Pore scale modeling of porous media flow including moving boundaries

Carina Bringedal Iuliu Sorin Pop, Manuela Bastidas, Sohely Sharmin

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KNOWLEDGE IN ACTION



- Geothermal energy extraction.
- Inject cold fluid into subsurface. Extract warm water.
- Model flow rates and heat transport.



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- Inject cold fluid into subsurface. Extract warm water.
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- Chemical reactions?



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- Mineral precipitation and dissolution can affect the fluid flow and heat transport through the reservoir.



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- Geothermal energy extraction.
- Inject cold fluid into subsurface. Extract warm water.
- Model flow rates and heat transport.
- Chemical reactions?
- Mineral precipitation and dissolution can affect the fluid flow and heat transport through the reservoir.
- If two fluids present: Their flow will affect each other.



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Darcy scale description

• Flow at reservoir scale usually modeled using Darcy's law:

$$\mathbf{v} = -\frac{\mathbf{K}}{\mu} \nabla P$$

• Permeability **K** gives effective description of the average flow through an elementary representative volume.



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- If zoom in: Detailed pore structure revealed.
- Not necessarily interested in detailed behavior, but in large scale effect.



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Darcy scale description

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- Permeability **K** gives effective description of the average flow through an elementary representative volume.
- If zoom in: Detailed pore structure revealed.
- Not necessarily interested in detailed behavior, but in large scale effect.
- Start with pore scale description \rightarrow Upscale to Darcy scale.

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Overview

Pore scale formulation

- Mineral precipitation and dissolution
- Two-phase flow
- Evolving domains

2 Upscaling using homogenization

- Asymptotic expansions
- Thin strip
- Periodic porous medium
- Iffective behavior on Darcy scale

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- Pore scale processes can affect fluid flow through the reservoir.
- Mineral precipitation and dissolution.



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- Pore scale processes can affect fluid flow through the reservoir.
- Mineral precipitation and dissolution.



• Two-phase/Unsaturated flow.



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- Formulate pore scale description including a moving boundary.
 - $\rightarrow\,$ Separate explicitly between grain and void space.
 - $\rightarrow\,$ Conservation equations in evolving domains.



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- How does the permeability and effective heat transfer change when a chemical reaction affects the pore geometry?



- Formulate pore scale description including a moving boundary.
 - $\rightarrow\,$ Separate explicitly between grain and void space.
 - $\rightarrow\,$ Conservation equations in evolving domains.
- How does the permeability and effective heat transfer change when a chemical reaction affects the pore geometry?
- How does the (relative) permeability change when two fluids are present?





- Scale separator: $\varepsilon = I/L$.
- Fluid domain: $\Omega^{\varepsilon}(t)$.
- Grain domain: $G^{\varepsilon}(t)$.
- Interface between them: $\Gamma^{\varepsilon}(t)$.



• In fluid-filled void space, mass and momentum conservation:

$$\partial_t \rho_f + \nabla \cdot (\rho_f \mathbf{q}^{\varepsilon}) = 0 \qquad \text{in } \Omega^{\varepsilon}(t)$$
 $\varepsilon^2 \Big(\partial_t (\rho_f \mathbf{q}^{\varepsilon}) + \nabla \cdot (\rho_f \mathbf{q}^{\varepsilon} \otimes \mathbf{q}^{\varepsilon}) \Big) = -\nabla p^{\varepsilon} + \varepsilon^2 \Big(\nabla \cdot (\mu \mathcal{D}(\mathbf{q}^{\varepsilon}) - \frac{2}{3} \nabla (\mu \nabla \cdot \mathbf{q}^{\varepsilon}) \Big) \qquad \text{in } \Omega^{\varepsilon}(t)$

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• If constant density and viscosity:

$$\varepsilon^2 \rho_f \Big(\partial_t \mathbf{q}^{\varepsilon} + \mathbf{q}^{\varepsilon} \cdot \nabla \mathbf{q}^{\varepsilon} \Big) = -\nabla p^{\varepsilon} + \varepsilon^2 \mu \nabla^2 \mathbf{q}^{\varepsilon} \quad \text{in } \Omega^{\varepsilon}(t)$$

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• In fluid-filled void space, mass and momentum conservation:

$$\partial_t \rho_f + \nabla \cdot (\rho_f \mathbf{q}^{\varepsilon}) = 0 \qquad \text{in } \Omega^{\varepsilon}(t)$$
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• If constant density and viscosity:

$$abla \cdot {f q}^arepsilon = 0 \qquad \qquad {
m in} \ \Omega^arepsilon(t)$$

$$\varepsilon^2 \rho_f \Big(\partial_t \mathbf{q}^{\varepsilon} + \mathbf{q}^{\varepsilon} \cdot \nabla \mathbf{q}^{\varepsilon} \Big) = -\nabla p^{\varepsilon} + \varepsilon^2 \mu \nabla^2 \mathbf{q}^{\varepsilon} \quad \text{in } \Omega^{\varepsilon}(t)$$

- Boundary conditions?
 - No-slip at grain wall.
 - ► Rankine-Hugoniot jump condition: $\mathbf{n}^{\varepsilon} \cdot [\mathbf{j}_a] = v_n[a]$ on $\Gamma^{\varepsilon}(t)$

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Mineral precipitation and dissolution

• Grain-fluid boundary moving due to chemical reactions:

$$\mathbf{n}^{\varepsilon} \cdot (-
ho_f \mathbf{q}^{\varepsilon}) = v_n (2
ho -
ho_f) \qquad \quad \text{on } \Gamma^{\varepsilon}(t)$$



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Mineral precipitation and dissolution

• Grain-fluid boundary moving due to chemical reactions:

$$\begin{split} \mathbf{n}^{\varepsilon} \cdot (-\rho_f \mathbf{q}^{\varepsilon}) &= v_n (2\rho - \rho_f) & \text{on } \Gamma^{\varepsilon}(t) \\ \mathbf{q}^{\varepsilon} &= v_n \frac{\rho_f - 2\rho}{\rho_f} \mathbf{n}^{\varepsilon} & \text{on } \Gamma^{\varepsilon}(t) \end{split}$$



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Mineral precipitation and dissolution

• Grain-fluid boundary moving due to chemical reactions:

$$\mathbf{n}^{\varepsilon} \cdot (-\rho_f \mathbf{q}^{\varepsilon}) = v_n (2\rho - \rho_f) \qquad \text{on } \Gamma^{\varepsilon}(t)$$
$$\mathbf{q}^{\varepsilon} = v_n \frac{\rho_f - 2\rho}{\rho_f} \mathbf{n}^{\varepsilon} \qquad \text{on } \Gamma^{\varepsilon}(t)$$
$$\mathbf{n}^{\varepsilon} \cdot (D\nabla u^{\varepsilon} - \mathbf{q}^{\varepsilon} u^{\varepsilon}) = v_n (\rho - u^{\varepsilon}) \qquad \text{on } \Gamma^{\varepsilon}(t)$$
$$\rho v_n = -\varepsilon f(u^{\varepsilon}, T_f^{\varepsilon}) \qquad \text{on } \Gamma^{\varepsilon}(t)$$



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Two-phase flow

• Fluid-fluid boundary moving due to surface tension:

$$\mathbf{q}_{I}^{\varepsilon} \cdot \mathbf{n}^{\varepsilon} = \mathbf{q}_{II}^{\varepsilon} \cdot \mathbf{n}^{\varepsilon} = \mathbf{v}_{n}$$
$$(\sigma_{I}^{\varepsilon} - \sigma_{II}^{\varepsilon}) \cdot \mathbf{n}^{\varepsilon} = \frac{\varepsilon^{3}}{Ca} \mathbf{n}^{\varepsilon}$$



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Evolving domains

- The domain formulation and evolution of them must also be accounted for.
- In the general case, use level set:

$$S^{arepsilon}(t,\mathbf{x}) = egin{cases} < 0 & ext{if } \mathbf{x} \in \Omega^{arepsilon}(t) \ 0 & ext{if } \mathbf{x} \in \Gamma^{arepsilon}(t) \ > 0 & ext{if } \mathbf{x} \in G^{arepsilon}(t) \ \mathbf{n}^{arepsilon} = rac{
abla S^{arepsilon}}{|
abla S^{arepsilon}|} \end{cases}$$

$$\partial_t S^{\varepsilon} + v_n |\nabla S^{\varepsilon}| = 0$$

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Evolving domains

- The domain formulation and evolution of them must also be accounted for.
- Can be simplified if considering a thin strip:



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Upscaling using homogenization

- Goal: Find effective description at Darcy scale of the pore scale formulation.
- Scale separator $\varepsilon = I/L$.



Asymptotic expansions

• Homogenization ansatz: $u(t, \mathbf{x}) = u_0(t, \mathbf{x}, \mathbf{y}) + \varepsilon u_1(t, \mathbf{x}, \mathbf{y}) + \dots$



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Asymptotic expansions

• Homogenization ansatz: $u(t, \mathbf{x}) = u_0(t, \mathbf{x}, \mathbf{y}) + \varepsilon u_1(t, \mathbf{x}, \mathbf{y}) + \dots$



- Scaling of local variable: $\nabla = \nabla_{\mathbf{x}} + \frac{1}{\varepsilon} \nabla_{\mathbf{y}}$.
- Insert expansions, collect dominating terms, account for moving boundaries and find effective quantities.

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- Dependence on transversal variable eliminated: 2D \rightarrow 1D.
- Coupled reactive and heat transport:





C. Bringedal, I. Berre, I.S. Pop, F.A. Radu, A model for non-isothermal flow and mineral precipitation and dissolution in a thin strip, Journal of Computational and Applied Mathematics, 2015.

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- Dependence on transversal variable eliminated: 2D \rightarrow 1D.
- Coupled reactive and heat transport:





$$\partial_t \left((1 - 2d_0)\rho_{f0} + 2d_0 2\rho \right) + \partial_x (\rho_{f0}\bar{q}_0) = 0$$

$$\overline{q}_0(x, t) = -\frac{(1 - 2d_0(x, t))^3}{12\mu_{f0}} \partial_x p_0(x, t)$$

$$\partial_t \left((1 - 2d_0)\rho_{f0}T_0 + 2d_0\varsigma\rho T_0 \right) + \partial_x (\rho_{f0}\overline{q}_0 T_0)$$

$$= \partial_x \left((1 - 2d_0)\kappa_f \partial_x T_0 + 2d_0\kappa_g \partial_x T_0 \right)$$

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- Dependence on transversal variable eliminated: 2D \rightarrow 1D.
- Two-phase flow with surface tension:



Ongoing work by Sohely Sharmin.

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- Dependence on transversal variable eliminated: 2D \rightarrow 1D.
- Two-phase flow with surface tension:



$$\begin{aligned} \partial_t d_0 &= -\partial_x \overline{q}_{w,0} & \partial_t d_0 = \partial_x \overline{q}_{o,0} \\ \overline{q}_{w,0} &= -\frac{d_0^3}{3} \partial_x p_{w,0} - \frac{d_0^2 (1 - d_0)}{2M} \partial_x p_{o,0} \\ \overline{q}_{o,0} &= -\frac{(1 - d_0)^3}{3} \partial_x p_{o,0} - \frac{d_0 (1 - d_0)^2}{M} \partial_x p_{o,0} - \frac{d_0^2 (1 - d_0)}{2} \partial_x p_{w,0} \\ \overline{Ca}_o p_{o,0} - \overline{Ca}_w p_{w,0} &= \partial_{xx} d_0 \end{aligned}$$

Ongoing work by Sohely Sharmin.

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- Two-scale model: Separation between macroscale variable **x** and microscale **y**.
- Coupled reactive and heat transport.
- In macroscale x, solve for $u_0(t, \mathbf{x})$, $p_0(t, \mathbf{x})$, $\overline{\mathbf{q}_0}(t, \mathbf{x})$, $T_0(t, \mathbf{x})$:

C. Bringedal, I. Berre, I.S. Pop, F.A. Radu, Upscaling of non-isothermal reactive porous media flow with changing porosity, Transport in Porous Media, 2016.

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- Two-scale model: Separation between macroscale variable **x** and microscale **y**.
- Coupled reactive and heat transport.
- In macroscale x, solve for $u_0(t, \mathbf{x})$, $p_0(t, \mathbf{x})$, $\overline{\mathbf{q}_0}(t, \mathbf{x})$, $T_0(t, \mathbf{x})$:

$$\begin{aligned} \partial_t \Big(|Y_0(t, \mathbf{x})| \rho_f + |G_0(t, \mathbf{x})| 2\rho \Big) + \nabla_{\mathbf{x}} \cdot \Big(\rho_f \overline{\mathbf{q}_0}\Big) &= 0\\ \overline{\mathbf{q}_0} &= -\frac{1}{\mu_f} \mathcal{K}(t, \mathbf{x}) \nabla_{\mathbf{x}} p_0\\ \partial_t \Big(|Y_0(t, \mathbf{x})| \rho_f T_0 + |G_0(t, \mathbf{x})| \varsigma \rho T_0 \Big) + \nabla_{\mathbf{x}} \cdot \Big(\rho_f \overline{\mathbf{q}_0} T_0 \Big)\\ &= \nabla_{\mathbf{x}} \cdot \Big(\kappa_f \mathcal{A}_f(t, \mathbf{x}) \nabla_{\mathbf{x}} T_0 + \kappa_g \mathcal{A}_g(t, \mathbf{x}) \nabla_{\mathbf{x}} T_0 \Big) \end{aligned}$$

C. Bringedal, I. Berre, I.S. Pop, F.A. Radu, Upscaling of non-isothermal reactive porous media flow with changing porosity, Transport in Porous Media, 2016.

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 For each macroscale point x, update level set equation and solve cell problems in y for components of matrices K, A_f and A_g:



$$\begin{split} k_{ij}(t,\mathbf{x}) &= \frac{1}{|Y_0|} \int_{Y_0} w_i^j(\mathbf{y}) d\mathbf{y} \\ \text{where } \mathbf{e}_j + \nabla_{\mathbf{y}} \Pi^j + \nabla_{\mathbf{y}}^2 \mathbf{w}^j = 0 \\ \text{and } \nabla_{\mathbf{y}} \cdot \mathbf{w}^j &= 0 \text{ in } Y_0, \\ \text{and } \mathbf{w}^j(y) &= 0 \text{ on } \Gamma_0. \end{split}$$

C. Bringedal, I. Berre, I.S. Pop, F.A. Radu, Upscaling of non-isothermal reactive porous media flow with changing porosity, Transport in Porous Media, 2016.

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 For each macroscale point x, update level set equation and solve cell problems in y for components of matrices K, A_f and A_g:

$$\begin{aligned} a_{ij}^{f} &= \int_{Y_{0}} (\delta_{ij} + \partial_{y_{i}} \Theta^{j}(y)) dy, \quad a_{ij}^{g} = \int_{G_{0}} (\delta_{ij} + \partial_{y_{i}} \Theta^{j}(y)) dy. \\ \text{where } \nabla_{y}^{2} \Theta_{f}^{j}(y) &= 0 \text{ in } Y_{0}(x, t) \text{ and } \nabla_{y}^{2} \Theta_{g}^{j}(y) = 0 \text{ in } G_{0}(x, t) \\ \text{and } \kappa_{f} \mathbf{n}_{0} \cdot (\mathbf{e}_{j} + \nabla_{y} \Theta_{f}^{j}(y)) = \kappa_{g} \mathbf{n}_{0} \cdot (\mathbf{e}_{j} + \nabla_{y} \Theta_{g}^{j}(y)) \\ \text{and } \Theta_{f}^{j}(y) &= \Theta_{g}^{j}(y) \text{ on } \Gamma_{0}(x, t), \end{aligned}$$

C. Bringedal, I. Berre, I.S. Pop, F.A. Radu, Upscaling of non-isothermal reactive porous media flow with changing porosity, Transport in Porous Media, 2016.

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- Effective behavior for flow and heat transport with changing porosity.
- Solve cell problems for various grain shapes/sizes.
- Obtain effective quantities as function of a parameter:

C. Bringedal, K. Kumar, Effective behavior near clogging in upscaled equations for non-isothermal reactive porous media flow, Transport in Porous Media, 2017.

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- Coupled pore scale Darcy scale implementation.
- Use cell problem formulation to upscale permeabilities.



Ongoing work by Manuela Bastidas.

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- Coupled pore scale Darcy scale implementation.
- Use cell problem formulation to upscale permeabilities.



* Porous media flow: Coupled processes relevant for geothermal energy, CO2 storage, groundwater contamination, etc.

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- * Porous media flow: Coupled processes relevant for geothermal energy, CO2 storage, groundwater contamination, etc.
- * Pore scale formulations including moving boundaries: Chemical reactions and two-phase flow.



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- * Porous media flow: Coupled processes relevant for geothermal energy, CO2 storage, groundwater contamination, etc.
- * Pore scale formulations including moving boundaries: Chemical reactions and two-phase flow.
- Upscaling for effective descriptions incorporating effect of pore scale processes.



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- * Porous media flow: Coupled processes relevant for geothermal energy, CO2 storage, groundwater contamination, etc.
- * Pore scale formulations including moving boundaries: Chemical reactions and two-phase flow.
- * Upscaling for effective descriptions incorporating effect of pore scale processes.
- * Understanding effective behavior and numerical upscaling.





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Thank you for your attention!



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A bit of advertisement

Summer school on hyperbolic conservation laws



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