

Study guide: Algorithms and implementations for exponential decay models

Hans Petter Langtangen^{1,2}

Center for Biomedical Computing, Simula Research Laboratory¹

Department of Informatics, University of Oslo²

Aug 4, 2015

- 1 INF5620 in a nutshell
- 2 Finite difference methods
- 3 Implementation
- 4 Verifying the implementation

- Numerical methods for partial differential equations (PDEs)
- How do we solve a PDE in practice and produce numbers?
- How do we trust the answer?
- Approach: *simplify, understand, generalize*

After the course

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

The new official six-point course description

After having completed INF5620 you

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

The new official six-point course description

After having completed INF5620 you

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

The new official six-point course description

After having completed INF5620 you

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

The new official six-point course description

After having completed INF5620 you

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

The new official six-point course description

After having completed INF5620 you

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

The new official six-point course description

After having completed INF5620 you

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

The new official six-point course description

After having completed INF5620 you

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

More specific contents: finite difference methods

- ODEs
- the wave equation $u_{tt} = u_{xx}$ in 1D, 2D, 3D
- the diffusion equation $u_t = u_{xx}$ in 1D, 2D, 3D
- write your own software from scratch
- understand how the methods work and why they fail

More specific contents: finite element methods

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

More specific contents: nonlinear and advanced problems

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

Philosophy: simplify, understand, generalize

- Start with simplified ODE/PDE problems
- Learn to reason about the discretization
- Learn to implement, verify, and experiment
- Understand the method, program, and results
- Generalize the problem, method, and program

This is the power of applied mathematics!

The exam

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

The exam

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

The exam

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

The exam

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

The exam

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

The exam

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

The exam

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

The exam

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

The exam

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

Required software

- Our software platform: Python (sometimes combined with Cython, Fortran, C, C++)
- Important Python packages: numpy, scipy, matplotlib, sympy, fenics, scitools, ...
- Suggested installation: Run [Ubuntu in a virtual machine](#)
- Alternative: run a [Vagrant machine](#)

Assumed/ideal background

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

Start-up example for the course

What if you don't have this ideal background?

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

ODE problem

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

where $a > 0$ is a constant.

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

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

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

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

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

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

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

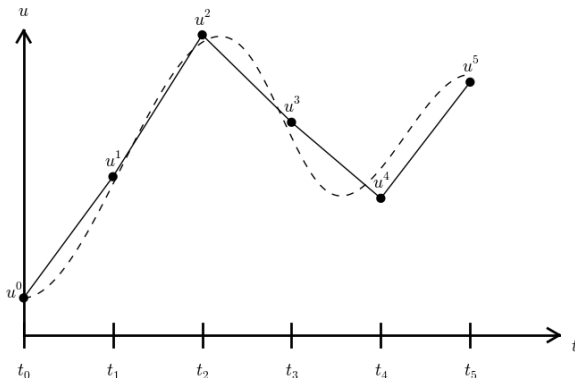
What to learn in the start-up example; generalizations

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

- 1 INF5620 in a nutshell
- 2 Finite difference methods**
- 3 Implementation
- 4 Verifying the implementation

Finite difference methods

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



Contents

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

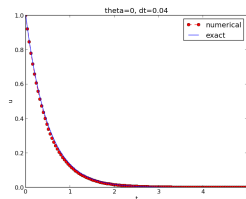
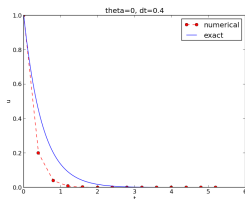
A basic model for exponential decay

The world's simplest (?) ODE:

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

Observation

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



The ODE model has a range of applications in many fields

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

See the [text](#) for details.

The ODE problem has a continuous and discrete version

Continuous problem.

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

(varies with a continuous t)

Discrete problem. Numerical methods applied to the continuous problem turns it into a discrete problem

$$u^{n+1} = \text{const} u^n, \quad n = 0, 1, \dots, N_t - 1, \quad u^0 = I \quad (2)$$

(varies with discrete mesh points t_n)

The steps in the finite difference method

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

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

Step 1: Discretizing the domain

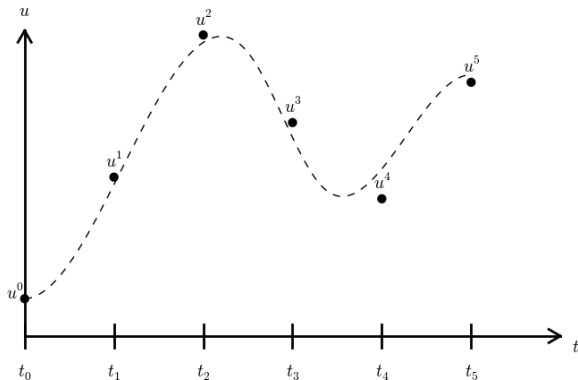
The time domain $[0, T]$ is represented by a *mesh*: a finite number of $N_t + 1$ points

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

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

Step 1: Discretizing the domain

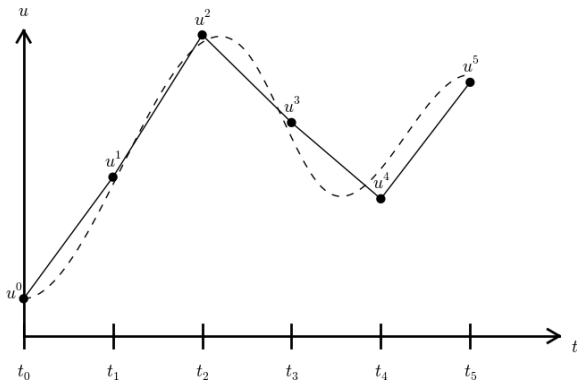
u^n is a mesh function, defined at the mesh points t_n , $n = 0, \dots, N_t$ only.



What about a mesh function between the mesh points?

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

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



Step 2: Fulfilling the equation at discrete time points

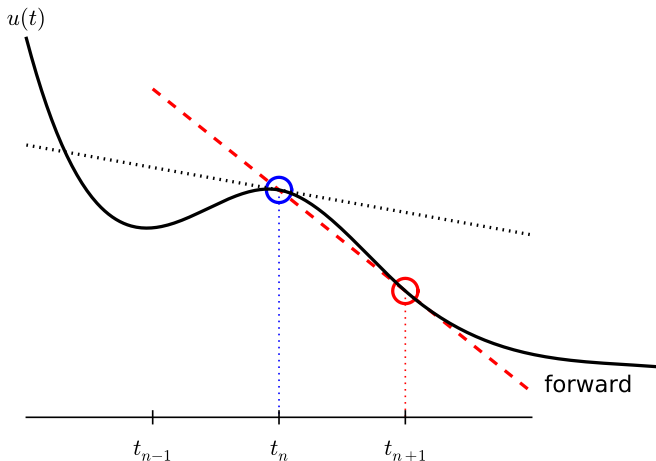
- The ODE holds for all $t \in (0, T]$ (infinite no of points)
- Idea: let the ODE be valid at the mesh points only (finite no of points)

$$u'(t_n) = -au(t_n), \quad n = 1, \dots, N_t \quad (4)$$

Step 3: Replacing derivatives by finite differences

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

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



Step 3: Replacing derivatives by finite differences

Inserting the finite difference approximation in

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

gives

$$\frac{u^{n+1} - u^n}{t_{n+1} - t_n} = -au^n, \quad n = 0, 1, \dots, N_t - 1 \quad (6)$$

(Known as *discrete equation*, or *discrete problem*, or *finite difference method/scheme*)

Step 4: Formulating a recursive algorithm

How can we actually compute the u^n values?

- given $u^0 = I$
- compute u^1 from u^0
- compute u^2 from u^1
- compute u^3 from u^2 (and so forth)

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

The Forward Euler scheme

Solve wrt u^{n+1} to get the computational formula:

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

Let us apply the scheme by hand

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

$$u_0 = l,$$

$$u_1 = u^0 - a\Delta t u^0 = l(1 - a\Delta t),$$

$$u_2 = l(1 - a\Delta t)^2,$$

$$u^3 = l(1 - a\Delta t)^3,$$

$$\vdots$$

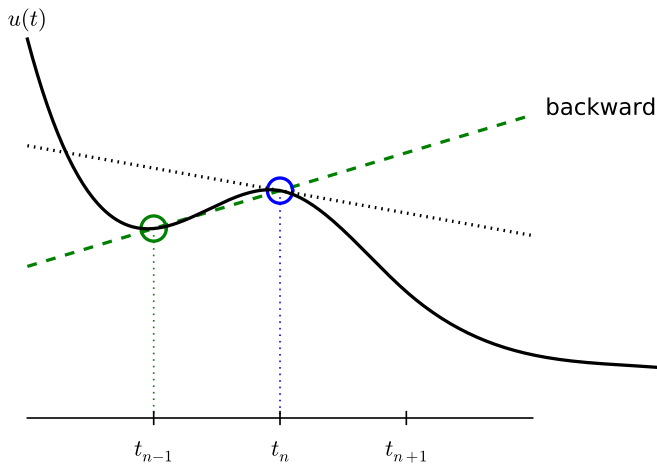
$$u^{N_t} = l(1 - a\Delta t)^{N_t}$$

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

A backward difference

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

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



The Backward Euler scheme

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

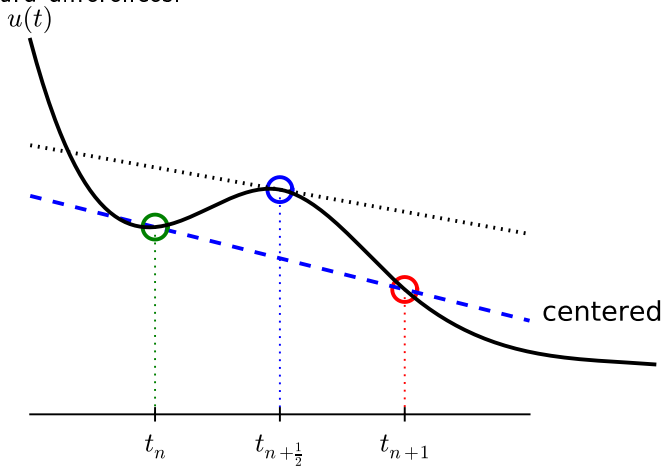
$$\frac{u^n - u^{n-1}}{t_n - t_{n-1}} = -au^n \quad (9)$$

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

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

A centered difference

Centered differences are better approximations than forward or backward differences.



The Crank-Nicolson scheme; ideas

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

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

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

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

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

Solution:

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

The Crank-Nicolson scheme; result

Result:

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

Solve wrt to u^{n+1} :

$$u^{n+1} = \frac{1 - \frac{1}{2}a(t_{n+1} - t_n)}{1 + \frac{1}{2}a(t_{n+1} - t_n)} u^n \quad (13)$$

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

The unifying θ -rule

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

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

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

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

$$u^{n+1} = \frac{1 - (1 - \theta)a(t_{n+1} - t_n)}{1 + \theta a(t_{n+1} - t_n)} \quad (15)$$

Constant time step

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

Summary of schemes for constant time step

$$u^{n+1} = (1 - a\Delta t)u^n \quad \text{Forward Euler} \quad (16)$$

$$u^{n+1} = \frac{1}{1 + a\Delta t} u^n \quad \text{Backward Euler} \quad (17)$$

$$u^{n+1} = \frac{1 - \frac{1}{2}a\Delta t}{1 + \frac{1}{2}a\Delta t} u^n \quad \text{Crank-Nicolson} \quad (18)$$

$$u^{n+1} = \frac{1 - (1 - \theta)a\Delta t}{1 + \theta a\Delta t} u^n \quad \text{The } \theta - \text{rule} \quad (19)$$

Test the understanding!

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

$$T' = -k(T - T_s), \quad T(0) = T_0, \quad t \in (0, t_{\text{end}}]$$

Physical quantities:

- $T(t)$: temperature of an object at time t
- k : parameter expressing heat loss to the surroundings
- T_s : temperature of the surroundings
- T_0 : initial temperature

Compact operator notation for finite differences

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

$$[D_t^- u = -au]^n \quad (20)$$

Specific notation for difference operators

Forward difference:

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

Centered difference:

$$[D_t u]^n = \frac{u^{n+\frac{1}{2}} - u^{n-\frac{1}{2}}}{\Delta t} \approx \frac{d}{dt} u(t_n), \quad (22)$$

Backward difference:

$$[D_t^- u]^n = \frac{u^n - u^{n-1}}{\Delta t} \approx \frac{d}{dt} u(t_n) \quad (23)$$

The Backward Euler scheme with operator notation

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

Common to put the whole equation inside square brackets:

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

$$[D_t^+ u = -au]^n \quad (25)$$

The Crank-Nicolson scheme with operator notation

Introduce an averaging operator:

$$[\bar{u}^t]^n = \frac{1}{2}(u^{n-\frac{1}{2}} + u^{n+\frac{1}{2}}) \approx u(t_n) \quad (26)$$

The Crank-Nicolson scheme can then be written as

$$[D_t u = -a\bar{u}^t]^{n+\frac{1}{2}} \quad (27)$$

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

- 1 INF5620 in a nutshell
- 2 Finite difference methods
- 3 Implementation**
- 4 Verifying the implementation

Implementation

Model:

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

Numerical method:

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

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

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

Requirements of a program

- Compute the numerical solution u^n , $n = 1, 2, \dots, N_t$
- Display the numerical and exact solution $u_e(t) = e^{-at}$
- Bring evidence to a correct implementation (*verification*)
- Compare the numerical and the exact solution in a plot
- computes the error $u_e(t_n) - u^n$
- computes the convergence rate of the numerical scheme
- reads its input data from the command line

Tools to learn

- Basic `Python` programming
- Array computing with `numpy`
- Plotting with `matplotlib.pyplot` and `scitools`
- File writing and reading

Notice

All programs are in the directory `src/decay`.

Why implement in Python?

- Python has a very clean, readable syntax (often known as "executable pseudo-code").
- Python code is very similar to MATLAB code (and MATLAB has a particularly widespread use for scientific computing).
- Python is 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++.

Why implement in Python?

- 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.

Algorithm

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

Translation to Python function

```
from numpy import *

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

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

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

Sample call:

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

Integer division

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

A safer solver function ($dt = \text{float}(dt)$ - guarantee float):

```
from numpy import *

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

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

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

```
def solver(I, a, T, dt, theta):  
    """  
    Solve  
  
         $u'(t) = -a*u(t),$   
  
    with initial condition  $u(0)=I$ , for  $t$  in the time interval  
     $(0, T]$ . The time interval is divided into time steps of  
    length  $dt$ .  
  
     $theta=1$  corresponds to the Backward Euler scheme,  $theta=0$   
    to the Forward Euler scheme, and  $theta=0.5$  to the Crank-  
    Nicolson method.  
    """  
    ...
```

Formatting of numbers

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

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

Or the alternative *format string syntax*:

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

Running the program

How to run the program `decay_v1.py`:

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

Can also run it as "normal" Unix programs: `./decay_v1.py` if the first line is

```
#!/usr/bin/env python
```

Then

```
Terminal> chmod a+rx decay_v1.py
```

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

Plotting the solution

Basic syntax:

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

Can (and should!) add labels on axes, title, legends.

Comparing with the exact solution

Python function for the exact solution $u_e(t) = Ie^{-at}$:

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

Quick plotting:

```
u_e = exact_solution(t, I, a)  
plot(t, u, t, u_e)
```

Problem: $u_e(t)$ applies the same mesh as u^n and looks as a piecewise linear function.

Remedy: Introduce a very fine mesh for u_e .

```
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  
     t,    u,    'r--o')       # red dashes w/circles
```

Add legends, axes labels, title, and wrap in a function

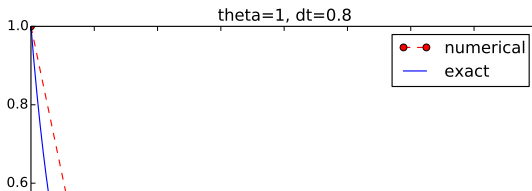
```
from matplotlib.pyplot import *

def plot_numerical_and_exact(theta, I, a, T, dt):
    """Compare the numerical and exact solution in a plot."""
    u, t = solver(I=I, a=a, T=T, dt=dt, theta=theta)

    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
         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('plot_%s_%g.png' % (theta, dt))
```

Complete code in `decay_v2.py`



Plotting with SciTools

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

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

```
from scitools.std import *

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

Change backend (plotting engine, Matplotlib by default):

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

- 1 INF5620 in a nutshell
- 2 Finite difference methods
- 3 Implementation
- 4 Verifying the implementation

Verifying the implementation

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

Simplest method: run a few algorithmic steps by hand

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

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

$$u^1 = Al = 0.0298245614035,$$

$$u^2 = Au^1 = 0.00889504462912,$$

$$u^3 = Au^2 = 0.00265290804728$$

See the function `verify_three_steps` in `decay_verf1.py`.

Comparison with an exact discrete solution

Best verification

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

Define

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

Repeated use of the θ -rule:

$$u^0 = I,$$

$$u^1 = Au^0 = AI$$

$$u^n = A^n u^{n-1} = A^n I$$

Making a test based on an exact discrete solution

The exact discrete solution is

$$u^n = I A^n \quad (28)$$

Question

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

Test if

$$\max_n |u^n - u_e(t_n)| < \epsilon \sim 10^{-15}$$

Implementation in `decay_verf2.py`.

Test the understanding!

Make a program for solving Newton's law of cooling

$$T' = -k(T - T_s), \quad T(0) = T_0, \quad t \in (0, t_{\text{end}}]$$

with the Forward Euler, Backward Euler, and Crank-Nicolson schemes (or a θ scheme). Verify the implementation.

Computing the numerical error as a mesh function

Task: compute the numerical error $e^n = u_e(t_n) - u^n$

Exact solution: $u_e(t) = Ie^{-at}$, implemented as

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

Compute e^n by

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

Array arithmetics - we compute on entire arrays!

- `exact_solution(t, I, a)` works with `t` as array
- Must have `exp` from `numpy` (not `math`)
- `e = u_e - u`: array subtraction
- Array arithmetics gives shorter and much faster code

Computing the norm of the error

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

Norms of a function $f(t)$:

$$\|f\|_{L^2} = \left(\int_0^T f(t)^2 dt \right)^{1/2} \quad (29)$$

$$\|f\|_{L^1} = \int_0^T |f(t)| dt \quad (30)$$

$$\|f\|_{L^\infty} = \max_{t \in [0, T]} |f(t)| \quad (31)$$

Norms of mesh functions

- Problem: $f^n = f(t_n)$ is a mesh function and hence not defined for all t . How to integrate f^n ?
- Idea: Apply a numerical integration rule, using only the mesh points of the mesh function.

The Trapezoidal rule:

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

Common simplification yields the L^2 norm of a mesh function:

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

Implementation of the norm of the error

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

Python w/array arithmetics:

```
e = exact_solution(t) - u  
E = sqrt(dt*sum(e**2))
```

Comment on array vs scalar computation

Scalar computing of $E = \sqrt{dt \cdot \sum(e^2)}$:

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

Obviously, scalar computing

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

Memory-saving implementation

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

Memory-saving solver function

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

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


Reading computed data from file

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

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

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

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

Usage of memory-saving code

```
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()  
        ...
```

Complete program: `decay_memsave.py`.