Multiscale Modeling and Simulation of Fluid Flows in Inelastic Media

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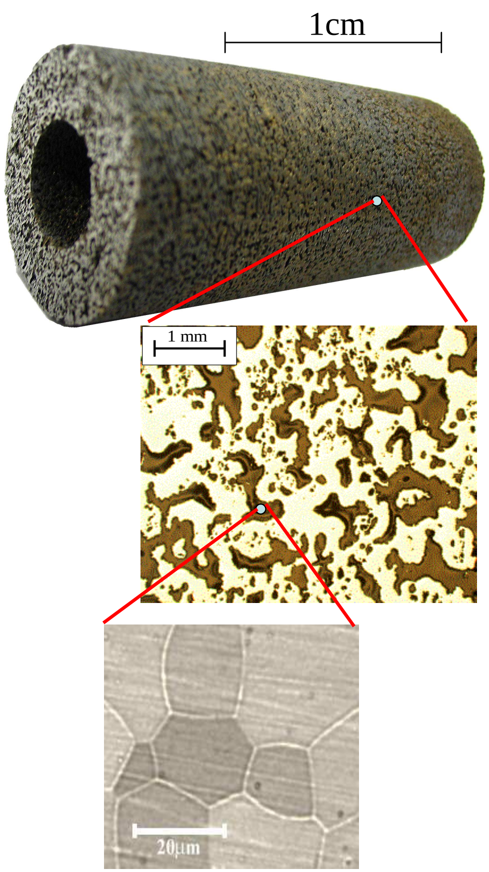
Introduction

- There are many processes that involve multiple scales:
  - Fluid flow in porous media (soil, porous rocks, etc.)
  - Elasticity problems in composite materials (adobe, concrete, asphalt, wood, etc.)
  - Modeling of suspensions, mixtures of several fluids, etc.
- Numerical simulations of fine-scale features is often impossible due to scale disparity
- Some type of upscaling method is needed.



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

Upscaling of flow in rigid porous media

- Assumptions: Rigid, impermeable skeleton, Stokes flow.
- Darcy, 1856 - a phenomenological theory suggesting that the macroscopic velocities $\mathbf{v}$ are proportional to the pressure gradient ∇p:

$$\mathbf{v} = -\frac{1}{\mu}\mathbf{K}^*\nabla p, \tag{1}$$

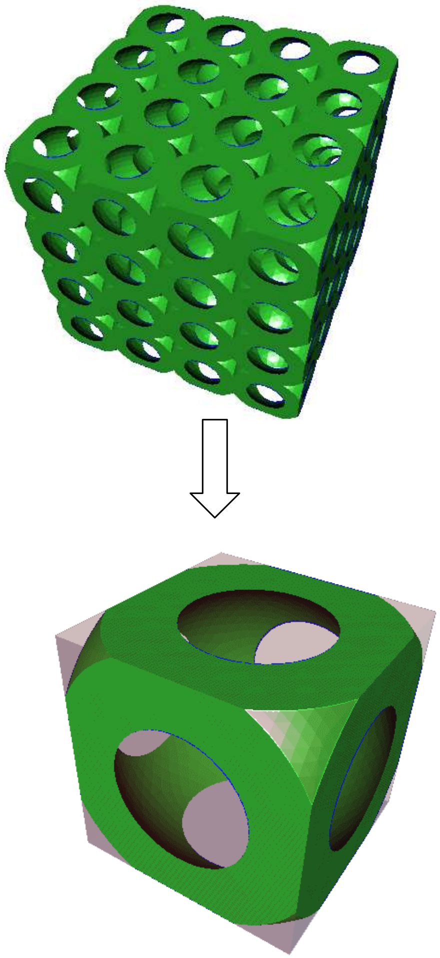
where $\mathbf{K}^*$ is a permeability tensor, as well as conservation of mass:

$$\nabla \cdot \mathbf{v} = 0 \iff \nabla \cdot (\mathbf{K}^*\nabla p) = 0. \tag{2}$$

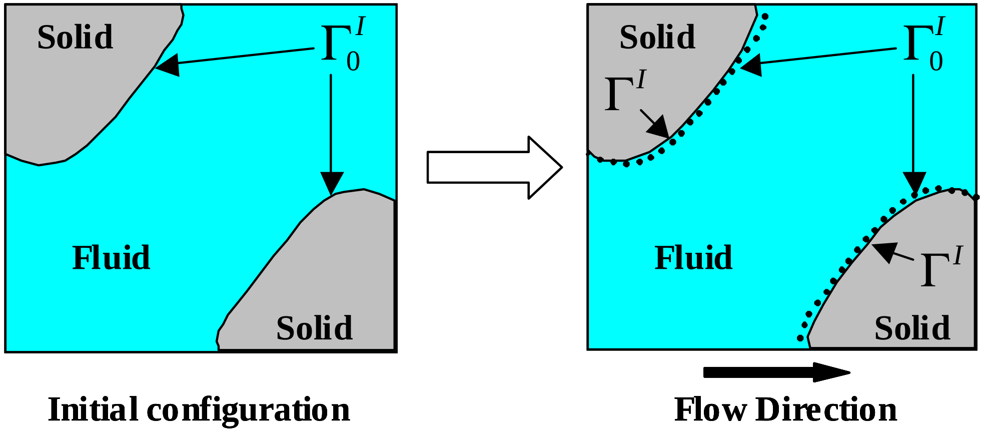
- Derivation of Darcy's law by can be done by asymptotic expansion [Sanchez-Palencia and Ene, 1975]:

$$\begin{aligned} \mathbf{v}_\varepsilon &= \varepsilon^2\mathbf{v}^0 + \varepsilon^3\mathbf{v}^1 + \ldots, \\ p_\varepsilon &= p^0 + \varepsilon p^1 + \ldots \end{aligned}$$

where ε is the small parameter of the problem.



Upscaling of deformable porous media



- Assumptions: elastic skeleton, small displacements of the interface compared to the pore size.
- The fine scale problem is the weakly coupled Fluid-Structure interaction problem.
- Biot [1941] - a phenomenological theory of consolidation
- Auriault and Sanchez-Palencia [1977] - Derivation of Biot's law by asymptotic expansion in the stationary case
- Sanchez-Palencia [1980], Burridge and Keller [1981] - Derivation in various time-dependent cases

Biot's law

- The macroscopic, quasi steady-state equations (ignoring acoustic effects in the skeleton) have the form:

$$\nabla \cdot \left(\mathcal{L}^* : \mathbf{e}(\mathbf{u}^{(0)}) - \mathbf{A}^* p^{(0)} \right) = \mathbf{0}, \tag{3}$$

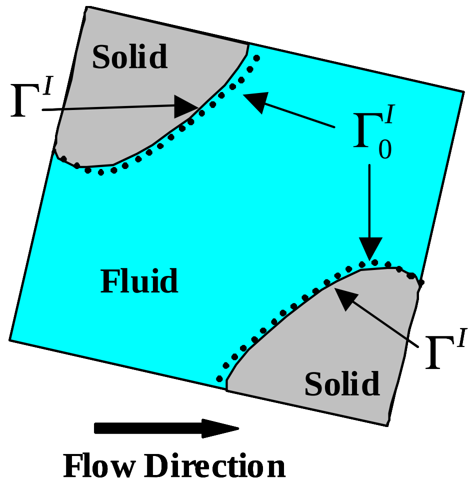
$$\nabla \cdot \left(\mathbf{K}^* \nabla p^{(0)} - \phi_f \frac{\partial \mathbf{u}^{(0)}}{\partial t} \right) = \mathbf{A}^* : \mathbf{e} \left(\frac{\partial \mathbf{u}^{(0)}}{\partial t} \right) + \beta^* \frac{\partial p^{(0)}}{\partial t}. \tag{4}$$

  where ϕ_f is the pore volume fraction. $\mathcal{L}^*$, $\mathbf{K}^*$, $\mathbf{A}^*$ and β^* are macroscopic coefficients obtained by solving 3 sets of cell problems.
- The macroscopic coefficients are:
  - $\mathcal{L}^*$ is the macroscopic elasticity tensor of the skeleton.
  - $\mathbf{K}^*$ is the skeleton's Darcy permeability.
  - $\mathbf{A}^*$, β^* are fluid-solid coupling coefficients.
- The macroscopic velocity $\mathbf{v}^{(0)}$ is given by:

$$\mathbf{v}^{(0)} = \phi_f \frac{\partial \mathbf{u}^{(0)}}{\partial t} - \mathbf{K}^* \nabla p^{(0)}. \tag{5}$$

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.



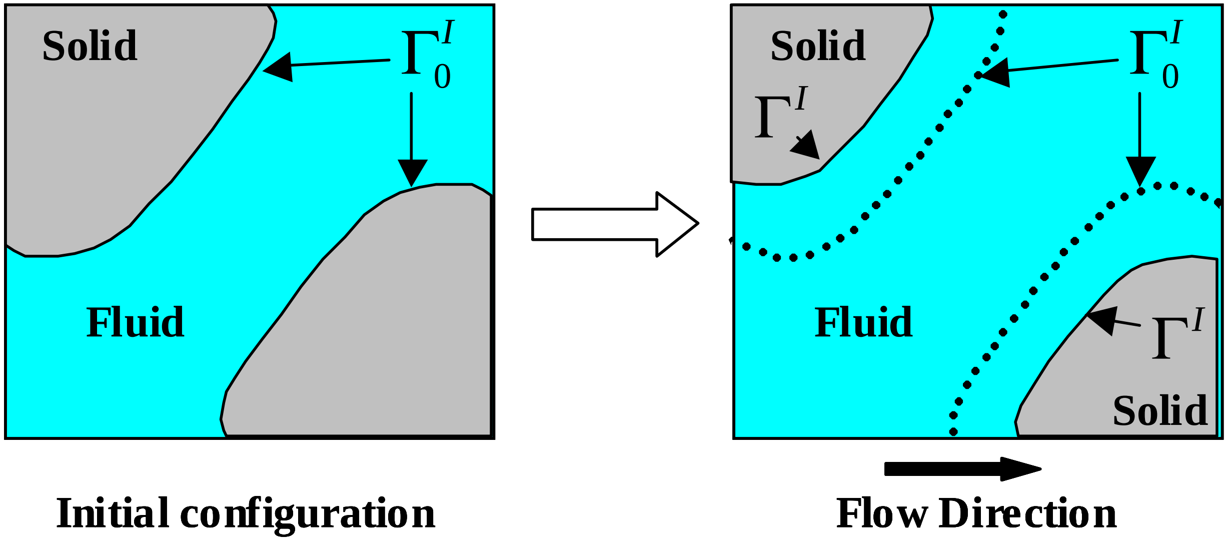
- The macroscopic equations then become nonlinear:

$$\nabla \cdot \left(\mathcal{L}^* : \mathbf{e}(\mathbf{u}^{(0)}) - \mathbf{A}^* p^{(0)}\right) = C\left(\mathbf{F}^* : \mathbf{e}(\mathbf{u}^{(0)}) + \boldsymbol{\alpha}^* p^{(0)}\right) : \nabla \mathbf{u}^{(0)} \tag{6}$$

$$\nabla \cdot \left(\mathbf{K}^* \nabla p^{(0)} - \phi_f \frac{\partial \mathbf{u}^{(0)}}{\partial t}\right) = \mathbf{A}^* : \mathbf{e}\left(\frac{\partial \mathbf{u}^{(0)}}{\partial t}\right) + \beta^* \frac{\partial p^{(0)}}{\partial t} + C\left(\mathbf{J}^* : \mathbf{e}(\mathbf{u}^{(0)}) + \mathbf{M}^* p^{(0)}\right) \nabla \mathbf{p}^{(0)} \tag{7}$$

Objectives

We consider an elastic skeleton, without restrictions on the displacements:



- Applications to filters, microfluidic devices, geomechanics problems.
- Present a numerical method for the solution of the coupled fluid-stricture problem at the microscale
- Derive an asymptotic solution for flows in simple channel geometries and verify against the numerics
- Present a hybrid Multiscale FEM model for upscaling general pore geometries

Fluid-structure interaction problem

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

$$\Gamma^I = \left\{ \mathbf{p} + \mathbf{u}(\mathbf{p}) | \forall \mathbf{p} \in \Gamma_0^I \right\}, \tag{8}$$

$$\begin{aligned} -\mu \Delta \mathbf{v} + \nabla p &= \mathbf{b} \quad \text{in } \Omega^f, \\ \nabla \cdot \mathbf{v} &= \mathbf{0} \quad \text{in } \Omega^f, \\ -\nabla \cdot \left(\mathbf{S} \left(\mathbf{e} \left(\mathbf{u} \right), \boldsymbol{\xi} \right) \right) &= \mathbf{b}_0 \quad \text{in } \Omega_0^s, \end{aligned} \tag{9}$$

$$\left(\mathbf{S} \left(\mathbf{e} \left(\mathbf{u} \right), \boldsymbol{\xi} \right) \right) \mathbf{n}_0 = \det \left(\nabla \mathbf{u} + \mathbf{I} \right) \left(-p\mathbf{I} + 2\mu \mathbf{e} \left(\mathbf{v} \right) \right) \right) \left(\nabla \mathbf{u} + \mathbf{I} \right)^{-T} \mathbf{n}_0 \text{ on } \Gamma_0^I. \tag{10}$$

Weak form of the coupled system

- Let is 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 (9)-(10) can be restated in a weak form:

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

$$\begin{aligned} D_{\Omega^f}(\mathbf{v},\mathbf{w}) - (p,\nabla\cdot\mathbf{w})_{\Omega^f} &= (\mathbf{b},\mathbf{w})_{\Omega^f}, \quad && \forall \mathbf{w} \in \left[H_0^1\left(\Omega^f\right)\right]^d, \\ -(\nabla\cdot\mathbf{v},q)_{\Omega^f} &= 0, && \forall q \in L^2(\Omega^f), \\ a_{\Omega_0^s}(\mathbf{u},\mathbf{w}) &= (\mathbf{b}_0,\mathbf{w})_{\Omega_0^s} + g_{\Gamma_0^I}(\mathbf{v},\mathbf{u},p,\mathbf{w}), && \forall \mathbf{w} \in \left[H_D^1\left(\Omega_0^s\right)\right]^d, \\ \Gamma &= \left\{\mathbf{p}+\mathbf{u}(\mathbf{p}) \middle| \forall \mathbf{p} \in \Gamma_0\right\}. \end{aligned} \tag{11}$$

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:

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

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

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

- 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 (11) lead to the nonlinear system of algebraic equations

$$\begin{pmatrix} \mathbf{A}(\mathbf{u}) & \mathbf{C}^T(\mathbf{u}) & \mathbf{0} \\ \mathbf{C}(\mathbf{u}) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{K} \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{p} \\ \mathbf{u} \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{0} \\ \mathbf{f}_2 + \mathbf{g}(\mathbf{u}, \mathbf{v}, \mathbf{p}) \end{pmatrix}, \tag{12}$$

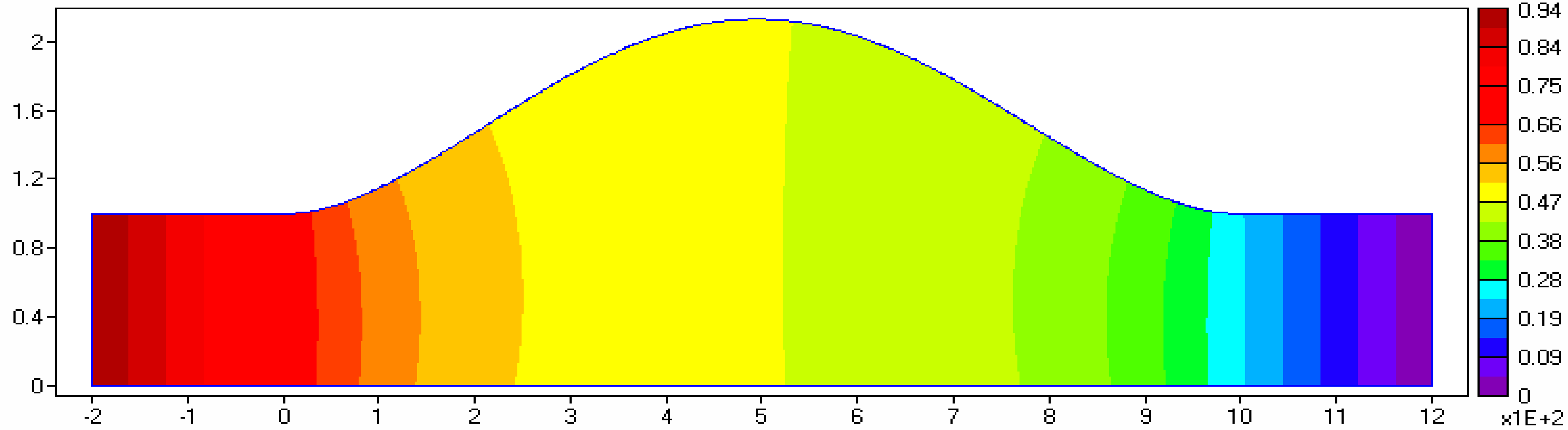
Direct iteration for the FSI problem

- Considering the following iterative approach for solving the FSI problem (11):
  - 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 (11):

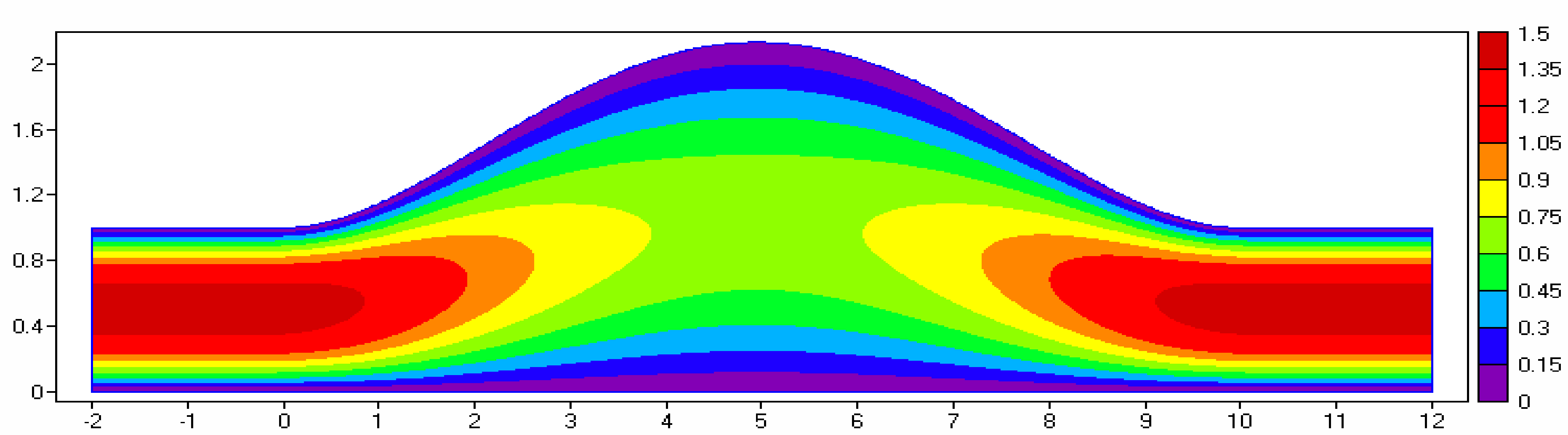
$$\begin{pmatrix} \mathbf{A}(\mathbf{u}_k) & \mathbf{C}^T(\mathbf{u}_k) & \mathbf{0} \\ \mathbf{C}(\mathbf{u}_k) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{K} \end{pmatrix} \begin{pmatrix} \mathbf{v}_{k+1} \\ \mathbf{p}_{k+1} \\ \mathbf{u}_{k+1} \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{0} \\ \mathbf{f}_2 + \mathbf{g}(\mathbf{u}_k, \mathbf{v}_{k+1}, \mathbf{p}_{k+1}) \end{pmatrix} \tag{13}$$

- 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]

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

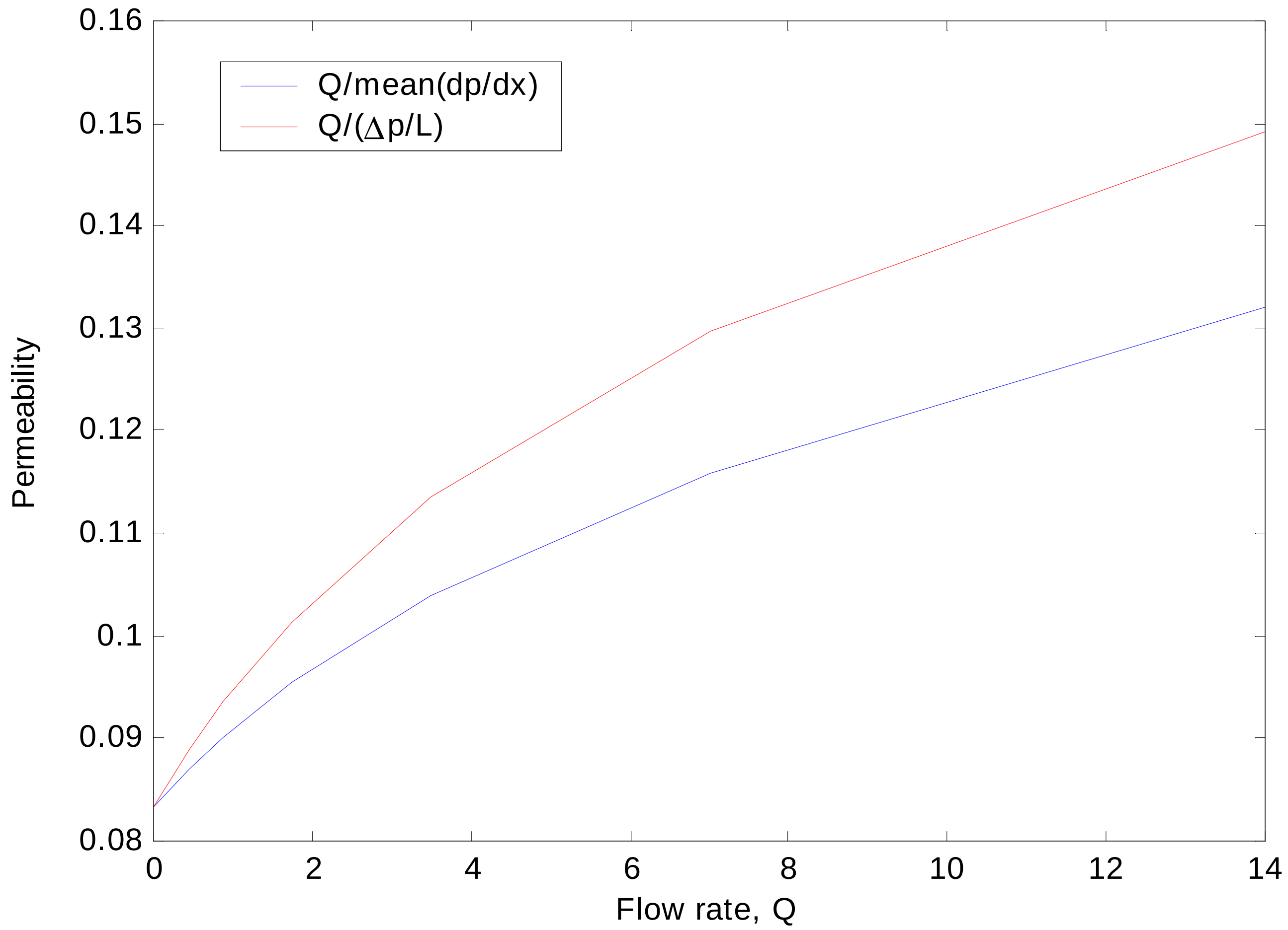
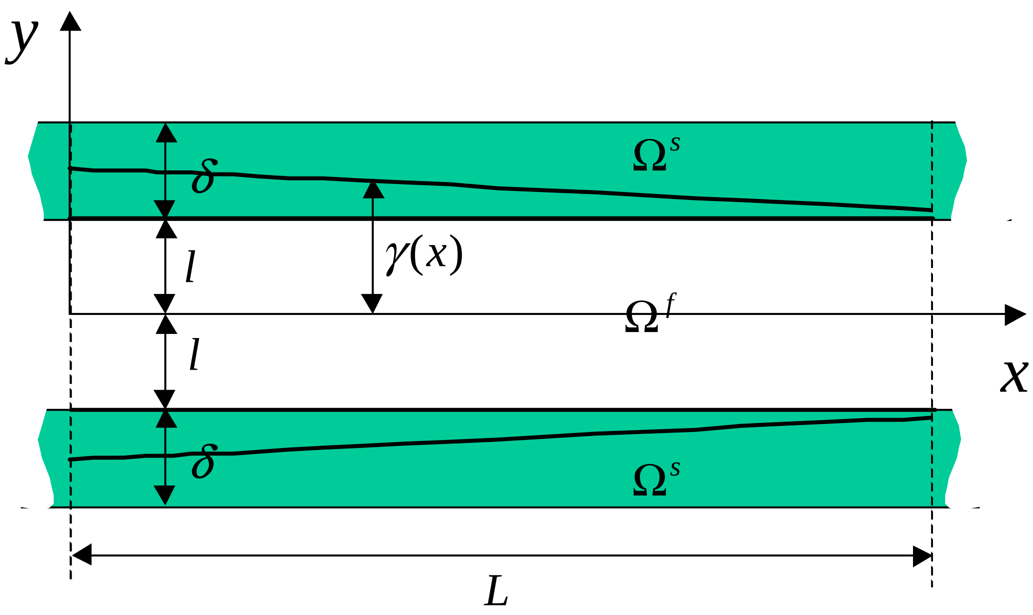


Figure 1: Channel permeability as a function of different flow rates.

Flow in elastic channel

- Consider a long channel with elastic walls



- The fluid and solid domains in the deformed configuration are defined as

$$\Omega_f = \{(x, y) : 0 < x < 1, \;\; 0 < y < \gamma(x))\},$$
$$\Omega_s = \{(x, y) : 0 < x < 1, \;\; \gamma(x) < y < 1 + \delta)\},$$

Asymptotic expansion of FSI problem

- Let the channel thickness $2l$ be much smaller than its length L and introduce the small parameter

$$\varepsilon = \frac{l}{L} \tag{14}$$

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

$$\begin{aligned}
v_1 &= v_1^0 + \varepsilon v_1^1 + \varepsilon^2 v_1^2 + \ldots \\
v_2 &= v_2^0 + \varepsilon v_2^1 + \varepsilon^2 v_2^2 + \ldots \\
p &= p^0 + \varepsilon p^1 + \varepsilon^2 p^2 + \ldots \\
u_1 &= u_1^0 + \varepsilon u_1^1 + \varepsilon^2 u_1^2 + \ldots \\
u_2 &= u_2^0 + \varepsilon u_2^1 + \varepsilon^2 u_2^2 + \ldots
\end{aligned}$$

The expansion is with respect to the deformed configuration.

Asymptotic expansion: The fluid domain

Substituting v_1, v_2 and p in the Stokes system and examining various powers of ε gives:

$$p^0 = p^0(x), \quad \frac{\partial}{\partial x}\left(\gamma^3(x)\frac{\partial p^0}{\partial x}\right) = 0 \tag{15}$$

- The above equations are independent of the solid type or interface displacements.
- The second equation can be interpreted as a 1D nonlinear Darcy law. Indeed, fix x and define, the $y-$average operator $\langle\cdot\rangle_y$:

$$\langle\phi(x,y)\rangle_y := \frac{1}{2}\int_{-\gamma(x)}^{\gamma(x)} \phi(x,y)dy \tag{16}$$

  One then obtains that

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

  that is, equation (15) can be interpreted as the conservation of mass for a flow with flux $\langle v_1(x)\rangle$, driven by a pressure gradient $\partial_x p^0(x)$. Also,

$$K := K(\gamma^3(x), x) = -\mu\frac{\langle v_1(x)\rangle}{\partial_x p^0(x)} = \frac{1}{3l}\gamma^3(x) \tag{17}$$

Asymptotic expansion (cont.)

- In order to evaluate the stresses in the solid, we assume a linear, isotropic material:

$$\mathbf{S} = \mathcal{L} : \mathbf{E} = \lambda_s : \mathrm{tr}(\mathbf{E})\mathbf{I} + 2\mu_s \mathbf{E}$$

- Under some additional assumptions on the solid ($\delta \sim l$ and both u_1 and u_2 are of order δ) on can solve the elasticity system and obtain the leading order terms in the stress tensor:

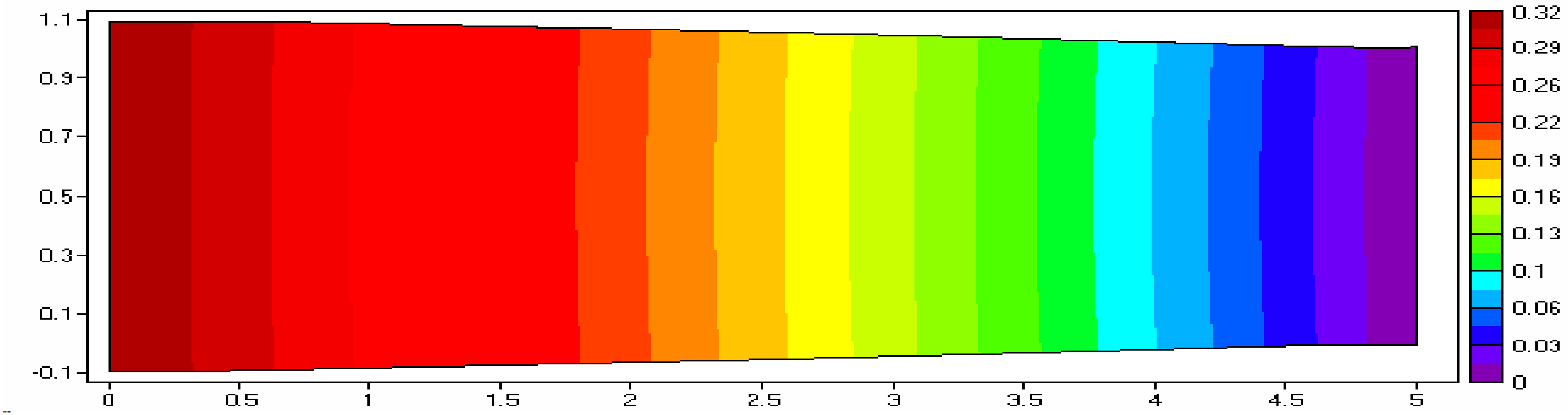
$$\mathbf{S}^s = \frac{\delta}{l} \begin{bmatrix} \lambda_s \dfrac{\partial u_2^0}{\partial y} & \mu_s \dfrac{\partial u_1^0}{\partial y} \\ \mu_s \dfrac{\partial u_1^0}{\partial y} & (\lambda_s + 2\mu_s) \dfrac{\partial u_2^0}{\partial y} \end{bmatrix} + \mathcal{O}\left(\varepsilon\right)$$

- On the other hand, $\mathbf{T}^f = -p^0(x)\mathbf{I} + \mathcal{O}\left(\varepsilon\right)$ and using the interface condition one gets:

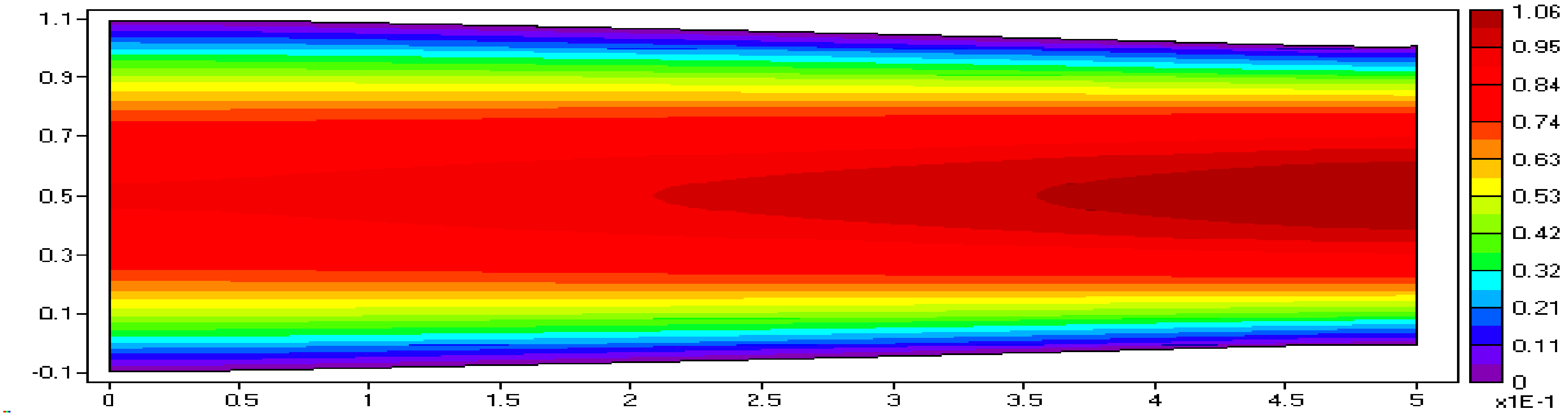
$$u_2^0 = 0 \quad \text{and} \quad \gamma(x) = l + \frac{l}{\lambda_s + 2\mu_s} p^0(x),$$

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

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

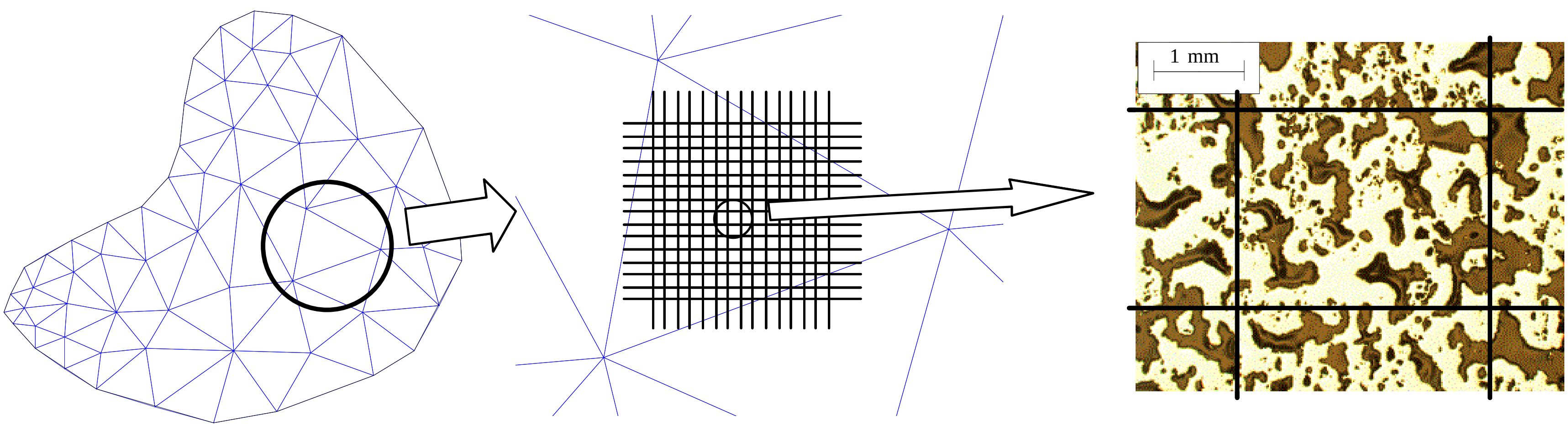
P^0	$\frac{\|\|\bar{\gamma}-\gamma\|\|_{L^2}}{\|\|\gamma\|\|_{L^2}}$		$\frac{\|\|\bar{K}-K\|\|_{L^2}}{\|\|K\|\|_{L^2}}$	
	$\varepsilon = \frac{1}{10}$	$\varepsilon = \frac{1}{20}$	$\varepsilon = \frac{1}{10}$	$\varepsilon = \frac{1}{20}$
0.32	2.41×10^{-3}	8.47×10^{-4}	6.63×10^{-3}	1.82×10^{-3}
0.16	1.19×10^{-3}	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}

Numerical upscaling

- Macroscopic model for general 2D/3D geometries (Diffusion only)

$$\nabla \cdot \left(\mathbf{K}\left(\mathbf{x}, p^*, \nabla p^*\right) \nabla p^*\right) = 0 \tag{18}$$

- Discretize the macroscopic problem using finite elements:



Macroscopic discretization

Microscopic RVE

- The mesh parameter h of the discretization is much bigger than the fine-scale geometry length-scale ε:

$$h >> \varepsilon \tag{19}$$

Numerical upscaling (cont.)

- Consider a fixed point iteration for the macroscopic equation:

$$\nabla \cdot \left(\mathbf{K} \left(\mathbf{x}, p^{*(n)}, \nabla p^{*(n)} \right) \nabla p^{*(n+1)} \right) = 0 \tag{20}$$

- The diffusion tensor $\mathbf{K}^{(n)} = \mathbf{K}\left(\mathbf{x}, p^{*(n)}, \nabla p^{*(n)}\right)$ is computed at each integration point. It is the Darcy permeability corresponding to the geometry $\tilde{\Gamma}_\varepsilon^{(n)}$, which, along with $\tilde{\mathbf{v}}_\varepsilon^{(n)}$, $\tilde{\mathbf{u}}_\varepsilon^{(n)}$ and $\tilde{p}_\varepsilon^{(n)}$ satisfies the FSI problem:

$$\tilde{\Gamma}_\varepsilon^{(n)} = \left\{ \mathbf{p} + \tilde{\mathbf{u}}_\varepsilon^{(n)}(\mathbf{p}) | \forall \mathbf{p} \in \Gamma_0^I \right\}, \tag{21}$$

$$-\nabla_y \tilde{p}_\varepsilon^{(n)} + \mu \Delta_y \tilde{\mathbf{v}}_\varepsilon^{(n)} + \mathbf{b} - \nabla_x p^{*(n)} = \mathbf{0} \quad \text{in } \Omega^f, \tag{22}$$

$$\nabla \cdot_y \tilde{\mathbf{v}}_\varepsilon^{(n)} = \mathbf{0} \quad \text{in } \Omega^f, \tag{23}$$

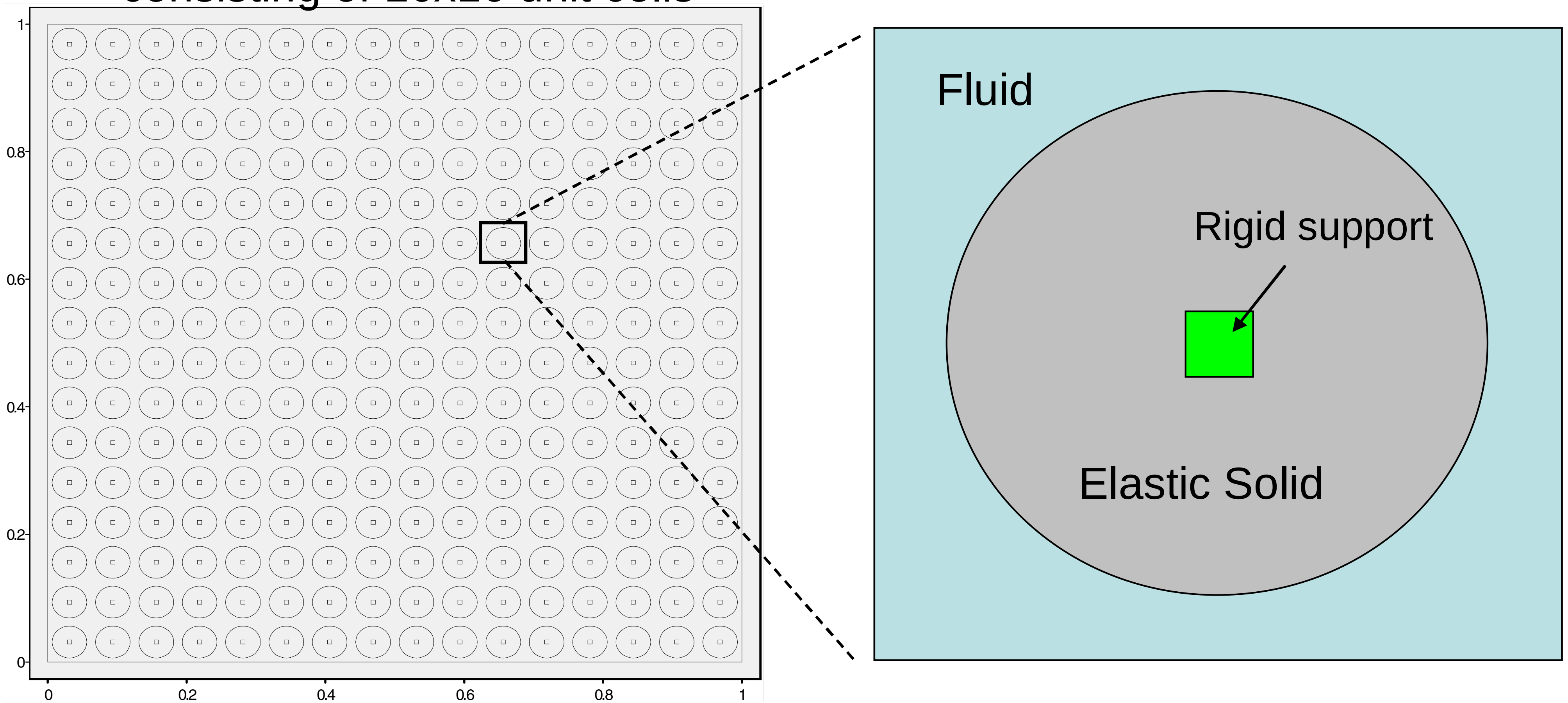
$$\left\langle \tilde{p}_\varepsilon^{(n)} \right\rangle = p^{*(n)}(\mathbf{x}) \tag{24}$$

$$\nabla \cdot_y \left(\mathbf{S}\left(\mathbf{e}_y \left(\tilde{\mathbf{u}}_\varepsilon^{(n)} \right), \boldsymbol{\xi} \right) \right) + \mathbf{b}_0 = \mathbf{0} \quad \text{in } \Omega_0^s, \tag{25}$$

Numerical upscaling: Example

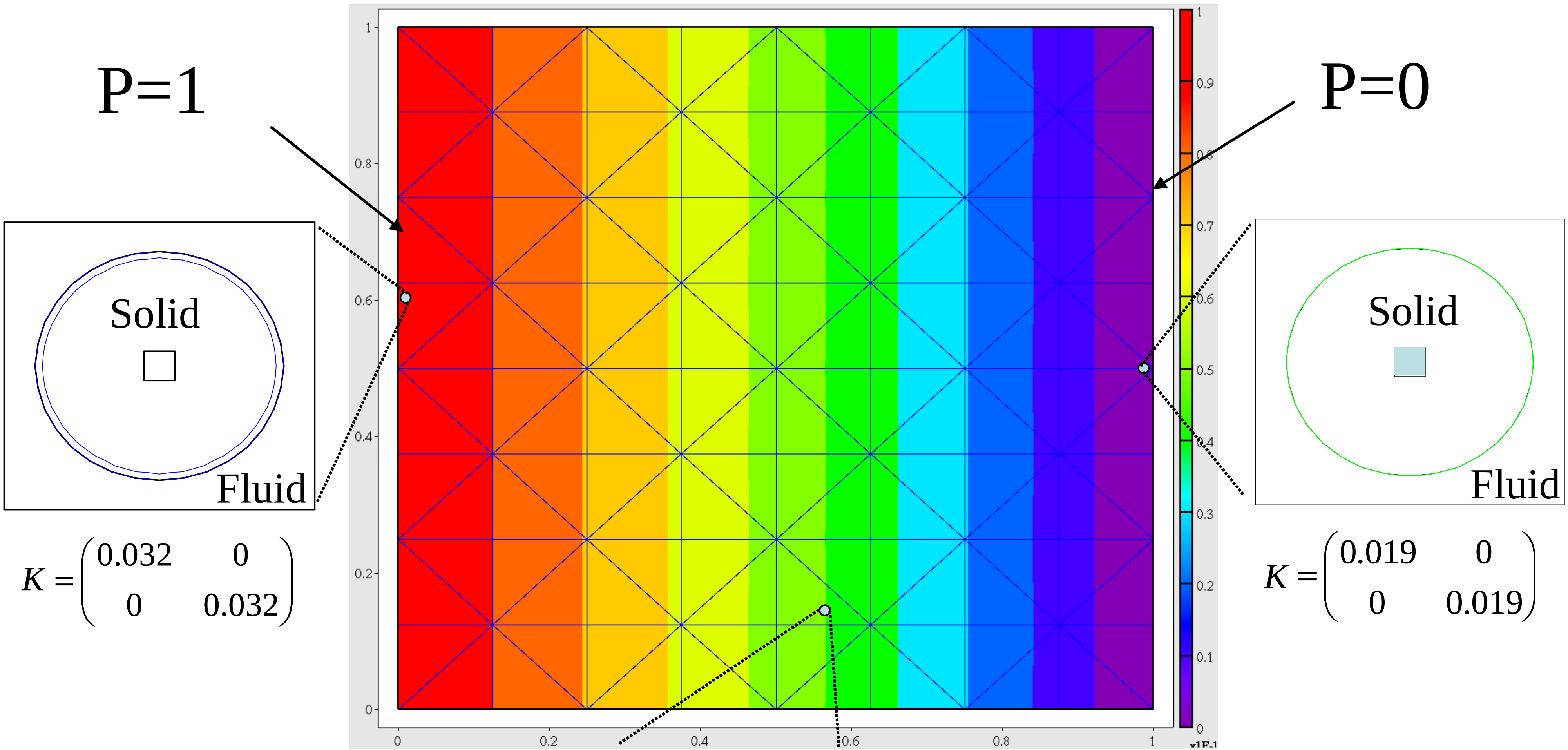
Macroscopic FSI problem consisting of 16x16 unit cells

Unit Cell Geometry



Numerical upscaling: Macroscale Solution

Pressure contour plot

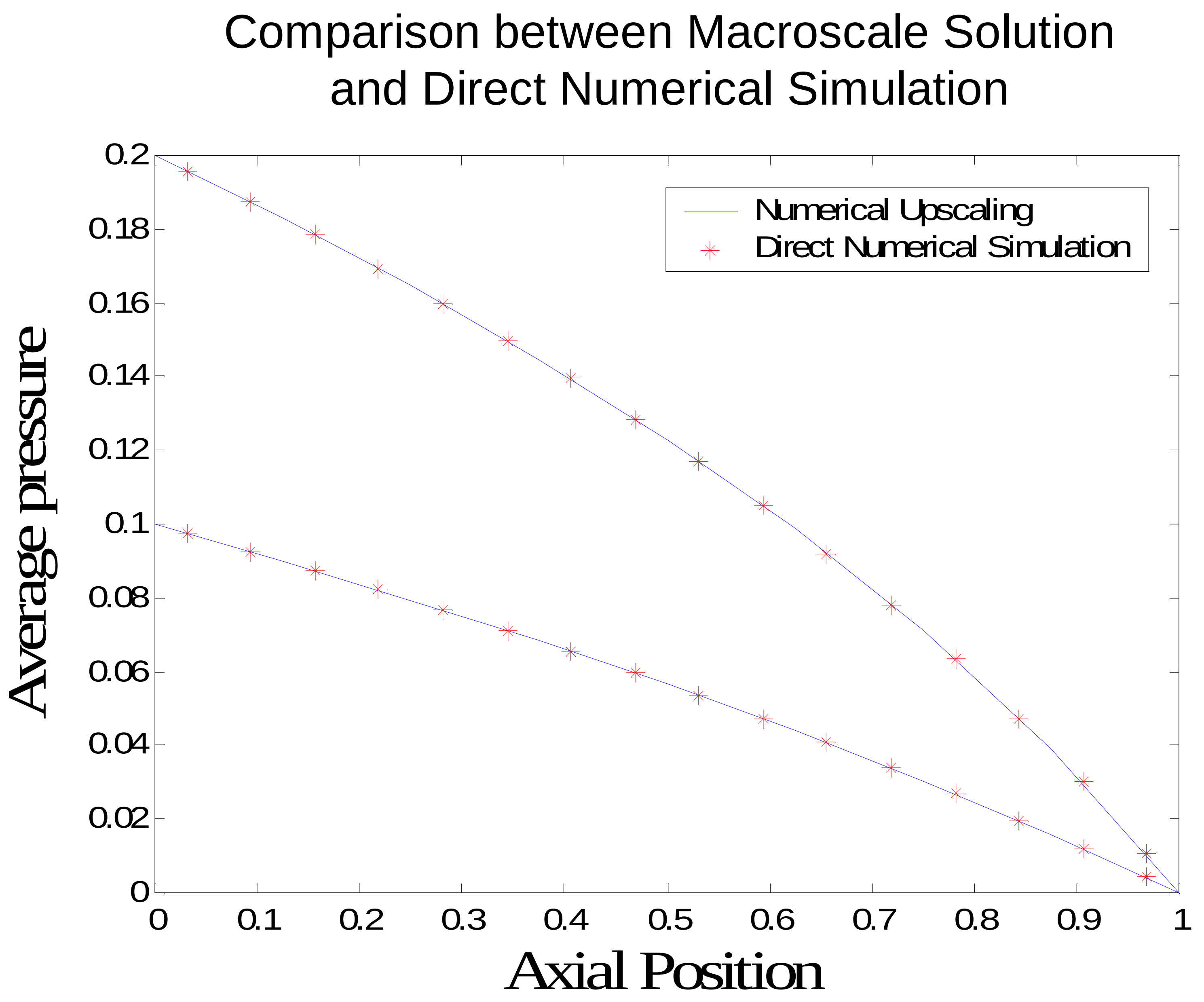


$$K = \begin{pmatrix} 0.032 & 0 \\ 0 & 0.032 \end{pmatrix}$$

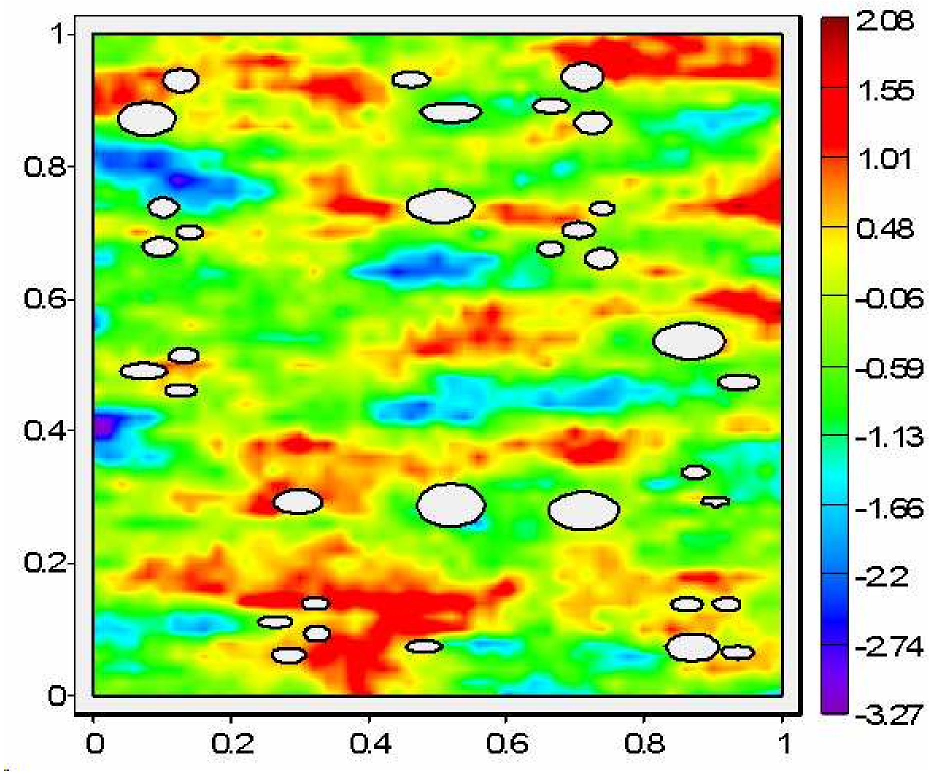
$$K = \begin{pmatrix} 0.019 & 0 \\ 0 & 0.019 \end{pmatrix}$$

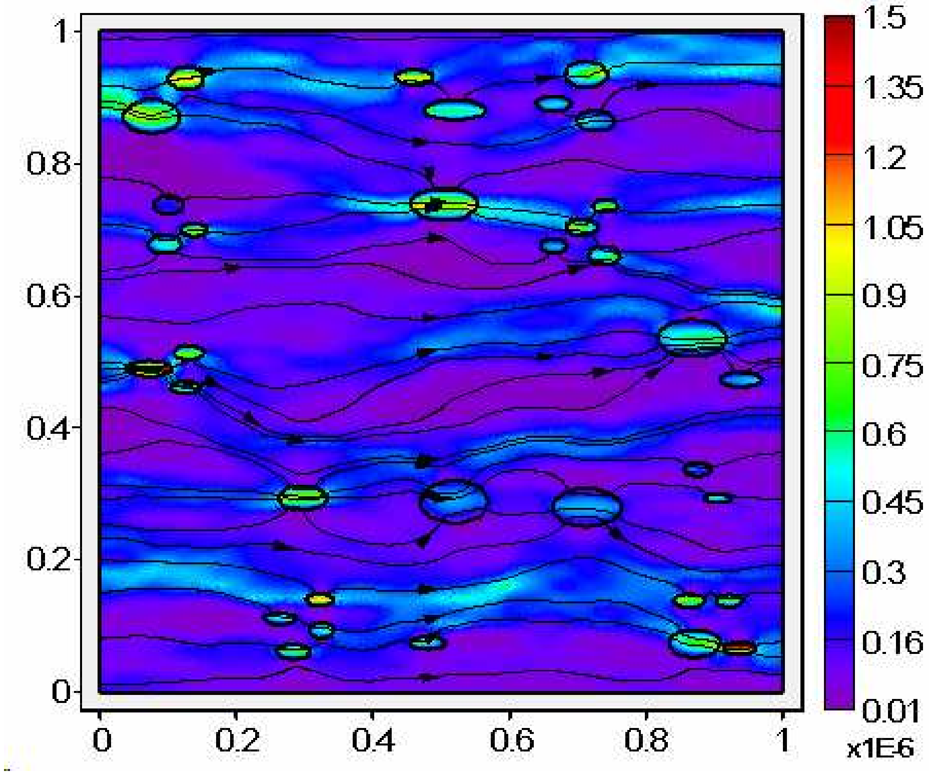
$$K = \begin{pmatrix} 0.025 & 0 \\ 0 & 0.025 \end{pmatrix}$$

Numerical upscaling: Comparison



Related Projects: Flow in vuggy reservoirs





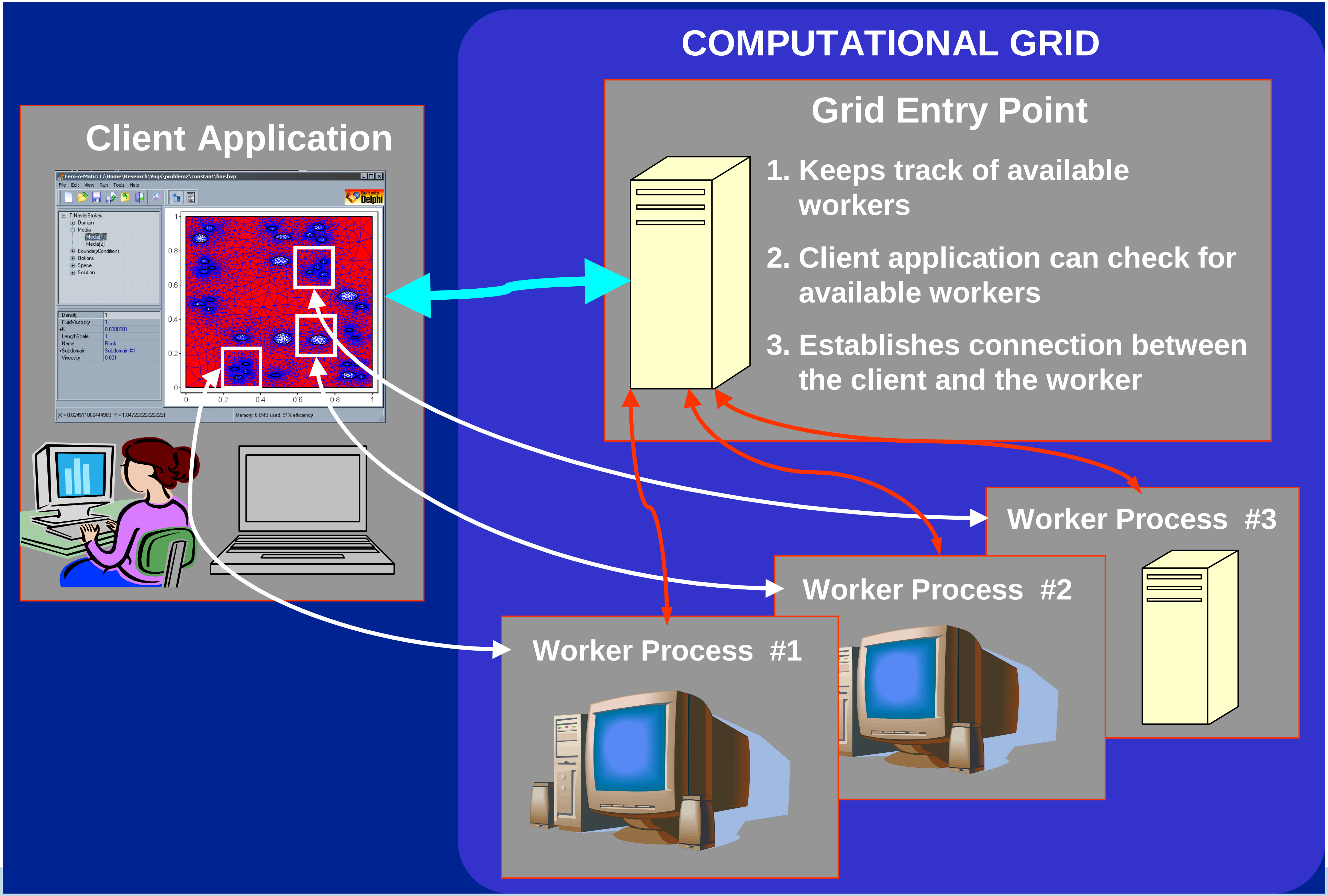
Current and Future Work

- Provide rigorous justification of the macroscopic model:
  - Linearize around the current position of the interface and estimate the error between the the upscaled and exact FSI solutions.
  - Compare the accumulated error for the entire nonlinear iteration process.
- Include elasticity in the numerical upscaling model
- Consider geometrically nonlinear solids
- Check the validity range of nonlinear extensions of Lee and Mei [1997] to Biot's equations and compare with multiscale model
- Upscaling of flow in vuggy, fractured carbonate reservoirs via the Stokes-Brinkman equations.

The End

Questions?

Distributed computation of local problems



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