

Multiscale Modeling and Simulation of Fluid Flows in Inelastic Media

Peter Popov

Institute for Scientific Computation
Texas A&M University
College Station, TX 77843

ppopov@tamu.edu

Yalchin Efendiev

Institute for Scientific Computation
Texas A&M University
College Station, TX 77843

efendiev@math.tamu.edu

Oleg Iliev

Fraunhofer Institut für
Techno- und Wirtschaftsmathematik
D-67657 Kaiserslautern, Germany

illiev@itwm.fhg.de

Presentation outline

- Brief overview of upscaling methods in deformable porous media
- The Fluid-Structure interaction (FSI) problem at the microscale and numerical methods for its solution
- An asymptotic upscaling result of the FSI problem in channel geometries and comparisons with computational solutions
- Numerical upscaling of flow in deformable porous media

Why homogenize

- Often solving a boundary value problem on the exact geometry is impossible. Some examples are fluid flow in porous media (e.g. soil), Elasticity equations in heterogeneous media (concrete, asphalt), etc.
- Consider a simple example:

$$\frac{\partial}{\partial x} \left(a(x/\varepsilon) \frac{\partial u^\varepsilon(x)}{\partial x} \right) = f(x),$$

$$u^\varepsilon(0) = 0 \quad u^\varepsilon(1) = 0.$$

- The aim of upscaling methods is to replace the above equation with one with smooth coefficients

$$\frac{\partial}{\partial x} \left(a^*(x) \frac{\partial u^*(x)}{\partial x} \right) = f(x),$$

whose solution $u^*(x)$ is close to $u^\varepsilon(x)$.

Answer: $a^*(x) = \left\langle \frac{1}{a(x/\varepsilon)} \right\rangle^{-1}$, where $\langle \phi \rangle = \frac{1}{\varepsilon} \int_x^{x+\varepsilon} \phi(y) dy$

Upscaling of flow in rigid porous media

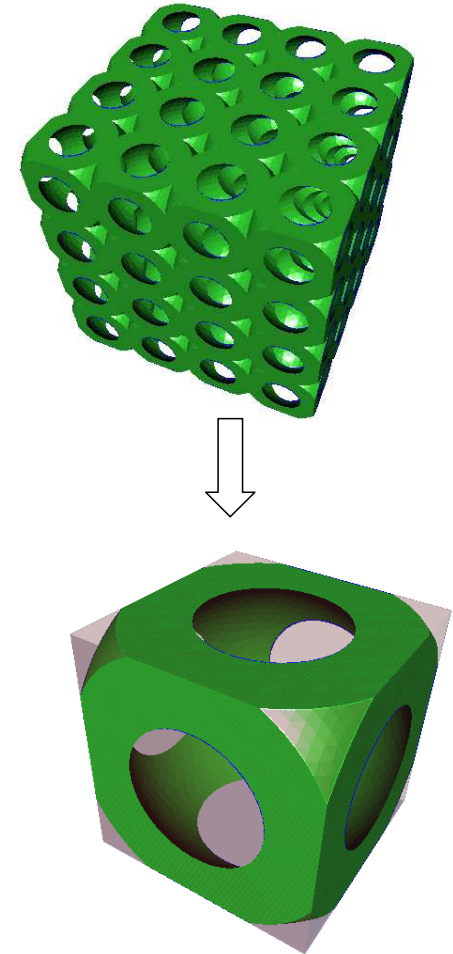
- Assumptions: Rigid skeleton, Stokes flow.
- Darcy, 1856 - a phenomenological theory suggesting that velocities are proportional to the pressure gradient:

$$\mathbf{v} = -\frac{1}{\mu} \mathbf{K} \nabla p,$$
$$\nabla \cdot \mathbf{v} = 0$$

- Derivation of Darcy's law by can be done by the asymptotic expansion method [Sanchez-Palencia and Ene, 1975]:

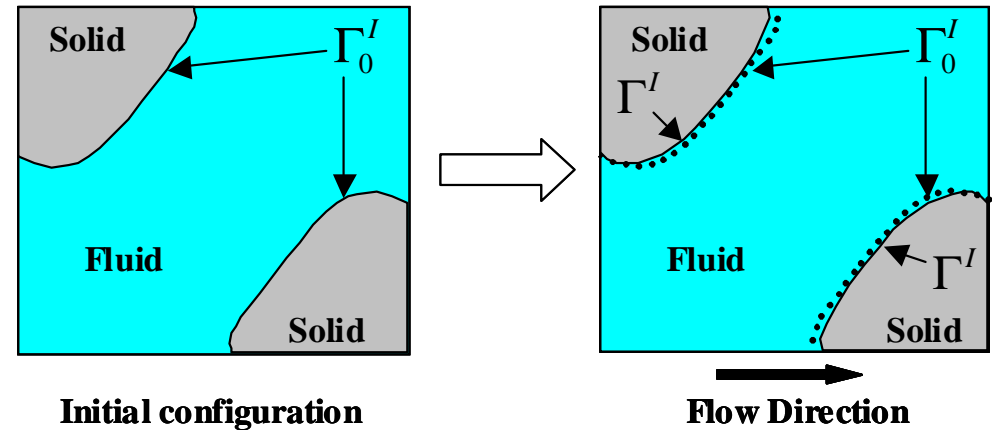
$$\mathbf{v}^\varepsilon = \varepsilon^2 \mathbf{v}^0 + \varepsilon^3 \mathbf{v}^1 + \dots,$$
$$p^\varepsilon = p^0 + \varepsilon p^1 + \dots$$

- Convergence proof can be found for example in Sanchez-Palencia [1980]



Upscaling of deformable porous media

- Elastic skeleton, small displacements of the interface compared to the pore size.
 - ◆ Biot [1941] - a phenomenological theory of consolidation:
 - ◆ Auriault and Sanchez-Palencia [1977] - Derivation of Biot's law by the homogenization method
 - ◆ Sanchez-Palencia [1980] - Derivation of Biot's law for time-dependent equations
- The macroscopic equations have the form:



$$\nabla \cdot \left(\mathcal{L}^* : \mathbf{e}(\mathbf{u}^{(0)}) - \mathbf{A}^* p^{(0)} \right) = \mathbf{0} \quad (1)$$

$$\nabla \cdot \left(\mathbf{K}^* \nabla p^{(0)} - n \frac{\partial \mathbf{u}^{(0)}}{\partial t} \right) = \boldsymbol{\gamma}^* : \mathbf{e} \left(\frac{\partial \mathbf{u}^{(0)}}{\partial t} \right) + \beta^* \frac{\partial p^{(0)}}{\partial t} \quad (2)$$

$$\mathbf{v}^{(0)} = n \frac{\partial \mathbf{u}^{(0)}}{\partial t} - \mathbf{K}^* \nabla p^{(0)} \quad (3)$$

Cell problems for Biot's law

- Standard cell problem for average elastic properties (\mathcal{L}^*):

$$\nabla \cdot (\mathcal{L} : \nabla \phi) = - (\nabla \cdot \mathcal{L}) : \mathbf{I}_4 \quad \text{in } \Omega^s \quad (4)$$

$$(\mathcal{L} : \nabla \phi) \mathbf{n}_0 = - (\mathcal{L} : \mathbf{I}_4) \mathbf{n}_0 \quad \text{on } \Gamma_0^I \quad (5)$$

- Pressure influence on the elasticity solution (\mathbf{A}^*):

$$\nabla \cdot (\mathcal{L} : \nabla \eta) = 0 \quad \text{in } \Omega^s \quad (6)$$

$$(\mathcal{L} : \nabla \eta) \mathbf{n}_0 = \mathbf{n}_0 \quad \text{on } \Gamma_0^I \quad (7)$$

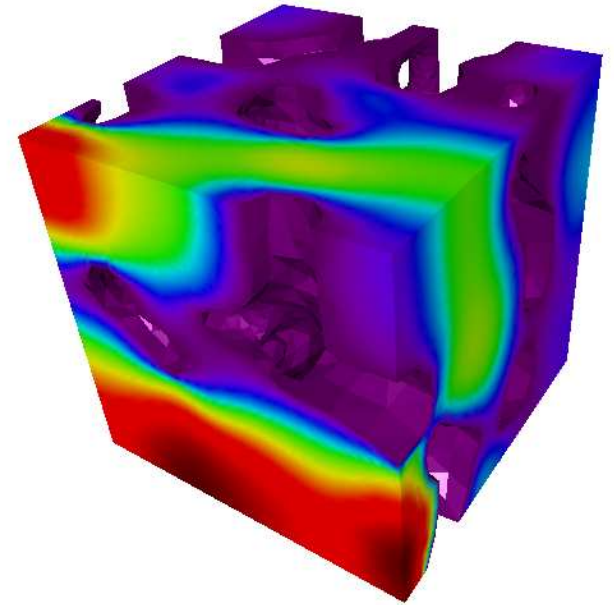
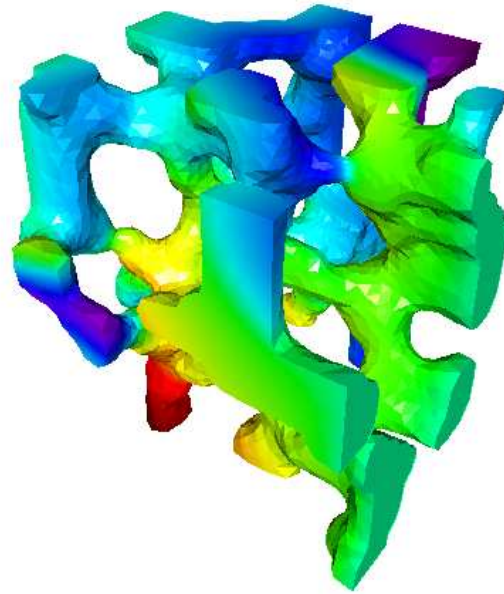
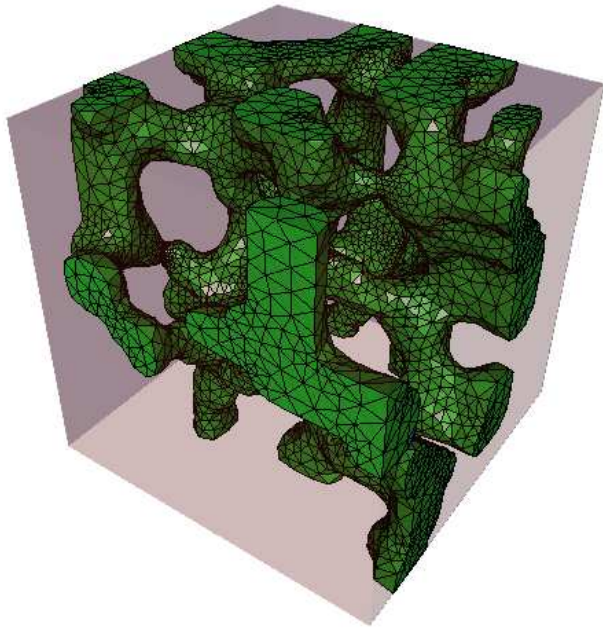
- Standard Darcy cell problem (\mathbf{K}^*):

$$\Delta \mathbf{w} + \nabla \mathbf{q} = -\mathbf{I} \quad \text{in } \Omega^f \quad (8)$$

$$\nabla \cdot \mathbf{w} = 0 \quad \text{in } \Omega^f \quad (9)$$

$$\mathbf{w} = \mathbf{0} \quad \text{on } \Gamma_0^I \quad (10)$$

Example: Nickel foam



Fluid-solid coupling term

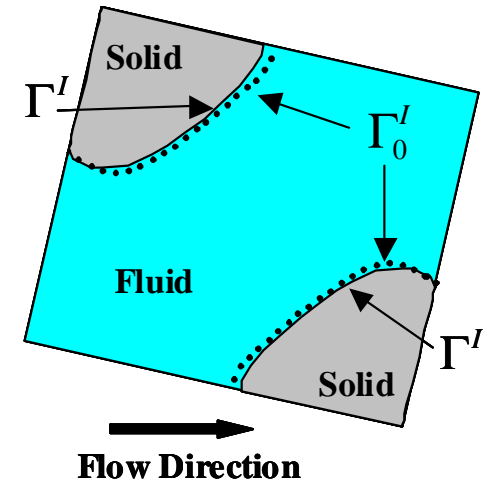
$$\mathbf{A}^* = \begin{pmatrix} 0.31 & 0.00 & 0.00 \\ 0.00 & 0.33 & 0.00 \\ 0.00 & 0.00 & 0.31 \end{pmatrix}$$

Darcy permeability

$$\mathbf{K}^* = \begin{pmatrix} 0.0045 & 0.0000 & 0.0000 \\ 0.0000 & 0.0025 & 0.0000 \\ 0.0000 & 0.0000 & 0.0043 \end{pmatrix}$$

Nonlinear extensions to Biot's law

- Various extensions have been proposed with less restrictive assumptions. For example, Lee and Mei [1997] assume:
 - ◆ Linear Elasticity.
 - ◆ Cell displacement can be decomposed into a rigid body motion + infinitely small deformation.
 - ◆ The rigid body motion is of the same order as the cell size.
- The macroscopic equations then become nonlinear:

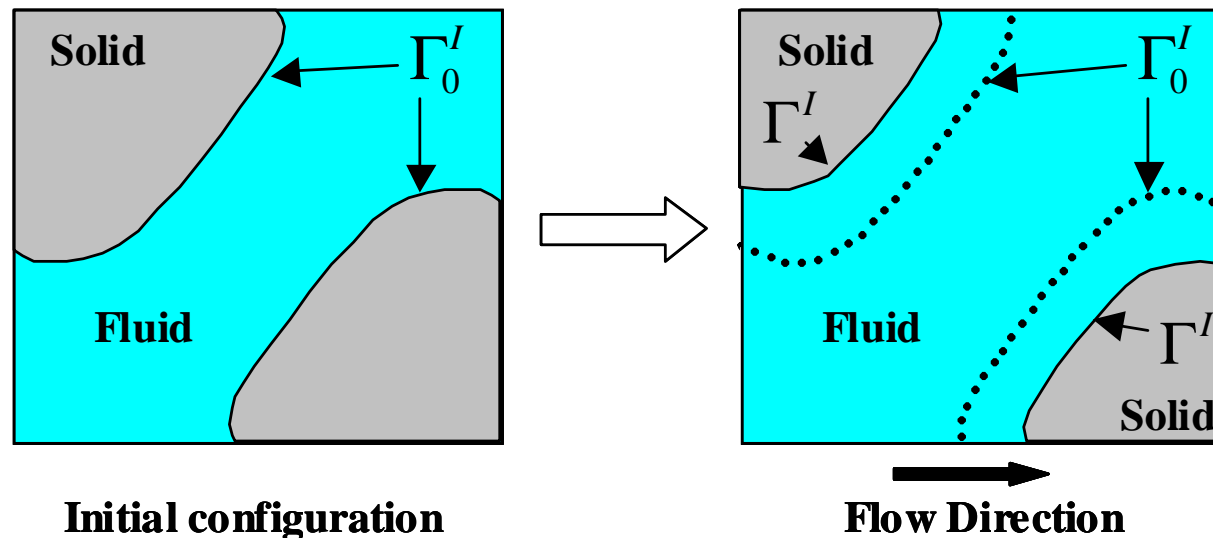


$$\nabla \cdot \left(\mathcal{L}^* : \mathbf{e}(\mathbf{u}^{(0)}) - \mathbf{A}^* p^{(0)} \right) = C \left(\mathbf{F}^* : \mathbf{e}(\mathbf{u}^{(0)}) + \boldsymbol{\alpha}^* p^{(0)} \right) : \nabla \mathbf{u}^{(0)} \quad (11)$$

$$\begin{aligned} \nabla \cdot \left(\mathbf{K}^* \nabla p^{(0)} - n \frac{\partial \mathbf{u}^{(0)}}{\partial t} \right) &= \gamma^* : \mathbf{e} \left(\frac{\partial \mathbf{u}^{(0)}}{\partial t} \right) + \beta^* \frac{\partial p^{(0)}}{\partial t} \\ &+ C \left(\mathbf{J}^* : \mathbf{e}(\mathbf{u}^{(0)}) + \mathbf{M}^* p^{(0)} \right) \nabla p^{(0)} \end{aligned} \quad (12)$$

Objectives

We consider an elastic skeleton, without restrictions on the displacements

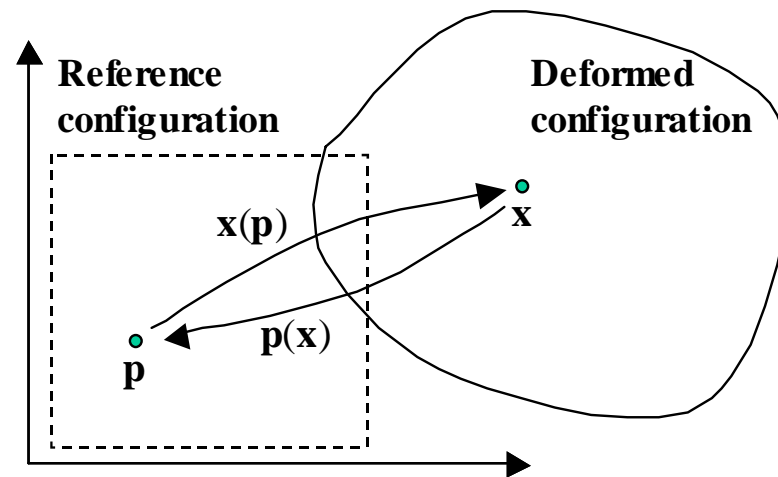


and we will:

- Present a numerical method for the solution of the coupled fluid-structure problem
- Derive an asymptotic solution for the flow in a long elastic channel
- Compare numerical results for a long channel with the asymptotic result

Reference and deformed configurations

- We associate the points of a continuum with points $\mathbf{p} \in \mathbb{R}^d$.
- The body undergoes a deformation $\mathbf{x} = \mathbf{x}(\mathbf{p})$:
- It's current state can be described either by *material* coordinates \mathbf{p} or *spatial* ones \mathbf{x} .
- Solid problems are typically defined on the reference (Lagrangian) configuration.
- Fluid problems are usually defined in the deformed (Eulerian) configuration.



Stress measures and conservation laws

- The (Cauchy) stress tensor $\mathbf{T}(\mathbf{x})$ is defined on the deformed configuration.
- the Piola-Kirchhoff stress tensor $\mathbf{S}(\mathbf{p})$ is defined in the reference configuration.
- The two are connected by

$$\mathbf{S}(\mathbf{p}) = \det(\mathbf{F}(\mathbf{p}))\mathbf{T}(\mathbf{x}(\mathbf{p}))\mathbf{F}^{-T}(\mathbf{p}). \quad (13)$$

- The balance of linear momentum reads:

$$-\nabla_{\mathbf{p}} \cdot \mathbf{S}(\mathbf{p}) = \mathbf{b}_0(\mathbf{p})$$

in the reference, and

$$-\nabla_{\mathbf{x}} \cdot \mathbf{T}(\mathbf{x}) = \mathbf{b}(\mathbf{x})$$

in the deformed configuration.

Elasticity problem

- Introducing the displacements and small strain tensor:

$$\mathbf{u}(\mathbf{p}) = \mathbf{x}(\mathbf{p}) - \mathbf{p}, \quad \mathbf{E}(\mathbf{p}) = \mathbf{e}(\mathbf{u}) = \frac{1}{2} (\nabla \mathbf{u}(\mathbf{p}) + \nabla \mathbf{u}(\mathbf{p})^T),$$

- A general nonlinear solid with internal variables is assumed:

$$\mathbf{S} = \frac{\partial W}{\partial \mathbf{F}}(\mathbf{F}, \boldsymbol{\xi}) \quad (14)$$

- The linearized elasticity problem is: *Find* $\mathbf{u}(\mathbf{p})$ *such that*

$$-\nabla \cdot (\mathbf{S}(\mathbf{E}, \boldsymbol{\xi})) = \mathbf{b}_0. \quad (15)$$

with Dirichlet

$$\mathbf{u} = \hat{\mathbf{u}} \text{ on } \Gamma_0^D \quad (16)$$

and/or Neumann

$$\mathbf{S} \mathbf{n}_0 = \hat{\mathbf{s}} \text{ on } \Gamma_0^N \quad (17)$$

boundary data with the usual conditions $\Gamma_0^D \cap \Gamma_0^N = \emptyset$ *and* $\Gamma_0^D \cup \Gamma_0^N = \Gamma_0$.

Fluid problem

- Given the symmetric part of the velocity gradient tensor

$$\mathbf{D}(\mathbf{x}) = \mathbf{e}(\mathbf{v}) = \frac{1}{2} (\nabla \mathbf{v}(\mathbf{x}) + \nabla \mathbf{v}(\mathbf{x})^T),$$

- A Newtonian fluid is one for which:

$$\mathbf{T} = -p\mathbf{I} + 2\mu\mathbf{D}.$$

- The fluid must satisfy the conservation of mass and momentum:

$$\begin{aligned}\nabla \cdot \mathbf{v} &= \mathbf{0}, \\ \rho(\mathbf{v} \cdot \nabla)\mathbf{v} &= -\nabla p + \mu\Delta\mathbf{v} + \mathbf{b}.\end{aligned}\tag{18}$$

- In the Stokes approximation, the quadratic term is disregarded:

$$-\mu\Delta\mathbf{v} + \nabla p = \mathbf{b}.\tag{19}$$

Fluid-Solid interface

- The velocity of the fluid on the interface Γ^I should be equal to the velocity of the interface itself:

$$\mathbf{v} = \mathbf{0} \text{ on } \Gamma^I. \quad (20)$$

- Continuity of normal component of the forces:

$$\mathbf{T}^f \mathbf{n} = \mathbf{T}^s \mathbf{n} \text{ on } \Gamma^I \quad (21)$$

where $\mathbf{n} = \mathbf{n}^s$ is the outward normal to the solid domain.

- The last equation, written on the (unknown) interface Γ^I reads:

$$-p\mathbf{n} + 2\mu\mathbf{D}\mathbf{n} = \det(\mathbf{F})^{-1}\mathbf{S}\mathbf{F}^T \mathbf{n} \text{ on } \Gamma^I \quad (22)$$

- Using equation (20), we can rewrite the last equation (22) as

$$\det(\nabla\mathbf{u} + \mathbf{I})(-p\mathbf{I} + 2\mu\mathbf{e}(\mathbf{v})) (\nabla\mathbf{u} + \mathbf{I})^{-T} \mathbf{n}_0 = (\mathbf{S}(\mathbf{e}(\mathbf{u}), \boldsymbol{\xi})) \mathbf{n}_0 \text{ on } \Gamma_0^I.$$

Fluid-structure interaction problem

■ Find Γ^I , \mathbf{v} , p and \mathbf{u} such that:

$$\Gamma^I = \{ \mathbf{p} + \mathbf{u}(\mathbf{p}) \mid \forall \mathbf{p} \in \Gamma_0^I \}, \quad (23)$$

$$\begin{aligned} -\mu \Delta \mathbf{v} + \nabla p &= \mathbf{b} && \text{in } \Omega^f, \\ \nabla \cdot \mathbf{v} &= 0 && \text{in } \Omega^f, \\ -\nabla \cdot (\mathbf{S}(\mathbf{e}(\mathbf{u}), \boldsymbol{\xi})) &= \mathbf{b}_0 && \text{in } \Omega_0^s, \end{aligned} \quad (24)$$

$$(\mathbf{S}(\mathbf{e}(\mathbf{u}), \boldsymbol{\xi})) \mathbf{n}_0 = \det(\nabla \mathbf{u} + \mathbf{I}) (-p \mathbf{I} + 2\mu \mathbf{e}(\mathbf{v})) (\nabla \mathbf{u} + \mathbf{I})^{-T} \mathbf{n}_0 \text{ on } \Gamma_0^I. \quad (25)$$

Weak form of the coupled system

- Let us introduce the form

$$g_{\Gamma_0^I}(\mathbf{v}, \mathbf{u}, p, \mathbf{w}) = \int_{\Gamma_0^I} \left\{ \det(\nabla \mathbf{u} + \mathbf{I})(-p\mathbf{I} + 2\mu \mathbf{e}(\mathbf{v})) (\nabla \mathbf{u} + \mathbf{I})^{-T} \right\} \mathbf{w} ds.$$

- The FSI problem (24)-(25) can be restated in a weak form:

Find the interface Γ^I , the deformed configuration of the fluid domain Ω^f , the displacements $\mathbf{u} \in [H^1(\Omega_0^s)]^d$, velocity $\mathbf{v} \in [H_0^1(\Omega^f)]^d$ and pressure $p \in L_0^2(\Omega^f)$ such that

$$\begin{aligned} D_{\Omega^f}(\mathbf{v}, \mathbf{w}) - (p, \nabla \cdot \mathbf{w})_{\Omega^f} &= (\mathbf{b}, \mathbf{w})_{\Omega^f}, & \forall \mathbf{w} \in [H_0^1(\Omega^f)]^d, \\ -(\nabla \cdot \mathbf{v}, q)_{\Omega^f} &= 0, & \forall q \in L^2(\Omega^f), \\ a_{\Omega_0^s}(\mathbf{u}, \mathbf{w}) &= (\mathbf{b}_0, \mathbf{w})_{\Omega_0^s} + g_{\Gamma_0^I}(\mathbf{v}, \mathbf{u}, p, \mathbf{w}), & \forall \mathbf{w} \in [H_D^1(\Omega_0^s)]^d, \\ \Gamma &= \{\mathbf{p} + \mathbf{u}(\mathbf{p}) \mid \forall \mathbf{p} \in \Gamma_0\}. \end{aligned} \tag{26}$$

Discretization of the FSI problem

- Let us introduce finite-dimensional subspaces $U_{\mathbf{v}}$, U_p and $U_{\mathbf{u}}$ for the velocity, pressure and displacements, respectively:

$$U_{\mathbf{v}} = \left[\left\{ v \in C^0(\Omega^f) \mid v \text{ is quadratic polynomial on } \forall \tau \in \mathcal{T}_h^f \right\} \right]^d \subset [H^1(\Omega^f)]^d,$$

$$U_p = \left\{ p \in C^0(\Omega^f) \mid p \text{ is linear on } \forall \tau \in \mathcal{T}_h^f \right\} \subset H^1(\Omega^f) \subset L^2(\Omega^f),$$

$$U_{\mathbf{u}} = \left[\left\{ u \in C^0(\Omega_0^s) \mid u \text{ is linear on } \forall \tau \in \mathcal{T}_h^s \right\} \right]^d \subset [H^1(\Omega_0^s)]^d.$$

- Conformity between the fluid \mathcal{T}_h^f and solid \mathcal{T}_h^s triangulations is maintained on the reference configuration of the interface Γ_0 .
- The first three equations in (26) lead to the nonlinear system of algebraic equations

$$\begin{pmatrix} \mathbf{A}(\mathbf{u}) & \mathbf{C}^T(\mathbf{u}) & \mathbf{0} \\ \mathbf{C}(\mathbf{u}) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{K} \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{p} \\ \mathbf{u} \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{0} \\ \mathbf{f}_2 + \mathbf{g}(\mathbf{u}, \mathbf{v}, \mathbf{p}) \end{pmatrix}, \quad (27)$$

Direct iteration for the FSI problem

- Considering the following iterative approach for solving the FSI problem (26):
 - ◆ Solve the Stokes equation in the fluid domain treating the solid as a rigid body;
 - ◆ Transfer the forces to the solid;
 - ◆ Calculate the displacement field in the solid and then **update** the fluid domain.
- Starting with $\mathbf{u}_0 = \mathbf{0}$, $\mathbf{v}_0 = \mathbf{0}$, $p_0 = 0$, use a fixed point iteration to solve (26):

$$\begin{pmatrix} \mathbf{A}(\mathbf{u}_k) & \mathbf{C}^T(\mathbf{u}_k) & \mathbf{0} \\ \mathbf{C}(\mathbf{u}_k) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{K} \end{pmatrix} \begin{pmatrix} \mathbf{v}_{k+1} \\ \mathbf{p}_{k+1} \\ \mathbf{u}_{k+1} \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{0} \\ \mathbf{f}_2 + \mathbf{g}(\mathbf{u}_k, \mathbf{v}_{k+1}, \mathbf{p}_{k+1}) \end{pmatrix} \quad (28)$$

- The algebraic systems of linear equations for both subproblems are solved by the Conjugate Gradient Method:
 - ◆ The elasticity matrix \mathbf{K} is preconditioned by a **MIC – 0 displacement decomposition** preconditioner [Blaheta, 1994]
 - ◆ A **pressure Schur complement** approach is used for the Stokes system [Turek, 1999]

Remeshing of the fluid domain

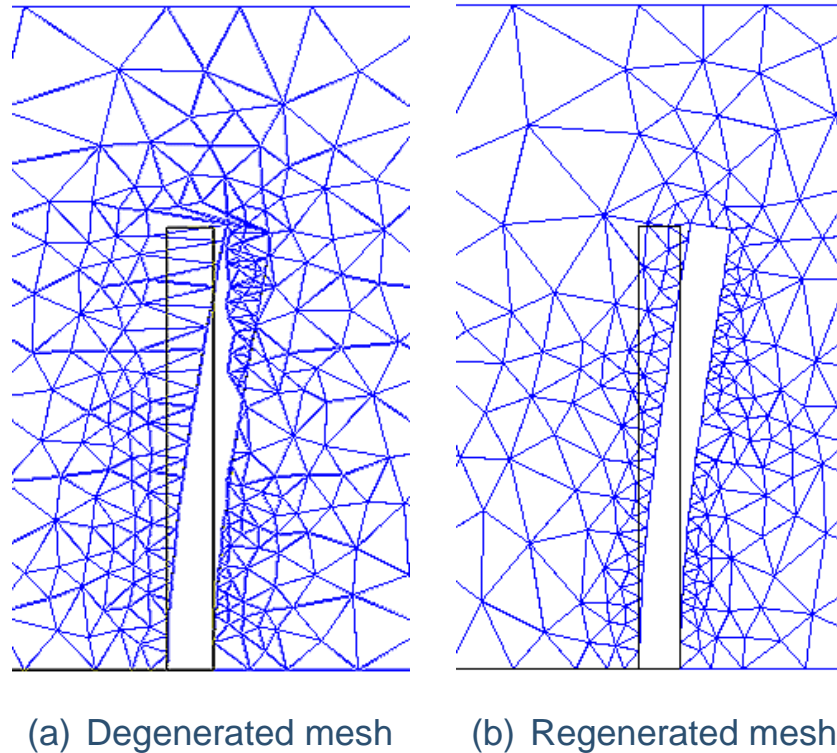
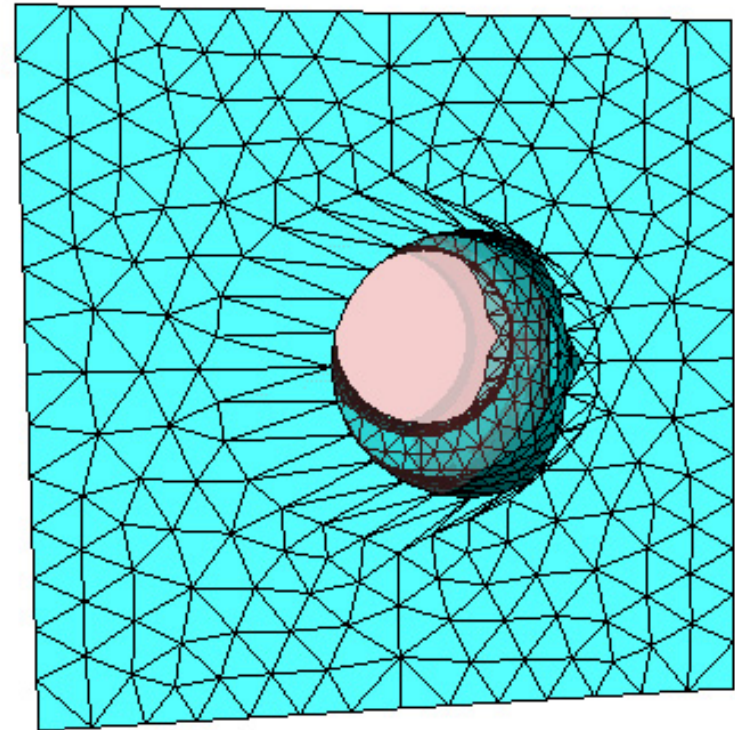


Figure 1: In this example an elastic obstacle deforms to the left in response to flow in the channel. The solid lines indicated its initial configuration. If only the boundary nodes of the fluid mesh are moved, it degenerates (left). The second mesh (right) is obtained after remeshing the fluid domain.

Remeshing of the fluid domain (cont.)



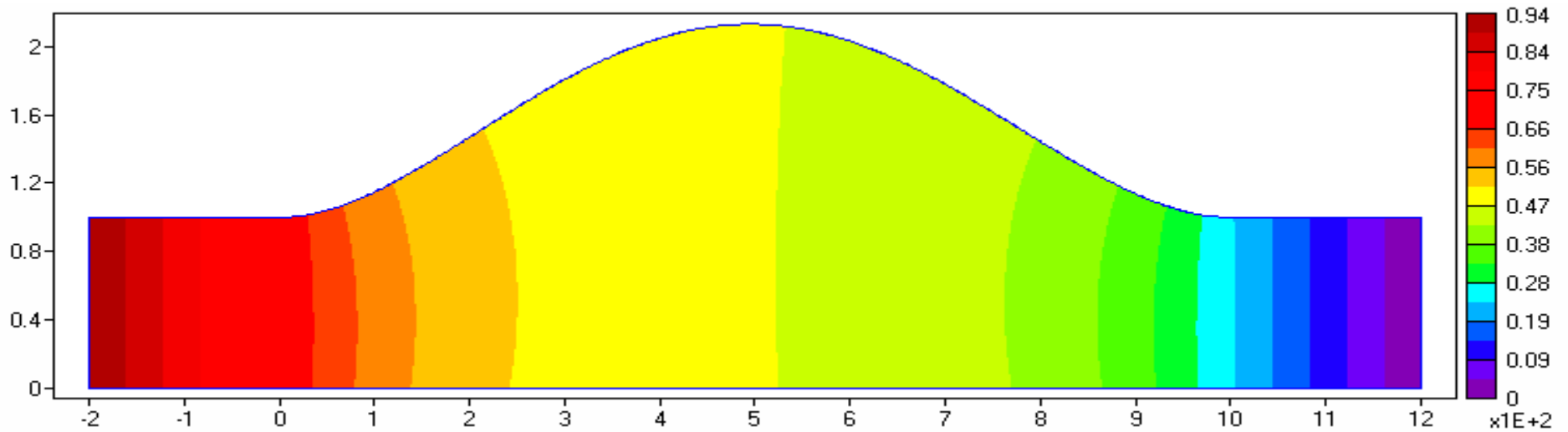
(a) Flow external to a elastic skeleton



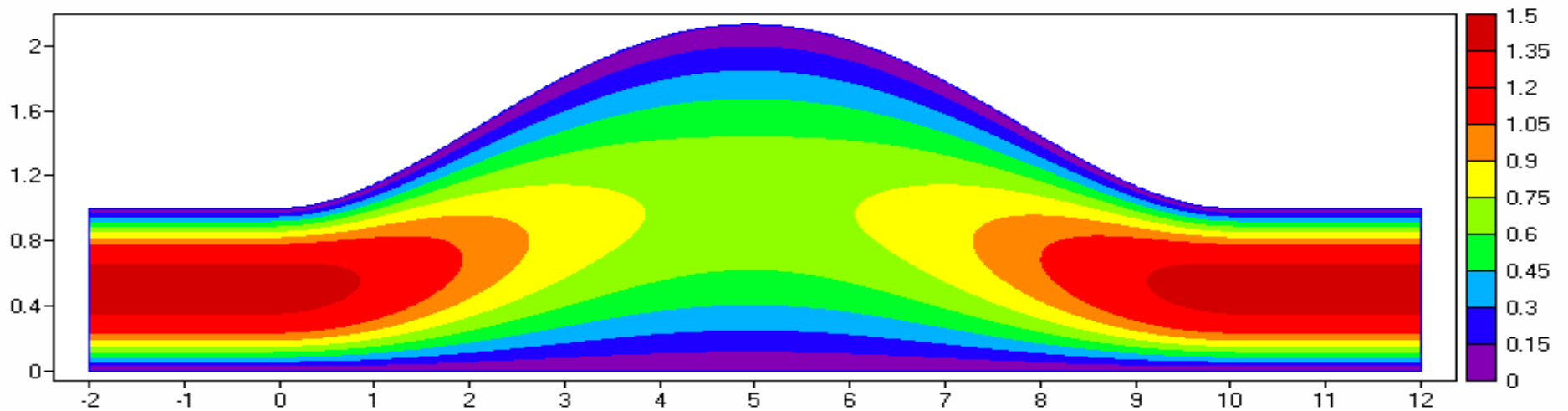
(b) Degenerated mesh after first iteration

Figure 2: Another case when the mesh degenerates after a new position of the interface is computed.

Channel with deformable segment



Final configuration of the fluid domain Ω^f and pressure profile. (Figure not drawn to scale).



Profile of the horizontal velocity component (Figure not drawn to scale).

Deformable segment: Flow rate vs. pressure

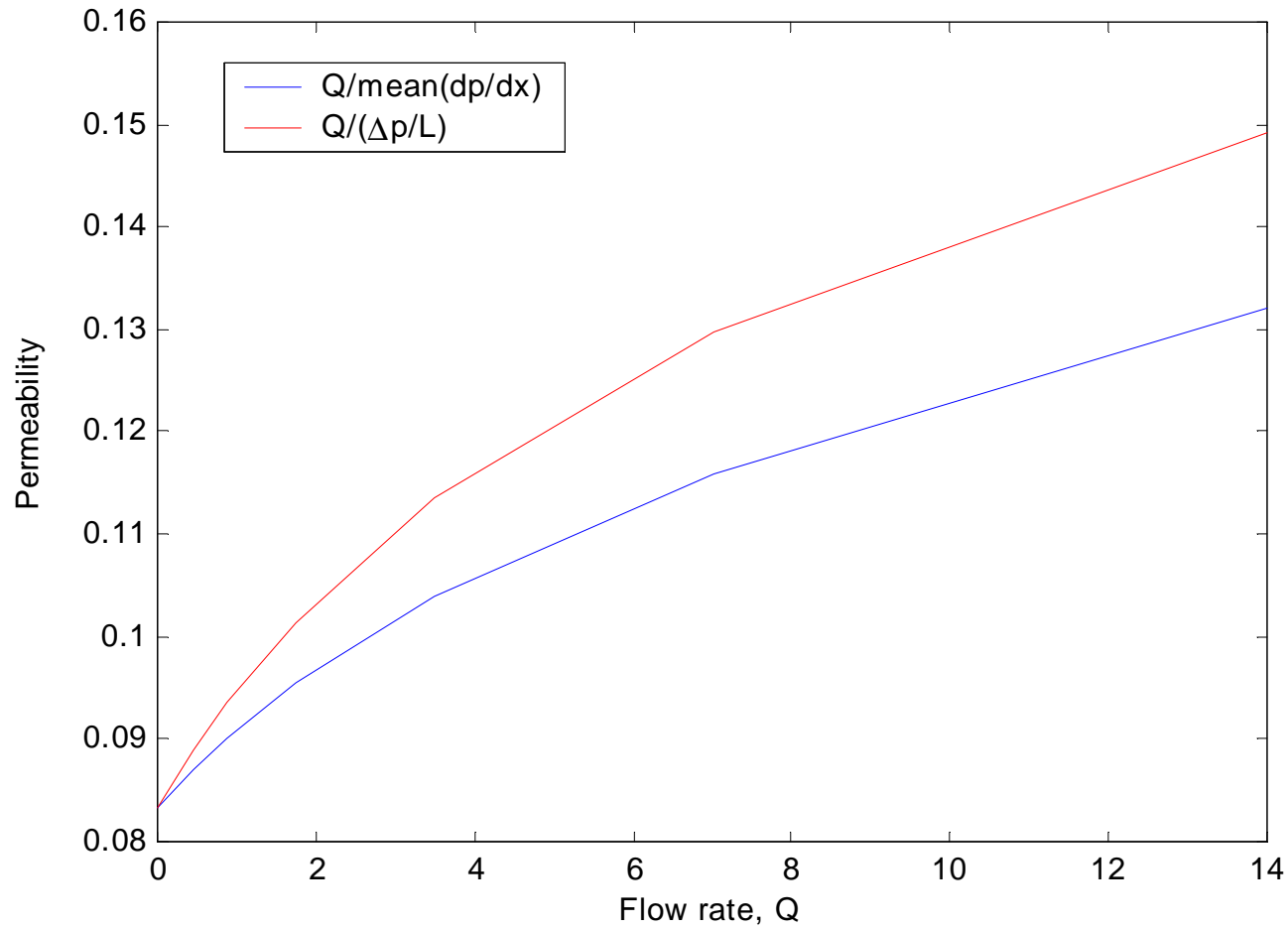
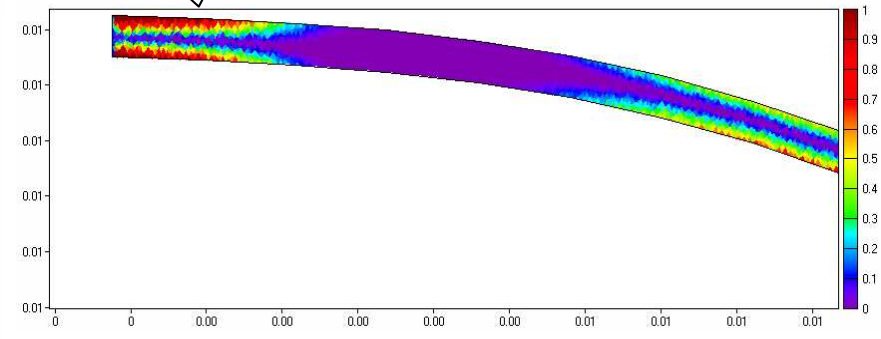
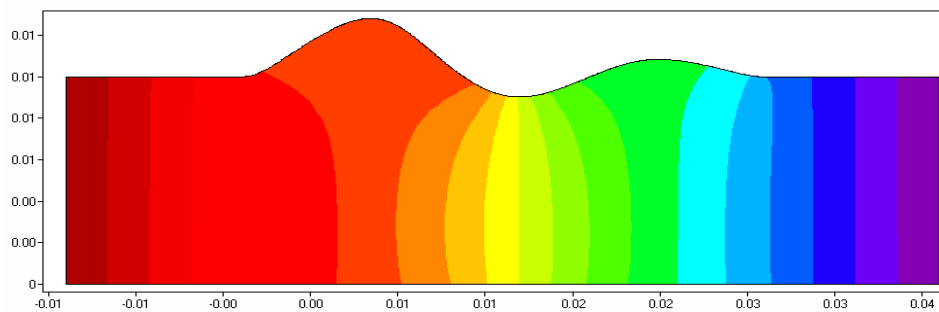
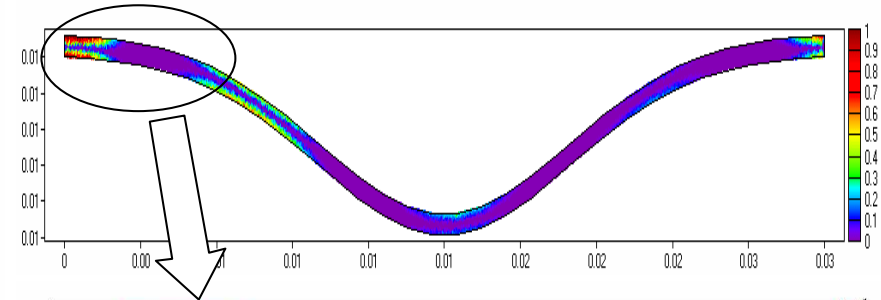
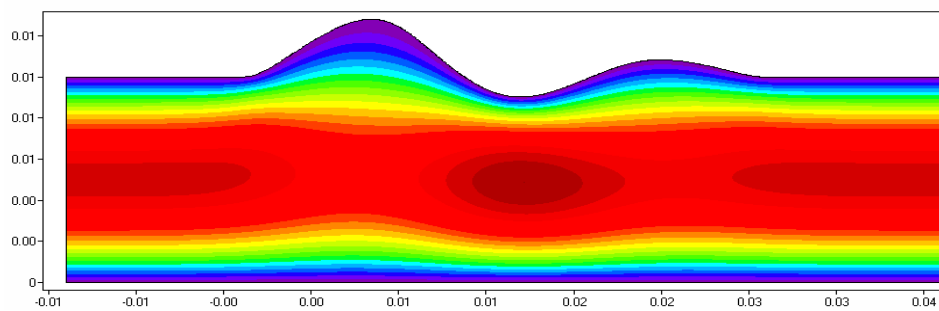
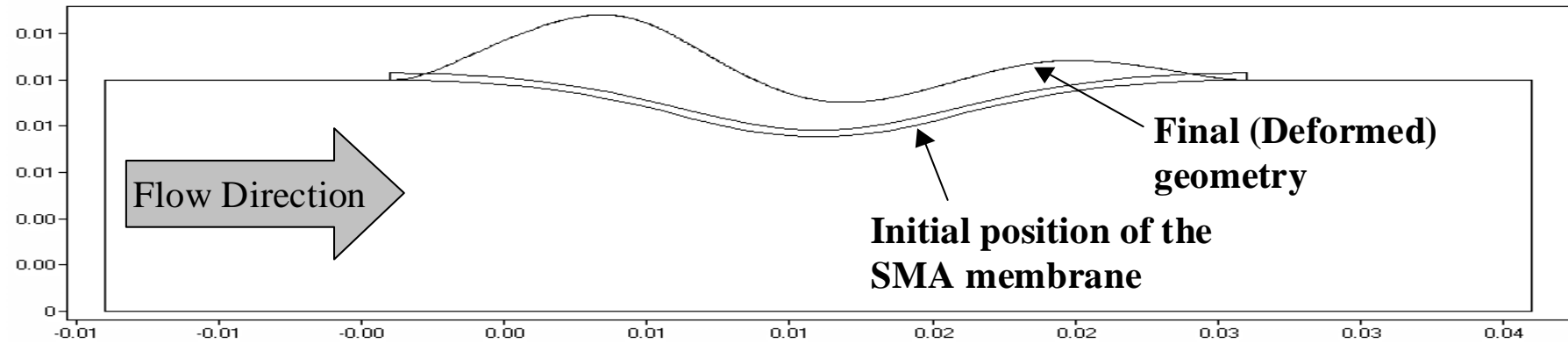
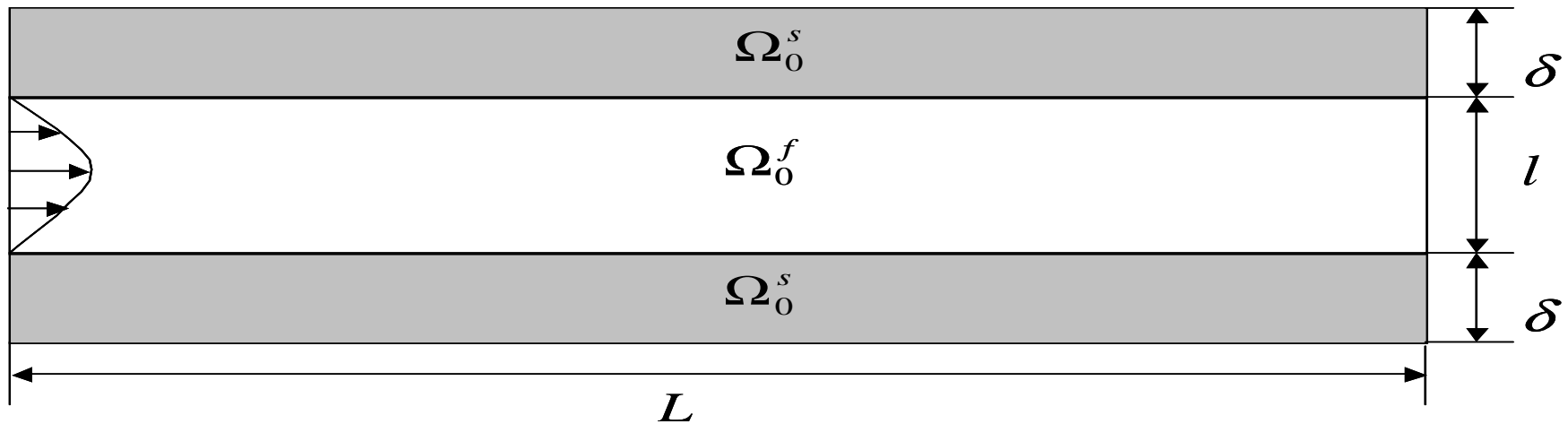


Figure 3: Channel permeability as a function of different flow rates.

Flow in a Channel with an SMA Segment



Flow in elastic channel



- Let the channel thickness l be much smaller than its length L and introduce the small parameter

$$\varepsilon = \frac{l}{L} \quad (29)$$

Asymptotic expansion of FSI problem

- Consider an asymptotic expansions with respect to ε of the field variables (velocity, pressure, displacement) of the **FSI problem**:

$$v_1 = v_1^0 + \varepsilon v_1^1 + \varepsilon^2 v_1^2 + \dots$$

$$v_2 = v_2^0 + \varepsilon v_2^1 + \varepsilon^2 v_2^2 + \dots$$

$$p = p^0 + \varepsilon p^1 + \varepsilon^2 p^2 + \dots$$

$$u_1 = u_1^0 + \varepsilon u_1^1 + \varepsilon^2 u_1^2 + \dots$$

$$u_2 = u_2^0 + \varepsilon u_2^1 + \varepsilon^2 u_2^2 + \dots$$

- Substituting in the Stokes system (18),(19), we get at the 0^{th} order

$$p^0 = p^0(x), \quad \langle v_1(x) \rangle = -\frac{1}{3} \gamma^3(x) \frac{\partial p^0}{\partial x}$$

$$\frac{\partial}{\partial x} \left(\gamma^3(x) \frac{\partial p^0}{\partial x} \right) = 0.$$

Asymptotic expansion (cont.)

- For the solid domain, assume that
 - ◆ Isotropic material ($\mathbf{S} = \mathcal{L} : \mathbf{E} = \lambda_s : \text{tr}(\mathbf{E})\mathbf{I} + 2\mu_s\mathbf{E}$)
 - ◆ $\delta \sim l$
 - ◆ both u_1 and u_2 are of order δ
- Then, one can solve the elasticity system at the zero order for ε and obtain

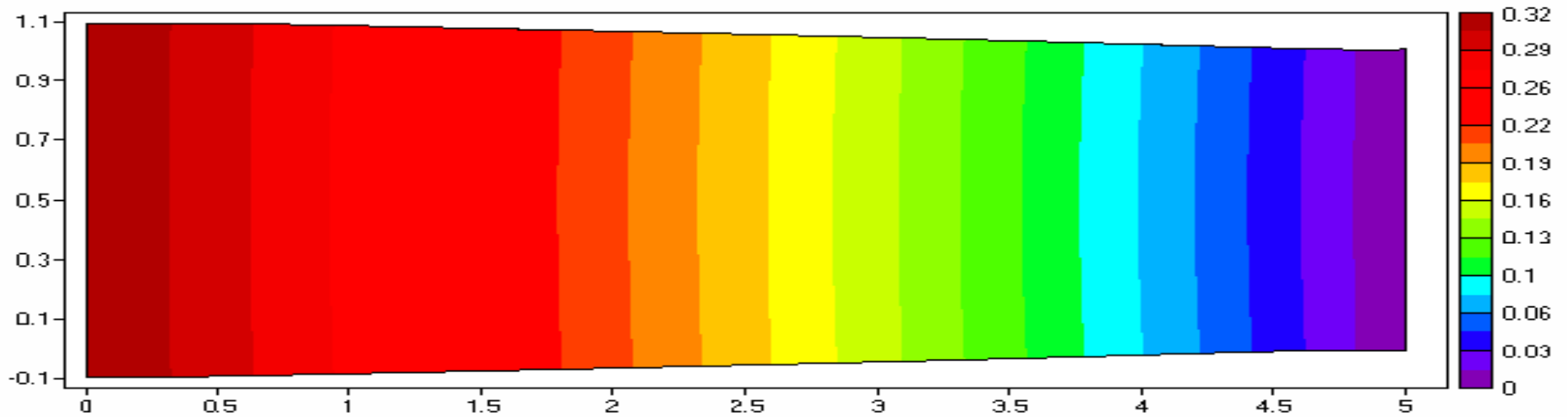
$$\sigma^{S,0} = \frac{\delta}{l} \begin{bmatrix} \frac{\lambda_s}{\lambda_s + 2\mu_s} c_2(x) & \frac{\mu_s}{\lambda_s + 2\mu_s} c_1(x) \\ \frac{\mu_s}{\lambda_s + 2\mu_s} c_1(x) & \frac{\lambda_s + 2\mu_s}{\lambda_s + 2\mu_s} c_2(x) \end{bmatrix}$$

- Using the interface condition, we get

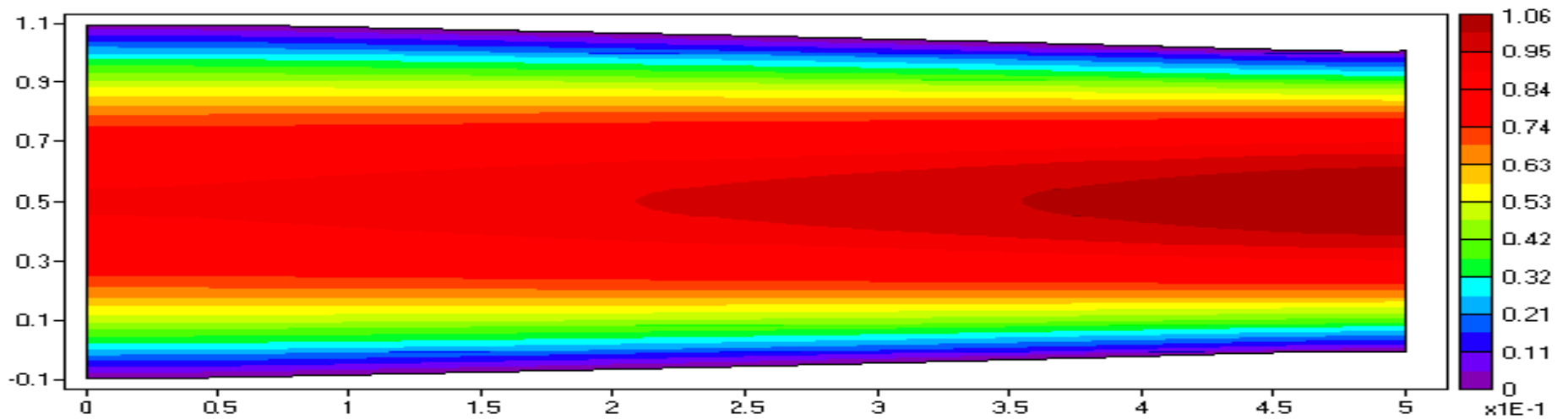
$$\gamma(x) \approx 1 + \delta \frac{1}{\lambda_s + 2\mu_s} p^0(x),$$

$$K = K(x, p^0(x)) = \frac{1}{3} \gamma^3(x) \approx \frac{1}{3} \left(1 + \delta \frac{1}{\lambda_s + 2\mu_s} p^0(x) \right)^3.$$

Long elastic channel: A typical solution



Final configuration of the fluid domain Ω^f and pressure profile.



Profile of the horizontal velocity component.

Numerical experiments

Table 1: Comparisons of asymptotic results with numerical values

P^0	$\frac{\ \bar{\gamma} - \gamma\ _{L^2}}{\ \gamma\ _{L^2}}$		$\frac{\ \bar{K} - K\ _{L^2}}{\ K\ _{L^2}}$	
	$\varepsilon = \frac{1}{10}$	$\varepsilon = \frac{1}{20}$	$\varepsilon = \frac{1}{10}$	$\varepsilon = \frac{1}{20}$
0.32	2.41×10^{-3}	8.47×10^{-4}	6.63×10^{-3}	1.82×10^{-3}
0.16	1.19×10^{-3}	4.21×10^{-4}	3.33×10^{-3}	1.06×10^{-3}
0.08	5.96×10^{-4}	2.10×10^{-4}	1.65×10^{-3}	5.34×10^{-4}
0.04	2.98×10^{-4}	1.05×10^{-4}	8.19×10^{-4}	2.68×10^{-4}

Long elastic channel: Permeability

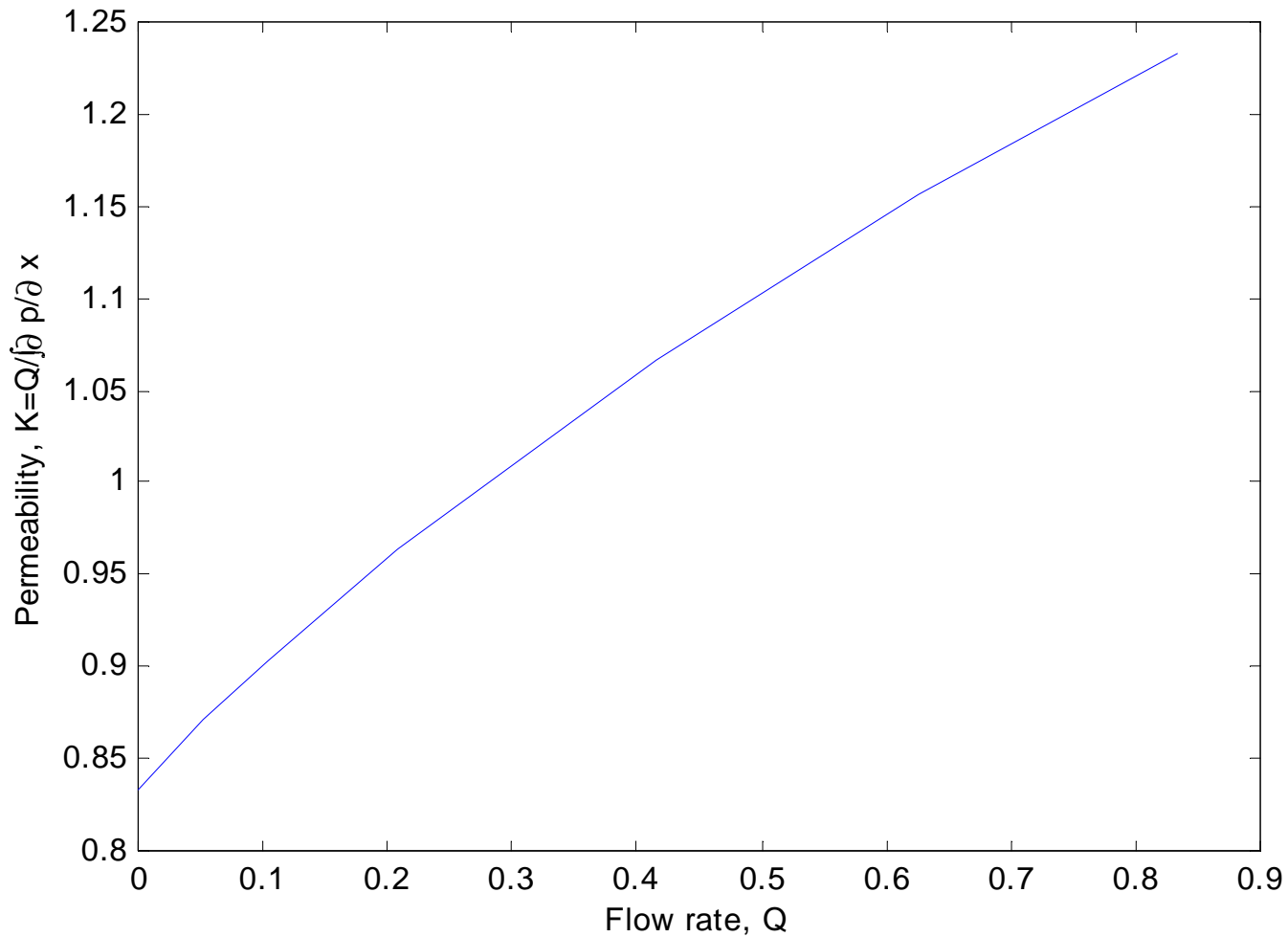


Figure 4: Channel permeability as a function of different flow rates.

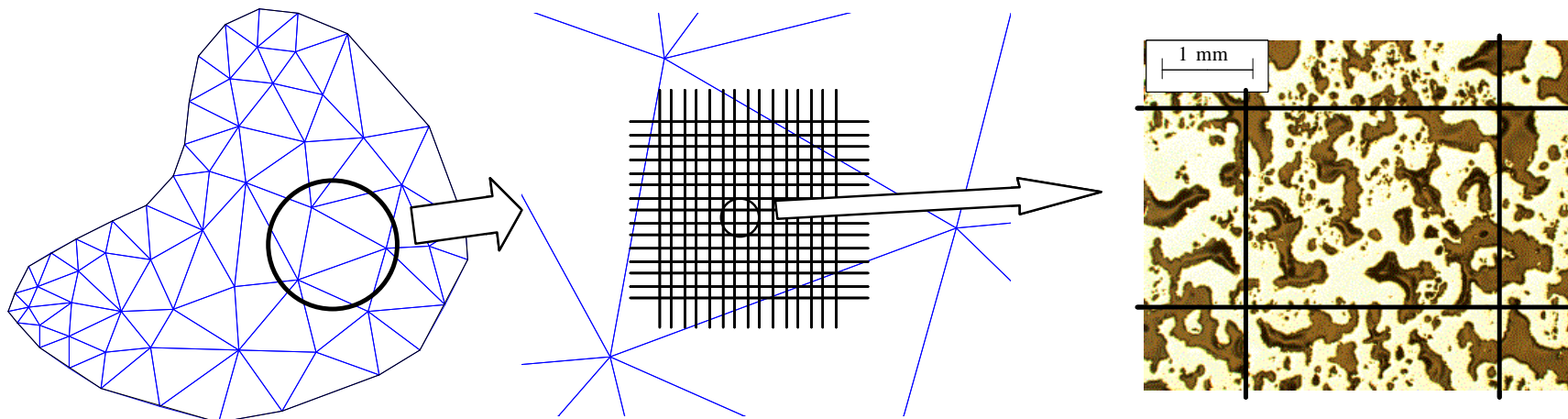
Numerical upscaling

- Macroscopic model for general 2D/3D geometries

$$\nabla \cdot (\mathbf{K}(\mathbf{x}, \langle p \rangle, \mathbf{e}(\langle \mathbf{u} \rangle)) \nabla \langle p \rangle) = f(\langle p \rangle, \nabla \langle p \rangle, \mathbf{e}(\langle \mathbf{u} \rangle)) \quad (\text{Diffusion}) \quad (30)$$

$$\nabla \cdot \mathbf{S}(\mathbf{e}(\langle \mathbf{u} \rangle), \langle p \rangle, \mathcal{Z}, \mathcal{P}) = \mathbf{b}(\langle p \rangle, \nabla \langle p \rangle, \mathbf{e}(\langle \mathbf{u} \rangle)) \quad (\text{Elasticity}) \quad (31)$$

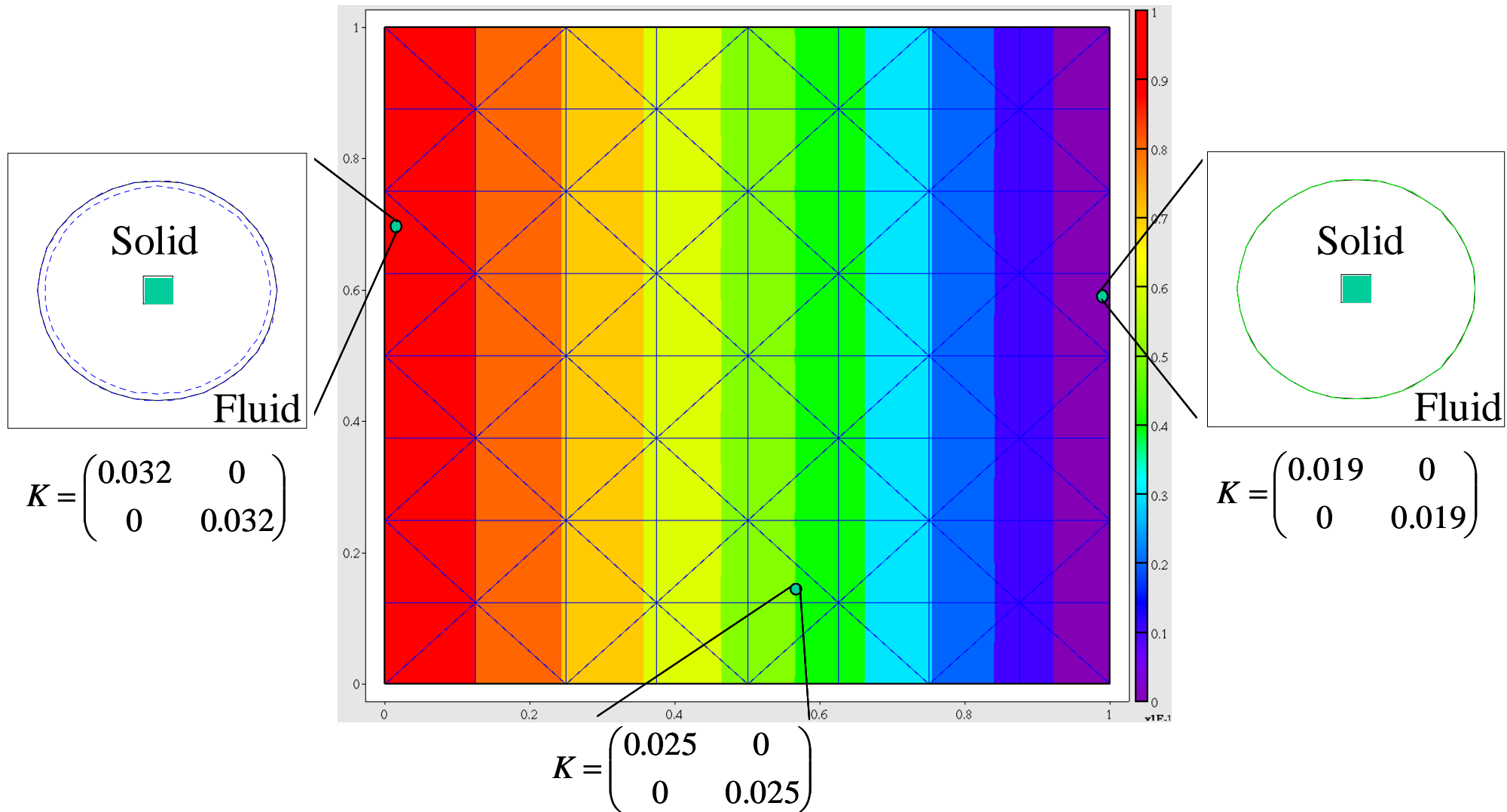
- Discretize the macroscopic problem using finite elements:



Macroscopic discretization

Microscopic RVE

Numerical upscaling: Example



Future Work

- Numerical upscaling: Macroscopic elasticity, rigorous justification of macroscopic model
- Determine the upscaling parameters for general 3D geometries ($\langle p \rangle$, $\nabla \langle p \rangle$, $e(\langle \mathbf{u} \rangle)$, ...)
- Validate models against microscale solutions
- Check the validity range of nonlinear extensions of Lee and Mei [1997] to Biot's equations

The End

Questions?

Direct iteration for the FSI problem (cont.)

Set $\mathbf{u}_0 = \mathbf{0}$. For $k = 0, 1, \dots$ until convergence do:

1. Find \mathbf{v}_k, p_k which satisfy the Stokes equations (18),(19) in Ω_k^f with the no-slip boundary condition on the interface Γ_k^I and the appropriate boundary conditions on $\partial\Omega_k^f \setminus \Gamma_k^I$.
2. Compute the traction $\mathbf{t}_k = \mathbf{T}\mathbf{n}_k$ on the interface Γ_k^I using equation (22).
3. Based on \mathbf{t}_k compute the tractions \mathbf{s}_k in the reference configuration of the interface, i.e. Γ_0^I using equation (13) and the current iterate for the displacements \mathbf{u}_k .
4. Find \mathbf{u}_{k+1} which satisfies the balance of linear momentum (15) in Ω_k^s with $\mathbf{S}\mathbf{n}_0 = \mathbf{s}_k$ and the appropriate boundary data on $\partial\Omega_k^s \setminus \Gamma_0^I$.
5. Compute $\Gamma_{k+1}^I = \{\mathbf{p} + \mathbf{u}_{k+1}(\mathbf{p}) | \forall p \in \Gamma_0^I\}$ and Ω_{k+1}^f :
6. Check convergence: $\|\mathbf{u}_{k+1} - \mathbf{u}_k\|_{\Gamma_{k+1}^I} < TOLERANCE * \|\mathbf{u}_{k+1}\|_{\Gamma_{k+1}^I}$. The norm is the discrete euclidian norm of the interface nodal values.

Weak form of the elasticity problem

- Let us introduce the bilinear form

$$a_{\Omega_0}(\mathbf{u}, \mathbf{w}) = \int_{\Omega_0} (\mathcal{L} : \mathbf{e}(\mathbf{u})) : \mathbf{e}(\mathbf{w}) dx.$$

- The weak form of the *linear* elasticity problem is:

Given $\hat{\mathbf{u}} \in [H^{1/2}(\Gamma^D)]^d$ and $\mathbf{b}_0 \in [H^{-1}(\Omega_0^s)]^d$, Find $\mathbf{u} \in [H^1(\Omega_0^s)]^d$ such that

$$\begin{aligned} a_{\Omega_0^s}(\mathbf{u}, \mathbf{w}) &= (\mathbf{b}_0, \mathbf{w})_{\Omega_0^s} + (\hat{\mathbf{s}}, \mathbf{w})_{\Gamma_0^N}, & \forall \mathbf{w} \in [H_D^1(\Omega_0^s)]^d, \\ \mathbf{u} &= \hat{\mathbf{u}}, & \text{on } \Gamma_0^D. \end{aligned} \quad (32)$$

- The problem (32) has unique solution iff Korn's inequality holds, i.e., $\exists C > 0$ such that

$$\int_{\Omega_0} \mathbf{e}(\mathbf{u}) : \mathbf{e}(\mathbf{u}) dx > C |\mathbf{u}|_1^2$$

Approximation to the elasticity problem

The Elasticity problem is solved by linear, triangular finite elements.

- Given a triangulation \mathcal{T}_h^s of Ω_0^s , the approximation space for the displacements is

$$U_{\mathbf{u}} = \left[\left\{ u \in C^0(\Omega_0^s) \mid u \text{ is linear on } \forall \tau \in \mathcal{T}_h^s \right\} \right]^d \subset \left[H^1(\Omega_0^s) \right]^d. \quad (33)$$

- Denote by ϕ_i^j , $i = 1 \dots N_v$, $j = 1 \dots d$ the nodal basis functions for the displacement space $U_{\mathbf{u}}$. The weak form (32) gives rise to the linear system

$$\mathbf{K}\mathbf{u} = \mathbf{b}, \quad (34)$$

$$\mathbf{K} = \begin{pmatrix} \mathbf{K}_{11} & \cdots & \mathbf{K}_{1d} \\ \vdots & \ddots & \vdots \\ \mathbf{K}_{d1} & \cdots & \mathbf{K}_{dd} \end{pmatrix}. \quad (35)$$

Solution to the elasticity linear system

The stiffness matrix \mathbf{K} is symmetric, positive definite and sparse, making it ideal for the application of the PCG method.

- Consider the matrix

$$\mathbf{K}_{SDC} = \text{diag}(\mathbf{K}_{11}, \dots, \mathbf{K}_{dd})$$

- It can be shown that \mathbf{K}_{SDC} is an optimal preconditioner for \mathbf{K} [Blaheta, 1994]:

$$\text{cond}((\mathbf{K}_{SDC})^{-1}\mathbf{K}) \leq \frac{d-1}{\gamma} \frac{1-\nu}{1-2\nu}, \quad (36)$$

- The application of $(\mathbf{K}_{SDC})^{-1}$ at each CG iteration for (34) can be done by multigrid in linear time, leading to an optimal method.
- We use a $MIC(0)$ factorization of \mathbf{K}_{SDC} which results in an $\mathcal{O}(h^{3/2})$ algorithm.

Weak form of the Stokes problem

- Let $D_{\Omega^f}(\mathbf{v}, \mathbf{w})$ be the vector Dirichlet form

$$D_{\Omega^f}(\mathbf{v}, \mathbf{w}) = \int_{\Omega^f} \mu \nabla \mathbf{v} : \nabla \mathbf{w} d\mathbf{x}.$$

- Find $\mathbf{v} \in [H_0^1(\Omega^f)]^d$, $p \in L_0^2(\Omega^f)$ such that

$$\begin{aligned} D_{\Omega^f}(\mathbf{v}, \mathbf{w}) - (p, \nabla \cdot \mathbf{w})_{\Omega^f} &= (\mathbf{b}, \mathbf{w})_{\Omega^f}, & \forall \mathbf{w} \in [H_0^1(\Omega^f)]^d, \\ -(\nabla \cdot \mathbf{v}, q)_{\Omega^f} &= 0, & \forall q \in L^2(\Omega^f). \end{aligned} \quad (37)$$

- The problem (37) has unique solution iff $\exists C > 0$ such that

$$\inf_{\forall p \in L_0^2(\Omega^f)} \sup_{\forall \mathbf{v} \in [H_0^1(\Omega^f)]^d} \frac{(p, \nabla \cdot \mathbf{v})_{\Omega^f}^2}{D_{\Omega^f}(\mathbf{v}, \mathbf{v})} > C \quad (38)$$

Approximation to the Stokes problem

The Stokes problem is solved using the LBB stable P_2P_1 (Taylor-Hood) element pair.

- Given a triangulation \mathcal{T}_h^f of Ω^f the approximation spaces for the velocity and pressure are:

$$U_{\mathbf{v}} = \left[\left\{ v \in C^0(\Omega^f) \mid v \text{ is quadratic polynomial on } \forall \tau \in \mathcal{T}_h^f \right\} \right]^d \subset [H^1(\Omega^f)]^d$$

$$U_p = \{ p \in C^0(\Omega^f) \mid p \text{ is linear on } \forall \tau \in \mathcal{T}_h \} \subset H^1(\Omega^f) \subset L^2(\Omega^f)$$

- By ordering the velocity unknowns first, followed by the pressure, the weak problem (37) results in a linear systems

$$\begin{pmatrix} \mathbf{A} & \mathbf{C}^T \\ \mathbf{C} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{d} \end{pmatrix}. \quad (39)$$

- From the discrete version of the LBB condition (38) it follows that (39) is nonsingular.

Solution to the Stokes linear system

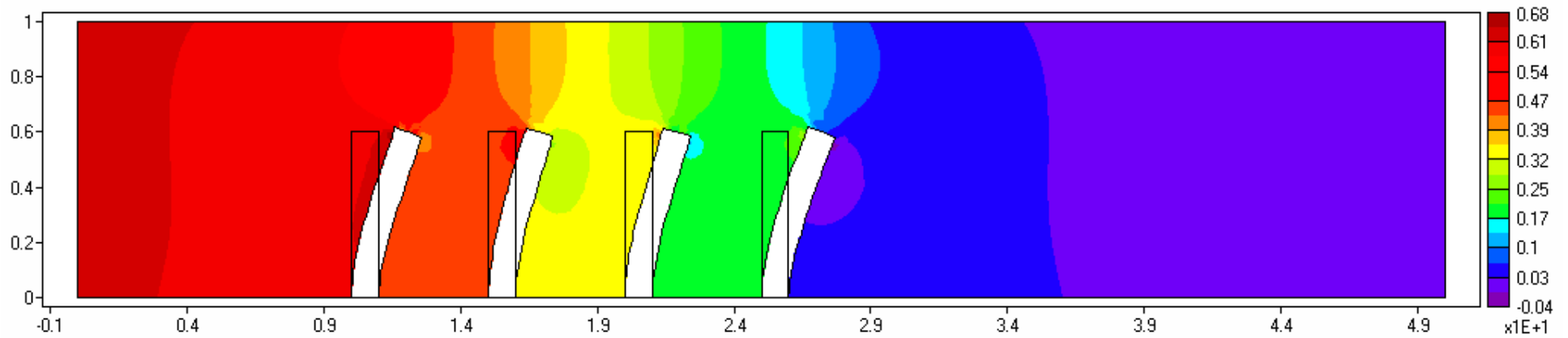
- Since \mathbf{A} is an invertible matrix one can eliminate the first row of (39) and obtain:

$$\mathbf{C}\mathbf{A}^{-1}\mathbf{C}^T\mathbf{p} = \mathbf{C}\mathbf{A}^{-1}\mathbf{f} - \mathbf{d}. \quad (40)$$

- The Schur complement $\mathbf{S} = \mathbf{C}\mathbf{A}^{-1}\mathbf{C}^T$ is a symmetric, positive definite system therefore we can solve (40) using the PCG method
- the PCG algorithm only requires the computation of the action of \mathbf{S} on a vector, and this can be done, provided that action of \mathbf{A}^{-1} can be computed efficiently.
- The velocity block \mathbf{A} is a block diagonal matrix, each block corresponding to a Laplacian stiffness matrix, and these can be inverted efficiently (in $\mathcal{O}(N)$ operations with multigrid, for example).
- Further, the Schur complement itself can be preconditioned by a mass matrix \mathbf{M}^p on the pressure space Turek [1999]:

$$M^p_{ij} = (\psi_i, \psi_j).$$

Flow in a channel with elastic obstacles



Numerical examples: A deformable segment

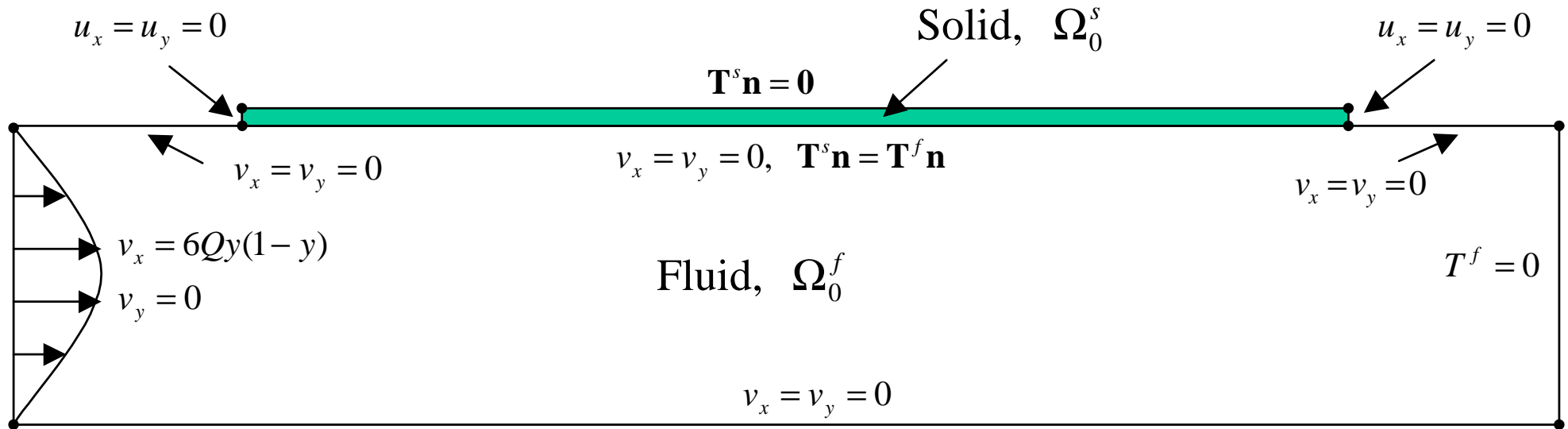


Figure 5: Geometry for flow through a channel with elastic segment (Figure not drawn to scale).

J.-L. Auriault and E. Sanchez-Palencia. Étude du comportement macroscopique d'un milieu poreux saturé déformable. *Journal de Mécanique*, 16:575–603, 1977.

M.A. Biot. General theory of three dimensional consolidation. *Journal of Applied Physics*, 12:155–164, 1941.

R. Blaheta. Displacement decomposition - incomplete factorization preconditioning techniques for linear elasticity problems. *Numerical Linear Algebra with Applications*, 1:107–128, 1994.

Cheo K. Lee and Chiang C. Mei. Re-examination of the equations of poroelasticity. *Int. J. Engng Sci.*, 35:329–352, 1997.

E. Sanchez-Palencia. *Non-Homogeneous Media and Vibration Theory*, volume 127 of *Lecture Notes in Physics*. Springer-Verlag, Berlin, 1980.

E. Sanchez-Palencia and H.I. Ene. Equations et phénomènes de surface pour l'écoulement dans un modèle de milieu poreux. *Journal de Mécanique*, 14:73–108, 1975.

S. Turek. *Efficient Solvers for Incompressible Flow Problems: An Algorithmic and Computational Approach*. Springer Verlag, 1999.