Algorithms and implementations for exponential decay models

MATMEK-4270

Prof. Mikael Mortensen, University of Oslo

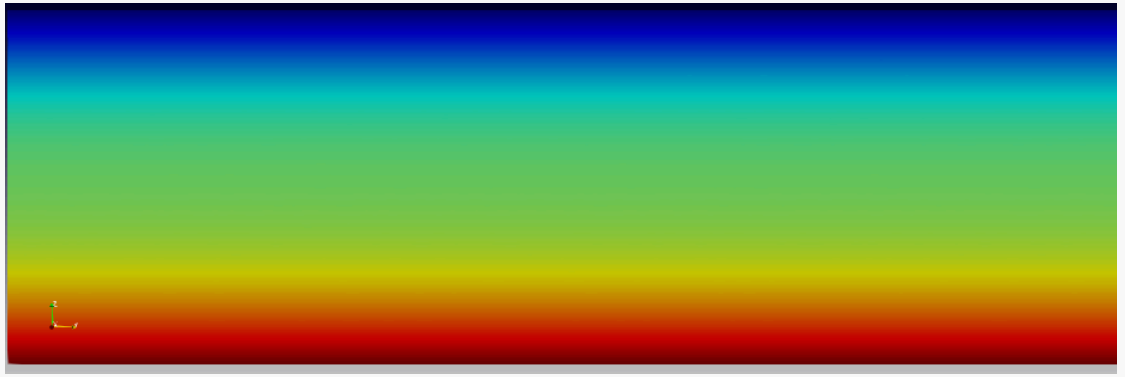
Hans Petter Langtangen 1962-2016

- 2011-2015 Editor-In-Chief SIAM J of Scientific Computing
- Author of 13 published books on scientific computing
- Professor of Mechanics, University of Oslo 1998
- Developed INF5620 (which became IN5270 and now MAT-MEK4270)
- Memorial page

A little bit about myself

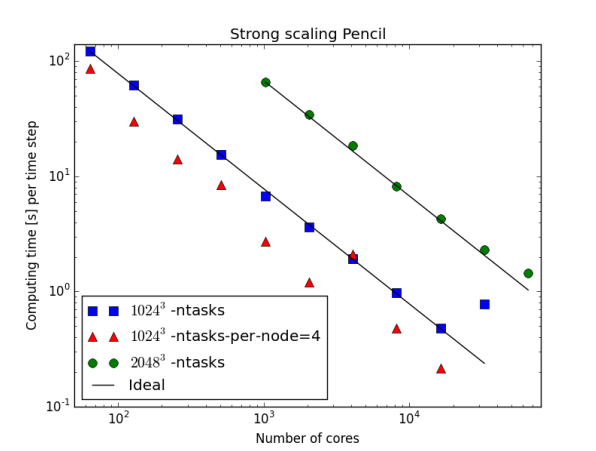
- Professor of mechanics (2019-)
- PhD (Chalmers University of Technology) in mathematical modelling of turbulent combustion
- Norwegian Defence Research Establishment (2007-2012)
- Computational Fluid Dynamics
- High Performance Computing
- Spectral methods

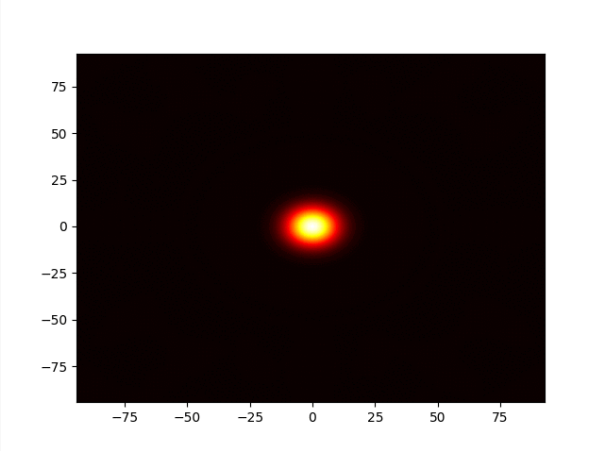
FFI Forsvarets forskningsinstitutt
Norwegian Defence Research Establishment

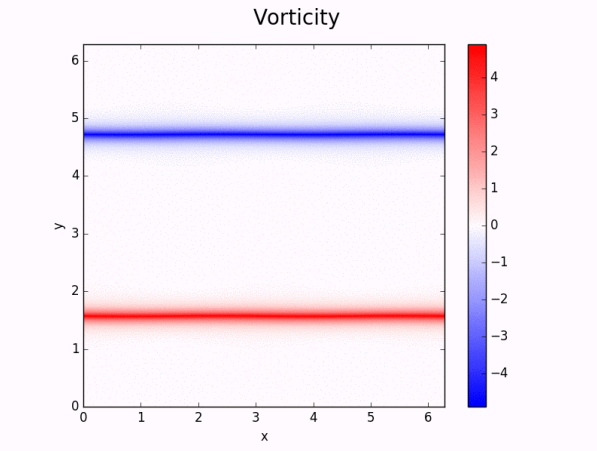


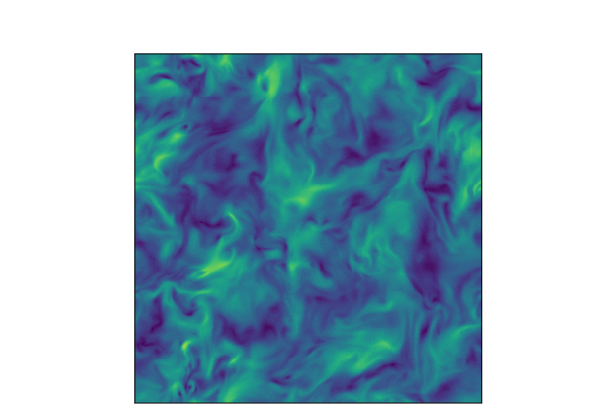
Principal developer of Shenfun

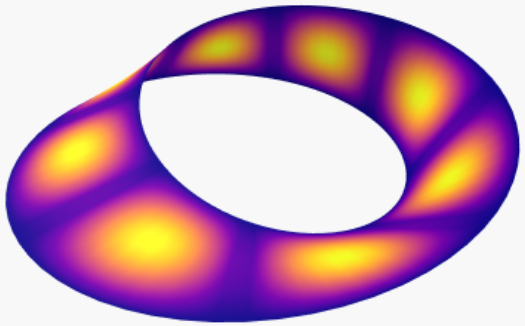
High performance computing platform for solving PDEs by the spectral Galerkin method. Written in Python (Cython). https://github.com/spectralDNS/shenfun

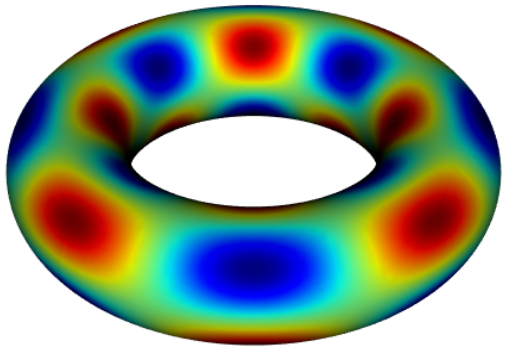












MAT-MEK4270 in a nutshell

- Numerical methods for partial differential equations (PDEs)
- How to solve the equations, not why
- How do we solve a PDE in practice?
- How do we trust the answer?
- Is the numerical scheme stable? accurate? consistent?
- Focus on programming (github, python, testing code)
- IN5670 -> IN5270 -> MAT-MEK4270 - Lots of old material

Syllabus

Important stuff

- Lecture notes
- Presentations (including this one)
- Github organization MATMEK-4270

Also important stuff, but less so as I will try to put all really important stuff in the lecture notes

- Langtangen, Finite Difference Computing with exponential decay - Chapters 1 and 2.
- Langtangen and Linge, Finite Difference Computing with PDEs - Parts of chapters 1 and 2.
- Langtangen and Mardal, Introduction to Numerical Methods for Variational Problems

Two major approaches

Finite differences

$$\frac{du(t)}{dt} \approx \frac{u(t+\Delta t) - u(t)}{\Delta t}$$

- Approximate in points
- Uniform grid
- Taylor expansions

Variational methods

$$\int_\Omega u'' v d\Omega = -\int_\Omega u' v' d\Omega + \int_\Gamma u' v d\Gamma$$

- Approximate weakly
- Finite element method
- Least squares method
- Galerkin method

We will use both approaches to first consider **function** approximations and then the approximation of **equations**.

Required software skills

- Our software platform: Python, Jupyter notebooks
- Important Python packages: `numpy`, `scipy`, `matplotlib`, `sympy`, `shenfun`, …
- Anaconda Python, conda environments

Assumed/ideal background

- IN1900: 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 - exponential decay

Exponential decay model

ODE problem

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

where $a > 0$ is a constant and $u(t)$ is the time-dependent solution.

- We study first a simple 1D ODE, because this will lead us to the building blocks that we need for solving PDEs!
- We can more easily study the concepts of stability, accuracy, convergence and consistency.

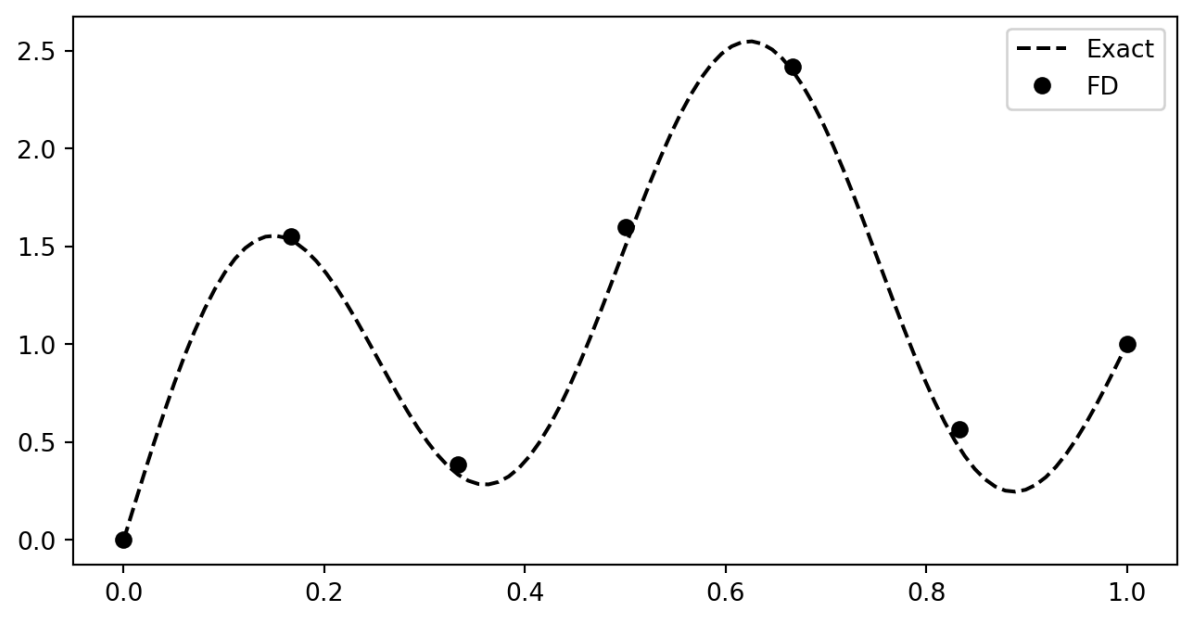
See Langtangen, Finite Difference Computing - Chapter 1

What to learn in the start-up example

- 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 optimize the code for computational speed
- How to plot the solutions
- How to compute numerical errors and convergence rates
- How to analyse the numerical solution

Finite difference methods

- The finite difference method is the simplest method for solving differential equations
- Satisfy the equations in discrete points, not continuously
- 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



The steps in the finite difference method

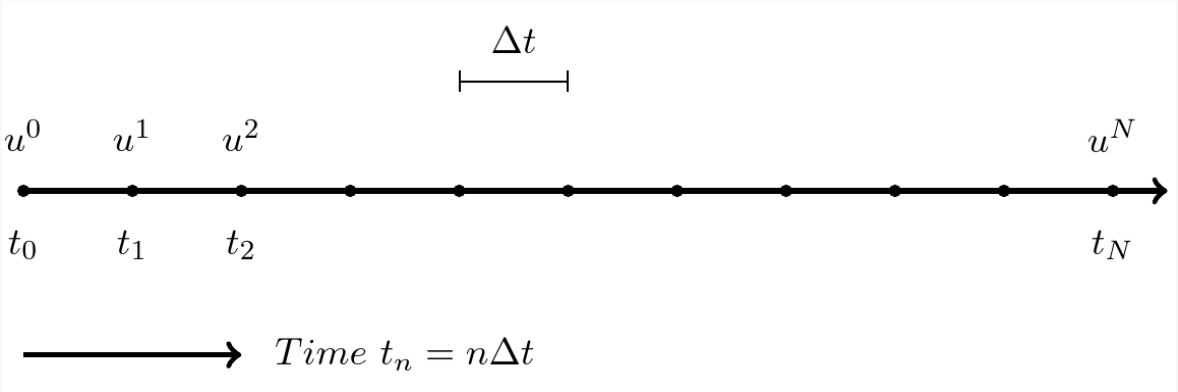
Solving a differential equation by a finite difference method consists of four steps:

1. discretizing the domain,
2. fulfilling the equation at discrete time points,
3. replacing derivatives by finite differences,
4. solve the discretized problem. (Often with a recursive algorithm in 1D)

Step 1: Discretizing the domain

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

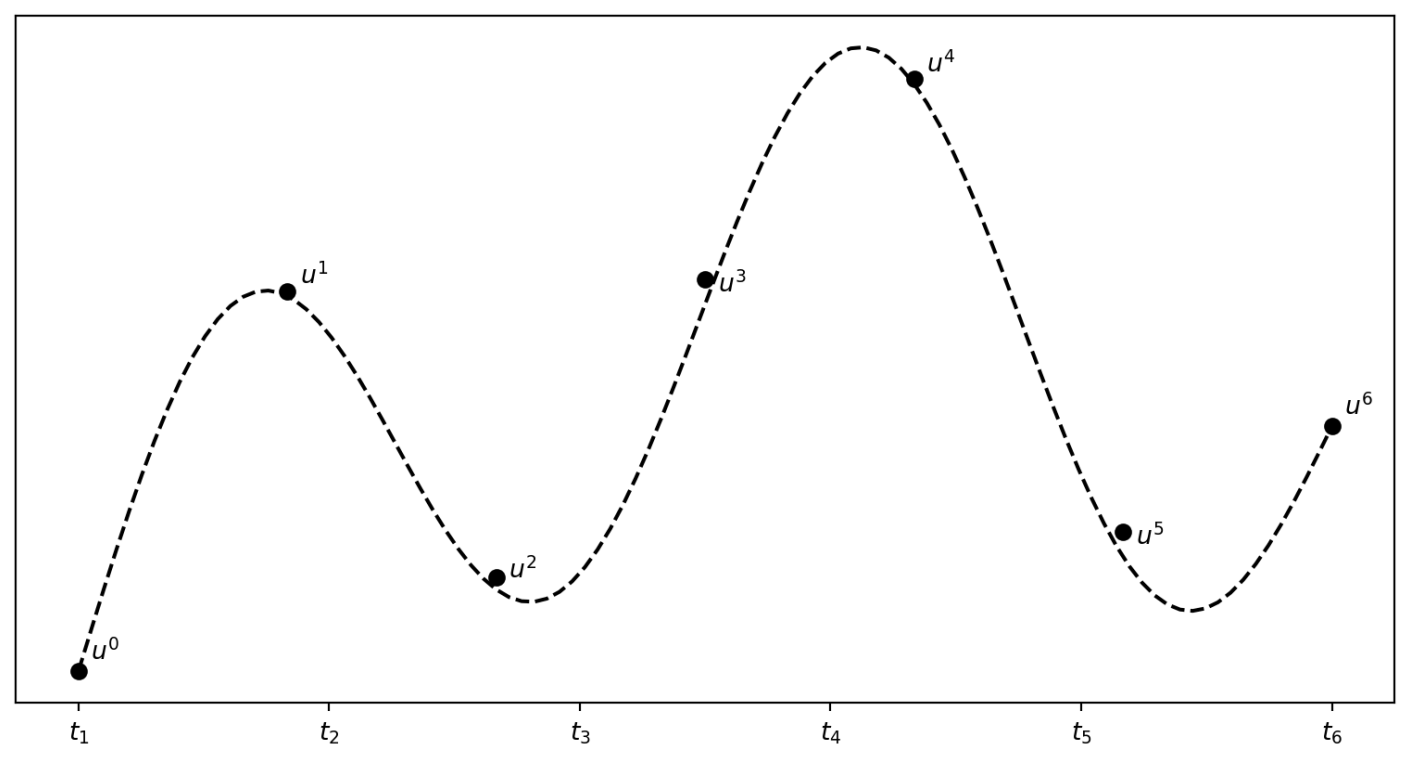
$$0 = t_0 < t_1 < t_2 < \cdots < t_{N_t - 1} < t_{N_t} = T$$



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

Step 1: Discretizing the domain

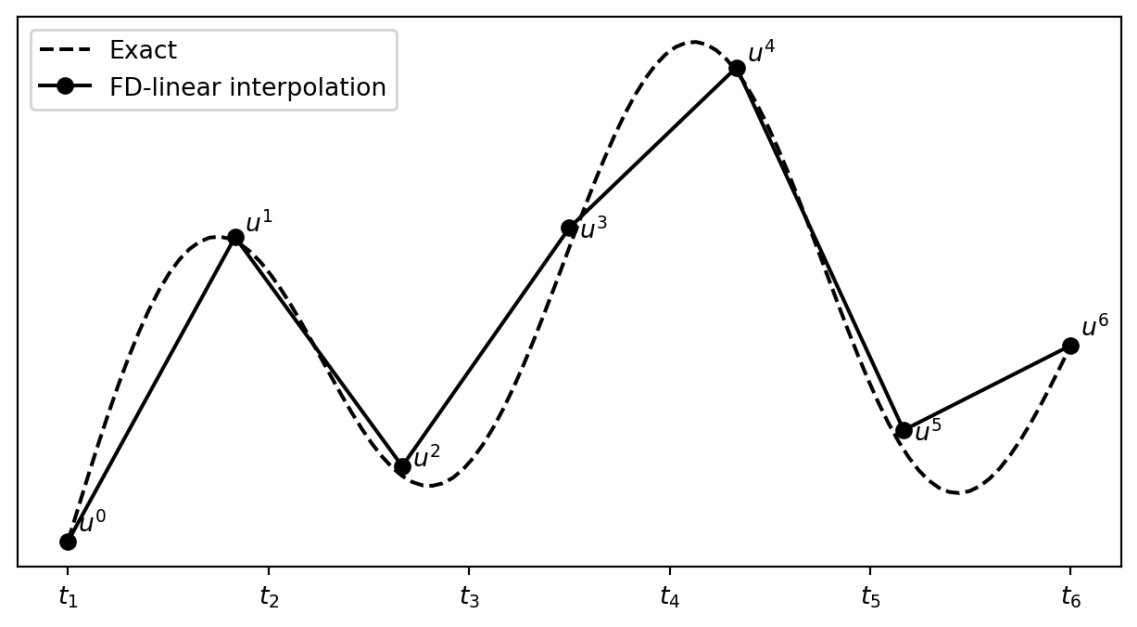
u^n is a **mesh function**, defined at the mesh points $t_n, n = 0, \ldots, N_t$ only.



What about a mesh function between the mesh points?

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

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



Step 2: Fulfilling the equation at discrete time points

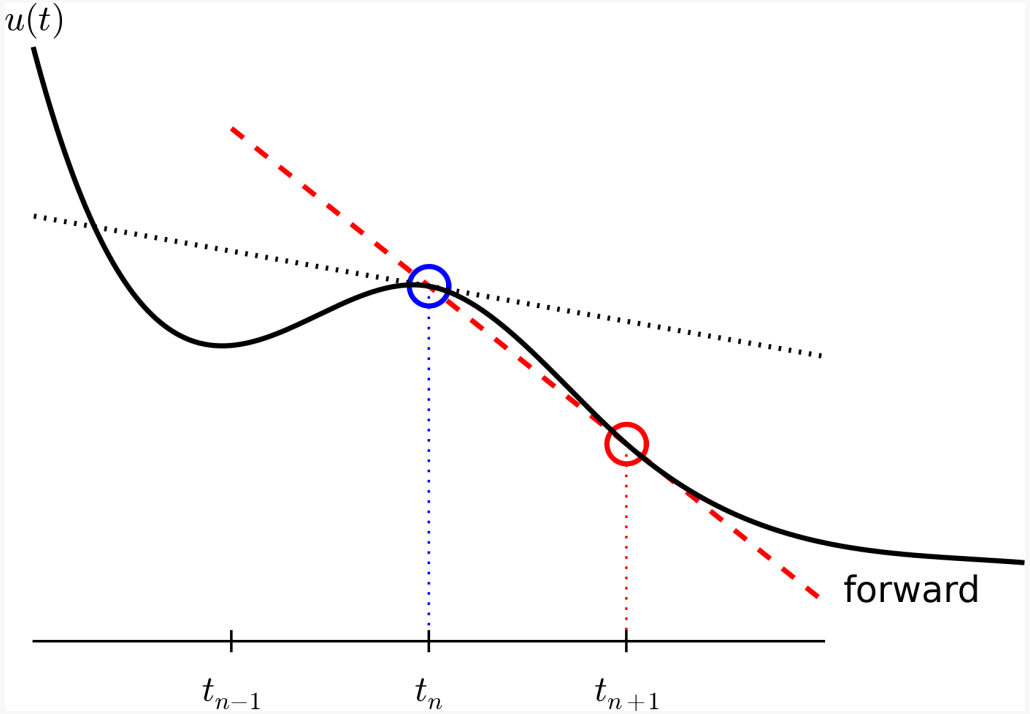
- The ODE holds for all $t \in (0, T]$ (infinite no of points)
- Idea: let the ODE be valid at the mesh points only (finite no of points)

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

Step 3: Replacing derivatives by finite differences

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

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



Step 3: Replacing derivatives by finite differences

Inserting the finite difference approximation in

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

gives

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

(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:

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

Let us apply the scheme by hand

Assume constant time spacing: $\Delta t = t_{n+1} - t_n = \text{const}$ such that $u^{n+1} = u^n(1 - a\Delta t)$

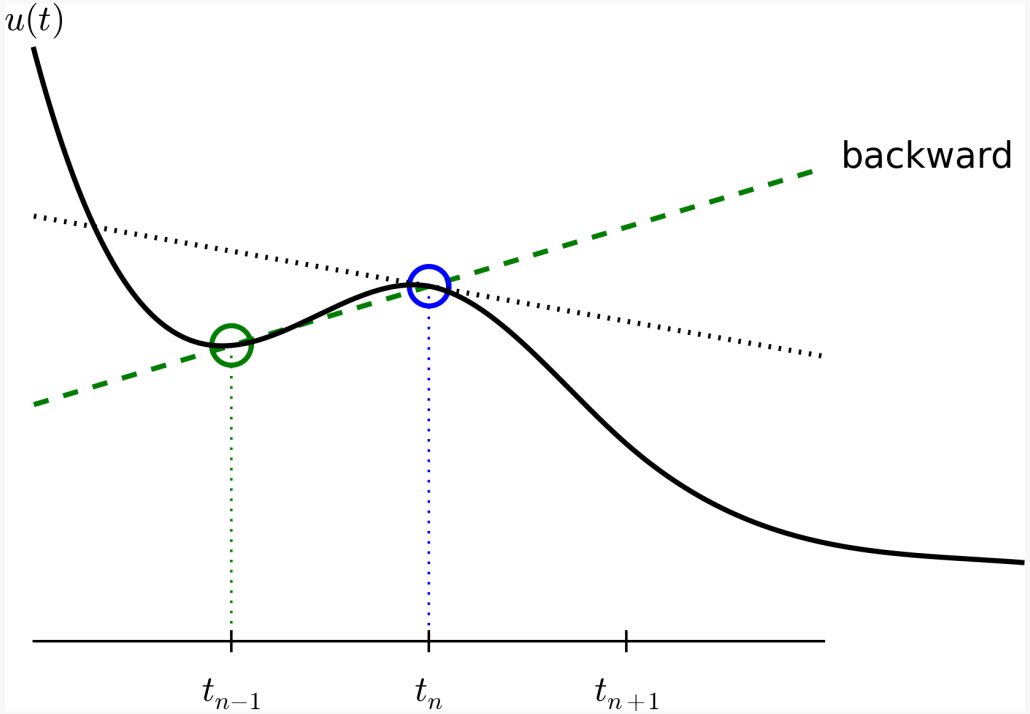
$$
\begin{aligned}
u^0 &= I, \\
u^1 &= I(1 - a\Delta t), \\
u^2 &= I(1 - a\Delta t)^2, \\
&\vdots \\
u^{N_t} &= I(1 - a\Delta t)^{N_t}
\end{aligned}
$$

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

A backward difference

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

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



The Backward Euler scheme

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

$$\frac{u^n - u^{n-1}}{t_n - t_{n-1}} = -au^n$$

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

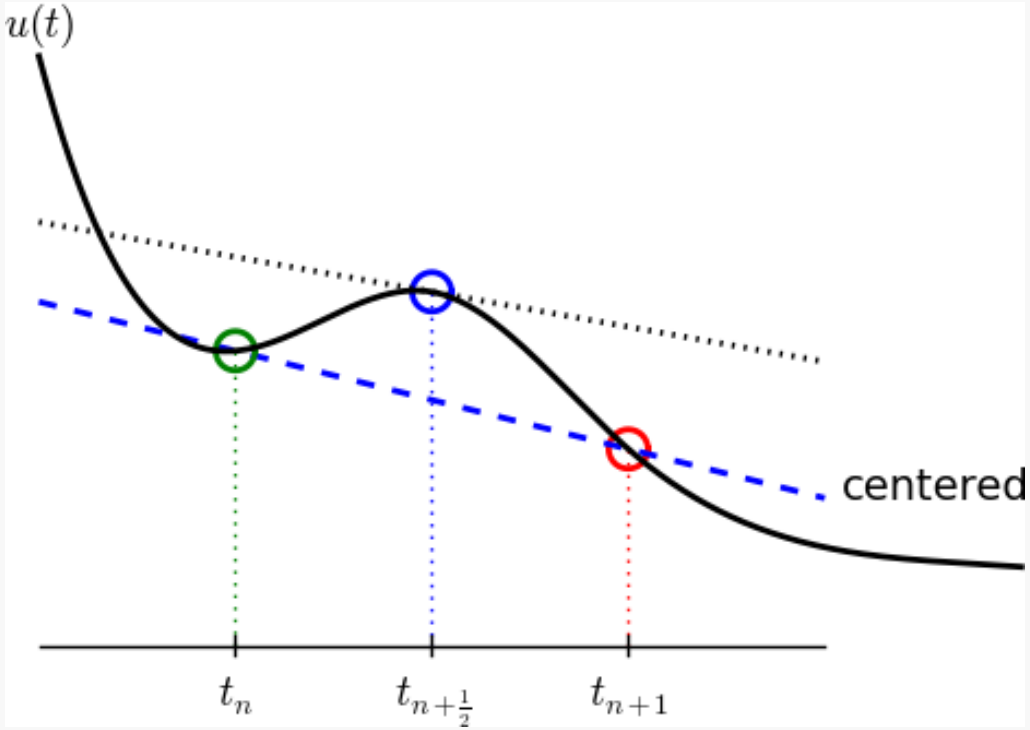
$$u^{n+1} = \frac{1}{1 + a(t_{n+1} - t_n)} u^n$$

Note

We use u^{n+1} as unknown and rename $u^n \longrightarrow u^{n+1}$ and $u^{n-1} \longrightarrow u^n$

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 $t_{n+\frac{1}{2}}$. With $N_t + 1$ points, that is N_t equations for $n = 0, 1, \ldots N_t - 1$

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

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

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

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 (linear interpolation):

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

The Crank-Nicolson scheme; result

Result:

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

Solve wrt to u^{n+1}:

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

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:

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

- $\theta = 0$: 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}:

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

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

$$u^{n+1} = (1 - a\Delta t)u^n \quad (\mathrm{FE})$$

$$u^{n+1} = \frac{1}{1 + a\Delta t}u^n \quad (\mathrm{BE})$$

$$u^{n+1} = \frac{1 - \frac{1}{2}a\Delta t}{1 + \frac{1}{2}a\Delta t}u^n \quad (\mathrm{CN})$$

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

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 $u^n, n = 1, 2, \ldots, N_t$
- 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
- Quantify the error $u_e(t_n) - u^n$ using **norms**
- Compute the **convergence rate** of the numerical scheme
- (Optimize for speed)

Algorithm

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

In Python

```python
import numpy as np
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 = np.zeros(Nt+1)           # array of u[n] values
    t = np.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

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

In Python

```python
import numpy as np
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 = np.zeros(Nt+1)           # array of u[n] values
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    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

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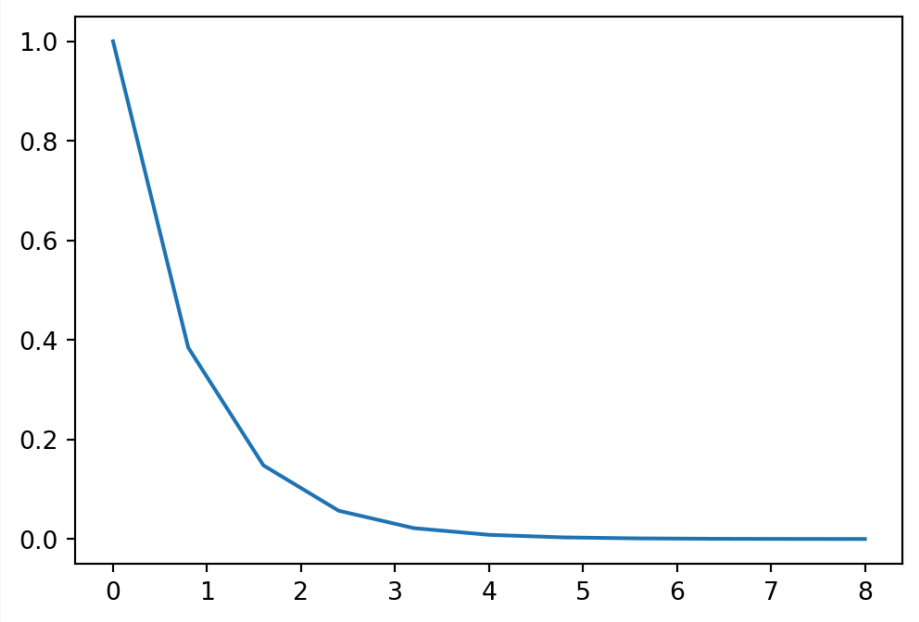

```
t= 0.000 u=1
t= 0.800 u=0.384615
t= 1.600 u=0.147929
t= 2.400 u=0.0568958
t= 3.200 u=0.021883
t= 4.000 u=0.00841653
t= 4.800 u=0.00323713
t= 5.600 u=0.00124505
t= 6.400 u=0.000478865
t= 7.200 u=0.000184179
t= 8.000 u=7.0838e-05
```

Plot the solution

We will also learn about plotting. It is very important to present data in a clear and consise manner. It is very easy to generate a *naked* plot

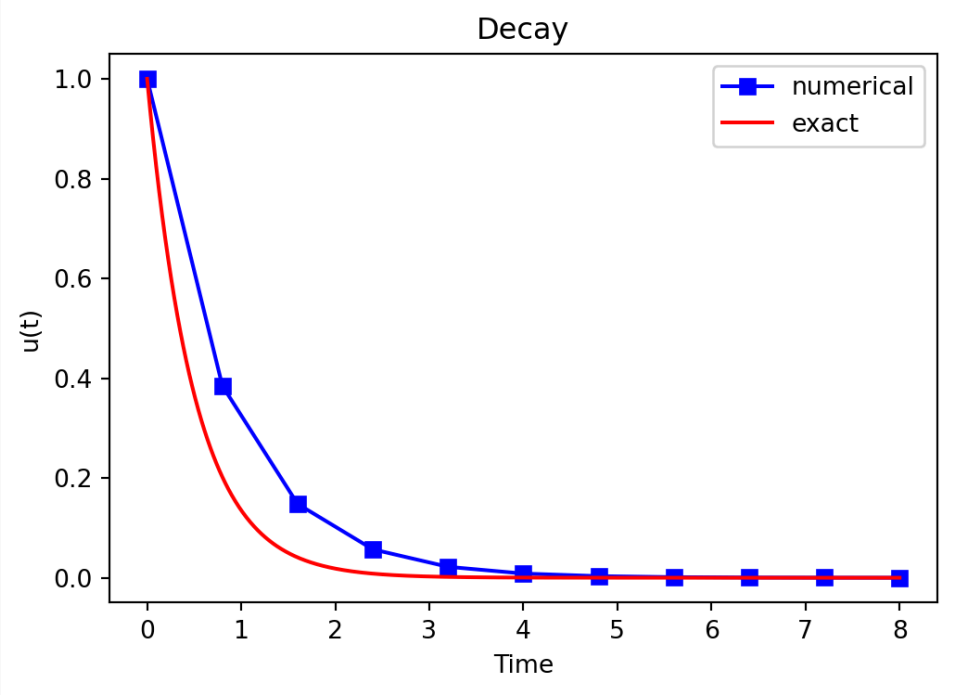
```
1 import matplotlib.pyplot as plt
2 I, a, T, dt, theta = 1, 2, 8, 0.8, 1
3 u, t = solver(I, a, T, dt, theta)
4 fig = plt.figure(figsize=(6, 4))
5 ax = fig.gca()
6 ax.plot(t, u)
```



Plot the solution

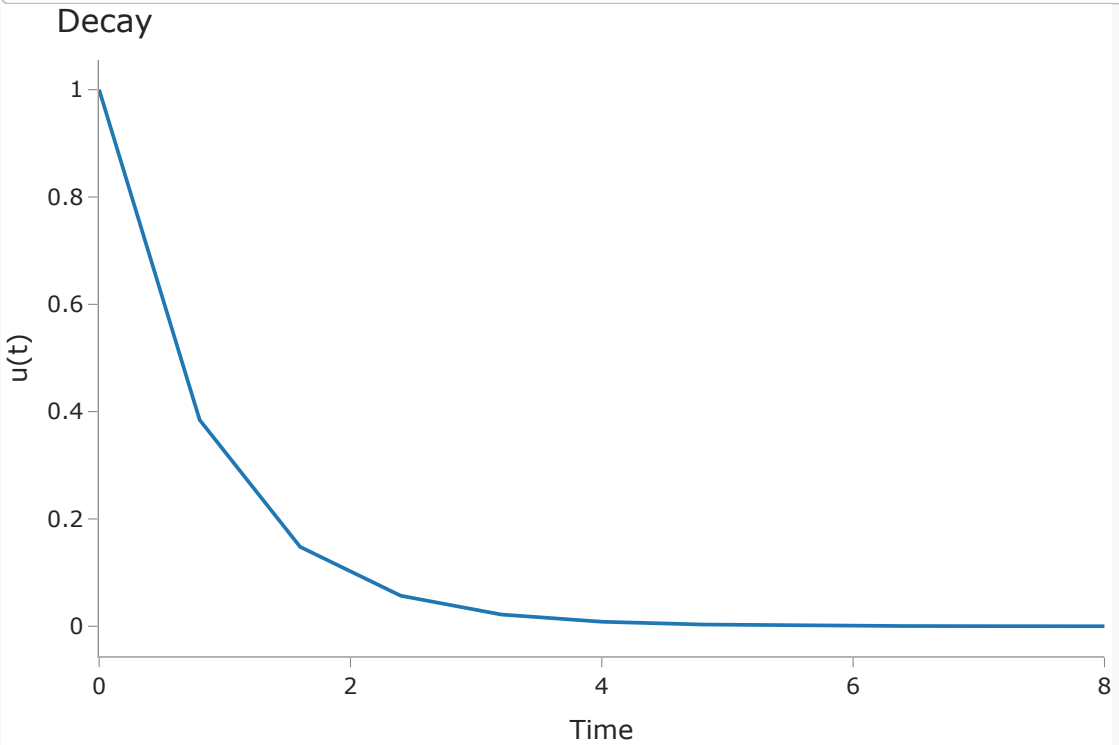
But you should always add legends, titles, exact solution, etc. Make the plot nice:-)

```
u_exact = lambda t, I, a: I*np.exp(-a*t)
u, t = solver(I=I, a=a, T=T, dt=0.8, theta=1)
te = np.linspace(0, T, 1000)
ue = u_exact(te, I, a)
fig = plt.figure(figsize=(6, 4))
plt.plot(t, u, 'bs-', te, ue, 'r')
plt.title('Decay')
plt.legend(['numerical', 'exact'])
plt.xlabel('Time'), plt.ylabel('u(t)');
```



Plotly is a very good alternative

```
1 import plotly.express as px
2 pfig = px.line(x=t, y=u, labels={'x': 'Time', 'y': 'u(t)'},
3                 width=600, height=400, title='Decay',
4                 template="simple_white")
5 pfig.show()
```



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
  - pytest
  - github actions

Comparison with exact numerical solution

What is exact?

There is a difference between exact numerical solution and exact solution!

Repeated use of the θ-rule gives exact numerical solution:

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

Exact solution on the other hand:

$$
u(t) = \exp(-at), \quad u(t_n) = \exp(-at_n)
$$

Making a test based on an exact numerical solution

The exact discrete solution is

$$u^n = IA^n$$

Test if your solver gives

$$\max_n |u^n - IA^n| < \epsilon \sim 10^{-15}$$

for a few precalculated steps.

Tip

Make sure you understand what n in u^n and in A^n means! n is not used as a power in u^n, but it is a power in A^n!

Run a few numerical steps by hand

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

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

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

The test based on exact numerical solution

```
def test_solver_three_steps(solver):
    """Compare three steps with known manual computations."""
    theta = 0.8
    a = 2
    I = 0.1
    dt = 0.8
    u_by_hand = np.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-14  # tolerance for comparing floats
    diff = abs(u - u_by_hand).max()
    success = diff < tol
    assert success, diff

test_solver_three_steps(solver)
```

Note

We do not use the **exact** solution because the numerical solution will not equal the exact!

Quantifying the error

Computing the norm of the error

- $e^n = u^n - u_e(t_n)$ is a **mesh function**
- Usually we want one number for the error
- Use a norm of e^n

Norms of a function $f(t)$:

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

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

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

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:

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

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

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

Norms - notice!

- The *continuous* norms use capital L^2, L^1, L^∞
- The *discrete* norm uses lowercase $\ell^2, \ell^1, \ell^\infty$

Implementation of the error norm

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

Python code for the norm:

```
1 u_exact = lambda t, I, a: I*np.exp(-a*t)
2 I, a, T, dt, theta = 1., 2., 8., 0.2, 1
3 u, t = solver(I, a, T, dt, theta)
4 en = u_exact(t, I, a) - u
5 E = np.sqrt(dt*np.sum(en**2))
6 print(f'Errornorm = {E}')
```

```
Errornorm = 0.0637716295205199
```

How about computational speed?

The code is naive and not very efficient. It is not vectorized!

Vectorization

Vectorization refers to the process of converting iterative operations on individual elements of an array (or other data structures) into batch operations on entire arrays.

For example, you have three arrays

$$\boldsymbol{u} = (u_i)_{i=0}^{N}, \boldsymbol{v} = (v_i)_{i=0}^{N}, \boldsymbol{w} = (w_i)_{i=0}^{N}$$

Now compute

$$w_i = u_i \cdot v_i, \quad \forall\, i = 0, 1, \ldots, N$$

How about computational speed?

The code is naive and not very efficient. It is not vectorized!

Vectorization

Vectorization refers to the process of converting iterative operations on individual elements of an array (or other data structures) into batch operations on entire arrays.

Regular (scalar) implementation:

```
N = 1000
u = np.random.random(N)
v = np.random.random(N)
w = np.zeros(N)

for i in range(N):
    w[i] = u[i] * v[i]
```

Vectorized:

```
w[:] = u * v
```

Numpy is heavily vectorized! So much so that mult, add, div, etc are vectorized by default!

How about computational speed?

The code is naive and not very efficient. It is not vectorized!

Vectorization

Vectorization refers to the process of converting iterative operations on individual elements of an array (or other data structures) into batch operations on entire arrays.

Vectorization warning

Pretty much all the code you will see and get access to in this course will be vectorized!

Vectorizing the decay solver

Get rid of the for-loop!

```
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]
```

How? Difficult because it is a **recursive** update and not regular **elementwise** multiplication. But remember

$$A = (1 - (1 - \theta)a\Delta t)/(1 + \theta\Delta t a)$$

$$\begin{aligned} u^1 &= Au^0, \\ u^2 &= Au^1, \\ &\vdots \\ u^{N_t} &= Au^{N_t-1} \end{aligned}$$

Vectorized code

```
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]
```

Can be implemented as

```
u[0] = I                  # assign initial condition
u[1:] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)
u[:] = np.cumprod(u)
```

Why vectorization?

- Python for-loops are slow!
- Python for-loops usually requires more lines of code.

```
def f0(u, I, theta, a, dt):
    u[0] = I
    u[1:] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)
    u[:] = np.cumprod(u)
    return u

def f1(u,  I, theta, a, dt):
    u[0] = I
    for n in range(0, len(u)-1):
        u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
    return u

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

assert np.allclose(f0(u.copy(), I, theta, a, dt),
                   f1(u.copy(), I, theta, a, dt))
```

Lets try some timings!

Why vectorization? Timings

```
def f0(u, I, theta, a, dt):
    u[0] = I
    u[1:] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)
    u[:] = np.cumprod(u)

def f1(u,  I, theta, a, dt):
    u[0] = I
    for n in range(0, len(u)-1):
        u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
```

Lets try some timings:

```
%timeit -q -o -n 1000 f0(u, I, theta, a, dt)
```

```
<TimeitResult : 2.34 µs ± 468 ns per loop (mean ± std. dev. of 7 runs, 1,000 loops each)>
```

```
%timeit -q -o -n 1000 f1(u, I, theta, a, dt)
```

```
<TimeitResult : 2.1 µs ± 87.5 ns per loop (mean ± std. dev. of 7 runs, 1,000 loops each)>
```

Hmm. Not really what's expected. Why? Because the array u is really short! Lets try a longer array

```
print(f"Length of u = {u.shape[0]}")
```

```
Length of u = 11
```

Longer array timings

```
dt = dt/10
u, t = solver(I, a, T, dt, theta)
print(f"Length of u = {u.shape[0]}")
```

```
Length of u = 101
```

```
%timeit -q -o -n 100 f0(u, I, theta, a, dt)
```

```
<TimeitResult : 2.86 µs ± 250 ns per loop (mean ± std. dev. of 7 runs, 100 loops each)>
```

```
%timeit -q -o -n 100 f1(u, I, theta, a, dt)
```

```
<TimeitResult : 19.9 µs ± 804 ns per loop (mean ± std. dev. of 7 runs, 100 loops each)>
```

Even longer array:

```
dt = dt/10
u, t = solver(I, a, T, dt, theta)
print(f"Length of u = {u.shape[0]}")
```

```
Length of u = 1001
```

```
%timeit -q -o -n 100 f0(u, I, theta, a, dt)
```

```
<TimeitResult : 3.45 µs ± 1.34 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)>
```

```
%timeit -q -o -n 100 f1(u, I, theta, a, dt)
```

```
<TimeitResult : 203 µs ± 4.98 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)>
```

Vectorized code takes the same time! Only overhead costs, not the actual computation.

What else is there? Numba

```
import numba as nb
@nb.jit
def f2(u,  I, theta, a, dt):
    u[0] = I
    for n in range(0, len(u)-1):
        u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
```

Time it once

```
%timeit -q -o -n 100 f2(u, I, theta, a, dt)
```

```
<TimeitResult : 45.7 µs ± 109 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)>
```

Slow because the code needs to be compiled. Try again

```
%timeit -q -o -n 100 f2(u, I, theta, a, dt)
```

```
<TimeitResult : 1.18 µs ± 16.7 ns per loop (mean ± std. dev. of 7 runs, 100 loops each)>
```

That is even faster than the vectorized code!

What else? Cython

```
%load_ext cython
```

```
The cython extension is already loaded. To reload it, use:
  %reload_ext cython
```

```
%%cython -a
#cython: boundscheck=False, wraparound=False, cdivision=True
cpdef void f3(double[::1] u, int  I, double theta, double a, double dt):
    cdef int n
    cdef int N = u.shape[0]
    u[0] = I
    for n in range(0, N-1):
        u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
    return
```

Generated by Cython 3.0.10

Yellow lines hint at Python interaction.

Click on a line that starts with a "+" to see the C code that Cython generated for it.

```
+1: #cython: boundscheck=False, wraparound=False, cdivision=True
+2: cpdef void f3(double[::1] u, int  I, double theta, double a, double dt):
 3:     cdef int n
+4:     cdef int N = u.shape[0]
+5:     u[0] = I
+6:     for n in range(0, N-1):
+7:         u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
+8:     return
```

Cython timing

```
1 %timeit -q -o -n 100 f3(u, I, theta, a, dt)
```

```
<TimeitResult : 1.23 µs ± 61.8 ns per loop (mean ± std. dev. of 7 runs, 100 loops each)>
```

Cython and Numba are both fast!

Cython and Numba are both as fast as pure C. Either one can be used to speed up critical routines with very little additional effort!

Note

Cython is very easy to use in notebooks, but requires some additional steps to be compiled used as extension modules with regular python programs.