Outlook finite elements and discussion of selected Additional optional problems

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Content

Plan

Problem 1

Consider the problem

$$
\begin{aligned}
-a\Delta u + \mathbf{b}\cdot\nabla u + cu &= f, && \text{in } \Omega,\\
u &= 0, && \text{on } \Gamma,
\end{aligned}
$$

with $a, c \in \mathbb{R}$, $\mathbf{b} \in \mathbb{R}^2$, $f \in L^2(\Omega)$ with $a > 0,\ c \geq 0$.

1. Where do problems of this type come from?
2. How can this be solved?
3. How can this be generalized?

Problem 1– Where do problems of this type come from?

The scalar elliptic equation

$$\begin{aligned} -a\Delta u + \mathbf{b}\cdot\nabla u + cu &= f, &\qquad \text{in } \Omega,\\ u &= 0, &\qquad \text{on } \Gamma, \end{aligned}$$

can be interpreted as a stationary solution (infinite time limit) of convection-diffusion equation (see e.g. Wikipedia):

$$\partial_t u - a\Delta u + \mathbf{b}\cdot\nabla u + cu = f.$$

Interpretation:

- u – material property, e.g. concentration, temperature,
- $\mathbf{b}$ – velocity, by which u is advected,
- c – sources and sinks.

Using $\mathbf{j}_{\mathrm{diff}} = -a\nabla u$ and $\mathbf{j}_{\mathrm{adv}} = u\mathbf{b}$ we can rewrite this equation as

$$\partial_t u + \nabla\cdot\mathbf{j} = R,$$

with total flux $\mathbf{j} = \mathbf{j}_{\mathrm{diff}} + \mathbf{j}_{\mathrm{adv}}$ and $R = -c\mathbf{u}$.

Problem 1– Where do problems of this type come from?

The heat equation/diffusion equation describes convective and diffusive transport of a quantity. In application it appears as ...

- Reaction-convection-diffusion equation (biology, chemistry)[1],
- Nernst-Planck equation (electrochemistry),
- Black scholes equation (financial markets),
- ...

[1] a.k.a. drift-diffusion equation

Problem 1– How can this be solved?

Example:

$$-au'' + bu' + cu = f, \qquad \text{in } (0,1) \tag{$\star$}$$

Weak form: Find $u \in V$ such that $a(u,v) = f(v)$ for all $v \in V$.

- If $(\star)$ comes with homogeneous Dirichlet condition, then $V = H_0^1(0,1)$

$$a(u,v) := \int au'v' + bu'v + cuv \,\mathrm{d}x = \int_0^1 fv \,\mathrm{d}x =: f(v)$$

- If $(\star)$ comes with $\mathbf{j} = 0$ at $x = 0, 1$, then $V = H^1(0,1)$ and

$$a(u,v) := \int au'v' - buv' + cuv \,\mathrm{d}x = \int_0^1 fv \,\mathrm{d}x =: f(v)$$

- If $(\star)$ comes with $\partial_x u = 0$ at $x = 0, 1$, then $V = H^1(0,1)$ and

$$a(u,v) := \int au'v' + bu'v + cuv \,\mathrm{d}x = \int_0^1 fv \,\mathrm{d}x =: f(v)$$

Problem 1– How can this be solved (numerically)?

Galerkin-method with linear elements:

$$a(u,v) := \int a u' v' - b u v' + c u v \, \mathrm{d}x = \int_0^1 f v \, \mathrm{d}x =: f(v)$$

- boundary condition in space (essential) or bilinear form (natural)
- well-posedness by Lax-Milgram (non-symmetric bilinear form)
- discretization by Galerkin method and FEM,

If b is constant and u_h, v_h piecewise linear, then

$$\int_{\Omega_k} b w_j w_i' \, \mathrm{d}x = b w_i' \int_{\Omega_k} w_j \, \mathrm{d}x = \frac{b}{2} w_i' \det F_k.$$

because $\int_{\Omega_k} w_i = \frac{1}{2} \det F_k$ for all k (prefactor depends on dimension).

Problem 1– How can this be generalized?

- Extension 1: Consider
$$\partial_t u + \nabla \cdot \mathbf{j} = R$$
where $\mathbf{j} = a(x)\nabla u + u\mathbf{b}(x)$ and $R = -c(x)u$.
- Extension 2: Nernst-Planck
$$\begin{aligned} &-\nabla \cdot (\epsilon(x)\nabla\phi) = e(z_+ n_+ + z_- n_-) \\ &\frac{\partial n_+}{\partial t} + \nabla \cdot \Big[-D_+ \nabla n_+ + \mathbf{b} n_+ + \frac{D_+ z_+ e}{k_B T} n_+ \nabla\phi \Big] = R_+ \\ &\frac{\partial n_-}{\partial t} + \nabla \cdot \Big[-D_- \nabla n_- + \mathbf{b} n_- + \frac{D_- z_- e}{k_B T} n_- \nabla\phi \Big] = R_- \end{aligned}$$
with electric potential ϕ, species density $n_\pm$, flow field $\mathbf{b}$. We have material constants $D_\pm$, $z_\pm$, e, $k_B T$.
- Extension 3: Allen-Cahn (nonlinear!)
$$\partial_t u - \Delta u + \varepsilon^{-1} W'(u) = 0$$
where $W(u) = \frac{1}{4}(u^2 - 1)^2$ describes phase transitions of order parameter.

Problem 1– example: Allen-Cahn

Finite differences-implicit Euler discretization of Allen-Cahn equation:

$$(\mathbb{I} + \tau A)u^{k+1} = \mathbb{I}(u^k - \tau W')$$

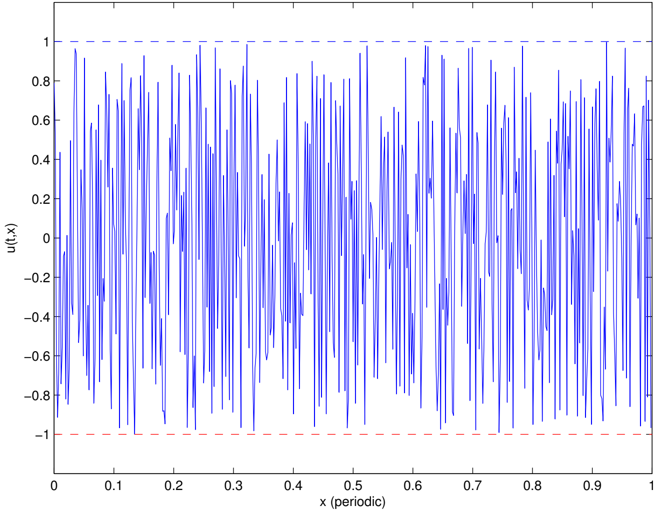
where $W' = \frac{1}{\varepsilon}((u^k)^3 - u^k)$.

```
% Example for lecture by Dirk Peschka
% Allen - Cahn equation by extension of
% assignment 5, exercise 3.
p     =    9; % space discretization
theta =    1; % theta=0 explicit theta=1 implicit
tau   = 1d-7; % time-step
flag  =    0; % usual 3-point Laplacian
eps   = 1d-5; % parameter in the model

[ xh,Ah,Mh ] = a05ex03getTheta(p,theta,tau,flag ); % *** Assignment 5, Exercise 3 ***
xh    = xh(:);
u     = 2*rand(size(xh))-1;               % *** random initial data ***
t     = 0;
I     = speye(2^p);
while t<1d-2
    % new piece of information enters here:
    % the nonlinearity is treated explicitly!
    u = Ah\(Mh*u - tau*I*(u.^3-u)/eps); % *** time-step ***
    t=t+tau;
    % output
    plot(xh,u,[0 1],[-1 -1],'r--',[0 1],[1 1],'b--');
    ylim([-1.2 1.2]);
    xlabel('x (periodic)');ylabel('u(t,x)');
    drawnow
end
```

Problem 1– example: Allen-Cahn

Solution of the Allen-Cahn equation:



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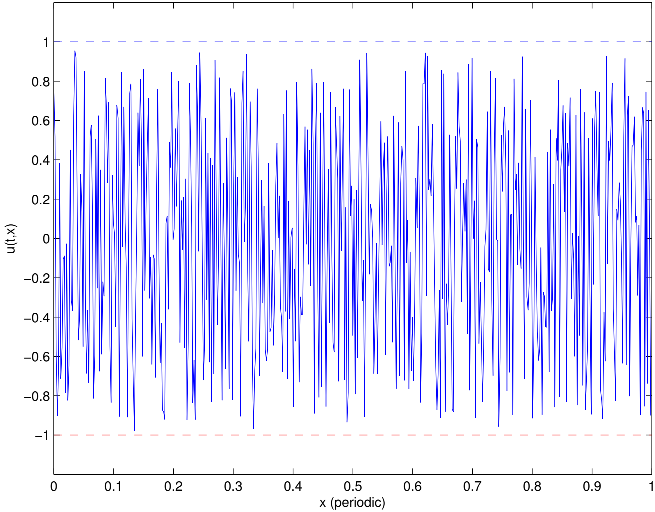

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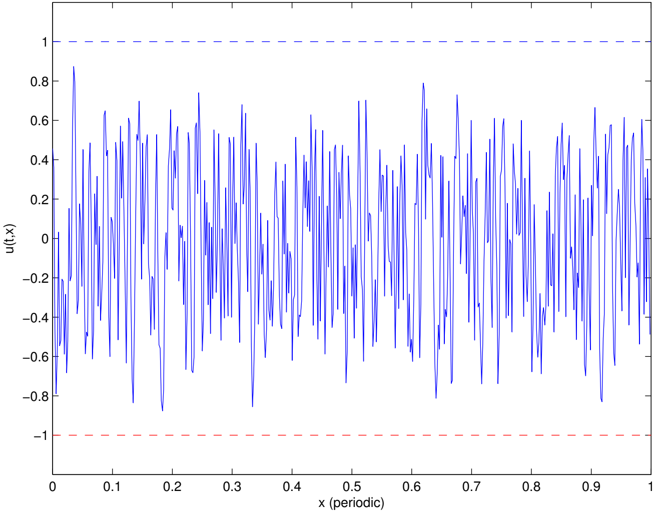

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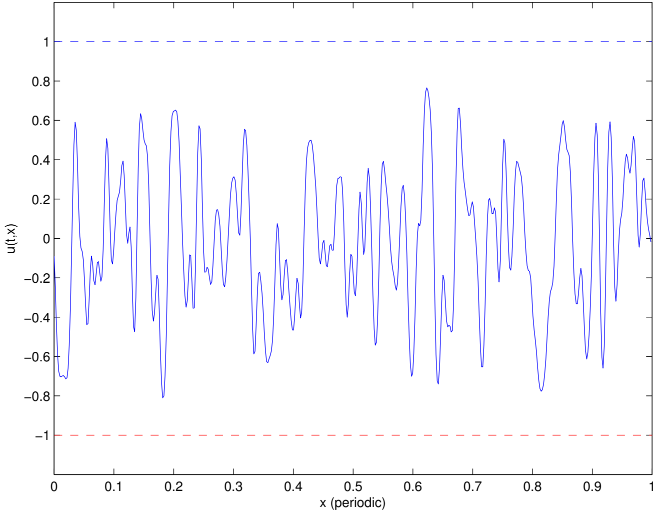

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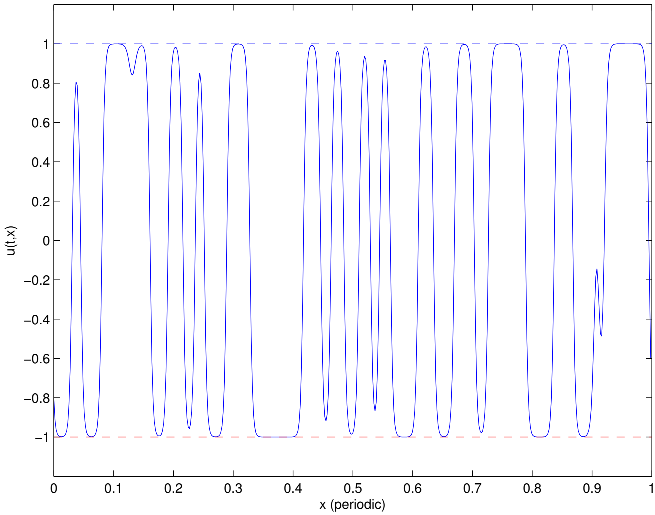

Problem 1– example: Allen-Cahn

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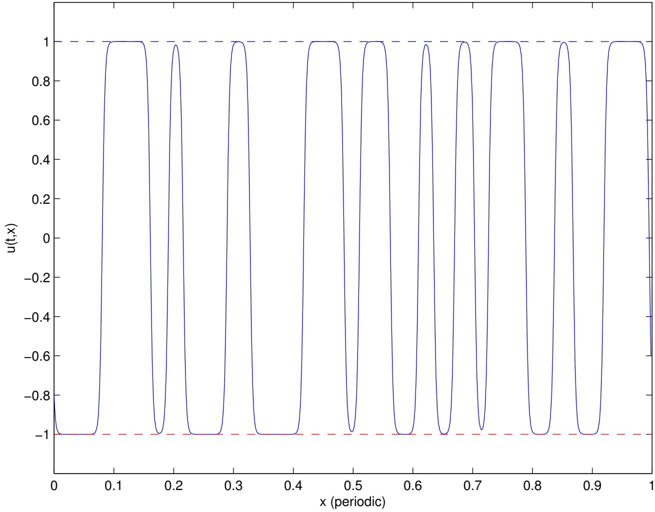

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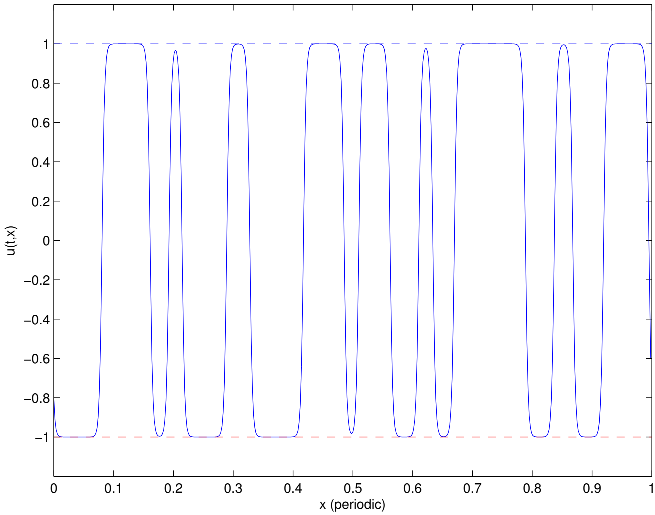
Solution of the Allen-Cahn equation:



Plan

Problem 3– Isoparametric elements

- Isoparametric elements $\Omega_k \subset \mathbb{R}$: Quadratic elements

$$F_k(s) = x(s) = a_1 + a_2 x + a_3 x^2$$

where $s \in (0,1) = \Omega_{\text{ref}}$ is the usual reference interval.

- Isoparametric elements $\Omega_k \subset \mathbb{R}^2$: Quadratic elements

$$F_k(s,t) = \begin{pmatrix} x(s,t) \\ y(s,t) \end{pmatrix} = \begin{pmatrix} a_1 + a_2 s + a_3 t + a_4 st + a_5 s^2 + a_6 t^2 \\ b_1 + b_2 s + b_3 t + b_4 st + b_5 s^2 + b_6 t^2 \end{pmatrix}$$

where $(s,t) \in \Omega_{\text{ref}} = \{(s,t) \in \mathbb{R}^2 : 0 < s < 1 - t; s, t > 0\}$ is the usual reference triangle.

We require F_k to be invertible, i.e. $\det \nabla F_k > 0$ for all $(s,t) \in \Omega_{\text{ref}}$.

Problem 3

How do we define basis functions on deformed triangles?

We have shape functions $\phi_m : \Omega_{\text{ref}} \to \mathbb{R}$, then

$$w_i(x, y) = \phi_m(F_k^{-1}(x, y))$$

for all $x, y \in \Omega_k$, where $i =$ `e2p(k,m)`.

Example 1D:

$$\Omega_{\text{ref}} = (0,1), \quad \Omega = (0,2)$$

$$F(s) = 2s + \alpha s(1-s)$$

for arbitrary s. If we want F to be invertible, $F' > 0$, i.e. $|\alpha| < 2$.

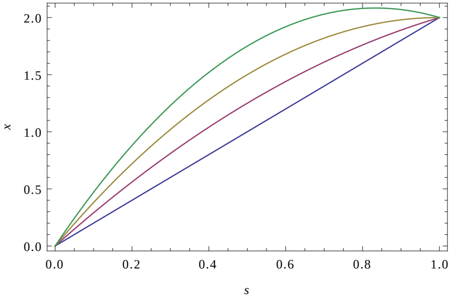


Figure: example with $\alpha = 0, 1, 2, 3$

Problem 3

Example 1D: Shape functions:

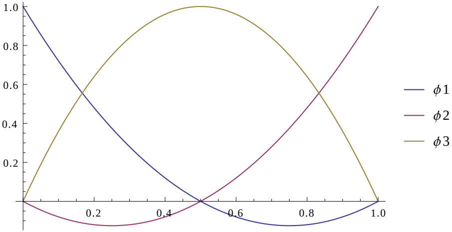
$$\phi_1(s) = 2(s-1)(s-\tfrac{1}{2}),$$
$$\phi_2(s) = 2s(s-\tfrac{1}{2}),$$
$$\phi_3(s) = 4s(1-s).$$

Basis functions for $F(s) = 2s + s(1-s)$ where $\alpha = 1$:

$$w_1(x) = \frac{1}{2}\left(11 - 3\sqrt{9-4x} - 4x\right),$$
$$w_2(x) = \frac{1}{2}\left(15 - 5\sqrt{9-4x} - 4x\right),$$
$$w_3(x) = 4(\sqrt{9-4x} + x - 3).$$

Remark: Note that w_i are no polynomials!

Problem 3



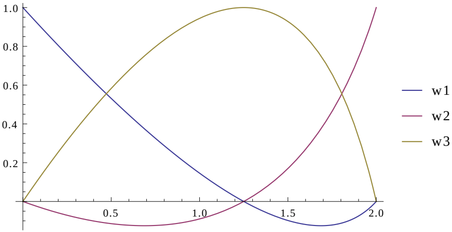


Figure: shape functions (left) and basis functions (right)

Note: Note that the points $p_1 = 0, p_2 = 1, p_3 = 1/2$ are mapped to different points $x_j = F(p_n)$ which satisfy $\delta_{mn} = \phi_m(p_n) = w_i(x_j) = \delta_{ij}$. We have $x_1 = 0, x_2 = 2, x_3 = 5/4$.

Problem 3

Question: Can we integrate

$$w_1(x) = \frac{1}{2}\left(11 - 3\sqrt{9-4x} - 4x\right),$$
$$w_2(x) = \frac{1}{2}\left(15 - 5\sqrt{9-4x} - 4x\right),$$
$$w_3(x) = 4(\sqrt{9-4x} + x - 3),$$

exactly, using Gauss integration, i.e.

$$I = \int_0^2 w_3(x) w_3(x)\,\mathrm{d}x?$$

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$$w_3(x) = 4(\sqrt{9-4x} + x - 3),$$

exactly, using Gauss integration, i.e.

$$I = \int_0^2 w_3(x) w_3(x)\,\mathrm{d}x?$$

Yes!

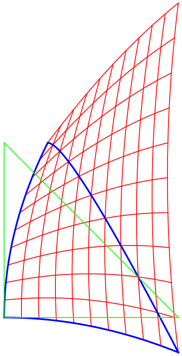
$$I = \int_0^1 \phi_3(s)\phi_3(s)F'(s)\,\mathrm{d}s$$

where $\phi_3(s)\phi_3(s)F'(s)$ is in P_5, i.e. 3-point Gauss quadrature is sufficient.

Problem 3

Example 2D:

$$F(s,t) = \begin{pmatrix} s \\ t \end{pmatrix} + \begin{pmatrix} (t^2 - st)/4 \\ -s^2/5 + st \end{pmatrix}$$

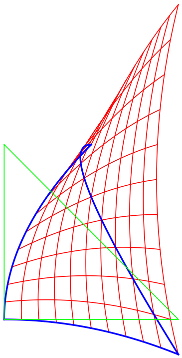


Question: Is the mapping invertible?

Problem 3

Example 2D:

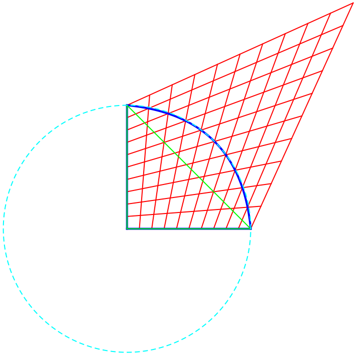
$$F(s,t) = \begin{pmatrix} s \\ t \end{pmatrix} + \begin{pmatrix} (t^2 - st)/2 \\ -s^2/5 + st \end{pmatrix}$$



Question: Is the mapping invertible?

Example 2D:

$$F(s,t) = \begin{pmatrix} s \\ t \end{pmatrix} + \begin{pmatrix} 2(\sqrt{2}-1)st \\ 2(\sqrt{2}-1)st \end{pmatrix}$$

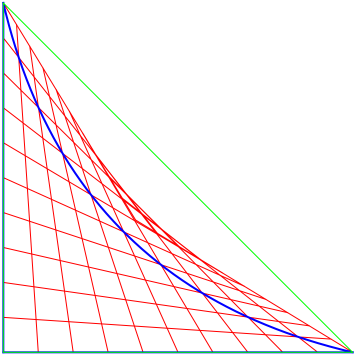


Question: Is the mapping invertible?

Problem 3

Example 2D:

$$F(s,t) = \begin{pmatrix} s \\ t \end{pmatrix} - \begin{pmatrix} \frac{3}{2}(\sqrt{2}-1)st \\ \frac{3}{2}(\sqrt{2}-1)st \end{pmatrix}$$



Question: Is the mapping invertible?

Problem 3

Example 2D: How to construct this in practice?
We have shape functions $\phi_m(s,t)$ with $\phi_m(p_n) = \delta_{mn}$.
If we want to map the points p_m to x_j we choose F according to

$$F_k(s,t) = \sum_{n=1}^{\mathtt{nphi}} \mathbf{x}_{\mathtt{e2p(k,n)}} \phi_n(s,t)$$

Question: Why does this work?
Question: Is this guaranteed to be invertible?

Example circle: $p_1 = (0,0), p_2 = (1,0), p_3 = (0,1), p_4 = (1/2,0), p_5 = (1,1)/2, p_6 = (0,1/2)$.

$$F = \begin{pmatrix} \phi_2 + \frac{1}{2}\phi_4 + \xi\phi_5 \\ \phi_3 + \frac{1}{2}\phi_6 + \xi\phi_5 \end{pmatrix}$$

where $\xi = 1/\sqrt{2}$.

Problem 3

In general we can expect F to be invertible, if F is sufficiently close to the identity

$$\mathrm{Id}(s,t) = \begin{pmatrix} s \\ t \end{pmatrix}.$$

The necessary and sufficient condition is $\nabla F > 0$ for all $(s,t) \in \bar{\Omega}_{\mathrm{ref}}$.

Problem 3

Summarizing, isoparametric elements:

- can give better approximations of boundaries,
- one needs to be careful that F_k is invertible,
- basis functions are defined

$$w_i(x,y) = \phi_n(F_k^{-1}(x,y)).$$

but integration is performed using, e.g.

$$\int_{\Omega_k} w_i w_j \,\mathrm{d}\Omega = \int_{\Omega_{\mathrm{ref}}} \phi_m \phi_n F' \mathrm{d}s\,\mathrm{d}t$$

which can be done exactly.

Plan

1. Problem 1
2. Problem 3
3. Problem 5

Problem 5

Many problems in physics are not single scalar equations, but systems of equations. Either because we have equations for various quantities (e.g. density and temperature and electric field), or the unknowns are vectors (velocity, vector potential, deformations).

- **Example 1**: Nernst-Planck (see before)
- **Example 2**: ~~Navier~~-Stokes equation

$$\begin{aligned} \xcancel{\rho\left(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}\right)} &= -\nabla p + \mu\Delta\mathbf{u} + \mathbf{f} \\ \nabla\cdot\mathbf{u} &= 0 \end{aligned}$$

  where $\mathbf{u}$ is the unknown velocity, p is the unknown pressure, $\mathbf{f}$ is a given force density, μ is the viscosity of the fluid.

- **Example 3**: Linear elasticity

$$\nabla\cdot\sigma + \mathbf{f} = 0$$

  where $\sigma = C : \varepsilon$ and $\varepsilon = \frac{1}{2}\left(\nabla\mathbf{u} + \nabla\mathbf{u}^\top\right)$, where C for isotropic materials is

$$C_{ijkl} = K\delta_{ij}\delta_{kl} + \mu\left(\delta_{ij}\delta_{jl} + \delta_{il}\delta jk - \frac{2}{3}\delta_{ij}\delta_{kl}\right).$$

Problem 5

Without constraints **example 2** and **example 3** are systems of elliptic equations, because the unknowns are vector-valued functions. In general we can expect the corresponding weak form to be of the type

$$a(\mathbf{u}, \mathbf{v}) = f(\mathbf{v})$$

where $\mathbf{u} = (u_1, u_2)$ and $u_1, u_2 \in V$, e.g. $V = H_0^1(\Omega)$.
Example:

$$\begin{aligned} a(\mathbf{u}, \mathbf{v}) &= \int_\Omega \nabla \mathbf{u} : \nabla \mathbf{v} + \mathbf{u} \cdot \mathbf{v} \,\mathrm{d}\Omega \\ &= \int_\Omega \sum_{i,j=1}^{2} \partial_i u_j \partial_i v_j + \sum_{i=1}^{2} u_i v_i \,\mathrm{d}\Omega = \int_\Omega \mathbf{f} \cdot \mathbf{v} \,\mathrm{d}\Omega \end{aligned}$$

We generally use the notation of the Frobenius inner product

$$A : B = \sum_{i,j} A_{ij} B_{ij}$$

Problem 5

Question: Which PDE does $\mathbf{u}$ satisfy for $V = H_0^1(\Omega)$?
Integration by parts on a gives

$$
\begin{aligned}
a(\mathbf{u}, \mathbf{v}) &= \int_\Omega \sum_{i,j=1}^{2} \partial_i u_j \partial_i v_j + \sum_{i=1}^{2} u_i v_i \,\mathrm{d}\Omega \\
&= \int_\Omega \sum_{i=1}^{2} \partial_x u_i \partial_x v_i + \partial_y u_i \partial_y v_i + u_i v_i \,\mathrm{d}\Omega \\
&= \int_\Omega \sum_{i=1}^{2} (-\Delta u_i + u_i) v_i \,\mathrm{d}\Omega + \int_\Gamma (\mathbf{n} \cdot \nabla u_i) v_i \,\mathrm{d}\Gamma
\end{aligned}
$$

Problem 5

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a(\mathbf{u},\mathbf{v}) &= \int_\Omega \sum_{i,j=1}^{2} \partial_i u_j \partial_i v_j + \sum_{i=1}^{2} u_i v_i \,\mathrm{d}\Omega \\
&= \int_\Omega \sum_{i=1}^{2} \partial_x u_i \partial_x v_i + \partial_y u_i \partial_y v_i + u_i v_i \,\mathrm{d}\Omega \\
&= \int_\Omega \sum_{i=1}^{2} (-\Delta u_i + u_i) v_i \,\mathrm{d}\Omega + \int_\Gamma (\mathbf{n}\cdot\nabla u_i) v_i \,\mathrm{d}\Gamma
\end{aligned}
$$

Therefore using the boundary conditions we get the PDE

$$
-\Delta u_i + u_i = f_i, \quad \text{in } \Omega, \qquad\qquad u_i = 0, \quad \text{on } \Gamma,
$$

which decouples, i.e., can be solved for $i = 1, 2$ independently.

Problem 5

How do we solve such a problem in practice?
Ansatz:

$$\mathbf{u} = \sum_{i=1}^{\dim V_h} (u_1^i \mathbf{e}_x + u_2^i \mathbf{e}_y) w_i(x, y)$$

Question 1: What are the unknowns and how many of those do we have?
Question 2: How should we organize them into a vector?

Problem 5

How do we solve such a problem in practice?
Ansatz:

$$\mathbf{u} = \sum_{i=1}^{\dim V_h} (u_1^i \mathbf{e}_x + u_2^i \mathbf{e}_y) w_i(x, y)$$

Question 1: What are the unknowns and how many of those do we have?
Question 2: How should we organize them into a vector?

$$\alpha = (u_1^1, u_1^2, u_1^3, ..., u_2^1, u_2^2, u_2^3, ...)^\top,$$
$$\alpha = (u_1^1, u_2^1, u_1^2, u_2^2, ...)^\top.$$

The first choice leads to a system of equation with a block-structure:

$$\mathbf{A}\alpha = \begin{pmatrix} A & B \\ C & A \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$$

Question 3: What is $A, B, C, \alpha_1, \alpha_2$?

Problem 5

How do we solve such a problem in practice?

Assume you have a MATLAB FE program, which creates the i, j indices and the values a for the matrix A, so that `A=sparse(i,j,a)`.

What does the following code do then

```
i1 = [i(:);ndof+i(:)];
j1 = [j(:);ndof+j(:)];
a1 = [a(:);a(:)];
A1 = sparse(i1,j1,a1);
```

where `ndof`$=\dim V_h$?

Question: How would you write a program, which creates `i1,j1,a1` right away, i.e. during the iteration over all elements?

Problem 5

Answer (prototypical):

```
ii = zeros(2,2,nelement,nphi^2);
jj = zeros(2,2,nelement,nphi^2);
aa = zeros(2,2,nelement,nphi^2);

for k=1:nelement

    ix = e2p(k,1:nphi);
    ...
    for i1=1:2
        for i2=1:2
            ii(i1,i2,k,:) = (i1-1)*ndof+[ix(1) ix(2) ...];
            jj(i1,i2,k,:) = (i2-1)*ndof+[ix(1) ix(1) ...];
        end
    end

    aa(1,1,k,:) = localstiff(...);
    aa(2,2,k,:) = localstiff(...);
    aa(1,2,k,:) =  ...
    aa(2,1,k,:) =  ...
end
A = sparse(ii(:),jj(:),aa(:));
```

Problem 5

How can this be generalized?

Stationary Stokes: Consider

$$\begin{aligned} a(\mathbf{u},\mathbf{v}) + b(p,\mathbf{v}) &= f(\mathbf{v}) \\ b(q,\mathbf{u}) &= 0 \end{aligned}$$

where

$$a(\mathbf{u},\mathbf{v}) = \int_\Omega \nabla\mathbf{u} : \nabla\mathbf{v}\,\mathrm{d}\Omega, \qquad b(q,\mathbf{u}) = \int_\Omega q\nabla\cdot\mathbf{u}\,\mathrm{d}\Omega.$$

This leads to the FEM discretization

$$\begin{pmatrix} \mathbf{A} & B^\top \\ B & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ p \end{pmatrix} = \begin{pmatrix} M\mathbf{f} \\ 0 \end{pmatrix}$$

Problem 5

How can this be generalized?
Instationary Stokes: Consider

$$\begin{aligned} \langle \partial_t \mathbf{u}(t), \mathbf{v} \rangle + a\big(\mathbf{u}(t), \mathbf{v}\big) + b(p, \mathbf{v}) &= f(\mathbf{v}) \\ b\big(q, \mathbf{u}(t)\big) &= 0 \end{aligned}$$

where

$$a(\mathbf{u}, \mathbf{v}) = \int_\Omega \nabla \mathbf{u} : \nabla \mathbf{v} \, \mathrm{d}\Omega, \qquad b(q, \mathbf{u}) = \int_\Omega q \nabla \cdot \mathbf{u} \, \mathrm{d}\Omega.$$

This leads to the implicit Euler (time) FEM (space) discretization

$$\begin{pmatrix} \mathbf{I} + \tau \mathbf{A} & B^\top \\ B & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u}^{k+1} \\ p \end{pmatrix} = \begin{pmatrix} M(\mathbf{u}^k + \tau \mathbf{f}) \\ 0 \end{pmatrix}$$

Problem 5

How can this be generalized?
Navier-Stokes: Consider

$$\begin{aligned} \langle \partial_t \mathbf{u}(t), \mathbf{v} \rangle + c(\mathbf{u}(t); \mathbf{u}(t), \mathbf{v}) + a\big(\mathbf{u}(t), \mathbf{v}\big) + b(p, \mathbf{v}) &= f(\mathbf{v}) \\ b\big(q, \mathbf{u}(t)\big) &= 0 \end{aligned}$$

where

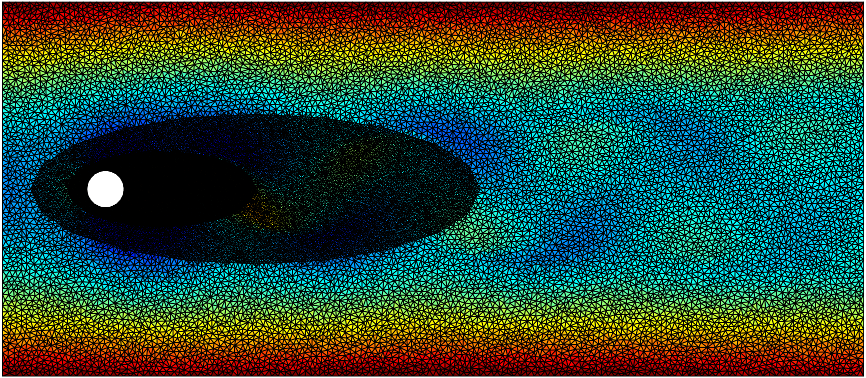
$$a(\mathbf{u}, \mathbf{v}) = \int_\Omega \nabla \mathbf{u} : \nabla \mathbf{v} \, \mathrm{d}\Omega, \qquad b(q, \mathbf{u}) = \int_\Omega q \nabla \cdot \mathbf{u} \, \mathrm{d}\Omega,$$
$$c(\mathbf{b}; \mathbf{u}, \mathbf{v}) = \int_\Omega (\mathbf{b} \cdot \nabla \mathbf{u}) \cdot \mathbf{v} \, \mathrm{d}\Omega.$$

This leads to the implicit Euler (time) FEM (space) discretization

$$\begin{pmatrix} \mathbf{I} + \tau \mathbf{A} & B^\top \\ B & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u}^{k+1} \\ p \end{pmatrix} = \begin{pmatrix} M(\mathbf{u}^k + \tau \mathbf{f}) + \tau \, c(\mathbf{u}^k; \mathbf{u}^k, \mathbf{v}) \\ 0 \end{pmatrix}$$

Solution of Navier-Stokes: Karman vortex street

27k points, 81k edges, $2 \times 108k + 27k = 243k$ unknowns
Taylor-Hood element P_2 for velocity, P_1 for pressure



Video

Problem 5

Solution of Navier-Stokes: Karman vortex street

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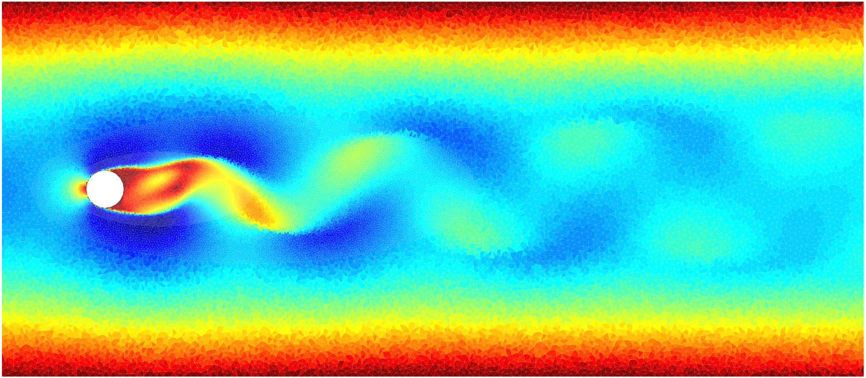

Video