

# Study guide: Solving nonlinear ODE and PDE problems

Hans Petter Langtangen<sup>1,2</sup>

Svein Linge<sup>3,1</sup>

<sup>1</sup>Center for Biomedical Computing, Simula Research Laboratory

<sup>2</sup>Department of Informatics, University of Oslo

<sup>3</sup>Department of Process, Energy and Environmental Technology, University College of Southeast Norway

Jun 27, 2016

## EDIT THESE SLIDES!

Remove everything with finite elements!

## What makes a differential equations nonlinear?

- In linear differential equations, the unknown  $u$  or its derivatives appear in linear terms  $au(t)$ ,  $au'(t)$ ,  $a\nabla^2 u$ , where  $a$  is independent of  $u$ .
- All other types of terms containing  $u$  are *nonlinear* and contain **products of  $u$  or its derivatives**.

## Examples on linear and nonlinear differential equations

Linear ODE:

$$u'(t) = a(t)u(t) + b(t)$$

Nonlinear ODE:

$$u'(t) = u(t)(1 - u(t)) = u(t) - u(t)^2$$

This (pendulum) ODE is also nonlinear:

$$u'' + \gamma \sin u = 0$$

because

$$\sin u = u - \frac{1}{6}u^3 + \mathcal{O}(u^5),$$

contains products of  $u$

## Introduction of basic concepts

- Logistic ODE as simple model for a nonlinear problem
- Introduction of basic techniques:
  - Explicit time integration (no nonlinearities)
  - Implicit time integration (nonlinearities)
  - Linearization and Picard iteration
  - Linearization via Newton's method
  - Linearization via a trick like geometric mean
- Numerical illustration of the performance

## The scaled logistic ODE

$$u'(t) = u(t)(1 - u(t)) = u - u^2$$

## Linearization by explicit time discretization

Forward Euler method:

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

gives a *linear* algebraic equation for the unknown value  $u^{n+1}$ !

Explicit time integration methods will (normally) linearize a nonlinear problem.

Another example: 2nd-order Runge-Kutta method

$$\begin{aligned} u^* &= u^n + \Delta t u^n(1 - u^n), \\ u^{n+1} &= u^n + \Delta t \frac{1}{2} (u^n(1 - u^n) + u^*(1 - u^*)) . \end{aligned}$$

## An implicit method: Backward Euler discretization

A backward time difference

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

gives a *nonlinear* algebraic equation for the unknown  $u^n$ . The equation is of quadratic type (which can easily be solved exactly):

$$\Delta t(u^n)^2 + (1 - \Delta t)u^n - u^{n-1} = 0$$

## Detour: new notation

To make formulas less overloaded and the mathematics as close as possible to computer code, a new notation is introduced:

- $u^{(1)}$  means  $u^{n-1}$
- In general:  $u^{(\ell)}$  means  $u^{n-\ell}$
- $u$  is the unknown ( $u^n$ )

Nonlinear equation to solve in new notation:

$$F(u) = \Delta t u^2 + (1 - \Delta t)u - u^{(1)} = 0$$

## Exact solution of quadratic nonlinear equations

Solution of  $F(u) = 0$ :

$$u = \frac{1}{2\Delta t} \left( -1 + \Delta t \pm \sqrt{(1 - \Delta t)^2 - 4\Delta t u^{(1)}} \right)$$

**Observation:** Nonlinear algebraic equations may have multiple solutions!

## How do we pick the right solution in this case?

Let's investigate the nature of the two roots:

```
>>> import sympy as sym
>>> dt, u_1, u = sym.symbols('dt u_1 u')
>>> r1, r2 = sym.solve(dt*u**2 + (1-dt)*u - u_1, u) # find roots
>>> r1
(dt - sqrt(dt**2 + 4*dt*u_1 - 2*dt + 1) - 1)/(2*dt)
>>> r2
(dt + sqrt(dt**2 + 4*dt*u_1 - 2*dt + 1) - 1)/(2*dt)
>>> print r1.series(dt, 0, 2)
-1/dt + 1 - u_1 + dt*(u_1**2 - u_1) + 0(dt**2)
>>> print r2.series(dt, 0, 2)
u_1 + dt*(-u_1**2 + u_1) + 0(dt**2)
```

The **r1** root behaves as  $1/\Delta t \rightarrow \infty$  as  $\Delta t \rightarrow 0$ ! Therefore, only the **r2** root is of relevance.

## Linearization

- In general, we cannot solve nonlinear algebraic equations with formulas
- We must *linearize* the equation, or create a recursive set of *linearized* equations whose solutions hopefully converge to the solution of the nonlinear equation
- Manual linearization may be an art
- Automatic linearization is possible (cf. Newton's method)

Examples will illustrate the points!

## Picard iteration

Nonlinear equation from Backward Euler scheme for logistic ODE:

$$F(u) = au^2 + bu + c = 0$$

Let  $u^-$  be an available approximation of the unknown  $u$ .  
Linearization of  $u^2$ :  $u^-u$

$$F(u) \approx \hat{F}(u) = au^-u + bu + c = 0$$

But

- Problem: the solution  $u$  of  $\hat{F}(u) = 0$  is not the exact solution of  $F(u) = 0$
- Solution: set  $u^- = u$  and repeat the procedure

## The algorithm of Picard iteration

At a time level, set  $u^- = u^{(1)}$  (solution at previous time level) and iterate:

$$u = -\frac{c}{au^- + b}, \quad u^- \leftarrow u$$

This technique is known as

- fixed-point iteration
- successive substitutions
- nonlinear Richardson iteration
- **Picard iteration**

## The algorithm of Picard iteration with classical math notation

- $u^k$ : computed approximation in iteration  $k$
- $u^{k+1}$  is the next approximation (unknown)

$$au^k u^{k+1} + bu^{k+1} + c = 0 \quad \Rightarrow \quad u^{k+1} = -\frac{c}{au^k + b}, \quad k = 0, 1, \dots$$

Or with a time level  $n$  too:

$$au^{n,k} u^{n,k+1} + bu^{n,k+1} - u^{n-1} = 0 \quad \Rightarrow \quad u^{n,k+1} = \frac{u^{n-1}}{au^{n,k} + b}, \quad k = 0, 1, \dots$$

## Stopping criteria

Using change in solution:

$$|u - u^-| \leq \epsilon_u$$

or change in residual:

$$|F(u)| = |au^2 + bu + c| < \epsilon_r$$

## A single Picard iteration

Common simple and cheap technique: perform 1 single Picard iteration

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

Inconsistent time discretization ( $u(1-u)$  must be evaluated for  $n$ ,  $n-1$ , or  $n-\frac{1}{2}$ ) - can produce quite inaccurate results, but is very popular.

## Implicit Crank-Nicolson discretization

Crank-Nicolson discretization:

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

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

Approximate  $u^{n+\frac{1}{2}}$  as usual by an arithmetic mean,

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

$$(u^{n+\frac{1}{2}})^2 \approx \frac{1}{4}(u^n + u^{n+1})^2 \quad (\text{nonlinear term})$$

which is nonlinear in the unknown  $u^{n+1}$ .

## Linearization by a geometric mean

Using a *geometric mean* for  $(u^{n+\frac{1}{2}})^2$  linearizes the nonlinear term  $(u^{n+\frac{1}{2}})^2$  (error  $\mathcal{O}(\Delta t^2)$ ) as in the discretization of  $u'$ :

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

Arithmetic mean on the linear  $u^{n+\frac{1}{2}}$  term and a geometric mean for  $(u^{n+\frac{1}{2}})^2$  gives a linear equation for  $u^{n+1}$ :

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

Note: Here we turned a nonlinear algebraic equation into a linear one. No need for iteration! (Consistent  $\mathcal{O}(\Delta t^2)$  approx.)

## Newton's method

Write the nonlinear algebraic equation as

$$F(u) = 0$$

Newton's method: linearize  $F(u)$  by two terms from the Taylor series,

$$\begin{aligned} F(u) &= F(u^-) + F'(u^-)(u - u^-) + \frac{1}{2}F''(u^-)(u - u^-)^2 + \dots \\ &\approx F(u^-) + F'(u^-)(u - u^-) \equiv \hat{F}(u) \end{aligned}$$

The linear equation  $\hat{F}(u) = 0$  has the solution

$$u = u^- - \frac{F(u^-)}{F'(u^-)}$$

Note that  $\hat{F}$  in Picard and Newton are different!

## Newton's method with an iteration index

$$u^{k+1} = u^k - \frac{F(u^k)}{F'(u^k)}, \quad k = 0, 1, \dots$$

Newton's method exhibits *quadratic convergence* if  $u^k$  is sufficiently close to the solution. Otherwise, the method may diverge.

## Using Newton's method on the logistic ODE

$$F(u) = au^2 + bu + c$$

$$F'(u) = 2au + b$$

The iteration method becomes

$$u = u^- + \frac{a(u^-)^2 + bu^- + c}{2au^- + b}, \quad u^- \leftarrow u$$

Start of iteration:  $u^- = u^{(1)}$

## Using Newton's method on the logistic ODE with typical math notation

Set iteration start as  $u^{n,0} = u^{n-1}$  and iterate with explicit indices for time ( $n$ ) and Newton iteration ( $k$ ):

$$u^{n,k+1} = u^{n,k} + \frac{\Delta t(u^{n,k})^2 + (1 - \Delta t)u^{n,k} - u^{n-1}}{2\Delta t u^{n,k} + 1 - \Delta t}$$

Compare notation with

$$u = u^- + \frac{\Delta t(u^-)^2 + (1 - \Delta t)u^- - u^{(1)}}{2\Delta t u^- + 1 - \Delta t}$$

## Relaxation may improve the convergence

- Problem: Picard and Newton iteration may change the solution too much
- Remedy: relaxation (less change in the solution)
- Let  $u^*$  be the suggested new value from Picard or Newton iteration

Relaxation with *relaxation parameter*  $\omega$  (weight old and new value):

$$u = \omega u^* + (1 - \omega)u^-, \quad \omega \leq 1$$

Simple formula when used in Newton's method:

$$u = u^- - \omega \frac{F(u^-)}{F'(u^-)}$$

## Implementation; part 1

Program `logistic.py`

```

def BE_logistic(u0, dt, Nt, choice='Picard',
               eps_r=1E-3, omega=1, max_iter=1000):
    if choice == 'Picard1':
        choice = 'Picard'; max_iter = 1

    u = np.zeros(Nt+1)
    iterations = []
    u[0] = u0
    for n in range(1, Nt+1):
        a = dt
        b = 1 - dt
        c = -u[n-1]

        if choice == 'Picard':

            def F(u):
                return a*u**2 + b*u + c

            u_ = u[n-1]
            k = 0
            while abs(F(u_)) > eps_r and k < max_iter:
                u_ = omega*(-c/(a*u_ + b)) + (1-omega)*u_
                k += 1
            u[n] = u_
            iterations.append(k)

```

## Implementation; part 2

```

def BE_logistic(u0, dt, Nt, choice='Picard',
               eps_r=1E-3, omega=1, max_iter=1000):
    ...
    elif choice == 'Newton':

        def F(u):
            return a*u**2 + b*u + c

        def dF(u):
            return 2*a*u + b

        u_ = u[n-1]
        k = 0
        while abs(F(u_)) > eps_r and k < max_iter:
            u_ = u_ - F(u_)/dF(u_)
            k += 1
        u[n] = u_
        iterations.append(k)

```



```
return u, iterations
```

### Implementation; part 3

The Crank-Nicolson method with a geometric mean:

```
def CN_logistic(u0, dt, Nt):
    u = np.zeros(Nt+1)
    u[0] = u0
    for n in range(0, Nt):
        u[n+1] = (1 + 0.5*dt)/(1 + dt*u[n] - 0.5*dt)*u[n]
    return u
```

### Experiments: accuracy of iteration methods

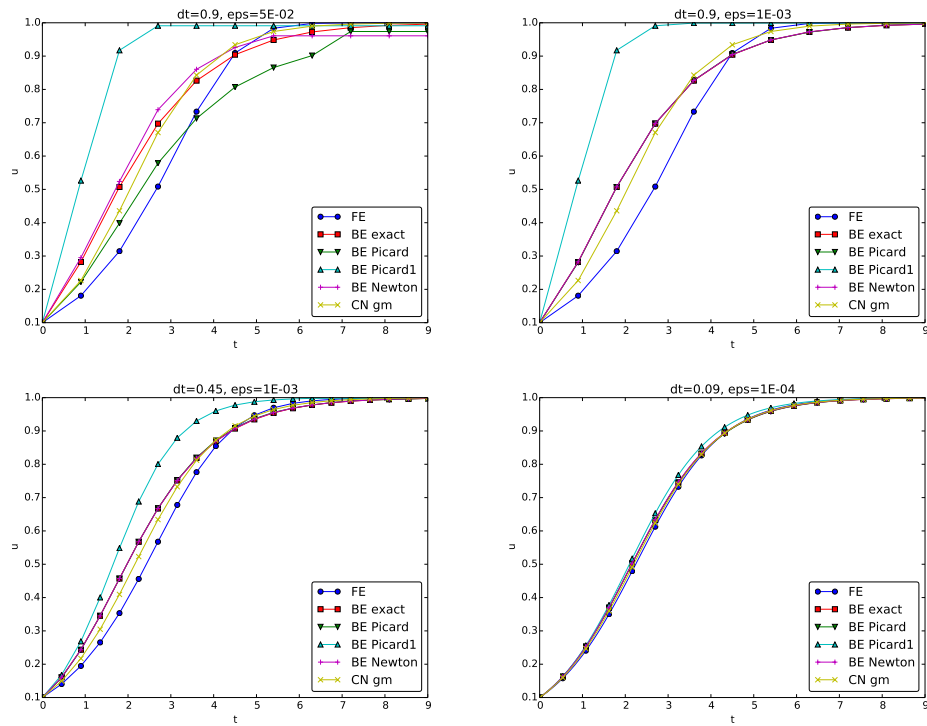


Figure 1: The impact of solution strategies and for four different time step lengths on the solution.

## Experiments: number of iterations

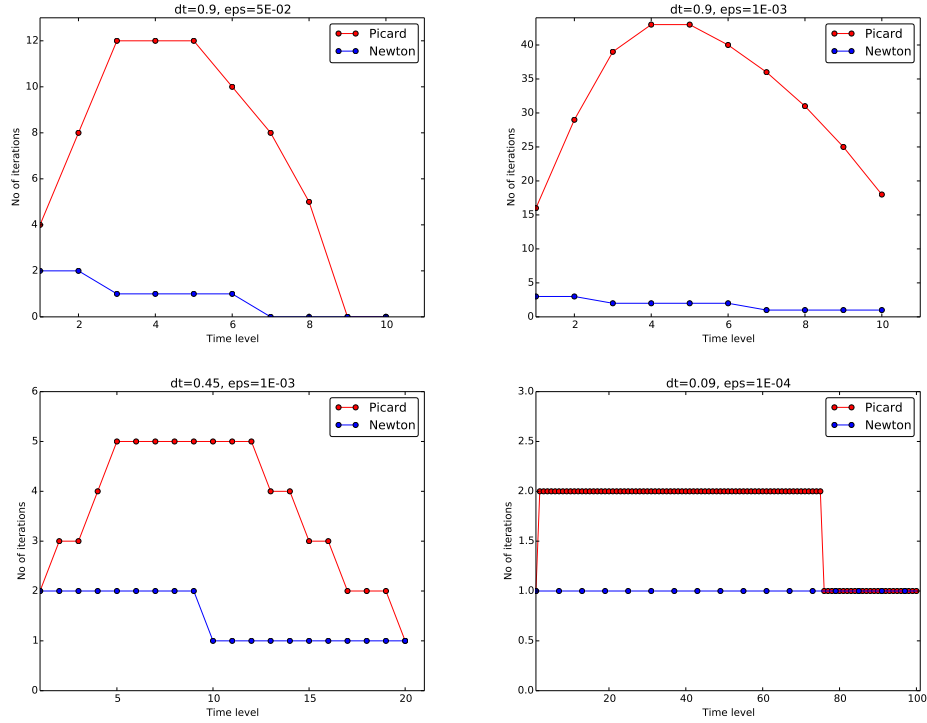


Figure 2: Comparison of the number of iterations at various time levels for Picard and Newton iteration.

## The effect of relaxation can potentially be great!

- $\Delta t = 0.9$ : Picard required 32 iterations on average
- $\omega = 0.8$ : 7 iterations
- $\omega = 0.5$ : 2 iterations (!) - optimal choice

Other  $\omega = 1$  experiments:

$\Delta t$	$\epsilon_r$	Picard	Newton
0.2	$10^{-7}$	5	2
0.2	$10^{-3}$	2	1
0.4	$10^{-7}$	12	3
0.4	$10^{-3}$	4	2
0.8	$10^{-7}$	58	3
0.8	$10^{-3}$	4	2

## Generalization to a general nonlinear ODE

$$u' = f(u, t)$$

Note:  $f$  is in general nonlinear in  $u$  so the ODE is nonlinear

## Explicit time discretization

Forward Euler and all explicit methods sample  $f$  with known values and all nonlinearities are gone:

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

## Backward Euler discretization

Backward Euler  $[D_t^- u = f]^n$  leads to nonlinear algebraic equations:

$$F(u^n) = u^n - \Delta t f(u^n, t_n) - u^{n-1} = 0$$

Alternative notation:

$$F(u) = u - \Delta t f(u, t_n) - u^{(1)} = 0$$

## Picard iteration for Backward Euler scheme

A simple Picard iteration, not knowing anything about the nonlinear structure of  $f$ , must approximate  $f(u, t_n)$  by  $f(u^-, t_n)$ :

$$\hat{F}(u) = u - \Delta t f(u^-, t_n) - u^{(1)}$$

The iteration starts with  $u^- = u^{(1)}$  and proceeds with repeating

$$u^* = \Delta t f(u^-, t_n) + u^{(1)}, \quad u = \omega u^* + (1 - \omega)u^-, \quad u^- \leftarrow u$$

until a stopping criterion is fulfilled.

## Manual linearization for a given $f(u, t)$

- $f(u^-, t)$ : *explicit* treatment of  $f$   
(as in time-discretization)
- $f(u, t)$ : *fully implicit* treatment of  $f$
- If  $f$  has some structure, say  $f(u, t) = u^3$ , we may think of a *partially implicit* treatment:  $(u^-)^2 u$
- More implicit treatment of  $f$  often gives faster convergence  
(as it gives more stable time discretizations)

Trick for partially implicit treatment of a general  $f(u, t)$ :

$$f(u^-, t) \frac{u}{u-1}$$

(Idea:  $u \approx u^-$ )

### Computational experiments with partially implicit treatment of $f$

- $f(u, t) = -u^3$ :
  - $(u^-)^3$  linearization: 22, 9, 6 iterations
  - $(u^-)^2 u$  linearization: 8, 5, 4 iterations
- $f(u, t) = e^{-u}$ : a trick  $f(u^-, t)u/u^-$  has no effect
- $f(u, t) = \sin(2(u+1))$ : a trick  $f(u^-, t)u/u^-$  has effect  
(7, 9, 11 iterations vs 17, 21, 20)

### Newton's method for Backward Euler scheme

Newton's method requires the computation of the derivative

$$F'(u) = 1 - \Delta t \frac{\partial f}{\partial u}(u, t_n)$$

**Algorithm for Newton's method for  $u' = f(u, t)$ .** Start with  $u^- = u^{(1)}$ , then iterate

$$u = u^- - \omega \frac{F(u^-)}{F'(u^-)} = u^- - \omega \frac{u^{(1)} + \Delta t f(u^-, t_n)}{1 - \Delta t \frac{\partial}{\partial u} f(u^-, t_n)}$$

### Crank-Nicolson discretization

The standard Crank-Nicolson scheme with arithmetic mean approximation of  $f$  reads

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

Nonlinear algebraic equation:

$$F(u) = u - u^{(1)} - \Delta t \frac{1}{2} f(u, t_{n+1}) - \Delta t \frac{1}{2} f(u^{(1)}, t_n) = 0$$

## Picard and Newton iteration in the Crank-Nicolson case

Picard iteration (for a general  $f$ ):

$$\hat{F}(u) = u - u^{(1)} - \Delta t \frac{1}{2} f(u^-, t_{n+1}) - \Delta t \frac{1}{2} f(u^{(1)}, t_n)$$

Newton's method:

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

$$F'(u) = 1 - \frac{1}{2} \Delta t \frac{\partial f}{\partial u}(u, t_{n+1})$$

## Systems of ODEs

$$\frac{d}{dt} u_0(t) = f_0(u_0(t), u_1(t), \dots, u_N(t), t)$$

$$\frac{d}{dt} u_1(t) = f_1(u_0(t), u_1(t), \dots, u_N(t), t),$$

$\vdots$

$$\frac{d}{dt} u_N(t) = f_N(u_0(t), u_1(t), \dots, u_N(t), t)$$

Introduce vector notation:

- $u = (u_0(t), u_1(t), \dots, u_N(t))$
- $(f_0(u, t), f_1(u, t), \dots, f_N(u, t))$

Vector form:

$$u' = f(u, t), \quad u(0) = U_0$$

Schemes: apply scalar scheme to each component

## A Backward Euler scheme for the vector ODE $u' = f(u, t)$

$$\frac{u_0^n - u_0^{n-1}}{\Delta t} = f_0(u^n, t_n)$$

$$\frac{u_1^n - u_1^{n-1}}{\Delta t} = f_1(u^n, t_n)$$

$\vdots$

$$\frac{u_N^n - u_N^{n-1}}{\Delta t} = f_N(u^n, t_n)$$

This can be written more compactly in vector form as

$$\frac{u^n - u^{n-1}}{\Delta t} = f(u^n, t_n)$$

This is a system of *nonlinear algebraic equations*,

$$u^n - \Delta t f(u^n, t_n) - u^{n-1} = 0,$$

or written out

$$u_0^n - \Delta t f_0(u^n, t_n) - u_0^{n-1} = 0,$$

$$\vdots$$

$$u_N^n - \Delta t f_N(u^n, t_n) - u_N^{n-1} = 0.$$

### Example: Crank-Nicolson scheme for the oscillating pendulum model

The scaled equations for an oscillating pendulum:

$$\dot{\omega} = -\sin \theta - \beta \omega |\omega|, \quad (1)$$

$$\dot{\theta} = \omega, \quad (2)$$

Set  $u_0 = \omega$ ,  $u_1 = \theta$

$$u'_0 = f_0(u, t) = -\sin u_1 - \beta u_0 |u_0|,$$

$$u'_1 = f_1(u, t) = u_0.$$

Crank-Nicolson discretization:

$$\frac{u_0^{n+1} - u_0^n}{\Delta t} = -\sin u_1^{n+\frac{1}{2}} - \beta u_0^{n+\frac{1}{2}} |u_0^{n+\frac{1}{2}}| \approx -\sin \left( \frac{1}{2}(u_1^{n+1} + u_1^n) \right) - \beta \frac{1}{4}(u_0^{n+1} + u_0^n) |u_0^{n+1} + u_0^n|, \quad (3)$$

$$\frac{u_1^{n+1} - u_1^n}{\Delta t} = u_0^{n+\frac{1}{2}} \approx \frac{1}{2}(u_0^{n+1} + u_0^n). \quad (4)$$

### The nonlinear $2 \times 2$ system

Introduce  $u_0$  and  $u_1$  for  $u_0^{n+1}$  and  $u_1^{n+1}$ , write  $u_0^{(1)}$  and  $u_1^{(1)}$  for  $u_0^n$  and  $u_1^n$ , and rearrange:

$$F_0(u_0, u_1) = \textcolor{red}{u}_0 - u_0^{(1)} + \Delta t \sin \left( \frac{1}{2}(\textcolor{red}{u}_1 + u_1^{(1)}) \right) + \frac{1}{4} \Delta t \beta (\textcolor{red}{u}_0 + u_0^{(1)}) |\textcolor{red}{u}_0 + u_0^{(1)}| = 0$$

$$F_1(u_0, u_1) = \textcolor{red}{u}_1 - u_1^{(1)} - \frac{1}{2} \Delta t (\textcolor{red}{u}_0 + u_0^{(1)}) = 0$$

## Systems of nonlinear algebraic equations

$$\begin{aligned}x \cos y + y^3 &= 0 \\ y^2 e^x + xy &= 2\end{aligned}$$

Systems of nonlinear algebraic equations arise from solving *systems of ODEs* or solving *PDEs*

### Notation for general systems of algebraic equations

$$F(u) = 0$$

where

$$u = (u_0, \dots, u_N), \quad F = (F_0, \dots, F_N)$$

Special linear system-type structure  
(arises frequently in PDE problems):

$$A(u)u = b(u)$$

### Picard iteration

Picard iteration for  $F(u) = 0$  is meaningless unless there is some structure so we can linearize. For  $A(u)u = b(u)$  we can linearize

$$A(u^-)u = b(u^-)$$

Note: we solve a system of nonlinear algebraic equations as a sequence of linear systems.

### Algorithm for relaxed Picard iteration

Given  $A(u)u = b(u)$  and an initial guess  $u^-$ , iterate until convergence:

1. solve  $A(u^-)u^* = b(u^-)$  with respect to  $u^*$
2.  $u = \omega u^* + (1 - \omega)u^-$
3.  $u^- \leftarrow u$

“Until convergence”:  $\|u - u^-\| \leq \epsilon_u$  or  $\|A(u)u - b\| \leq \epsilon_r$

## Newton's method for $F(u) = 0$

Linearization of  $F(u) = 0$  equation via multi-dimensional Taylor series:

$$F(u) = F(u^-) + J(u^-) \cdot (u - u^-) + \mathcal{O}(\|u - u^-\|^2)$$

where  $J$  is the *Jacobian* of  $F$ , sometimes denoted  $\nabla_u F$ , defined by

$$J_{i,j} = \frac{\partial F_i}{\partial u_j}$$

Approximate the original nonlinear system  $F(u) = 0$  by

$$\hat{F}(u) = F(u^-) + J(u^-) \cdot \delta u = 0, \quad \delta u = u - u^-$$

which is linear vector equation in  $u$

## Algorithm for Newton's method

$$\underline{F(u^-)}_{\text{vector}} + \underline{J(u^-)}_{\text{matrix}} \cdot \underline{\delta u}_{\text{vector}} = 0$$

Solution by a two-step procedure:

1. solve linear system  $J(u^-)\delta u = -F(u^-)$  wrt  $\delta u$
2. update  $u = u^- + \delta u$

Relaxed update:

$$u = \omega(u^- + \delta u) + (1 - \omega)u^- = u^- + \omega\delta u$$

## Newton's method for $A(u)u = b(u)$

For

$$F_i = \sum_k A_{i,k}(u)u_k - b_i(u)$$

one gets

$$J_{i,j} = \frac{\partial F_i}{\partial u_j} = \sum_k \frac{\partial A_{i,k}}{\partial u_j} u_k + A_{i,j} - \frac{\partial b_i}{\partial u_j}$$

Matrix form:

$$(A + A'u + b')\delta u = -Au + b$$

$$(A(u^-) + A'(u^-)u^- + b'(u^-))\delta u = -A(u^-)u^- + b(u^-)$$



## Comparison of Newton and Picard iteration

Newton:

$$(A(u^-) + A'(u^-)u^- + b'(u^-))\delta u = -A(u^-)u^- + b(u^-)$$

Rewrite:

$$\underbrace{A(u^-)(u^- + \delta u) - b(u^-)}_{\text{Picard system}} + \gamma(A'(u^-)u^- + b'(u^-))\delta u = 0$$

All the “Picard terms” are contained in the Newton formulation.

## Combined Picard-Newton algorithm

**Idea:** Write a common Picard-Newton algorithm so we can trivially switch between the two methods (e.g., start with Picard, get faster convergence with Newton when  $u$  is closer to the solution)

**Algorithm:** Given  $A(u)$ ,  $b(u)$ , and an initial guess  $u^-$ , iterate until convergence:

1. solve  $(A + \gamma(A'(u^-)u^- + b'(u^-)))\delta u = -A(u^-)u^- + b(u^-)$  with respect to  $\delta u$
2.  $u = u^- + \omega\delta u$
3.  $u^- \leftarrow u$

Note:

- $\gamma = 1$ : Newton’s method
- $\gamma = 0$ : Picard iteration

## Stopping criteria

Let  $\|\cdot\|$  be the standard Euclidian vector norm. Several termination criteria are much in use:

- Absolute change in solution:  $\|u - u^-\| \leq \epsilon_u$
- Relative change in solution:  $\|u - u^-\| \leq \epsilon_u \|u_0\|$ , where  $u_0$  denotes the start value of  $u^-$  in the iteration
- Absolute residual:  $\|F(u)\| \leq \epsilon_r$
- Relative residual:  $\|F(u)\| \leq \epsilon_r \|F(u_0)\|$
- Max no of iterations: stop when  $k > k_{\max}$

## Combination of absolute and relative stopping criteria

Problem with relative criterion: a small  $\|F(u_0)\|$  (because  $u_0 \approx u$ , perhaps because of small  $\Delta t$ ) must be significantly reduced. Better with absolute criterion.

- Can make combined absolute-relative criterion
- $\epsilon_{rr}$ : tolerance for relative part
- $\epsilon_{ra}$ : tolerance for absolute part

$$\|F(u)\| \leq \epsilon_{rr}\|F(u_0)\| + \epsilon_{ra}$$

$$\|F(u)\| \leq \epsilon_{rr}\|F(u_0)\| + \epsilon_{ra} \quad \text{or} \quad \|\delta u\| \leq \epsilon_{ur}\|u_0\| + \epsilon_{ua} \quad \text{or} \quad k > k_{\max}$$

## Example: A nonlinear ODE model from epidemiology

Spreading of a disease (e.g., a flu) can be modeled by a  $2 \times 2$  ODE system

$$\begin{aligned} S' &= -\beta SI \\ I' &= \beta SI - \nu I \end{aligned}$$

Here:

- $S(t)$  is the number of people who can get ill (susceptibles)
- $I(t)$  is the number of people who are ill (infected)
- Must know  $\beta > 0$  (danger of getting ill) and  $\nu > 0$  ( $1/\nu$ : expected recovery time)

## Implicit time discretization

A Crank-Nicolson scheme:

$$\begin{aligned} \frac{S^{n+1} - S^n}{\Delta t} &= -\beta[SI]^{n+\frac{1}{2}} \approx -\frac{\beta}{2}(S^n I^n + S^{n+1} I^{n+1}) \\ \frac{I^{n+1} - I^n}{\Delta t} &= \beta[SI]^{n+\frac{1}{2}} - \nu I^{n+\frac{1}{2}} \approx \frac{\beta}{2}(S^n I^n + S^{n+1} I^{n+1}) - \frac{\nu}{2}(I^n + I^{n+1}) \end{aligned}$$

New notation:  $S$  for  $S^{n+1}$ ,  $S^{(1)}$  for  $S^n$ ,  $I$  for  $I^{n+1}$ ,  $I^{(1)}$  for  $I^n$

$$\begin{aligned} F_S(S, I) &= S - S^{(1)} + \frac{1}{2}\Delta t\beta(S^{(1)}I^{(1)} + SI) = 0 \\ F_I(S, I) &= I - I^{(1)} - \frac{1}{2}\Delta t\beta(S^{(1)}I^{(1)} + SI) + \frac{1}{2}\Delta t\nu(I^{(1)} + I) = 0 \end{aligned}$$

## A Picard iteration

- We have approximations  $S^-$  and  $I^-$  to  $S$  and  $I$ .
- Linearize  $SI$  in  $S$  ODE as  $I^- S$  (linear equation in  $S$ !)
- Linearize  $SI$  in  $I$  ODE as  $S^- I$  (linear equation in  $I$ !)

$$S = \frac{S^{(1)} - \frac{1}{2}\Delta t \beta S^{(1)} I^{(1)}}{1 + \frac{1}{2}\Delta t \beta I^-}$$

$$I = \frac{I^{(1)} + \frac{1}{2}\Delta t \beta S^{(1)} I^{(1)} - \frac{1}{2}\Delta t \nu I^{(1)}}{1 - \frac{1}{2}\Delta t \beta S^- + \frac{1}{2}\Delta t \nu}$$

Before a new iteration:  $S^- \leftarrow S$  and  $I^- \leftarrow I$

## Newton's method

$$F(u) = 0, \quad F = (F_S, F_I), \quad u = (S, I)$$

Jacobian:

$$J = \begin{pmatrix} \frac{\partial}{\partial S} F_S & \frac{\partial}{\partial I} F_S \\ \frac{\partial}{\partial S} F_I & \frac{\partial}{\partial I} F_I \end{pmatrix} = \begin{pmatrix} 1 + \frac{1}{2}\Delta t \beta I & \frac{1}{2}\Delta t \beta S \\ -\frac{1}{2}\Delta t \beta I & 1 - \frac{1}{2}\Delta t \beta S + \frac{1}{2}\Delta t \nu \end{pmatrix}$$

Newton system:  $J(u^-)\delta u = -F(u^-)$

$$\begin{pmatrix} 1 + \frac{1}{2}\Delta t \beta I^- & \frac{1}{2}\Delta t \beta S^- \\ -\frac{1}{2}\Delta t \beta I^- & 1 - \frac{1}{2}\Delta t \beta S^- + \frac{1}{2}\Delta t \nu \end{pmatrix} \begin{pmatrix} \delta S \\ \delta I \end{pmatrix} =$$

$$\begin{pmatrix} S^- - S^{(1)} + \frac{1}{2}\Delta t \beta (S^{(1)} I^{(1)} + S^- I^-) \\ I^- - I^{(1)} - \frac{1}{2}\Delta t \beta (S^{(1)} I^{(1)} + S^- I^-) - \frac{1}{2}\Delta t \nu (I^{(1)} + I^-) \end{pmatrix}$$

**Actually no need to bother with nonlinear algebraic equations for this particular model...**

**Remark:** For this particular system of ODEs, explicit time integration methods work very well. Even a Forward Euler scheme is fine, but the 4-th order Runge-Kutta method is an excellent balance between high accuracy, high efficiency, and simplicity.

## Linearization at the differential equation level

Goal: linearize a PDE like

$$\frac{\partial u}{\partial t} = \nabla \cdot (\alpha(u) \nabla u) + f(u)$$

## PDE problem

$$\begin{aligned}\frac{\partial u}{\partial t} &= \nabla \cdot (\alpha(u) \nabla u) + f(u), & \mathbf{x} \in \Omega, \ t \in (0, T] \\ -\alpha(u) \frac{\partial u}{\partial n} &= g, & \mathbf{x} \in \partial\Omega_N, \ t \in (0, T] \\ u &= u_0, & \mathbf{x} \in \partial\Omega_D, \ t \in (0, T]\end{aligned}$$

## Explicit time integration

Explicit time integration methods remove the nonlinearity

Forward Euler method:

$$[D_t^+ u = \nabla \cdot (\alpha(u) \nabla u) + f(u)]^n$$

$$\frac{u^{n+1} - u^n}{\Delta t} = \nabla \cdot (\alpha(u^n) \nabla u^n) + f(u^n)$$

This is a *linear equation* in the unknown  $u^{n+1}(\mathbf{x})$ , with solution

$$u^{n+1} = u^n + \Delta t \nabla \cdot (\alpha(u^n) \nabla u^n) + \Delta t f(u^n)$$

Disadvantage:  $\Delta t \leq (\max \alpha)^{-1}(\Delta x^2 + \Delta y^2 + \Delta z^2)$

## Backward Euler scheme

Backward Euler scheme:

$$[D_t^- u = \nabla \cdot (\alpha(u) \nabla u) + f(u)]^n$$

Written out:

$$\frac{u^n - u^{n-1}}{\Delta t} = \nabla \cdot (\alpha(u^n) \nabla u^n) + f(u^n)$$

This is a nonlinear, stationary PDE for the unknown function  $u^n(\mathbf{x})$

## Picard iteration for Backward Euler scheme

We have

$$\frac{u^n - u^{n-1}}{\Delta t} = \nabla \cdot (\alpha(u^n) \nabla u^n) + f(u^n)$$

Picard iteration:

$$\frac{u^{n,k+1} - u^{n-1}}{\Delta t} = \nabla \cdot (\alpha(u^{n,k}) \nabla u^{n,k+1}) + f(u^{n,k})$$

Start iteration with  $u^{n,0} = u^{n-1}$

### Picard iteration with alternative notation

$$\frac{u^{n,k+1} - u^{n-1}}{\Delta t} = \nabla \cdot (\alpha(u^{n,k}) \nabla u^{n,k+1}) + f(u^{n,k})$$

Rewrite with a simplified, implementation-friendly notation:

- $u$  means the unknown  $u^{n,k+1}$  to solve for
- $u^-$  means the most recent approximation to  $u$
- $u^{(1)}$  means  $u^{n-1}$  ( $u^{(\ell)}$  means  $u^{n-\ell}$ )

$$\frac{u - u^{(1)}}{\Delta t} = \nabla \cdot (\alpha(u^-) \nabla u) + f(u^-)$$

Start iteration with  $u^- = u^{(1)}$ ; update with  $u^-$  to  $u$ .

### Backward Euler scheme and Newton's method

Normally, Newton's method is defined for systems of *algebraic equations*, but the idea of the method can be applied at the PDE level too!

Let  $u^{n,k}$  be an approximation to the unknown  $u^n$ . We seek a better approximation

$$u^n = u^{n,k} + \delta u$$

- Insert  $u^n = u^{n,k} + \delta u$  in the PDE
- Taylor expand the nonlinearities and keep only terms that are linear in  $\delta u$

Result: linear PDE for the *approximate* correction  $\delta u$

### Calculation details of Newton's method at the PDE level

Insert  $u^{n,k} + \delta u$  for  $u^n$  in PDE:

$$\frac{u^{n,k} + \delta u - u^{n-1}}{\Delta t} = \nabla \cdot (\alpha(u^{n,k} + \delta u) \nabla (u^{n,k} + \delta u)) + f(u^{n,k} + \delta u)$$

Taylor expand  $\alpha(u^{n,k} + \delta u)$  and  $f(u^{n,k} + \delta u)$ :

$$\begin{aligned} \alpha(u^{n,k} + \delta u) &= \alpha(u^{n,k}) + \frac{d\alpha}{du}(u^{n,k})\delta u + \mathcal{O}(\delta u^2) \approx \alpha(u^{n,k}) + \alpha'(u^{n,k})\delta u \\ f(u^{n,k} + \delta u) &= f(u^{n,k}) + \frac{df}{du}(u^{n,k})\delta u + \mathcal{O}(\delta u^2) \approx f(u^{n,k}) + f'(u^{n,k})\delta u \end{aligned}$$

## Calculation details of Newton's method at the PDE level

Inserting linear approximations of  $\alpha$  and  $f$ :

$$\begin{aligned} \frac{u^{n,k} + \delta u - u^{n-1}}{\Delta t} &= \nabla \cdot (\alpha(u^{n,k}) \nabla u^{n,k}) + f(u^{n,k}) + \\ &\quad \nabla \cdot (\alpha(u^{n,k}) \nabla \delta u) + \nabla \cdot (\alpha'(u^{n,k}) \delta u \nabla u^{n,k}) + \\ &\quad \nabla \cdot (\alpha'(u^{n,k}) \underbrace{\delta u \nabla \delta u}_{\text{dropped}}) + f'(u^{n,k}) \delta u \end{aligned}$$

Note:  $\alpha'(u^{n,k}) \delta u \nabla \delta u$  is  $\mathcal{O}(\delta u^2)$  and therefore omitted.

## Result of Newton's method at the PDE level

$$\delta F(\delta u; u^{n,k}) = -F(u^{n,k})$$

with

$$\begin{aligned} F(u^{n,k}) &= \frac{u^{n,k} - u^{n-1}}{\Delta t} - \nabla \cdot (\alpha(u^{n,k}) \nabla u^{n,k}) + f(u^{n,k}) \\ \delta F(\delta u; u^{n,k}) &= -\frac{1}{\Delta t} \delta u + \nabla \cdot (\alpha(u^{n,k}) \nabla \delta u) + \\ &\quad \nabla \cdot (\alpha'(u^{n,k}) \delta u \nabla u^{n,k}) + f'(u^{n,k}) \delta u \end{aligned}$$

Note:

- $\delta F$  is linear in  $\delta u$
- $F$  contains only known terms

## Similarity with Picard iteration

Rewrite the PDE for  $\delta u$  using  $u^{n,k} + \delta u = u^{n,k+1}$ :

$$\begin{aligned} \frac{u^{n,k+1} - u^{n-1}}{\Delta t} &= \nabla \cdot (\alpha(u^{n,k}) \nabla u^{n,k+1}) + f(u^{n,k}) \\ &\quad + \nabla \cdot (\alpha'(u^{n,k}) \delta u \nabla u^{n,k}) + f'(u^{n,k}) \delta u \end{aligned}$$

Note:

- The first line is the same PDE as arise in the Picard iteration
- The remaining terms arise from the differentiations in Newton's method

## Using new notation for implementation

- $u$  for  $u^n$
- $u^-$  for  $u^{n,k}$
- $u^{(1)}$  for  $u^{n-1}$

$$\delta F(\delta u; u^-) = -F(u^-) \quad (\text{PDE})$$

$$\begin{aligned} F(u^-) &= \frac{u^- - u^{(1)}}{\Delta t} - \nabla \cdot (\alpha(u^-) \nabla u^-) + f(u^-) \\ \delta F(\delta u; u^-) &= -\frac{1}{\Delta t} \delta u + \nabla \cdot (\alpha(u^-) \nabla \delta u) + \\ &\quad \nabla \cdot (\alpha'(u^-) \delta u \nabla u^-) + f'(u^-) \delta u \end{aligned}$$

## Combined Picard and Newton formulation

$$\begin{aligned} \frac{u - u^{(1)}}{\Delta t} &= \nabla \cdot (\alpha(u^-) \nabla u) + f(u^-) + \\ &\quad \gamma (\nabla \cdot (\alpha'(u^-) (u - u^-) \nabla u^-) + f'(u^-) (u - u^-)) \end{aligned}$$

Observe:

- $\gamma = 0$ : Picard iteration
- $\gamma = 1$ : Newton's method

Why is this formulation convenient? Easy to switch (start with Picard, use Newton close to solution)

## Crank-Nicolson discretization

Crank-Nicolson discretization applies a centered difference at  $t_{n+\frac{1}{2}}$ :

$$[D_t u = \nabla \cdot (\alpha(u) \nabla u) + f(u)]^{n+\frac{1}{2}}.$$

Many choices of formulating an arithmetic means:

$$\begin{aligned} [f(u)]^{n+\frac{1}{2}} &\approx f\left(\frac{1}{2}(u^n + u^{n+1})\right) = [f(\bar{u}^t)]^{n+\frac{1}{2}} \\ [f(u)]^{n+\frac{1}{2}} &\approx \frac{1}{2}(f(u^n) + f(u^{n+1})) = [\overline{f(u)}^t]^{n+\frac{1}{2}} \\ [\alpha(u) \nabla u]^{n+\frac{1}{2}} &\approx \alpha\left(\frac{1}{2}(u^n + u^{n+1})\right) \nabla\left(\frac{1}{2}(u^n + u^{n+1})\right) = \alpha(\bar{u}^t) \nabla \bar{u}^t]^{n+\frac{1}{2}} \\ [\alpha(u) \nabla u]^{n+\frac{1}{2}} &\approx \frac{1}{2}(\alpha(u^n) + \alpha(u^{n+1})) \nabla\left(\frac{1}{2}(u^n + u^{n+1})\right) = [\overline{\alpha(u)}^t \nabla \bar{u}^t]^{n+\frac{1}{2}} \\ [\alpha(u) \nabla u]^{n+\frac{1}{2}} &\approx \frac{1}{2}(\alpha(u^n) \nabla u^n + \alpha(u^{n+1}) \nabla u^{n+1}) = [\overline{\alpha(u) \nabla u}^t]^{n+\frac{1}{2}} \end{aligned}$$

### Arithmetic means: which variant is best?

Is there any differences in accuracy between

1. two factors of arithmetic means
2. the arithmetic mean of a product

More precisely,

$$\begin{aligned}[PQ]^{n+\frac{1}{2}} &= P^{n+\frac{1}{2}}Q^{n+\frac{1}{2}} \approx \frac{1}{2}(P^n + P^{n+1})\frac{1}{2}(Q^n + Q^{n+1}) \\ [PQ]^{n+\frac{1}{2}} &\approx \frac{1}{2}(P^nQ^n + P^{n+1}Q^{n+1})\end{aligned}$$

It can be shown (by Taylor series around  $t_{n+\frac{1}{2}}$ ) that both approximations are  $\mathcal{O}(\Delta t^2)$

### Solution of nonlinear equations in the Crank-Nicolson scheme

No big difference from the Backward Euler case, just more terms:

- Identify the  $F(u) = 0$  for the unknown  $u^{n+1}$
- Apply Picard iteration or Newton's method to the PDE
- Identify the sequence of linearized PDEs and iterate

### Discretization of 1D stationary nonlinear differential equations

Differential equation:

$$-(\alpha(u)u')' + au = f(u), \quad x \in (0, L)$$

Boundary conditions:

$$\alpha(u(0))u'(0) = C, \quad u(L) = D$$

### Relevance of this stationary 1D problem

1. As stationary limit of a diffusion PDE

$$u_t = (\alpha(u)u_x)_x + au + f(u)$$

$$(u_t \rightarrow 0)$$



2. The time-discrete problem at each time level arising from a Backward Euler scheme for a diffusion PDE

$$u_t = (\alpha(u)u_x)_x + f(u)$$

( $au$  comes from  $u_t$ ,  $a \sim 1/\Delta t$ ,  $f(u) := f(u) - u^{n-1}/\Delta t$ )

### Finite difference discretizations

The nonlinear term  $(\alpha(u)u')'$  behaves just as a variable coefficient term  $(\alpha(x)u')'$  wrt discretization:

$$[-D_x \alpha D_x u + au = f]_i$$

Written out at internal points:

$$-\frac{1}{\Delta x^2} \left( \alpha_{i+\frac{1}{2}}(u_{i+1} - u_i) - \alpha_{i-\frac{1}{2}}(u_i - u_{i-1}) \right) + au_i = f(u_i)$$

$\alpha_{i+\frac{1}{2}}$ : two choices

$$\alpha_{i+\frac{1}{2}} \approx \alpha\left(\frac{1}{2}(u_i + u_{i+1})\right) = [\alpha(\bar{u}^x)]^{i+\frac{1}{2}}$$

$$\alpha_{i+\frac{1}{2}} \approx \frac{1}{2}(\alpha(u_i) + \alpha(u_{i+1})) = [\overline{\alpha(u)}^x]^{i+\frac{1}{2}}$$

### Finite difference scheme

$$\alpha_{i+\frac{1}{2}} \approx \frac{1}{2}(\alpha(u_i) + \alpha(u_{i+1})) = [\overline{\alpha(u)}^x]^{i+\frac{1}{2}}$$

results in

$$[-D_x \bar{\alpha}^x D_x u + au = f]_i.$$

$$-\frac{1}{2\Delta x^2} ((\alpha(u_i) + \alpha(u_{i+1}))(u_{i+1} - u_i) - (\alpha(u_{i-1}) + \alpha(u_i))(u_i - u_{i-1})) + au_i = f(u_i)$$

### Boundary conditions

- At  $i = N_x$ :  $u_i = 0$ .
- At  $i = 0$ :  $\alpha(u)u' = C$

$$[\alpha(u)D_{2x}u = C]_0$$

$$\alpha(u_0)\frac{u_1 - u_{-1}}{2\Delta x} = C$$

The fictitious value  $u_{-1}$  can, as usual, be eliminated with the aid of the scheme at  $i = 0$

## The structure of the equation system

Structure of nonlinear algebraic equations:

$$A(u)u = b(u)$$

$$\begin{aligned} A_{i,i} &= \frac{1}{2\Delta x^2}(-\alpha(u_{i-1}) + 2\alpha(u_i) - \alpha(u_{i+1})) + a \\ A_{i,i-1} &= -\frac{1}{2\Delta x^2}(\alpha(u_{i-1}) + \alpha(u_i)) \\ A_{i,i+1} &= -\frac{1}{2\Delta x^2}(\alpha(u_i) + \alpha(u_{i+1})) \\ b_i &= f(u_i) \end{aligned}$$

Note:

- $A(u)$  is tridiagonal:  $A_{i,j} = 0$  for  $j > i + 1$  and  $j < i - 1$ .
- The  $i = 0$  and  $i = N_x$  equation must incorporate boundary conditions

## The equation for the Neumann boundary condition

$i = 0$ : insert

$$u_{-1} = u_1 - \frac{2\Delta x}{\alpha(u_0)}$$

in  $A_{0,0}$ . The expression for  $A_{i,i+1}$  applies for  $i = 0$ , and  $A_{i,i-1}$  for  $i = 0$  does not enter the system.

## The equation for the Dirichlet boundary condition

1. For  $i = N_x$  we can use the Dirichlet condition as a separate equation

$$u_i = D, \quad i = N_x$$

2. Alternative: for  $i = N_x$  we can substitute  $u_{N_x}$  in  $A_{i,i}$  by  $D$  and have  $N_x - 1$  equations.

## Nonlinear equations for a mesh with two cells

Let's do all the details! We omit a separate equation for the  $u = D$  condition at  $i = N_x$ . Starting point is then

$$\begin{aligned} A_{0,-1}u_{-1} + A_{0,0}u_0 + A_{0,1}u_1 &= b_0 \\ A_{1,0}u_0 + A_{1,1}u_1 + A_{1,2}u_2 &= b_1 \end{aligned}$$

Must

- write out the  $A_{i,j}$  and  $b_i$  expressions
- replace  $u_{-1}$  from the Neumann condition
- use  $D$  for  $u_2$  (boundary condition)

### Picard iteration

Use the most recently computed value  $u^-$  of  $u$  in  $A(u)$  and  $b(u)$ :

$$A(u^-)u = b(u^-)$$

$$\begin{aligned} \frac{1}{2\Delta x^2} & \left( -(\alpha(u_{-1}^-) + 2\alpha(u_0^- + \alpha(u_1^-))u_1 + \right. \\ & \left. (\alpha(u_{-1}^-) + 2\alpha(u_0^-) + \alpha(u_1^-))u_0 + au_0 \right) \\ & = f(u_0^-) - \frac{1}{\alpha(u_0^-)\Delta x}(\alpha(u_{-1}^-) + \alpha(u_0^-))C, \end{aligned}$$

$$\begin{aligned} \frac{1}{2\Delta x^2} & \left( -(\alpha(u_0^-) + \alpha(u_1^-))u_0 + \right. \\ & \left. (\alpha(u_0^-) + 2\alpha(u_1^-) + \alpha(D))u_1 + au_1 \right) \\ & = f(u_1^-) + \frac{1}{2\Delta x^2}(\alpha(u_1^-) + \alpha(D))D. \end{aligned}$$

### The matrix systems to be solved

Eliminating the Dirichlet condition at  $i = N_x$ :

$$\begin{pmatrix} B_{0,0} & B_{0,1} \\ B_{1,0} & B_{1,1} \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \end{pmatrix} = \begin{pmatrix} d_0 \\ d_1 \end{pmatrix}$$

Including the equation for  $i = N_x$ :

$$\begin{pmatrix} B_{0,0} & B_{0,1} & 0 \\ B_{1,0} & B_{1,1} & B_{1,2} \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} d_0 \\ d_1 \\ D \end{pmatrix}$$

### Newton's method; Jacobian (1)

Nonlinear eq.no  $i$  has the structure

$$\begin{aligned} F_i = & A_{i,i-1}(u_{i-1}, u_i)u_{i-1} + A_{i,i}(u_{i-1}, u_i, u_{i+1})u_i + \\ & A_{i,i+1}(u_i, u_{i+1})u_{i+1} - b_i(u_i) \end{aligned}$$

Need Jacobian, i.e., need to differentiate  $F(u) = A(u)u - b(u)$  wrt  $u$ . Example:

$$\begin{aligned}
\frac{\partial}{\partial u_i}(A_{i,i}(u_{i-1}, u_i, u_{i+1})u_i) &= \frac{\partial A_{i,i}}{\partial u_i}u_i + A_{i,i} \frac{\partial u_i}{\partial u_i} \\
&= \frac{\partial}{\partial u_i} \left( \frac{1}{2\Delta x^2} (-\alpha(u_{i-1}) + 2\alpha(u_i) - \alpha(u_{i+1})) + a \right) u_i + \\
&\quad \frac{1}{2\Delta x^2} (-\alpha(u_{i-1}) + 2\alpha(u_i) - \alpha(u_{i+1})) + a \\
&= \frac{1}{2\Delta x^2} (2\alpha'(u_i)u_i - \alpha(u_{i-1}) + 2\alpha(u_i) - \alpha(u_{i+1})) + a
\end{aligned}$$

### Newton's method; Jacobian (2)

The complete Jacobian becomes (make sure you get this!)

$$\begin{aligned}
J_{i,i} &= \frac{\partial F_i}{\partial u_i} = \frac{\partial A_{i,i-1}}{\partial u_i}u_{i-1} + \frac{\partial A_{i,i}}{\partial u_i}u_i + A_{i,i} + \frac{\partial A_{i,i+1}}{\partial u_i}u_{i+1} - \frac{\partial b_i}{\partial u_i} \\
&= \frac{1}{2\Delta x^2} (-\alpha'(u_i)u_{i-1} + 2\alpha'(u_i)u_i - \alpha(u_{i-1}) + 2\alpha(u_i) - \alpha(u_{i+1})) + \\
&\quad a - \frac{1}{2\Delta x^2} \alpha'(u_i)u_{i+1} - b'(u_i) \\
J_{i,i-1} &= \frac{\partial F_i}{\partial u_{i-1}} = \frac{\partial A_{i,i-1}}{\partial u_{i-1}}u_{i-1} + A_{i-1,i} + \frac{\partial A_{i,i}}{\partial u_{i-1}}u_i - \frac{\partial b_i}{\partial u_{i-1}} \\
&= \frac{1}{2\Delta x^2} (-\alpha'(u_{i-1})u_{i-1} - (\alpha(u_{i-1}) + \alpha(u_i)) + \alpha'(u_{i-1})u_i) \\
J_{i,i+1} &= \frac{\partial A_{i,i+1}}{\partial u_{i+1}}u_{i+1} + A_{i+1,i} + \frac{\partial A_{i,i}}{\partial u_{i+1}}u_i - \frac{\partial b_i}{\partial u_{i+1}} \\
&= \frac{1}{2\Delta x^2} (-\alpha'(u_{i+1})u_{i+1} - (\alpha(u_i) + \alpha(u_{i+1})) + \alpha'(u_{i+1})u_i)
\end{aligned}$$

### Newton's method; nonlinear equations at the end points

$$\begin{aligned}
F_i &= -\frac{1}{2\Delta x^2} ((\alpha(u_i) + \alpha(u_{i+1}))(u_{i+1} - u_i) - (\alpha(u_{i-1}) + \alpha(u_i)) \times \\
&\quad (u_i - u_{i-1})) + au_i - f(u_i) = 0
\end{aligned}$$

At  $i = 0$ , replace  $u_{-1}$  by formula from Neumann condition.

1. Exclude Dirichlet condition as separate equation: replace  $u_i$ ,  $i = N_x$ , by  $D$  in  $F_i$ ,  $i = N_x - 1$
2. Include Dirichlet condition as separate equation:

$$F_{N_x}(u_0, \dots, u_{N_x}) = u_{N_x} - D = 0.$$

Note: The size of the Jacobian depends on 1 or 2.

## Galerkin-type discretizations

- $V$ : function space with basis functions  $\psi_i(x)$ ,  $i \in \mathcal{I}_s$
- Dirichlet condition at  $x = L$ :  $\psi_i(L) = 0$ ,  $i \in \mathcal{I}_s$  ( $v(L) = 0 \forall v \in V$ )
- $u = D + \sum_{j \in \mathcal{I}_s} c_j \psi_j$

Galerkin's method for  $-(\alpha(u)u')' + au = f(u)$ :

$$\int_0^L \alpha(u)u'v' dx + \int_0^L auv dx = \int_0^L f(u)v dx + [\alpha(u)u'v]_0^L, \quad \forall v \in V$$

Insert Neumann condition:

$$[\alpha(u)u'v]_0^L = \alpha(u(L))u'(L)v(L) - \alpha(u(0))u'(0)v(0) = -Cv(0)$$

## The nonlinear algebraic equations

Find  $u \in V$  such that

$$\int_0^L \alpha(u)u'v' dx + \int_0^L auv dx = \int_0^L f(u)v dx - Cv(0), \quad \forall v \in V$$

$\forall v \in V \Rightarrow \forall i \in \mathcal{I}_s, v = \psi_i$ . Inserting  $u = D + \sum_j c_j \psi_j$  and sorting terms:

$$\sum_j \left( \int_0^L \alpha(D + \sum_k c_k \psi_k) \psi_j' \psi_i' dx \right) c_j = \int_0^L f(D + \sum_k c_k \psi_k) \psi_i dx - C\psi_i(0)$$

This is a *nonlinear algebraic system*

**Fundamental integration problem: how to deal with  $\int f(\sum_k c_k \psi_k) \psi_i dx$  for unknown  $c_k$ ?**

- We do not know  $c_k$  in  $\int_0^L f(\sum_k c_k \psi_k) \psi_i dx$  and  $\int_0^L \alpha(\sum_k c_k \psi_k) \psi_i' \psi_j' dx$
- Solution: numerical integration with approximations to  $c_k$ , as in  $\int_0^L f(u^-) \psi_i dx$

Next: want to do *symbolic integration* of such terms to see the structure of nonlinear finite element equations (to compare with finite differences)

### We choose $\psi_i$ as finite element basis functions

$$\psi_i = \varphi_{\nu(i)}, \quad i \in \mathcal{I}_s$$

Degree of freedom number  $\nu(i)$  in the mesh corresponds to unknown number  $i$  ( $c_i$ ).

Model problem:  $\nu(i) = i$ ,  $\mathcal{I}_s = \{0, \dots, N_n - 2\}$  (last node excluded)

$$u = D + \sum_{j \in \mathcal{I}_s} c_j \varphi_{\nu(j)}$$

or with  $\varphi_i$  in the boundary function:

$$u = D\varphi_{N_n-1} + \sum_{j \in \mathcal{I}_s} c_j \varphi_j$$

### The group finite element method

Since  $u$  is represented by  $\sum_j \varphi_j u(x_j)$ , we may use the same approximation for  $f(u)$ :

$$f(u) \approx \sum_j f(x_j) \varphi_j$$

$f(x_j)$ : value of  $f$  at node  $j$ . With  $u_j$  as  $u(x_j)$ , we can write

$$f(u) \approx \sum_j f(u_j) \varphi_j$$

This approximation is known as the *group finite element method* or the *product approximation* technique. The index  $j$  runs over all node numbers in the mesh.

### What is the point with the group finite element method?

1. Complicated nonlinear expressions can be simplified to increase the efficiency of numerical computations.
2. One can derive *symbolic forms* of the difference equations arising from the finite element method in nonlinear problems. The symbolic form is useful for comparing finite element and finite difference equations of nonlinear differential equation problems.

## Simplified problem for symbolic calculations

Simple nonlinear problem:  $-u'' = u^2$ ,  $u'(0) = 1$ ,  $u'(L) = 0$ .

$$\int_0^L u' v' dx = \int_0^L u^2 v dx - v(0), \quad \forall v \in V$$

Now,

- Focus on  $\int u^2 v dx$
- Set  $c_j = u(x_j) = u_j$   
(to mimic finite difference interpretation of  $u_j$ )
- That is,  $u = \sum_j u_j \varphi_j$

## Integrating very simple nonlinear functions results in complicated expressions in the finite element method

Consider  $\int u^2 v dx$  with  $u = \sum_k u_k \varphi_k$  and  $v = \varphi_i$ :

$$\int_0^L (\sum_k u_k \varphi_k)^2 \varphi_i dx$$

Tedious exact evaluation on uniform P1 elements:

$$\frac{h}{12} (u_{i-1}^2 + 2u_i(u_{i-1} + u_{i+1}) + 6u_i^2 + u_{i+1}^2)$$

Finite difference counterpart:  $u_i^2$  (!)

## Application of the group finite element method

$$\int_0^L f(u) \varphi_i dx \approx \int_0^L (\sum_j \varphi_j f(u_j)) \varphi_i dx = \sum_j (\underbrace{\int_0^L \varphi_i \varphi_j dx}_{\text{mass matrix } M_{i,j}}) f(u_j)$$

Corresponding part of difference equation for P1 elements:

$$\frac{h}{6} (f(u_{i-1}) + 4f(u_i) + f(u_{i+1}))$$

Rewrite as “finite difference form plus something”:

$$\frac{h}{6} (f(u_{i-1}) + 4f(u_i) + f(u_{i+1})) = h[f(\textcolor{red}{u}) - \frac{h^2}{6} D_x D_x f(u)]_i$$

This is like the finite difference discretization of  $-u'' = f(u) - \frac{h^2}{6} f''(u)$

## Lumping the mass matrix gives finite difference form

Lumped mass matrix (integrate at the nodes):  $M$  becomes diagonal and the finite element and difference method's treatment of  $f(u)$  becomes identical!

## Alternative: evaluation of finite element terms at nodes gives great simplifications

Idea: integrate  $\int f(u)v \, dx$  numerically with a rule that samples  $f(u)v$  at the nodes only. This involves great simplifications, since

$$\sum_k u_k \varphi_k(x_\ell) = u_\ell$$

and

$$f \varphi_i(x_\ell) = f\left(\sum_k u_k \underbrace{\varphi_k(x_\ell)}_{\delta_{k\ell}}\right) \underbrace{\varphi_i(x_\ell)}_{\delta_{i\ell}} = f(u_\ell) \delta_{i\ell} \quad \neq 0 \text{ only for } f(u_i)$$

$$(\delta_{ij} = 0 \text{ if } i \neq j \text{ and } \delta_{ij} = 1 \text{ if } i = j)$$

## Numerical integration of nonlinear terms

Trapezoidal rule with the nodes only gives the finite difference form of  $[f(u)]_i$ :

$$\int_0^L f\left(\sum_k u_k \varphi_k(x)\right) \varphi_i(x) \, dx \approx h \sum_{\ell=0}^{N_n-1} f(u_\ell) \delta_{i\ell} - \mathcal{C} = h \mathbf{f}(\mathbf{u}_i)$$

( $\mathcal{C}$ : boundary adjustment of rule,  $i = 0, N_n - 1$ )

## Finite elements for a variable coefficient Laplace term

Consider the term  $(\alpha u')'$ , with the group finite element method:  $\alpha(u) \approx \sum_k \alpha(u_k) \varphi_k$ , and the variational counterpart

$$\int_0^L \alpha\left(\sum_k c_k \varphi_k\right) \varphi'_i \varphi'_j \, dx \approx \sum_k \left(\int_0^L \varphi_k \varphi'_i \varphi'_j \, dx\right) \alpha(u_k) = \dots$$

Further calculations (see text) lead to

$$-\frac{1}{h} \left( \frac{1}{2} (\alpha(u_i) + \alpha(u_{i+1})) (u_{i+1} - u_i) - \frac{1}{2} (\alpha(u_{i-1}) + \alpha(u_i)) (u_i - u_{i-1}) \right)$$

= standard finite difference discretization of  $-(\alpha(u)u)'$  with an arithmetic mean of  $\alpha(u)$



## Numerical integration at the nodes

Instead of the group finite element method and exact integration, use Trapezoidal rule in the nodes for  $\int_0^L \alpha(\sum_k u_k \varphi_k) \varphi'_i \varphi'_j dx$ .

Work at the cell level (most convenient with discontinuous  $\varphi'_i$ ):

$$\begin{aligned}
 \int_{-1}^1 \alpha(\sum_t \tilde{u}_t \tilde{\varphi}_t) \tilde{\varphi}'_r \tilde{\varphi}'_s \frac{h}{2} dX &= \int_{-1}^1 \alpha(\sum_{t=0}^1 \tilde{u}_t \tilde{\varphi}_t) \frac{2}{h} \frac{d\tilde{\varphi}_r}{dX} \frac{2}{h} \frac{d\tilde{\varphi}_s}{dX} \frac{h}{2} dX \\
 &= \frac{1}{2h} (-1)^r (-1)^s \int_{-1}^1 \alpha(\sum_{t=0}^1 u_t \tilde{\varphi}_t(X)) dX \\
 &\approx \frac{1}{2h} (-1)^r (-1)^s \alpha(\sum_{t=0}^1 \tilde{\varphi}_t(-1) \tilde{u}_t) + \alpha(\sum_{t=0}^1 \tilde{\varphi}_t(1) \tilde{u}_t) \\
 &= \frac{1}{2h} (-1)^r (-1)^s (\alpha(\tilde{u}_0) + \alpha(\tilde{u}^{(1)}))
 \end{aligned}$$

## Summary of finite element vs finite difference nonlinear algebraic equations

$$-(\alpha(u)u')' + au = f(u)$$

Uniform P1 finite elements:

- Group finite element or Trapezoidal integration at nodes:  
 $-(\alpha(u)u')'$  becomes  $-h[D_x \alpha(u)]_i^x D_x u|_i$
- $f(u)$  becomes  $hf(u_i)$  with Trapezoidal integration  
or the “mass matrix” representation  $h[f(u) - \frac{h}{6} D_x D_x f(u)]_i$  if group finite elements
- $au$  leads to the “mass matrix” form  $ah[u - \frac{h}{6} D_x D_x u]_i$

## Real computations utilize accurate numerical integration

- Previous group finite element or Trapezoidal integration examples had one aim: derive symbolic expressions for finite element equations
- Real world computations apply numerical integration
- How to define Picard iteration and Newton’s method from a variational form with numerical integration in real world computations?

### Picard iteration defined from the variational form

$$-(\alpha(u)u')' + au = f(u), \quad x \in (0, L), \quad \alpha(u(0))u'(0) = C, \quad u(L) = D$$

Variational form ( $v = \psi_i$ ):

$$F_i = \int_0^L \alpha(u)u'\psi'_i \, dx + \int_0^L au\psi_i \, dx - \int_0^L f(u)\psi_i \, dx + C\psi_i(0) = 0$$

Picard iteration: use “old value”  $u^-$  in  $\alpha(u)$  and  $f(u)$  and integrate numerically:

$$F_i = \int_0^L (\alpha(u^-)u'\psi'_i + au\psi_i) \, dx - \int_0^L f(u^-)\psi_i \, dx + C\psi_i(0)$$

### The linear system in Picard iteration

$$F_i = \int_0^L (\alpha(u^-)u'\psi'_i + au\psi_i) \, dx - \int_0^L f(u^-)\psi_i \, dx + C\psi_i(0)$$

This is a linear problem  $a(u, v) = L(v)$  with bilinear and linear forms

$$a(u, v) = \int_0^L (\alpha(u^-)u'v' + auv) \, dx, \quad L(v) = \int_0^L f(u^-)v \, dx - Cv(0)$$

The linear system now is computed the standard way.

### The equations in Newton's method

$$F_i = \int_0^L (\alpha(u)u'\psi'_i + au\psi_i - f(u)\psi_i) \, dx + C\psi_i(0) = 0, \quad i \in \mathcal{I}_s$$

Easy to evaluate right-hand side  $-F_i(u^-)$  by numerical integration:

$$F_i = \int_0^L (\alpha(u^-)u'\psi'_i + au\psi_i - f(u^-)\psi_i) \, dx + C\psi_i(0) = 0$$

(just known functions)

### Useful formulas for computing the Jacobian

$$\begin{aligned} \frac{\partial u}{\partial c_j} &= \frac{\partial}{\partial c_j} \sum_k c_k \psi_k = \psi_j \\ \frac{\partial u'}{\partial c_j} &= \frac{\partial}{\partial c_j} \sum_k c_k \psi'_k = \psi'_j \end{aligned}$$

## Computing the Jacobian

$$\begin{aligned}
J_{i,j} &= \frac{\partial F_i}{\partial c_j} = \int_0^L \frac{\partial}{\partial c_j} (\alpha(u)u'\psi'_i + au\psi_i - f(u)\psi_i) dx \\
&= \int_0^L ((\alpha'(u)\frac{\partial u}{\partial c_j}u' + \alpha(u)\frac{\partial u'}{\partial c_j})\psi'_i + a\frac{\partial u}{\partial c_j}\psi_i - f'(u)\frac{\partial u}{\partial c_j}\psi_i) dx \\
&= \int_0^L ((\alpha'(u)\psi_ju' + \alpha(u)\psi'_j\psi'_i + a\psi_j\psi_i - f'(u)\psi_j\psi_i) dx \\
&= \int_0^L (\alpha'(u)u'\psi'_i\psi_j + \alpha(u)\psi'_i\psi'_j + (a - f(u))\psi_i\psi_j) dx
\end{aligned}$$

Use  $\alpha'(u^-)$ ,  $\alpha(u^-)$ ,  $f'(u^-)$ ,  $f(u^-)$  and integrate expressions numerically (only known functions)

## Computations in a reference cell $[-1, 1]$

$$\begin{aligned}
\tilde{F}_r^{(e)} &= \int_{-1}^1 (\alpha(\tilde{u}^-)\tilde{u}^{-'}\tilde{\varphi}'_r + (a - f(\tilde{u}^-))\tilde{\varphi}_r) \det J dX - C\tilde{\varphi}_r(0) \\
\tilde{J}_{r,s}^{(e)} &= \int_{-1}^1 (\alpha'(\tilde{u}^-)\tilde{u}^{-'}\tilde{\varphi}'_r\tilde{\varphi}'_s + \alpha(\tilde{u}^-)\tilde{\varphi}'_r\tilde{\varphi}'_s + (a - f(\tilde{u}^-))\tilde{\varphi}_r\tilde{\varphi}_s) \det J dX
\end{aligned}$$

$r, s \in I_d$  (local degrees of freedom)

## How to handle Dirichlet conditions in Newton's method

- Newton's method solves  $J(u^-)\delta u = -F(u^-)$
- $\delta u$  is a *correction* to  $u^-$
- If  $u(x_i)$  has Dirichlet condition  $D$ , set  $u_i^- = D$  in prior to the first iteration
- Set  $\delta u_i = 0$  (no change for Dirichlet conditions)

## Multi-dimensional PDE problems

$$u_t = \nabla \cdot (\alpha(u)\nabla u) + f(u)$$

## Backward Euler and variational form

$$u_t = \nabla \cdot (\alpha(u)\nabla u) + f(u)$$

Backward Euler time discretization:

$$u^n - \Delta t \nabla \cdot (\alpha(u^n)\nabla u^n) + f(u^n) = u^{n-1}$$

Alternative notation ( $u$  for  $u^n$ ,  $u^{(1)}$  for  $u^{n-1}$ ):

$$u - \Delta t \nabla \cdot (\alpha(u) \nabla u) - \Delta t f(u) = u^{(1)}$$

Boundary conditions:  $\partial u / \partial n = 0$  for simplicity. Variational form:

$$\int_{\Omega} (uv + \Delta t \alpha(u) \nabla u \cdot \nabla v - \Delta t f(u)v - u^{(1)}v) \, dx = 0$$

### Nonlinear algebraic equations arising from the variational form

$$\int_{\Omega} (uv + \Delta t \alpha(u) \nabla u \cdot \nabla v - \Delta t f(u)v - u^{(1)}v) \, dx = 0$$

$$F_i = \int_{\Omega} (u\psi_i + \Delta t \alpha(u) \nabla u \cdot \nabla \psi_i - \Delta t f(u)\psi_i - u^{(1)}\psi_i) \, dx = 0$$

Picard iteration:

$$F_i \approx \hat{F}_i = \int_{\Omega} (u\psi_i + \Delta t \alpha(u^-) \nabla u \cdot \nabla \psi_i - \Delta t f(u^-)\psi_i - u^{(1)}\psi_i) \, dx = 0$$

This is a variable coefficient problem like  $au - \nabla \cdot \alpha(\mathbf{x}) \nabla u = f(\mathbf{x}, t)$  and results in a linear system

### A note on our notation and the different meanings of $u$ (1)

PDE problem:  $u(\mathbf{x}, t)$  is the exact solution of

$$u_t = \nabla \cdot (\alpha(u) \nabla u) + f(u)$$

Time discretization:  $u(\mathbf{x})$  is the exact solution of the time-discrete spatial equation

$$u - \Delta t \nabla \cdot (\alpha(u^n) \nabla u) - \Delta t f(u) = u^{(1)}$$

The same  $u(\mathbf{x})$  is the exact solution of the (continuous) variational form:

$$\int_{\Omega} (uv + \Delta t \alpha(u) \nabla u \cdot \nabla v - \Delta t f(u)v - u^{(1)}v) \, dx, \quad \forall v \in V$$

## A note on our notation and the different meanings of $u$ (2)

Or we may approximate  $u$ :  $u(\mathbf{x}) = \sum_j c_j \psi_j(\mathbf{x})$  and let this spatially discrete  $u$  enter the variational form,

$$\int_{\Omega} (uv + \Delta t \alpha(u) \nabla u \cdot \nabla v - \Delta t f(u) v - u^{(1)} v) \, dx, \quad \forall v \in V$$

Picard iteration:  $u(\mathbf{x})$  solves the *approximate* variational form

$$\int_{\Omega} (uv + \Delta t \alpha(u^-) \nabla u \cdot \nabla v - \Delta t f(u^-) v - u^{(1)} v) \, dx$$

Could introduce

- $u_e(\mathbf{x}, t)$  for the exact solution of the PDE problem
- $u_e(\mathbf{x})^n$  for the exact solution after time discretization
- $u^n(\mathbf{x})$  for the spatially discrete solution  $\sum_j c_j \psi_j$
- $u^{n,k}$  for approximation in Picard/Newton iteration no  $k$  to  $u^n(\mathbf{x})$

## Newton's method (1)

Need to evaluate  $F_i(u^-)$ :

$$F_i \approx \hat{F}_i = \int_{\Omega} (u^- \psi_i + \Delta t \alpha(u^-) \nabla u^- \cdot \nabla \psi_i - \Delta t f(u^-) \psi_i - u^{(1)} \psi_i) \, dx$$

To compute the Jacobian we need

$$\begin{aligned} \frac{\partial u}{\partial c_j} &= \sum_k \frac{\partial}{\partial c_j} c_k \psi_k = \psi_j \\ \frac{\partial \nabla u}{\partial c_j} &= \sum_k \frac{\partial}{\partial c_j} c_k \nabla \psi_k = \nabla \psi_j \end{aligned}$$

## Newton's method (2)

The Jacobian becomes

$$J_{i,j} = \frac{\partial F_i}{\partial c_j} = \int_{\Omega} (\psi_j \psi_i + \Delta t \alpha'(u) \psi_j \nabla u \cdot \nabla \psi_i + \Delta t \alpha(u) \nabla \psi_j \cdot \nabla \psi_i - \Delta t f'(u) \psi_j \psi_i) \, dx$$

Evaluation of  $J_{i,j}$  as the coefficient matrix in the Newton system  $J \delta u = -F$  means  $J(u^-)$ :

$$J_{i,j} = \int_{\Omega} (\psi_j \psi_i + \Delta t \alpha'(u^-) \psi_j \nabla u^- \cdot \nabla \psi_i + \Delta t \alpha(u^-) \nabla \psi_j \cdot \nabla \psi_i - \Delta t f'(u^-) \psi_j \psi_i) \, dx$$

## Non-homogeneous Neumann conditions

A natural physical flux condition:

$$-\alpha(u) \frac{\partial u}{\partial n} = g, \quad \mathbf{x} \in \partial\Omega_N$$

Integration by parts gives the boundary term

$$\int_{\partial\Omega_N} \alpha(u) \frac{\partial u}{\partial n} v \, ds$$

Inserting the nonlinear Neumann condition:

$$- \int_{\partial\Omega_N} g v \, ds$$

(no nonlinearity)

## Robin condition

Heat conduction problems often apply a kind of Newton's cooling law, also known as a Robin condition, at the boundary:

$$-\alpha(u) \frac{\partial u}{\partial n} = h(u)(u - T_s(t)), \quad \mathbf{x} \in \partial\Omega_R$$

Here:

- $h(u)$ : heat transfer coefficient between the body ( $\Omega$ ) and its surroundings
- $T_s$ : temperature of the surroundings

Inserting the condition in the boundary integral  $\int_{\partial\Omega_N} \alpha(u) \frac{\partial u}{\partial n} v \, ds$ :

$$\int_{\partial\Omega_R} h(u)(u - T_s(T)) v \, ds$$

Use  $h(u^-)(u - T_s)$  for Picard, differentiate for Newton

## Finite difference discretization in a 2D problem

$$u_t = \nabla \cdot (\alpha(u) \nabla u) + f(u)$$

Backward Euler in time, centered differences in space:

$$[D_t^- u = D_x \overline{\alpha(u)}^x D_x u + D_y \overline{\alpha(u)}^y D_y u + f(u)]_{i,j}^n$$

$$\begin{aligned} u_{i,j}^n - \frac{\Delta t}{h^2} & \left( \frac{1}{2} (\alpha(u_{i,j}^n) + \alpha(u_{i+1,j}^n)) (u_{i+1,j}^n - u_{i,j}^n) \right. \\ & - \frac{1}{2} (\alpha(u_{i-1,j}^n) + \alpha(u_{i,j}^n)) (u_{i,j}^n - u_{i-1,j}^n) \\ & + \frac{1}{2} (\alpha(u_{i,j}^n) + \alpha(u_{i,j+1}^n)) (u_{i,j+1}^n - u_{i,j}^n) \\ & \left. - \frac{1}{2} (\alpha(u_{i,j-1}^n) + \alpha(u_{i,j}^n)) (u_{i,j}^n - u_{i,j-1}^n) \right) - \Delta t f(u_{i,j}^n) = u_{i,j}^{n-1} \end{aligned}$$

Nonlinear algebraic system on the form  $A(u)u = b(u)$

## Picard iteration

- Use the most recently computed values  $u^-$  of  $u^n$  in  $\alpha$  and  $f$
- Or:  $A(u^-)u = b(u^-)$
- Like solving  $u_t = \nabla \cdot (\alpha(\mathbf{x}) \nabla u) + f(\mathbf{x}, t)$

Picard iteration in operator notation:

$$[D_t^- u = D_x \overline{\alpha(u^-)}^x D_x u + D_y \overline{\alpha(u^-)}^y D_y u + f(u^-)]_{i,j}^n$$

## Newton's method: the nonlinear algebraic equations

Define the nonlinear equations (use  $u$  for  $u^n$ ,  $u^{(1)}$  for  $u^{n-1}$ ):

$$\begin{aligned} F_{i,j} = u_{i,j} - \frac{\Delta t}{h^2} & \left( \frac{1}{2} (\alpha(u_{i,j}) + \alpha(u_{i+1,j})) (u_{i+1,j} - u_{i,j}) - \right. \\ & \frac{1}{2} (\alpha(u_{i-1,j}) + \alpha(u_{i,j})) (u_{i,j} - u_{i-1,j}) + \\ & \frac{1}{2} (\alpha(u_{i,j}) + \alpha(u_{i,j+1})) (u_{i,j+1} - u_{i,j}) - \\ & \left. \frac{1}{2} (\alpha(u_{i,j-1}) + \alpha(u_{i,j})) (u_{i,j} - u_{i,j-1}) \right) - \Delta t f(u_{i,j}) - u_{i,j}^{(1)} = 0 \end{aligned}$$

### Newton's method: the Jacobian and its sparsity

$$J_{i,j,r,s} = \frac{\partial F_{i,j}}{\partial u_{r,s}}$$

Newton system:

$$\sum_{r \in \mathcal{I}_x} \sum_{s \in \mathcal{I}_y} J_{i,j,r,s} \delta u_{r,s} = -F_{i,j}, \quad i \in \mathcal{I}_x, \quad j \in \mathcal{I}_y.$$

But  $F_{i,j}$  contains only  $u_{i\pm 1,j}$ ,  $u_{i,j\pm 1}$ , and  $u_{i,j}$ . We get nonzero contributions only for  $J_{i,j,i-1,j}$ ,  $J_{i,j,i+1,j}$ ,  $J_{i,j,i,j-1}$ ,  $J_{i,j,i,j+1}$ , and  $J_{i,j,i,j}$ . The Newton system collapses to

$$J_{i,j,r,s} \delta u_{r,s} = J_{i,j,i,j} \delta u_{i,j} + J_{i,j,i-1,j} \delta u_{i-1,j} + J_{i,j,i+1,j} \delta u_{i+1,j} + J_{i,j,i,j-1} \delta u_{i,j-1} + J_{i,j,i,j+1} \delta u_{i,j+1}$$

### Newton's method: details of the Jacobian

$$\begin{aligned} J_{i,j,i-1,j} &= \frac{\partial F_{i,j}}{\partial u_{i-1,j}} \\ &= \frac{\Delta t}{h^2} (\alpha'(u_{i-1,j})(u_{i,j} - u_{i-1,j}) + \alpha(u_{i-1,j})(-1)), \\ J_{i,j,i+1,j} &= \frac{\partial F_{i,j}}{\partial u_{i+1,j}} \\ &= \frac{\Delta t}{h^2} (-\alpha'(u_{i+1,j})(u_{i+1,j} - u_{i,j}) - \alpha(u_{i+1,j})), \\ J_{i,j,i,j-1} &= \frac{\partial F_{i,j}}{\partial u_{i,j-1}} \\ &= \frac{\Delta t}{h^2} (\alpha'(u_{i,j-1})(u_{i,j} - u_{i,j-1}) + \alpha(u_{i,j-1})(-1)), \\ J_{i,j,i,j+1} &= \frac{\partial F_{i,j}}{\partial u_{i,j+1}} \\ &= \frac{\Delta t}{h^2} (-\alpha'(u_{i,j+1})(u_{i,j+1} - u_{i,j}) - \alpha(u_{i,j+1})). \end{aligned}$$

**Good exercise at this point:**  $J_{i,j,i,j}$

Compute  $J_{i,j,i,j}$ :



$$\begin{aligned}
F_{i,j} &= u_{i,j} - \frac{\Delta t}{h^2} \left( \frac{1}{2}(\alpha(u_{i,j}) + \alpha(u_{i+1,j}))(u_{i+1,j} - u_{i,j}) - \right. \\
&\quad \frac{1}{2}(\alpha(u_{i-1,j}) + \alpha(u_{i,j}))(u_{i,j} - u_{i-1,j}) + \\
&\quad \frac{1}{2}(\alpha(u_{i,j}) + \alpha(u_{i,j+1}))(u_{i,j+1} - u_{i,j}) - \\
&\quad \left. \frac{1}{2}(\alpha(u_{i,j-1}) + \alpha(u_{i,j}))(u_{i,j} - u_{i,j-1}) \right) - \Delta t f(u_{i,j}) - u_{i,j}^{(1)} = 0 \\
J_{i,j,i,j} &= \frac{\partial F_{i,j}}{\partial u_{i,j}}
\end{aligned}$$

## Continuation methods

- Picard iteration or Newton's method may diverge
- Relaxation with  $\omega < 1$  may help
- If not, resort to *continuation methods*

## Continuation method: solve difficult problem as a sequence of simpler problems

- Introduce a *continuation parameter*  $\Lambda$
- $\Lambda = 0$ : simple version of the PDE problem
- $\Lambda = 1$ : desired PDE problem
- Increase  $\Lambda$  in steps:  $\Lambda_0 = 0, \Lambda_1 < \dots < \Lambda_n = 1$
- Use the solution from  $\Lambda_{i-1}$  as initial guess for the iterations for  $\Lambda_i$

## Example on a continuation method

$$-\nabla \cdot (||\nabla u||^q \nabla u) = f,$$

Pseudo-plastic fluids may be  $q = -0.8$ , which is a difficult problem for Picard/Newton iteration.

$$\Lambda \in [0, 1] : \quad q = -\Lambda 0.8$$

$$-\nabla \cdot (||\nabla u||^{-\Lambda 0.8} \nabla u) = f$$

Start with  $\Lambda = 0$ , increase in steps to  $\Lambda = 1$ , use previous solution as initial guess for Newton or Picard