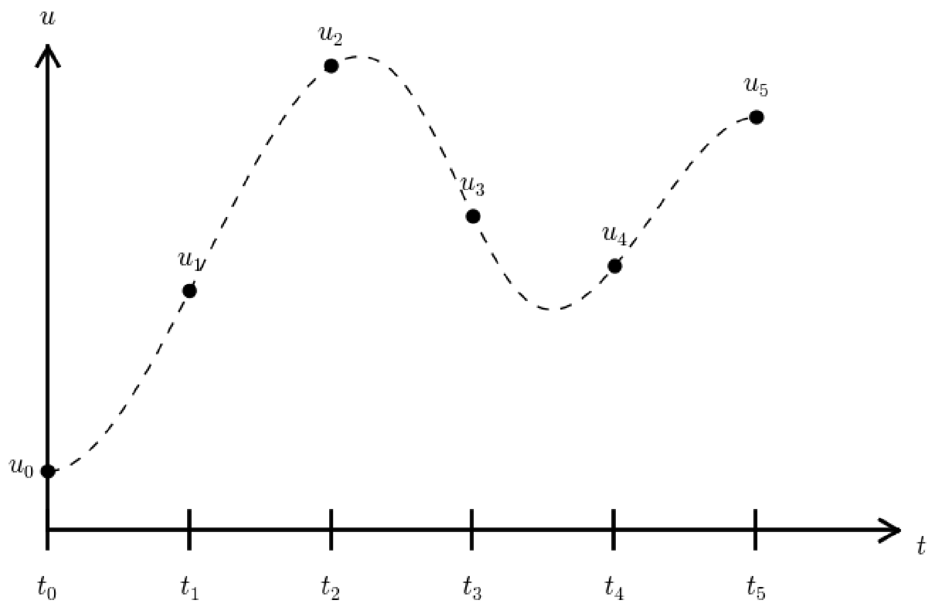
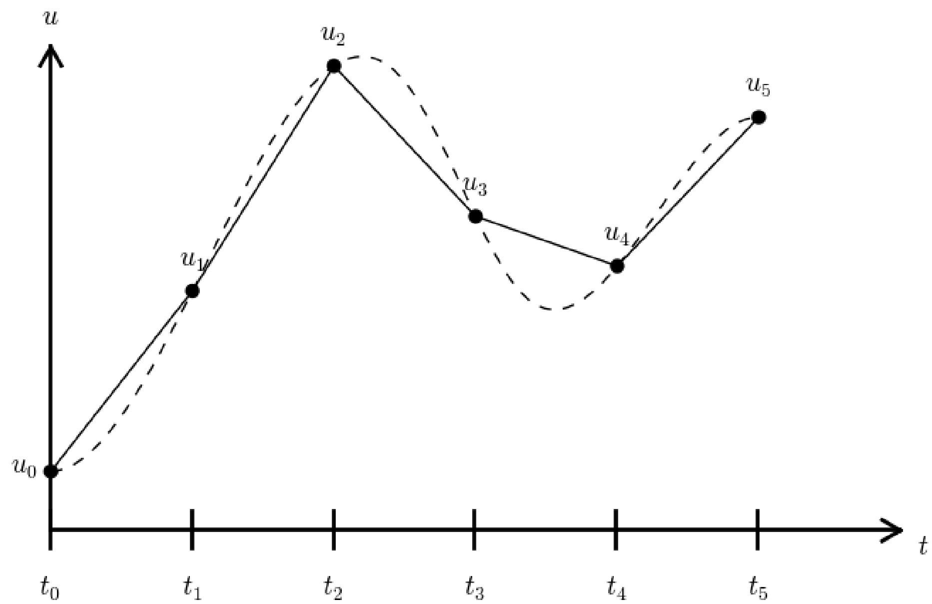


Figure 1: Time mesh with the numerical solution as a mesh function.

2.9 What about a mesh function between the mesh points?

Can extend the mesh function to yield values between mesh points by *linear interpolation*:

$$u(t) \approx u^n + \frac{u^{n+1} - u^n}{t_{n+1} - t_n}(t - t_n)\,. \tag{2}$$



2.10 Step 2: Fulfilling the equation at discrete time points

- The ODE holds for all $t \in (0, T]$ (infinite no of points)

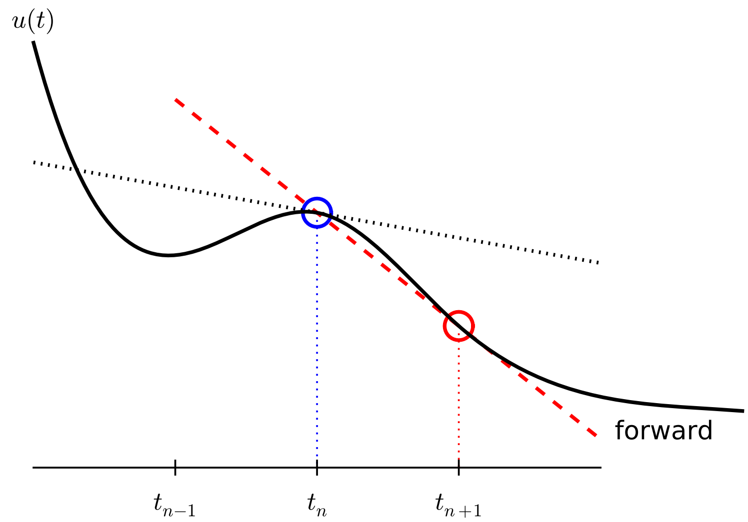
- Idea: let the ODE be valid at the mesh points only (finite no of points)

$$u'(t_n) = -au(t_n), \quad n = 1, \ldots, N_t \,. \tag{3}$$

2.11 Step 3: Replacing derivatives by finite differences

Now it is time for the *finite difference* approximations of derivatives:

$$u'(t_n) \approx \frac{u^{n+1} - u^n}{t_{n+1} - t_n} \,. \tag{4}$$



2.12 Step 3: Replacing derivatives by finite differences

Inserting the finite difference approximation in

$$u'(t_n) = -au(t_n),$$

gives

$$\frac{u^{n+1} - u^n}{t_{n+1} - t_n} = -au^n, \quad n = 0, 1, \ldots, N_t - 1\,. \tag{5}$$

This is the

- discrete equation
- discrete problem
- finite difference method
- finite difference scheme

2.13 Step 4: Formulating a recursive algorithm

- How can we actually compute the u^n values?
- Fundamental structure:
  - given $u^0 = I$
  - compute u^1 from u^0
  - compute u^2 from u^1
  - compute u^3 from u^2 (and so forth)

- In general: we have u^n and seek u^{n+1}

The Forward Euler scheme.
Solve wrt u^{n+1} to get the computational formula:

$$u^{n+1} = u^n - a(t_{n+1} - t_n)u^n\,. \tag{6}$$

2.14 Let us apply the scheme

Assume constant time spacing: $\Delta t = t_{n+1} - t_n = \text{const}$

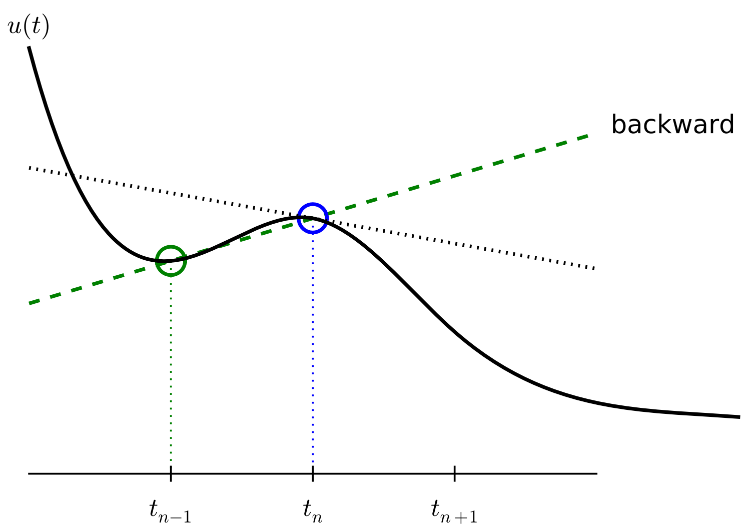
$$\begin{aligned}
u_0 &= I,\\
u_1 &= u^0 - a\Delta t u^0 = I(1 - a\Delta t),\\
u_2 &= I(1 - a\Delta t)^2,\\
u^3 &= I(1 - a\Delta t)^3,\\
&\vdots\\
u^{N_t} &= I(1 - a\Delta t)^{N_t}\,.
\end{aligned}$$

Ooops - we can find the numerical solution by hand (in this simple example)! No need for a computer (yet)...

2.15 A backward difference

Here is another finite difference approximation to the derivative (backward difference):

$$u'(t_n) \approx \frac{u^n - u^{n-1}}{t_n - t_{n-1}}\,. \tag{7}$$



2.16 The Backward Euler scheme

Inserting the finite difference approximation in $u'(t_n) = -au(t_n)$ yields the Backward Euler (BE) scheme:

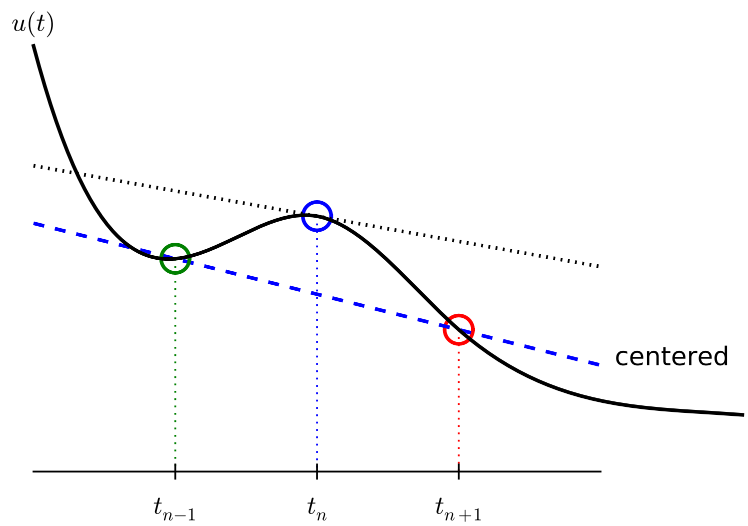
$$\frac{u^n - u^{n-1}}{t_n - t_{n-1}} = -au^n\,. \tag{8}$$

Solve with respect to the unknown u^{n+1}:

$$u^{n+1} = \frac{1}{1 + a(t_{n+1} - t_n)}u^n\,. \tag{9}$$

2.17 A centered difference

Centered differences are better approximations than forward or backward differences.



2.18 The Crank-Nicolson scheme; part 1

Idea 1: let the ODE hold at $t_{n+1/2}$

$$u'(t_{n+1/2} = -au(t_{n+1/2})\,.$$

Idea 2: approximate $u'(t_{n+1/2}$ by a centered difference

$$u'(t_{n+\frac{1}{2}}) \approx \frac{u^{n+1} - u^n}{t_{n+1} - t_n}\,. \tag{10}$$

Problem: $u(t_{n+1/2})$ is not defined, only $u^n = u(t_n)$ and $u^{n+1} = u(t_{n+1})$

Solution:

$$u(t_{n+1/2}) \approx \frac{1}{2}(u^n + u^{n+1})$$

2.19 The Crank-Nicolson scheme; part 2

Result:

$$\frac{u^{n+1} - u^n}{t_{n+1} - t_n} = -a\frac{1}{2}(u^n + u^{n+1})\,. \tag{11}$$

Solve wrt to u^{n+1}:

$$u^{n+1} = \frac{1 - \frac{1}{2}a(t_{n+1} - t_n)}{1 + \frac{1}{2}a(t_{n+1} - t_n)}u^n\,. \tag{12}$$

This is a Crank-Nicolson (CN) scheme or a midpoint or centered scheme.

2.20 The unifying θ-rule

The Forward Euler, Backward Euler, and Crank-Nicolson schemes can be formulated as one scheme with a varying parameter θ:

$$\frac{u^{n+1} - u^n}{t_{n+1} - t_n} = -a(\theta u^{n+1} + (1-\theta)u^n)\,. \tag{13}$$

- $\theta = 0$: Forward Euler
- $\theta = 1$: Backward Euler
- $\theta = 1/2$: Crank-Nicolson
- We may alternatively choose any $\theta \in [0, 1]$.

u^n is known, solve for u^{n+1}:

$$u^{n+1} = \frac{1 - (1-\theta)a(t_{n+1} - t_n)}{1 + \theta a(t_{n+1} - t_n)}\,. \tag{14}$$

This scheme is known as the θ-rule.

2.21 Constant time step

Very common assumption (not important, but exclusively used for simplicity hereafter): constant time step $t_{n+1} - t_n \equiv \Delta t$

Summary of schemes for constant time step.

$$u^{n+1} = (1 - a\Delta t)u^n \qquad \text{Forward Euler} \qquad (15)$$

$$u^{n+1} = \frac{1}{1 + a\Delta t}u^n \qquad \text{Backward Euler} \qquad (16)$$

$$u^{n+1} = \frac{1 - \frac{1}{2}a\Delta t}{1 + \frac{1}{2}a\Delta t}u^n \qquad \text{Crank-Nicolson} \qquad (17)$$

$$u^{n+1} = \frac{1 - (1-\theta)a\Delta t}{1 + \theta a\Delta t}u^n \qquad \text{The } \theta-\text{rule} \qquad (18)$$

2.22 Test the understanding!

Derive Forward Euler, Backward Euler, and Crank-Nicolson schemes for Newton's law of cooling:

$$u' = -k(u - u_S), \quad u(0) = I,\ t \in (0, T]\,.$$

Physical quantities:

- $u(t)$: temperature of an object at time t
- k: parameter expressing heat loss to the surroundings
- u_S: temperature of the surroundings
- I: initial temperature

2.23 Compact operator notation for finite differences

- Finite difference formulas can be tedious to write and read/understand
- Handy tool: finite difference operator notation
- Advantage: communicates the nature of the difference in a compact way

$$[D_t^- u = -au]^n\,. \qquad (19)$$

2.24 Compact operator notation for difference operators

Forward difference:

$$[D_t^+ u]^n = \frac{u^{n+1} - u^n}{\Delta t} \approx \frac{d}{dt}u(t_n)\,. \qquad (20)$$

Centered difference:

$$[D_t u]^n = \frac{u^{n+\frac{1}{2}} - u^{n-\frac{1}{2}}}{\Delta t} \approx \frac{d}{dt}u(t_n), \qquad (21)$$

Backward difference:

$$[D_t^- u]^n = \frac{u^n - u^{n-1}}{\Delta t} \approx \frac{d}{dt}u(t_n) \qquad (22)$$

2.25 The Backward Euler scheme with operator notation

$$[D_t^- u]^n = -au^n\,.$$

Common to put the whole equation inside square brackets:

$$[D_t^- u = -au]^n\,. \tag{23}$$

2.26 The Forward Euler scheme with operator notation

$$[D_t^+ u = -au]^n\,. \tag{24}$$

2.27 The Crank-Nicolson scheme with operator notation

Introduce an averaging operator:

$$[\overline{u}^t]^n = \frac{1}{2}(u^{n-\frac{1}{2}} + u^{n+\frac{1}{2}}) \approx u(t_n) \tag{25}$$

The Crank-Nicolson scheme can then be written as

$$[D_t u = -a\overline{u}^t]^{n+\frac{1}{2}}\,. \tag{26}$$

Test: use the definitions and write out the above formula to see that it really is the Crank-Nicolson scheme!

3 Implementation

Model:

$$u'(t) = -au(t), \quad t \in (0,T], \quad u(0) = I,$$

Numerical method:

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

for $\theta \in [0,1]$. Note

- $\theta = 0$ gives Forward Euler
- $\theta = 1$ gives Backward Euler
- $\theta = 1/2$ gives Crank-Nicolson

3.1 Requirements of a program

- Compute the numerical solution u^n, $n = 1, 2, \ldots, N_t$
- Display the numerical and exact solution $u_e(t) = e^{-at}$
- Brings evidence to a correct implementation (*verification*)
- Compare the numerical and the exact solution in a plot
- computes the error $u_e(t_n) - u^n$

- computes the convergence rate of the numerical scheme
- reads its input data from the command line

3.2 Tools to learn

- Basic Python[1] programming
- Array computing with `numpy`[2]
- Plotting with `matplotlib.pyplot`[3] and `scitools`[4] (equivalent)
- File writing and reading
- Making command-line user interface via `argparse.ArgumentParser`
- Making graphical user interfaces via Parampool[5]

Notice.
All programs are in the directory `src/decay`[a].

[a] `http://tinyurl.com/jvzzcfn/decay`

3.3 Why implement in Python?

- Python has a very clean, readable syntax (often known as "executable pseudo-code").
- Python code is very similar to MATLAB code (and MATLAB has a particularly widespread use for scientific computing).
- Python is similar to, but much simpler to work with and results in more reliable code than C++.
- Python is a full-fledged, very powerful programming language.
- Python has a rich set of modules for scientific computing, and its popularity in scientific computing is rapidly growing.
- Python was made for being combined with compiled languages (C, C++, Fortran) to reuse existing numerical software and to reach high computational performance of new implementations.
- Python has extensive support for administrative task needed when doing large-scale computational investigations.

[1] `http://python.org`
[2] `http://numpy.org/`
[3] `http://matplotlib.sourceforge.net/`
[4] `http://code.google.com/p/scitools/`
[5] `https://github.com/hplgit/parampool`

- Python has extensive support for graphics (visualization, user interfaces, web applications).
- FEniCS, a very powerful tool for solving PDEs by the finite element method, is most human-efficient to operate from Python.

3.4 Algorithm

- Store u^n, $n = 0, 1, \ldots, N_t$ in an array `u`.
- Algorithm:
  1. initialize u^0
  2. for $t = t_n$, $n = 1, 2, \ldots, N_t$: compute u_n using the θ-rule formula

3.5 Translation to Python function

```
from numpy import *

def solver(I, a, T, dt, theta):
    """Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt."""
    Nt = int(T/dt)            # no of time intervals
    T = Nt*dt                 # adjust T to fit time step dt
    u = zeros(Nt+1)           # array of u[n] values
    t = linspace(0, T, Nt+1)  # time mesh

    u[0] = I                  # assign initial condition
    for n in range(0, Nt):    # n=0,1,...,Nt-1
        u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
    return u, t
```

Note about the `for` loop: `range(0, Nt, s)` generates all integers from `0` to `Nt` in steps of `s` (default 1), *but not including* `Nt` (!).

Sample call:

```
u, t = solver(I=1, a=2, T=8, dt=0.8, theta=1)
```

3.6 Integer division

Python applies integer division: `1/2` is 0, while `1./2` or `1.0/2` or `1/2.` or `1/2.0` or `1.0/2.0` all give 0.5.

A safer `solver` function (`dt = float(dt)` - guarantee float):

```
from numpy import *

def solver(I, a, T, dt, theta):
    """Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt."""
    dt = float(dt)            # avoid integer division
    Nt = int(round(T/dt))     # no of time intervals
    T = Nt*dt                 # adjust T to fit time step dt
    u = zeros(Nt+1)           # array of u[n] values
```

```
    t = linspace(0, T, Nt+1)  # time mesh

    u[0] = I                  # assign initial condition
    for n in range(0, Nt):    # n=0,1,...,Nt-1
        u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
    return u, t
```

3.7 Doc strings

- First string after the function heading
- Used for documenting the function
- Automatic documentation tools can make fancy manuals for you
- Can be used for automatic testing

```
def solver(I, a, T, dt, theta):
    """
    Solve

        u'(t) = -a*u(t),

    with initial condition u(0)=I, for t in the time interval
    (0,T]. The time interval is divided into time steps of
    length dt.

    theta=1 corresponds to the Backward Euler scheme, theta=0
    to the Forward Euler scheme, and theta=0.5 to the Crank-
    Nicolson method.
    """
    ...
```

3.8 Formatting of numbers

Can control formatting of reals and integers through the *printf* format:

```
print 't=%6.3f u=%g' % (t[i], u[i])
```

Or the alternative *format string syntax*:

```
print 't={t:6.3f} u={u:g}'.format(t=t[i], u=u[i])
```

3.9 Running the program

How to run the program decay_v1.py[6]:

```
Terminal> python decay_v1.py
```

[6] https://github.com/hplgit/INF5620/blob/gh-pages/src/decay/decay_v1.py

Can also run it as "normal" Unix programs: `./decay_v1.py`:

1. Insert first line `#!/usr/bin/env python` (program to interpret the file)
2. Run `chmod a+rx decay_v1.py`

Then this works:

```
Terminal> ./decay_v1.py
```

4 Verifying the implementation

- Verification = bring evidence that the program works
- Find suitable test problems
- Make function for each test problem
- Later: put the verification tests in a professional testing framework

4.1 Simplest method: run a few algorithmic steps by hand

Use a calculator ($I = 0.1$, $\theta = 0.8$, $\Delta t = 0.8$):

$$A \equiv \frac{1-(1-\theta)a\Delta t}{1+\theta a\Delta t} = 0.298245614035$$

$$\begin{aligned} u^1 &= AI = 0.0298245614035, \\ u^2 &= Au^1 = 0.00889504462912, \\ u^3 &= Au^2 = 0.00265290804728 \end{aligned}$$

See the function `verify_three_steps` in `decay_verf1.py`[7].

4.2 Comparison with an exact discrete solution

Best verification.
Compare computed numerical solution with a closed-form *exact discrete solution* (if possible)

Define

$$A = \frac{1-(1-\theta)a\Delta t}{1+\theta a\Delta t}\,.$$

[7] http://tinyurl.com/jvzzcfn/decay/decay_verf1.py

Repeated use of the θ-rule:

$$\begin{aligned}
u^0 &= I,\\
u^1 &= Au^0 = AI,\\
u^2 &= Au^1 = A^2 I,\\
&\vdots\\
u^n &= A^n u^{n-1} = A^n I\,.
\end{aligned}$$

The exact discrete solution as

$$u^n = IA^n\,. \tag{27}$$

Question.
Understand what n in u^n and in A^n means!

Test if $\max_n |u^n - u_{\rm e}(t_n)| < \epsilon \sim 10^{-15}$. Implementation in `decay_verf2.py`[8].

4.3 Computing the numerical error

Task: compute the numerical error $e^n = u_{\rm e}(t_n) - u^n$
Exact solution: $u_{\rm e}(t) = Ie^{-at}$, implemented as

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

Compute e^n by

```
u, t = solver(I, a, T, dt, theta)  # Numerical solution
u_e = exact_solution(t, I, a)
e = u_e - u
```

Array arithmetics - we compute on entire arrays!

- Array `e` is the problem's discrete *error function*
- Sometimes convenient with a scalar error measure (one number)
- Can integrate e^n

4.4 Computing the norm of the error

- e^n is a mesh function
- Usually we want one number for the error

[8] `http://tinyurl.com/jvzzcfn/decay/decay_verf2.py`

- Use a norm of e^n

Norms for a function $f(t)$:

$$||f||_{L^2} = \left(\int_0^T f(t)^2 dt\right)^{1/2}, \tag{28}$$

$$||f||_{L^1} = \int_0^T |f(t)| dt, \tag{29}$$

$$||f||_{L^\infty} = \max_{t\in[0,T]} |f(t)|\,. \tag{30}$$

Problem: $f^n = f(t_n)$ is a mesh function and hence not defined for all t. How to integrate f^n?

4.5 Norms of mesh functions

Idea: Apply a numerical integration rule, using only the mesh points of the mesh function.

The Trapezoidal rule:

$$||f^n|| = \left(\Delta t\left(\frac{1}{2}(f^0)^2 + \frac{1}{2}(f^{N_t})^2 + \sum_{n=1}^{N_t-1}(f^n)^2\right)\right)^{1/2}$$

Common approximation of this formula:

$$||f^n||_{\ell^2} = \left(\Delta t\sum_{n=0}^{N_t}(f^n)^2\right)^{1/2}.$$

This is the L^2 norm for a mesh function.

4.6 Implementation of the norm

$$E = ||e^n||_{\ell^2} = \sqrt{\Delta t\sum_{n=0}^{N_t}(e^n)^2}$$

Python:

```
E = sqrt(dt*sum(e**2))
```

4.7 Comment on array vs scalar computation

Array (vector) computing (`e` is vector, `sqrt` and `sum` from `numpy`):

```
E = sqrt(dt*sum(e**2))
```

Similar scalar computing (element by element operations in Python):

```
m = len(u)     # length of u array (alt: u.size)
u_e = zeros(m)
t = 0
for i in range(m):
    u_e[i] = exact_solution(t, a, I)
    t = t + dt
e = zeros(m)
for i in range(m):
    e[i] = u_e[i] - u[i]
s = 0  # summation variable
for i in range(m):
    s = s + e[i]**2
error = sqrt(dt*s)
```

Obviously, scalar computing

- takes more code
- is less readable
- runs much slower

Rule.
Compute on entire arrays (when possible)!

5 Plotting solutions

Basic plotting with Matplotlib is very like MATLAB syntax

```
from matplotlib.pyplot import *
plot(t, u)
show()
```

Compare `u` curve with $u_{\mathrm{e}}(t)$:

```
t_e = linspace(0, T, 1001)      # fine mesh
u_e = exact_solution(t_e, I, a)
plot(t,   u,   'r-')            # red  line for u
plot(t_e, u_e, 'b-')            # blue line for u_e
```

5.1 Decorating a plot

- Use different line types
- Add axis labels
- Add curve legends
- Add plot title
- Save plot to file

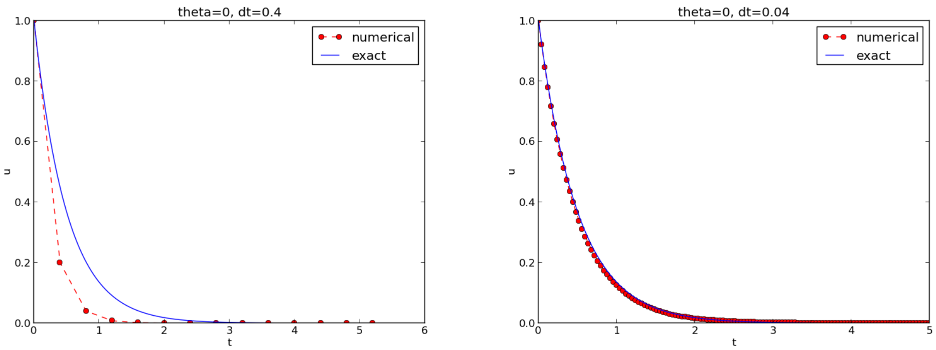


Figure 2: The Forward Euler scheme for two values of the time step.

```
from matplotlib.pyplot import *

figure()                          # create new plot
t_e = linspace(0, T, 1001)        # fine mesh for u_e
u_e = exact_solution(t_e, I, a)
plot(t,   u,   'r--o')            # red dashes w/circles
plot(t_e, u_e, 'b-')              # blue line for exact sol.
legend(['numerical', 'exact'])
xlabel('t')
ylabel('u')
title('theta=%g, dt=%g' % (theta, dt))
savefig('%s_%g.png' % (theta, dt))
show()
```

See complete code in `decay_plot_mpl.py`[9].

5.2 How the plots look like

5.3 Plotting with SciTools

SciTools[10] provides a unified plotting interface (Easyviz) to many different plotting packages: Matplotlib, Gnuplot, Grace, VTK, OpenDX, ...

Can use Matplotlib (MATLAB-like) syntax, or a more compact `plot` function syntax:

```
from scitools.std import *

plot(t,   u,   'r--o',           # red dashes w/circles
     t_e, u_e, 'b-',             # blue line for exact sol.
     legend=['numerical', 'exact'],
     xlabel='t',
     ylabel='u',
     title='theta=%g, dt=%g' % (theta, dt),
     savefig='%s_%g.png' % (theta2name[theta], dt),
     show=True)
```

[9] http://tinyurl.com/jvzzcfn/decay/decay_plot_mpl.py

[10] http://code.google.com/p/scitools

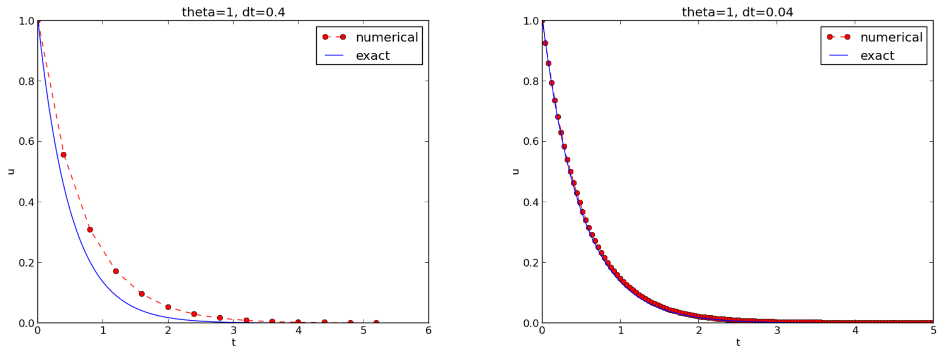


Figure 3: The Backward Euler scheme for two values of the time step.

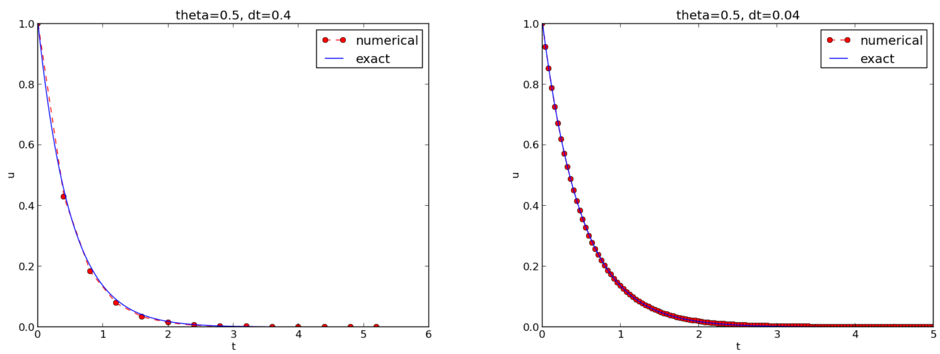


Figure 4: The Crank-Nicolson scheme for two values of the time step.

Complete code in decay_plot_st.py[11].
Change backend (plotting engine, Matplotlib by default):

```
Terminal> python decay_plot_st.py --SCITOOLS_easyviz_backend gnuplot
Terminal> python decay_plot_st.py --SCITOOLS_easyviz_backend grace
```

6 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

[11] https://github.com/hplgit/INF5620/blob/gh-pages/src/decay/decay_plot_st.py

6.1 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
```

6.2 Reading a sequence of command-line arguments

The program `decay_plot_mpl.py`[12] needs this input:

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

Give these on the command line in correct sequence

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

6.3 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
```

[12] http://tinyurl.com/jvzzcfn/decay/decay_plot_mpl.py

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`[13].

6.4 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:

```
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)

6.5 Reading option-values pairs

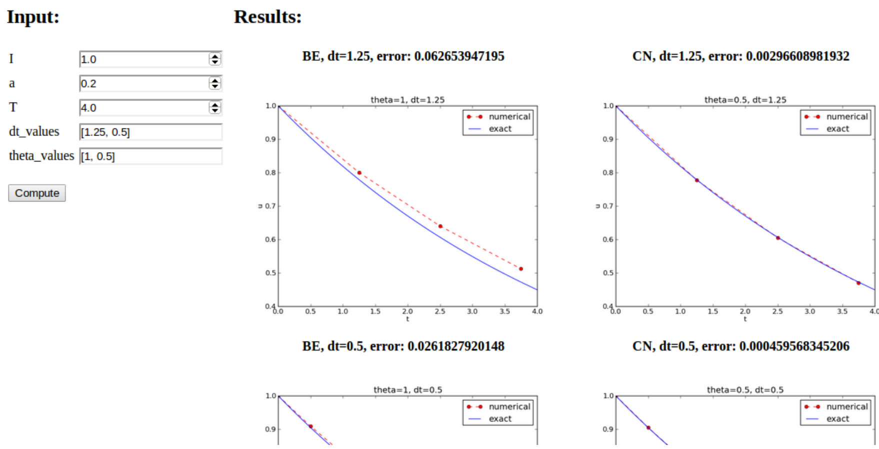
`argparse.ArgumentParser` parses the command-line arguments:

```
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`[14].

[13] http://tinyurl.com/jvzzcfn/decay/decay_cml.py
[14] http://tinyurl.com/jvzzcfn/decay/decay_argparse.py

6.6 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 15 seconds (!)

6.7 The Parampool package

- Parampool[15] is a package for handling a large pool of input parameters in simulation programs
- Parampool can automatically create sophisticated graphical web user interfaces to set parameters and view solutions
- 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)

6.8 Making a compute function

- What we have: `decay_plot_mpl.py`[16]
- `main` function carries out simulations and plotting for a series of Δt values
- Goal: steer and view these experiments from a web GUI
- Means:
  - create a compute function
  - call `parampool` functionality

[15] `https://github.com/hplgit/parampool`
[16] `http://tinyurl.com/jvzzcfn/decay/decay_plot_mpl.py`

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]):
```

6.9 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
- 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 and the error:

```
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
```

6.10 The HTML coding in detail

Embed a PNG plot in HTML code:

```
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.

6.11 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!

6.12 Running the web application

Start the GUI

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

Open a web browser at `127.0.0.1:5000`

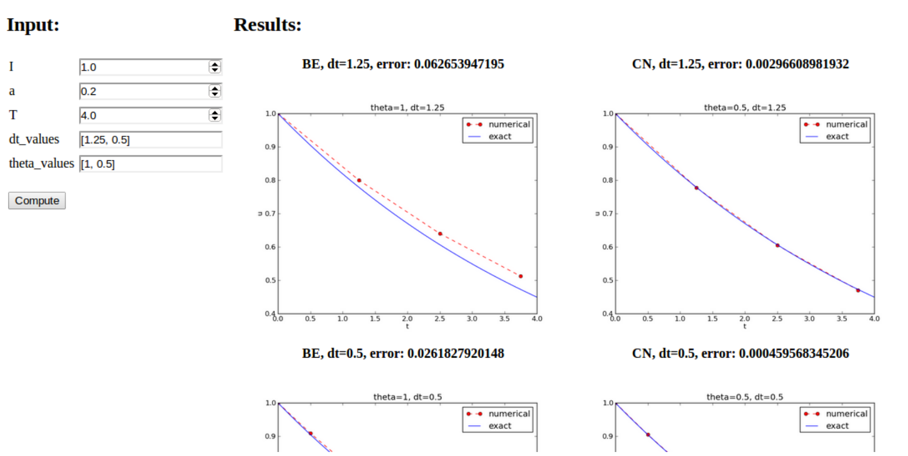


Figure 5: Automatically generated graphical web interface.

6.13 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

7 Computing convergence rates

Frequent assumption on the relation between the numerical error E and some discretization parameter Δt:

$$E = C\Delta t^r, \tag{31}$$

Unknown: C and r.

Estimating the convergence rate r. Perform numerical experiments: $(\Delta t_i, E_i)$, $i = 0, \ldots, m-1$.

1. Take the logarithm of (31), $\ln E = r \ln \Delta t + \ln C$, 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

$$r_{i-1} = \frac{\ln(E_{i-1}/E_i)}{\ln(\Delta t_{i-1}/\Delta t_i)} \tag{32}$$

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[17].

Example on 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
```

Verification. 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 $r \approx 0$:

[17] `https://github.com/hplgit/INF5620/blob/gh-pages/src/decay/decay_convrate.py`

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

7.1 Memory-saving implementation

- Note 1: we store the entire array `u`, i.e., u^n for $n = 0, 1, \ldots, N_t$
- Note 2: the formula for u^{n+1} needs u^n only, not u^{n-1}, u^{n-2}, ...
- No need to store more than u^{n+1} and u^n
- Extremely important when solving PDEs
- No practical importance here (much memory available)
- But let's illustrate how to do save memory!
- Idea 1: store u^{n+1} in `u`, u^n in `u_1` (`float`)
- Idea 2: store `u` in a file, read file later for plotting

```
def solver_memsave(I, a, T, dt, theta, filename='sol.dat'):
    """
    Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt.
    Minimum use of memory. The solution is stored in a file
    (with name filename) for later plotting.
    """
    dt = float(dt)         # avoid integer division
    Nt = int(round(T/dt))  # no of intervals

    outfile = open(filename, 'w')
    # u: time level n+1, u_1: time level n
    t = 0
    u_1 = I
    outfile.write('%.16E  %.16E\n' % (t, u_1))
    for n in range(1, Nt+1):
        u = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u_1
        u_1 = u
        t += dt
        outfile.write('%.16E  %.16E\n' % (t, u))
    outfile.close()
    return u, t
```

Reading the computed data:

```
def read_file(filename='sol.dat'):
    infile = open(filename, 'r')
    u = [];  t = []
    for line in infile:
        words = line.split()
        if len(words) != 2:
            print 'Found more than two numbers on a line!', words
            sys.exit(1)  # abort
        t.append(float(words[0]))
        u.append(float(words[1]))
    return np.array(t), np.array(u)
```

Simpler code with numpy functionality for reading/writing tabular data:

```
def read_file_numpy(filename='sol.dat'):
    data = np.loadtxt(filename)
    t = data[:,0]
    u = data[:,1]
    return t, u
```

Similar function np.savetxt, but then we need all u^n and t^n values in a two-dimensional array (which we try to prevent now!).

Usage:

```
def explore(I, a, T, dt, theta=0.5, makeplot=True):
    filename = 'u.dat'
    u, t = solver_minmem(I, a, T, dt, theta, filename)

    t, u = read_file(filename)
    u_e = exact_solution(t, I, a)
    e = u_e - u
    E = np.sqrt(dt*np.sum(e**2))
    if makeplot:
        plt.figure()
        ...
```

Complete program: decay_memsave.py[18].

8 Software engineering

Goal: make more professional numerical software.

Topics:

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

8.1 Making a module

- Previous programs: much repetitive code (esp. solver)
- DRY (Don' 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 of
  - solver
  - verify_three_steps

[18] https://github.com/hplgit/INF5620/blob/gh-pages/src/decay/decay_memsave.py

- 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:

```
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():
    ...

def exact_solution(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:

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

Test block:

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

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:

```
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()
```

8.2 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`? Or is it our own function?

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: math line $e^{-at}\sin(2\pi t)$ 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)
```

8.3 Doctests

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

```
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
    """
    ...
```

8.4 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.

8.5 Another example on using doctests

```
def explore(I, a, T, dt, theta=0.5, makeplot=True):
    """
    Run a case with the solver, compute error measure,
    and plot the numerical and exact solutions (if makeplot=True).

    >>> for theta in 0, 0.5, 1:
    ...     E = explore(I=1.9, a=2.1, T=5, dt=0.1, theta=theta,
    ...                 makeplot=False)
    ...     print '%.10E' % E
    ...
    7.3565079236E-02
    2.4183893110E-03
    6.5013039886E-02
    """
    ...
```

Complete program: decay_mod_doctest.py[19].

Caution.
Avoid doctests in functions using `sys.argv` and `print` (possible, but needs careful coding).

8.6 Unit testing with nose

- Nose is a very user-friendly testing framework
- Based on *unit testing*
- Identify small units of code
- Test each unit
- Nose automates running all tests
- Good habit: make a small edit in a code, run all tests
- Even better habit: write tests before the code
- Unit testing in scientific computing is not well so established

[19] http://tinyurl.com/jvzzcfn/decay/decay_mod_doctest.py

8.7 Basic use of nose

1. Implement tests in functions with names starting with `test_`.
2. Test functions perform assertions on computed results using `assert` functions from the `nose.tools` module.
3. Test functions can be in the source code files or be collected in separate files, usually with names starting with `test_`.

8.8 Example: nose test in a module

Very simple module `mymod`:

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

Either in `mymod.py` or in a new file `test_mymod.py`, implement a test that `double` works:

```
import nose.tools as nt

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

(Need `import mymod` if the test is in `test_mymod.py`.)

Running

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

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

Running

```
Terminal> nosetests -s
```

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

8.9 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():
    ...
    nt.assert_equal(result, 8)    # alternative 1
    assert result == 8            # alternative 2
    if result != 8:               # alternative 3
        raise AssertionError()
```

8.10 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

8.11 Demonstrating nose

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.

```
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_against_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)
```

8.12 Floats as test results

- 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: np.array(
            [  8.00000000e-01,   3.20000000e-01,
               1.28000000e-01,   5.12000000e-02,
               2.04800000e-02,   8.19200000e-03,
               3.27680000e-03,   1.31072000e-03,
               5.24288000e-04]),
        1: np.array(
            [ 0.8       ,  0.5       ,  0.3125    ,  0.1953125 ,
              0.12207031,  0.07629395,  0.04768372,  0.02980232,
              0.01862645]),
        }
    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)
```

8.13 Testing for 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
```

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 (!)
```

Unit test for this issue:

```
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)
```

8.14 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()
    # Suppress output from decay_mod.main()
    stdout = sys.stdout  # save standard output for later use
    scratchfile = open('.tmp', 'w')  # fake standard output
    sys.stdout = scratchfile

    r = decay_mod.main()
    for theta in r:
        nt.assert_true(r[theta])  # check for non-empty list

    scratchfile.close()
    sys.stdout = stdout  # restore standard output

    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)

# no need for any main
```

Complete program: `test_decay_nose.py`[20].

8.15 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

[20] http://tinyurl.com/jvzzcfn/decay/tests/test_decay_nose.py

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

8.16 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()
```

8.17 Demonstration of unittest

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

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_against_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[21].

9 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 compliex scientific applications

9.1 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

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

[21] http://tinyurl.com/jvzzcfn/decay/tests/test_decay_nose.py

Basic usage:

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

9.3 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)
```

Observe

- Can utilize user's `ArgumentParser`, or make one
- `None` is used to indicate an "empty" (non-initialized) variable

9.4 The solver class

- Store numerical data Δt, θ
- 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)

    def error(self):
        u_e = self.problem.exact_solution(self.t)
        e = u_e - self.u
        E = sqrt(self.dt*sum(e**2))
        return E
```

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

9.5 The visualizer class

- Store data about what to plot (if any)
- Offer different types of plots
- Here: make just the same plot as in the previous `explore` function

Implementation:

```
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
```

Remarks:

- The `plt` object in `plot` adds a new curve to a plot, which enables comparing different solutions from different runs of `Solver.solve`
- Such different curves gets different colors

9.6 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`[22].

10 Implementing more advanced problem and solver classes

- The previous `Problem` and `Solver` classes soon contain much repetitive code when the number of parameters increases

[22] http://tinyurl.com/jvzzcfn/decay/decay_class.py

- 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`

10.1 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`[23].

10.2 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',
```

[23]http://tinyurl.com/jvzzcfn/decay/class_decay_verf1.py

```
                     T='end time of simulation')

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

10.3 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
```

10.4 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`

11 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

Problem:

$$u'(t) = -au(t), \quad u(0) = I,\ 0 < t \leq T, \tag{33}$$

Solution method (θ-rule):

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

Tasks:

- Plot u^n against $u_{\mathrm{e}} = Ie^{-at}$ for various choices of the parameters I, a, Δt, and θ
- How does the discrete solution compare with the exact solution when Δt is varied and $\theta = 0, 0.5, 1$?
- Use the `decay_mod.py`[24] module (little modification of the plotting, see `experiments/decay_mod.py`[25])
- 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` (Δt values on the command line)

```
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
```

[24] http://tinyurl.com/jvzzcfn/decay/decay_mod.py
[25] http://tinyurl.com/jvzzcfn/decay/experiments/decay_mod.py

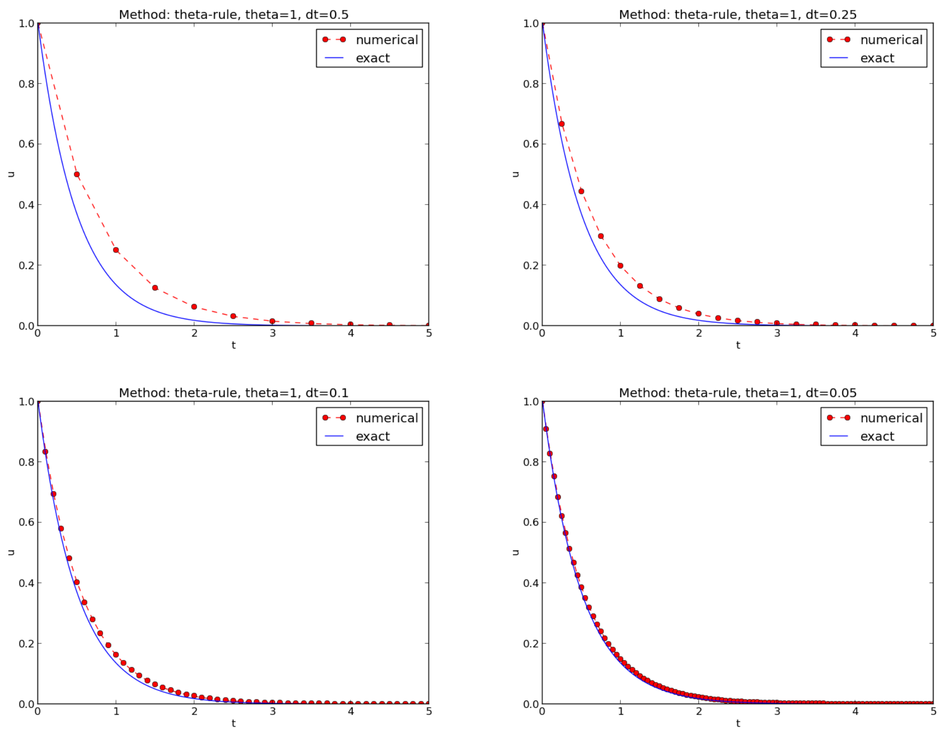


Figure 6: Illustration of the Backward Euler method for four time step values.

```
    # 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`[26].

Many useful constructs in the program above:

- `[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`

[26] `http://tinyurl.com/jvzzcfn/decay/experiments/decay_exper0.py`

11.1 Interpreting output from other programs

Programs that run other programs, like `decay_exper0.py` does, will often need to interpret output from the other programs. For example,

```
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 θ value
- plot E versus Δt, for each θ, in a log-log plot

Must replace `os.system(cmd)` by use of the `subprocess` module:

```
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)
```

Note: The command stored in `cmd` is run and all text that is written to the standard output *and* the standard error is available in the string `output`. The text in `output` is what appeared in the terminal window while running `cmd`.

Next tasks:

- Run through the `output` string, line by line
- If the current line prints θ, Δt, 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 θ 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)
```

- Plot E versus Δt for $\theta = 0, 0.5, 1$

```
import matplotlib.pyplot as plt
#import scitools.std as plt
plt.loglog(errors['dt'], errors[0], 'ro-')
plt.hold('on')  # MATLAB style...
plt.loglog(errors['dt'], errors[0.5], 'b+-')
plt.loglog(errors['dt'], errors[1], 'gx-')
plt.legend(['FE', 'CN', 'BE'], loc='upper left')
plt.xlabel('log(time step)')
plt.ylabel('log(error)')
plt.title('Error vs time step')
plt.savefig('error_BE_CN_FE.png')
```

This is a log-log plot because we expect $E \sim \Delta t^r$.

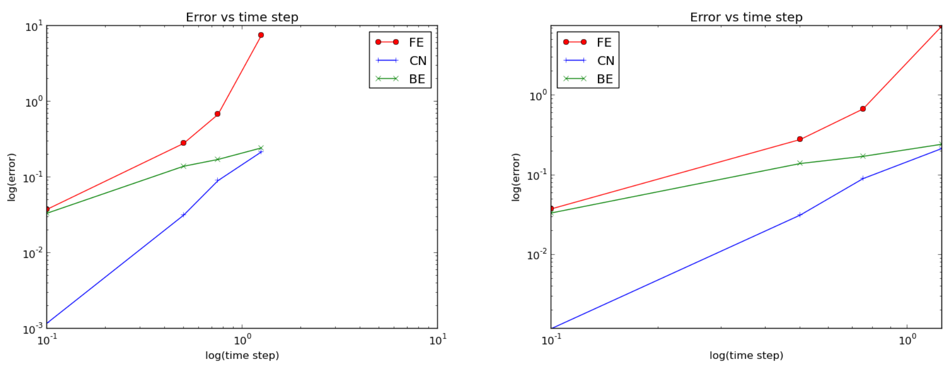


Figure 7: Default plot (left) and manually adjusted plot (right).

Complete program: `experiments/decay_exper1.py`[27]. 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

11.2 Making a report

- Scientific investigations are best documented in a report!
- A sample report[28]
- How can we write such a report?

[27] http://tinyurl.com/jvzzcfn/decay/experiments/decay_exper1.py
[28] http://hplgit.github.com/INF5620/doc/writing_reports/sphinx-cloud/

- First problem: what format should I write in?
- Plain HTML[29], generated by `decay_exper1_html.py`[30]
- HTML with MathJax[31], generated by `decay_exper1_mathjax.py`[32]
- LaTeX PDF[33], based on LaTeX source[34]
- Sphinx HTML[35], based on reStructuredText[36]
- Markdown, MediaWiki, ...
- Doconce[37] can generate LaTeX, HTML w/MathJax, Sphinx, Markdown, MediaWiki, ... (Doconce source[38] for the examples above, and Python program for generating the Doconce source[39])
- Examples on different report formats[40]

11.3 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[41]

12 Analysis of finite difference equations

Model:

$$u'(t) = -au(t), \quad u(0) = I, \tag{34}$$

Method:

$$u^{n+1} = \frac{1 - (1-\theta)a\Delta t}{1 + \theta a\Delta t} u^n \tag{35}$$

[29] http://hplgit.github.com/INF5620/doc/writing_reports/report_html.html
[30] http://tinyurl.com/jvzzcfn/decay/experiments/decay_exper1_html.py
[31] http://hplgit.github.com/INF5620/doc/writing_reports/report_html_mathjax.html
[32] http://tinyurl.com/jvzzcfn/decay/experiments/decay_exper1_html.py
[33] http://hplgit.github.com/INF5620/doc/writing_reports/report.pdf
[34] http://hplgit.github.com/INF5620/doc/writing_reports/report.tex.html
[35] http://hplgit.github.com/INF5620/doc/writing_reports/sphinx-cloud/index.html
[36] http://hplgit.github.com/INF5620/doc/writing_reports/report_sphinx.rst.html
[37] http://code.google.com/p/doconce
[38] http://hplgit.github.com/INF5620/doc/writing_reports/report.do.txt.html
[39] http://tinyurl.com/jvzzcfn/decay/experiments/decay_exper1_do.py
[40] http://hplgit.github.com/INF5620/doc/writing_reports/
[41] http://hplgit.github.com/teamods/bitgit/html/

Problem setting.
How good is this method? Is it safe to use it?

12.1 Encouraging numerical solutions

$I = 1$, $a = 2$, $\theta = 1, 0.5, 0$, $\Delta t = 1.25, 0.75, 0.5, 0.1$.

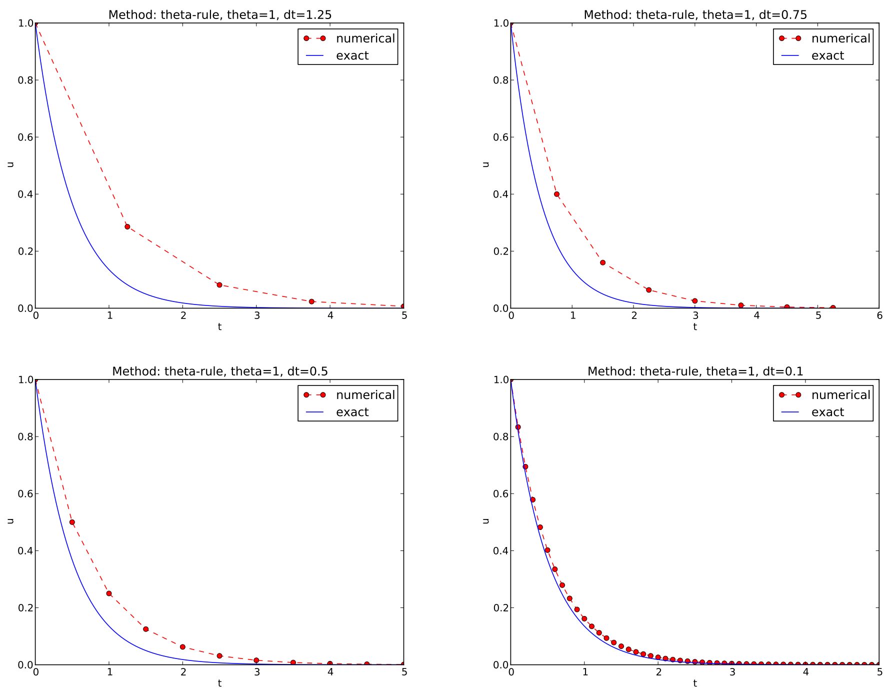


Figure 8: Backward Euler.

12.2 Discouraging numerical solutions; Crank-Nicolson

12.3 Discouraging numerical solutions; Forward Euler

12.4 Summary of observations

The characteristics of the displayed curves can be summarized as follows:

- The Backward Euler scheme always give a monotone solution, lying above the exact curve.
- The Crank-Nicolson scheme gives the most accurate results, but for $\Delta t = 1.25$ the solution oscillates.

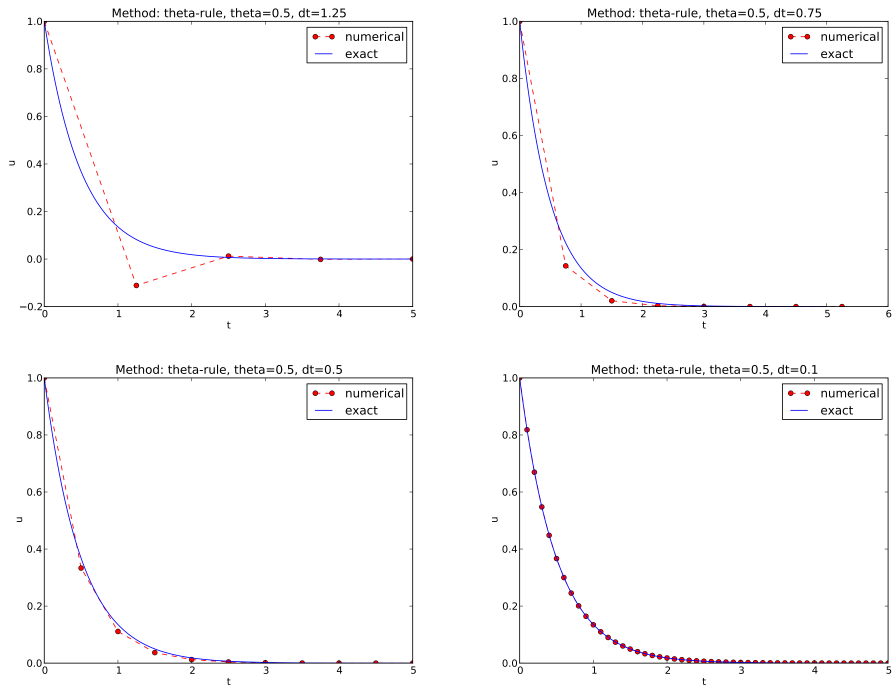


Figure 9: Crank-Nicolson.

- The Forward Euler scheme gives a growing, oscillating solution for $\Delta t = 1.25$; a decaying, oscillating solution for $\Delta t = 0.75$; a strange solution $u^n = 0$ for $n \geq 1$ when $\Delta t = 0.5$; and a solution seemingly as accurate as the one by the Backward Euler scheme for $\Delta t = 0.1$, but the curve lies below the exact solution.

12.5 Problem setting

Goal.
We ask the question

- Under what circumstances, i.e., values of the input data I, a, and Δt will the Forward Euler and Crank-Nicolson schemes result in undesired oscillatory solutions?

Techniques of investigation:

- Numerical experiments
- Mathematical analysis

Another question to be raised is

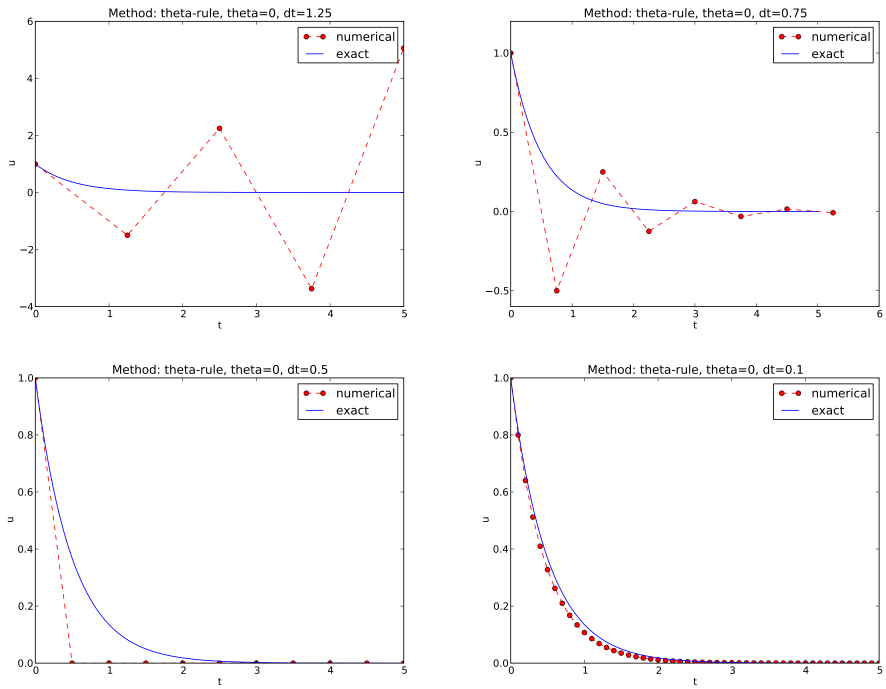


Figure 10: Forward Euler.

- How does Δt impact the error in the numerical solution?

12.6 Experimental investigation of oscillatory solutions

The solution is oscillatory if

$$u^n > u^{n-1},$$

Seems that $a\Delta t < 2$ for CN, and 1 for FE.

12.7 Exact numerical solution

Starting with $u^0 = I$, the simple recursion (35) can be applied repeatedly n times, with the result that

$$u^{n+1} = IA^n, \quad A = \frac{1 - (1-\theta)a\Delta t}{1 + \theta a\Delta t}\,. \tag{36}$$

Such an exact discrete solution is unusual, but very handy since it allows a much more detailed mathematical analysis that what is normally possible.

12.8 Stability

Since $u^n \sim A^n$,

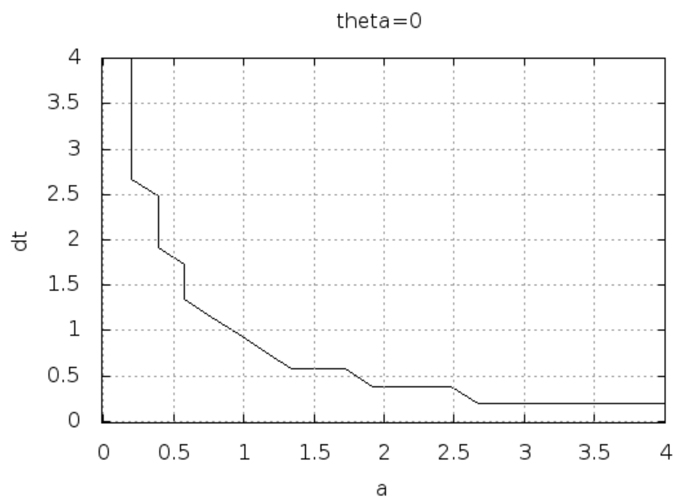


Figure 11: Forward Euler scheme: oscillatory solutions occur for points above the curve.

- $A < 0$ will give a factor $(-1)^n$ and oscillatory solutions
- $|A| > 1$ will give growing solutions
- Recall: the exact solution is monotone decaying
- If these qualitative properties are not met, we say that the numerical is *unstable*

$A < 0$ if

$$\frac{1 - (1-\theta)a\Delta t}{1 + \theta a \Delta t} < 0 \,. \tag{37}$$

To avoid oscillatory solutions we must have $A > 0$ and

$$\Delta t < \frac{1}{(1-\theta)a} \,. \tag{38}$$

- Always fulfilled for Backward Euler
- $\Delta t \leq 1/a$ for Forward Euler
- $\Delta t \leq 2/a$ for Crank-Nicolson

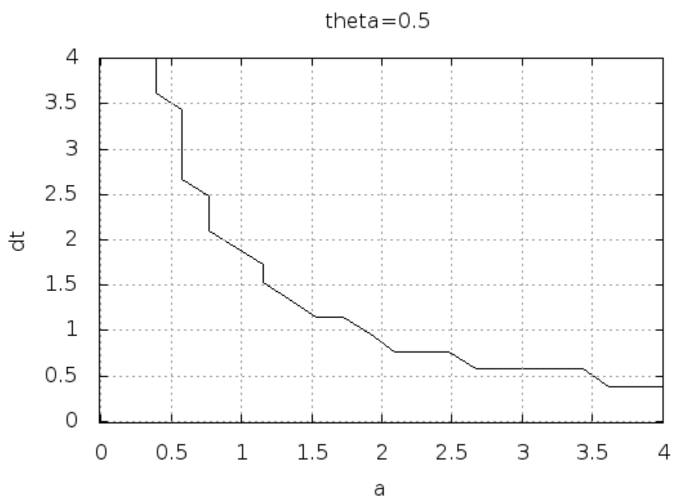
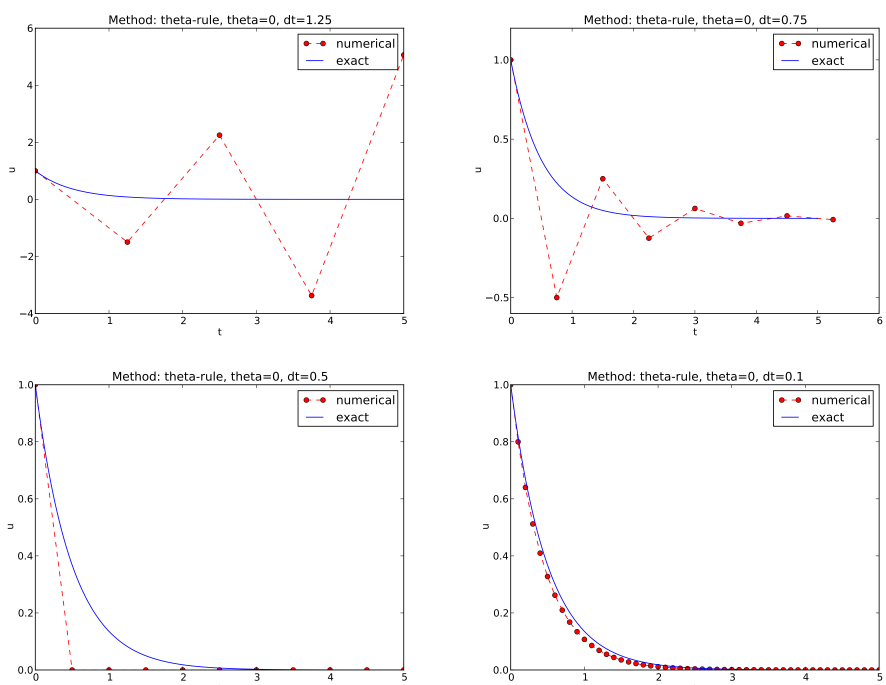


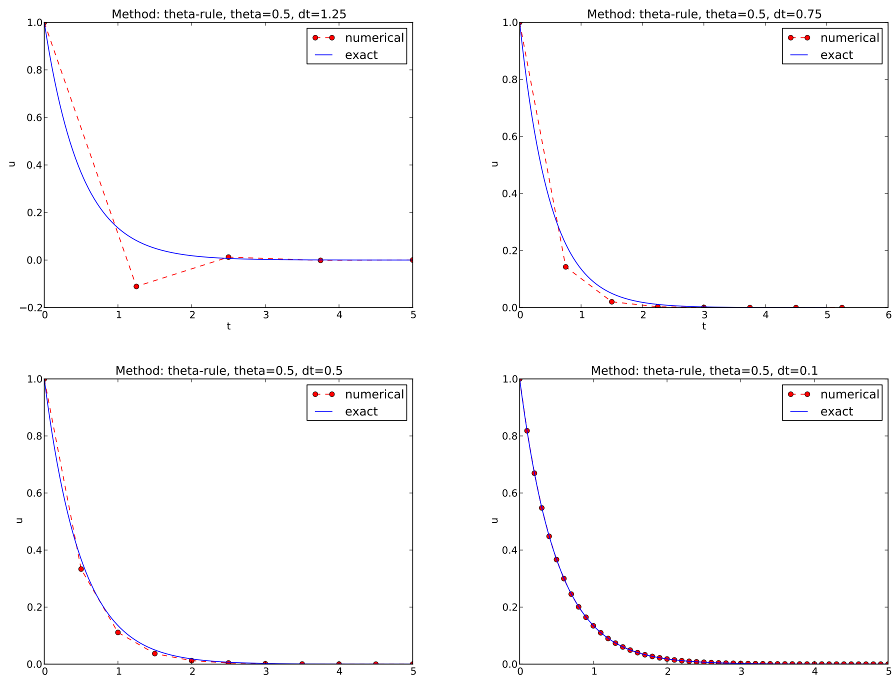
Figure 12: Crank-Nicolson scheme: oscillatory solutions occur for points above the curve.

12.9 Explanation of problems with Forward Euler



- $a\Delta t = 2 \cdot 1.25 = 2.5$ and $A = -1.5$: oscillations and growth
- $a\Delta t = 2 \cdot 0.75 = 1.5$ and $A = -0.5$: oscillations and decay
- $\Delta t = 0.5$ and $A = 0$: $u^n = 0$ for $n > 0$
- Smaller *Deltat*: qualitatively correct solution

12.10 Explanation of problems with Crank-Nicolson



- $\Delta t = 1.25$ and $A = -0.25$: oscillatory solution
- Never any growing solution

12.11 Summary of stability

1. Forward Euler is *conditionally stable*
   - $\Delta t < 2/a$ for avoiding growth
   - $\Delta t \leq 1/a$ for avoiding oscillations

2. The Crank-Nicolson is *unconditionally stable* wrt growth and conditionally stable wrt oscillations
    - $\Delta t < 2/a$ for avoiding oscillations
3. Backward Euler is unconditionally stable

12.12 Comparing amplification factors

Exact solution:

$$u(t_{n+1}) = A_{\mathrm{e}} u(t_n), \quad A_{\mathrm{e}} = e^{-a\Delta t}$$

Numerical solution:

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

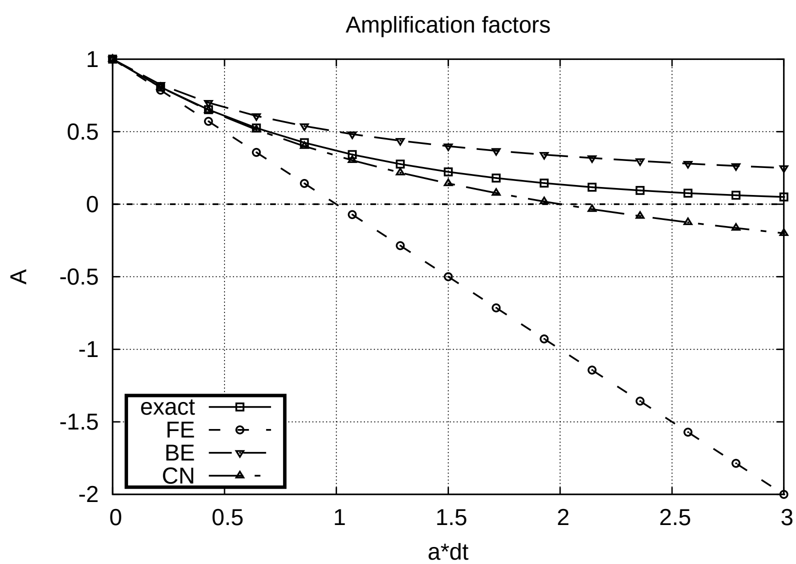


Figure 13: Comparison of amplification factors as functions of $p = a\Delta t$.

12.13 Series expansion of amplification factors

To better see the similarties of A_{e} and A mathematically, we can Taylor expand $A_{\mathrm{e}}(p)$ and $A(p)$, $p = a\Delta t$.

```
>>> from sympy import *
>>> # Create p as a mathematical symbol with name 'p'
>>> p = Symbol('p')
>>> # Create a mathematical expression with p
```

```
>>> A_e = exp(-p)
>>>
>>> # Find the first 6 terms of the Taylor series of A_e
>>> A_e.series(p, 6)
1 + (1/2)*p**2 - p - 1/6*p**3 - 1/120*p**5 + (1/24)*p**4 + O(p**6)

>>> theta = Symbol('theta')
>>> A = (1-(1-theta)*p)/(1+theta*p)
>>> FE = A_e.series(p, 4) - A.subs(theta, 0).series(p, 4)
>>> BE = A_e.series(p, 4) - A.subs(theta, 1).series(p, 4)
>>> CN = A_e.series(p, 4) - A.subs(theta, half).series(p, 4)
>>> FE
(1/2)*p**2 - 1/6*p**3 + O(p**4)
>>> BE
-1/2*p**2 + (5/6)*p**3 + O(p**4)
>>> CN
(1/12)*p**3 + O(p**4)
```

12.14 Error in amplification factors

Focus: the error measure $A - A_{\rm e}$ as function of Δt ($p = a\Delta t$):

$$A - A_{\rm e} = \left\{ \begin{array}{ll} \mathcal{O}(\Delta t^2), & \hbox{Forward and Backward Euler},\\ \mathcal{O}(\Delta t^3), & \hbox{Crank-Nicolson} \end{array}\right. \tag{39}$$

12.15 The fraction of numerical and exact amplification factors

Focus: the error measure $1 - A/A_{\rm e}$ as function of $p = a\Delta t$:

```
>>> FE = 1 - (A.subs(theta, 0)/A_e).series(p, 4)
>>> BE = 1 - (A.subs(theta, 1)/A_e).series(p, 4)
>>> CN = 1 - (A.subs(theta, half)/A_e).series(p, 4)
>>> FE
(1/2)*p**2 + (1/3)*p**3 + O(p**4)
>>> BE
-1/2*p**2 + (1/3)*p**3 + O(p**4)
>>> CN
(1/12)*p**3 + O(p**4)
```

Same leading-order terms as for the error measure $A - A_{\rm e}$.

12.16 The true/global error at a point

Focus: the global error $e^n = u_{\rm e}(t_n) - u^n$

```
>>> n = Symbol('n')
>>> u_e = exp(-p*n)   # I=1
>>> u_n = A**n        # I=1
>>> FE = u_e.series(p, 4) - u_n.subs(theta, 0).series(p, 4)
>>> BE = u_e.series(p, 4) - u_n.subs(theta, 1).series(p, 4)
>>> CN = u_e.series(p, 4) - u_n.subs(theta, half).series(p, 4)
>>> FE
(1/2)*n*p**2 - 1/2*n**2*p**3 + (1/3)*n*p**3 + O(p**4)
>>> BE
(1/2)*n**2*p**3 - 1/2*n*p**2 + (1/3)*n*p**3 + O(p**4)
>>> CN
(1/12)*n*p**3 + O(p**4)
```

Substitute n by $t/\Delta t$:

- Forward and Backward Euler: leading order term $\frac{1}{2}ta^2t\Delta t$
- Crank-Nicolson: leading order term $\frac{1}{12}ta^3\Delta t^2$

12.17 Convergence

The numerical scheme is convergent if the global error $e^n \to 0$ as $\Delta t \to 0$. If the error has a leading order term Δt^r, the convergence rate is of order r.

12.18 Integrated errors

Focus: norm of the numerical error

$$||e^n||_{\ell^2} = \sqrt{\Delta t \sum_{n=0}^{N_t} (u_{\mathrm{e}}(t_n) - u^n)^2}\,.$$

Forward and Backward Euler:

$$||e^n||_{\ell^2} = \frac{1}{4}\sqrt{\frac{T^3}{3}}a^2\Delta t\,.$$

Crank-Nicolson:

$$||e^n||_{\ell^2} = \frac{1}{4}\sqrt{\frac{T^3}{3}}a^2\Delta t\,.$$

Summary of errors.

Analysis of both the pointwise and the time-integrated true errors:

- 1st order for Forward and Backward Euler
- 2nd order for Crank-Nicolson

12.19 Truncation error

- How good is the discrete equation?
- Possible answer: see how well u_{e} fits the discrete equation

$$[D_t u = -au]^n,$$

i.e.,

Forward Euler:

$$\frac{u^{n+1} - u^n}{\Delta t} = -au^n\,.$$

Insert u_{e} (which does not in general fulfill this equation):

$$\frac{u_{\mathrm{e}}(t_{n+1}) - u_{\mathrm{e}}(t_n)}{\Delta t} + au_{\mathrm{e}}(t_n) = R^n \neq 0\,. \tag{40}$$

- The residual R^n is the *truncation error.*

- How does R^n vary with Δt?

Tool: Taylor expand u_{e} around the point where the ODE is sampled (here t_n)

$$u_{\mathrm{e}}(t_{n+1}) = u_{\mathrm{e}}(t_n) + u_{\mathrm{e}}'(t_n)\Delta t + \frac{1}{2}u_{\mathrm{e}}''(t_n)\Delta t^2 + \cdots$$

Inserting this Taylor series in (40) gives

$$R^n = u_{\mathrm{e}}'(t_n) + \frac{1}{2}u_{\mathrm{e}}''(t_n)\Delta t + \ldots + au_{\mathrm{e}}(t_n)\,.$$

Now, u_{e} solves the ODE $u_{\mathrm{e}}' = -au_{\mathrm{e}}$, and then

$$R^n \approx \frac{1}{2}u_{\mathrm{e}}''(t_n)\Delta t\,.$$

This is a mathematical expression for the truncation error.

Backward Euler:

$$R^n \approx -\frac{1}{2}u_{\mathrm{e}}''(t_n)\Delta t,$$

Crank-Nicolson:

$$R^{n+1/2} \approx \frac{1}{24}u_{\mathrm{e}}'''(t_{n+\frac{1}{2}})\Delta t^2\,.$$

12.20 Consistency, stability, and convergence

- Truncation error measures the residual in the difference equations. The scheme is *consistent* if the truncation error goes to 0 as $\Delta t \to 0$. Importance: the difference equations approaches the differential equation as $\Delta t \to 0$.

- *Stability* means that the numerical solution exhibits the same qualitative properties as the exact solution. Here: monotone, decaying function.

- *Convergence* implies that the true (global) error $e^n = u_{\mathrm{e}}(t_n) - u^n \to 0$ as $\Delta t \to 0$. This is really what we want!

The Lax equivalence theorem for *linear* differential equations: consistency + stability is equivalent with convergence.

(Consistency and stability is in most problems much easier to establish than convergence.)

13 Model extensions

13.1 Extension to a variable coefficient

$$u'(t) = -a(t)u(t), \quad t \in (0, T], \quad u(0) = I\,. \tag{41}$$

The Forward Euler scheme:

$$\frac{u^{n+1} - u^n}{\Delta t} = -a(t_n)u^n\,. \tag{42}$$

The Backward Euler scheme:

$$\frac{u^{n} - u^{n-1}}{\Delta t} = -a(t_n)u^n\,. \tag{43}$$

The Crank-Nicolson scheme (evaluting $a(t_{n+\frac{1}{2}})$ and using an average for u):

$$\frac{u^{n+1} - u^n}{\Delta t} = -a(t_{n+\frac{1}{2}})\frac{1}{2}(u^n + u^{n+1})\,. \tag{44}$$

The Crank-Nicolson scheme (using using an average for a and u):

$$\frac{u^{n+1} - u^n}{\Delta t} = -\frac{1}{2}(a(t_n)u^n + a(t_{n+1})u^{n+1})\,. \tag{45}$$

The θ-rule unifies the three mentioned schemes,

$$\frac{u^{n+1} - u^n}{\Delta t} = -a((1-\theta)t_n + \theta t_{n+1})((1-\theta)u^n + \theta u^{n+1})\,. \tag{46}$$

or,

$$\frac{u^{n+1} - u^n}{\Delta t} = -(1-\theta)a(t_n)u^n - \theta a(t_{n+1})u^{n+1}\,. \tag{47}$$

Operator notation:

$$
\begin{aligned}
&[D_t^+ u = -au]^n,\\
&[D_t^- u = -au]^n,\\
&[D_t u = -a\overline{u}^{t}]^{n+\frac{1}{2}},\\
&[D_t u = -\overline{au}^{t}]^{n+\frac{1}{2}},\\
&[D_t u = -a\overline{u}^{t,\theta}]^{n+\theta},\\
&[D_t u = -\overline{au}^{t,\theta}]^{n+\theta}\,.
\end{aligned}
$$

13.2 Extension to a source term

$$u'(t) = -a(t)u(t) + b(t), \quad t \in (0, T], \quad u(0) = I\,. \tag{48}$$

Schemes.

$$[D_t^+ u = -au + b]^n,$$
$$[D_t^- u = -au + b]^n,$$
$$[D_t u = -a\overline{u}^t + b]^{n+\frac{1}{2}},$$
$$[D_t u = \overline{-au + b}^t]^{n+\frac{1}{2}},$$
$$[D_t u = -a\overline{u}^{t,\theta} + b]^{n+\theta},$$
$$[D_t u = \overline{-au + b}^{t,\theta}]^{n+\theta}\,.$$

13.3 Implementation of the generalized model problem

$$u^{n+1} = ((1 - \Delta t(1-\theta)a^n)u^n + \Delta t(\theta b^{n+1} + (1-\theta)b^n))(1 + \Delta t\theta a^{n+1})^{-1}\,. \quad (49)$$

The Python code. Implementation where $a(t)$ and $b(t)$ are given as Python functions (see file decay_vc.py[42]):

```
def solver(I, a, b, T, dt, theta):
    """
    Solve u'=-a(t)*u + b(t), u(0)=I,
    for t in (0,T] with steps of dt.
    a and b are Python functions of t.
    """
    dt = float(dt)            # avoid integer division
    Nt = int(round(T/dt))     # no of time intervals
    T = Nt*dt                 # adjust T to fit time step dt
    u = zeros(Nt+1)           # array of u[n] values
    t = linspace(0, T, Nt+1)  # time mesh

    u[0] = I                  # assign initial condition
    for n in range(0, Nt):    # n=0,1,...,Nt-1
        u[n+1] = ((1 - dt*(1-theta)*a(t[n]))*u[n] + \
                  dt*(theta*b(t[n+1]) + (1-theta)*b(t[n])))/\
                  (1 + dt*theta*a(t[n+1]))
    return u, t
```

Implementations of variable coefficients. Plain functions:

```
def a(t):
    return a_0 if t < tp else k*a_0

def b(t):
    return 1
```

Better implementation: class with the parameters `a0`, `tp`, and `k` as attributes and a *special method* `__call__` for evaluating $a(t)$:

```
class A:
    def __init__(self, a0=1, k=2):
        self.a0, self.k = a0, k
```

[42] https://github.com/hplgit/INF5620/blob/gh-pages/src/decay/decay_vc.py

```
    def __call__(self, t):
        return self.a0 if t < self.tp else self.k*self.a0

a = A(a0=2, k=1)  # a behaves as a function a(t)
```

Use one-liner *lambda function*:

```
a = lambda t: a_0 if t < tp else k*a_0
```

In general,

```
f = lambda arg1, arg2, ...: expressin
```

is equivalent to

```
def f(arg1, arg2, ...):
    return expression
```

One can use lambda functions directly in calls:

```
u, t = solver(1, lambda t: 1, lambda t: 1, T, dt, theta)
```

for a problem $u' = -u + 1$, $u(0) = 1$.

A lambda function can appear anywhere where a variable can appear.

13.4 Verification via trivial solutions

- Start debugging of a new code with trying a problem where $u = \text{const} \neq 0$.
- Choose $u = C$ (a constant). Choose any $a(t)$ and set $b = a(t)C$ and $I = C$.
- "All" numerical methods will reproduce $u =_{\text{const}}$ exactly (machine precision).
- Often $u = C$ eases debugging.
- In this example: *any error* in the formula for u^{n+1} make $u \neq C$!

Verification function as a nose test:

```
import nose.tools as nt

def test_constant_solution():
    """
    Test problem where u=u_const is the exact solution, to be
    reproduced (to machine precision) by any relevant method.
    """
    def exact_solution(t):
        return u_const

    def a(t):
        return 2.5*(1+t**3)  # can be arbitrary
```

```
def b(t):
    return a(t)*u_const

u_const = 2.15
theta = 0.4; I = u_const; dt = 4
Nt = 4  # enough with a few steps
u, t = solver(I=I, a=a, b=b, T=Nt*dt, dt=dt, theta=theta)
print u
u_e = exact_solution(t)
difference = abs(u_e - u).max()  # max deviation
nt.assert_almost_equal(difference, 0, places=14)
```

13.5 Verification via manufactured solutions

- Choose *any* formula for $u(t)$.
- Fit I, $a(t)$, and $b(t)$ in $u' = -au + b$, $u(0) = I$, to make the chosen formula a solution of the ODE problem.
- Then we can always have an analytical solution (!).
- Ideal for verification: testing convergence rates.
- Called the *method of manufactured solutions* (MMS)
- Special case: u linear in t, because all sound numerical methods will reproduce a linear u exactly (machine precision).
- $u(t) = ct + d$. $u(0) = 0$ means $d = I$.
- ODE implies $c = -a(t)u + b(t)$.
- Choose $a(t)$ and c, and set $b(t) = c + a(t)(ct + I)$.
- Any error in the formula for u^{n+1} makes $u \neq ct + I$!

We can easily show that a linear $u^n = ct_n + I$ fulfills the discrete equations for the Forward Euler, Backward Euler, and Crank-Nicolson schemes. First,

$$[D_t^+ t]^n = \frac{t_{n+1} - t_n}{\Delta t} = 1, \tag{50}$$

$$[D_t^- t]^n = \frac{t_n - t_{n-1}}{\Delta t} = 1, \tag{51}$$

$$[D_t t]^n = \frac{t_{n+\frac{1}{2}} - t_{n-\frac{1}{2}}}{\Delta t} = \frac{(n+\frac{1}{2})\Delta t - (n-\frac{1}{2})\Delta t}{\Delta t} = 1\,. \tag{52}$$

The difference equation for the Forward Euler scheme

$$[D^+ u = -au + b]^n,$$

with $a^n = a(t_n)$, $b^n = c + a(t_n)(ct_n + I)$, and $u^n = ct_n + I$ then results in

$$c = -a(t_n)(ct_n + I) + c + a(t_n)(ct_n + I) = c$$

Verification function as a nose test:

```
def test_linear_solution():
    """
    Test problem where u=c*t+I is the exact solution, to be
    reproduced (to machine precision) by any relevant method.
    """
    def exact_solution(t):
        return c*t + I

    def a(t):
        return t**0.5  # can be arbitrary

    def b(t):
        return c + a(t)*exact_solution(t)

    theta = 0.4; I = 0.1; dt = 0.1; c = -0.5
    T = 4
    Nt = int(T/dt)  # no of steps
    u, t = solver(I=I, a=a, b=b, T=Nt*dt, dt=dt, theta=theta)
    u_e = exact_solution(t)
    difference = abs(u_e - u).max()  # max deviation
    print difference
    # No of decimal places for comparison depend on size of c
    nt.assert_almost_equal(difference, 0, places=14)
```

13.6 Extension to systems of ODEs

Sample system:

$$u' = -a_u u + a_v v, \tag{53}$$
$$v' = -a_v v + a_u u, \tag{54}$$

for constants $a_u, a_v > 0$.

The Forward Euler method:

$$u^{n+1} = u^n + \Delta t(-a_u u^n + a_v v^n), \tag{55}$$
$$v^{n+1} = u^n + \Delta t(-a_v v^n + a_u u^n)\,. \tag{56}$$

The Backward Euler scheme:

$$u^{n+1} = u^n + \Delta t(-a_u u^{n+1} + a_v v^{n+1}), \tag{57}$$
$$v^{n+1} = v^n + \Delta t(-a_v v^{n+1} + a_u u^{n+1}),\,. \tag{58}$$

which is a 2×2 linear system: in

$$(1 + \Delta t a_u)u^{n+1} + a_v v^{n+1}) = u^n, \tag{59}$$
$$a_u u^{n+1} + (1 + \Delta t a_v)v^{n+1} = v^n\,. \tag{60}$$

14 General first-order ODEs

14.1 Generic form

The standard form for ODEs:

$$u' = f(u,t), \quad u(0) = I, \tag{61}$$

u and f: scalar or vector.
Vectors in case of ODE systems:

$$u(t) = (u^{(0)}(t), u^{(1)}(t), \ldots, u^{(m-1)}(t)) .$$

$$\begin{aligned} f(u,t) = (&f^{(0)}(u^{(0)}(t), \ldots, u^{(m-1)}(t)),\\ &f^{(1)}(u^{(0)}(t), \ldots, u^{(m-1)}(t)),\\ &\vdots\\ &f^{(m-1)}(u^{(0)}(t), \ldots, u^{(m-1)}(t))) . \end{aligned}$$

Higher-order ODEs are most often expressed as first-order systems.

14.2 The Odespy software

Odespy[43] features simple Python implementations of the most fundamental schemes as well as Python interfaces to several famous packages for solving ODEs: ODEPACK[44], Vode[45], rkc.f[46], rkf45.f[47], Radau5[48], as well as the ODE solvers in SciPy[49], SymPy[50], and odelab[51].

Typical usage:

```
def f(u, t):
    return -a*u

import odespy
import numpy as np

I = 1; a = 2; T = 6; dt = 1

solver = odespy.RK4(f)
solver.set_initial_condition(I)

t_mesh = np.linspace(0, T, Nt+1)

u, t = solver.solve(t_mesh)
```

[43] https://github.com/hplgit/odespy
[44] https://computation.llnl.gov/casc/odepack/odepack_home.html
[45] https://computation.llnl.gov/casc/odepack/odepack_home.html
[46] http://www.netlib.org/ode/rkc.f
[47] http://www.netlib.org/ode/rkf45.f
[48] http://www.unige.ch/ hairer/software.html
[49] http://docs.scipy.org/doc/scipy/reference/generated/scipy.integrate.ode.html
[50] http://docs.sympy.org/dev/modules/mpmath/calculus/odes.html
[51] http://olivierverdier.github.com/odelab/

14.3 Example: Runge-Kutta methods

```
solvers = [odespy.RK2(f),
           odespy.RK3(f),
           odespy.RK4(f),
           odespy.BackwardEuler(f, nonlinear_solver='Newton')]

for solver in solvers:
    solver.set_initial_condition(I)
    u, t = solver.solve(t)

# + lots of plot code...
```

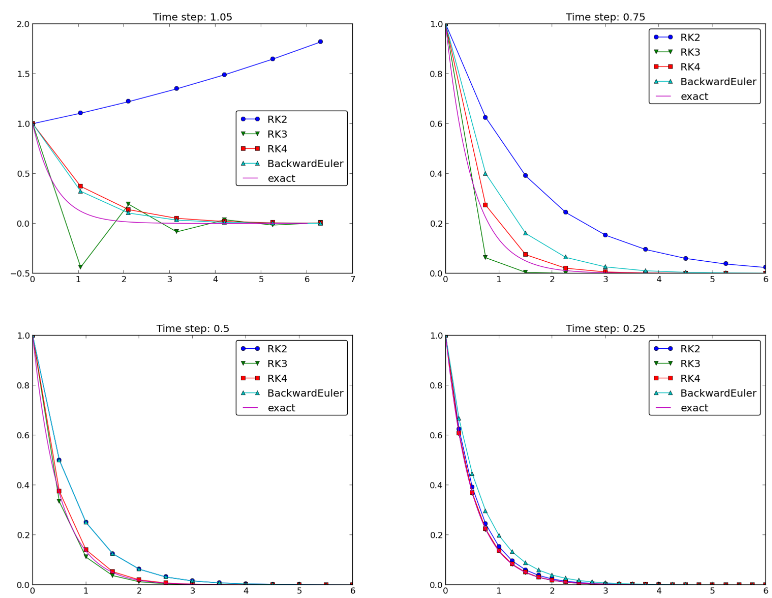


Figure 14: Behavior of different schemes for the decay equation.

The 4-th order Runge-Kutta method (`RK4`) is the method of choice!

14.4 Example: Adaptive Runge-Kutta methods

- Adaptive methods find "optimal" locations of the mesh points to ensure that the error is less than a given tolerance.
- Downside: approximate error estimation, not always optimal location of points.
- "Industry standard ODE solver": Dormand-Prince 4/5-th order Runge-Kutta (MATLAB's famous `ode45`).

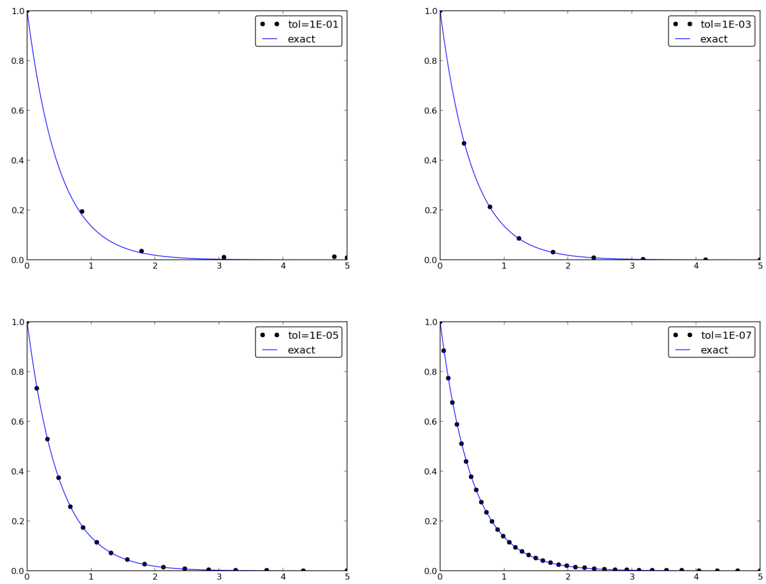


Figure 15: Choice of adaptive time mesh by the Dormand-Prince method for difference tolerances.

15 Other schemes

15.1 Implicit 2-step backward scheme

$$u'(t_{n+1}) \approx \frac{3u^{n+1} - 4u^n + u^{n-1}}{2\Delta t},$$

Scheme:

$$u^{n+1} = \frac{4}{3}u^n - \frac{1}{3}u^{n-1} + \frac{2}{3}\Delta t f(u^{n+1}, t_{n+1})\,.$$

15.2 The Leapfrog scheme

$$u'(t_n) \approx \frac{u^{n+1} - u^{n-1}}{2\Delta t} = [D_{2t}u]^n, \qquad (62)$$

Scheme:

$$[D_{2t}u = -a + b]^n,$$

or, if we write out and solve for the unknown u^{n+1},

$$u^{n+1} = u^{n-1} + \Delta t f(u^n, t_n)\,. \qquad (63)$$

- Some other scheme must be used as starter (u^1).

- Leapfrog is an explicit scheme - a nonlinear f (in u) is trivial to handle.
- Leapfrog is unstable after some time.

15.3 The filtered Leapfrog scheme

After computing u^{n+1}, stabilize Leapfrog by

$$u^n \;\leftarrow\; u^n + \gamma(u^{n-1} - 2u^n + u^{n+1})\,. \tag{64}$$

15.4 2nd-order Runge-Kutta scheme

Forward-Euler + approximate Crank-Nicolson:

$$u^* = u^n + \Delta t f(u^n, t_n), \tag{65}$$

$$u^{n+1} = u^n + \Delta t \frac{1}{2}\left(f(u^n, t_n) + f(u^*, t_{n+1})\right), \tag{66}$$

15.5 2nd-order Adams-Bashforth scheme

$$u^{n+1} = u^n + \frac{1}{2}\Delta t \left(3f(u^n, t_n) - f(u^{n-1}, t_{n-1})\right)\,. \tag{67}$$

15.6 3rd-order Adams-Bashforth scheme

$$u^{n+1} = u^n + \frac{1}{12}\left(23f(u^n, t_n) - 16f(u^{n-1}, t_{n-1}) + 5f(u^{n-2}, t_{n-2})\right)\,. \tag{68}$$

Index