Introduction to computing with finite difference methods

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Note: **PRELIMINARY VERSION**

Contents

List of Exercises, Problems, and Projects

Finite difference methods for partial differential equations (PDEs) employ a range of concepts and tools that can be introduced and illustrated in the context of simple ordinary differential equation (ODE) examples. This is what we do in the present document. By first working with ODEs, we keep the mathematical problems to be solved as simple as possible (but no simpler), thereby allowing full focus on understanding the key concepts and tools. The choice of topics in the forthcoming treatment of ODEs is therefore solely dominated by what carries over to numerical methods for PDEs.

Theory and practice are primarily illustrated by solving the very simple ODE $u' = -au$, $u(0) = I$, where $a > 0$ is a constant, but we also address the generalized problem $u' = -a(t)u + b(t)$ and the nonlinear problem $u' = f(u, t)$. The following topics are introduced:

- 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
- 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
- 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
- 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 the model equation $u' = -au$ arises in a wide range of phenomena in physics, biology, and finance

The exposition in a nutshell.
Everything we cover is put into a practical, hands-on context. All mathematics is translated into working computing codes, and all the mathematical theory of finite difference methods presented here is motivated from a strong need to understand strange behavior of programs. Two fundamental questions saturate the text:

- How to we solve a differential equation problem and produce numbers?
- How to we trust the answer?

1 Finite difference methods

Goal.
We explain the basic ideas of finite difference methods using a simple ordinary differential equation $u' = -au$ as primary example. Emphasis is put on the reasoning when discretizing the problem and introduction of key concepts such as mesh, mesh function, finite difference approximations, averaging in a mesh, deriation of algorithms, and discrete operator notation.

1.1 A basic model for exponential decay

Our model problem is perhaps the simplest ordinary differential equation (ODE):

$$u'(t) = -au(t),$$

Here, $a > 0$ is a constant and $u'(t)$ means differentiation with respect to time t. This type of equation arises in a number of widely different phenomena where some quantity u undergoes exponential reduction. Examples include radioactive decay, population decay, investment decay, cooling of an object, pressure decay in the atmosphere, and retarded motion in fluids (for some of these models, a can be negative as well), see Section 11 for details and motivation. We have chosen this particular ODE not only because its applications are relevant, but even more because studying numerical solution methods for this simple ODE gives important insight that can be reused in much more complicated settings, in particular when solving diffusion-type partial differential equations.

The analytical solution of the ODE is found by the method of separation of variables, which results in

$$u(t) = Ce^{-at},$$

for any arbitrary constant C. To formulate a mathematical problem for which there is a unique solution, we need a condition to fix the value of C. This condition is known as the *initial condition* and stated as $u(0) = I$. That is, we know the value I of u when the process starts at $t = 0$. The exact solution is then $u(t) = Ie^{-at}$.

We seek the solution $u(t)$ of the ODE for $t \in (0, T]$. The point $t = 0$ is not included since we know u here and assume that the equation governs u for $t > 0$. The complete ODE problem then reads: find $u(t)$ such that

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

This is known as a *continuous problem* because the parameter t varies continuously from 0 to T. For each t we have a corresponding $u(t)$. There are hence infinitely many values of t and $u(t)$. The purpose of a numerical method is to formulate a corresponding *discrete* problem whose solution is characterized by a finite number of values, which can be computed in a finite number of steps on a computer.

1.2 The Forward Euler scheme

Solving an ODE like (1) by a finite difference method consists of the following 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.

Step 1: Discretizing the domain. The time domain $[0, T]$ is represented by a finite number of $N_t + 1$ points

$$0 = t_0 < t_1 < t_2 < \cdots < t_{N_t - 1} < t_{N_t} = T\,. \tag{2}$$

The collection of points $t_0, t_1, \ldots, t_{N_t}$ constitutes a *mesh* or *grid*. Often the mesh points will be uniformly spaced in the domain $[0, T]$, which means that the spacing $t_{n+1} - t_n$ is the same for all n. This spacing is often denoted by Δt, in this case $t_n = n\Delta t$.

We seek the solution u at the mesh points: $u(t_n)$, $n = 1, 2, \ldots, N_t$. Note that u^0 is already known as I. A notational short-form for $u(t_n)$, which will be used extensively, is u^n. More precisely, we let u^n be the *numerical approximation* to the exact solution $u(t_n)$ at $t = t_n$. The numerical approximation is a *mesh function*, here defined only at the mesh points. When we need to clearly distinguish between the numerical and the exact solution, we often place a subscript e on the exact solution, as in $u_{\rm e}(t_n)$. Figure 1 shows the t_n and u_n points for $n = 0, 1, \ldots, N_t = 7$ as well as $u_{\rm e}(t)$ as the dashed line. The goal of a numerical method for ODEs is to compute the mesh function by solving a finite set of *algebraic equations* derived from the original ODE problem.

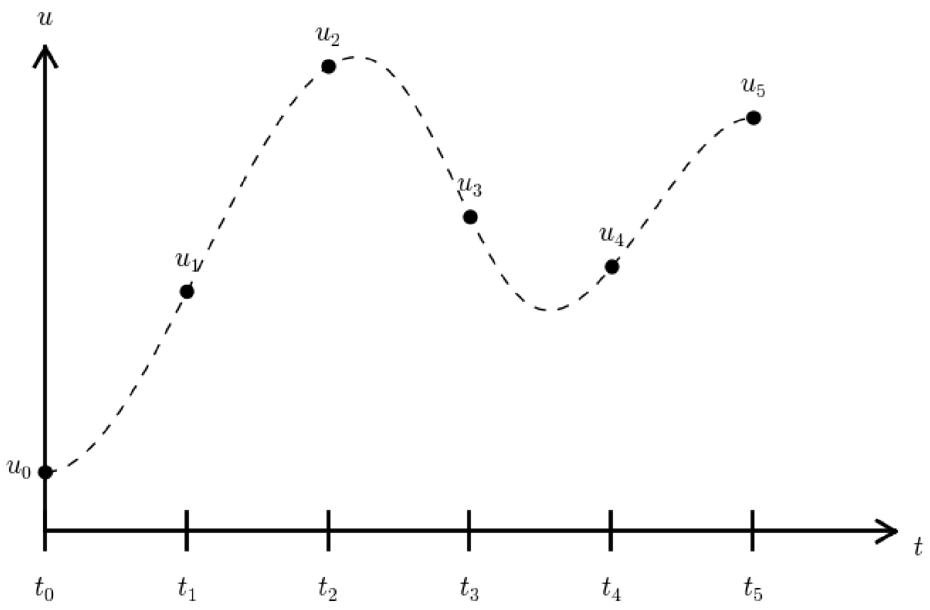


Figure 1: Time mesh with discrete solution values.

Since finite difference methods produce solutions at the mesh points only, it is an open question what the solution is between the mesh points. One can use methods for interpolation to compute the value of u between mesh points. The simplest (and most widely used) interpolation method is to assume that u varies linearly between the mesh points, see Figure 2. Given u^n and u^{n+1}, the value of u at some $t \in [t_n, t_{n+1}]$ is by linear interpolation

$$u(t) \approx u^n + \frac{u^{n+1} - u^n}{t_{n+1} - t_n}(t - t_n)\,. \tag{3}$$

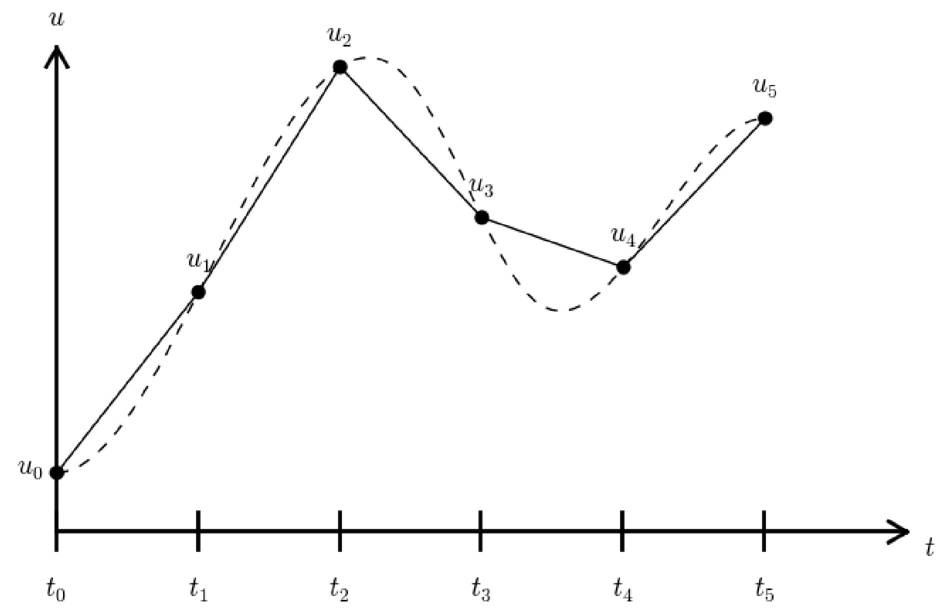


Figure 2: Linear interpolation between the discrete solution values (dashed curve is exact solution).

Step 2: Fulfilling the equation at discrete time points. The ODE is supposed to hold for all $t \in (0, T]$, i.e., at an infinite number of points. Now we relax that requirement and require that the ODE is fulfilled at a finite set of discrete points in time. The mesh points $t_1, t_2, \ldots, t_{N_t}$ are a natural choice of points. The original ODE is then reduced to the following N_t equations:

$$u'(t_n) = -au(t_n), \quad n = 1, \ldots, N_t\,. \tag{4}$$

Step 3: Replacing derivatives by finite differences. The next and most essential step of the method is to replace the derivative u' by a finite difference approximation. Let us first try a one-sided difference approximation (see Figure 3),

$$u'(t_n) \approx \frac{u^{n+1} - u^n}{t_{n+1} - t_n}\,. \tag{5}$$

Inserting this approximation in (4) results in

$$\frac{u^{n+1} - u^n}{t_{n+1} - t_n} = -au^n, \quad n = 0, 1, \ldots, N_t - 1\,. \tag{6}$$

This equation is the discrete counterpart to the original ODE problem (1), and often referred to as *finite difference scheme* or more generally as the *discrete* *equations* of the problem. The fundamental feature of these equations is that they are *algebraic* and can hence be straightforwardly solved to produce the mesh function, i.e., the values of u at the mesh points (u^n, $n = 1, 2, \ldots, N_t$).

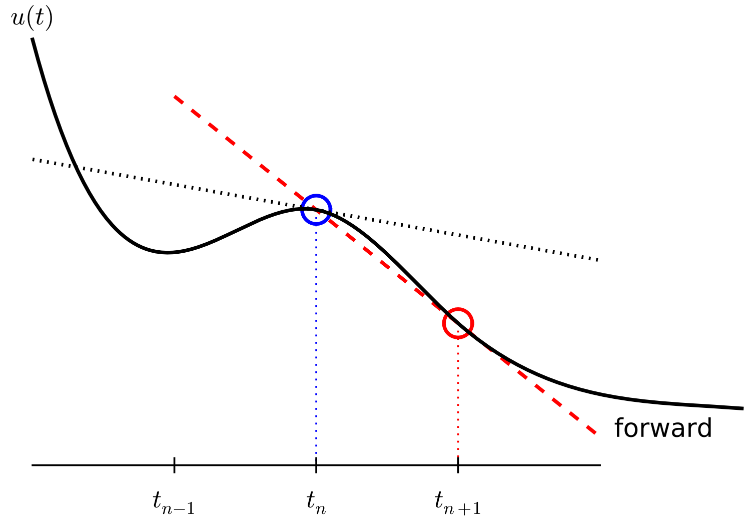


Figure 3: Illustration of a forward difference.

Step 4: Formulating a recursive algorithm. The final step is to identify the computational algorithm to be implemented in a program. The key observation here is to realize that (6) can be used to compute u^{n+1} if u^n is known. Starting with $n = 0$, u^0 is known since $u^0 = u(0) = I$, and (6) gives an equation for u^1. Knowing u^1, u^2 can be found from (6). In general, u^n in (6) can be assumed known, and then we can easily solve for the unknown u^{n+1}:

$$u^{n+1} = u^n - a(t_{n+1} - t_n)u^n \,. \tag{7}$$

We shall refer to (7) as the Forward Euler (FE) scheme for our model problem. From a mathematical point of view, equations of the form (7) are known as *difference equations* since they express how differences in u, like $u^{n+1} - u^n$, evolve with n. The finite difference method can be viewed as a method for turning a differential equation into a difference equation.

Computation with (7) is straightforward:

$$\begin{aligned}
&u_0 = I,\\
&u_1 = u^0 - a(t_1 - t_0)u^0 = I(1 - a(t_1 - t_0)),\\
&u_2 = u^1 - a(t_2 - t_1)u^1 = I(1 - a(t_1 - t_0))(1 - a(t_2 - t_1)),\\
&u^3 = u^2 - a(t_3 - t_2)u^2 = I(1 - a(t_1 - t_0))(1 - a(t_2 - t_1))(1 - a(t_3 - t_2)),
\end{aligned}$$

and so on until we reach u^{N_t}. Very often, $t_{n+1} - t_n$ is constant for all n, so we can introduce the common symbol Δt for the time step: $\Delta t = t_{n+1} - t_n$, $n = 0, 1, \ldots, N_t - 1$. Using a constant time step Δt in the above calculations gives

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

This means that we have found a closed formula for u^n, and there is no need to let a computer generate the sequence $u^1, u^2, u^3, \ldots$. However, finding such a formula for u^n is possible only for a few very simple problems, so in general finite difference equations must be solved on a computer.

As the next sections will show, the scheme (7) is just one out of many alternative finite difference (and other) methods for the model problem (1).

1.3 The Backward Euler scheme

There are several choices of difference approximations in step 3 of the finite difference method as presented in the previous section. Another alternative is

$$u'(t_n) \approx \frac{u^n - u^{n-1}}{t_n - t_{n-1}}\,. \tag{8}$$

Since this difference is based on going backward in time (t_{n-1}) for information, it is known as the Backward Euler difference. Figure 4 explains the idea.

Inserting (8) in (4) yields the Backward Euler (BE) scheme:

$$\frac{u^n - u^{n-1}}{t_n - t_{n-1}} = -au^n\,. \tag{9}$$

We assume, as explained under step 4 in Section 1.2, that we have computed $u^0, u^1, \ldots, u^{n-1}$ such that (9) can be used to compute u^n. For direct similarity with the Forward Euler scheme (7) we replace n by $n+1$ in (9) and solve for the unknown value u^{n+1}:

$$u^{n+1} = \frac{1}{1 + a(t_{n+1} - t_n)}u^n\,. \tag{10}$$

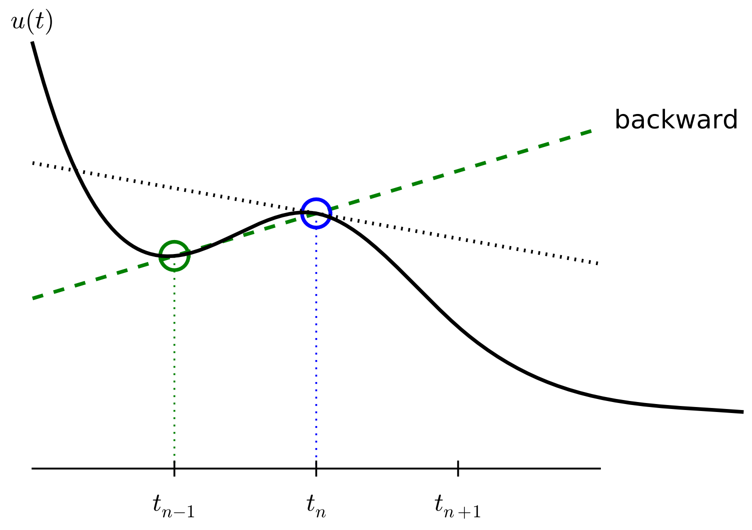


Figure 4: Illustration of a backward difference.

1.4 The Crank-Nicolson scheme

The finite difference approximations used to derive the schemes (7) and (10) are both one-sided differences, known to be less accurate than central (or midpoint) differences. We shall now construct a central difference at $t_{n+1/2} = \frac{1}{2}(t_n + t_{n+1})$, or $t_{n+1/2} = (n+\frac{1}{2})\Delta t$ if the mesh spacing is uniform in time. The approximation reads

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

Note that the fraction on the right-hand side is the same as for the Forward Euler approximation (5) and the Backward Euler approximation (8) (with n replaced by $n+1$). The accuracy of this fraction as an approximation to the derivative of u depends on *where* we seek the derivative: in the center of the interval $[t_n, t_{n+1}]$ or at the end points.

With the formula (11), where u' is evaluated at $t_{n+1/2}$, it is natural to demand the ODE to be fulfilled at the time points between the mesh points:

$$u'(t_{n+\frac{1}{2}}) = -au(t_{n+\frac{1}{2}}), \quad n = 0, \ldots, N_t - 1\,. \tag{12}$$

Using (11) in (12) results in

$$\frac{u^{n+1} - u^n}{t_{n+1} - t_n} = -au^{n+\frac{1}{2}}, \tag{13}$$

where $u^{n+\frac{1}{2}}$ is a short form for $u(t_{n+\frac{1}{2}})$. The problem is that we aim to compute u^n for integer n, implying that $u^{n+\frac{1}{2}}$ is not a quantity computed by our method.

It must therefore be expressed by the quantities that we actually produce, i.e., the numerical solution at the mesh points. One possibility is to approximate $u^{n+\frac{1}{2}}$ as an arithmetic mean of the u values at the neighboring mesh points:

$$u^{n+\frac{1}{2}} \approx \frac{1}{2}(u^n + u^{n+1})\,. \tag{14}$$

Using (14) in (13) results in

$$\frac{u^{n+1} - u^n}{t_{n+1} - t_n} = -a\frac{1}{2}(u^n + u^{n+1})\,. \tag{15}$$

Figure 5 sketches the geometric interpretation of such a centered difference.

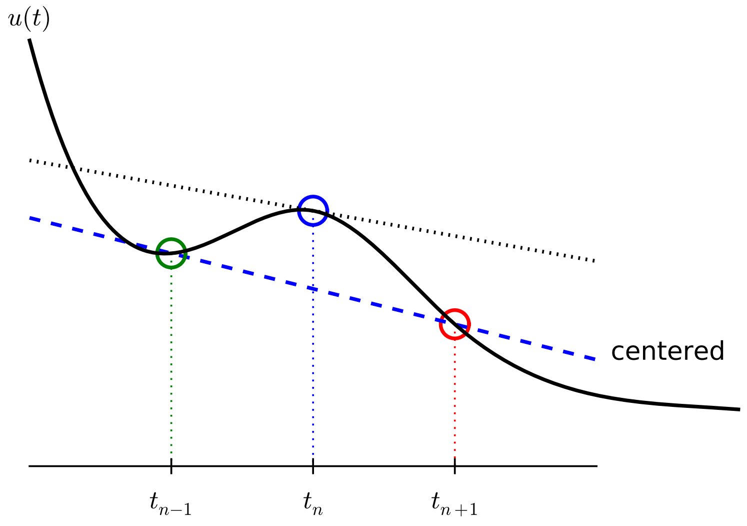


Figure 5: Illustration of a centered difference.

We assume that u^n is already computed so that u^{n+1} is the unknown, which we can solve for:

$$u^{n+1} = \frac{1 - \frac{1}{2}a(t_{n+1} - t_n)}{1 + \frac{1}{2}a(t_{n+1} - t_n)}u^n\,. \tag{16}$$

The finite difference scheme (16) is often called the Crank-Nicolson (CN) scheme or a midpoint or centered scheme.

1.5 The unifying θ-rule

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

$$\frac{u^{n+1} - u^n}{t_{n+1} - t_n} = -a(\theta u^{n+1} + (1-\theta)u^n)\,. \tag{17}$$

Observe:

- $\theta = 0$ gives the Forward Euler scheme
- $\theta = 1$ gives the Backward Euler scheme, and
- $\theta = \frac{1}{2}$ gives the Crank-Nicolson scheme.
- We may alternatively choose any other value of θ in $[0, 1]$.

As before, u^n is considered known and u^{n+1} unknown, so we solve for the latter:

$$u^{n+1} = \frac{1 - (1-\theta)a(t_{n+1} - t_n)}{1 + \theta a(t_{n+1} - t_n)}\,. \tag{18}$$

This scheme is known as the θ-rule, or alternatively written as the "theta-rule".

Derivation.
We start with replacing u' by the fraction

$$\frac{u^{n+1} - u^n}{t_{n+1} - t_n},$$

in the Forward Euler, Backward Euler, and Crank-Nicolson schemes. Then we observe that the difference between the methods concerns which point this fraction approximates the derivative. Or in other words, at which point we sample the ODE. So far this has been the end points or the midpoint of $[t_n, t_{n+1}]$. However, we may choose any point $\tilde{t} \in [t_n, t_{n+1}]$. The difficulty is that evaluating the right-hand side $-au$ at an arbitrary point faces the same problem as in Section 1.4: the point value must be expressed by the discrete u quantities that we compute by the scheme, i.e., u^n and u^{n+1}. Following the averaging idea from Section 1.4, the value of u at an arbitrary point $\tilde{t}$ can be calculated as a *weighted average*, which generalizes the arithmetic mean $\frac{1}{2}u^n + \frac{1}{2}u^{n+1}$. If we express $\tilde{t}$ as a weighted average

$$t_{n+\theta} = \theta t_{n+1} + (1-\theta)t_n,$$

where $\theta \in [0, 1]$ is the weighting factor, we can write

$$u(\tilde{t}) = u(\theta t_{n+1} + (1-\theta)t_n) \approx \theta u^{n+1} + (1-\theta)u^n\,. \tag{19}$$

We can now let the ODE hold at the point $\tilde{t} \in [t_n, t_{n+1}]$, approximate u' by the fraction $(u^{n+1} - u^n)/(t_{n+1} - t_n)$, and approximate the right-hand side $-au$ by the weighted average (19). The result is (17).

1.6 Constant time step

All schemes up to now have been formulated for a general non-uniform mesh in time: $t_0, t_1, \ldots, t_{N_t}$. Non-uniform meshes are highly relevant since one can use many points in regions where u varies rapidly, and save points in regions where u is slowly varying. This is the key idea of *adaptive* methods where the spacing of the mesh points are determined as the computations proceed.

However, a uniformly distributed set of mesh points is very common and sufficient for many applications. It therefore makes sense to present the finite difference schemes for a uniform point distribution $t_n = n\Delta t$, where Δt is the constant spacing between the mesh points, also referred to as the *time step*. The resulting formulas look simpler and are perhaps more well known.

Summary of schemes for constant time step.

$$u^{n+1} = (1 - a\Delta t)u^n \qquad \text{Forward Euler} \tag{20}$$

$$u^{n+1} = \frac{1}{1 + a\Delta t}u^n \qquad \text{Backward Euler} \tag{21}$$

$$u^{n+1} = \frac{1 - \frac{1}{2}a\Delta t}{1 + \frac{1}{2}a\Delta t}u^n \qquad \text{Crank-Nicolson} \tag{22}$$

$$u^{n+1} = \frac{1 - (1 - \theta)a\Delta t}{1 + \theta a\Delta t}u^n \qquad \text{The } \theta - \text{rule} \tag{23}$$

Not surprisingly, we present these three alternative schemes because they have different pros and cons, both for the simple ODE in question (which can easily be solved as accurately as desired), and for more advanced differential equation problems.

Test the understanding.
At this point it can be good training to apply the explained finite difference discretization techniques to a slightly different equation. Exercise 1 is therefore highly recommended to check that the key concepts are understood.

1.7 Compact operator notation for finite differences

Finite difference formulas can be tedious to write and read, especially for differential equations with many terms and many derivatives. To save space and help the reader of the scheme to quickly see the nature of the difference approximations, we introduce a compact notation. A forward difference approximation is denoted by the D_t^+ operator:

$$[D_t^+ u]^n = \frac{u^{n+1} - u^n}{\Delta t} \approx \frac{d}{dt}u(t_n)\,. \tag{24}$$

The notation consists of an operator that approximates differentiation with respect to an independent variable, here t. The operator is built of the symbol D, with the variable as subscript and a superscript denoting the type of difference. The superscript $^+$ indicates a forward difference. We place square brackets around the operator and the function it operates on and specify the mesh point, where the operator is acting, by a superscript.

The corresponding operator notation for a centered difference and a backward difference reads

$$[D_t u]^n = \frac{u^{n+\frac{1}{2}} - u^{n-\frac{1}{2}}}{\Delta t} \approx \frac{d}{dt}u(t_n), \tag{25}$$

and

$$[D_t^- u]^n = \frac{u^n - u^{n-1}}{\Delta t} \approx \frac{d}{dt}u(t_n)\,. \tag{26}$$

Note that the superscript $^-$ denotes the backward difference, while no superscript implies a central difference.

An averaging operator is also convenient to have:

$$[\overline{u}^t]^n = \frac{1}{2}(u^{n-\frac{1}{2}} + u^{n+\frac{1}{2}}) \approx u(t_n) \tag{27}$$

The superscript t indicates that the average is taken along the time coordinate. The common average $(u^n + u^{n+1})/2$ can now be expressed as $[\overline{u}^t]^{n+\frac{1}{2}}$. (When also spatial coordinates enter the problem, we need the explicit specification of the coordinate after the bar.)

The Backward Euler finite difference approximation to $u' = -au$ can be written as follows utilizing the compact notation:

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

In difference equations we often place the square brackets around the whole equation, to indicate at which mesh point the equation applies, since each term is supposed to be approximated at the same point:

$$[D_t^- u = -au]^n\,. \tag{28}$$

The Forward Euler scheme takes the form

$$[D_t^+ u = -au]^n, \tag{29}$$

while the Crank-Nicolson scheme is written as

$$[D_t u = -a\overline{u}^t]^{n+\frac{1}{2}}\,. \tag{30}$$

Question.

Apply (25) and (27) and write out the expressions to see that (30) is indeed the Crank-Nicolson scheme.

The θ-rule can be specified by

$$[\bar{D}_t u = -a\overline{u}^{t,\theta}]^{n+\theta}, \tag{31}$$

if we define a new time difference and a *weighted averaging operator*:

$$[\bar{D}_t u]^{n+\theta} = \frac{u^{n+1}-u^n}{t^{n+1}-t^n}, \tag{32}$$

$$[\overline{u}^{t,\theta}]^{n+\theta} = (1-\theta)u^n + \theta u^{n+1} \approx u(t_{n+\theta}), \tag{33}$$

where $\theta \in [0,1]$. Note that for $\theta = \frac{1}{2}$ we recover the standard centered difference and the standard arithmetic mean. The idea in (31) is to sample the equation at $t_{n+\theta}$, use a skew difference at that point $[\bar{D}_t u]^{n+\theta}$, and a skew mean value. An alternative notation is

$$[D_t u]^{n+\frac{1}{2}} = \theta[-au]^{n+1} + (1-\theta)[-au]^n\,.$$

Looking at the various examples above and comparing them with the underlying differential equations, we see immediately which difference approximations that have been used and at which point they apply. Therefore, the compact notation effectively communicates the reasoning behind turning a differential equation into a difference equation.

2 Implementation

Goal.
We want make a computer program for solving

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

by finite difference methods. The program should also display the numerical solution as a curve on the screen, preferably together with the exact solution. We shall also be concerned with program testing, user interfaces, and computing convergence rates.

All programs referred to in this section are found in the `src/decay` directory (we use the classical Unix term *directory* for what many others nowadays call *folder*).

Mathematical problem. We want to explore the Forward Euler scheme, the Backward Euler, and the Crank-Nicolson schemes applied to our model problem. From an implementational point of view, it is advantageous to implement the θ-rule

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

since it can generate the three other schemes by various of choices of θ: $\theta = 0$ for Forward Euler, $\theta = 1$ for Backward Euler, and $\theta = 1/2$ for Crank-Nicolson. Given a, $u^0 = I$, T, and Δt, our task is to use the θ-rule to compute $u^1, u^2, \ldots, u^{N_t}$, where $t_{N_t} = N_t\Delta t$, and N_t the closest integer to $T/\Delta t$.

Computer Language: Python. Any programming language can be used to generate the u^{n+1} values from the formula above. However, in this document we shall mainly make use of Python of several reasons:

- 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 a full-fledged, very powerful programming language.
- Python is similar to, but much simpler to work with and results in more reliable code than C++.
- 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.
- 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.

Learning Python is easy. Many newcomers to the language will probably learn enough from the forthcoming examples to perform their own computer experiments. The examples start with simple Python code and gradually make use of more powerful constructs as we proceed. As long as it is not inconvenient for the problem at hand, our Python code is made as close as possible to MATLAB code for easy transition between the two languages.

Readers who feel the Python examples are too hard to follow will probably benefit from read a tutorial, e.g.,

- The Official Python Tutorial
- Python Tutorial on tutorialspoint.com
- Interactive Python tutorial site
- A Beginner’s Python Tutorial

The author also has a book [4] that introduces scientific programming with Python.

2.1 Making a solver function

We choose to have an array `u` for storing the u^n values, $n = 0, 1, \ldots, N_t$. The algorithmic steps are

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

Function for computing the numerical solution. The following Python function takes the input data of the problem (I, a, T, Δt, θ) as arguments and returns two arrays with the solution $u^0, \ldots, u^{N_t}$ and the mesh points $t_0, \ldots, t_{N_t}$, respectively:

```
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
```

The `numpy` library contains a lot of functions for array computing. Most of the function names are similar to what is found in the alternative scientific computing language MATLAB. Here we make use of

- `zeros(Nt+1)` for creating an array of a size `Nt+1` and initializing the elements to zero
- `linspace(0, T, Nt+1)` for creating an array with `Nt+1` coordinates uniformly distributed between `0` and `T`

The `for` loop deserves a comment, especially for newcomers to Python. The construction `range(0, Nt, s)` generates all integers from `0` to `Nt` in steps of `s`, *but not including* `Nt`. Omitting `s` means `s=1`. For example, `range(0, 6, 3)` gives `0` and `3`, while `range(0, Nt)` generates `0`, `1`, ..., `Nt-1`. Our loop implies the following assignments to `u[n+1]`: `u[1]`, `u[2]`, ..., `u[Nt]`, which is what we want since `u` has length `Nt+1`. The first index in Python arrays or lists is *always* `0` and the last is then `len(u)-1`. The length of an array `u` is obtained by `len(u)` or `u.size`.

To compute with the `solver` function, we need to *call* it. Here is a sample call:

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

Integer division. The shown implementation of the `solver` may face problems and wrong results if `T`, `a`, `dt`, and `theta` are given as integers, see Exercises 4 and 5. The problem is related to *integer division* in Python (as well as in Fortran, C, C++, and many other computer languages): `1/2` becomes `0`, while `1.0/2`, `1/2.0`, or `1.0/2.0` all become `0.5`. It is enough that at least the nominator or the denominator is a real number (i.e., a `float` object) to ensure correct mathematical division. Inserting a conversion `dt = float(dt)` guarantees that `dt` is `float` and avoids problems in Exercise 5.

Another problem with computing $N_t = T/\Delta t$ is that we should round N_t to the nearest integer. With `Nt = int(T/dt)` the `int` operation picks the largest integer smaller than `T/dt`. Correct mathematical rounding as known from school is obtained by

```
Nt = int(round(T/dt))
```

The complete version of our improved, safer `solver` function then becomes

```
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
```

Doc strings. Right below the header line in the `solver` function there is a Python string enclosed in triple double quotes `"""`. The purpose of this string object is to document what the function does and what the arguments are. In this case the necessary documentation do not span more than one line, but with triple double quoted strings the text may span several lines:

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

Such documentation strings appearing right after the header of a function are called *doc strings*. There are tools that can automatically produce nicely formatted documentation by extracting the definition of functions and the contents of doc strings.

It is strongly recommended to equip any function whose purpose is not obvious with a doc string. Nevertheless, the forthcoming text deviates from this rule if the function is explained in the text.

Formatting of numbers. Having computed the discrete solution `u`, it is natural to look at the numbers:

```
# Write out a table of t and u values:
for i in range(len(t)):
    print t[i], u[i]
```

This compact `print` statement gives unfortunately quite ugly output because the `t` and `u` values are not aligned in nicely formatted columns. To fix this problem, we recommend to use the *printf format*, supported most programming languages inherited from C. Another choice is Python's recent *format string syntax*.

Writing `t[i]` and `u[i]` in two nicely formatted columns is done like this with the printf format:

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

The percentage signs signify "slots" in the text where the variables listed at the end of the statement are inserted. For each "slot" one must specify a format for how the variable is going to appear in the string: `s` for pure text, `d` for an integer, `g` for a real number written as compactly as possible, `9.3E` for scientific notation with three decimals in a field of width 9 characters (e.g., `-1.351E-2`), or `.2f` for standard decimal notation with two decimals formatted with minimum width. The printf syntax provides a quick way of formatting tabular output of numbers with full control of the layout.

The alternative *format string syntax* looks like

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

As seen, this format allows logical names in the "slots" where `t[i]` and `u[i]` are to be inserted. The "slots" are surrounded by curly braces, and the logical name is followed by a colon and then the printf-like specification of how to format real numbers, integers, or strings.

Running the program. The function and main program shown above must be placed in a file, say with name decay_v1.py (v1 stands for "version 1" - we shall make numerous different versions of this program). Make sure you write the code with a suitable text editor (Gedit, Emacs, Vim, Notepad++, or similar). The program is run by executing the file this way:

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

The text `Terminal>` just indicates a prompt in a Unix/Linux or DOS terminal window. After this prompt, which will look different in your terminal window, depending on the terminal application and how it is set up, commands like `python decay_v1.py` can be issued. These commands are interpreted by the operating system.

We strongly recommend to run Python programs within the IPython shell. First start IPython by typing `ipython` in the terminal window. Inside the IPython shell, our program `decay_v1.py` is run by the command `run decay_v1.py`:

```
Terminal> ipython

In [1]: run decay_v1.py
t= 0.000 u=1
t= 0.800 u=0.384615
t= 1.600 u=0.147929
t= 2.400 u=0.0568958
t= 3.200 u=0.021883
t= 4.000 u=0.00841653
t= 4.800 u=0.00323713
t= 5.600 u=0.00124505
t= 6.400 u=0.000478865
t= 7.200 u=0.000184179
t= 8.000 u=7.0838e-05

In [2]:
```

The advantage of running programs in IPython are many: previous commands are easily recalled with the up arrow, `%pdb` turns on debugging so that variables can be examined if the program aborts due to an exception, output of commands are stored in variables, programs and statements can be profiled, any operating system command can be executed, modules can be loaded automatically and other customizations can be performed when starting IPython – to mention a few of the most useful features.

Although running programs in IPython is strongly recommended, most execution examples in the forthcoming text use the standard Python shell with prompt `>>>` and run programs through a typesetting like

```
Terminal> python programname
```

The reason is that such typesetting makes the text more compact in the vertical direction than showing sessions with IPython syntax.

2.2 Verifying the implementation

It is easy to make mistakes while deriving and implementing numerical algorithms, so we should never believe in the printed u values before they have been thoroughly verified. The most obvious idea is to compare the computed solution with the exact solution, when that exists, but there will always be a discrepancy between these two solutions because of the numerical approximations. The challenging question is whether we have the mathematically correct discrepancy or if we have another, maybe small, discrepancy due to both an approximation error and an error in the implementation.

The purpose of *verifying* a program is to bring evidence for the property that there are no errors in the implementation. To avoid mixing unavoidable approximation errors and undesired implementation errors, we should try to make tests where we have some exact computation of the discrete solution or at least parts of it. Examples will show how this can be done.

Running a few algorithmic steps by hand. The simplest approach to produce a correct reference for the discrete solution u of finite difference equations is to compute a few steps of the algorithm by hand. Then we can compare the hand calculations with numbers produced by the program.

A straightforward approach is to use a calculator and compute u^1, u^2, and u^3. With $I = 0.1$, $\theta = 0.8$, and $\Delta t = 0.8$ we get

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

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

Comparison of these manual calculations with the result of the `solver` function is carried out in the function

```
def verify_three_steps():
    """Compare three steps with known manual computations."""
    theta = 0.8; a = 2; I = 0.1; dt = 0.8
    u_by_hand = array([I,
                       0.0298245614035,
                       0.00889504462912,
                       0.00265290804728])

    Nt = 3  # number of time steps
    u, t = solver(I=I, a=a, T=Nt*dt, dt=dt, theta=theta)

    tol = 1E-15  # tolerance for comparing floats
    difference = abs(u - u_by_hand).max()
    success = difference <= tol
    return success
```

The main program, where we call the `solver` function and print `u`, is now put in a separate function `main`:

```
def main():
    u, t = solver(I=1, a=2, T=8, dt=0.8, theta=1)
    # Write out a table of t and u values:
    for i in range(len(t)):
        print 't=%6.3f u=%g' % (t[i], u[i])
        # or print 't={t:6.3f} u={u:g}'.format(t=t[i], u=u[i])
```

The main program in the file may now first run the verification test and then go on with the real simulation (`main()`) only if the test is passed:

```
if verify_three_steps():
    main()
else:
    print 'Bug in the implementation!'
```

Since the verification test is always done, future errors introduced accidentally in the program have a good chance of being detected.

Caution: choice of parameter values.

For the choice of values of parameters in verification tests one should stay away from integers, especially 0 and 1, as these can simplify formulas too much for test purposes. For example, with $\theta = 1$ the nominator in the formula for u^n will be the same for all a and Δt values. One should therefore choose more "arbitrary" values, say $\theta = 0.8$ and $I = 0.1$.

It is essential that verification tests can be automatically run at *any* time. For this purpose, there are test frameworks and corresponding programming rules that allow us to request running through a suite of test cases (see Section 3.4), but in this very early stage of program development we just implement and run the verification in our own code so that every detail is visible and understood.

The complete program including the `verify_three_steps*` functions is found in the file `decay_verf1.py` (`verf1` is a short name for "verification, version 1").

Comparison with an exact discrete solution. Sometimes it is possible to find a closed-form *exact discrete solution* that fulfills the discrete finite difference equations. The implementation can then be verified against the exact discrete solution. This is usually the best technique for verification.

Define

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

Manual computations with the θ-rule results in

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

We have then established the exact discrete solution as

$$u^n = IA^n\,. \tag{34}$$

Caution.
One should be conscious about the different meanings of the notation on the left- and right-hand side of (34): on the left, n in u^n is a superscript reflecting a counter of mesh points (t_n), while on the right, n is the power in the exponentiation A^n.

Comparison of the exact discrete solution and the computed solution is done in the following function:

```
def verify_exact_discrete_solution():

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

    theta = 0.8; a = 2; I = 0.1; dt = 0.8
    Nt = int(8/dt)  # no of steps
    u, t = solver(I=I, a=a, T=Nt*dt, dt=dt, theta=theta)
    u_de = array([exact_discrete_solution(n, I, a, theta, dt)
                  for n in range(Nt+1)])
    difference = abs(u_de - u).max()  # max deviation
    tol = 1E-15  # tolerance for comparing floats
    success = difference <= tol
    return success
```

The complete program is found in the file `decay_verf2.py` (`verf2` is a short name for "verification, version 2").

Local functions.
One can define a function inside another function, here called a *local function* (also known as *closure*) inside a *parent function.* A local function is invisible outside the parent function. A convenient property is that any local function has access to all variables defined in the parent function, also if we send the local function to some other function as argument (!). In the present example, it means that the local function `exact_discrete_solution` does not need its five arguments as the values can alternatively be accessed through the local variables defined in the

parent function `verify_exact_discrete_solution`. We can send such an `exact_discrete_solution` without arguments to any other function and `exact_discrete_solution` will still have access to `n`, `I`, `a`, and so forth defined in its parent function.

2.3 Computing the numerical error as a mesh function

Now that we have evidence for a correct implementation, we are in a position to compare the computed u^n values in the `u` array with the exact u values at the mesh points, in order to study the error in the numerical solution.

Let us first make a function for the analytical solution $u_{\mathrm{e}}(t) = Ie^{-at}$ of the model problem:

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

A natural way to compare the exact and discrete solutions is to calculate their difference as a mesh function:

$$e^n = u_{\mathrm{e}}(t_n) - u^n, \quad n = 0, 1, \ldots, N_t\,. \tag{35}$$

We may view $u_{\mathrm{e}}^n = u_{\mathrm{e}}(t_n)$ as the representation of $u_{\mathrm{e}}(t)$ as a mesh function rather than a continuous function defined for all $t \in [0, T]$ (u_{e}^n is often called the *representative* of u_{e} on the mesh). Then, $e^n = u_{\mathrm{e}}^n - u^n$ is clearly the difference of two mesh functions. This interpretation of e^n is natural when programming.

The error mesh function e^n can be computed by

```
u, t = solver(I, a, T, dt, theta)  # Numerical sol.
u_e = exact_solution(t, I, a)      # Representative of exact sol.
e = u_e - u
```

Note that the mesh functions `u` and `u_e` are represented by arrays and associated with the points in the array `t`.

Array arithmetics.

The last statements

```
u_e = exact_solution(t, I, a)
e = u_e - u
```

are primary examples of array arithmetics: `t` is an array of mesh points that we pass to `exact_solution`. This function evaluates `-a*t`, which is a scalar times an array, meaning that the scalar is multiplied with each array element. The result is an array, let us call it `tmp1`. Then `exp(tmp1)` means applying the exponential function to each element in `tmp`, resulting an array, say `tmp2`. Finally, `I*tmp2` is computed (scalar times array) and `u_e` refers to this array returned from `exact_solution`. The expression `u_e - u` is the difference between two arrays, resulting in a new array referred to by `e`.

2.4 Computing the norm of the numerical error

Instead of working with the error e^n on the entire mesh, we often want one number expressing the size of the error. This is obtained by taking the norm of the error function.

Let us first define norms of a function $f(t)$ defined for all $t \in [0, T]$. Three common norms are

$$||f||_{L^2} = \left(\int_0^T f(t)^2 dt \right)^{1/2}, \tag{36}$$

$$||f||_{L^1} = \int_0^T |f(t)| dt, \tag{37}$$

$$||f||_{L^\infty} = \max_{t \in [0,T]} |f(t)| . \tag{38}$$

The L^2 norm (36) ("L-two norm") has nice mathematical properties and is the most popular norm. It is a generalization of the well-known Eucledian norm of vectors to functions. The L^∞ is also called the max norm or the supremum norm. In fact, there is a whole family of norms,

$$||f||_{L^p} = \left(\int_0^T f(t)^p dt \right)^{1/p}, \tag{39}$$

with p real. In particular, $p = 1$ corresponds to the L^1 norm above while $p = \infty$ is the L^∞ norm.

Numerical computations involving mesh functions need corresponding norms. Given a set of function values, f^n, and some associated mesh points, t_n, a numerical integration rule can be used to calculate the L^2 and L^1 norms defined above. Imagining that the mesh function is extended to vary linearly between the mesh points, the Trapezoidal rule is in fact an exact integration rule. A possible modification of the L^2 norm for a mesh function f^n on a uniform mesh with spacing Δt is therefore the well-known Trapezoidal integration formula

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

A common approximation of this expression, motivated by the convenience of having a simpler formula, is

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

This is called the discrete L^2 norm and denoted by ℓ^2. The error in $||f||^2_{\ell^2}$ compared with the Trapezoidal integration formula is $\Delta t((f^0)^2 + (f^{N_t})^2)/2$, which means perturbed weights at the end points of the mesh function, and the error goes to zero as $\Delta t \to 0$. As long as we are consistent and stick to one kind of integration rule for the norm of a mesh function, the details and accuracy of this rule is not of concern.

The three discrete norms for a mesh function f^n, corresponding to the L^2, L^1, and L^∞ norms of $f(t)$ defined above, are defined by

$$||f^n||_{\ell^2} \left(\Delta t \sum_{n=0}^{N_t} (f^n)^2\right)^{1/2}, \tag{40}$$

$$||f^n||_{\ell^1} \Delta t \sum_{n=0}^{N_t} |f^n| \tag{41}$$

$$||f^n||_{\ell^\infty} \max_{0\leq n\leq N_t} |f^n|\,. \tag{42}$$

Note that the L^2, L^1, ℓ^2, and ℓ^1 norms depend on the length of the interval of interest (think of $f = 1$, then the norms are proportional to $\sqrt{T}$ or T). In some applications it is convenient to think of a mesh function as just a vector of function values and neglect the information of the mesh points. Then we can replace Δt by T/N_t and drop T. Moreover, it is convenient to divide by the total length of the vector, $N_t + 1$, instead of N_t. This reasoning gives rise to the *vector norms* for a vector $f = (f_0, \ldots, f_N)$:

$$||f||_2 = \left(\frac{1}{N+1} \sum_{n=0}^{N} (f_n)^2\right)^{1/2}, \tag{43}$$

$$||f||_1 = \frac{1}{N+1} \sum_{n=0}^{N} |f_n| \tag{44}$$

$$||f||_{\ell^\infty} = \max_{0\leq n\leq N} |f_n|\,. \tag{45}$$

Here we have used the common vector component notation with subscripts (f_n) and N as length. We will mostly work with mesh functions and use the discrete ℓ^2 norm (40) or the max norm ℓ^∞ (42), but the corresponding vector norms (43)-(45) are also much used in numerical computations, so it is important to know the different norms and the relations between them.

A single number that expresses the size of the numerical error will be taken as $||e^n||_{\ell^2}$ and called E:

$$E = \sqrt{\Delta t \sum_{n=0}^{N_t} (e^n)^2} \tag{46}$$

The corresponding Python code, using array arithmetics, reads

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

The `sum` function comes from `numpy` and computes the sum of the elements of an array. Also the `sqrt` function is from `numpy` and computes the square root of each element in the array argument.

Scalar computing. Instead of doing array computing `sqrt(dt*sum(e**2))` we can compute with one element at a time:

```
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)
```

Such element-wise computing, often called *scalar* computing, takes more code, is less readable, and runs much slower than what we can achieve with array computing.

2.5 Plotting solutions

Having the `t` and `u` arrays, the approximate solution `u` is visualized by the intuitive command `plot(t, u)`:

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

Plotting multiple curves. It will be illustrative to also plot $u_e(t)$ for comparison. Doing a `plot(t, u_e)` is not exactly what we want: the `plot` function draws straight lines between the discrete points `(t[n], u_e[n])` while $u_e(t)$ varies as an exponential function between the mesh points. The technique for showing the "exact" variation of $u_e(t)$ between the mesh points is to introduce a very fine mesh for $u_e(t)$:

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

With more than one curve in the plot we need to associate each curve with a legend. We also want appropriate names on the axis, a title, and a file containing the plot as an image for inclusion in reports. The Matplotlib package (`matplotlib.pyplot`) contains functions for this purpose. The names of the functions are similar to the plotting functions known from MATLAB. A complete plot session then becomes

```
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()
```

Note that `savefig` here creates a PNG file whose name reflects the values of θ and Δt so that we can easily distinguish files from different runs with θ and Δt.

A bit more sophisticated and easy-to-read filename can be generated by mapping the θ value to acronyms for the three common schemes: FE (Forward Euler, $\theta = 0$), BE (Backward Euler, $\theta = 1$), CN (Crank-Nicolson, $\theta = 0.5$). A Python dictionary is ideal for such a mapping from numbers to strings:

```
theta2name = {0: 'FE', 1: 'BE', 0.5: 'CN'}
savefig('%s_%g.png' % (theta2name[theta], dt))
```

Experiments with computing and plotting. Let us wrap up the computation of the error measure and all the plotting statements in a function `explore`. This function can be called for various θ and Δt values to see how the error varies with the method and the mesh resolution:

```
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).
    """
    u, t = solver(I, a, T, dt, theta)    # Numerical solution
    u_e = exact_solution(t, I, a)
    e = u_e - u
    E = sqrt(dt*sum(e**2))
    if makeplot:
        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))
        theta2name = {0: 'FE', 1: 'BE', 0.5: 'CN'}
        savefig('%s_%g.png' % (theta2name[theta], dt))
        savefig('%s_%g.pdf' % (theta2name[theta], dt))
        savefig('%s_%g.eps' % (theta2name[theta], dt))
        show()
    return E
```

The `figure()` call is key here: without it, a new `plot` command will draw the new pair of curves in the same plot window, while we want the different pairs to appear in separate windows and files. Calling `figure()` ensures this.

The `explore` function stores the plot in three different image file formats: PNG, PDF, and EPS (Encapsulated PostScript). The PNG format is aimed at being included in HTML files, the PDF format in pdfLaTeX documents, and the EPS format in LaTeX documents. Frequently used viewers for these image files on Unix systems are `gv` (comes with Ghostscript) for the PDF and EPS formats and `display` (from the ImageMagick) suite for PNG files:

```
Terminal> gv BE_0.5.pdf
Terminal> gv BE_0.5.eps
Terminal> display BE_0.5.png
```

The complete code containing the functions above resides in the file `decay_plot_mpl.py`. Running this program results in

```
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
```

We observe that reducing Δt by a factor of 10 increases the accuracy for all three methods (θ values). We also see that the combination of $\theta = 0.5$ and a small time step $\Delta t = 0.04$ gives a much more accurate solution, and that $\theta = 0$ and $\theta = 1$ with $\Delta t = 0.4$ result in the least accurate solutions.

Figure 6 demonstrates that the numerical solution for $\Delta t = 0.4$ clearly lies below the exact curve, but that the accuracy improves considerably by reducing the time step by a factor of 10.

Combining plot files. Mounting two PNG files, as done in the figure, is easily done by the `montage` program from the ImageMagick suite:

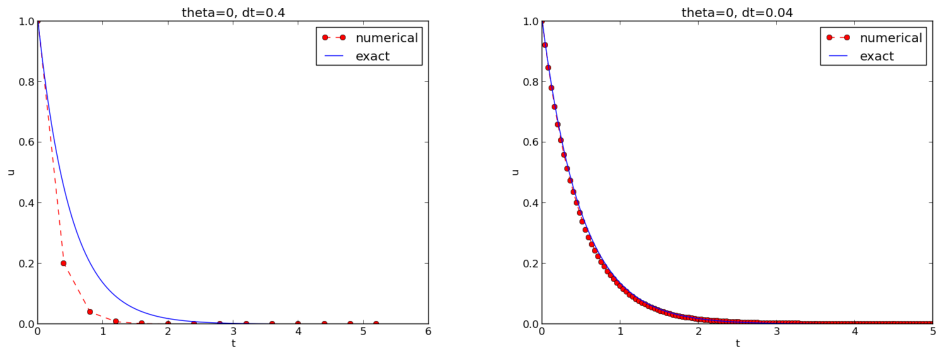


Figure 6: The Forward Euler scheme for two values of the time step.

```
Terminal> montage -background white -geometry 100% -tile 2x1 \
          FE_0.4.png FE_0.04.png FE1.png
Terminal> convert -trim FE1.png FE1.png
```

The `-geometry` argument is used to specify the size of the image, and here we preserve the individual sizes of the images. The `-tile HxV` option specifies `H` images in the horizontal direction and `V` images in the vertical direction. A series of image files to be combined are then listed, with the name of the resulting combined image, here `FE1.png` at the end. The `convert -trim` command removes surrounding white areas in the figure (an operation usually known as *cropping* in image manipulation programs).

For LaTeX reports it is not recommended to use `montage` and PNG files as the result has too low resolution. Instead, plots should be made in the PDF format and combined using the `pdftk`, `pdfnup`, and `pdfcrop` tools (on Linux/Unix):

```
Terminal> pdftk FE_0.4.png FE_0.04.png output tmp.pdf
Terminal> pdfnup --nup 2x1 tmp.pdf     # output in tmp-nup.pdf
Terminal> pdfcrop tmp-nup.pdf FE1.png  # output in FE1.png
```

Here, `pdftk` combines images into a multi-page PDF file, `pdfnup` combines the images in individual pages to a table of images (pages), and `pdfcrop` removes white margins in the resulting combined image file.

The behavior of the two other schemes is shown in Figures 7 and 8. Crank-Nicolson is obviously the most accurate scheme from this visual point of view.

Plotting with SciTools. The SciTools package provides a unified plotting interface, called Easyviz, to many different plotting packages, including Matplotlib, Gnuplot, Grace, MATLAB, VTK, OpenDX, and VisIt. The syntax is very similar to that of Matplotlib and MATLAB. In fact, the plotting commands

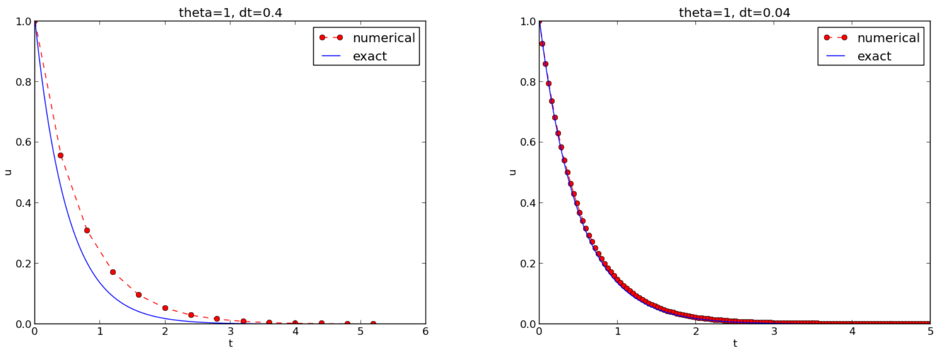


Figure 7: The Backward Euler scheme for two values of the time step.

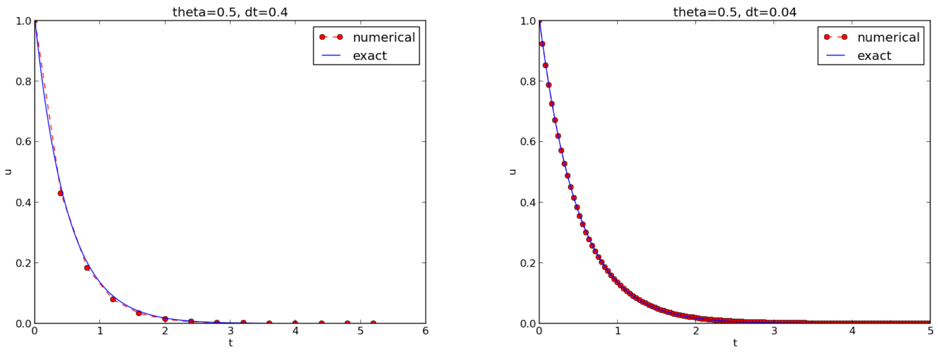


Figure 8: The Crank-Nicolson scheme for two values of the time step.

shown above look the same in SciTool's Easyviz interface, apart from the import statement, which reads

```
from scitools.std import *
```

This statement performs a `from numpy import *` as well as an import of the most common pieces of the Easyviz (`scitools.easyviz`) package, along with some additional numerical functionality.

With Easyviz one can merge several plotting commands into a single one using keyword arguments:

```
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)
```

The `decay_plot_st.py` file contains such a demo.

By default, Easyviz employs Matplotlib for plotting, but Gnuplot and Grace are viable alternatives:

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

The backend used for creating plots (and numerous other options) can be permanently set in SciTool's configuration file.

All the Gnuplot windows are launched without any need to kill one before the next one pops up (as is the case with Matplotlib) and one can press the key 'q' anywhere in a plot window to kill it. Another advantage of Gnuplot is the automatic choice of sensible and distinguishable line types in black-and-white PDF and PostScript files.

Regarding functionality for annotating plots with title, labels on the axis, legends, etc., we refer to the documentation of Matplotlib and SciTools for more detailed information on the syntax. The hope is that the programming syntax explained so far suffices for understanding the code and learning more from a combination of the forthcoming examples and other resources such as books and web pages.

Test the understanding.

Exercise 2 asks you to implement a solver for a problem that is slightly different from the one above. You may use the `solver` and `explore` functions explained above as a starting point. Apply the new solver to Exercise 3.

2.6 Creating command-line interfaces

It is good programming practice to let programs read input from the user rather than require the user to edit the source code when trying out new values of input parameters. Reading input from the command line is a simple and flexible way of interacting with the user. Python stores all the command-line arguments in the list `sys.argv`, and there are, in principle, two ways of programming with command-line arguments in Python:

- Decide upon a sequence of parameters on the command line and read their values directly from the `sys.argv[1:]` list (`sys.argv[0]` is the just program name).
- Use option-value pairs (`--option value`) on the command line to override default values of input parameters, and utilize the `argparse.ArgumentParser` tool to interact with the command line.

Both strategies will be illustrated next.

Reading a sequence of command-line arguments. The decay_plot_mpl.py program needs the following input data: I, a, T, an option to turn the plot on or off (makeplot), and a list of Δt values.

The simplest way of reading this input from the command line is to say that the first four command-line arguments correspond to the first four points in the list above, in that order, and that the rest of the command-line arguments are the Δt values. The input given for makeplot can be a string among 'on', 'off', 'True', and 'False'. The code for reading this input is most conveniently put in a function:

```
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
```

One should note the following about the constructions in the program above:

- Everything on the command line ends up in a *string* in the list sys.argv. Explicit conversion to, e.g., a float object is required if the string as a number we want to compute with.
- The value of makeplot is determined from a boolean expression, which becomes True if the command-line argument is either 'on' or 'True', and False otherwise.
- It is easy to build the list of Δt values: we simply run through the rest of the list, sys.argv[5:], convert each command-line argument to float, and collect these float objects in a list, using the compact and convenient *list comprehension* syntax in Python.

The loops over θ and Δt values can be coded in a main function:

```
def main():
    I, a, T, makeplot, dt_values = read_command_line()
    for theta in 0, 0.5, 1:
        for dt in dt_values:
            E = explore(I, a, T, dt, theta, makeplot)
            print '%3.1f %6.2f: %12.3E' % (theta, dt, E)
```

The complete program can be found in decay_cml.py.

Working with an argument parser. Python's `ArgumentParser` tool in the `argparse` module makes it easy to create a professional command-line interface to any program. The documentation of `ArgumentParser` demonstrates its versatile applications, so we shall here just list an example containing basic features. On the command line we want to specify option-value pairs for I, a, and T, e.g., `--a 3.5 --I 2 --T 2`. Including `--makeplot` turns the plot on and excluding this option turns the plot off. The Δt values can be given as `--dt 1 0.5 0.25 0.1 0.01`. Each parameter must have a sensible default value so that we specify the option on the command line only when the default value is not suitable.

We introduce a function for defining the mentioned command-line options:

```
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
```

Each command-line option is defined through the `parser.add_argument` method. Alternative options, like the short `--I` and the more explaining version `--initial_condition` can be defined. Other arguments are `type` for the Python object type, a default value, and a help string, which gets printed if the command-line argument `-h` or `--help` is included. The `metavar` argument specifies the value associated with the option when the help string is printed. For example, the option for I has this help output:

```
Terminal> python decay_argparse.py -h
  ...
  --I I, --initial_condition I
                        initial condition, u(0)
  ...
```

The structure of this output is

```
--I metavar, --initial_condition metavar
                      help-string
```

The `--makeplot` option is a pure flag without any value, implying a true value if the flag is present and otherwise a false value. The `action='store_true'` makes an option for such a flag.

Finally, the `--dt` option demonstrates how to allow for more than one value (separated by blanks) through the `nargs='+'` keyword argument. After the command line is parsed, we get an object where the values of the options are stored as attributes. The attribute name is specified by the `dist` keyword argument, which for the `--dt` option is `dt_values`. Without the `dest` argument, the value of an option `--opt` is stored as the attribute `opt`.

The code below demonstrates how to read the command line and extract the values for each option:

```
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
```

The `main` function remains the same as in the `decay_cml.py` code based on reading from `sys.argv` directly. A complete program featuring the demo above of `ArgumentParser` appears in the file `decay_argparse.py`.

2.7 Creating a graphical web user interface

The Python package Parampool can be used to automatically generate a web-based *graphical user interface* (GUI) for our simulation program. Although the programming technique dramatically simplifies the efforts to create a GUI, the forthcoming material on equipping our `decay_mod` module with a GUI is quite technical and of significantly less importance than knowing how to make a command-line interface (Section 2.6). There is no danger in jumping right to Section 2.8.

Making a compute function. The first step is to identify a function that performs the computations and that takes the necessary input variables as arguments. This is called the *compute function* in Parampool terminology. We may start with a copy of the basic file `decay_plot_mpl.py`, which has a `main` function displayed in Section 2.5 for carrying out simulations and plotting for a series of Δt values. Now we want to control and view the same experiments from a web GUI.

To tell Parampool what type of input data we have, we assign default values of the right type to all arguments in the main function and call it `main_GUI`:

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

The compute function must return the HTML code we want for displaying the result in a web page. Here we want to show plots of the numerical and exact solution for different methods and Δt values. The plots can be organized in a table with θ (methods) varying through the columns and Δt varying through the rows. Assume now that a new version of the `explore` function not only returns the error `E` but also HTML code containing the plot. Then we can write the `main_GUI` function as

```
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
```

Rather than creating plot files and showing the plot on the screen, the new version of the `explore` function makes a string with the PNG code of the plot and embeds that string in HTML code. This action is conveniently performed by Parampool's `save_png_to_str` function:

```
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)
```

Note that we now write `plt.plot`, `plt.xlabel`, etc. The `html_text` string is long and contains all the characters that build up the PNG file of the current plot. The new `explore` function can make use of the above code snippet and return `html_text` along with `E`.

Generating the user interface. The web GUI is automatically generated by the following code, placed in 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 the `decay_GUI_generate.py` program results in three new files whose names are specified in the call to `generate`:

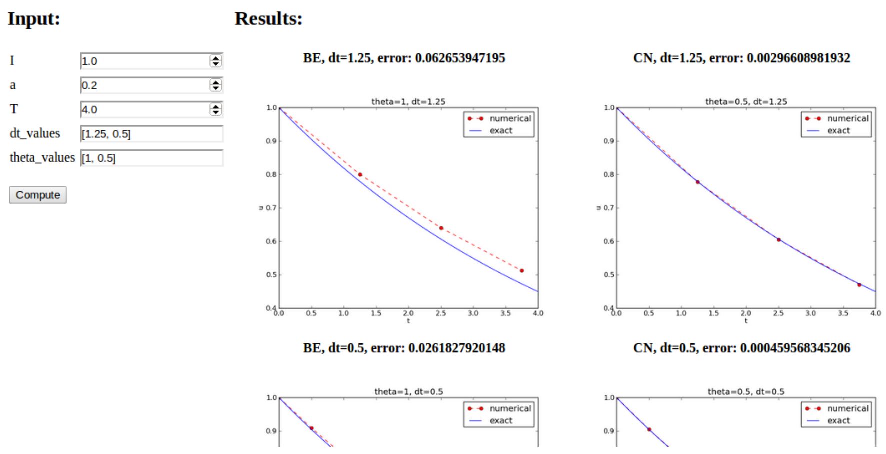
1. `decay_GUI_model.py` defines HTML widgets to be used to set input data in the web interface,
2. `templates/decay_GUI_views.py` defines the layout of the web page,
3. `decay_GUI_controller.py` runs the web application.

We only need to run the last program, and there is no need to look into these files.

Running the web application. The web GUI is started by

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

Open a web browser at the location `127.0.0.1:5000`. Input fields for `I`, `a`, `T`, `dt_values`, and `theta_values` are presented. Setting the latter two to `[1.25, 0.5]` and `[1, 0.5]`, respectively, and pressing *Compute* results in four plots, see Figure 9. With the techniques demonstrated here, one can easily create a tailored web GUI for a particular type of application and use it to interactively explore physical and numerical effects.


Input:

I	1.0
a	0.2
T	4.0
dt_values	[1.25, 0.5]
theta_values	[1, 0.5]

Results:

BE, dt=1.25, error: 0.062653947195

CN, dt=1.25, error: 0.00296608981932

BE, dt=0.5, error: 0.0261827920148

CN, dt=0.5, error: 0.000459568345206

Figure 9: Automatically generated graphical web interface.

2.8 Computing convergence rates

We expect that the error E in the numerical solution is reduced if the mesh size Δt is decreased. More specifically, many numerical methods obey a power-law relation between E and Δt:

$$E = C\Delta t^r, \tag{47}$$

where C and r are (usually unknown) constants independent of Δt. The formula (47) is viewed as an asymptotic model valid for sufficiently small Δt. How small is normally hard to estimate without doing numerical estimations of r.

The parameter r is known as the *convergence rate*. For example, if the convergence rate is 2, halving Δt reduces the error by a factor of 4. Diminishing Δt then has a greater impact on the error compared with methods that have $r = 1$. For a given value of r, we refer to the method as of r-th order. First- and second-order methods are most common in scientific computing.

Estimating r. There are two alternative ways of estimating C and r based on a set of m simulations with corresponding pairs $(\Delta t_i, E_i)$, $i = 0, \ldots, m-1$, and $\Delta t_i < \Delta t_{i-1}$ (i.e., decreasing cell size).

1. Take the logarithm of (47), $\ln E = r \ln \Delta t + \ln C$, 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

$$r_{i-1} = \frac{\ln(E_{i-1}/E_i)}{\ln(\Delta t_{i-1}/\Delta t_i)} \tag{48}$$

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

The disadvantage of method 1 is that (47) might not be valid for the coarsest meshes (largest Δt values). Fitting a line to all the data points is then misleading. Method 2 computes convergence rates for pairs of experiments and allows us to see if the sequence r_i converges to some value as $i \rightarrow m-2$. The final r_{m-2} can then be taken as the convergence rate. If the coarsest meshes have a differing rate, the corresponding time steps are probably too large for (47) to be valid. That is, those time steps lie outside the asymptotic range of Δt values where the error behaves like (47).

Implementation. It is straightforward to extend the `main` function in the program `decay_argparse.py` with statements for computing $r_0, r_1, \ldots, r_{m-2}$ from (47):

```
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
```

The program containing this `main` function is called `decay_convrate.py`.

The `r` object is a *dictionary of lists*. The keys in this dictionary are the θ values. For example, `r[1]` holds the list of the r_i values corresponding to $\theta = 1$. In the loop `for theta in r`, the loop variable `theta` takes on the values of the keys in the dictionary `r` (in an undetermined ordering). We could simply do a `print r[theta]` inside the loop, but this would typically yield output of the convergence rates with 16 decimals:

```
[1.331919482274763, 1.1488178494691532, ...]
```

Instead, we format each number with 2 decimals, using a list comprehension to turn the list of numbers, `r[theta]`, into a list of formatted strings. Then we join these strings with a space in between to get a sequence of rates on one line in the terminal window. More generally, `d.join(list)` joins the strings in the list `list` to one string, with `d` as delimiter between `list[0]`, `list[1]`, etc.

Here is an example on the outcome of the convergence rate computations:

```
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
```

The Forward and Backward Euler methods seem to have an r value which stabilizes at 1, while the Crank-Nicolson seems to be a second-order method with $r = 2$.

Very often, we have some theory that predicts what r is for a numerical method. Various theoretical error measures for the θ-rule point to $r = 2$ for $\theta = 0.5$ and $r = 1$ otherwise. The computed estimates of r are in very good agreement with these theoretical values.

Why convergence rates are important.

The strong practical application of computing convergence rates is for verification: wrong convergence rates point to errors in the code, and correct convergence rates brings evidence that the implementation is correct. Experience shows that bugs in the code easily destroy the expected convergence rate.

Debugging via convergence rates. Let us experiment with bugs and see the implication on the convergence rate. We may, for instance, forget to multiply by `a` in the denominator in the updating formula for `u[n+1]`:

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

Running the same `decay_convrate.py` command as above gives the expected convergence rates (!). Why? The reason is that we just specified the Δt values are relied on default values for other parameters. The default value of a is 1. Forgetting the factor `a` has then no effect. This example shows how important it is to avoid parameters that are 1 or 0 when verifying implementations. Running the code `decay_v0.py` with $a = 2.1$ and $I = 0.1$ yields

```
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
```

This time we see that the expected convergence rates for the Crank-Nicolson and Backward Euler methods are not obtained, while $r = 1$ for the Forward Euler method. The reason for correct rate in the latter case is that $\theta = 0$ and the wrong `theta*dt` term in the denominator vanishes anyway.

The error

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

manifests itself through wrong rates $r \approx 0$ for all three methods. About the same results arise from an erroneous initial condition, `u[0] = 1`, or wrong loop limits, `range(1,Nt)`. It seems that in this simple problem, most bugs we can think of are detected by the convergence rate test, provided the values of the input data do not hide the bug.

A `verify_convergence_rate` function could compute the dictionary of list via `main` and check if the final rate estimates (r_{m-2}) are sufficiently close to the expected ones. A tolerance of 0.1 seems appropriate, given the uncertainty in estimating r:

```
def verify_convergence_rate():
    r = main()
    tol = 0.1
    expected_rates = {0: 1, 1: 1, 0.5: 2}
    for theta in r:
        r_final = r[theta][-1]
        diff = abs(expected_rates[theta] - r_final)
        if diff > tol:
            return False
    return True  # all tests passed
```

We remark that `r[theta]` is a list and the last element in any list can be extracted by the index `-1`.

2.9 Memory-saving implementation

The computer memory requirements of our implementations so far consists mainly of the `u` and `t` arrays, both of length $N_t + 1$, plus some other temporary arrays that Python needs for intermediate results if we do array arithmetics in our program (e.g., `I*exp(-a*t)` needs to store `a*t` before `-` can be applied to it and then `exp`). The extremely modest storage requirements of simple ODE problems put no restrictions on the formulations of the algorithm and implementation. Nevertheless, when the methods for ODEs used here are applied to three-dimensional partial differential equation (PDE) problems, memory storage requirements suddenly become an issue.

The PDE counterpart to our model problem $u' = -a$ is a diffusion equation $u_t = a\nabla^2 u$ posed on a space-time domain. The discrete representation of this domain may in 3D be a spatial mesh of M^3 points and a time mesh of N_t points. A typical desired value for M is 100 in many applications, or even 1000. Storing all the computed u values, like we have done in the programs so far, demands storage of some arrays of size $M^3 N_t$, giving a factor of M^3 larger storage demands compared to our ODE programs. Each real number in the array for u requires 8 bytes (b) of storage. With $M = 100$ and $N_t = 1000$, there is a storage demand of $(10^3)^3 \cdot 1000 \cdot 8 = 8$ Gb for the solution array. Fortunately, we can usually get rid of the N_t factor, resulting in 8 Mb of storage. Below we explain how this is done, and the technique is almost always applied in implementations of PDE problems.

Let us critically evaluate how much we really need to store in the computer's memory in our implementation of the θ method. To compute a new u^{n+1}, all we need is u^n. This implies that the previous $u^{n-1}, u^{n-2}, \ldots, u^0$ values do not need to be stored in an array, although this is convenient for plotting and data analysis in the program. Instead of the u array we can work with two variables for real numbers, u and u_1, representing u^{n+1} and u^n in the algorithm, respectively. At each time level, we update u from u_1 and then set u_1 = u so that the computed u^{n+1} value becomes the "previous" value u^n at the next time level. The downside is that we cannot plot the solution after the simulation is done since only the last two numbers are available. The remedy is to store computed values in a file and use the file for visualizing the solution later.

We have implemented this memory saving idea in the file decay_memsave.py, which is a merge of the decay_plot_mpl.py and decay_argparse.py programs, using module prefixes np for numpy and plt for matplotlib.pyplot.

The following function demonstrates how we work with the two most recent values of the unknown:

```
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
```

This code snippet serves as a quick introduction to file writing in Python. Reading the data in the file into arrays t and u are done by the function

```
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)
```

This type of file with numbers in rows and columns is very common, and numpy has a function loadtxt which loads such tabular data into a two-dimensional array, say with name data. The number in row i and column j is then data[i,j].

The whole column number j can be extracted by data[:,j]. A version of read_file using np.loadtxt reads

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

The present counterpart to the explore function from decay_plot_mpl.py must run solver_memsave and then load data from file before we can compute the error measure and make the plot:

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

The decay_memsave.py file also includes command-line options --I, --a, --T, --dt, --theta, and --makeplot for controlling input parameters and making a single run. For example,

```
Terminal> python decay_memsave.py --T 10 --theta 1 --dt 2
```

results in the output

```
I=1.0, a=1.0, T=10.0, makeplot=True, theta=1.0, dt=2.0
theta=1.0 dt=2 Error=3.136E-01
```

3 Software engineering

Goal.
Efficient use of differential equation models requires software that is easy to test and flexible for setting up extensive numerical experiments. This section introduces three important concepts:

- Modules
- Testing frameworks
- Implementation with classes

The concepts are introduced using the differential equation problem $u' = -au$, $u(0) = I$, as example.

3.1 Making a module

The DRY principle.
The previous sections have outlined numerous different programs, all of them having their own copy of the `solver` function. Such copies of the same piece of code is against the important *Don't Repeat Yourself* (DRY) principle in programming. If we want to change the `solver` function there should be *one and only one* place where the change needs to be performed.

To clean up the repetitive code snippets scattered among the `decay_*.py` files, we start by collecting the various functions we want to keep for the future in one file, now called `decay_mod.py` (`mod` stands for "module"). The following functions are copied to this file:

- `solver` for computing the numerical solution
- `verify_three_steps` for verifying the first three solution points against hand calculations
- `verify_discrete_solution` for verifying the entire computed solution against an exact formula for the numerical solution
- `explore` for computing and plotting the solution
- `define_command_line_options` for defining option-value pairs on the command line
- `read_command_line` for reading input from the command line, now extended to work both with `sys.argv` directly and with an `ArgumentParser` object
- `main` for running experiments with $\theta = 0, 0.5, 1$ and a series of Δt values, and computing convergence rates
- `main_GUI` for doing the same as the `main` function, but modified for automatic GUI generation
- `verify_convergence_rate` for verifying the computed convergence rates against the theoretically expected values

We use Matplotlib for plotting. A sketch of the `decay_mod.py` file, with complete versions of the modified functions, looks as follows:

```
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):
    if use_argparse:
        parser = define_command_line_options()
        args = parser.parse_args()
        print 'I={}, a={}, makeplot={}, dt_values={}'.format(
            args.I, args.a, args.makeplot, args.dt_values)
        return args.I, args.a, args.makeplot, args.dt_values
    else:
        if len(sys.argv) < 6:
            print 'Usage: %s I a on/off dt1 dt2 dt3 ...' % \
                  sys.argv[0]; sys.exit(1)

        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, makeplot, dt_values

def main():
    ...
```

This `decay_mod.py` file is already a module such that we can import desired functions in other programs. For example, we can in a file do

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

However, it should also be possible to both use `decay_mod.py` as a module *and* execute the file as a program that runs `main()`. This is accomplished by ending the file with a *test block*:

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

When `decay_mod.py` is used as a module, `__name__` equals the module name `decay_mod`, while `__name__` equals `'__main__'` when the file is run as a program. Optionally, we could run the verification tests if the word `verify` is present on the command line and `verify_convergence_rate` could be tested if `verify_rates` is found on the command line. The `verify_rates` argument must be removed before we read parameter values from the command line, otherwise the `read_command_line` function (called by `main`) will not work properly.

```
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()
```

3.2 Prefixing imported functions by the module name

Import statements of the form `from module import *` import functions and variables in `module.py` into the current file. For example, when doing

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

we get mathematical functions like `sin` and `exp` as well as MATLAB-style functions like `linspace` and `plot`, which can be called by these well-known names. Unfortunately, it sometimes becomes confusing to know where a particular function comes from. Is it from `numpy`? Or `matplotlib.pyplot`? Or is it our own function?

An alternative import is

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

and such imports require functions to be prefixed by the module name, e.g.,

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

This is normally regarded as a better habit because it is explicitly stated from which module a function comes from.

The modules `numpy` and `matplotlib.pyplot` are so frequently used, and their full names quite tedious to write, so two standard abbreviations have evolved in the Python scientific computing community:

```
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)
```

A version of the `decay_mod` module where we use the `np` and `plt` prefixes is found in the file `decay_mod_prefix.py`.

The downside of prefixing functions by the module name is that mathematical expressions like $e^{-at}\sin(2\pi t)$ get 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)
```

Such an expression looks like `exp(-a*t)*sin(2*pi*t)` in most other programming languages. Similarly, `np.linspace` and `plt.plot` look less familiar to people who are used to MATLAB and who have not adopted Python's prefix style. Whether to do `from module import *` or `import module` depends on personal taste and the problem at hand. In these writings we use `from module import` in shorter programs where similarity with MATLAB could be an advantage, and where a one-to-one correspondence between mathematical formulas and Python expressions is important. The style `import module` is preferred inside Python modules (see Exercise 11 for a demonstration).

3.3 Doctests

We have emphasized how important it is to be able to run tests in the program at any time. This was solved by calling various `verify*` functions in the previous examples. However, there exists well-established procedures and corresponding tools for automating the execution of tests. We shall briefly demonstrate two important techniques: *doctest* and *unit testing*. The corresponding files are the modules `decay_mod_doctest.py` and `decay_mod_nosetest.py`.

A doc string (the first string after the function header) is used to document the purpose of functions and their arguments. Very often it is instructive to include an example on how to use the function. Interactive examples in the Python shell are most illustrative as we can see the output resulting from function calls. For example, we can in the `solver` function include an example on calling this function and printing the computed `u` and `t` arrays:

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

When such interactive demonstrations are inserted in doc strings, Python's doctest module can be used to automate running all commands in interactive sessions and compare new output with the output appearing in the doc string. All we have to do in the current example is to write

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

This command imports the `doctest` module, which runs all tests. No additional command-line argument is allowed when running doctests. If any test fails, the problem is reported, e.g.,

```
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.
```

Note that in the output of `t` and `u` we write `u` with 14 digits. Writing all 16 digits is not a good idea: if the tests are run on different hardware, round-off errors might be different, and the `doctest` module detects that the numbers are not precisely the same and reports failures. In the present application, where $0 < u(t) \leq 0.8$, we expect round-off errors to be of size 10^{-16}, so comparing 15 digits would probably be reliable, but we compare 14 to be on the safe side.

Doctests are highly encouraged as they do two things: 1) demonstrate how a function is used and 2) test that the function works.

Here is an example on a doctest in the `explore` function:

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

This time we limit the output to 10 digits.

Caution.
Doctests requires careful coding if they use command-line input or print results to the terminal window. Command-line input must be simulated by filling `sys.argv` correctly, e.g., `sys.argv = '--I 1.0 --a 5'.split`. The output lines of print statements must be copied exactly as they appear when running the statements in an interactive Python shell.

3.4 Unit testing with nose

The unit testing technique consists of identifying small units of code, usually functions (or classes), and write one or more tests for each unit. One test should, ideally, not depend on the outcome of other tests. For example, the doctest in function `solver` is a unit test, and the doctest in function `explore` as well, but the latter depends on a working `solver`. Putting the error computation and plotting in `explore` in two separate functions would allow independent unit tests. In this way, the design of unit tests impacts the design of functions. The recommended practice is actually to design and write the unit tests first and *then* implement the functions!

In scientific computing it is not always obvious how to best perform unit testing. The units is naturally larger than in non-scientific software. Very often the solution procedure of a mathematical problem identifies a unit.

Basic use of nose. The `nose` package is a versatile tool for implementing unit tests in Python. Here is a short explanation of the usage of nose:

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

Here comes a very simple illustration of the three points. Assume that we have this function in a module `mymod`:

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

Either in this file, or in a separate file `test_mymod.py`, we implement a test function whose purpose is to test that the function `double` works as intended:

```
import nose.tools as nt

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

Notice that `test_double` has no arguments. We need to do an `import mymod` or `from mymod import double` if this test resides in a separate file. Running

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

makes the `nose` tool run all functions with names matching `test_*()` in `mymod.py`. Alternatively, if the test functions are in some `test_mymod.py` file, we can just write `nosetests -s`. The nose tool will then look for all files with names mathching `test*.py` and run all functions `test_*()` in these files.

When you have nose tests in separate test files with names `test*.py` it is common to collect these files in a subdirectory `tests`, or `*_tests` if you have several test subdirectories. Running `nosetests -s` will then recursively look for all `tests` and `*_tests` subdirectories and run all functions `test_*()` in all files `test_*.py` in these directories. Just one command can then launch a series of tests in a directory tree!

An example of a `tests` directory with different types of `test*.py` files are found in src/decay/tests. Note that these perform imports of modules in the parent directory. These imports works well because the tests are supposed to be run by `nosetests -s` executed in the parent directory (`decay`).

Tip.

The `-s` option to `nosetests` assures that any print statement in the `test_*` functions appears in the output. Without this option, `nosetests` suppressed whatever the tests writes to the terminal window (standard output). Such behavior is annoying, especially when developing and testing tests.

The number of failed tests and their details are reported, or an `OK` is printed if all tests passed.

The advantage with the `nose` package is two-fold:

1. tests are written and collected in a structured way, and
2. large collections of tests, scattered throughout a tree of directories, can be executed with one command `nosetests -s`.

Alternative assert statements. In case the `nt.assert_equal` function finds that the two arguments are equal, the test is a success, otherwise it is a failure and an exception of type `AssertionError` is raised. The particular exception is the indicator that a test has failed.

Instead of calling the convenience function `nt.assert_equal`, we can use Python's plain `assert` statement, which tests if a boolean expression is true and raises an `AssertionError` otherwise. Here, the statement is `assert result == 8`.

A completely manual alternative is to explicitly raise an `AssertionError` exception if the computed result is wrong:

```
if result != 8:
    raise AssertionError()
```

Applying nose. Let us illustrate how to use the `nose` tool for testing key functions in the `decay_mod` module. Or more precisely, the module is called `decay_mod_unittest` with all the `verify*` functions removed as these now are outdated by the unit tests.

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 code in the previously shown `verify*` functions. We start with comparing u^n, as computed by the function `solver`, to the formula for the exact discrete solution:

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

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

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

The `nt.assert_almost_equal` is the relevant function for comparing two real numbers. The `delta` argument specifies a tolerance for the comparison. Alternatively, one can specify a `places` argument for the number of decimal places to be used in the comparison.

After having carefully verified the implementation, we may store correctly computed numbers in the test program or in files for use in future tests. Here is an example on how the outcome from the `solver` function can be compared to what is considered to be correct results:

```
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)
```

The `precomputed` object is a dictionary with four keys: `'t'` for the time mesh, and three θ values for u^n solutions corresponding to $\theta = 0, 0.5, 1$.

Testing for special type of input data that may cause trouble constitutes a common way of constructing unit tests. For example, the updating formula for u^{n+1} may be incorrectly evaluated because of unintended integer divisions. With

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

the nominator and denominator in the updating expression,

```
(1 - (1-theta)*a*dt)
(1 + theta*dt*a)
```

evaluate to 1 and 3, respectively, and the fraction `1/3` will call up integer division and consequently lead to `u[n+1]=0`. We construct a unit test to make sure `solver` is smart enough to avoid this problem:

```
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)
```

The final test is to see that the convergence rates corresponding to $\theta = 0, 0.5, 1$ are 1, 2, and 1, respectively:

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

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

Nothing more is needed in the test_decay_nose.py file where the tests reside. Running nosetests -s will report Ran 3 tests and an OK for success. Everytime we modify the decay_mod_unittest module we can run nosetests to quickly see if the edits have any impact on the verification tests.

Installation of nose. The nose package does not come with a standard Python distribution and must therefore be installed separately. The procedure is standard and described on Nose's web pages. On Debian-based Linux systems the command is sudo apt-get install python-nose, and with MacPorts you run sudo port install py27-nose.

Using nose to test modules with doctests. Assume that mod is the name of some module that contains doctests. We may let nose run these doctests and report errors in the standard way using the code set-up

```
import doctest
import mod

def test_mod():
    failure_count, test_count = doctest.testmod(m=mod)
    nt.assert_equal(failure_count, 0,
                    msg='%d tests out of %d failed' %
                    (failure_count, test_count))
```

The call to doctest.testmod runs all doctests in the module file mod.py and returns the number of failures (failure_count) and the total number of tests (test_count). A real example is found in the file test_decay_doctest.py.

3.5 Classical class-based unit testing

The classical way of implementing unit tests derives from the JUnit tool in Java where all tests are methods in a class for testing. Python comes with a module unittest for doing this type of unit tests. While nose allows simple functions for unit tests, unittest requires deriving a class Test* from unittest.TestCase and implementing each test as methods with names test_* in that class. I strongly recommend to use nose over unittest, because it is much simpler and more convenient, but class-based unit testing is a very classical subject that computational scientists should have some knowledge about. That is why a short introduction to unittest is included below.

Basic use of unittest. We apply the double function in the mymod module introduced in the previous section as example. Unit testing with the aid of the unittest module consists of writing a file test_mymod.py with the content

```
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()
```

The test is run by executing the test file `test_mymod.py` as a standard Python program. There is no support in `unittest` for automatically locating and running all tests in all test files in a directory tree.

Those who have experience with object-oriented programming will see that the difference between using `unittest` and `nose` is minor.

Demonstration of unittest. The same tests as shown for the nose framework are reimplemented with the `TestCase` classes in the file `test_decay_unittest.py`. The tests are identical, the only difference being that with `unittest` we must write the tests as methods in a class and the assert functions have slightly different names.

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

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

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

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

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

3.6 Implementing simple problem and solver classes

The θ-rule was compactly and conveniently implemented in a function `solver` in Section 2.1. In more complicated problems it might be beneficial to use classes and introduce a class `Problem` to hold the definition of the physical problem, a class `Solver` to hold the data and methods needed to numerically solve the problem, and a class `Visualizer` to make plots. This idea will now be illustrated, resulting in code that represents an alternative to the `solver` and `explore` functions found in the `decay_mod` module.

Explaining the details of class programming in Python is considered beyond the scope of this text. Readers who are unfamiliar with Python class programming should first consult one of the many electronic Python tutorials or textbooks to come up to speed with concepts and syntax of Python classes before reading on. The author has a gentle introduction to class programming for scientific applications in [4], see Chapter 7 and 9 and Appendix E. Other useful resources are

- The Python Tutorial: `http://docs.python.org/2/tutorial/classes.html`
- Wiki book on Python Programming: `http://en.wikibooks.org/wiki/Python_Programming/Classes`
- tutorialspoint.com: `http://www.tutorialspoint.com/python/python_classes_objects.htm`

The problem class. The purpose of the problem class is to store all information about the mathematical model. This usually means all the physical parameters in the problem. In the current example with exponential decay we may also add the exact solution of the ODE to the problem class. The simplest form of a problem class is therefore

```
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
        return I*exp(-a*t)
```

We could in the `exact_solution` method have written `self.I*exp(-self.a*t)`, but using local variables `I` and `a` allows the formula `I*exp(-a*t)` which looks closer to the mathematical expression Ie^{-at}. This is not an important issue with the current compact formula, but is beneficial in more complicated problems with longer formulas to obtain the closest possible relationship between code and mathematics. My coding style is to strip off the `self` prefix when the code expresses mathematical formulas.

The class data can be set either as arguments in the constructor or at any time later, e.g.,

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

(Some programmers prefer `set` and `get` functions for setting and getting data in classes, often implemented via *properties* in Python, but I consider that overkill when we just have a few data items in a class.)

It would be convenient if class `Problem` could also initialize the data from the command line. To this end, we add a method for defining a set of command-line options and a method that sets the local attributes equal to what was found on the command line. The default values associated with the command-line options are taken as the values provided to the constructor. Class `Problem` now becomes

```
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 that if the user already has an `ArgumentParser` object it can be supplied, but if she does not have any, class `Problem` makes one. Python's `None` object is used to indicate that a variable is not initialized with a proper value.

The solver class. The solver class stores data related to the numerical solution method and provides a function `solve` for solving the problem. A problem object must be given to the constructor so that the solver can easily look up physical data. In the present example, the data related to the numerical solution method consists of Δt and θ. We add, as in the problem class, functionality for reading Δt and θ from the command line:

```
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 that we here simply reuse the implementation of the numerical method from the `decay_mod` module. The `solve` function is just a *wrapper* of the previously developed stand-alone `solver` function.

The visualizer class. The purpose of the visualizer class is to plot the numerical solution stored in class `Solver`. We also add the possibility to plot the exact solution. Access to the problem and solver objects is required when making plots so the constructor must hold references to these objects:

```
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
```

The plt object in the plot method is worth a comment. The idea is that plot can add a numerical solution curve to an existing plot. Calling plot with a plt object (which has to be a matplotlib.pyplot or scitools.std object in this implementation), will just add the curve self.solver.u as a dashed line with circles at the mesh points (leaving the color of the curve up to the plotting tool). This functionality allows plots with several solutions: just make a loop where new data is set in the problem and/or solver classes, the solver's solve() method is called, and the most recent numerical solution is plotted by the plot(plt) method in the visualizer object Exercise 12 describes a problem setting where this functionality is explored.

Combining the objects. Eventually we need to show how the classes 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()
```

The file decay_class.py constitutes a module with the three classes and the main function.

Test the understanding.

Implement the problem in Exercise 29 in terms of problem, solver, and visualizer classes. Equip the classes and their methods with doc strings with tests. Also include nose tests.

3.7 Improving the problem and solver classes

The previous `Problem` and `Solver` classes containing parameters soon get much repetitive code when the number of parameters increases. Much of this code can be parameterized and be made more compact. For this purpose, we decide to 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. Provided a problem, solver, or visualizer class defines these three dictionaries in the constructor, using default or user-supplied values of the parameters, we can create a super class `Parameters` with general code for defining command-line options and reading them as well as methods for setting and getting a parameter. A `Problem` or `Solver` class will then inherit command-line functionality and the set/get methods from the `Parameters` class.

A generic class for parameters. A simplified version of the parameter class looks as follows:

```
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)
```

The file `class_decay_oo.py` contains a slightly more advanced version of class `Parameters` where we in the `set` and `get` functions test for valid parameter names and raise exceptions with informative messages if any name is not registered.

The problem class. A class `Problem` for the problem $u' = -au$, $u(0) = I$, $t \in (0, T]$, with parameters input a, I, and T can now be coded as

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

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

The solver class. Also the solver class is derived from class `Parameters` and works with the `prms`, `types`, and `help` dictionaries in the same way as class `Problem`. Otherwise, the code is very similar to class `Solver` in the `decay_class.py` file:

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

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

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

The visualizer class. Class `Visualizer` can be identical to the one in the `decay_class.py` file since the class does not need any parameters. However, a few adjustments in the `plot` method is necessary since parameters are accessed as, e.g., `problem.get('T')` rather than `problem.T`. The details are found in the file `class_decay_oo.py`.

Finally, we need a function that solves a real problem using the classes `Problem`, `Solver`, and `Visualizer`. This function can be just like `main` in the `decay_class.py` file.

The advantage with the `Parameters` class is that it scales to problems with a large number of physical and numerical parameters: as long as the parameters are defined once via a dictionary, the compact code in class `Parameters` can handle any collection of parameters of any size.

4 Performing scientific experiments

Goal.
This section explores the behavior of a numerical method for a differential equation through computer experiments. In particular, it is shown how scientific experiments can be set up and reported. We address the ODE problem

$$u'(t) = -au(t), \quad u(0) = I, \quad t \in (0, T], \tag{49}$$

numerically discretized by the θ-rule:

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

Our aim is to plot $u^0, u^1, \ldots, u^N$ together with the exact solution $u_e = Ie^{-at}$ for various choices of the parameters in this numerical problem: I, a, Δt, and θ. We are especially interested in how the discrete solution compares with the exact solution when the Δt parameter is varied and θ takes on the three values corresponding to the Forward Euler, Backward Euler, and Crank-Nicolson schemes ($\theta = 0, 1, 0.5$, respectively).

4.1 Software

A verified implementation for computing the numerical solution u^n and plotting it together with the exact solution u_e is found in the file `decay_mod.py`. This program admits command-line arguments to specify a series of Δt values and will run a loop over these values and $\theta = 0, 0.5, 1$. We make a slight edit of how the plots are designed: the numerical solution is specified with line type `'r--o'` (dashed red lines with dots at the mesh points), and the `show()` command is removed to avoid a lot of plot windows popping up on the computer screen (but hardcopies of the plot are still stored in files via `savefig`). The slightly modified program has the name `experiments/decay_mod.py`. All files associated with the scientific investigation are collected in a subdirectory `experiments`.

Running the experiments is easy since the `decay_mod.py` program already has the loops over θ and Δt implemented. An experiment with $I = 1$, $a = 2$, $T = 5$, and $dt = 0.5, 0.25, 0.1, 0.05$ is run by

```
Terminal> python decay_mod.py --I 1 --a 2 --makeplot \
          --T 5 --dt 0.5 0.25 0.1 0.05
```

4.2 Combining plot files

The `decay_mod.py` program generates a lot of image files, e.g., `FE_*.png`, `BE_*.png`, and `CN_*.png`. We want to combine all the `FE_*.png` files in a table fashion in one file, with two images in each row, starting with the largest Δt in the upper left corner and decreasing the value as we go to the right and down. This can be done using the `montage` program. The often occurring white areas around the plots can be cropped away by the `convert -trim` command. The remaining white can be made transparent for HTML pages with a non-white background by the command `convert -transparent white`.

Also plot files in the PDF format with names `FE_*.pdf`, `BE_*.pdf`, and `CN_*.pdf` are generated and these should be combined using other tools: `pdftk` to combine individual plots into one file with one plot per page, and `pdfnup` to combine the pages into a table with multiple plots per page. The resulting image often has some extra surrounding white space that can be removed by the `pdfcrop` program. The code snippets below contain all details about the usage of `montage`, `convert`, `pdftk`, `pdfnup`, and `pdfcrop`.

Running manual commands is boring, and errors may easily sneak in. Both for automating manual work and documenting the operating system commands we actually issued in the experiment, we should write a *script* (little program). An alternative is to write the commands into an IPython notebook and use the notebook as the script. A plain script as a standard Python program in a separate text file will be used here.

Reproducible science.

A script that automates running our computer experiments will ensure that the experiments can easily be rerun by ourselves or others in the future, either to check the results or redo the experiments with other input data. Also, whatever we did to produce the results is documented in every detail in the script. Automating scripts are therefore essential to making our research *reproducible*, which is a fundamental principle in science.

The script takes a list of Δt values on the command line as input and makes three combined images, one for each θ value, displaying the quality of the numerical solution as Δt varies. For example,

```
Terminal> python decay_exper0.py 0.5 0.25 0.1 0.05
```

results in images `FE.png`, `CN.png`, `BE.png`, `FE.pdf`, `CN.pdf`, and `BE.pdf`, each with four plots corresponding to the four Δt values. Each plot compares the numerical solution with the exact one. The latter image is shown in Figure 10.

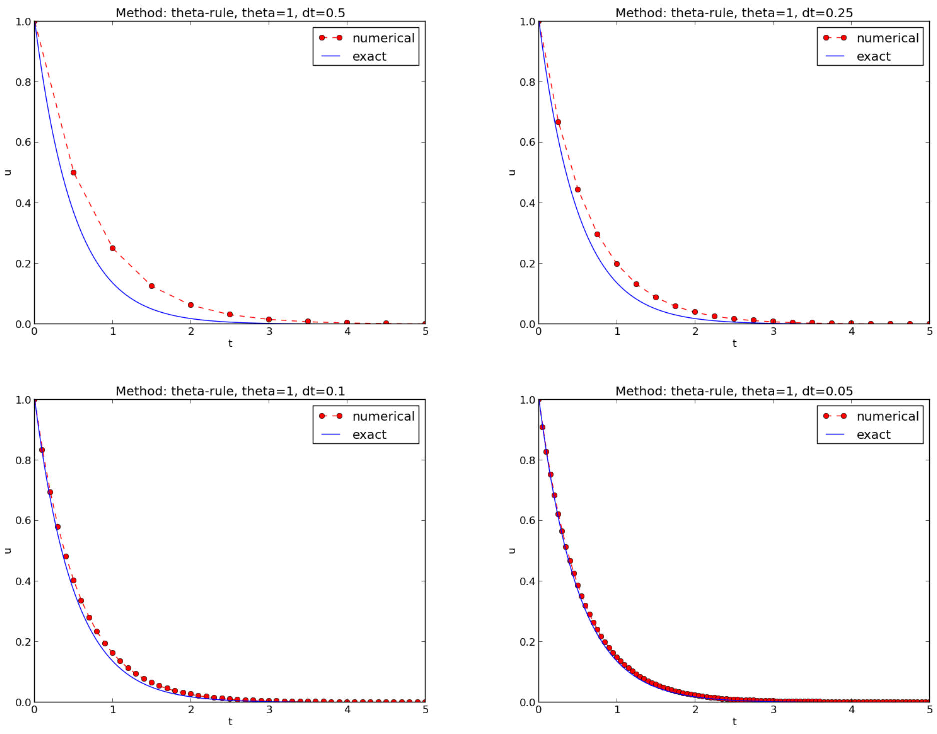


Figure 10: Illustration of the Backward Euler method for four time step values.

Ideally, the script should be scalable in the sense that it works for any number of Δt values, which is the case for this particular implementation:

```
import os, sys

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

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

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

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

    # Remove the files generated above and by decay_mod.py
    from glob import glob
    filenames = glob('*_*.png') + glob('*_*.pdf') + \
                glob('*_*.eps') + glob('tmp*.pdf')
    for filename in filenames:
        os.remove(filename)

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

This file is available as `experiments/decay_exper0.py`.

We may comment upon many useful constructs in this script:

- `[float(arg) for arg in sys.argv[1:]]` builds a list of real numbers from all the command-line arguments.
- `failure = os.system(cmd)` runs an operating system command, e.g., another program. The execution is successful only if `failure` is zero.
- Unsuccessful execution usually makes it meaningless to continue the program, and therefore we abort the program with `sys.exit(1)`. Any argument different from 0 signifies to the computer's operating system that our program stopped with a failure.

- `['%s_%s.png' % (method, dt) for dt in dt_values]` builds a list of filenames from a list of numbers (`dt_values`).
- All `montage`, `convert`, `pdftk`, `pdfnup`, and `pdfcrop` commands for creating composite figures are stored in a list and later executed in a loop.
- `glob('*_*.png')` returns a list of the names of all files in the current directory 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`.

4.3 Interpreting output from other programs

Programs that run other programs, like `decay_exper0.py` does, will often need to interpret output from those programs. Let us demonstrate how this is done in Python by extracting the relations between θ, Δt, and the error E as written to the terminal window by the `decay_mod.py` program, when being executed by `decay_exper0.py`. We will

- 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

The simple `os.system(cmd)` call does not allow us to read the output from running `cmd`. Instead we need to invoke a bit more involved procedure:

```
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)
```

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`. Or in other words, the text in `output` is what appeared in the terminal window while running `cmd`.

Our next task is to run through the `output` string, line by line, and if the current line prints θ, Δt, and E, we split the line into these three pieces and store the data. The chosen storage structure is a dictionary `errors` with keys `dt` to hold the Δt values in a list, and three θ keys to hold the corresponding E values in a list. The relevant code lines are

```
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)
```

Note that we do not bother to store the Δt values as we read them from `output`, because we already have these values in the `dt_values` list.

We are now ready to plot E versus Δt for $\theta = 0, 0.5, 1$:

```
import matplotlib.pyplot as plt
plt.loglog(errors['dt'], errors[0], 'ro-')
plt.hold('on')
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.png')
plt.savefig('error.pdf')
```

Plots occasionally need some manual adjustments. Here, the axis of the log-log plot look nicer if we adapt them strictly to the data, see Figure 11. To this end, we need to compute $\min E$ and $\max E$, and later specify the extent of the axes:

```
# Find min/max for the axis
E_min = 1E+20; E_max = -E_min
for theta in 0, 0.5, 1:
    E_min = min(E_min, min(errors[theta]))
    E_max = max(E_max, max(errors[theta]))

plt.loglog(errors['dt'], errors[0], 'ro-')
...
plt.axis([min(dt_values), max(dt_values), E_min, E_max])
...
```

The complete program, incorporating the code snippets above, is found in `experiments/decay_exper1.py`. This example can hopefully act as template for numerous other occasions where one needs to run experiments, extract data from the output of programs, make plots, and combine several plots in a figure file. The `decay_exper1.py` program is organized as a module, and other files can then easily extend the functionality, as illustrated in the next section.

4.4 Making a report

The results of running computer experiments are best documented in a little report containing the problem to be solved, key code segments, and the plots from a series of experiments. At least the part of the report containing the plots should be automatically generated by the script that performs the set of

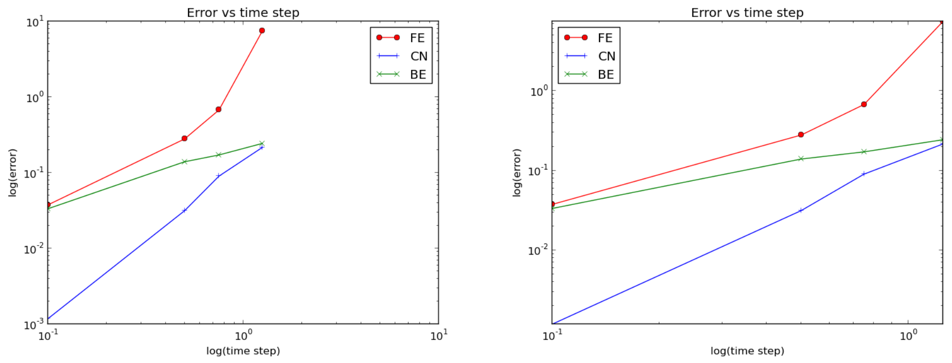


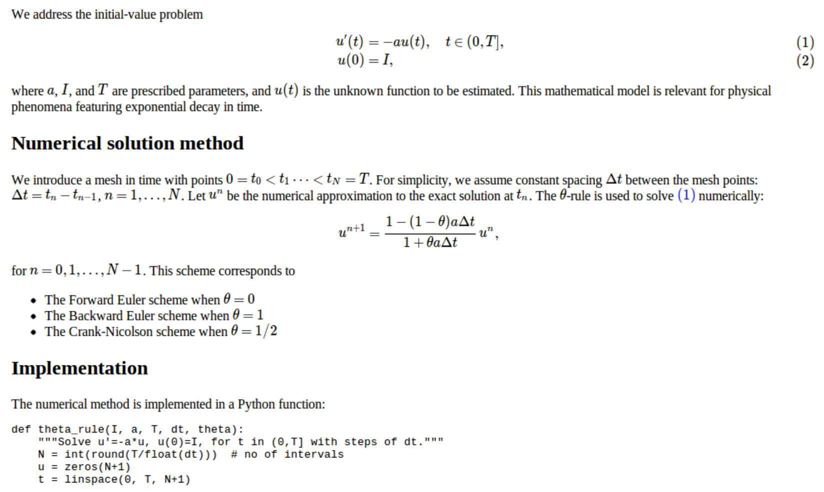
Figure 11: Default plot (left) and manually adjusted axes (right).

experiments, because in that script we know exactly which input data that were used to generate a specific plot, thereby ensuring that each figure is connected to the right data. Take a look at an example at `http://tinyurl.com/k3sdbuv/writing_reports//sphinx-cloud/` to see what we have in mind.

Plain HTML. Scientific reports can be written in a variety of formats. Here we begin with the HTML format which allows efficient viewing of all the experiments in any web browser. The program `decay_exper1_html.py` calls `decay_exper1.py` to perform the experiments and then runs statements for creating an HTML file with a summary, a section on the mathematical problem, a section on the numerical method, a section on the `solver` function implementing the method, and a section with subsections containing figures that show the results of experiments where Δt is varied for $\theta = 0, 0.5, 1$. The mentioned Python file contains all the details for writing this HTML report. You can view the report on `http://tinyurl.com/k3sdbuv/writing_reports//_static/report_html.html`.

HTML with MathJax. Scientific reports usually need mathematical formulas and hence mathematical typesetting. In plain HTML, as used in the `decay_exper1_html.py` file, we have to use just the keyboard characters to write mathematics. However, there is an extension to HTML, called MathJax, which allows formulas and equations to be typeset with LaTeX syntax and nicely rendered in web browsers, see Figure 12. A relatively small subset of LaTeX environments is supported, but the syntax for formulas is quite rich. Inline formulas are look like `\( u'=-au \)` while equations are surrounded by `$$` signs. Inside such signs, one can use `\[ u'=-au \]` for unnumbered equations, or `\begin{equation}` and `\end{equation}` surrounding `u'=-au` for numbered equations, or `\begin{align}` and `\end{align}` for multiple aligned equations. You need to be familiar with mathematical typesetting in LaTeX.

The file `decay_exper1_mathjax.py` contains all the details for turning the previous plain HTML report into web pages with nicely typeset mathematics. The corresponding HTML code be studied to see all details of the mathematical typesetting.



We address the initial-value problem

$$u'(t) = -au(t), \quad t \in (0,T], \qquad (1)$$
$$u(0) = I, \qquad (2)$$

where a, I, and T are prescribed parameters, and $u(t)$ is the unknown function to be estimated. This mathematical model is relevant for physical phenomena featuring exponential decay in time.

Numerical solution method

We introduce a mesh in time with points $0 = t_0 < t_1 \cdots < t_N = T$. For simplicity, we assume constant spacing Δt between the mesh points: $\Delta t = t_n - t_{n-1}$, $n = 1, \ldots, N$. Let u^n be the numerical approximation to the exact solution at t_n. The θ-rule is used to solve (1) numerically:

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

for $n = 0, 1, \ldots, N-1$. This scheme corresponds to

- The Forward Euler scheme when $\theta = 0$
- The Backward Euler scheme when $\theta = 1$
- The Crank-Nicolson scheme when $\theta = 1/2$

Implementation

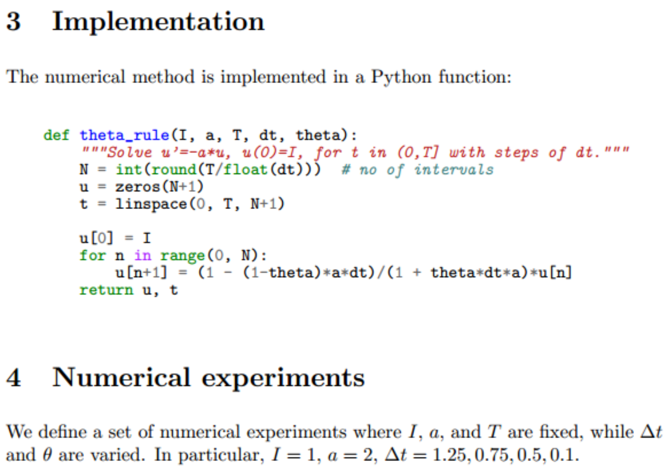
The numerical method is implemented in a Python function:

```
def theta_rule(I, a, T, dt, theta):
    """Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt."""
    N = int(round(T/float(dt)))  # no of intervals
    u = zeros(N+1)
    t = linspace(0, T, N+1)
```

Figure 12: Report in HTML format with MathJax.

LaTeX. The *de facto* language for mathematical typesetting and scientific report writing is LaTeX. A number of very sophisticated packages have been added to the language over a period of three decades, allowing very fine-tuned layout and typesetting. For output in the PDF format, see Figure 13 for an example, LaTeX is the definite choice when it comes to quality. The LaTeX language used to write the reports has typically a lot of commands involving backslashes and braces. For output on the web, using HTML (and not the PDF directly in the browser window), LaTeX struggles with delivering high quality typesetting. Other tools, especially Sphinx, give better results and can also produce nice-looking PDFs. The file `decay_exper1_latex.py` shows how to generate the LaTeX source from a program.

Sphinx. Sphinx is a typesetting language with similarities to HTML and LaTeX, but with much less tagging. It has recently become very popular for software documentation and mathematical reports. Sphinx can utilize LaTeX for mathematical formulas and equations (via MathJax or PNG images). Unfortunately, the subset of LaTeX mathematics supported is less than in full MathJax (in particular, numbering of multiple equations in an `align` type environment is not supported). The Sphinx syntax is an extension of the reStructuredText language. An attractive feature of Sphinx is its rich support for fancy layout of web pages. In particular, Sphinx can easily be combined with various layout



3 Implementation

The numerical method is implemented in a Python function:

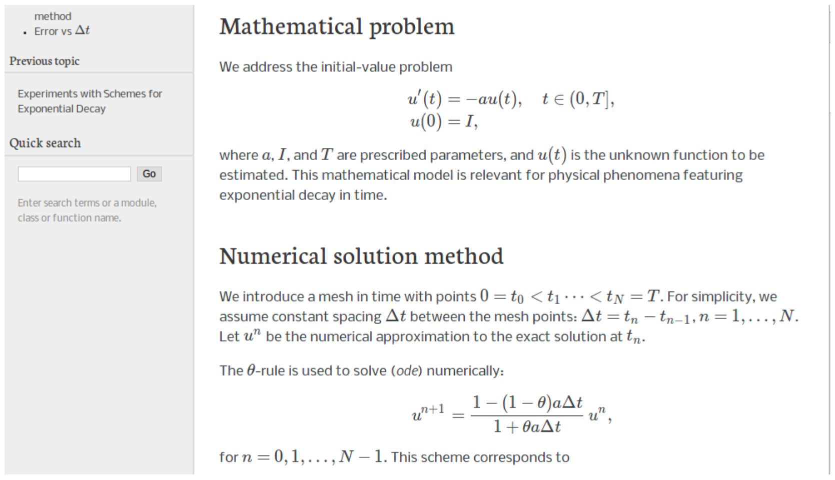
```
def theta_rule(I, a, T, dt, theta):
    """Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt."""
    N = int(round(T/float(dt)))  # no of intervals
    u = zeros(N+1)
    t = linspace(0, T, N+1)

    u[0] = I
    for n in range(0, N):
        u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
    return u, t
```

4 Numerical experiments

We define a set of numerical experiments where I, a, and T are fixed, while Δt and θ are varied. In particular, $I = 1$, $a = 2$, $\Delta t = 1.25, 0.75, 0.5, 0.1$.

Figure 13: Report in PDF format generated from LaTeX source.

themes that give a certain look and feel to the web site and that offers table of contents, navigation, and search facilities, see Figure 14.


method
• Error vs Δt
Previous topic
Experiments with Schemes for Exponential Decay
Quick search
Go
Enter search terms or a module, class or function name.

Mathematical problem

We address the initial-value problem

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

where a, I, and T are prescribed parameters, and $u(t)$ is the unknown function to be estimated. This mathematical model is relevant for physical phenomena featuring exponential decay in time.

Numerical solution method

We introduce a mesh in time with points $0 = t_0 < t_1 \cdots < t_N = T$. For simplicity, we assume constant spacing Δt between the mesh points: $\Delta t = t_n - t_{n-1}, n = 1, \ldots, N$. Let u^n be the numerical approximation to the exact solution at t_n.

The θ-rule is used to solve (*ode*) numerically:

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

for $n = 0, 1, \ldots, N-1$. This scheme corresponds to

Figure 14: Report in HTML format generated from Sphinx source.

Markdown. A recently popular format for easy writing of web pages is Markdown. Text is written very much like one would do in email, using spacing and special characters to naturally format the code instead of heavily tagging the text as in LaTeX and HTML. With the tool Pandoc one can go from Markdown to a variety of formats. HTML is a common output format, but LaTeX, epub, XML, OpenOffice, MediaWiki, and MS Word are some other possibilities.

Wiki formats. A range of wiki formats are popular for creating notes on the web, especially documents which allow groups of people to edit and add content. Apart from MediaWiki (the wiki format used for Wikipedia), wiki formats have no support for mathematical typesetting and also limited tools for displaying computer code in nice ways. Wiki formats are therefore less suitable for scientific reports compared to the other formats mentioned here.

Doconce. Since it is difficult to choose the right tool or format for writing a scientific report, it is advantageous to write the content in a format that easily translates to LaTeX, HTML, Sphinx, Markdown, and various wikis. Doconce is such a tool. It is similar to Pandoc, but offers some special convenient features for writing about mathematics and programming. The tagging is modest, somewhere between LaTeX and Markdown. The program `decay_exper_do.py` demonstrates how to generate (and write) Doconce code for a report.

Worked example. The HTML, LaTeX (PDF), Sphinx, and Doconce formats for the scientific report whose content is outlined above, are exemplified with source codes and results at the web pages associated with this teaching material: `http://tinyurl.com/k3sdbuv/writing_reports/`.

4.5 Publishing a complete project

A report documenting scientific investigations should be accompanied by all the software and data used for the investigations so that others have a possibility to redo the work and assess the qualify of the results. This possibility is important for *reproducible research* and hence reaching reliable scientific conclusions.

One way of documenting a complete project is to make a directory tree with all relevant files. Preferably, the tree is published at some project hosting site like Bitbucket, GitHub, or Googlecode so that others can download it as a tarfile, zipfile, or clone the files directly using a version control system like Mercurial or Git. For the investigations outlined in Section 4.4, we can create a directory tree with files

```
setup.py
./src:
   decay_mod.py
./doc:
   ./src:
      decay_exper1_mathjax.py
      make_report.sh
      run.sh
   ./pub:
      report.html
```

The `src` directory holds source code (modules) to be reused in other projects, the `setup.py` builds and installs such software, the `doc` directory contains the documentation, with `src` for the source of the documentation and `pub` for ready-made, published documentation. The `run.sh` file is a simple Bash script listing the `python` command we used to run `decay_exper1_mathjax.py` to generate the experiments and the `report.html` file.

5 Exercises and Problems

Exercise 1: Derive schemes for Newton's law of cooling

Show in detail how we can apply the ideas of the Forward Euler, Backward Euler, Crank-Nicolson, and θ-rule discretizations to derive explicit computational formulas for new temperature values in Newton's law of cooling (see Section 11.5):

$$\frac{dT}{dt} = -k(T - T_s), \quad T(0) = T_0\,. \tag{50}$$

Here, T is the temperature of the body, T_s is the temperature of the surroundings, t is time, k is the heat transfer coefficient, and T_0 is the initial temperature of the body.

Filename: `schemes_cooling.pdf`.

Exercise 2: Implement schemes for Newton's law of cooling

Formulate a θ-rule for the three schemes in Exercise 1 such that you can get the three schemes from a single formula by varying the θ parameter. Implement the θ scheme in a function `cooling(T0, k, T_s, t_end, dt, theta=0.5)`, where `T0` is the initial temperature, `k` is the heat transfer coefficient, `T_s` is the temperature of the surroundings, `t_end` is the end time of the simulation, `dt` is the time step, and `theta` corresponds to θ. The `cooling` function should return the temperature as an array `T` of values at the mesh points and the time mesh `t`. Construct verification examples to check that the implementation works.

Hint. For verification, try to find an exact solution of the discrete equations. A trick is to introduce $u = T - T_s$, observe that $u^n = (T_0 - T_s)A^n$ for some amplification factor A, and then express this formula in terms of T^n.

Filename: `cooling.py`.

Exercise 3: Find time of murder from body temperature

A detective measures the temperature of a dead body to be 26.7 C at 2 pm. One hour later the temperature is 25.8 C. The question is when death occurred.

Assume that Newton's law of cooling (120) is an appropriate mathematical model for the evolution of the temperature in the body. First, determine k in (120) by formulating a Forward Euler approximation with one time steep from time 2 am to time 3 am, where knowing the two temperatures allows for finding k. Assume the temperature in the air to be 20 C. Thereafter, simulate the temperature evolution from the time of murder, taken as $t = 0$, when

$T = 37$ C, until the temperature reaches 25.8 C. The corresponding time allows for answering when death occurred. Filename: `detective.py`.

Exercise 4: Experiment with integer division

Explain what happens in the following computations, where some are mathematically unexpected:

```
>>> dt = 3
>>> T = 8
>>> Nt = T/dt
>>> Nt
2
>>> theta = 1; a = 1
>>> (1 - (1-theta)*a*dt)/(1 + theta*dt*a)
0
```

Filename: `pyproblems.txt`.

Exercise 5: Experiment with wrong computations

Consider the `solver` function in the `decay_v1.py` file and the following call:

```
u, t = solver(I=1, a=1, T=7, dt=2, theta=1)
```

The output becomes

```
    t= 0.000 u=1
    t= 2.000 u=0
    t= 4.000 u=0
    t= 6.000 u=0
```

Print out the result of all intermediate computations and use `type(v)` to see the object type of the result stored in `v`. Examine the intermediate calculations and explain why `u` is wrong and why we compute up to $t = 6$ only even though we specified $T = 7$. Filename: `decay_v1_err.py`.

Exercise 6: Plot the error function

Solve the problem $u' = -au$, $u(0) = I$, using the Forward Euler, Backward Euler, and Crank-Nicolson schemes. For each scheme, plot the error function $e^n = u_e(t_n) - u^n$ for Δt, $\frac{1}{4}\Delta t$, and $\frac{1}{8}\Delta t$, where u_e is the exact solution of the ODE and u^n is the numerical solution at mesh point t_n. Filename: `decay_plot_error.py`.

Exercise 7: Compare methods for a given time mesh

Make a program that imports the `solver` function from the `decay_mod` module and offers a function `compare(dt, I, a)` for comparing, in a plot, the methods corresponding to $\theta = 0, 0.5, 1$ and the exact solution. This plot shows the accuracy of the methods for a given time mesh. Read input data for the problem from the command line using appropriate functions in the `decay_mod` module (the `--dt` option for giving several time step values can be reused: just use the first time step value for the computations). Filename: `decay_compare_theta.py`.

Exercise 8: Change formatting of numbers and debug

The decay_memsave.py program writes the time values and solution values to a file which looks like

```
0.0000000000000000E+00  1.0000000000000000E+00
2.0000000000000001E-01  8.3333333333333337E-01
4.0000000000000002E-01  6.9444444444444453E-01
6.0000000000000009E-01  5.7870370370370383E-01
8.0000000000000004E-01  4.8225308641975323E-01
1.0000000000000000E+00  4.0187757201646102E-01
1.2000000000000000E+00  3.3489797668038418E-01
1.3999999999999999E+00  2.7908164723365347E-01
```

Modify the file output such that it looks like

```
0.000  1.00000
0.200  0.83333
0.400  0.69444
0.600  0.57870
0.800  0.48225
1.000  0.40188
1.200  0.33490
1.400  0.27908
```

Run the modified program

```
Terminal> python decay_memsave_v2.py --T 10 --theta 1 \
          --dt 0.2 --makeplot
```

The program just prints `Bug in the implementation!` and does not show the plot. What went wrong? Filename: `decay_memsave_v2.py`.

Problem 9: Write a doctest

Type in the following program and equip the `roots` function with a doctest:

```
import sys
# This sqrt(x) returns real if x>0 and complex if x<0
from numpy.lib.scimath import sqrt

def roots(a, b, c):
    """
    Return the roots of the quadratic polynomial
    p(x) = a*x**2 + b*x + c.

    The roots are real or complex objects.
    """
    q = b**2 - 4*a*c
    r1 = (-b + sqrt(q))/(2*a)
    r2 = (-b - sqrt(q))/(2*a)
    return r1, r2

a, b, c = [float(arg) for arg in sys.argv[1:]]
print roots(a, b, c)
```

Make sure to test both real and complex roots. Write out numbers with 14 digits or less. Filename: `doctest_roots.py`.

Problem 10: Write a nose test

Make a nose test for the `roots` function in Problem 9. Filename: `test_roots.py`.

Problem 11: Make a module

Let

$$q(t) = \frac{RAe^{at}}{R + A(e^{at} - 1)}\,.$$

Make a Python module `q_module` containing two functions `q(t)` and `dqdt(t)` for computing $q(t)$ and $q'(t)$, respectively. Perform a `from numpy import *` in this module. Import `q` and `dqdt` in another file using the "star import" construction `from q_module import *`. All objects available in this file is given by `dir()`. Print `dir()` and `len(dir())`. Then change the import of `numpy` in `q_module.py` to `import numpy as np`. What is the effect of this import on the number of objects in `dir()` in a file that does `from q_module import *`?

Filename: `q_module.py`.

Exercise 12: Make use of a class implementation

We want to solve the exponential decay problem $u' = -au$, $u(0) = I$, for several Δt values and $\theta = 0, 0.5, 1$. For each Δt value, we want to make a plot where the three solutions corresponding to $\theta = 0, 0.5, 1$ appear along with the exact solution. Write a function `experiment` to accomplish this. The function should import the classes `Problem`, `Solver`, and `Visualizer` from the `decay_class` module and make use of these. A new command-line option `--dt_values` must be added to allow the user to specify the Δt values on the command line (the options `--dt` and `--theta` implemented by the `decay_class` module have then no effect when running the `experiment` function). Note that the classes in the `decay_class` module should *not* be modified. Filename: `decay_class_exper.py`.

Exercise 13: Generalize a class implementation

Consider the file `decay_class.py` where the exponential decay problem $u' = -au$, $u(0) = I$, is implemented via the classes `Problem`, `Solver`, and `Visualizer`. Extend the classes to handle the more general problem

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

using the θ-rule for discretization.

In the case with arbitrary functions $a(t)$ and $b(t)$ the problem class is no longer guaranteed to provide an exact solution. Let the `exact_solution` in class `Problem` return `None` if the exact solution for the particular problem is not available. Modify classes `Solver` and `Visualizer` accordingly.

Add test functions `test_*()` for the nose testing tool in the module. Also add a demo example where the environment suddenly changes (modeled as an abrupt change in the decay rate a):

$$a(t) = \begin{cases} 1, & 0 \leq t \leq t_p, \\ k, & t > t_p, \end{cases}$$

where t_p is the point of time the environment changes. Take $t_p = 1$ and make plots that illustrate the effect of having $k \gg 1$ and $k \ll 1$. Filename: `decay_class2.py`.

Exercise 14: Generalize an advanced class implementation

Solve Exercise 13 by utilizing the class implementations in `decay_class_oo.py`. Filename: `decay_class3.py`.

6 Analysis of finite difference equations

We address the ODE for exponential decay,

$$u'(t) = -au(t), \quad u(0) = I, \tag{51}$$

where a and I are given constants. This problem is solved by the θ-rule finite difference scheme, resulting in the recursive equations

$$u^{n+1} = \frac{1 - (1-\theta)a\Delta t}{1 + \theta a\Delta t}u^n \tag{52}$$

for the numerical solution u^{n+1}, which approximates the exact solution u_{e} at time point t_{n+1}. For constant mesh spacing, which we assume here, $t_{n+1} = (n+1)\Delta t$.

Discouraging numerical solutions. Choosing $I = 1$, $a = 2$, and running experiments with $\theta = 1, 0.5, 0$ for $\Delta t = 1.25, 0.75, 0.5, 0.1$, gives the results in Figures 15, 16, and 17.

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

- The Backward Euler scheme always gives 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.
- 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.

Since the exact solution of our model problem is a monotone function, $u(t) = Ie^{-at}$, some of these qualitatively wrong results are indeed alarming!

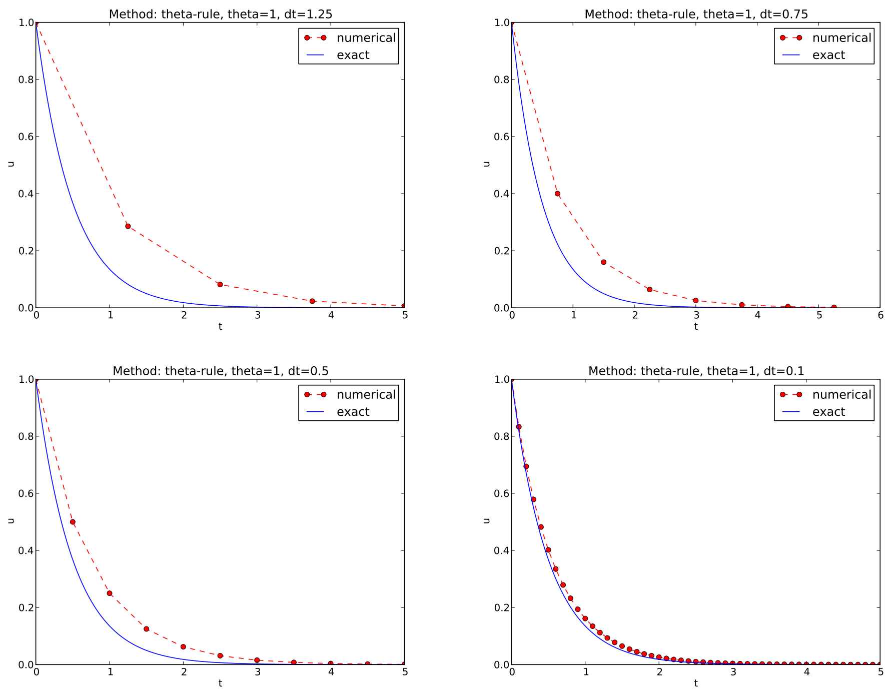


Figure 15: Backward Euler.

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?

The question will be investigated both by numerical experiments and by precise mathematical theory. The latter will help establish general critera on Δt for avoiding non-physical oscillatory or growing solutions.

Another question to be raised is

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

For our simple model problem we can answer this question very precisely, but we will also look at simplified formulas for small Δt and touch upon important concepts such as *convergence rate* and *the order of a scheme*. Other fundamental concepts mentioned are stability, consistency, and convergence.

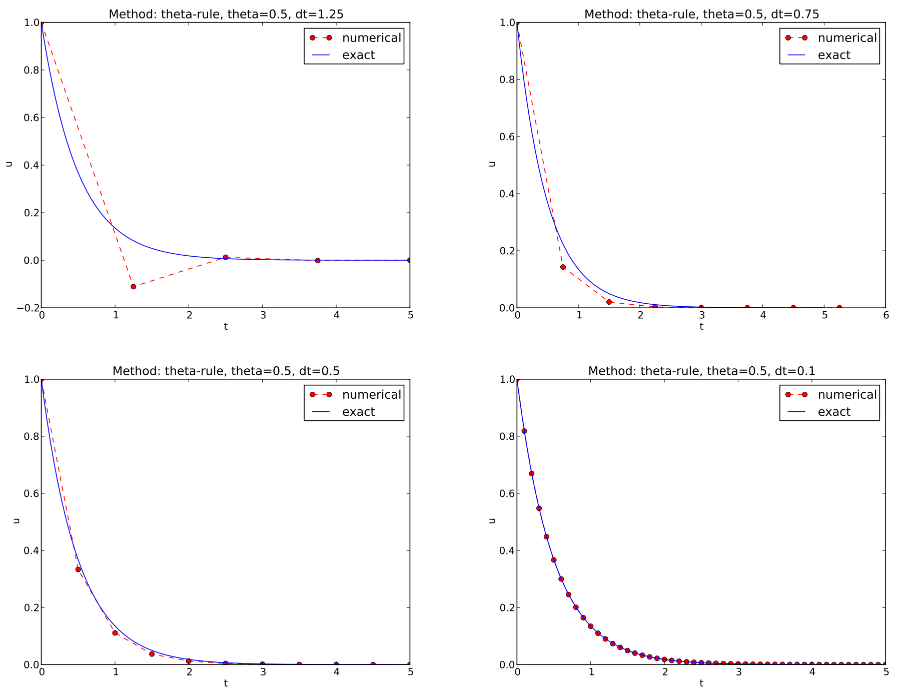


Figure 16: Crank-Nicolson.

6.1 Experimental investigation of oscillatory solutions

To address the first question above, we may set up an experiment where we loop over values of I, a, and Δt. For each experiment, we flag the solution as oscillatory if

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

for some value of n, since we expect u^n to decay with n, but oscillations make u increase over a time step. We will quickly see that oscillations are independent of I, but do depend on a and Δt. Therefore, we introduce a two-dimensional function $B(a, \Delta t)$ which is 1 if oscillations occur and 0 otherwise. We can visualize B as a contour plot (lines for which $B = \text{const}$). The contour $B = 0.5$ corresponds to the borderline between oscillatory regions with $B = 1$ and monotone regions with $B = 0$ in the $a, \Delta t$ plane.

The B function is defined at discrete a and Δt values. Say we have given P a values, $a_0, \ldots, a_{P-1}$, and Q Δt values, $\Delta t_0, \ldots, \Delta t_{Q-1}$. These a_i and Δt_j values, $i = 0, \ldots, P-1$, $j = 0, \ldots, Q-1$, form a rectangular mesh of $P \times Q$ points in the plane. At each point $(a_i, \Delta t_j)$, we associate the corresponding value of $B(a_i, \Delta t_j)$, denoted B_{ij}. The B_{ij} values are naturally stored in a two-dimensional array. We can thereafter create a plot of the contour line $B_{ij} = 0.5$ dividing the oscillatory and monotone regions. The file `decay_osc_regions.py` `osc_regions` stands

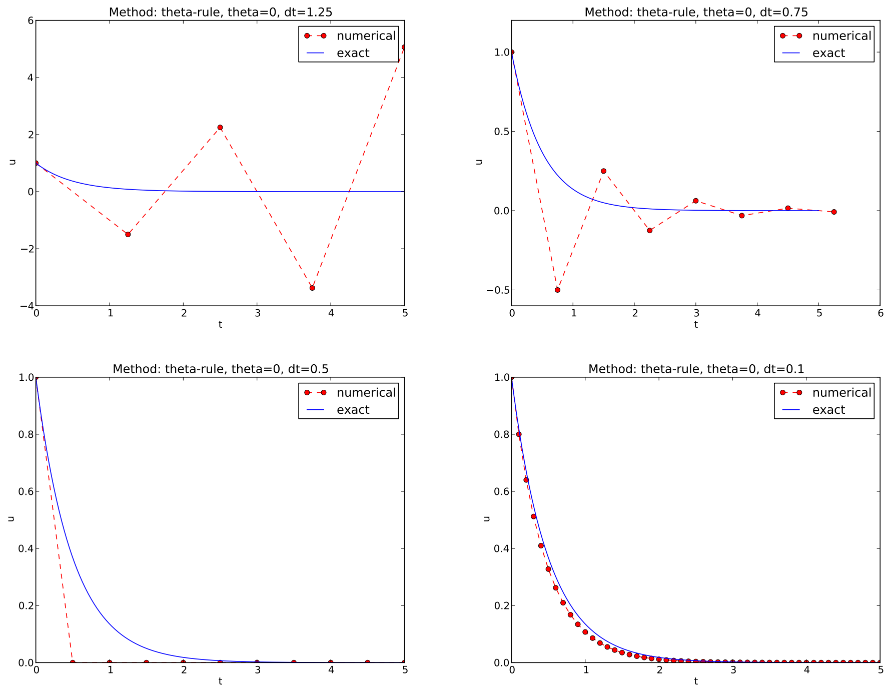


Figure 17: Forward Euler.

for "oscillatory regions") contains all nuts and bolts to produce the $B = 0.5$ line in Figures 18 and 19. The oscillatory region is above this line.

```
from decay_mod import solver
import numpy as np
import scitools.std as st

def non_physical_behavior(I, a, T, dt, theta):
    """
    Given lists/arrays a and dt, and numbers I, dt, and theta,
    make a two-dimensional contour line B=0.5, where B=1>0.5
    means oscillatory (unstable) solution, and B=0<0.5 means
    monotone solution of u'=-au.
    """
    a = np.asarray(a); dt = np.asarray(dt)  # must be arrays
    B = np.zeros((len(a), len(dt)))         # results
    for i in range(len(a)):
        for j in range(len(dt)):
            u, t = solver(I, a[i], T, dt[j], theta)
            # Does u have the right monotone decay properties?
            correct_qualitative_behavior = True
            for n in range(1, len(u)):
                if u[n] > u[n-1]:  # Not decaying?
                    correct_qualitative_behavior = False
                    break  # Jump out of loop
            B[i,j] = float(correct_qualitative_behavior)
    a_, dt_ = st.ndgrid(a, dt)  # make mesh of a and dt values
    st.contour(a_, dt_, B, 1)
    st.grid('on')
    st.title('theta=%g' % theta)
    st.xlabel('a'); st.ylabel('dt')
    st.savefig('osc_region_theta_%s.png' % theta)
    st.savefig('osc_region_theta_%s.pdf' % theta)

non_physical_behavior(
    I=1,
    a=np.linspace(0.01, 4, 22),
    dt=np.linspace(0.01, 4, 22),
    T=6,
    theta=0.5)
```

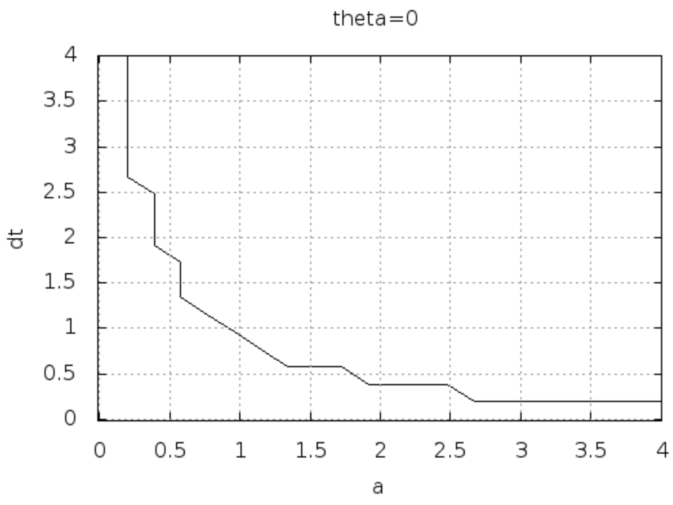


Figure 18: Forward Euler scheme: oscillatory solutions occur for points above the curve.

By looking at the curves in the figures one may guess that $a\Delta t$ must be less than a critical limit to avoid the undesired oscillations. This limit seems to be about 2 for Crank-Nicolson and 1 for Forward Euler. We shall now establish a precise mathematical analysis of the discrete model that can explain the observations in our numerical experiments.

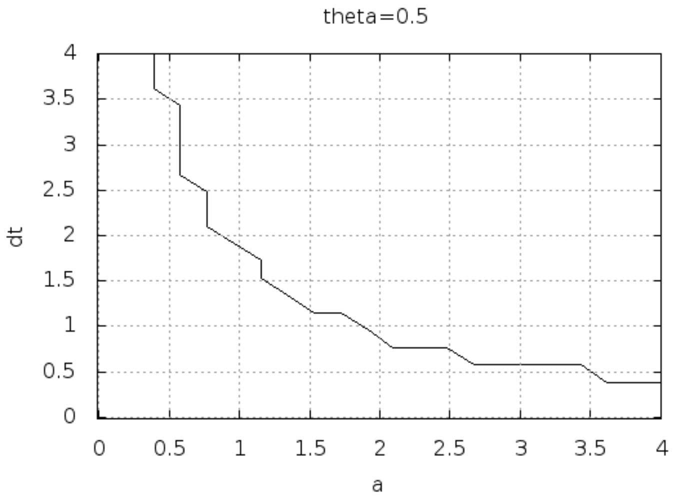


Figure 19: Crank-Nicolson scheme: oscillatory solutions occur for points above the curve.

6.2 Exact numerical solution

Starting with $u^0 = I$, the simple recursion (52) can be applied repeatedly n times, with the result that

$$u^n = IA^n, \quad A = \frac{1-(1-\theta)a\Delta t}{1+\theta a\Delta t}\,. \tag{53}$$

Solving difference equations.

Difference equations where all terms are linear in u^{n+1}, u^n, and maybe u^{n-1}, u^{n-2}, etc., are called *homogeneous, linear* difference equations, and their solutions are generally of the form $u^n = A^n$. Inserting this expression and dividing by A^{n+1} gives a polynomial equation in A. In the present case we get

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

This is a solution technique of wider applicability than repeated use of the recursion (52).

Regardless of the solution approach, we have obtained a formula for u^n. This formula can explain everything what we see in the figures above, but it also gives us a more general insight into accuracy and stability properties of the three schemes.

6.3 Stability

Since u^n is a factor A raised to an integer power n, we realize that $A < 0$ will for odd powers imply $u^n < 0$ and for even power result in $u^n > 0$. That is, the solution oscillates between the mesh points. We have oscillations due to $A < 0$ when

$$(1-\theta)a\Delta t > 1\,. \tag{54}$$

Since $A > 0$ is a requirement for having a numerical solution with the same basic property (monotonicity) as the exact solution, we may say that $A > 0$ is a *stability criterion*. Expressed in terms of Δt the stability criterion reads

$$\Delta t < \frac{1}{(1-\theta)a}\,. \tag{55}$$

The Backward Euler scheme is always stable since $A < 0$ is impossible for $\theta = 1$, while non-oscillating solutions for Forward Euler and Crank-Nicolson demand $\Delta t \leq 1/a$ and $\Delta t \leq 2/a$, respectively. The relation between Δt and a look reasonable: a larger a means faster decay and hence a need for smaller time steps.

Looking at Figure 17, we see that with $a\Delta t = 2 \cdot 1.25 = 2.5$, $A = -1.5$, and the solution $u^n = (-1.5)^n$ oscillates *and* grows. With $a\Delta t = 2 \cdot 0.75 = 1.5$, $A = -0.5$, $u^n = (-0.5)^n$ decays but oscillates. The peculiar case $\Delta t = 0.5$, where the Forward Euler scheme produces a solution that is stuck on the t axis, corresponds to $A = 0$ and therefore $u^0 = I = 1$ and $u^n = 0$ for $n \geq 1$. The decaying oscillations in the Crank-Nicolson scheme for $\Delta t = 1.25$ are easily explained by the fact that $A \approx -0.11 < 0$.

The factor A is called the *amplification factor* since the solution at a new time level is A times the solution at the previous time level. For a decay process, we must obviously have $|A| \leq 1$, which is fulfilled for all Δt if $\theta \geq 1/2$. Arbitrarily large values of u can be generated when $|A| > 1$ and n is large enough. The numerical solution is in such cases totally irrelevant to an ODE modeling decay processes! To avoid this situation, we must for $\theta < 1/2$ have

$$\Delta t \leq \frac{2}{(1-2\theta)a}, \tag{56}$$

which means $\Delta t < 2/a$ for the Forward Euler scheme.

Stability properties.
We may summarize the stability investigations as follows:

1. The Forward Euler method is a *conditionally stable* scheme because it requires $\Delta t < 2/a$ for avoiding growing solutions and $\Delta t < 1/a$ for avoiding oscillatory solutions.

2. The Crank-Nicolson is *unconditionally stable* with respect to growing solutions, while it is conditionally stable with the criterion $\Delta t < 2/a$ for avoiding oscillatory solutions.
3. The Backward Euler method is unconditionally stable with respect to growing and oscillatory solutions - any Δt will work.

Much literature on ODEs speaks about L-stable and A-stable methods. In our case A-stable methods ensures non-growing solutions, while L-stable methods also avoids oscillatory solutions.

6.4 Comparing amplification factors

After establishing how A impacts the qualitative features of the solution, we shall now look more into how well the numerical amplification factor approximates the exact one. The exact solution reads $u(t) = Ie^{-at}$, which can be rewritten as

$$u_{\rm e}(t_n) = Ie^{-an\Delta t} = I(e^{-a\Delta t})^n \,. \tag{57}$$

From this formula we see that the exact amplification factor is

$$A_{\rm e} = e^{-a\Delta t} \,. \tag{58}$$

We realize that the exact and numerical amplification factors depend on a and Δt through the product $a\Delta t$. Therefore, it is convenient to introduce a symbol for this product, $p = a\Delta t$, and view A and $A_{\rm e}$ as functions of p. Figure 20 shows these functions. Crank-Nicolson is clearly closest to the exact amplification factor, but that method has the unfortunate oscillatory behavior when $p > 2$.

6.5 Series expansion of amplification factors

As an alternative to the visual understanding inherent in Figure 20, there is a strong tradition in numerical analysis to establish formulas for the approximation errors when the discretization parameter, here Δt, becomes small. In the present case we let p be our small discretization parameter, and it makes sense to simplify the expressions for A and $A_{\rm e}$ by using Taylor polynomials around $p = 0$. The Taylor polynomials are accurate for small p and greatly simplifies the comparison of the analytical expressions since we then can compare polynomials, term by term.

Calculating the Taylor series for $A_{\rm e}$ is easily done by hand, but the three versions of A for $\theta = 0, 1, \frac{1}{2}$ lead to more cumbersome calculations. Nowadays, analytical computations can benefit greatly by symbolic computer algebra software. The Python package `sympy` represents a powerful computer algebra system, not yet as sophisticated as the famous Maple and Mathematica systems, but free and very easy to integrate with our numerical computations in Python.

When using `sympy`, it is convenient to enter the interactive Python mode where we can write expressions and statements and immediately see the results.

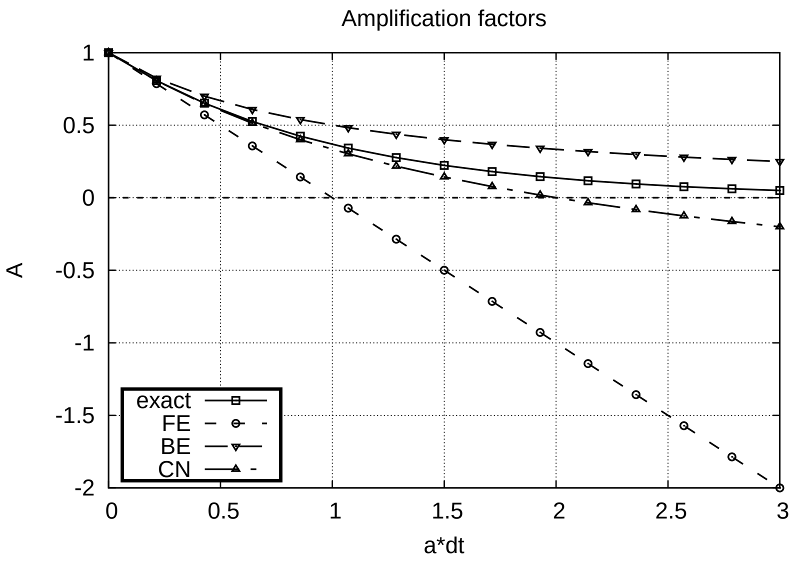


Figure 20: Comparison of amplification factors.

Here is a simple example. We strongly recommend to use `isympy` (or `ipython`) for such interactive sessions.

Let us illustrate `sympy` with a standard Python shell syntax (`>>>` prompt) to compute a Taylor polynomial approximation to e^{-p}:

```
>>> 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, 0, 6)
1 + (1/2)*p**2 - p - 1/6*p**3 - 1/120*p**5 + (1/24)*p**4 + O(p**6)
```

Lines with `>>>` represent input lines and lines without this prompt represents the result of computations (note that `isympy` and `ipython` apply other prompts, but in this text we always apply `>>>` for interactive Python computing). Apart from the order of the powers, the computed formula is easily recognized as the beginning of the Taylor series for e^{-p}.

Let us define the numerical amplification factor where p and θ enter the formula as symbols:

```
>>> theta = Symbol('theta')
>>> A = (1-(1-theta)*p)/(1+theta*p)
```

To work with the factor for the Backward Euler scheme we can substitute the value 1 for `theta`:

```
>>> A.subs(theta, 1)
1/(1 + p)
```

Similarly, we can replace `theta` by $1/2$ for Crank-Nicolson, preferably using an exact rational representation of $1/2$ in `sympy`:

```
>>> half = Rational(1,2)
>>> A.subs(theta, half)
1/(1 + (1/2)*p)*(1 - 1/2*p)
```

The Taylor series of the amplification factor for the Crank-Nicolson scheme can be computed as

```
>>> A.subs(theta, half).series(p, 0, 4)
1 + (1/2)*p**2 - p - 1/4*p**3 + O(p**4)
```

We are now in a position to compare Taylor series:

```
>>> FE = A_e.series(p, 0, 4) - A.subs(theta, 0).series(p, 0, 4)
>>> BE = A_e.series(p, 0, 4) - A.subs(theta, 1).series(p, 0, 4)
>>> CN = A_e.series(p, 0, 4) - A.subs(theta, half).series(p, 0, 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)
```

From these expressions we see that the error $A - A_{\rm e} \sim \mathcal{O}(p^2)$ for the Forward and Backward Euler schemes, while $A - A_{\rm e} \sim \mathcal{O}(p^3)$ for the Crank-Nicolson scheme. It is the *leading order term*, i.e., the term of the lowest order (polynomial degree), that is of interest, because as $p \rightarrow 0$, this term is (much) bigger than the higher-order terms (think of $p = 0.01$: p is a hundred times larger than p^2).

Now, a is a given parameter in the problem, while Δt is what we can vary. One therefore usually writes the error expressions in terms Δt. When then have

$$A - A_{\rm e} = \left\{ \begin{array}{ll} \mathcal{O}(\Delta t^2), & \hbox{Forward and Backward Euler}, \\ \mathcal{O}(\Delta t^3), & \hbox{Crank-Nicolson} \end{array}\right. \tag{59}$$

We say that the Crank-Nicolson scheme has an error in the amplification factor of order Δt^3, while the two other schemes are of order Δt^2 in the same quantity. What is the significance of the order expression? If we halve Δt, the error in amplification factor at a time level will be reduced by a factor of 4 in the Forward and Backward Euler schemes, and by a factor of 8 in the Crank-Nicolson scheme. That is, as we reduce Δt to obtain more accurate results, the Crank-Nicolson scheme reduces the error more efficiently than the other schemes.

6.6 The fraction of numerical and exact amplification factors

An alternative comparison of the schemes is to look at the ratio $A/A_{\rm e}$, or the error $1 - A/A_{\rm e}$ in this ratio:

```
>>> FE = 1 - (A.subs(theta, 0)/A_e).series(p, 0, 4)
>>> BE = 1 - (A.subs(theta, 1)/A_e).series(p, 0, 4)
>>> CN = 1 - (A.subs(theta, half)/A_e).series(p, 0, 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)
```

The leading-order terms have the same powers as in the analysis of $A - A_{\rm e}$.

6.7 The global error at a point

The error in the amplification factor reflects the error when progressing from time level t_n to t_{n-1}. To investigate the real error at a point, known as the *global error*, we look at $e^n = u^n - u_{\rm e}(t_n)$ for some n and Taylor expand the mathematical expressions as functions of $p = a\Delta t$:

```
>>> n = Symbol('n')
>>> u_e = exp(-p*n)
>>> u_n = A**n
>>> FE = u_e.series(p, 0, 4) - u_n.subs(theta, 0).series(p, 0, 4)
>>> BE = u_e.series(p, 0, 4) - u_n.subs(theta, 1).series(p, 0, 4)
>>> CN = u_e.series(p, 0, 4) - u_n.subs(theta, half).series(p, 0, 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)
```

For a fixed time t, the parameter n in these expressions increases as $p \rightarrow 0$ since $t = n\Delta t = \text{const}$ and hence n must increase like Δt^{-1}. With n substituted by $t/\Delta t$ in the leading-order error terms, these become $\frac{1}{2}na^2\Delta t^2 = \frac{1}{2}ta^2\Delta t$ for the Forward and Backward Euler scheme, and $\frac{1}{12}na^3\Delta t^3 = \frac{1}{12}ta^3\Delta t^2$ for the Crank-Nicolson scheme. The global error is therefore of second order (in Δt) for the latter scheme and of first order for the former schemes.

When the global error $e^n \rightarrow 0$ as $\Delta t \rightarrow 0$, we say that the scheme is *convergent*. It means that the numerical solution approaches the exact solution as the mesh is refined, and this is a much desired property of a numerical method.

6.8 Integrated errors

It is common to study the norm of the numerical error, as explained in detail in Section 2.4. The L^2 norm can be computed by treating e^n as a function of t in `sympy` and performing symbolic integration. For the Forward Euler scheme we have

```
p, n, a, dt, t, T, theta = symbols('p n a dt t T 'theta')
A = (1-(1-theta)*p)/(1+theta*p)
u_e = exp(-p*n)
u_n = A**n
error = u_e.series(p, 0, 4) - u_n.subs(theta, 0).series(p, 0, 4)
# Introduce t and dt instead of n and p
error = error.subs('n', 't/dt').subs(p, 'a*dt')
error = error.as_leading_term(dt) # study only the first term
print error
error_L2 = sqrt(integrate(error**2, (t, 0, T)))
print error_L2
```

The output reads

```
sqrt(30)*sqrt(T**3*a**4*dt**2*(6*T**2*a**2 - 15*T*a + 10))/60
```

which means that the L^2 error behaves like $a^2\Delta t$.

Strictly speaking, the numerical error is only defined at the mesh points so it makes most sense to compute the ℓ^2 error

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

We have obtained an exact analytical expressions for the error at $t = t_n$, but here we use the leading-order error term only since we are mostly interested in how the error behaves as a polynomial in Δt, and then the leading order term will dominate. For the Forward Euler scheme, $u_{\mathrm{e}}(t_n) - u^n \approx \frac{1}{2}np^2$, and we have

$$||e^n||_{\ell^2}^2 = \Delta t \sum_{n=0}^{N_t} \frac{1}{4}n^2p^4 = \Delta t \frac{1}{4}p^4 \sum_{n=0}^{N_t} n^2\,.$$

Now, $\sum_{n=0}^{N_t} n^2 \approx \frac{1}{3}N_t^3$. Using this approximation, setting $N_t = T/\Delta t$, and taking the square root gives the expression

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

Calculations for the Backward Euler scheme are very similar and provide the same result, while the Crank-Nicolson scheme leads to

$$||e^n||_{\ell^2} = \frac{1}{12}\sqrt{\frac{T^3}{3}}a^3\Delta t^2\,.$$

Summary of errors.

Both the point-wise and the time-integrated true errors are of second order in Δt for the Crank-Nicolson scheme and of first order in Δt for the Forward Euler and Backward Euler schemes.

6.9 Truncation error

The truncation error is a very frequently used error measure for finite difference methods. It is defined as *the error in the difference equation that arises when inserting the exact solution.* Contrary to many other error measures, e.g., the true error $e^n = u_{\rm e}(t_n) - u^n$, the truncation error is a quantity that is easily computable.

Let us illustrate the calculation of the truncation error for the Forward Euler scheme. We start with the difference equation on operator form,

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

i.e.,

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

The idea is to see how well the exact solution $u_{\rm e}(t)$ fulfills this equation. Since $u_{\rm e}(t)$ in general will not obey the discrete equation, error in the discrete equation, called a *residual*, denoted here by R^n:

$$R^n = \frac{u_{\rm e}(t_{n+1}) - u_{\rm e}(t_n)}{\Delta t} + au_{\rm e}(t_n)\,. \tag{60}$$

The residual is defined at each mesh point and is therefore a mesh function with a superscript n.

The interesting feature of R^n is to see how it depends on the discretization parameter Δt. The tool for reaching this goal is to Taylor expand $u_{\rm e}$ around the point where the difference equation is supposed to hold, here $t = t_n$. We have that

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

Inserting this Taylor series in (60) gives

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

Now, $u_{\rm e}$ fulfills the ODE $u_{\rm e}' = -au_{\rm e}$ such that the first and last term cancels and we have

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

This R^n is the *truncation error*, which for the Forward Euler is seen to be of first order in Δt.

The above procedure can be repeated for the Backward Euler and the Crank-Nicolson schemes. We start with the scheme in operator notation, write it out in detail, Taylor expand $u_{\rm e}$ around the point $\tilde{t}$ at which the difference equation is defined, collect terms that correspond to the ODE (here $u_{\rm e}' + au_{\rm e}$), and identify the remaining terms as the residual R, which is the truncation error. The Backward Euler scheme leads to

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

while the Crank-Nicolson scheme gives

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

The *order* r of a finite difference scheme is often defined through the leading term Δt^r in the truncation error. The above expressions point out that the Forward and Backward Euler schemes are of first order, while Crank-Nicolson is of second order. We have looked at other error measures in other sections, like the error in amplification factor and the error $e^n = u_{\rm e}(t_n) - u^n$, and expressed these error measures in terms of Δt to see the order of the method. Normally, calculating the truncation error is more straightforward than deriving the expressions for other error measures and therefore the easiest way to establish the order of a scheme.

6.10 Consistency, stability, and convergence

Three fundamental concepts when solving differential equations by numerical methods are consistency, stability, and convergence. We shall briefly touch these concepts below in the context of the present model problem.

Consistency means that the error in the difference equation, measured through the truncation error, goes to zero as $\Delta t \rightarrow 0$. Since the truncation error tells how well the exact solution fulfills the difference equation, and the exact solution fulfills the differential equation, consistency ensures that the difference equation approaches the differential equation in the limit. The expressions for the truncation errors in the previous section are all proportional to Δt or Δt^2, hence they vanish as $\Delta t \rightarrow 0$, and all the schemes are consistent. Lack of consistency implies that we actually solve a different differential equation in the limit $\Delta t \rightarrow 0$ than we aim at.

Stability means that the numerical solution exhibits the same qualitative properties as the exact solution. This is obviously a feature we want the numerical solution to have. In the present exponential decay model, the exact solution is monotone and decaying. An increasing numerical solution is not in accordance with the decaying nature of the exact solution and hence unstable. We can also say that an oscillating numerical solution lacks the property of monotonicity of the exact solution and is also unstable. We have seen that the Backward Euler scheme always leads to monotone and decaying solutions, regardless of Δt, and is hence stable. The Forward Euler scheme can lead to increasing solutions and oscillating solutions if Δt is too large and is therefore unstable unless Δt is sufficiently small. The Crank-Nicolson can never lead to increasing solutions and has no problem to fulfill that stability property, but it can produce oscillating solutions and is unstable in that sense, unless Δt is sufficiently small.

Convergence implies that the global (true) error mesh function $e^n = u_{\rm e}(t_n) - u^n \rightarrow 0$ as $\Delta t \rightarrow 0$. This is really what we want: the numerical solution gets as close to the exact solution as we request by having a sufficiently fine mesh.

Convergence is hard to establish theoretically, except in quite simple problems like the present one. Stability and consistency are much easier to calculate. A major breakthrough in the understanding of numerical methods for differential equations came in 1956 when Lax and Richtmeyer established equivalence between convergence on one hand and consistency and stability on the other (the Lax equivalence theorem). In practice it meant that one can first establish that a method is stable and consistent, and then it is automatically convergent (which is much harder to establish). The result holds for linear problems only, and in the world of nonlinear differential equations the relations between consistency, stability, and convergence are much more complicated.

We have seen in the previous analysis that the Forward Euler, Backward Euler, and Crank-Nicolson schemes are convergent ($e^n \rightarrow 0$), that they are consistent ($R^n \rightarrow 0$, and that they are stable under certain conditions on the size of Δt. We have also derived explicit mathematical expressions for e^n, the truncation error, and the stability criteria.

7 Exercises

Exercise 15: Visualize the accuracy of finite differences $u = e^{-at}$

The purpose of this exercise is to visualize the accuracy of finite difference approximations of the derivative of a given function. For any finite difference approximation, take the Forward Euler difference as an example, and any specific function, take $u = e^{-at}$, we may introduce an error fraction specific

$$E = \frac{[D_t^+ u]^n}{u'(t_n)} = \frac{\exp\left(-a(t_n + \Delta t)\right) - \exp\left(-at_n\right)}{-a\exp\left(-at_n\right)} = -\frac{1}{a\Delta t}\left(\exp\left(-a\Delta t\right) - 1\right),$$

and view E as a function of Δt. We expect that $\lim_{\Delta t\rightarrow 0} E = 1$, while E may deviate significantly from unit for large Δt. How the error depends on Δt is best visualized in a graph where we use a logarithmic scale on for Δt, so we can cover many orders of magnitude of that quantity. Here is a code segment creating an array of 100 intervals, on the logarithmic scale, ranging from 10^{-6} to 1 and then plotting E versus $p = a\Delta t$ with logarithmic scale on the Δt axis:

```
from numpy import logspace, exp
from matplotlib.pyplot import plot
p = logspace(-6, 1, 101)
```

```
y = -(exp(-p)-1)/p
semilog(p, y)
```

Illustrate such errors for the finite difference operators $[D_t^+ u]^n$ (forward), $[D_t^- u]^n$ (backward), and $[D_t u]^n$ (centered).

Perform a Taylor series expansions of the error fractions and find the leading order r in the expressions of type $1+C\Delta t^r + \mathcal{O}(\Delta t^{r+1})$, where C is some constant. Filename: `decay_plot_fd_exp_error.py`.

Exercise 16: Explore the θ-rule for exponential growth

This exercise asks you to solve the ODE $u' = -au$ with $a < 0$ such that the ODE models exponential growth instead of exponential decay. A central theme is to investigate numerical artifacts and non-physical solution behavior.

a) Run experiments with θ and Δt to uncover numerical artifacts (the exact solution is a monotone, growing function). Use the insight to design a set of experiments that aims to demonstrate all types of numerical artifacts for different choices of Δt while a is fixed.

Hint. Modify the `decay_exper1.py` code to suit your needs.
Filename: `growth_exper.py`.

b) Write a scientific report about the findings.

Hint. Use examples from Section 4.4 to see how scientific reports can be written.
Filenames: `growth_exper.pdf`, `growth_exper.html`.

c) Plot the amplification factors for the various schemes together with the exact one for $a < 0$ and use the plot to explain the observations made in the experiments.

Hint. Modify the `decay_ampf_plot.py` code.
Filename: `growth_ampf.py`.

8 Model extensions

It is time to consider generalizations of the simple decay model $u = -au$ and also to look at additional numerical solution methods.

8.1 Generalization: including a variable coefficient

In the ODE for decay, $u' = -au$, we now consider the case where a depends on time:

$$u'(t) = -a(t)u(t), \quad t \in (0, T], \quad u(0) = I\,. \tag{61}$$

A Forward Euler scheme consist of evaluating (61) at $t = t_n$ and approximating the derivative with a forward difference $[D_t^+ u]^n$:

$$\frac{u^{n+1} - u^n}{\Delta t} = -a(t_n)u^n\,. \tag{62}$$

The Backward Euler scheme becomes

$$\frac{u^n - u^{n-1}}{\Delta t} = -a(t_n)u^n\,. \tag{63}$$

The Crank-Nicolson method builds on sampling the ODE at $t_{n+\frac{1}{2}}$. We can evaluate a at $t_{n+\frac{1}{2}}$ and use an average for u at times t_n and t_{n+1}:

$$\frac{u^{n+1} - u^n}{\Delta t} = -a(t_{n+\frac{1}{2}})\frac{1}{2}(u^n + u^{n+1})\,. \tag{64}$$

Alternatively, we can use an average for the product au:

$$\frac{u^{n+1} - u^n}{\Delta t} = -\frac{1}{2}(a(t_n)u^n + a(t_{n+1})u^{n+1})\,. \tag{65}$$

The θ-rule unifies the three mentioned schemes. One version is to have a evaluated at $t_{n+\theta}$,

$$\frac{u^{n+1} - u^n}{\Delta t} = -a((1-\theta)t_n + \theta t_{n+1})((1-\theta)u^n + \theta u^{n+1})\,. \tag{66}$$

Another possibility is to apply a weighted average for the product au,

$$\frac{u^{n+1} - u^n}{\Delta t} = -(1-\theta)a(t_n)u^n - \theta a(t_{n+1})u^{n+1}\,. \tag{67}$$

With the finite difference operator notation the Forward Euler and Backward Euler schemes can be summarized as

$$[D_t^+ u = -au]^n, \tag{68}$$

$$[D_t^- u = -au]^n\,. \tag{69}$$

The Crank-Nicolson and θ schemes depend on whether we evaluate a at the sample point for the ODE or if we use an average. The various versions are written as

$$[D_t u = -a\overline{u}^t]^{n+\frac{1}{2}}, \tag{70}$$

$$[D_t u = -\overline{au}^t]^{n+\frac{1}{2}}, \tag{71}$$

$$[D_t u = -a\overline{u}^{t,\theta}]^{n+\theta}, \tag{72}$$

$$[D_t u = -\overline{au}^{t,\theta}]^{n+\theta}\,. \tag{73}$$

8.2 Generalization: including a source term

A further extension of the model ODE is to include a source term $b(t)$:

$$u'(t) = -a(t)u(t) + b(t), \quad t \in (0, T], \quad u(0) = I\,. \tag{74}$$

Schemes. The time point where we sample the ODE determines where $b(t)$ is evaluated. For the Crank-Nicolson scheme and the θ-rule we have a choice of whether to evaluate $a(t)$ and $b(t)$ at the correct point or use an average. The chosen strategy becomes particularly clear if we write up the schemes in the operator notation:

$$[D_t^+ u = -au + b]^n, \tag{75}$$

$$[D_t^- u = -au + b]^n, \tag{76}$$

$$[D_t u = -a\overline{u}^t + b]^{n+\frac{1}{2}}, \tag{77}$$

$$[D_t u = \overline{-au + b}^t]^{n+\frac{1}{2}}, \tag{78}$$

$$[D_t u = -a\overline{u}^{t,\theta} + b]^{n+\theta}, \tag{79}$$

$$[D_t u = \overline{-au + b}^{t,\theta}]^{n+\theta}\,. \tag{80}$$

8.3 Implementation of the generalized model problem

Deriving the θ-rule formula. Writing out the θ-rule in (80), using (32) and (33), we get

$$\frac{u^{n+1} - u^n}{\Delta t} = \theta(-a^{n+1}u^{n+1} + b^{n+1})) + (1-\theta)(-a^n u^n + b^n)), \tag{81}$$

where a^n means evaluating a at $t = t_n$ and similar for a^{n+1}, b^n, and b^{n+1}. We solve for u^{n+1}:

$$u^{n+1} = ((1 - \Delta t(1-\theta)a^n)u^n + \Delta t(\theta b^{n+1} + (1-\theta)b^n))(1 + \Delta t\theta a^{n+1})^{-1}\,. \tag{82}$$

The Python code. Here is a suitable implementation of (81) where $a(t)$ and $b(t)$ are given as Python functions:

```
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
```

This function is found in the file `decay_vc.py` (`vc` stands for "variable coefficients").

Coding of variable coefficients. The `solver` function shown above demands the arguments `a` and `b` to be Python functions of time `t`, say

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

def b(t):
    return 1
```

Here, `a(t)` has three parameters `a0`, `tp`, and `k`, which must be global variables. A better implementation is to represent `a` by a class where the parameters are attributes and a *special method* `__call__` evaluates $a(t)$:

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

    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)
```

For quick tests it is cumbersome to write a complete function or a class. The *lambda function* construction in Python is then convenient. For example,

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

is equivalent to the `def a(t):` definition above. In general,

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

is equivalent to

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

One can use lambda functions directly in calls. Say we want to solve $u' = -u + 1$, $u(0) = 2$:

```
u, t = solver(2, lambda t: 1, lambda t: 1, T, dt, theta)
```

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

8.4 Verifying a constant solution

A very useful partial verification method is to construct a test problem with a very simple solution, usually $u = \text{const}$. Especially the initial debugging of a program code can benefit greatly from such tests, because 1) all relevant numerical methods will exactly reproduce a constant solution, 2) many of the intermediate calculations are easy to control for a constant u, and 3) even a constant u can uncover many bugs in an implementation.

The only constant solution for the problem $u' = -au$ is $u = 0$, but too many bugs can escape from that trivial solution. It is much better to search for a problem where $u = C = \text{const} \neq 0$. Then $u' = -a(t)u + b(t)$ is more appropriate: with $u = C$ we can choose any $a(t)$ and set $b = a(t)C$ and $I = C$. An appropriate nose test is

```
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)
```

An interesting question is what type of bugs that will make the computed u^n deviate from the exact solution C. Fortunately, the updating formula and the initial condition must be absolutely correct for the test to pass! Any attempt to make a wrong indexing in terms like `a(t[n])` or any attempt to introduce an erroneous factor in the formula creates a solution that is different from C.

8.5 Verification via manufactured solutions

Following the idea of the previous section, we can choose any formula as the exact solution, insert the formula in the ODE problem and fit the data $a(t)$, $b(t)$, and I to make the chosen formula fulfill the equation. This powerful technique for generating exact solutions is very useful for verification purposes and known as the *method of manufactured solutions*, often abbreviated MMS.

One common choice of solution is a linear function in the independent variable(s). The rationale behind such a simple variation is that almost any relevant numerical solution method for differential equation problems is able to reproduce the linear function exactly to machine precision (if u is about unity in size; precision is lost if u take on large values, see Exercise 17). The linear solution also makes some stronger demands to the numerical method and the implementation than the constant solution used in Section 8.4, at least in more complicated applications. However, the constant solution is often ideal for initial debugging before proceeding with a linear solution.

We choose a linear solution $u(t) = ct + d$. From the initial condition it follows that $d = I$. Inserting this u in the ODE results in

$$c = -a(t)u + b(t)\,.$$

Any function $u = ct + I$ is then a correct solution if we choose

$$b(t) = c + a(t)(ct + I)\,.$$

With this $b(t)$ there are no restrictions on $a(t)$ and c.

Let prove that such a linear solution obeys the numerical schemes. To this end, we must check that $u^n = ca(t_n)(ct_n + I)$ fulfills the discrete equations. For these calculations, and later calculations involving linear solutions inserted in finite difference schemes, it is convenient to compute the action of a difference operator on a linear function t:

$$[D_t^+ t]^n = \frac{t_{n+1} - t_n}{\Delta t} = 1, \tag{83}$$

$$[D_t^- t]^n = \frac{t_n - t_{n-1}}{\Delta t} = 1, \tag{84}$$

$$[D_t t]^n = \frac{t_{n+\frac{1}{2}} - t_{n-\frac{1}{2}}}{\Delta t} = \frac{(n+\frac{1}{2})\Delta t - (n-\frac{1}{2})\Delta t}{\Delta t} = 1\,. \tag{85}$$

Clearly, all three finite difference approximations to the derivative are exact for $u(t) = t$ or its mesh function counterpart $u^n = t_n$.

The difference equation for the Forward Euler scheme

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

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

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

which is always fulfilled. Similar calculations can be done for the Backward Euler and Crank-Nicolson schemes, or the θ-rule for that matter. In all cases, $u^n = ct_n + I$ is an exact solution of the discrete equations. That is why we should expect that $u^n - u_e(t_n) = 0$ mathematically and $|u^n - u_e(t_n)|$ less than a small number about the machine precision for $n = 0, \ldots, N_t$.

The following function offers an implementation of this verification test based on a linear exact solution:

```
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)
```

Any error in the updating formula makes this test fail!

Choosing more complicated formulas as the exact solution, say $\cos(t)$, will not make the numerical and exact solution coincide to machine precision, because finite differencing of $\cos(t)$ does not exactly yield the exact derivative $-\sin(t)$. In such cases, the verification procedure must be based on measuring the convergence rates as exemplified in Section 2.8. Convergence rates can be computed as long as one has an exact solution of a problem that the solver can be tested on, but this can always be obtained by the method of manufactured solutions.

8.6 Extension to systems of ODEs

Many ODE models involves more than one unknown function and more than one equation. Here is an example of two unknown functions $u(t)$ and $v(t)$:

$$u' = au + bv, \tag{86}$$

$$v' = cu + dv, \tag{87}$$

for constants a, b, c, d. Applying the Forward Euler method to each equation results in simple updating formula

$$u^{n+1} = u^n + \Delta t(au^n + bv^n), \tag{88}$$
$$v^{n+1} = u^n + \Delta t(cu^n + dv^n)\,. \tag{89}$$

On the other hand, the Crank-Nicolson or Backward Euler schemes result in a 2×2 linear system for the new unknowns. The latter schemes gives

$$u^{n+1} = u^n + \Delta t(au^{n+1} + bv^{n+1}), \tag{90}$$
$$v^{n+1} = v^n + \Delta t(cu^{n+1} + dv^{n+1})\,. \tag{91}$$

Collecting u^{n+1} as well as v^{n+1} on the left-hand side results in

$$(1 - \Delta ta)u^{n+1} + bv^{n+1} = u^n, \tag{92}$$
$$cu^{n+1} + (1 - \Delta td)v^{n+1} = v^n, \tag{93}$$

which is a system of two coupled, linear, algebraic equations in two unknowns.

9 General first-order ODEs

We now turn the attention to general, nonlinear ODEs and systems of such ODEs. Our focus is on numerical methods that can be readily reused for time-discretization PDEs, and diffusion PDEs in particular. The methods are just briefly listed, and we refer to the rich literature for more detailed descriptions and analysis - the books [6, 1, 2, 3] are all excellent resources on numerical methods for ODEs. We also demonstrate the Odespy Python interface to a range of different software for general first-order ODE systems.

9.1 Generic form

ODEs are commonly written in the generic form

$$u' = f(u, t), \quad u(0) = I, \tag{94}$$

where $f(u, t)$ is some prescribed function. As an example, our most general exponential decay model (74) has $f(u, t) = -a(t)u(t) + b(t)$.

The unknown u in (94) may either be a scalar function of time t, or a vector valued function of t in case of a *system of ODEs* with m unknown components:

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

In that case, the right-hand side is vector-valued function with m components,

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

Actually, any system of ODEs can be written in the form (94), but higher-order ODEs then need auxiliary unknown functions to enable conversion to a first-order system.

Next we list some well-known methods for $u' = f(u,t)$, valid both for a single ODE (scalar u) and systems of ODEs (vector u). The choice of methods is inspired by the kind of schemes that are popular also for partial differential equations.

9.2 The θ-rule

The θ-rule scheme applied to $u' = f(u,t)$ becomes

$$\frac{u^{n+1}-u^n}{\Delta t} = \theta f(u^{n+1},t_{n+1}) + (1-\theta)f(u^n,t_n)\,. \tag{95}$$

Bringing the unknown u^{n+1} to the left-hand side and the known terms on the right-hand side gives

$$u^{n+1} - \Delta t\theta f(u^{n+1},t_{n+1}) = u^n + \Delta t(1-\theta)f(u^n,t_n)\,. \tag{96}$$

For a general f (not linear in u), this equation is *nonlinear* in the unknown u^{n+1} unless $\theta = 0$. For a scalar ODE ($m = 1$), we have to solve a single nonlinear algebraic equation for u^{n+1}, while for a system of ODEs, we get a system of coupled, nonlinear algebraic equations. Newton's method is a popular solution approach in both cases. Note that with the Forward Euler scheme ($\theta = 0$) we do not have to deal with nonlinear equations, because in that case we have an explicit updating formula for u^{n+1}. This is known as an *explicit* scheme. With $\theta \neq 1$ we have to solve systems of algebraic equations, and the scheme is said to be *implicit*.

9.3 An implicit 2-step backward scheme

The implicit backward method with 2 steps applies a three-level backward difference as approximation to $u'(t)$,

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

which is an approximation of order Δt^2 to the first derivative. The resulting scheme for $u' = f(u, t)$ reads

$$u^{n+1} = \frac{4}{3}u^n - \frac{1}{3}u^{n-1} + \frac{2}{3}\Delta t f(u^{n+1}, t_{n+1})\,. \tag{97}$$

Higher-order versions of the scheme (97) can be constructed by including more time levels. These schemes are known as the Backward Differentiation Formulas (BDF), and the particular version (97) is often referred to as BDF2.

Note that the scheme (97) is implicit and requires solution of nonlinear equations when f is nonlinear in u. The standard 1st-order Backward Euler method or the Crank-Nicolson scheme can be used for the first step.

9.4 Leapfrog schemes

The ordinary Leapfrog scheme. The derivative of u at some point t_n can be approximated by a central difference over two time steps,

$$u'(t_n) \approx \frac{u^{n+1} - u^{n-1}}{2\Delta t} = [D_{2t}u]^n \tag{98}$$

which is an approximation of second order in Δt. The scheme can then be written as

$$[D_{2t}u = f(u, t)]^n,$$

in operator notation. Solving for u^{n+1} gives

$$u^{n+1} = u^{n-1} + \Delta t f(u^n, t_n)\,. \tag{99}$$

Observe that (99) is an explicit scheme, and that a nonlinear f (in u) is trivial to handle since it only involves the known u^n value. Some other scheme must be used as starter to compute u^1, preferably the Forward Euler scheme since it is also explicit.

The filtered Leapfrog scheme. Unfortunately, the Leapfrog scheme (99) will develop growing oscillations with time (see Problem 22)[[[. A remedy for such undesired oscillations is to introduce a *filtering technique*. First, a standard Leapfrog step is taken, according to (99), and then the previous u^n value is adjusted according to

$$u^n \ \leftarrow\ u^n + \gamma(u^{n-1} - 2u^n + u^{n+1})\,. \tag{100}$$

The γ-terms will effectively damp oscillations in the solution, especially those with short wavelength (like point-to-point oscillations). A common choice of γ is 0.6 (a value used in the famous NCAR Climate Model).

9.5 The 2nd-order Runge-Kutta scheme

The two-step scheme

$$u^* = u^n + \Delta t f(u^n, t_n), \tag{101}$$

$$u^{n+1} = u^n + \Delta t \frac{1}{2}\left(f(u^n, t_n) + f(u^*, t_{n+1})\right), \tag{102}$$

essentially applies a Crank-Nicolson method (102) to the ODE, but replaces the term $f(u^{n+1}, t_{n+1})$ by a prediction $f(u^*, t_{n+1})$ based on a Forward Euler step (101). The scheme (101)-(102) is known as Huen's method, but is also a 2nd-order Runge-Kutta method. The scheme is explicit, and the error is expected to behave as Δt^2.

9.6 A 2nd-order Taylor-series method

One way to compute u^{n+1} given u^n is to use a Taylor polynomial. We may write up a polynomial of 2nd degree:

$$u^{n+1} = u^n + u'(t_n)\Delta t + \frac{1}{2}u''(t_n)\Delta t^2 .$$

From the equation $u' = f(u, t)$ it follows that the derivatives of u can be expressed in terms of f and its derivatives:

$$\begin{aligned}
u'(t_n) &= f(u^n, t_n),\\
u''(t_n) &= \frac{\partial f}{\partial u}(u^n, t_n)u'(t_n) + \frac{\partial f}{\partial t}\\
&= f(u^n, t_n)\frac{\partial f}{\partial u}(u^n, t_n) + \frac{\partial f}{\partial t},
\end{aligned}$$

resulting in the scheme

$$u^{n+1} = u^n + f(u^n, t_n)\Delta t + \frac{1}{2}\left(f(u^n, t_n)\frac{\partial f}{\partial u}(u^n, t_n) + \frac{\partial f}{\partial t}\right)\Delta t^2 . \tag{103}$$

More terms in the series could be included in the Taylor polynomial to obtain methods of higher order than 2.

9.7 The 2nd- and 3rd-order Adams-Bashforth schemes

The following method is known as the 2nd-order Adams-Bashforth scheme:

$$u^{n+1} = u^n + \frac{1}{2}\Delta t\left(3f(u^n, t_n) - f(u^{n-1}, t_{n-1})\right) . \tag{104}$$

The scheme is explicit and requires another one-step scheme to compute u^1 (the Forward Euler scheme or Heun's method, for instance). As the name implies, the scheme is of order Δt^2.

Another explicit scheme, involving four time levels, is the 3rd-order Adams-Bashforth scheme

$$u^{n+1} = u^n + \frac{1}{12}\left(23f(u^n,t_n) - 16f(u^{n-1},t_{n-1}) + 5f(u^{n-2},t_{n-2})\right) . \qquad (105)$$

The numerical error is of order Δt^3, and the scheme needs some method for computing u^1 and u^2.

More general, higher-order Adams-Bashforth schemes (also called *explicit Adams methods*) compute u^{n+1} as a linear combination of f at k previous time steps:

$$u^{n+1} = u^n + \sum_{j=0}^{k} \beta_j f(u^{n-j}, t_{n-j}),$$

where β_j are known coefficients.

9.8 4th-order Runge-Kutta scheme

The perhaps most widely used method to solve ODEs is the 4th-order Runge-Kutta method, often called RK4. Its derivation is a nice illustration of common numerical approximation strategies, so let us go through the steps in detail.

The starting point is to integrate the ODE $u' = f(u,t)$ from t_n to t_{n+1}:

$$u(t_{n+1}) - u(t_n) = \int\limits_{t_n}^{t_{n+1}} f(u(t),t)dt\,.$$

We want to compute $u(t_{n+1})$ and regard $u(t_n)$ as known. The task is to find good approximations for the integral, since the integrand involves the unknown u between t_n and t_{n+1}.

The integral can be approximated by the famous Simpson's rule:

$$\int\limits_{t_n}^{t_{n+1}} f(u(t),t)dt \approx \frac{\Delta t}{6}\left(f^n + 4f^{n+\frac{1}{2}} + f^{n+1}\right) .$$

The problem now is that we do not know $f^{n+\frac{1}{2}} = f(u^{n+\frac{1}{2}}, t_{n+1/2})$ and $f^{n+1} = (u^{n+1}, t_{n+1})$ as we know only u^n and hence f^n. The idea is to use various approximations for $f^{n+\frac{1}{2}}$ and f^{n+1} based on using well-known schemes for the ODE in the intervals $[t_n, t_{n+1/2}]$ and $[t_n, t_{n+1}]$. We split the integral approximation into four terms:

$$\int\limits_{t_n}^{t_{n+1}} f(u(t),t)dt \approx \frac{\Delta t}{6}\left(f^n + 2\hat{f}^{n+\frac{1}{2}} + 2\tilde{f}^{n+\frac{1}{2}} + \bar{f}^{n+1}\right),$$

where $\hat{f}^{n+\frac{1}{2}}$, $\tilde{f}^{n+\frac{1}{2}}$, and $\bar{f}^{n+1}$ are approximations to $f^{n+\frac{1}{2}}$ and f^{n+1} that can be based on already computed quantities. For $\hat{f}^{n+\frac{1}{2}}$ we can apply an approximation to $u^{n+\frac{1}{2}}$ using the Forward Euler method with step $\frac{1}{2}\Delta t$:

$$\hat{f}^{n+\frac{1}{2}} = f(u^n + \frac{1}{2}\Delta t f^n, t_{n+1/2}) \qquad (106)$$

Since this gives us a prediction of $f^{n+\frac{1}{2}}$, we can for $\tilde{f}^{n+\frac{1}{2}}$ try a Backward Euler method to approximate $u^{n+\frac{1}{2}}$:

$$\tilde{f}^{n+\frac{1}{2}} = f(u^n + \frac{1}{2}\Delta t \hat{f}^{n+\frac{1}{2}}, t_{n+1/2})\,. \qquad (107)$$

With $\tilde{f}^{n+\frac{1}{2}}$ as a hopefully good approximation to $f^{n+\frac{1}{2}}$, we can for the final term $\bar{f}^{n+1}$ use a Crank-Nicolson method to approximate u^{n+1}:

$$\bar{f}^{n+1} = f(u^n + \Delta t \hat{f}^{n+\frac{1}{2}}, t_{n+1})\,. \qquad (108)$$

We have now used the Forward and Backward Euler methods as well as the Crank-Nicolson method in the context of Simpson's rule. The hope is that the combination of these methods yields an overall time-stepping scheme from t_n to t_n+1 that is much more accurate than the $\mathcal{O}(\Delta t)$ and $\mathcal{O}(\Delta t^2)$ of the individual steps. This is indeed true: the overall accuracy is $\mathcal{O}(\Delta t^4)$!

To summarize, the 4th-order Runge-Kutta method becomes

$$u^{n+1} = u^n + \frac{\Delta t}{6}\left(f^n + 2\hat{f}^{n+\frac{1}{2}} + 2\tilde{f}^{n+\frac{1}{2}} + \bar{f}^{n+1}\right), \qquad (109)$$

where the quantities on the right-hand side are computed from (106)-(108). Note that the scheme is fully explicit so there is never any need to solve linear or nonlinear algebraic equations. However, the stability is conditional and depends on f. There is a whole range of *implicit* Runge-Kutta methods that are unconditionally stable, but require solution of algebraic equations involving f at each time step.

The simplest way to explore more sophisticated methods for ODEs is to apply one of the many high-quality software packages that exist, as the next section explains.

9.9 The Odespy software

A wide range of the methods and software exist for solving (94). Many of methods are accessible through a unified Python interface offered by the Odespy package. Odespy features simple Python implementations of the most fundamental schemes as well as Python interfaces to several famous packages for solving ODEs: ODEPACK, Vode, rkc.f, rkf45.f, Radau5, as well as the ODE solvers in SciPy, SymPy, and odelab.

The usage of Odespy follows this setup for the ODE $u' = -au$, $u(0) = I$, $t \in (0, T]$, here solved by the famous 4th-order Runge-Kutta method, using $\Delta t = 1$ and $N_t = 6$ steps:

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

import odespy
import numpy as np

I = 1; a = 0.5; Nt = 6; dt = 1
solver = odespy.RK4(f)
solver.set_initial_condition(I)
t_mesh = np.linspace(0, Nt*dt, Nt+1)
u, t = solver.solve(t_mesh)
```

The previously listed methods for ODEs are all accessible in Odespy:

- the θ-rule: `ThetaRule`
- special cases of the θ-rule: `ForwardEuler`, `BackwardEuler`, `CrankNicolson`
- the 2nd- and 4th-order Runge-Kutta methods: `RK2` and `RK4`
- The BDF methods and the Adam-Bashforth methods: `Vode`, `Lsode`, `Lsoda`, `lsoda_scipy`
- The Leapfrog scheme: `Leapfrog` and `LeapfrogFiltered`

9.10 Example: Runge-Kutta methods

Since all solvers have the same interface in Odespy, modulo different set of parameters to the solvers' constructors, one can easily make a list of solver objects and run a loop for comparing (a lot of) solvers. The code below, found in complete form in `decay_odespy.py`, compares the famous Runge-Kutta methods of orders 2, 3, and 4 with the exact solution of the decay equation $u' = -au$. Since we have quite long time steps, we have included the only relevant θ-rule for large time steps, the Backward Euler scheme ($\theta = 1$), as well. Figure 21 shows the results.

```
import numpy as np
import scitools.std as plt
import sys

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

I = 1; a = 2; T = 6
dt = float(sys.argv[1]) if len(sys.argv) >= 2 else 0.75
Nt = int(round(T/dt))
t = np.linspace(0, Nt*dt, Nt+1)

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

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

    plt.plot(t, u)
    plt.hold('on')
    legends.append(solver.__class__.__name__)

# Compare with exact solution plotted on a very fine mesh
t_fine = np.linspace(0, T, 10001)
u_e = I*np.exp(-a*t_fine)
plt.plot(t_fine, u_e, '-') # avoid markers by specifying line type
legends.append('exact')

plt.legend(legends)
plt.title('Time step: %g' % dt)
plt.show()
```

Visualization tip.

We use SciTools for plotting here, but importing `matplotlib.pyplot` as `plt` instead also works. However, plain use of Matplotlib as done here results in curves with different colors, which may be hard to distinguish on black-and-white paper. Using SciTools, curves are automatically given colors *and* markers, thus making curves easy to distinguish on screen with colors and on black-and-white paper. The automatic adding of markers is normally a bad idea for a very fine mesh since all the markers get cluttered, but SciTools limits the number of markers in such cases. For the exact solution we use a very fine mesh, but in the code above we specify the line type as a solid line (`-`), which means no markers and just a color to be automatically determined by the backend used for plotting (Matplotlib by default, but SciTools gives the opportunity to use other backends to produce the plot, e.g., Gnuplot or Grace).

Also note the that the legends are based on the class names of the solvers, and in Python the name of a the class type (as a string) of an object `obj` is obtained by `obj.__class__.__name__`.

The runs in Figure 21 and other experiments reveal that the 2nd-order Runge-Kutta method (`RK2`) is unstable for $\Delta t > 1$ and decays slower than the Backward Euler scheme for large and moderate Δt (see Exercise 21 for an analysis). However, for fine $\Delta t = 0.25$ the 2nd-order Runge-Kutta method approaches the exact solution faster than the Backward Euler scheme. That is, the latter scheme does a better job for larger Δt, while the higher order scheme is superior for smaller Δt. This is a typical trend also for most schemes for ordinary and partial differential equations.

The 3rd-order Runge-Kutta method (`RK3`) has also artifacts in form of oscillatory behavior for the larger Δt values, much like that of the Crank-Nicolson scheme. For finer Δt, the 3rd-order Runge-Kutta method converges quickly to the exact solution.

The 4th-order Runge-Kutta method (`RK4`) is slightly inferior to the Backward Euler scheme on the coarsest mesh, but is then clearly superior to all the other schemes. It is definitely the method of choice for all the tested schemes.

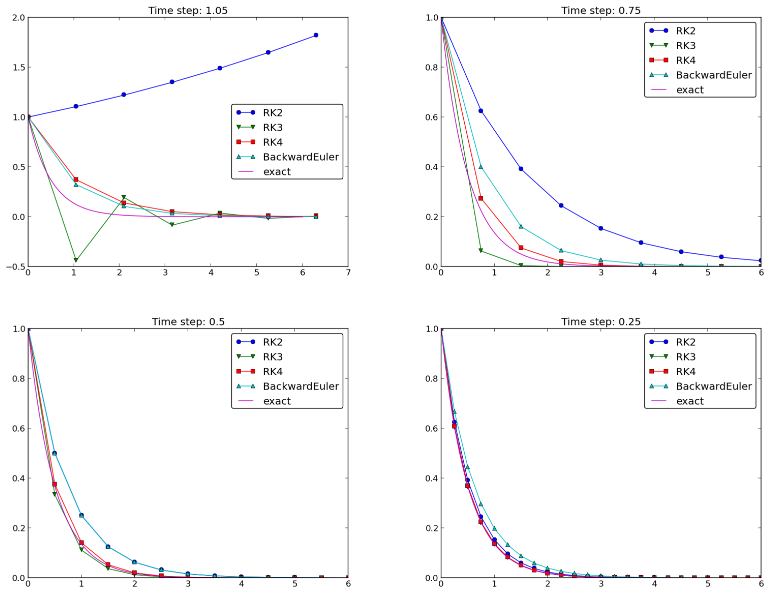


Figure 21: Behavior of different schemes for the decay equation.

Remark about using the θ-rule in Odespy. The Odespy package assumes that the ODE is written as $u' = f(u,t)$ with an f that is possibly nonlinear in u. The θ-rule for $u' = f(u,t)$ leads to

$$u^{n+1} = u^n + \Delta t \left(\theta f(u^{n+1}, t_{n+1}) + (1-\theta) f(u^n, t_n)\right),$$

which is a *nonlinear equation* in u^{n+1}. Odespy's implementation of the θ-rule (`ThetaRule`) and the specialized Backward Euler (`BackwardEuler`) and Crank-Nicolson (`CrankNicolson`) schemes must invoke iterative methods for solving the nonlinear equation in u^{n+1}. This is done even when f is linear in u, as in the model problem $u' = -au$, where we can easily solve for u^{n+1} by hand. Therefore, we need to specify use of Newton's method to the equations. (Odespy allows other methods than Newton's to be used, for instance Picard iteration, but that method is not suitable. The reason is that it applies the Forward Euler scheme to generate a start value for the iterations. Forward Euler may give very wrong solutions for large Δt values. Newton's method, on the other hand, is insensitive to the start value in *linear problems*.)

9.11 Example: Adaptive Runge-Kutta methods

Odespy offers solution methods that can adapt the size of Δt with time to match a desired accuracy in the solution. Intuitively, small time steps will be chosen in areas where the solution is changing rapidly, while larger time steps can be used where the solution is slowly varying. Some kind of *error estimator* is used to adjust the next time step at each time level.

A very popular adaptive method for solving ODEs is the Dormand-Prince Runge-Kutta method of order 4 and 5. The 5th-order method is used as a reference solution and the difference between the 4th- and 5th-order methods is used as an indicator of the error in the numerical solution. The Dormand-Prince method is the default choice in MATLAB's widely used `ode45` routine.

We can easily set up Odespy to use the Dormand-Prince method and see how it selects the optimal time steps. To this end, we request only one time step from $t = 0$ to $t = T$ and ask the method to compute the necessary non-uniform time mesh to meet a certain error tolerance. The code goes like

```
import odespy
import numpy as np
import decay_mod
import sys
#import matplotlib.pyplot as plt
import scitools.std as plt

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

def exact_solution(t):
    return I*np.exp(-a*t)

I = 1; a = 2; T = 5
tol = float(sys.argv[1])
solver = odespy.DormandPrince(f, atol=tol, rtol=0.1*tol)

Nt = 1  # just one step - let the scheme find its intermediate points
t_mesh = np.linspace(0, T, Nt+1)
t_fine = np.linspace(0, T, 10001)

solver.set_initial_condition(I)
u, t = solver.solve(t_mesh)

# u and t will only consist of [I, u^Nt] and [0,T]
# solver.u_all and solver.t_all contains all computed points
plt.plot(solver.t_all, solver.u_all, 'ko')
plt.hold('on')
plt.plot(t_fine, exact_solution(t_fine), 'b-')
plt.legend(['tol=%.0E' % tol, 'exact'])
plt.savefig('tmp_odespy_adaptive.png')
plt.show()
```

Running four cases with tolerances 10^{-1}, 10^{-3}, 10^{-5}, and 10^{-7}, gives the results in Figure 22. Intuitively, one would expect denser points in the beginning of the decay and larger time steps when the solution flattens out.

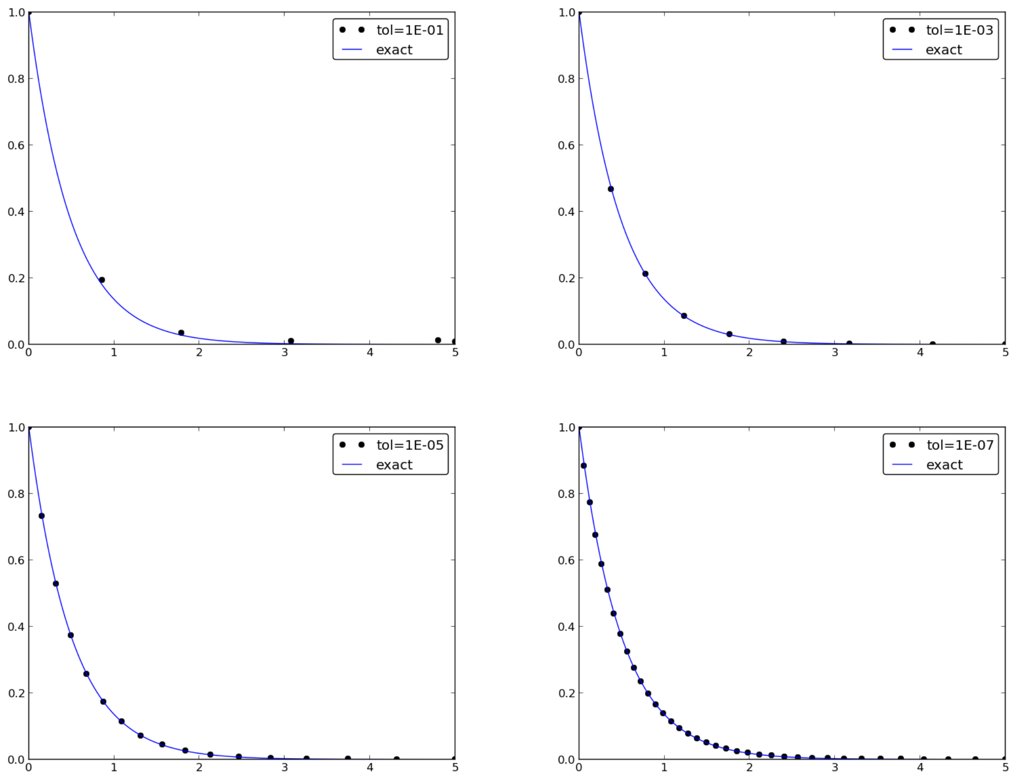


Figure 22: Choice of adaptive time mesh by the Dormand-Prince method for different tolerances.

10 Exercises

Exercise 17: Experiment with precision in tests and the size of u

It is claimed in Section 8.5 that most numerical methods will reproduce a linear exact solution to machine precision. Test this assertion using the nose test function `test_linear_solution` in the `decay_vc.py` program. Vary the parameter `c` from very small, via `c=1` to many larger values, and print out the maximum difference between the numerical solution and the exact solution. What is the relevant value of the `places` (or `delta`) argument to `nose.tools.assert_almost_equal` in each case? Filename: `test_precision.py`.

Exercise 18: Implement the 2-step backward scheme

Implement the 2-step backward method (97) for the model $u'(t) = -a(t)u(t) + b(t)$, $u(0) = I$. Allow the first step to be computed by either the Backward Euler scheme or the Crank-Nicolson scheme. Verify the implementation by choosing $a(t)$ and $b(t)$ such that the exact solution is linear in t (see Section 8.5). Show mathematically that a linear solution is indeed a solution of the discrete equations.

Compute convergence rates (see Section 2.8) in a test case $a = \text{const}$ and $b = 0$, where we easily have an exact solution, and determine if the choice of a first-order scheme (Backward Euler) for the first step has any impact on the overall accuracy of this scheme. The expected error goes like $\mathcal{O}(\Delta t^2)$. Filename: `decay_backward2step.py`.

Exercise 19: Implement the 2nd-order Adams-Bashforth scheme

Implement the 2nd-order Adams-Bashforth method (104) for the decay problem $u' = -a(t)u + b(t)$, $u(0) = I$, $t \in (0, T]$. Use the Forward Euler method for the first step such that the overall scheme is explicit. Verify the implementation using an exact solution that is linear in time. Analyze the scheme by searching for solutions $u^n = A^n$ when $a = \text{const}$ and $b = 0$. Compare this second-order secheme to the Crank-Nicolson scheme. Filename: `decay_AdamsBashforth2.py`.

Exercise 20: Implement the 3rd-order Adams-Bashforth scheme

Implement the 3rd-order Adams-Bashforth method (105) for the decay problem $u' = -a(t)u + b(t)$, $u(0) = I$, $t \in (0, T]$. Since the scheme is explicit, allow it to be started by two steps with the Forward Euler method. Investigate experimentally the case where $b = 0$ and a is a constant: Can we have oscillatory solutions for large Δt? Filename: `decay_AdamsBashforth3.py`.

Exercise 21: Analyze explicit 2nd-order methods

Show that the schemes (102) and (103) are identical in the case $f(u, t) = -a$, where $a > 0$ is a constant. Assume that the numerical solution reads $u^n = A^n$ for some unknown amplification factor A to be determined. Find A and derive stability criteria. Can the scheme produce oscillatory solutions of $u' = -au$? Plot the numerical and exact amplification factor. Filename: `decay_RK2_Taylor2.py`.

Problem 22: Implement and investigate the Leapfrog scheme

A Leapfrog scheme for the ODE $u'(t) = -a(t)u(t) + b(t)$ is defined by

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

A separate method is needed to compute u^1. The Forward Euler scheme is a possible candidate.

a) Implement the Leapfrog scheme for the model equation. Plot the solution in the case $a = 1$, $b = 0$, $I = 1$, $\Delta t = 0.01$, $t \in [0, 4]$. Compare with the exact solution $u_{\mathrm{e}}(t) = e^{-t}$.

b) Show mathematically that a linear solution in t fulfills the Forward Euler scheme for the first step and the Leapfrog scheme for the subsequent steps. Use this linear solution to verify the implementation, and automate the verification through a nose test.

Hint. It can be wise to automate the calculations such that it is easy to redo the calculations for other types of solutions. Here is a possible `sympy` function that takes a symbolic expression `u` (implemented as a Python function of `t`), fits the `b` term, and checks if `u` fulfills the discrete equations:

```
import sympy as sp

def analyze(u):
    t, dt, a = sp.symbols('t dt a')

    print 'Analyzing u_e(t)=%s' % u(t)
    print 'u(0)=%s' % u(t).subs(t, 0)

    # Fit source term to the given u(t)
    b = sp.diff(u(t), t) + a*u(t)
    b = sp.simplify(b)
    print 'Source term b:', b

    # Residual in discrete equations; Forward Euler step
    R_step1 = (u(t+dt) - u(t))/dt + a*u(t) - b
    R_step1 = sp.simplify(R_step1)
    print 'Residual Forward Euler step:', R_step1

    # Residual in discrete equations; Leapfrog steps
    R = (u(t+dt) - u(t-dt))/(2*dt) + a*u(t) - b
    R = sp.simplify(R)
    print 'Residual Leapfrog steps:', R

def u_e(t):
    return c*t + I

analyze(u_e)
# or short form: analyze(lambda t: c*t + I)
```

c) Show that a second-order polynomial in t cannot be a solution of the discrete equations. However, if a Crank-Nicolson scheme is used for the first step, a second-order polynomial solves the equations exactly.

d) Create a manufactured solution $u(t) = \sin(t)$ for the ODE $u' = -au + b$. Compute the convergence rate of the Leapfrog scheme using this manufactured solution. The expected convergence rate of the Leapfrog scheme is $\mathcal{O}(\Delta t^2)$. Does the use of a 1st-order method for the first step impact the convergence rate?

e) Set up a set of experiments to demonstrate that the Leapfrog scheme (99) is associated with numerical artifacts (instabilities). Document the main results from this investigation.

f) Analyze and explain the instabilities of the Leapfrog scheme (99):

1. Choose $a = \text{const}$ and $b = 0$. Assume that an exact solution of the discrete equations has the form $u^n = A^n$, where A is an amplification factor to be determined. Derive an equation for A by inserting $u^n = A^n$ in the Leapfrog scheme.
2. Compute A either by hand and/or with the aid of `sympy`. The polynomial for A has two roots, A_1 and A_2. Let u^n be a linear combination $u^n = C_1 A_1^n + C_2 A_2^n$.
3. Show that one of the roots is the explanation of the instability.
4. Compare A with the exact expression, using a Taylor series approximation.
5. How can C_1 and C_2 be determined?

g) Since the original Leapfrog scheme is unconditionally unstable as time grows, it demands some stabilization. This can be done by filtering, where we first find u^{n+1} from the original Leapfrog scheme and then replace u^n by $u^n + \gamma(u^{n-1} - 2u^n + u^{n+1})$, where γ can be taken as 0.6. Implement the filtered Leapfrog scheme and check that it can handle tests where the original Leapfrog scheme is unstable.

Filenames: `decay_leapfrog.py`, `decay_leapfrog.pdf`.

Problem 23: Make a unified implementation of many schemes

Consider the linear ODE problem $u'(t) = -a(t)u(t) + b(t)$, $u(0) = I$. Explicit schemes for this problem can be written in the general form

$$u^{n+1} = \sum_{j=0}^{m} c_j u^{n-j}, \tag{110}$$

for some choice of $c_0, \ldots, c_m$. Find expressions for the c_j coefficients in case of the θ-rule, the three-level backward scheme, the Leapfrog scheme, the 2nd-order Runge-Kutta method, and the 3rd-order Adams-Bashforth scheme.

Make a class `ExpDecay` that implements the general updating formula (110). The formula cannot be applied for $n < m$, and for those n values, other schemes must be used. Assume for simplicity that we just repeat Crank-Nicolson steps until (110) can be used. Use a subclass to specify the list $c_0, \ldots, c_m$ for a particular method, and implement subclasses for all the mentioned schemes. Verify the implementation by testing with a linear solution, which should be exactly reproduced by all methods. Filename: `decay_schemes_oo.py`.

11 Applications of exponential decay models

This section presents many mathematical models that all end up with ODEs of the type $u' = -au + b$. The applications are taken from biology, finance, and physics, and cover population growth or decay, compound interest and inflation, radioactive decay, cooling of objects, compaction of geological media, pressure variations in the atmosphere, and air resistance on falling or rising bodies.

11.1 Scaling

Real applications of a model $u' = -au + b$ will often involve a lot of parameters in the expressions for a and b. It can be quite a challenge to find relevant values of all parameters. In simple problems, however, it turns out that it is not always necessary to estimate all parameters because we can lump them into one or a few *dimensionless* numbers by using a very attractive technique called scaling. It simply means to stretch the u and t axis is the present problem - and suddenly all parameters in the problem are lumped one parameter if $b \neq 0$ and no parameter when $b = 0$!

Scaling means that we introduce a new function $\bar{u}(\bar{t})$, with

$$\bar{u} = \frac{u - u_m}{u_c}, \quad \bar{t} = \frac{t}{t_c},$$

where u_m is a characteristic value of u, u_c is a characteristic size of the range of u values, and t_c is a characteristic size of the range of t_c where u varies significantly. Choosing u_m, u_c, and t_c is not always easy and often an art in complicated problems. We just state one choice first:

$$u_c = I, \quad u_m = b/a, \quad t_c = 1/a\,.$$

Inserting $u = u_m + u_c\bar{u}$ and $t = t_c\bar{t}$ in the problem $u' = -au + b$, assuming a and b are constants, results after some algebra in the *scaled problem*

$$\frac{d\bar{u}}{d\bar{t}} = -\bar{u}, \quad \bar{u}(0) = 1 - \beta,$$

where β is a dimensionless number

$$\beta = \frac{b}{Ia}\,.$$

That is, only the special combination of $b/(Ia)$ matters, not what the individual values of b, a, and I are. Moreover, if $b = 0$, the scaled problem is independent of a and I! In practice this means that we can perform one numerical simulation of the scaled problem and recover the solution of any problem for a given a and I by stretching the axis in the plot: $u = I\bar{u}$ and $t = \bar{t}/a$. For $b \neq 0$, we simulate the scaled problem for a few β values and recover the physical solution u by translating and stretching the u axis and stretching the t axis.

The scaling breaks down if $I = 0$. In that case we may choose $u_m = 0$, $u_c = b/a$, and $t_c = 1/b$, resulting in a slightly different scaled problem:

$$\frac{d\bar{u}}{d\bar{t}} = 1 - \bar{u}, \quad \bar{u}(0) = 0\,.$$

As with $b = 0$, the case $I = 0$ has a scaled problem with no physical parameters!

It is common to drop the bars after scaling and write the scaled problem as $u' = -u$, $u(0) = 1 - \beta$, or $u' = 1 - u$, $u(0) = 0$. Any implementation of the problem $u' = -au + b$, $u(0) = I$, can be reused for the scaled problem by setting $a = 1$, $b = 0$, and $I = 1 - \beta$ in the code, if $I \neq 0$, or one sets $a = 1$, $b = 1$, and $I = 0$ when the physical I is zero. Falling bodies in fluids, as described in Section 11.8, involves $u' = -au + b$ with seven physical parameters. All these vanish in the scaled version of the problem if we start the motion from rest!

11.2 Evolution of a population

Let N be the number of individuals in a population occupying some spatial domain. Despite N being an integer in this problem, we shall compute with N as a real number and view $N(t)$ as a continuous function of time. The basic model assumption is that in a time interval Δt the number of newcomers to the populations (newborns) is proportional to N, with proportionality constant $\bar{b}$. The amount of newcomers will increase the population and result in to

$$N(t + \Delta t) = N(t) + \bar{b}N(t)\,.$$

It is obvious that a long time interval Δt will result in more newcomers and hence a larger $\bar{b}$. Therefore, we introduce $b = \bar{b}/\Delta t$: the number of newcomers per unit time and per individual. We must then multiply b by the length of the time interval considered and by the population size to get the total number of new individuals, $b\Delta t N$.

If the number of removals from the population (deaths) is also proportional to N, with proportionality constant $d\Delta t$, the population evolves according to

$$N(t + \Delta t) = N(t) + b\Delta t N(t) - d\Delta t N(t)\,.$$

Dividing by Δt and letting $\Delta t \to 0$, we get the ODE

$$N' = (b - d)N, \quad N(0) = N_0\,. \tag{111}$$

In a population where the death rate (d) is larger than then newborn rate (b), $a > 0$, and the population experiences exponential decay rather than exponential growth.

In some populations there is an immigration of individuals into the spatial domain. With I individuals coming in per time unit, the equation for the population change becomes

$$N(t+\Delta t) = N(t) + b\Delta t N(t) - d\Delta t N(t) + \Delta t I\,.$$

The corresponding ODE reads

$$N' = (b-d)N + I, \quad N(0) = N_0\,. \tag{112}$$

Some simplification arises if we introduce a fractional measure of the population: $u = N/N_0$ and set $r = b - d$. The ODE problem now becomes

$$u' = ru + f, \quad u(0) = 1, \tag{113}$$

where $f = I/N_0$ measures the net immigration per time unit as the fraction of the initial population. Very often, r is approximately constant, but f is usually a function of time.

The growth rate r of a population decreases if the environment has limited resources. Suppose the environment can sustain at most $N_{\max}$ individuals. We may then assume that the growth rate approaches zero as N approaches $N_{\max}$, i.e., as u approaches $M = N_{\max}/N_0$. The simplest possible evolution of r is then a linear function: $r(t) = r_0(1 - u(t)/M)$, where r_0 is the initial growth rate when the population is small relative to the maximum size and there is enough resources. Using this $r(t)$ in (113) results in the *logistic model* for the evolution of a population (assuming for the moment that $f = 0$):

$$u' = r_0(1 - u/M)u, \quad u(0) = 1\,. \tag{114}$$

Initially, u will grow at rate r_0, but the growth will decay as u approaches M, and then there is no more change in u, causing $u \to M$ as $t \to \infty$. Note that the logistic equation $u' = r_0(1 - u/M)u$ is *nonlinear* because of the quadratic term $-u^2 r_0/M$.

11.3 Compound interest and inflation

Say the annual interest rate is r percent and that the bank adds the interest once a year to your investment. If u^n is the investment in year n, the investment in year u^{n+1} grows to

$$u^{n+1} = u^n + \frac{r}{100}u^n\,.$$

In reality, the interest rate is added every day. We therefore introduce a parameter m for the number of periods per year when the interest is added. If n counts the periods, we have the fundamental model for compound interest:

$$u^{n+1} = u^n + \frac{r}{100m}u^n\,. \tag{115}$$

This model is a *difference equation*, but it can be transformed to a continuous differential equation through a limit process. The first step is to derive a formula for the growth of the investment over a time t. Starting with an investment u^0, and assuming that r is constant in time, we get

$$\begin{aligned} u^{n+1} &= \left(1 + \frac{r}{100m}\right) u^n \\ &= \left(1 + \frac{r}{100m}\right)^2 u^{n-1} \\ &\vdots \\ &= \left(1 + \frac{r}{100m}\right)^{n+1} u^0 \end{aligned}$$

Introducing time t, which here is a real-numbered counter for years, we have that $n = mt$, so we can write

$$u^{mt} = \left(1 + \frac{r}{100m}\right)^{mt} u^0 \,.$$

The second step is to assume *continuous compounding*, meaning that the interest is added continuously. This implies $m \to \infty$, and in the limit one gets the formula

$$u(t) = u_0 e^{rt/100}, \tag{116}$$

which is nothing but the solution of the ODE problem

$$u' = \frac{r}{100} u, \quad u(0) = u_0 \,. \tag{117}$$

This is then taken as the ODE model for compound interest if $r > 0$. However, the reasoning applies equally well to inflation, which is just the case $r < 0$. One may also take the r in (117) as the net growth of an investemt, where r takes both compound interest and inflation into account. Note that for real applications we must use a time-dependent r in (117).

Introducing $a = \frac{r}{100}$, continuous inflation of an initial fortune I is then a process exhibiting exponential decay according to

$$u' = -au, \quad u(0) = I \,.$$

11.4 Radioactive Decay

An atomic nucleus of an unstable atom may lose energy by emitting ionizing particles and thereby be transformed to a nucleus with a different number of protons and neutrons. This process is known as radioactive decay. Actually, the process is stochastic when viewed for a single atom, because it is impossible to predict exactly when a particular atom emits a particle. Nevertheless, with a large number of atoms, N, one may view the process as deterministic and compute the mean behavior of the decay. Below we reason intuitively about an ODE for the mean behavior. Thereafter, we show mathematically that a detailed stochastic model for single atoms leads the same mean behavior.

Deterministic model. Suppose at time t, the number of the original atom type is $N(t)$. A basic model assumption is that the transformation of the atoms of the original type in a small time interval Δt is proportional to N, so that

$$N(t+\Delta t) = N(t) - a\Delta t N(t),$$

where $a > 0$ is a constant. Introducing $u = N(t)/N(0)$, dividing by Δt and letting $\Delta t \to 0$ gives the following ODE:

$$u' = -au, \quad u(0) = 1\,. \tag{118}$$

The parameter a can for a given nucleus be expressed through the *half-life* $t_{1/2}$, which is the time taken for the decay to reduce the initial amount by one half, i.e., $u(t_{1/2}) = 0.5$. With $u(t) = e^{-at}$, we get $t_{1/2} = a^{-1}\ln 2$ or $a = \ln 2/t_{1/2}$.

Stochastic model. We have originally N_0 atoms. Each atom may have decayed or survived at a particular time t. We want to count how many original atoms that are left, i.e., how many atoms that have survived. The survival of a single atom at time t is a random event. Since there are only two outcomes, survival or decay, we have a Bernoulli trial. Let p be the probability of survival (implying that the probability of decay is $1-p$). If each atom survives independently of the others, and the probability of survival is the same for every atom, we have N_0 statistically Bernoulli trials, known as a *binomial experiment* from probability theory. The probability $P(N)$ that N out of the N_0 atoms have survived at time t is then given by the famous *binomial distribution*

$$P(N) = \frac{N_0!}{N!(N_0-N)!}p^N(1-p)^{N_0-N}\,.$$

The mean (or expected) value $\mathrm{E}[P]$ of $P(N)$ is known to be $N_0 p$.

It remains to estimate p. Let the interval $[0,t]$ be divided into m small subintervals of length Δt. We make the assumption that the probability of decay of a single atom in an interval of length Δt is $\tilde{p}$, and that this probability is proportional to Δt: $\tilde{p} = \lambda\Delta t$ (it sounds natural that the probability of decay increases with Δt). The corresponding probability of survival is $1-\lambda\Delta t$. Believing that λ is independent of time, we have, for each interval of length Δt, a Bernoulli trial: the atom either survives or decays in that interval. Now, p should be the probability that the atom survives in all the intervals, i.e., that we have m successful Bernoulli trials in a row and therefore

$$p = (1-\lambda\Delta t)^m\,.$$

The expected number of atoms of the original type at time t is

$$\mathrm{E}[P] = N_0 p = N_0(1-\lambda\Delta t)^m, \quad m = t/\Delta t\,. \tag{119}$$

To see the relation between the two types of Bernoulli trials and the ODE above, we go to the limit $\Delta t \to t$, $m \to \infty$. One can show that

$$p = \lim_{m\to\infty}(1-\lambda\Delta t)^m = \lim_{m\to\infty}\left(1-\lambda\frac{t}{m}\right)^m = e^{-\lambda t}$$

This is the famous exponential waiting time (or arrival time) distribution for a Poisson process in probability theory (obtained here, as often done, as the limit of a binomial experiment). The probability of decay, $1-e^{-\lambda t}$, follows an exponential distribution. The limit means that m is very large, hence Δt is very small, and $\tilde{p} = \lambda\Delta t$ is very small since the intensity of the events, λ, is assumed finite. This situation corresponds to a very small probability that an atom will decay in a very short time interval, which is a reasonable model. The same model occurs in lots of different applications, e.g., when waiting for a taxi, or when finding defects along a rope.

Relation between stochastic and deterministic models. With $p = e^{-\lambda t}$ we get the expected number of original atoms at t as $N_0 p = N_0 e^{-\lambda t}$, which is exactly the solution of the ODE model $N' = -\lambda N$. This gives also an interpretation of a via λ or vice versa. Our important finding here is that the ODE model captures the mean behavior of the underlying stochastic model. This is, however, not always the common relation between microscopic stochastic models and macroscopic "averaged" models.

Also of interest is to see that a Forward Euler discretization of $N' = -\lambda N$, $N(0) = N_0$, gives $N^m = N_0(1-\lambda\Delta t)^m$ at time $t_m = m\Delta t$, which is exactly the expected value of the stochastic experiment with N_0 atoms and m small intervals of length Δt, where each atom can decay with probability $\lambda\Delta t$ in an interval.

A fundamental question is how accurate the ODE model is. The underlying stochastic model fluctuates around its expected value. A measure of the fluctuations is the standard deviation of the binomial experiment with N_0 atoms, which can be shown to be $\mathrm{Std}[P] = \sqrt{N_0 p(1-p)}$. Compared to the size of the expectation, we get the normalized standard deviation

$$\frac{\sqrt{\mathrm{Var}[P]}}{\mathrm{E}[P]} = N_0^{-1/2}\sqrt{p^{-1}-1} = N_0^{-1/2}\sqrt{(1-e^{-\lambda t})^{-1}-1} \approx (N_0\lambda t)^{-1/2},$$

showing that the normalized fluctuations are very small if N_0 is very large, which is usually the case.

11.5 Newton's law of cooling

When a body at some temperature is placed in a cooling environment, experience shows that the temperature falls rapidly in the beginning, and then the changes in temperature levels off until the body's temperature equals that of the surroundings. Newton carried out some experiments on cooling hot iron and found that the temperature evolved as a "geometric progression at times in arithmetic progression", meaning that the temperature decayed exponentially.

Later, this result was formulated as a differential equation: the rate of change of the temperature in a body is proportional to the temperature difference between the body and its surroundings. This statement is known as *Newton's law of cooling*, which can be mathematically expressed as

$$\frac{dT}{dt} = -k(T - T_s), \tag{120}$$

where T is the temperature of the body, T_s is the temperature of the surroundings, t is time, and k is a positive constant. Equation (120) is primarily viewed as an empirical law, valid when heat is efficiently convected away from the surface of the body by a flowing fluid such as air at constant temperature T_s. The *heat transfer coefficient* k reflects the transfer of heat from the body to the surroundings and must be determined from physical experiments.

We must obviously have an initial condition $T(0) = T_0$ in addition to the cooling law (120).

11.6 Decay of atmospheric pressure with altitude

Vertical equilibrium of air in the atmosphere is governed by the equation

$$\frac{dp}{dz} = -\varrho g\,. \tag{121}$$

Here, $p(z)$ is the air pressure, ϱ is the density of air, and $g = 9.807$ m/s^2 is a standard value of the acceleration of gravity. (Equation (121) follows directly from the general Navier-Stokes equations for fluid motion, with the assumption that the air does not move.)

The pressure is related to density and temperature through the ideal gas law

$$\varrho = \frac{Mp}{R^*T}, \tag{122}$$

where M is the molar mass of the Earth's air (0.029 kg/mol), R^* is the universal gas constant (8.314 Nm/(mol K)), and T is the temperature. All variables p, ϱ, and T vary with the height z. Inserting (122) in (121) results in an ODE with a variable coefficient:

$$\frac{dp}{dz} = -\frac{Mg}{R^*T(z)}p\,. \tag{123}$$

Multiple atmospheric layers. The atmosphere can be approximately modeled by seven layers. In each layer, (123) is applied with a linear temperature of the form

$$T(z) = \bar{T}_i + L_i(z - h_i),$$

where $z = h_i$ denotes the bottom of layer number i, having temperature $\bar{T}_i$, and L_i is a constant in layer number i. The table below lists h_i (m), $\bar{T}_i$ (K), and L_i (K/m) for the layers $i = 0, \ldots, 6$.

i	h_i	$\bar{T}_i$	L_i
0	0	288	-0.0065
1	11,000	216	0.0
2	20,000	216	0.001
3	32,000	228	0.0028
4	47,000	270	0.0
5	51,000	270	-0.0028
6	71,000	214	-0.002

For implementation it might be convenient to write (123) on the form

$$\frac{dp}{dz} = -\frac{Mg}{R^*(\bar{T}(z) + L(z)(z - h(z)))}p, \tag{124}$$

where $\bar{T}(z)$, $L(z)$, and $h(z)$ are piecewise constant functions with values given in the table. The value of the pressure at the sea level $z = 0$, $p_0 = p(0)$, is 101325 Pa.

Simplification: $L = 0$. One commonly used simplification is to assume that the temperature is constant within each layer. This means that $L = 0$.

Simplification: one-layer model. Another commonly used approximation is to work with one layer instead of seven. This one-layer model is based on $T(z) = T_0 - Lz$, with sea level standard temperature $T_0 = 288$ K and temperature lapse rate $L = 0.0065$ K/m.

11.7 Compaction of sediments

Sediments, originally made from materials like sand and mud, get compacted through geological time by the weight of new material that is deposited on the sea bottom. The porosity ϕ of the sediments tells how much void (fluid) space there is between the sand and mud grains. The porosity reduces with depth because the weight of the sediments above and causes the void space to shrink and thereby increase the compaction.

A typical assumption is that the change in ϕ at some depth z is negatively proportional to ϕ. This assumption leads to the differential equation problem

$$\frac{d\phi}{dz} = -c\phi, \quad \phi(0) = \phi_0, \tag{125}$$

where the z axis points downwards, $z = 0$ is the surface with known porosity, and $c > 0$ is a constant.

The upper part of the Earth's crust consists of many geological layers stacked on top of each other, as indicated in Figure 23. The model (125) can be applied for each layer. In layer number i, we have the unknown porosity function $\phi_i(z)$ fulfilling $\phi_i'(z) = -c_i z$, since the constant c in the model (125) depends on the type of sediment in the layer. From the figure we see that new layers of sediments are deposited on top of older ones as time progresses. The compaction, as measured by ϕ, is rapid in the beginning and then decreases (exponentially) with depth in each layer.

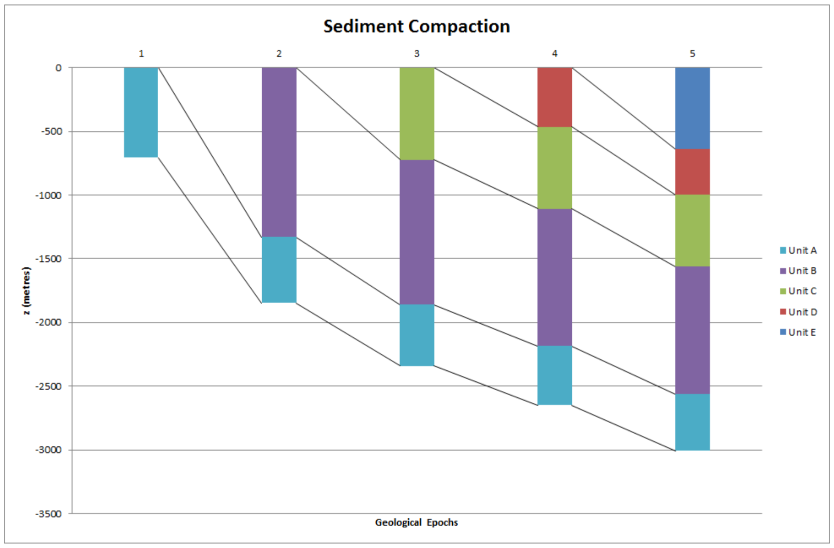


Figure 23: Illustration of the compaction of geological layers (with different colors) through time.

When we drill a well at present time through the right-most column of sediments in Figure 23, we can measure the thickness of the sediment in (say) the bottom layer. Let L_1 be this thickness. Assuming that the volume of sediment remains constant through time, we have that the initial volume, $\int_0^{L_{1,0}} \phi_1 dz$, must equal the volume seen today, $\int_{\ell-L_1}^{\ell} \phi_1 dz$, where ℓ is the depth of the bottom of the sediment in the present day configuration. After having solved for ϕ_1 as a function of z, we can then find the original thickness $L_{1,0}$ of the sediment from the equation

$$\int_0^{L_{1,0}} \phi_1 dz = \int_{\ell-L_1}^{\ell} \phi_1 dz \,.$$

In hydrocarbon exploration it is important to know $L_{1,0}$ and the compaction history of the various layers of sediments.

11.8 Vertical motion of a body in a viscous fluid

A body moving vertically through a fluid (liquid or gas) is subject to three different types of forces: the gravity force, the drag force, and the buoyancy force.

Overview of forces. The gravity force is $F_g = -mg$, where m is the mass of the body and g is the acceleration of gravity. The uplift or buoyancy force ("Archimedes force") is $F_b = \varrho g V$, where ϱ is the density of the fluid and V is the volume of the body. Forces and other quantities are taken as positive in the upward direction.

The drag force is of two types, depending on the Reynolds number

$$\mathrm{Re} = \frac{\varrho d|v|}{\mu}, \tag{126}$$

where d is the diameter of the body in the direction perpendicular to the flow, v is the velocity of the body, and μ is the dynamic viscosity of the fluid. When $\mathrm{Re} < 1$, the drag force is fairly well modeled by the so-called Stokes' drag, which for a spherical body of diameter d reads

$$F_d^{(S)} = -3\pi d\mu v\,. \tag{127}$$

For large Re, typically $\mathrm{Re} > 10^3$, the drag force is quadratic in the velocity:

$$F_d^{(q)} = -\frac{1}{2}C_D \varrho A|v|v, \tag{128}$$

where C_D is a dimensionless drag coefficient depending on the body's shape, and A is the cross-sectional area as produced by a cut plane, perpendicular to the motion, through the thickest part of the body. The superscripts ^{q} and ^{S} in $F_d^{(S)}$ and $F_d^{(q)}$ indicate Stokes drag and quadratic drag, respectively.

Equation of motion. All the mentioned forces act in the vertical direction. Newton's second law of motion applied to the body says that the sum of these forces must equal the mass of the body times its acceleration a in the vertical direction.

$$ma = F_g + F_d^{(S)} + F_b\,.$$

Here we have chosen to model the fluid resistance by the Stokes drag. Inserting the expressions for the forces yields

$$ma = -mg - 3\pi d\mu v + \varrho g V\,.$$

The unknowns here are v and a, i.e., we have two unknowns but only one equation. From kinematics in physics we know that the acceleration is the time derivative of the velocity: $a = dv/dt$. This is our second equation. We can easily eliminate a and get a single differential equation for v:

$$m\frac{dv}{dt} = -mg - 3\pi d\mu v + \varrho g V\,.$$

A small rewrite of this equation is handy: We express m as $\varrho_b V$, where ϱ_b is the density of the body, and we divide by the mass to get

$$v'(t) = -\frac{3\pi d\mu}{\varrho_b V} v + g\left(\frac{\varrho}{\varrho_b} - 1\right) . \tag{129}$$

We may introduce the constants

$$a = \frac{3\pi d\mu}{\varrho_b V}, \quad b = g\left(\frac{\varrho}{\varrho_b} - 1\right), \tag{130}$$

so that the structure of the differential equation becomes obvious:

$$v'(t) = -av(t) + b\,. \tag{131}$$

The corresponding initial condition is $v(0) = v_0$ for some prescribed starting velocity v_0.

This derivation can be repeated with the quadratic drag force $F_d^{(q)}$, leading to the result

$$v'(t) = -\frac{1}{2}C_D\frac{\varrho A}{\varrho_b V}|v|v + g\left(\frac{\varrho}{\varrho_b} - 1\right) . \tag{132}$$

Defining

$$a = \frac{1}{2}C_D\frac{\varrho A}{\varrho_b V}, \tag{133}$$

and b as above, we can write (132) as

$$v'(t) = -a|v|v + b\,. \tag{134}$$

Terminal velocity. An interesting aspect of (131) and (134) is whether v will approach a final constant value, the so-called *terminal velocity* v_T, as $t \to \infty$. A constant v means that $v'(t) \to 0$ as $t \to \infty$ and therefore the terminal velocity v_T solves

$$0 = -av_T + b$$

and

$$0 = -a|v_T|v_T + b\,.$$

The former equation implies $v_T = b/a$, while the latter has solutions $v_T = -\sqrt{|b|/a}$ for a falling body ($v_T < 0$) and $v_T = \sqrt{b/a}$ for a rising body ($v_T > 0$).

A Crank-Nicolson scheme. Both governing equations, the Stokes' drag model (131) and the quadratic drag model (134), can be readily solved by the Forward Euler scheme. For higher accuracy one can use the Crank-Nicolson method, but a straightforward application this method results a nonlinear equation in the new unknown value v^{n+1} when applied to (134):

$$\frac{v^{n+1} - v^n}{\Delta t} = -a\frac{1}{2}(|v^{n+1}|v^{n+1} + |v^n|v^n) + b\,. \tag{135}$$

However, instead of approximating the term $-|v|v$ by an arithmetic average, we can use a *geometric mean*:

$$(|v|v)^{n+\frac{1}{2}} \approx |v^n|v^{n+1}\,. \tag{136}$$

The error is of second order in Δt, just as for the arithmetic average and the centered finite difference approximation in (135). With this approximation trick, the discrete equation

$$\frac{v^{n+1} - v^n}{\Delta t} = -a|v^n|v^{n+1} + b$$

becomes a *linear* equation in v^{n+1}, and we can therefore easily solve for v^{n+1}:

$$v^{n+1} = \frac{v_n + \Delta t b^{n+\frac{1}{2}}}{1 + \Delta t a^{n+\frac{1}{2}}|v^n|}\,. \tag{137}$$

Physical data. Suitable values of μ are $1.8\cdot 10^{-5}$ Pa s for air and $8.9\cdot 10^{-4}$ Pa s for water. Densities can be taken as 1.2 kg/m^3 for air and as $1.0\cdot 10^3$ kg/m^3 for water. For considerable vertical displacement in the atmosphere one should take into account that the density of air varies with the altitude, see Section 11.6. One possible density variation arises from the one-layer model in the mentioned section.

Any density variation makes b time dependent and we need $b^{n+\frac{1}{2}}$ in (137). To compute the density that enters $b^{n+\frac{1}{2}}$ we must also compute the vertical position $z(t)$ of the body. Since $v = dz/dt$, we can use a centered difference approximation:

$$\frac{z^{n+\frac{1}{2}} - z^{n-\frac{1}{2}}}{\Delta t} = v^n \quad \Rightarrow \quad z^{n+\frac{1}{2}} = z^{n-\frac{1}{2}} + \Delta t\, v^n\,.$$

This $z^{n+\frac{1}{2}}$ is used in the expression for b to compute $\varrho(z^{n+\frac{1}{2}})$ and then $b^{n+\frac{1}{2}}$.

The drag coefficient C_D depends heavily on the shape of the body. Some values are: 0.45 for a sphere, 0.42 for a semi-sphere, 1.05 for a cube, 0.82 for a long cylinder (when the center axis is in the vertical direction), 0.75 for a rocket, 1.0-1.3 for a man in upright position, 1.3 for a flat plate perpendicular to the flow, and 0.04 for a streamlined, droplet-like body.

Verification. To verify the program, one may assume a heavy body in air such that the F_b force can be neglected, and further assume a small velocity such that the air resistance F_d can also be neglected. This can be obtained by setting μ and ϱ to zero. The motion then leads to the velocity $v(t) = v_0 - gt$, which is linear in t and therefore should be reproduced to machine precision (say tolerance 10^{-15}) by any implementation based on the Crank-Nicolson or Forward Euler schemes.

Another verification, but not as powerful as the one above, can be based on computing the terminal velocity and comparing with the exact expressions. The advantage of this verification is that we can also the test situation $\varrho \neq 0$.

As always, the method of manufactured solutions can be applied to test the implementation of all terms in the governing equation, but the solution then has no physical relevance in general.

Scaling. Applying scaling, as described in Section 11.1, will for the linear case reduce the need to estimate values for seven parameters down to choosing one value of a single dimensionless parameter

$$\beta = \frac{\varrho_b g V \left(\frac{\varrho}{\varrho_b} - 1\right)}{3\pi d\mu I},$$

provided $I \neq 0$. If the motion starts from rest, $I = 0$, the scaled problem $\bar{u}' = 1 - \bar{u}$, $\bar{u}(0) = 0$, has no need for estimating physical parameters. This means that there is a single universal solution to the problem of a falling body starting from rest: $\bar{u}(t) = 1 - e^{-\bar{t}}$. All real physical cases correspond to stretching the $\bar{t}$ axis and the $\bar{u}$ axis in this dimensionless solution. More precisely, the physical velocity $u(t)$ is related to the dimensionless velocity $\bar{u}(\bar{t})$ through

$$u = \frac{\varrho_b g V \left(\frac{\varrho}{\varrho_b} - 1\right)}{3\pi d\mu} \bar{u}(t/(g(\varrho/\varrho_b - 1)))\,.$$

11.9 Decay ODEs from solving a PDE by Fourier expansions

Suppose we have a partial differential equation

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + f(x,t),$$

with boundary conditions $u(0,t) = u(L,t) = 0$ and initial condition $u(x,0) = I(x)$. One may express the solution as

$$u(x,t) = \sum_{k=1}^{m} A_k(t) e^{ikx\pi/L},$$

for appropriate unknown functions A_k, $k = 1,\ldots,m$. We use the complex exponential $e^{ikx\pi/L}$ for easy algebra, but the physical u is taken as the real part of any complex expression. Note that the expansion in terms of $e^{ikx\pi/L}$ is compatible with the boundary conditions: all functions $e^{ikx\pi/L}$ vanish for $x = 0$ and $x = L$. Suppose we can express $I(x)$ as

$$I(x) = \sum_{k=1}^{m} I_k e^{ikx\pi/L}\,.$$

Such an expansion can be computed by well-known Fourier expansion techniques, but the details are not important here. Also, suppose we can express the given $f(x,t)$ as

$$f(x,t) = \sum_{k=1}^{m} b_k(t) e^{ikx\pi/L}\,.$$

Inserting the expansions for u and f in the differential equations demands that all terms corresponding to a given k must be equal. The calculations results in the follow system of ODEs:

$$A_k'(t) = -\alpha\frac{k^2\pi^2}{L^2} + b_k(t), \quad k = 1,\ldots,m\,.$$

From the initial condition

$$u(x,0) = \sum_k A_k(0)e^{ikx\pi/L} = I(x) = \sum_k I_k e^{(ikx\pi/L)},$$

it follows that $A_k(0) = I_k$, $k = 1,\ldots,m$. We then have m equations of the form $A_k' = -aA_k + b$, $A_k(0) = I_k$, for appropriate definitions of a and b. These ODE problems independent each other such that we can solve one problem at a time. The outline technique is a quite common approach for solving partial differential equations.

Remark. Since a_k depends on k and the stability of the Forward Euler scheme demands $a_k\Delta t \leq 1$, we get that $\Delta t \leq \alpha^{-1}L^2\pi^{-2}k^{-2}$. Usually, quite large k values are needed to accurately represent the given functions I and f and then Δt needs to be very small for these large values of k. Therefore, the Crank-Nicolson and Backward Euler schemes, which allow larger Δt without any growth in the solutions, are more popular choices when creating time-stepping algorithms for partial differential equations of the type considered in this example.

12 Exercises and Projects

Exercise 24: Simulate an oscillating cooling process

The surrounding temperature T_s in Newton's law of cooling (120) may vary in time. Assume that the variations are periodic with period P and amplitude a around a constant mean temperature T_m:

$$T_s(t) = T_m + a\sin\left(\frac{2\pi}{P}t\right)\,. \tag{138}$$

Simulate a process with the following data: $k = 20$ min^{-1}, $T(0) = 5$ C, $T_m = 25$ C, $a = 2.5$ C, and $P = 1$ h. Also experiment with $P = 10$ min and $P = 3$ h. Plot T and T_s in the same plot. Filename: `osc_cooling.py`.

Exercise 25: Radioactive decay of Carbon-14

The Carbon-14 isotope, whose radioactive decay is used extensively in dating organic material that is tens of thousands of years old, has a half-life of $5,730$ years. Determine the age of an organic material that contains 8.4 percent of its initial amount of Carbon-14. Use a time unit of 1 year in the computations. The uncertainty in the half time of Carbon-14 is ± 40 years. What is the corresponding uncertainty in the estimate of the age?

Hint. Use simulations with $5,730 \pm 40$ y as input and find the corresponding interval for the result.

Filename: `carbon14.py`.

Exercise 26: Simulate stochastic radioactive decay

The purpose of this exercise is to implement the stochastic model described in Section 11.4 and show that its mean behavior approximates the solution of the corresponding ODE model.

The simulation goes on for a time interval $[0, T]$ divided into N_t intervals of length Δt. We start with N_0 atoms. In some time interval, we have N atoms that have survived. Simulate N Bernoulli trials with probability $\lambda\Delta t$ in this interval by drawing N random numbers, each being 0 (survival) or 1 (decay), where the probability of getting 1 is $\lambda\Delta t$. We are interested in the number of decays, d, and the number of survived atoms in the next interval is then $N - d$. The Bernoulli trials are simulated by drawing N uniformly distributed real numbers on $[0, 1]$ and saying that 1 corresponds to a value less than $\lambda\Delta t$:

```
# Given lambda_, dt, N
import numpy as np
uniform = np.random.uniform(N)
Bernoulli_trials = np.asarray(uniform < lambda_*dt, dtype=np.int)
d = Bernoulli_trials.size
```

Observe that `uniform < lambda_*dt` is a boolean array whose true and false values become 1 and 0, respectively, when converted to an integer array.

Repeat the simulation over $[0, T]$ a large number of times, compute the average value of N in each interval, and compare with the solution of the corresponding ODE model. Filename: `stochastic_decay.py`.

Exercise 27: Radioactive decay of two substances

Consider two radioactive substances A and B. The nuclei in substance A decay to form nuclei of type B with a half-life $A_{1/2}$, while substance B decay to form type A nuclei with a half-life $B_{1/2}$. Letting u_A and u_B be the fractions of the initial amount of material in substance A and B, respectively, the following system of ODEs governs the evolution of $u_A(t)$ and $u_B(t)$:

$$\frac{1}{\ln 2}u_A' = u_B/B_{1/2} - u_A/A_{1/2}, \tag{139}$$

$$\frac{1}{\ln 2}u_B' = u_A/A_{1/2} - u_B/B_{1/2}, \tag{140}$$

with $u_A(0) = u_B(0) = 1$.

Make a simulation program that solves for $u_A(t)$ and $u_B(t)$. Verify the implementation by computing analytically the limiting values of u_A and u_B as $t \to \infty$ (assume $u_A', u_B' \to 0$) and comparing these with those obtained numerically.

Run the program for the case of $A_{1/2} = 10$ minutes and $B_{1/2} = 50$ minutes. Use a time unit of 1 minute. Plot u_A and u_B versus time in the same plot. Filename: `radioactive_decay_2subst.py`.

Exercise 28: Simulate the pressure drop in the atmosphere

We consider the models for atmospheric pressure in Section 11.6. Make a program with three functions,

- one computing the pressure $p(z)$ using a seven-layer model and varying L,
- one computing $p(z)$ using a seven-layer model, but with constant temperature in each layer, and
- one computing $p(z)$ based on the one-layer model.

How can these implementations be verified? Should ease of verification impact how you code the functions? Compare the three models in a plot. Filename: `atmospheric_pressure.py`.

Exercise 29: Make a program for vertical motion in a fluid

Implement the Stokes' drag model (129) and the quadratic drag model (132) from Section 11.8, using the Crank-Nicolson scheme and a geometric mean for $|v|v$ as explained, and assume constant fluid density. At each time level, compute the Reynolds number Re and choose the Stokes' drag model if $\text{Re} < 1$ and the quadratic drag model otherwise.

The computation of the numerical solution should take place either in a stand-alone function (as in Section 2.1) or in a solver class that looks up a problem class for physical data (as in Section 3.6). Create a module (see Section 3.1) and equip it with nose tests (see Section 3.4) for automatically verifying the code.

Verification tests can be based on

- the terminal velocity (see Section 11.8),
- the exact solution when the drag force is neglected (see Section 11.8),

- the method of manufactured solutions (see Section 8.5) combined with computing convergence rates (see Section 2.8).

Use, e.g., a quadratic polynomial for the velocity in the method of manufactured solutions. The expected error is $\mathcal{O}(\Delta t^2)$ from the centered finite difference approximation and the geometric mean approximation for $|v|v$.

A solution that is linear in t will also be an exact solution of the discrete equations in many problems. Show that this is true for linear drag (by adding a source term that depends on t), but not for quadratic drag because of the geometric mean approximation. Use the method of manufactured solutions to add a source term *in the discrete equations for quadratic drag* such that a linear function of t is a solution. Add a nose test for checking that the linear function is reproduced to machine precision in the case of both linear and quadratic drag.

Apply the software to a case where a ball rises in water. The buoyancy force is here the driving force, but the drag will be significant and balance the other forces after a short time. A soccer ball has radius 11 cm and mass 0.43 kg. Start the motion from rest, set the density of water, ϱ, to 1000 kg/m^3, set the dynamic viscosity, μ, to 10^{-3} Pa s, and use a drag coefficient for a sphere: 0.45. Plot the velocity of the rising ball. Filename: `vertical_motion.py`.

Project 30: Simulate parachuting

The aim of this project is to develop a general solver for the vertical motion of a body with quadratic air drag, verify the solver, apply the solver to a skydiver in free fall, and finally apply the solver to a complete parachute jump.

All the pieces of software implemented in this project should be realized as Python functions and/or classes and collected in one module.

a) Set up the differential equation problem that governs the velocity of the motion. The parachute jumper is subject to the gravity force and a quadratic drag force. Assume constant density. Add an extra source term be used for program verification. Identify the input data to the problem.

b) Make a Python module for computing the velocity of the motion. Also equip the module with functionality for plotting the velocity.

Hint 1. Use the Crank-Nicolson scheme with a geometric mean of $|v|v$ in time to linearize the equation of motion with quadratic drag.

Hint 2. You can either use functions or classes for implementation. If you choose functions, make a function `solver` that takes all the input data in the problem as arguments and that returns the velocity (as a mesh function) and the time mesh. In case of a class-based implementation, introduce a problem class with the physical data and a solver class with the numerical data and a `solve` method that stores the velocity and the mesh in the class.

Allow for a time-dependent area and drag coefficient in the formula for the drag force.

c) Show that a linear function of t does not fulfill the discrete equations because of the geometric mean approximation used for the quadratic drag term. Fit a source term, as in the method of manufactured solutions, such that a linear function of t is a solution of the discrete equations. Make a nose test to check that this solution is reproduced to machine precision.

d) The expected error in this problem goes like Δt^2 because we use a centered finite difference approximation with error $\mathcal{O}(\Delta t^2)$ and a geometric mean approximation with error $\mathcal{O}(\Delta t^2)$. Use the method of manufactured solutions combined with computing convergence rate to verify the code. Make a nose test for checking that the convergence rate is correct.

e) Compute the drag force, the gravity force, and the buoyancy force as a function of time. Create a plot with these three forces.

Hint. You can either make a function `forces(v, t, plot=None)` that returns the forces (as mesh functions) and `t` and shows a plot on the screen and also saves the plot to a file with name `plot` if `plot` is not `None`, or you can extend the solver class with computation of forces and include plotting of forces in the visualization class.

f) Compute the velocity of a skydiver in free fall before the parachute opens.

Hint. Meade and Struthers [5] provide some data relevant to skydiving. The mass of the human body and equipment can be set to 100 kg. A skydiver in spread-eagle formation has a cross-section of 0.5 m^2 in the horizontal plane. The density of air decreases varies altitude, but can be taken as constant, 1 kg/m^3, for altitudes relevant to skydiving (0-4000 m). The drag coefficient for a man in upright position can be set to 1.2. Start with a zero velocity. A free fall typically has a terminating velocity of 45 m/s. (This value can be used to tune other parameters.)

g) The next task is to simulate a parachute jumper during free fall and after the parachute opens. At time t_p, the parachute opens and the drag coefficient and the cross-sectional area change dramatically. Use the program to simulate a jump from $z = 3000$ m to the ground $z = 0$. What is the maximum acceleration, measured in units of g, experienced by the jumper?

Hint. Following Meade and Struthers [5], one can set the cross-section area perpendicular to the motion to 44 m^2 when the parachute is open. Assume that it takes 8 s to increase the area linearly from the original to the final value.

The drag coefficient for an open parachute can be taken as 1.8, but tuned using the known value of the typical terminating velocity reached before landing: 5.3 m/s. One can take the drag coefficient as a piecewise constant function with an abrupt change at t_p. The parachute is typically released after $t_p = 60$ s, but larger values of t_p can be used to make plots more illustrative.

Filename: `skydiving.py`.

Exercise 31: Formulate vertical motion in the atmosphere

Vertical motion of a body in the atmosphere needs to take into account a varying air density if the range of altitudes is many kilometers. In this case, ϱ varies with the altitude z. The equation of motion for the body is given in Section 11.8. Let us assume quadratic drag force (otherwise the body has to be very, very small). A differential equation problem for the air density, based on the information for the one-layer atmospheric model in Section 11.6, can be set up as

$$p'(z) = -\frac{Mg}{R^*(T_0 + Lz)}p, \tag{141}$$

$$\varrho = p\frac{M}{R^*T}\,. \tag{142}$$

To evaluate $p(z)$ we need the altitude z. From the principle that the velocity is the derivative of the position we have that

$$z'(t) = v(t), \tag{143}$$

where v is the velocity of the body.

Explain in detail how the governing equations can be discretized by the Forward Euler and the Crank-Nicolson methods. Filename: `falling_in_variable_density.pdf`.

Exercise 32: Simulate vertical motion in the atmosphere

Implement the Forward Euler or the Crank-Nicolson scheme derived in Exercise 31. Demonstrate the effect of air density variation on a falling human, e.g., the famous fall of Felix Baumgartner. The drag coefficient can be set to 1.2.

Remark. In the Crank-Nicolson scheme one must solve a 3×3 system of equations at each time level, since p, ϱ, and v are coupled, while each equation can be stepped forward at a time with the Forward Euler scheme. Filename: `falling_in_variable_density.py`.

Exercise 33: Compute $y = |x|$ by solving an ODE

Consider the ODE problem

$$y'(x) = \begin{cases} -1, & x < 0, \\ 1, & x \geq 0 \end{cases} \qquad x \in (-1, 1], \quad y(1-) = 1,$$

which has the solution $y(x) = |x|$. Using a mesh $x_0 = -1$, $x_1 = 0$, and $x_2 = 1$, calculate by hand y_1 and y_2 from the Forward Euler, Backward Euler, Crank-Nicolson, and Leapfrog methods. Use all of the former three methods for computing the y_1 value to be used in the Leapfrog calculation of y_2. Thereafter, visualize how these schemes perform for a uniformly partitioned mesh with $N = 10$ and $N = 11$ points. Filename: `signum.py`.

Exercise 34: Simulate growth of a fortune with random interest rate

The goal of this exercise is to compute the value of a fortune subject to inflation and a random interest rate. Suppose that the inflation is constant at i percent per year and that the annual interest rate, p, changes randomly at each time step, starting at some value p_0 at $t = 0$. The random change is from a value p^n at $t = t_n$ to $p_n + \Delta p$ with probability 0.25 and $p_n - \Delta p$ with probability 0.25. No change occurs with probability 0.5. There is also no change if p^{n+1} exceeds 15 or becomes below 1. Use a time step of one month, $p_0 = i$, initial fortune scaled to 1, and simulate 1000 scenarios of length 20 years. Compute the mean evolution of one unit of money and the corresponding standard deviation. Plot the mean curve along with the mean plus one standard deviation and the mean minus one standard deviation. This will illustrate the uncertainty in the mean curve.

Hint 1. The following code snippet computes p^{n+1}:

```python
import random

def new_interest_rate(p_n, dp=0.5):
    r = random.random()  # uniformly distr. random number in [0,1)
    if 0 <= r < 0.25:
        p_np1 = p_n + dp
    elif 0.25 <= r < 0.5:
        p_np1 = p_n - dp
    else:
        p_np1 = p_n
    return (p_np1 if 1 <= p_np1 <= 15 else p_n)
```

Hint 2. If $u_i(t)$ is the value of the fortune in experiment number i, $i = 0, \ldots, N-1$, the mean evolution of the fortune is

$$\bar{u}(t) = \frac{1}{N} \sum_{i=0}^{N-1} u_i(t),$$

and the standard deviation is

$$s(t) = \sqrt{\frac{1}{N-1} \left(-(\bar{u}(t))^2 + \sum_{i=0}^{N-1} (u_i(t))^2 \right)}\,.$$

Suppose $u_i(t)$ is stored in an array `u`. The mean and the standard deviation of the fortune is most efficiently computed by using two accumulation arrays, `sum_u` and `sum_u2`, and performing `sum_u += u` and `sum_u2 += u**2` after every experiment. This technique avoids storing all the $u_i(t)$ time series for computing the statistics.

Filename: `random_interest.py`.

Exercise 35: Simulate a population in a changing environment

We shall study a population modeled by (113) where the environment, represented by r and f, undergoes changes with time.

a) Assume that there is a sudden drop (increase) in the birth (death) rate at time $t = t_r$, because of limited nutrition or food supply:

$$a(t) = \begin{cases} r_0, & t < t_r, \\ r_0 - A, & t \geq t_r, \end{cases}$$

This drop in population growth is compensated by a sudden net immigration at time $t_f > t_r$:

$$f(t) = \begin{cases} 0, & t < t_f, \\ f_0, & t \geq t_a, \end{cases}$$

Start with r_0 and make $A > r_0$. Experiment with these and other parameters to illustrate the interplay of growth and decay in such a problem. Filename: `population_drop.py`.

b) Now we assume that the environmental conditions changes periodically with time so that we may take

$$r(t) = r_0 + A\sin\left(\frac{2\pi}{P}t\right) .$$

That is, the combined birth and death rate oscillates around r_0 with a maximum change of $\pm A$ repeating over a period of length P in time. Set $f = 0$ and experiment with the other parameters to illustrate typical features of the solution. Filename: `population_osc.py`.

Exercise 36: Simulate logistic growth

Solve the logistic ODE (114) using a Crank-Nicolson scheme where $(u^{n+\frac{1}{2}})^2$ is approximated by a *geometric mean*:

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

This trick makes the discrete equation linear in u^{n+1}. Filename: `logistic_CN.py`.

Exercise 37: Rederive the equation for continuous compound interest

The ODE model (117) was derived under the assumption that r was constant. Perform an alternative derivation without this assumption: 1) start with (115); 2) introduce a time step Δt instead of m: $\Delta t = 1/m$ if t is measured in years; 3) divide by Δt and take the limit $\Delta t \rightarrow 0$. Simulate a case where the inflation is at a constant level I percent per year and the interest rate oscillates: $r = -I/2 + r_0 \sin(2\pi t)$. Compare solutions for $r_0 = I, 3I/2, 2I$. Filename: `interest_modeling.py`.

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