Homogenization and Nonlinearity in Deforming Heterogeneous Media

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Motivation: nonlinear effcts & efficient computation

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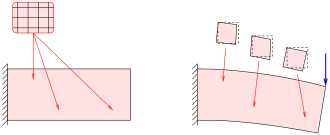
Biot – Darcy model — by homogenization of fluid-structure interaction

$$-\nabla \cdot (\mathbb{A}\nabla^S \mathbf{u} - \mathbf{B}p) = \mathbf{f}^s \;,$$
$$\mathbf{B} : \nabla^S \dot{\mathbf{u}} - \nabla \cdot \mathbf{K}(\nabla p - \mathbf{f}^f) + M\dot{p} = 0 \;,$$

Idea

. . . an extension of the first order theory, whereby the linear strain kinematics still holds and the initial domain is taken as the reference.

- Quasi-periodic structures: evolving locally with deformation
- Effect of deforming microstructure ⇒ homogenized coefficients (HC)
- Using sensitivity analysis ⇒ linear expansion formulas for HC

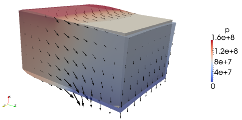


Avoid $(\mathrm{FEM})^2$!

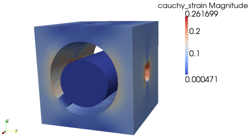
Outline

- Quasistatic Biot – Darcy model by homogenization
- Sensitivity and expansion formulas for the homogenized coefficients
  [E.R. Sensitivity strategies in modelling heterogeneous media undergoing finite deformation.

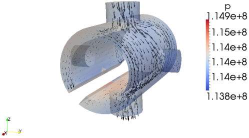
  Math. Comp. Simulation (2003) **61**:261–270.]
- Weakly nonlinear model of porous medium



macro



local / solid



local / fluid

- Outlook: nonlinear kinematics / Conlusions

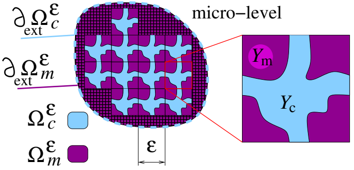
E. Rohan, V. Lukeš, Modeling flows in periodically heterogeneous porous media with deformation-dependent permeability, in: Proc. of COMPLAS 2013, 2013, p. http://congress.cimne.upc.es/complas2013/proceedings/.

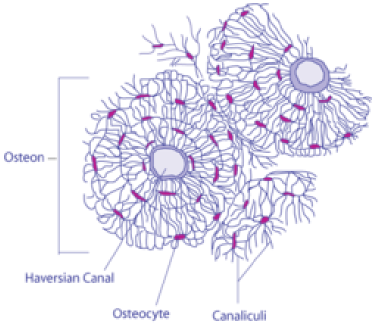
E. Rohan, V. Lukeš, On modelling nonlinear phenomena in deforming heterogeneous media using homogenization and sensitivity analysis concepts, in: Proc. of CST 2014, Coburg-Sax Publ., 2014, pp. 1–20.

Micromodel of poroelasticity — fluid & solid

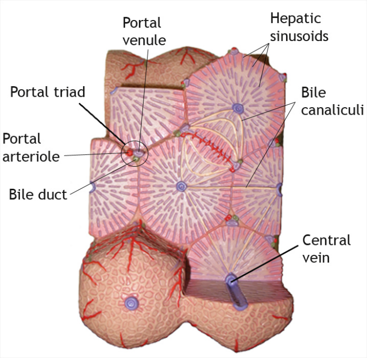
Domain split – matrix & channels

$\Omega = \Omega_m^\varepsilon \cup \Omega_c^\varepsilon \cup \Gamma^\varepsilon$





osteon – cortical bone



liver lobes

Micromodel of poroelasticity — fluid & solid

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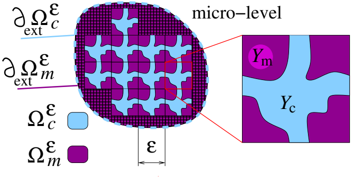

Quasistatic problem — decoupling

2 homogenization problems:

- Porous (elastic/viscoelastic) skeleton + "static" (compressible) fluid $\Rightarrow$ Biot poroelastic coefficients $\mathbb{A}, \mathbf{B}, M$
- Stokes (steady) flow $\Rightarrow$ Darcy flow, permeability $\mathbf{K}$

Even for acoustic problem the poroelastic coefficients computed using the same "auxiliary" microscopic problems as for this quasistatic situation

J.-L. Auriault, C. Boutin. Transp. Porous Media, 10(2):153–169, 1993.
J.L. Ferrín, A. Mikelić. Math. Meth. Appl. Sci., 26:831–859, 2003.
E. Rohan, S. Shaw, J.R. Whiteman. Comp. Geosci., 2013.

Micromodel of poroelasticity — fluid & solid

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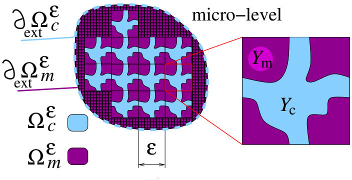


1) Fluid-Structure interaction — static

$$-\nabla \cdot (\mathbb{D}^\varepsilon \nabla^S \mathbf{u}^\varepsilon) = \mathbf{f}^\varepsilon , \quad \text{in } \Omega_m^\varepsilon ,$$
$$\mathbf{n}^{[m]} \cdot \mathbb{D}^\varepsilon \nabla^S \mathbf{u}^\varepsilon = \mathbf{g}^\varepsilon , \quad \text{on } \partial_{\mathrm{ext}}\Omega_m^\varepsilon ,$$
$$\mathbf{n}^{[m]} \cdot \mathbb{D}^\varepsilon \nabla^S \mathbf{u}^\varepsilon = -\bar{p}^\varepsilon \mathbf{n}^{[m]} , \quad \text{on } \Gamma^\varepsilon ,$$

mass conservation of the fluid filling the channels

$$-J^\varepsilon := -\int_{\partial_{\mathrm{ext}}\Omega_c^\varepsilon} \mathbf{w}^\varepsilon \cdot \mathbf{n}^{[c]} \,\mathrm{dS}_x = \int_{\partial\Omega_c^\varepsilon} \tilde{\mathbf{u}}^\varepsilon \cdot \mathbf{n}^{[c]} \,\mathrm{dS}_x + \gamma \bar{p}^\varepsilon |\Omega_c^\varepsilon| ,$$

J^ε ... relative flow outside Ω_c^ε. γ ... fluid compressibility.

Weak formulation: Find $(\mathbf{u}^\varepsilon, \bar{p}^\varepsilon) \in \mathbf{H}^1(\Omega_m^\varepsilon)/\mathcal{R}(\Omega_m^\varepsilon) \times \mathbb{R}$ such that

$$\int_{\Omega_m^\varepsilon} (\mathbb{D}^\varepsilon \nabla^S \mathbf{u}^\varepsilon) : \nabla^S \mathbf{v} + \bar{p}^\varepsilon \int_{\Gamma^\varepsilon} \mathbf{n}^{[m]} \cdot \mathbf{v} \, \mathrm{dS}_x = \int_{\partial_{\mathrm{ext}} \Omega_m^\varepsilon} \mathbf{g}^\varepsilon \cdot \mathbf{v} \, \mathrm{dS}_x \,,$$

$$\int_{\partial \Omega_c^\varepsilon} \tilde{\mathbf{u}}^\varepsilon \cdot \mathbf{n}^{[c]} \, \mathrm{dS}_x + \gamma \bar{p}^\varepsilon |\Omega_c^\varepsilon| = -J^\varepsilon \,, \quad \forall \mathbf{v} \in \mathbf{H}^1(\Omega_m^\varepsilon) \,.$$

Convergence result: $\exists \mathbf{u}(x) \in \mathbf{H}^1(\Omega)$, $\mathbf{u}^{1,}(x,y) \in \mathbf{L}^2(\Omega; \mathbf{H}^1_\#(Y))$, and $\bar{p} \in \mathbb{R}$

$$\bar{p}^\varepsilon \to \bar{p} \,,$$

$$\widetilde{\mathbf{u}^\varepsilon} \stackrel{2}{\rightharpoonup} \mathbf{u} \,,$$

$$\nabla \widetilde{\mathbf{u}^\varepsilon} \stackrel{2}{\rightharpoonup} \nabla_x \mathbf{u} + \nabla_y \mathbf{u}^1 \,,$$

$\Rightarrow$ recovery sequences of test functions (displacements) $\mathbf{v}^\varepsilon$,

$$\widetilde{\mathbf{v}^\varepsilon} \stackrel{2}{\to} \mathbf{v} \,,$$

$$\nabla \widetilde{\mathbf{v}^\varepsilon} \stackrel{2}{\to} \nabla_x \mathbf{v} + \nabla_y \mathbf{v}^1 \,,$$

Convergence of traction forces on $\partial\Omega$

$$\int_{\partial\Omega} \mathbf{v}^\varepsilon \cdot (-p\mathbf{n}\bar{\chi}_c^\varepsilon + \bar{\chi}_m^\varepsilon \mathbf{g}^\varepsilon)\, \mathrm{dS}_x \to \int_{\partial\Omega} \overline{\mathbf{g}}(p) \cdot \mathbf{v}\, \mathrm{dS}_x \;,$$

where $\bar{\chi}_m^\varepsilon \mathbf{g}^\varepsilon \rightharpoonup (1-\phi_S)\mathbf{g} \equiv \hat{\mathbf{g}}$ ... effective traction related to solid

$\overline{\mathbf{g}}(p) = \hat{\mathbf{g}} - p\mathbf{n}\phi_S$ ... mean traction stress

Interface integrals on Γ^ε

Let ϕ_S and ϕ be the surface and the volume fractions, respectively, then

$$\int_{\Gamma^\varepsilon} \mathbf{v}^\varepsilon \cdot \mathbf{n}^{[m]}\, \mathrm{dS}_x \to \int_{\partial\Omega} \phi_S \mathbf{v} \cdot \mathbf{n}\, \mathrm{dS}_x - \int_\Omega \phi \operatorname{div}_x \mathbf{v} + \int_\Omega \fint_{\Gamma_Y} \mathbf{v}^1 \cdot \mathbf{n}^{[m]}\, \mathrm{dS}_y \;.$$

If $\phi = \phi_S$ on $\partial\Omega$, then (Γ_Y ... the interface within Y)

$$\int_{\Gamma^\varepsilon} \mathbf{v}^\varepsilon \cdot \mathbf{n}^{[m]}\, \mathrm{dS}_x \to \int_\Omega \mathbf{v} \cdot \nabla_x \phi + \int_\Omega \fint_{\Gamma_Y} \mathbf{v}^1 \cdot \mathbf{n}^{[m]}\, \mathrm{dS}_y \;,$$

Two-scale limit problem

Find $(\mathbf{u}, \mathbf{u}^{1,}) \in \mathbf{H}^1(\Omega) \times \mathbf{L}^2(\Omega; \mathbf{H}^1_\#(Y))$ and $\bar{p} \in \mathbb{R}$ such that *(no volume forces)*

$$\fint_{\Omega \times Y_m} \left(\nabla^S_x \mathbf{v} + \nabla^S_y \mathbf{v}^1\right) : \mathbb{D} \left(\nabla^S_x \mathbf{u} + \nabla^S_y \mathbf{u}^1\right)$$

$$-\bar{p} \int_\Omega \left(\phi \operatorname{div} \mathbf{v} - \fint_{\Gamma_Y} \mathbf{v}^1 \cdot \mathbf{n}^{[m]} \, \mathrm{dS}_y\right) = \int_{\partial\Omega} \overline{\mathbf{g}}(\bar{p}) \cdot \mathbf{v} \, \mathrm{dS}_x \;,$$

$$\int_\Omega \left(\phi \operatorname{div} \mathbf{u} - \fint_{\Gamma_Y} \mathbf{u}^1 \cdot \mathbf{n}^{[m]} \, \mathrm{dS}_y\right) + \bar{p} \gamma \phi |\Omega| = -J \;,$$

for all $\mathbf{v} \in \mathbf{H}^1(\Omega), \mathbf{v}^1 \in L^2(\Omega; \mathbf{H}^1_\#(Y))$, where $J^\varepsilon \to J$

- Local — Microscopic problems: take $\mathbf{v} \equiv 0$, $\Rightarrow$ problems in Y.
- Global – Macroscopic problem: take $\mathbf{v}^1 \equiv 0$, $\Rightarrow$ problems in Ω.

Local problems

$$\fint_{Y_m} \nabla_y^S \mathbf{v}^1 : \mathbb{D} \nabla_y^S \left(\mathbf{u}^1 + \mathbf{\Pi}^{ij} \partial_j^x u_i \right) + \bar{p} \fint_{\Gamma_Y} \mathbf{v}^1 \cdot \mathbf{n}^{[m]} \, \mathrm{dS}_y = 0 \quad \forall \mathbf{v}^1 \in \mathbf{H}_\#^1(Y) \,,$$

"homog. deformation modes" $\mathbf{\Pi}^{ij} = (\Pi_k^{ij})$, $\Pi_k^{ij} = y_j \delta_{ik}$, $i, j, k = 1, 2, 3$

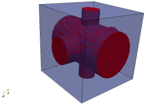
Corrector functions $\boldsymbol{\omega}^{ij}(y)$, $\boldsymbol{\omega}^P(y) \in \widetilde{\mathbf{H}_\#^1}(Y_m)$

$$\mathbf{u}^1(x, y) = \boldsymbol{\omega}^{ij}(y) \, \partial_j^x u_i(x) - \bar{p} \boldsymbol{\omega}^P(y)$$

1. $\boldsymbol{\omega}^{ij}$ ... response to unit homog. strain

$$\fint_{Y_m} \left(\mathbb{D} \nabla_y^S (\boldsymbol{\omega}^{ij} + \mathbf{\Pi}^{ij}) \right) : \nabla_y^S \mathbf{v} = 0 \,, \quad \forall \mathbf{v} \in \mathbf{H}_\#^1(Y_m) \,.$$

Micro-channel Y_c



matrix Y_m — solid

2. $\boldsymbol{\omega}^P$ ... response to unit pressure in Y_c

$$\fint_{Y_m} (\mathbb{D} \nabla_y^S \boldsymbol{\omega}^P) : \nabla_y^S \mathbf{v} = \fint_{\Gamma_Y} \mathbf{v} \cdot \mathbf{n}^{[m]} \, \mathrm{dS}_y \,, \quad \forall \mathbf{v} \in \mathbf{H}_\#^1(Y$$

Upscaled microlevel model — Homogenized problem

Homogenized coefficients (depend on correctors $\boldsymbol{\omega}^{ij}, \boldsymbol{\omega}^P$)

$$
\begin{aligned}
A_{ijkl} &= \fint_{Y_m} \left(\mathbb{D}\nabla_y^S(\boldsymbol{\omega}^{ij} + \boldsymbol{\Pi}^{ij})\right) : \nabla_y^S(\boldsymbol{\omega}^{kl} + \boldsymbol{\Pi}^{kl}) \;, \\
B_{ij} &= \phi\delta_{ij} - \fint_{Y_m} \mathrm{div}_y \boldsymbol{\omega}^{ij} \;, \\
M &= \gamma\phi + \fint_{Y_m} \left(\mathbb{D}\nabla_y^S \boldsymbol{\omega}^P\right) : \nabla_y^S \boldsymbol{\omega}^P \;,
\end{aligned}
$$

where $\boldsymbol{\Pi}^{rs} = (\Pi_i^{rs}) = (y_s\delta_{ir})$
Macroscopic equations for $\mathbf{u} \in \mathbf{H}^1(\Omega)/\mathcal{R}(\Omega)$ and $p \in \mathbb{R}$:

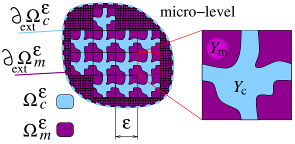
$$
\begin{aligned}
&\int_\Omega \left(\mathbb{A}\nabla_x^S \mathbf{u} - p\mathbf{B}\right) : \nabla_x^S \mathbf{v} = \int_\Omega (1-\phi)\mathbf{f}\cdot\mathbf{v} + \int_{\partial\Omega} \overline{\mathbf{g}}(p)\cdot\mathbf{v}\,\mathrm{dS}_x \;, \quad \forall\, \mathbf{v} \in \mathbf{H}^1(\Omega) \\
&\int_\Omega \mathbf{B} : \nabla_x^S \frac{\mathrm{d}}{\mathrm{d}\,t}\mathbf{u} + |\Omega| M \frac{\mathrm{d}}{\mathrm{d}\,t} p = -\dot{J},
\end{aligned}
$$

$\dot{J} = \mathrm{div}\mathbf{w}$ is the fluid content increase.

2) Upscaling Stokes flow $\rightarrow$ Darcy law

Homogenization of the Stokes flow in Ω_c^ε. For a while, any deformation of the skeleton is disregarded. Flow velocity $\mathbf{w}^\varepsilon$ and pressure p satisfy:

$$
\begin{aligned}
-\eta^\varepsilon \nabla^2 \mathbf{w}^\varepsilon + \nabla p^\varepsilon &= \mathbf{f}^\varepsilon \,, \quad \text{in } \Omega_c^\varepsilon \,, \\
\nabla \cdot \mathbf{w}^\varepsilon &= 0 \,, \quad \text{in } \Omega_c^\varepsilon \,, \\
\mathbf{w}^\varepsilon &= 0 \quad \text{on } \Gamma^\varepsilon \,, \\
-p^\varepsilon \mathbf{n}^{[c]} + \eta^\varepsilon \mathbf{n}^{[c]} \cdot \nabla \mathbf{w}^\varepsilon &= \mathbf{g}^\varepsilon \,, \quad \text{on } \partial_{\mathrm{ext}} \Omega_c^\varepsilon \,,
\end{aligned}
$$



where $\eta^\varepsilon = \varepsilon^2 \bar{\eta}$ is the viscosity (nonvanishing flow when $\varepsilon \rightarrow 0$).

Weak formulation

Find $(\mathbf{w}^\varepsilon, p^\varepsilon) \in \mathbf{V}(\Omega_c^\varepsilon) \times L^2(\Omega_c^\varepsilon)$ so that

$$
\int_{\Omega_c^\varepsilon} \varepsilon^2 \bar{\eta} \nabla \mathbf{w}^\varepsilon : \nabla \mathbf{v} - \int_{\Omega_c^\varepsilon} p^\varepsilon \nabla \cdot \mathbf{v} = \int_{\Omega_c^\varepsilon} \mathbf{f}^\varepsilon \cdot \mathbf{v} + \int_{\partial_{\mathrm{ext}} \Omega_c^\varepsilon} \mathbf{g}^\varepsilon \cdot \mathbf{v} \quad \forall \mathbf{v} \in \mathbf{V}(\Omega_c^\varepsilon) \,,
$$

$$
\int_{\Omega_c^\varepsilon} q \nabla \cdot \mathbf{w}^\varepsilon = 0 \quad \forall q \in L^2(\Omega_c^\varepsilon) \,.
$$

[Sanchez-Palencia, Allaire,...]

Limit model — Darcy law

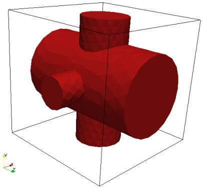
Homogenized (mean) flow velocity $\mathbf{w} = \fint_{Y_c} \tilde{\mathbf{w}}$ satisfies

$$\mathbf{w} = -\frac{\mathbf{K}}{\bar{\eta}} \left(\nabla_x p^0 - \mathbf{f} \right), \qquad \text{where } K_{ij} = \fint_{Y_c} \psi_i^j = \fint_{Y_c} \nabla_y \boldsymbol{\psi}^i : \nabla_y \boldsymbol{\psi}^i$$

is the intrinsic permeability depending on the local corrector problem:
Find $(\boldsymbol{\psi}^i, \pi^i) \in \mathbf{H}^1_\#(Y_c) \times L^2(Y_c)$, $i = 1, 2, 3$ such that

$$\int_{Y_c} \nabla_y \boldsymbol{\psi}^k : \nabla_y \mathbf{v} - \int_{Y_c} \pi^k \nabla \cdot \mathbf{v} = \int_{Y_c} v_k \quad \forall \mathbf{v} \in \mathbf{H}^1_\#(Y_c)\,,$$

$$\int_{Y_c} q \nabla_y \cdot \boldsymbol{\psi}^k = 0 \quad \forall q \in L^2(Y_c)\,.$$



channel Y_c

Coupled flow deformation problem

The Biot model of poroelastic media for quasi-static problems is constituted by the following equations imposed in Ω

$$-\nabla \cdot \boldsymbol{\sigma} = \mathbf{f}^s \,, \qquad \boldsymbol{\sigma} = \mathbb{A}\nabla^S \mathbf{u} - \mathbf{B}p \,,$$
$$\mathbf{B} : \nabla^S \dot{\mathbf{u}} + M\dot{p} = -\nabla \cdot \mathbf{w} \,, \qquad \mathbf{w} = -\frac{\mathbf{K}}{\bar{\eta}} \left(\nabla p - \mathbf{f}^f\right) \,.$$

The homogenized coefficients can be perturbed by the deformation!

Boundary conditions:

$$\mathbf{u} = 0 \,, \quad \text{on } \partial_u \Omega \,, \qquad \mathbf{n} \cdot \boldsymbol{\sigma} = \mathbf{g}^s \,, \quad \text{on } \partial_\sigma \Omega \,,$$
$$p = p_\partial \,, \quad \text{on } \partial_p \Omega \,, \qquad \mathbf{n} \cdot \mathbf{w} = w_n \,, \quad \text{on } \partial_w \Omega \,,$$

whereby the decomposition of $\partial\Omega$ into disjoint parts is considered

$$\text{skeleton:} \quad \partial\Omega = \partial_\sigma \Omega \cup \partial_u \Omega \,, \quad \partial_\sigma \Omega \cap \partial_u \Omega = \emptyset \,,$$
$$\text{fluid:} \quad \partial\Omega = \partial_w \Omega \cup \partial_p \Omega \,, \quad \partial_w \Omega \cap \partial_p \Omega = \emptyset \,.$$

Conception of a weakly non-linear model

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Linear theory approach:

- poroelastic model (static problem, locally constant pressure) $\Rightarrow$ $\mathbb{A}, \mathbf{B}, M$
- flow in (rigid) porous medium $\Rightarrow$ $\mathbf{K}$
- "Biot's" coupling "flow & deformation": through the mass conservation eq.

Extension beyond the linear theory – ingredients:

- 1st order approximation of the deforming local microstructures using corrector result of homogenization
  $\Rightarrow$ convection material velocity field $\vec{\mathcal{V}}$,
- sensitivity of the homogenized coefficients w.r.t. deformation by $\vec{\mathcal{V}}$
- linearization schemes for incerementa formulation

Perturbation of microstructures

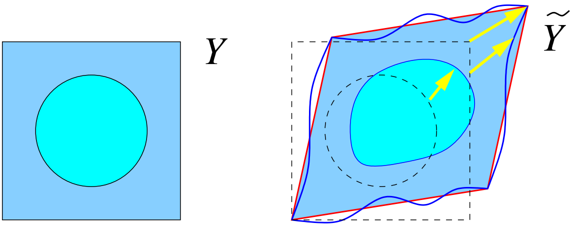
Using the corrector result of homogenization we introduce $\vec{\mathcal{V}}(x,y)$:

$$\text{affine part of displacement:} \quad \bar{\mathbf{u}}(x,y) = \mathbf{\Pi}^{ij}(y) e_{ij}^x(\mathbf{u}(x)) \,,$$

$$\text{fluctuating part of displacement:} \quad \mathbf{u}^1(x,y) = \boldsymbol{\omega}^{ij}(y) e_{ij}^x(\mathbf{u}(x)) - \boldsymbol{\omega}^P(y) p(x) \,,$$

$$\text{total perturbation:} \quad \tilde{\mathbf{u}}(x,y) = \bar{\mathbf{u}}(x,y) + \mathbf{u}^1(x,y) = \tilde{\tau} \vec{\mathcal{V}}(x,y) \,.$$

where $x \in \Omega$ and $y \in Y_m$.



$$\tilde{\mathbf{u}}(x,y) = \bar{\mathbf{u}}(x,y) + \mathbf{u}^1(x,y)$$

Perturbation of microstructures

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Using the corrector result of homogenization we introduce $\vec{\mathcal{V}}(x,y)$:

affine part of displacement: $\bar{\mathbf{u}}(x,y) = \boldsymbol{\Pi}^{ij}(y) e^x_{ij}(\mathbf{u}(x))$,

fluctuating part of displacement: $\mathbf{u}^1(x,y) = \boldsymbol{\omega}^{ij}(y) e^x_{ij}(\mathbf{u}(x)) - \boldsymbol{\omega}^P(y) p(x)$,

total perturbation: $\tilde{\mathbf{u}}(x,y) = \bar{\mathbf{u}}(x,y) + \mathbf{u}^1(x,y) = \tilde{\tau}\vec{\mathcal{V}}(x,y)$.

where $x \in \Omega$ and $y \in Y_m$.

Local perturbed homogenized coefficients:

- $\tilde{\mathcal{M}}(\tilde{\mathbf{u}}(x,\cdot), Y)$ associated with domain $\tilde{Y}(x) = Y + \{\tilde{\mathbf{u}}(x,\cdot)\}_{y \in Y}$
- perturbed homogenized coefficients $H(\tilde{\mathcal{M}}(\tilde{\mathbf{u}}, Y))$ can be approximated using the sensititvity analysis:

$$H(\tilde{\mathcal{M}}(\tilde{\mathbf{u}}(x,\cdot), Y)) \approx \tilde{H}(\mathcal{M}(Y), \tilde{\mathbf{u}}) = H^0(\mathcal{M}(Y)) + \delta H^0(\mathcal{M}(Y)) \circ \tilde{\tau}\vec{\mathcal{V}}(x,\cdot)$$
$$= H^0 + \delta_{\mathbf{e}} H^0 : \mathbf{e}(\mathbf{u}) + \delta_p H^0 p \ , \ .$$

where $$(\delta_{\mathbf{e}} H^0)_{ij} := (\partial_{\mathbf{e}} \delta H^0 \circ \tilde{\mathbf{u}})_{ij} = \delta H^0 \circ (\boldsymbol{\omega}^{ij} + \boldsymbol{\Pi}^{ij}) \ ,$$
$$\delta_p H^0 := \partial_p \delta H^0 \circ \tilde{\mathbf{u}} = \delta H^0 \circ (-\boldsymbol{\omega}^P) \ .$$

Sensitivity of microstructures

- Convection velocity field ⇒ perturbed microstructure: $\vec{\mathcal{V}} : \overline{Y} \longrightarrow \mathbb{R}^3$, $z_i(y,\tau) = y_i + \tau \mathcal{V}_i(y)$, $y \in Y$, $i = 1, 2$,
- Domain method of differentiation:

  $\delta(\cdot)$ ... total (*material*) derivative

  $\delta_\tau(\cdot)$ ... partial (*local*) derivative *w.r.t.* "time" τ .

  ...as used in shape optimization...

- General functional $\Phi(\varphi) = |Y|^{-1} \int_{Y_d} F(\varphi)$ where $Y_d \stackrel{\text{B.V.P.}}{\rightarrow} \varphi$
  Using the chain rule differentiation,

$$\delta\Phi(\varphi) = \delta_\varphi \Phi(\varphi) \circ \delta\varphi + \delta_\tau \Phi(\varphi) \;,$$

$$\text{where } \delta_\tau \Phi(\varphi) = \fint_{Y_d} F(\varphi) \left(\nabla_y \cdot \mathcal{V} - \fint_Y \nabla_y \cdot \mathcal{V} \right) + \fint_{Y_d} \delta_\tau F(\varphi) \;,$$

$\delta\varphi$ can be eliminated due to the local corrector problems.

Sensitivity of the permeability K

Recall $K_{ij} = \fint_{Y_c} \psi^i_j$, hence:

$$\delta K_{ij} = \delta_\tau \fint_{Y_c} \psi^i_j + \fint_{Y_c} \delta\psi^i_j \,.$$

Use the local corrector problem (and its differentiated form) to eliminate $\delta\psi^i_j$. Finally

$$\begin{aligned}\delta K_{ij} = & \fint_{Y_c} \left(\psi^j_i + \psi^i_j - \nabla_y \boldsymbol{\psi}^i : \nabla_y \boldsymbol{\psi}^j + \pi^i \nabla_y \cdot \boldsymbol{\psi}^j + \pi^j \nabla_y \cdot \boldsymbol{\psi}^i \right) \nabla_y \cdot \mathcal{V} \\ & - \fint_{Y} \nabla_y \cdot \mathcal{V} \fint_{Y_c} \nabla_y \boldsymbol{\psi}^i : \nabla_y \boldsymbol{\psi}^j \\ & + \fint_{Y_c} \left(\partial^y_l \mathcal{V}_r \partial^y_r \psi^i_k \partial^y_l \psi^j_k + \partial^y_l \mathcal{V}_r \partial^y_r \psi^j_k \partial^y_l \psi^i_k - \pi^i \partial^y_k \mathcal{V}_r \partial^y_r \psi^j_k - \pi^j \partial^y_k \mathcal{V}_r \partial^y_r \psi^i_k \right)\end{aligned}$$

…and similarly for $\delta A_{ijkl}, \delta B_{ij}, \delta M$

Weakly nonlinear model of FSPM

Find the couple $(\mathbf{u}, p) \in \mathbf{U}(\Omega) \times P(\Omega)$ satisfying

$$\int_\Omega \left(\tilde{\mathbb{A}} \mathbf{e}(\mathbf{u}) - p \tilde{\mathbf{B}} \right) : \mathbf{e}(\mathbf{v}) = \int_\Omega \tilde{\mathbf{f}}^s \cdot \mathbf{v} + \int_{\partial\Omega} \tilde{\mathbf{g}}^s \cdot \mathbf{v} \, \mathrm{dS}_x \,, \quad \forall \mathbf{v} \in \mathbf{U}(\Omega) \,,$$

$$\int_\Omega q \left(\tilde{\mathbf{B}} : \mathbf{e}(\frac{\mathrm{d}}{\mathrm{d}\, t} \mathbf{u}) + \frac{\mathrm{d}}{\mathrm{d}\, t} p \tilde{M} \right) + \int_\Omega \frac{\tilde{\mathbf{K}}}{\bar{\eta}} (\nabla_x p - \mathbf{f}) \cdot \nabla_x q = 0 \quad \forall q \in P_0(\Omega) \,,$$

where the generic form holds: $\tilde{H} = H^0 + \delta_{\mathbf{e}} H^0 : \mathbf{e}(\mathbf{u}) + \delta_p H^0 p$.

Incremental formulation

Given $(\mathbf{u}^0, p^0) \approx \big(\mathbf{u}(t - \Delta t, \cdot), p(t - \Delta t, \cdot)\big)$, compute $(\mathbf{u}, p) \approx \big(\mathbf{u}(t, \cdot), p(t, \cdot)\big)$, so that $\Psi^t((\mathbf{u}, p), (\mathbf{v}, q)) = 0$ for any $(\mathbf{v}, q) \in \mathbf{U}_0(\Omega) \times P_0(\Omega)$, where the nonlinear residuum of the non-steady formulation is given as

$$\Psi^t((\mathbf{u}, p), (\mathbf{v}, q)) = \int_\Omega \left(\tilde{\mathbb{A}} \mathbf{e}(\mathbf{u}) - p \tilde{\mathbf{B}} \right) : \mathbf{e}(\mathbf{v}) + \int_\Omega q \left(\tilde{\mathbf{B}} \mathbf{e}(\mathbf{u} - \mathbf{u}^0) + \tilde{M}(p - p^0) \right)$$
$$+ \frac{\Delta t}{\bar{\eta}} \int_\Omega \tilde{\mathbf{K}} (\nabla_x p - \mathbf{f}(t)) \cdot \nabla_x q - \int_\Omega \tilde{\mathbf{f}}^s(t) \cdot \mathbf{v} - \int_{\partial\Omega} \tilde{\mathbf{g}}^s(t) \cdot \mathbf{v} \,.$$

Linearization scheme I/III

Incremental step problem

compute $(\delta \mathbf{u}, \delta p) \in \mathbf{U}_0(\Omega) \times P_0(\Omega)$ for a given $(\bar{\mathbf{u}}, \bar{p})$,

$$\delta \Psi^t((\bar{\mathbf{u}}, \bar{p}), (\mathbf{v}, q)) \circ (\delta \mathbf{u}, \delta p) = -\Psi^t((\bar{\mathbf{u}}, \bar{p}), (\mathbf{v}, q)) \quad \forall (\mathbf{v}, q) \in \mathbf{U}_0(\Omega) \times P_0(\Omega) \, .$$

where the differentiation of Ψ^t yields

$$\begin{aligned} \delta \Psi^t((\bar{\mathbf{u}}, \bar{p}), (\mathbf{v}, q)) \circ (\delta \mathbf{u}, \delta p) = & \int_\Omega \left(\overline{\mathbb{A}} \mathbf{e}(\delta \mathbf{u}) - \delta p \overline{\mathbf{B}}\right) : \mathbf{e}(\mathbf{v}) \\ & - \int_\Omega \left(\partial_{\mathbf{e}} \mathbf{f}^s \circ \mathbf{e}(\delta \mathbf{u}) + \partial_p \mathbf{f}^s \circ \delta p\right) \cdot \mathbf{v} \\ & - \int_{\partial\Omega} \left(\partial_{\mathbf{e}} \mathbf{g}^s \circ \mathbf{e}(\delta \mathbf{u}) + \partial_p \mathbf{g}^s \circ \delta p\right) \cdot \mathbf{v} \\ & + \frac{\Delta t}{\bar{\eta}} \int_\Omega \nabla q \cdot \left(\overline{\mathbf{K}} \nabla \delta p + \overline{\mathbf{G}} : \mathbf{e}(\delta \mathbf{u}) + \overline{\mathbf{Q}} \delta p\right) \\ & + \int_\Omega q \left(\overline{\mathbf{D}} : \mathbf{e}(\delta \mathbf{u}) + \overline{M} \delta p\right) \, , \end{aligned}$$

coeffs. $\overline{\mathbb{A}}, \overline{\mathbf{B}}, \overline{\mathbf{K}}, \overline{\mathbf{G}}, \overline{\mathbf{Q}}, \overline{\mathbf{D}}$, and $\overline{M}$ are defined using sensitivity expressions:

Linearization scheme II/III

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Coefficients for the corrector step – based on the sensitivity analysis involving deformation of the microstructures

$$\bar{\partial}\mathbb{A}^0 = \partial_{\mathbf{e}}\mathbb{A}^0 \circ \mathbf{e}(\bar{\mathbf{u}}) + \partial_p\mathbb{A}^0 \circ \bar{p} \,, \quad \bar{\partial}\mathbf{B}^0 = \partial_{\mathbf{e}}\mathbf{B}^0 \circ \mathbf{e}(\bar{\mathbf{u}}) + \partial_p\mathbf{B}^0 \circ \bar{p} \,,$$
$$\bar{\partial}M^0 = \partial_{\mathbf{e}}M^0 \circ \mathbf{e}(\bar{\mathbf{u}}) + \partial_p M^0 \circ \bar{p} \,, \quad \bar{\partial}\mathbf{K}^0 = \partial_{\mathbf{e}}\mathbf{K}^0 \circ \mathbf{e}(\bar{\mathbf{u}}) + \partial_p\mathbf{K}^0 \circ \bar{p} \,,$$

$$\begin{aligned}
\overline{\mathbb{A}}(\bar{\mathbf{u}}, \bar{p}) &= \mathbb{A}^0 + \bar{\partial}\mathbb{A}^0 + \partial_{\mathbf{e}}(\mathbb{A}^0\mathbf{e}(\bar{\mathbf{u}})) \circ \langle\ \rangle_{\mathbf{e}} - \partial_{\mathbf{e}}(\mathbf{B}^0\bar{p}) \circ \langle\ \rangle_{\mathbf{e}} \\
\overline{\mathbf{B}}(\bar{\mathbf{u}}, \bar{p}) &= \mathbf{B}^0 + \bar{\partial}\mathbf{B}^0 + \partial_p(\mathbf{B}^0\bar{p}) \circ \langle\ \rangle_p - \partial_p(\mathbb{A}^0\mathbf{e}(\bar{\mathbf{u}})) \circ \langle\ \rangle_p \\
\overline{\mathbf{D}}(\bar{\mathbf{u}}, \bar{p}, \mathbf{u}^0, p^0) &= \mathbf{B}^0 + \bar{\partial}\mathbf{B}^0 + \partial_{\mathbf{e}}\mathbf{B}^0 : (\mathbf{e}(\bar{\mathbf{u}}) - \mathbf{e}(\mathbf{u}^0)) \circ \langle\ \rangle_{\mathbf{e}} + \partial_{\mathbf{e}}M^0(\bar{p} - p^0) \circ \langle\ \rangle_{\mathbf{e}} \\
\overline{M}(\bar{\mathbf{u}}, \bar{p}, \mathbf{u}^0, p^0) &= M^0 + \bar{\partial}M^0 + \partial_p M^0(\bar{p} - p^0) \circ \langle\ \rangle_p + \partial_p\mathbf{B}^0 : (\mathbf{e}(\bar{\mathbf{u}}) - \mathbf{e}(\mathbf{u}^0)) \circ \langle\ \rangle_p \,, \\
\overline{\mathbf{K}}(\bar{\mathbf{u}}, \bar{p}) &= \mathbf{K}^0 + \bar{\partial}\mathbf{K}^0 \,, \\
\overline{\mathbf{G}} &= \partial_{\mathbf{e}}\mathbf{K}^0(\nabla\bar{p} - \mathbf{f}) \circ \langle\ \rangle_{\mathbf{e}} \,, \\
\overline{\mathbf{Q}} &= \partial_p\mathbf{K}^0(\nabla\bar{p} - \mathbf{f})) \circ \langle\ \rangle_p \,,
\end{aligned}$$

Linearization scheme III/III

Given $(\mathbf{u}^0, p^0) \approx (\mathbf{u}(t - \Delta t, \cdot), p(t - \Delta t, \cdot))$, compute $(\mathbf{u}, p) \approx (\mathbf{u}(t, \cdot), p(t, \cdot))$:

- step 0 set $(\bar{\mathbf{u}}, \bar{p}) = (\mathbf{u}^0, p^0)$
- **step 1**: use $(\bar{\mathbf{u}}, \bar{p})$ to define the perturbed homogenized coefficients $\tilde{H}(\bar{\mathbf{u}}, \bar{p})$ and residual $r(\cdot) := \Psi^t((\bar{\mathbf{u}}, \bar{p}), \cdot)$, and **compute** $(\delta\mathbf{u}, \delta p) \in \mathbf{U}_0(\Omega) \times P_0(\Omega)$:

$$\delta\Psi^t((\bar{\mathbf{u}}, \bar{p}), (\mathbf{v}, q)) \circ (\delta\mathbf{u}, \delta p) = -r(\mathbf{v}, q) \quad \forall (\mathbf{v}, q) \in \mathbf{U}_0(\Omega) \times P_0(\Omega) \, .$$

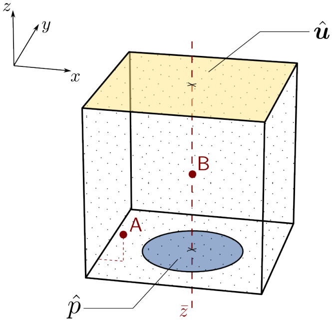
- **step 2**: update

$$\begin{aligned} \bar{\mathbf{u}} &:= \mathbf{u} = \bar{\mathbf{u}} + \delta\mathbf{u} \, , \\ \bar{p} &:= p = \bar{p} + \delta p \, , \\ \text{residual} \quad r(\cdot) &:= \Psi^t((\bar{\mathbf{u}}, \bar{p}), \cdot) \, , \end{aligned}$$

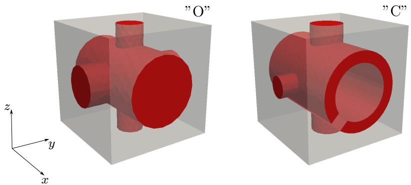
  and GOTO step 1, unless residuum $|r(\cdot)|$ is "small enough"
- step 3: GOTO the next time level with

$$\mathbf{u}^0 := \mathbf{u} \, , \quad p^0 := p \, .$$

Example: perfused block / confined compression



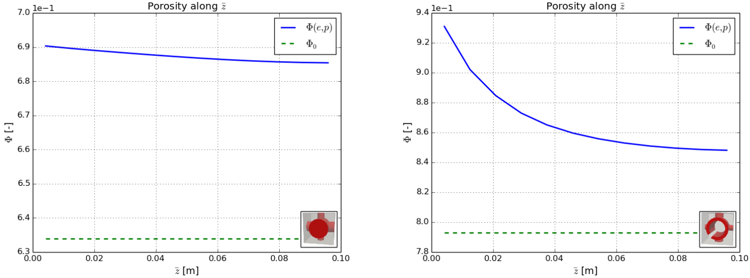
"macro" Ω



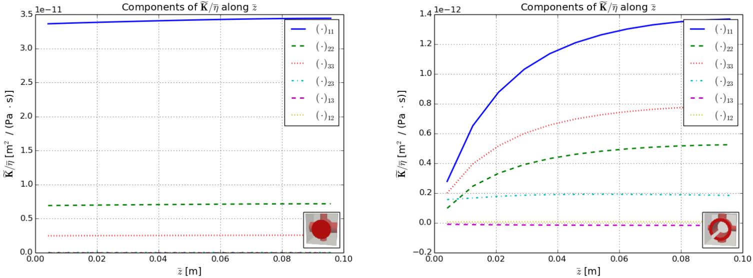
fluid channels Y_c in "micro-cell" Y

- compression by ramp-and-hold test displacements $\hat{\mathbf{u}}$
- material properties:
  - matrix = *polystyrene*: $E = 3.0 \times 10^9$, $\nu = 0.34$
  - fluid = *glycerine*: $\gamma \approx 10^{-9}$, $\eta = 0.95$
- scale: $\varepsilon_0 = 0.001$
- SW: in-house FEM in Python: SfePy, `sfepy.org`

Example: comparison: lin. / non-lin.

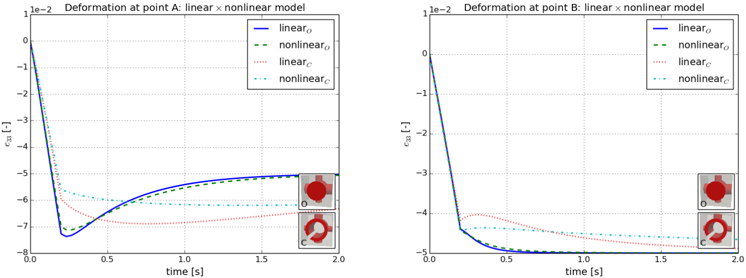


porosity along the central axis z in domain Ω (steady state)

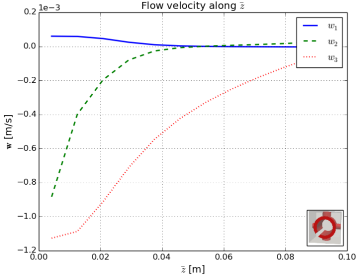


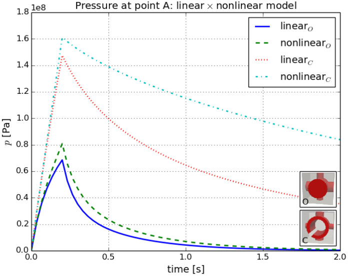
permeability $K_{ij}/\bar{\eta}$ along the central axis z in domain Ω (steady state)

Example: comparison: lin. / non-lin.



deformation e_{33} at points A and B in domain Ω

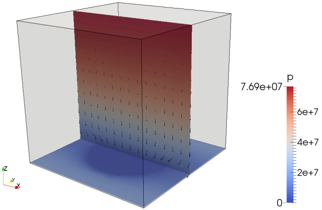


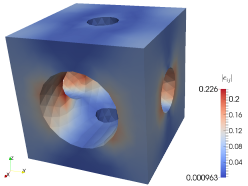


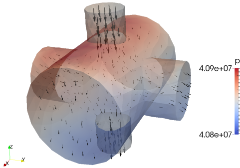
fluid perfusion flow along central axis z pressure at point A

Example: effects of microstructure

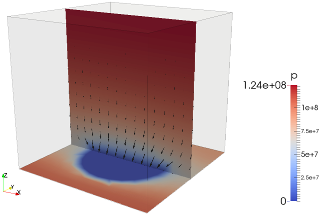
macro: | micro: solid skeleton | micro: fluid channel

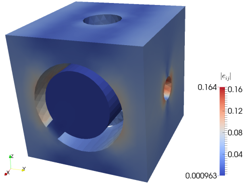


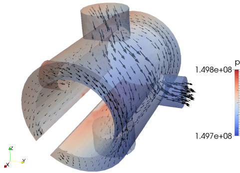




pressure / velocity | strain | pressure / velocity







non-symmetric flow!

Eulerian formulation — "residual-based formulation"

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Weak formulation

Admissibility sets *(Dirichlet BCs)*

$$V(t) = \{\mathbf{v}|\ \mathbf{v} = \mathbf{u}^\partial \text{ on } \partial_u\Omega(t) \subset \partial\Omega(t)\}\ ,$$
$$Q(t) = \{q|\ q = p^\partial \text{ on } \partial_p\Omega(t) \subset \partial\Omega(t)\}\ .$$

Define:

$$\Phi_t((\mathbf{u},p);(\mathbf{v},0)) = \int_{\Omega(t)} \boldsymbol{\sigma} : \nabla\mathbf{v} - \int_{\Omega(t)} \rho\mathbf{b}\cdot\mathbf{v} \quad \forall V_0(t)\ ,$$
$$\Phi_t((\mathbf{u},p);(0,q)) = \int_{\Omega(t)} (\nabla\cdot\dot{\mathbf{u}}q + \mathbf{K}\nabla p\cdot\nabla q) - \mathcal{J}_t(q) \quad \forall q \in Q_0(t)\ ,$$

Find $(\mathbf{u},p) \in V(t) \times Q(t)$ such that

$$\Phi_t((\mathbf{u},p);(\mathbf{v},q)) = 0 \quad \forall(\mathbf{v},q) \in V_0(t) \times Q_0(t)\ .$$

Differentiation of residual – "moving configuration"

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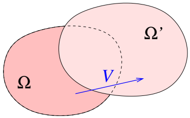
Incremental (Updated Lagrangian) formulation (ULF)

Given $(\bar{\mathbf{u}}, \bar{p})$ at time $t \geq 0$, compute a new state $(\mathbf{u}, p)$ at time $t + \delta t$ such that

$$\Phi_{t+\delta t}((\mathbf{u}, p); (\mathbf{v}, q)) \approx \Phi_t((\bar{\mathbf{u}}, \bar{p}); (\mathbf{v}, q)) + \delta\Phi_t((\bar{\mathbf{u}}, \bar{p}); (\mathbf{v}, q)) \circ (\delta\mathbf{u}, \delta p, \delta t\mathcal{V}) \,,$$

where $\delta\Phi_t((\bar{\mathbf{u}}, \bar{p}); (\mathbf{v}, q)) \circ (\delta\mathbf{u}, \delta p, \delta t\mathcal{V})$ is the increment due to the material derivative associated with convection field $\mathcal{V}$,

$$\mathbf{u} = \bar{\mathbf{u}} + \delta\mathbf{u} \,, p = \bar{p} + \delta p \,,$$
$$\text{where} \quad \delta\mathbf{u} = \dot{\mathbf{u}}\delta t \,, \quad \delta p = \dot{p}\delta t \,,$$
$$\Omega(t + \delta t) = \Omega(t) + \delta t\{\mathcal{V}\}_{\Omega(t)}$$



Lie derivative of the Cauchy stress $\boldsymbol{\sigma} = J^{-1}\mathbf{FSF}^T = \boldsymbol{\sigma}^{\text{eff}} - p\mathbf{I}$

$$\dot{\boldsymbol{\sigma}} = -\boldsymbol{\sigma}\nabla\cdot\mathcal{V} + \nabla\mathcal{V}\boldsymbol{\sigma} + \boldsymbol{\sigma}(\nabla\mathcal{V})^T + \pounds_{\mathcal{V}}\,\boldsymbol{\sigma} \,,$$
$$\pounds_{\mathcal{V}}\,\boldsymbol{\sigma}^p = p(\nabla\mathcal{V} + (\nabla\mathcal{V})^T) - p\nabla\cdot\mathcal{V}\mathbf{I} - \dot{p}\mathbf{I} \,,$$
$$\pounds_{\mathcal{V}}\,\boldsymbol{\sigma}^{\text{eff}} = J^{-1}\mathbf{F}\dot{\mathbf{S}}\mathbf{F}^T = \mathbb{D}^{\text{eff}} e(\dot{\mathbf{u}}) \,.$$

ULF — perturbed residuals

reference state	$(\hat{\mathbf{u}}, \hat{p})$
test fields	$(\mathbf{v}, q)$
state and domain perturbation rates	$(\dot{\mathbf{u}}, \dot{p}, \mathcal{V})$

$$\delta\Phi_t((\hat{\mathbf{u}}, \hat{p}); (\mathbf{v}, 0)) \circ (\dot{\mathbf{u}}, \dot{p}, \mathcal{V}) =$$
$$\int_\Omega \mathbb{D}^{\text{eff}} e(\dot{\mathbf{u}}) : e(\mathbf{v}) + \int_\Omega \nabla\mathcal{V}\boldsymbol{\sigma}^{\text{eff}} : \nabla\mathbf{v}$$
$$- \int_\Omega (p(\nabla\cdot\mathbf{v})(\nabla\cdot\mathcal{V}) - p\nabla\mathbf{v}\nabla\mathcal{V} : \mathbf{I} + \dot{p}\nabla\cdot\mathbf{v}) - \int_\Omega \rho\dot{\mathbf{b}}\cdot\mathbf{v} \,,$$

$$\delta\Phi_t((\hat{\mathbf{u}}, \hat{p}); (0, q)) \circ (\dot{\mathbf{u}}, \dot{p}, \mathcal{V}) =$$
$$\int_\Omega (q(\nabla\cdot\dot{\mathbf{u}})(\nabla\cdot\mathcal{V}) - q\nabla\dot{\mathbf{u}}\nabla\mathcal{V} : \mathbf{I} + q\nabla\cdot\dot{\mathbf{u}})$$
$$+ \int_\Omega (\mathbf{K}\nabla p\cdot\nabla q)\,\nabla\cdot\mathcal{V} + \int_\Omega (\mathbf{K}\nabla\dot{p}\cdot\nabla q)$$
$$- \int_\Omega \mathbf{K}(\nabla p\nabla\mathcal{V})\cdot\nabla q - \int_\Omega \mathbf{K}\nabla p\cdot(\nabla q\nabla\mathcal{V}) + \int_\Omega \dot{\mathbf{K}}\nabla p\cdot\nabla q - \dot{\mathcal{J}}_t(q) \,.$$

Incremental formulation — nonlinear kinematics

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For a given new load functional $L^{k+1}(\cdot)$, find increments $(\mathbf{u}, p) \in \delta\mathbf{U}(\Omega(t_{k+1})) \times \delta P(\Omega(t_{k+1}))$ which satisfy

$$\int_\Omega \tilde{\mathbb{A}}^{\text{eff}}\mathbf{e}(\mathbf{u}) : \mathbf{e}(\mathbf{v}) + \int_\Omega \tilde{\boldsymbol{\Sigma}}^{\text{eff}} : (\nabla\mathbf{u})^T\nabla\mathbf{v} - \int_\Omega p[\tilde{\mathbf{B}} + \tilde{\mathbf{B}}_\triangledown(\bar{\mathbf{u}})] : \mathbf{e}(\mathbf{v})$$
$$= \int_\Omega \hat{p}[\tilde{\mathbf{B}} + \tilde{\mathbf{B}}_\triangledown(\bar{\mathbf{u}})] : \mathbf{e}(\mathbf{v}) + \int_\Omega \hat{p}\delta\mathbf{B} : \mathbf{e}(\mathbf{v}) - \int_\Omega \boldsymbol{\Sigma}^k : \mathbf{e}(\mathbf{v}) + L^{k+1}(\mathbf{v})$$

for all $\mathbf{v} \in \delta\mathbf{U}_0(\Omega(t_k))$ and

$$\int_\Omega q[\tilde{\mathbf{B}} + \tilde{\mathbf{B}}_\triangledown(\bar{\mathbf{u}})] : \mathbf{e}(\mathbf{u}) + \int_\Omega q(\tilde{M} + \tilde{M}_\triangledown(\bar{\mathbf{u}}))p + \delta t\int_\Omega \left(\tilde{\mathbf{K}} + \tilde{\mathbf{K}}_\triangledown(\bar{\mathbf{u}})\right)\nabla p \cdot \nabla q$$
$$= \int_\Omega q\left[\tilde{\mathbf{B}} - \delta\mathbf{B}\right] : \mathbf{e}(\bar{\mathbf{u}}) + \int_\Omega q(\tilde{M} - \delta M)\bar{p} + \delta t\mathcal{J}^{k+1}(q)$$
$$- \delta t\int_\Omega \left(\tilde{\mathbf{K}} + \tilde{\mathbf{K}}_\triangledown(\bar{\mathbf{u}}) + \delta\mathbf{K}\right)\nabla\hat{p} \cdot \nabla q\,,$$

for all $q \in \delta P_0(\Omega(t_k))$ where $\tilde{\mathbf{H}}$ depend on the perturbed microstructure and

$$\tilde{\mathbf{B}}_\triangledown(\mathbf{v}) = \tilde{\mathbf{B}}(\nabla\cdot\mathbf{v} - (\nabla\mathbf{v})^T)\,,$$
$$\tilde{\mathbf{K}}_\triangledown(\mathbf{v}) = (\nabla\cdot\mathbf{v})\tilde{\mathbf{K}} - \tilde{\mathbf{K}}(\nabla\mathbf{v})^T - (\nabla\mathbf{v})\tilde{\mathbf{K}}^T\,,$$
$$\tilde{M}_\triangledown(\mathbf{v}) = \tilde{M}\nabla\cdot\mathbf{v}\,,$$

Conclusions

- Proposed a Weakly Nonlinear "Biot" model (WNB) which provides correction of effective material parameters w.r.t. *state variables*
- WNB is based on sensitivity and linear expansions of the poroelastic coefficients & permeability w.r.t. *state variables*;
- WNB:
  - accounts for important nonlinear effects (depends on micro-geom.!)
  - well adaptable for modelling of *functionally graded materials*

Outlook

- Time integration / linearization / dissipation ... to be checked;
- Adaptation of this approach for nonlinear kinematics (ULF);
- Extensions: dynamics / wave propagation electrochemical interactions, multi-porous media

Thanks for your attention