Mini-course on Stationary Iterative Methods

Lecture 1 – Multiphysics problems

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2021 CRM Summer School: Solving large systems efficiently in multi-physics numerical simulations

What is a multiphysics problem ?

- Multiphysics is the opposite of “single physics”
- Typical single physics problems :
  - Heat transfer
  - Convection/advection
  - Wave propagation
  - Elastic deformations
  - ...
- Many types of multiphysics :
  - Interacting objects with different dynamics
  - Different properties of the same object interacting
  - Different approximations of the same physical phenomenon
  - ...

Multiphysics simulations

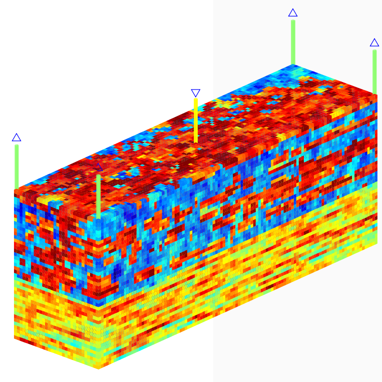
- Single physics problems often have specialized discretizations and solvers that exploit specific properties of such problems
  - Heat transfer : fast Poisson solvers, multigrid, ...
  - Wave propagation : ray tracing, sweeping preconditioners, ...
  - Advection : Upwinding, streamline methods, approximate Riemann solvers, ordering methods, ...
  - ...
- Such specialized approaches cannot be applied blindly to multiphysics problems !

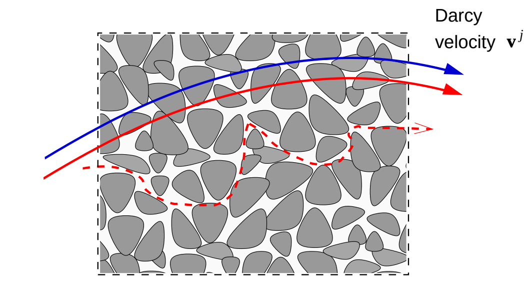
Outline

Multiphysics problem 1 :
Two-phase flow in porous media

Flow in porous media

- Goal : Track the evolution of underground fluids (groundwater, crude oil, natural gas, . . .) as well as the concentrations of dissolved chemicals (salinity, contaminants, . . .)
- Applications : oil & gas production, carbon sequestration, contaminant tracking, ground subsidence,. . .

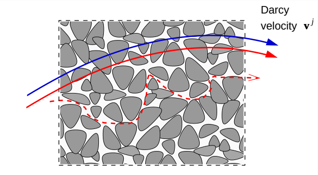




Darcy flow model

- **Single** phase flow : one fluid only
- Fluid velocity is proportional to the negative pressure gradient :

$$\mathbf{v} = -K(\mathbf{x})\nabla p$$



- Conservation of mass :

$$(\text{Accumulation}) = (\text{Mass in}) - (\text{Mass out})$$

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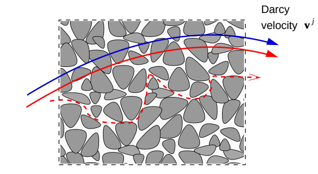


- Conservation of mass :

$$\frac{\partial}{\partial t}(\phi\rho) = \nabla \cdot (K(\mathbf{x})\,\rho\nabla p) + q,$$

where

- $\phi =$ porosity
- $\rho = \rho(p) =$ fluid density (as a function of p)
- $q =$ sources (injection/productdion wells, chemical reactions, ...)

Two-phase flow

- Two immiscible phases, e.g., oil and water
- Define :

$$S_w = \text{saturation of water (i.e., fraction of pore space occupied by water)}$$
$$S_o = \text{saturation of oil (i.e., fraction of pore space occupied by oil)}$$

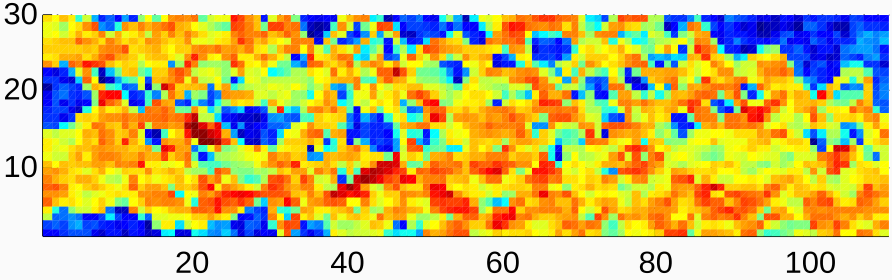
- Pores are saturated : $S_o = 1 - S_w$
- Flow of each phase interferes each other : fluid velocity depends on saturation

$$\mathbf{v}_w = -K(\mathbf{x})\lambda_w(S_w)\nabla p, \qquad \mathbf{v}_o = -K(\mathbf{x})\lambda_o(S_w)\nabla p$$

- Mass conservation, one per phase (write $S = S_w$ from now on) :

$$\text{Water :} \qquad \frac{\partial}{\partial t}(\phi\rho_w S) = \nabla\cdot(K(\mathbf{x})\rho_w\lambda_w(S)\,\nabla p) + q_w,$$
$$\text{Oil :} \qquad \frac{\partial}{\partial t}(\phi\rho_o(1-S)) = \nabla\cdot(K(\mathbf{x})\rho_o\lambda_o(S)\,\nabla p) + q_o,$$

Two immiscible phases



(Source : K. & Tchelepi, JCP 2007)

Where is the multiphysics ?

$$\boxed{\begin{array}{ll} \text{Water :} & \dfrac{\partial}{\partial t}(\phi\rho_w S) = \nabla\cdot(K(\mathbf{x})\rho_w\lambda_w(S)\,\nabla p) + q_w, \\ \text{Oil :} & \dfrac{\partial}{\partial t}(\phi\rho_o(1-S)) = \nabla\cdot(K(\mathbf{x})\rho_o\lambda_o(S)\,\nabla p) + q_o, \end{array}}$$

- Assume rock and fluids are incompressible, i.e., ϕ, ρ_w and ρ_o are constant
- Add both equations and get

$$0 = \nabla\cdot(K(\mathbf{x})(\lambda_w(S)+\lambda_o(S))\nabla p) + \frac{q_w}{\rho_w} + \frac{q_o}{\rho_o}.$$

This is an elliptic equation of the form

$$-\nabla\cdot(K_T(\mathbf{x},S)\nabla p) = \tilde{q} \qquad (*)$$

where the permeability depends on S.

- Define the **total fluid velocity** $\mathbf{v}_T = -K(\mathbf{x})(\lambda_w(S) + \lambda_o(S))\nabla p$
- $\mathbf{v}_T$ depends on S and p, but often varies **slowly** in time
- Special case : in 1D and with $q_w = q_o = 0$, $(*)$ becomes

$$\frac{d}{dx}(\mathbf{v}_T) = 0 \implies \mathbf{v}_T = const.!$$

- The water velocity $\mathbf{v}_w = -K(\mathbf{x})\lambda_w(S)\nabla p$ is proportional to $\mathbf{v}_T$:

$$\mathbf{v}_w = \frac{\lambda_w(S)}{\lambda_w(S) + \lambda_o(S)}\mathbf{v}_T =: f(S)\mathbf{v}_T$$

- Rewrite water equation as

$$\frac{\partial}{\partial t}(\phi S) + \nabla \cdot (f(S)\mathbf{v}_T) = \frac{q_w}{\rho_w}.$$

- When $q_w = 0$ and $\mathbf{v}_T$ is constant, this is a hyperbolic conservation law !
- The two problems are coupled, since K_T depends on S and $\mathbf{v}_T$ on ∇p

Problem summary

- Unknowns : $p =$ pressure, $S =$ saturation
- In the incompressible limit, we have

$$
\begin{aligned}
-\nabla \cdot (K_T \nabla p) &= \tilde{q} \\
\frac{\partial}{\partial t}(\phi S) + \nabla \cdot (f(S)\mathbf{v}_T) &= \frac{q_w}{\rho_w}
\end{aligned}
$$

- For fixed S, pressure satisfies a **linear elliptic** equation
- For fixed $\mathbf{v}_T$, saturation satisfies a **nonlinear hypberbolic** conservation law
- The two equations require very different discretizations and solvers !

Elliptic vs. hyperbolic problems

Elliptic problems

Our pressure equation is an elliptic problem is of the form

$$-\nabla \cdot (K(\mathbf{x})\nabla p) = \tilde{q} \qquad \text{for } \mathbf{x} \in \Omega$$

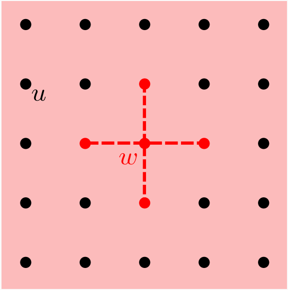
together with boundary conditions :

- Dirichlet : $p = g(\mathbf{x})$ on the boundary (or part of the boundary)
- Neumann : $K(\mathbf{x})\frac{\partial p}{\partial n} = g$
- Robin : $K(\mathbf{x})\frac{\partial p}{\partial n} + \alpha p = g$

To approximate $p(\mathbf{x})$, we **discretize** the PDE using finite difference, finite volumes or finite element methods.

Example : At a grid point $\mathbf{x} = \mathbf{x}_{ij}$, approximate derivatives $p_{ij} \approx p(\mathbf{x}_{ij})$ using finite differences :

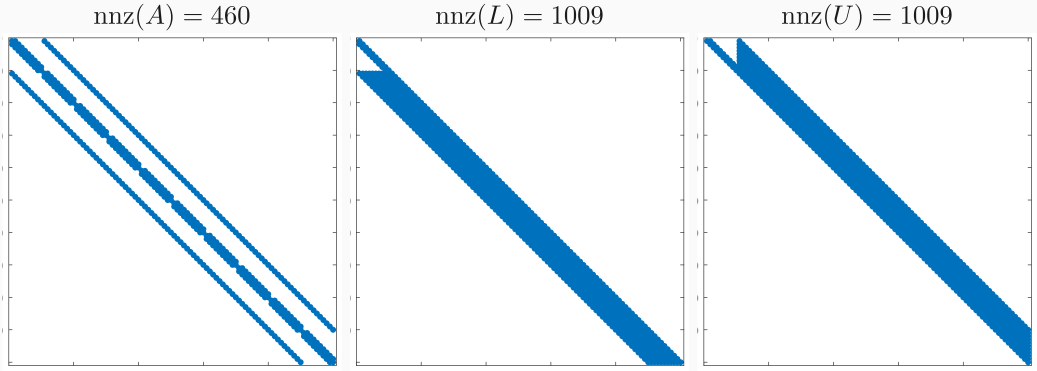
$$\frac{\partial}{\partial x}\left(K\frac{\partial p}{\partial x}\right)(\mathbf{x}_{ij}) \approx \frac{K_{i+1/2,j}(p_{i+1,j} - p_{ij}) - K_{i-1/2,j}(p_{ij} - p_{i-1,j})}{h^2}$$



Important properties of this elliptic problem :

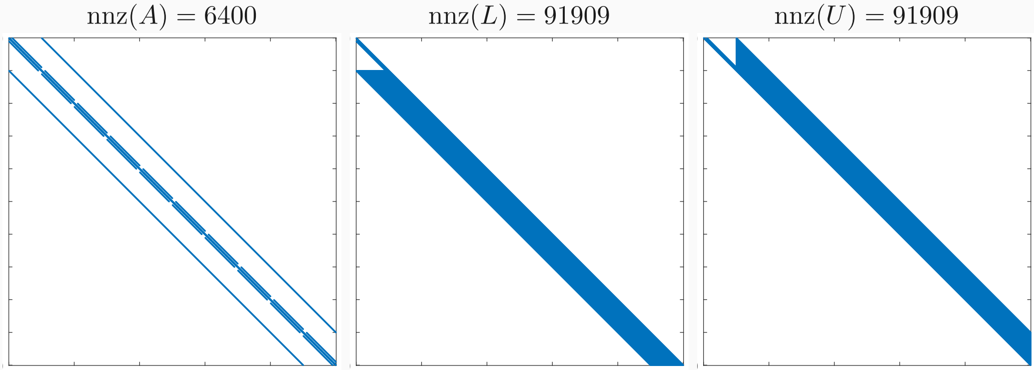
- Operator is isotropic : no preferential direction
- Operator is local : sparse matrix
- Operator is **unbounded** : ill-conditioned matrices
- Solution is smooth when K is continuous
- Infinite speed of propagation : solution at $\mathbf{x}_{ij}$ depends on data everywhere in the domain

Non-zero pattern of the matrix : 2D problem



- LU factors are about twice as dense as A

Non-zero pattern of the matrix : 3D problem

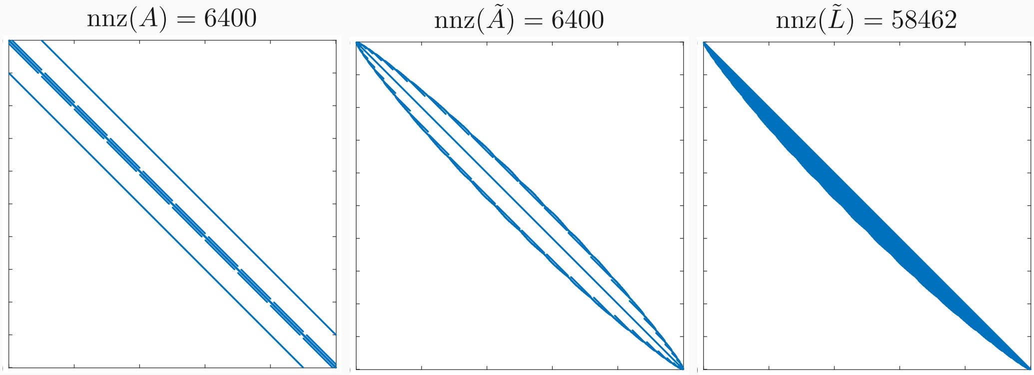


- LU factors are about 14 times as dense as A !

Solution methods

- Direct methods, i.e., Gaussian elimination
  - Factorization step : costs roughly between $O(|L+U|)$ to $O(|L+U|^{1.5})$
  - Substitution step : costs $O(|L+U|)$
  - Reordering is important : minimal degree ordering, multi-frontal methods,...
  - Works well for "small" problems, some parallelism possible (MUMPS)
  - Less competitive for 3D problems because of more fill-in

Reordered matrix



- LU factors are “only” 9 times as dense as $\tilde{A}$ after reordering

Solution methods

- Iterative methods : generate a sequence of successively better approximations to the solution
  - Subdivide into smaller problems based on "subdomains", then iterate to convergence $\Longrightarrow$ Domain Decomposition Methods (mini-course Victorita Dolean, Wednesday to Friday)
  - Work on problem on many grids of different resolutions $\Longrightarrow$ multigrid methods (mini-course by Scott MacLachlan, Tuesday to Thursday next week)
- Such methods often requires only matrix-vector multiplications $\Longrightarrow$ work proportional to number of non-zeros in the matrix, matrix-free implementations
- Speed of convergence matters !

Hyperbolic Problems

- The saturation variable S in our two-phase problem satisfies the **transport** equation

$$\frac{\partial}{\partial t}(\phi S) + \nabla \cdot (f(S)\mathbf{v}_T) = \frac{q_w}{\rho_w}.$$

- When $q_w = 0$, the equation is an example of a **hyperbolic conservation law**.
- The simplest example is the **advection equation**, when $f(S) = S$ and $\phi = 1$:

$$\frac{\partial S}{\partial t} + \nabla \cdot (S\mathbf{v}_T) = 0.$$

- If $\mathbf{v}_T$ is fixed in time and divergence free ($\nabla \cdot \mathbf{v}_T = 0$), then the exact solution is

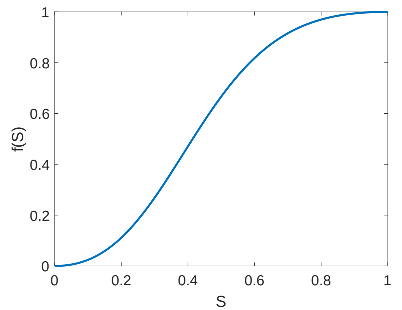
$$S(\mathbf{x}, t) = g(\mathbf{x} - t \cdot \mathbf{v}_T),$$

where $g(\mathbf{x}) = S(\mathbf{x}, 0)$ is the initial state.
- In other words, solution values just get transported, with speed and direction given by $\mathbf{v}_T$.

Nonlinear conservation law

- In many gas applications, $f(S)$ is nonlinear.
  Example from oil & gas :

$$f(S) = \frac{S^2}{S^2 + M(1-S)^2}$$



- When $f(S)$ is nonlinear, discontinuities can develop from smooth initial states $\implies$ shock waves

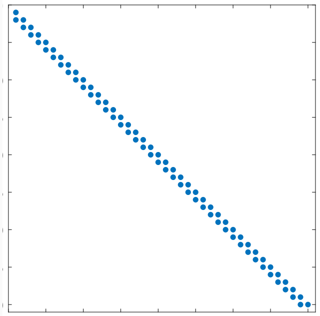
- Other properties :
  - Directional propagation : upwind discretizations
  - Finite speed of propagation : short-range communication
  - For explicit time discretizations : stability limit (CFL condition)
  - Nonlinearities may cause problems with convergence
  - Mass conservation is a must

Nonlinear conservation law

Example : implicit in time, upwind discretization in 1D, $v_T > 0$:

$$\frac{S_j^{n+1} - S_j^n}{\Delta t} + v_T \cdot \frac{f(S_j^{n+1}) - f(S_{j-1}^{n+1})}{\Delta x} = 0.$$

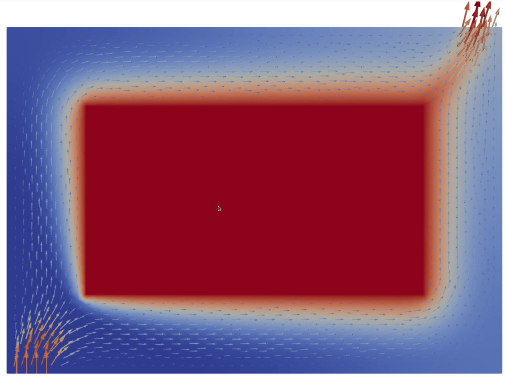
- After linearization, matrix is lower triangular !
- In higher dimensions, this isn't always true (e.g. recirculation zones), but reordering can often help with limiting fill-in and/or finding sparse approximations for preconditioning (see later)



Multiphysics problem 2 : Cooling by fluid injection

Cooling by fluid injection

- Another type of multiphysics problems actually involves different physics in different parts of the domain
- Example : a heated metal object is cooled by a fluid that enters the domain at a prescribed speed and temperature



Define

- Ω_s = part of the domain containing the solid
- $\Omega_f = \Omega \setminus \Omega_s$ = part of the domain containing the fluid
- Γ = solid-fluid interface

Within the solid, heat flow is modelled by Fourier's law of heat conduction :

$$\text{(Heat flux)} = -K_s \nabla T$$

$$\text{(Accumulation)} = \text{(Heat in)} - \text{(Heat out)} + \text{(Heat source)}$$

$$\frac{\partial}{\partial t}(\rho_s C_s T) = \nabla \cdot (K_s \nabla T) + q$$

where T = temperature (unknown)

K_s = heat conductivity,

C_s = specific heat capacity,

ρ_s = density,

q = heat source.

Within the fluid part of the domain, the conservation of energy needs to take into account heat being carried into our out of the control volume due to fluid flow :

$$
\begin{aligned}
(\text{Heat flux}) &= -K_f \nabla T + \mathbf{v}\, \rho_f C_f T \\
(\text{Accumulation}) &= (\text{Heat in}) - (\text{Heat out}) \\
\frac{\partial}{\partial t}(\rho_f C_f T) + \nabla \cdot (\mathbf{v}\, \rho_f C_f T) &= \nabla \cdot (K_f \nabla T)
\end{aligned}
$$

where T = temperature (unknown),

K_s = heat conductivity,

C_s = specific heat capacity,

ρ_s = density,

$\mathbf{v}$ = fluid velocity (unknown).

A large convective term can lead to boundary layers and other issues that affect the discretization and the solver.

The fluid velocity $\mathbf{v}$ is determined by the Navier-Stokes equation, which is appropriate for fluids with low viscosity. For mass conservation, we have

$$\frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f \mathbf{v}) = 0$$

For momentum conservation, we define the Cauchy stress tensor $\boldsymbol{\sigma}$:

$$\boldsymbol{\sigma} = -pI + 2\eta \nabla^s \mathbf{v},$$

where $\eta =$ viscosity,

$$\nabla^s \mathbf{v} = \frac{1}{2}(\nabla \mathbf{v} + (\nabla \mathbf{v})^T) = \text{symmetric gradient of } \mathbf{v}.$$

Any change in momentum must be balanced out by a velocity change. Writing the conservation law on a volume **moving with the fluid** gives

$$\nabla \cdot \boldsymbol{\sigma} = \rho_f \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} \right)$$

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$$\nabla \cdot (2\eta \nabla^s \mathbf{v}) - \nabla p = \rho_f \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right)$$

Conservation laws – summary

$$\begin{aligned}
&\text{Momentum :} && \nabla\cdot(2\eta\nabla^s\mathbf{v}) - \nabla p = \rho_f\left(\frac{\partial\mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v}\right) && \text{in } \Omega_f,\\
&\text{Mass :} && \frac{\partial\rho_f}{\partial t} + \nabla\cdot(\rho_f\mathbf{v}) = 0 && \text{in } \Omega_f,\\
&\text{Heat :} && \frac{\partial}{\partial t}(\rho_f C_f T) + \nabla\cdot(\mathbf{v}\,\rho_f C_f T) = \nabla\cdot(K_f\nabla T) && \text{in } \Omega_f,\\
&\text{Heat :} && \frac{\partial}{\partial t}(\rho_s C_s T) = \nabla\cdot(K_s\nabla T) + q && \text{in } \Omega_s.
\end{aligned}$$

$+$ boundary conditions on $\mathbf{v}$ and T.

Heat transfer between solid and fluid is modelled by the **coupling equation**

$$K_s\nabla T\cdot\mathbf{n}_s + K_f\nabla T\cdot\mathbf{n}_f = 0, \qquad T \text{ continuous on } \Gamma.$$

Conservation laws – steady state

Assuming that a steady state solution can be reached, we can set all time-derivative terms to zero and get

$$
\begin{aligned}
&\text{Momentum :} && \nabla\cdot(2\eta\nabla^s\mathbf{v}) - \rho_f(\mathbf{v}\cdot\nabla)\mathbf{v} - \nabla p = 0 && \text{in } \Omega_f,\\
&\text{Mass :} && \nabla\cdot(\rho_f\mathbf{v}) = 0 && \text{in } \Omega_f,\\
&\text{Heat :} && -\nabla\cdot(K_f\nabla T) + \nabla\cdot(\mathbf{v}\,\rho_f C_f T) = 0 && \text{in } \Omega_f,\\
&\text{Heat :} && -\nabla\cdot(K_s\nabla T) = q && \text{in } \Omega_s,\\
&\text{Coupling :} && K_s\nabla T\cdot\mathbf{n}_s + K_f\nabla T\cdot\mathbf{n}_f = 0 && \text{on } \Gamma.
\end{aligned}
$$

Here, there are different physics within each region,

- Navier-Stokes on Ω_f (coupling to T via ρ and η),
- Diffusion on Ω_s (coupled to T in Ω_f),
- Advection-diffusion on Ω_f (coupled to T in Ω_f and to $\mathbf{v}$ in N-S).

- The Navier-Stokes problem itself has two variables of different types, the velocity $\mathbf{v}$ and pressure p.
- Any stable finite element discretization must respect an inf-sup condition. One possibility is to use piecewise quadratic approximations for $\mathbf{v}$ and piecewise linear approximations for p.
- Once discretized, we get a saddle-point problem

$$\begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{g} \end{bmatrix}.$$

- There are techniques for partially decoupling the velocity and pressure problems and using specialized solvers for each of them, see e.g.
    - H. Elman, D. Silvester and A. Wathen. Finite Elements and Fast Iterative Solvers : with Applications in Incompressible Fluid Dynamics, 2nd Edition, Oxford University Press, 2014.