Upscaling: perforated domains

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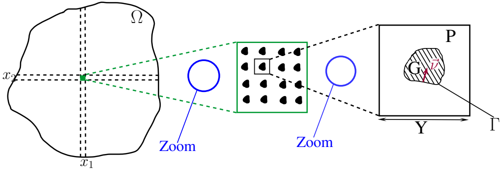
KNOWLEDGE IN ACTION

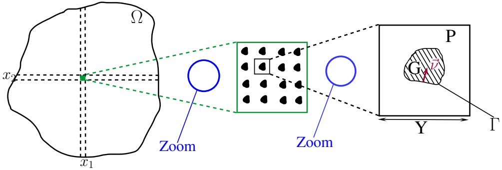
CMAT

Perforated domains



Porous medium (macro-scale, Darcy): $\Omega \subset \mathbb{R}^2$, (or $\Omega \subset \mathbb{R}^d$, $d \geq 1$)

Perforated domains



Porous medium (macro-scale, Darcy): $\Omega \subset \mathbb{R}^2$, (or $\Omega \subset \mathbb{R}^d, d \geq 1$)

Pore space (micro-scale, pores): $\Omega^\varepsilon \subset \Omega$ $(0 < \varepsilon << 1)$

With $Y = [0,1]^2$ (unit cell), decompose $Y = \mathcal{P} \cup \mathcal{G} \cup \Gamma$ (*pore, grain, wall*);

For $\mathrm{k} = (k_1, k_2)^T \in \mathbb{Z}^2$, define $\Theta_\mathrm{k} = \{x + \mathrm{k} / x \in \Theta\}$, and

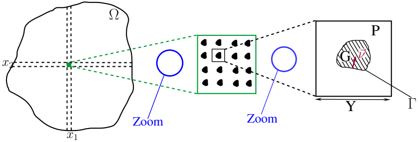
$$\varepsilon\Theta = \{\varepsilon x / x \in \Theta\} \text{ (with } \Theta \in \{\mathcal{P}, \mathcal{G}, \Gamma\})$$

Assume $\bar{\Omega} = \cup \left\{\varepsilon(\mathrm{k} + \bar{Y}) / \mathrm{k} \in \mathcal{K}_\varepsilon\right\}$, with $\mathcal{K}_\varepsilon$ - set of indices;

Define

$$\Omega^\varepsilon = \cup \{\varepsilon(\mathrm{k} + \mathcal{P}) / \mathrm{k} \in \mathcal{K}_\varepsilon\} \text{ (the total pore/void space)}$$
$$\Gamma^\varepsilon = \cup \{\varepsilon(\mathrm{k} + \Gamma) / \mathrm{k} \in \mathcal{K}_\varepsilon\} \text{ (the grain boundaries/pore walls)}$$

Main ideas



1. *Two scales*:

$$x \longrightarrow (x, y), \text{ with } y = \frac{x}{\varepsilon}$$

2. *Homogenization ansatz*:

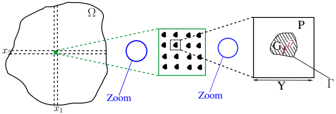
$$u^{\varepsilon}(x) = u_0(x, y) + \varepsilon u_1(x, y) + \varepsilon^2 u_2(x, y) + \ldots,$$

with u_k being Y-periodic (w.r.t. y) ($k = 0, 1, \ldots$).

3. *Derivatives*: Consider $g^{\epsilon}(x) := g\left(x, \frac{x}{\varepsilon}\right) = g(x, y)$; then

$$\frac{\partial g}{\partial x_i}(x, y) \quad \text{becomes} \quad \frac{dg^{\epsilon}}{dx_i}(x) = \frac{\partial g}{\partial x_i}(x, y) + \frac{\partial y_i}{\partial x_i}\frac{\partial g}{\partial y_i}(x, y) = \frac{\partial g}{\partial x_i}(x, y) + \frac{1}{\varepsilon}\frac{\partial g}{\partial y_i}(x, y)$$

Periodicity and micro-scale model



Let $A^\varepsilon : \mathbb{R}^2 \to \mathbb{R}$ - rapidly oscillating scalar function (can be extended to matrices) - defined by $A^\varepsilon(x) = A\big(x, \frac{x}{\varepsilon}\big)$ for all $x = (x_1, x_2)^T \in \mathbb{R}^2$, where $A : \mathbb{R}^4 \to \mathbb{R}$ satisfies for all $x = (x_1, x_2)^T$ and $y = (y_1, y_2)^T$

$$\text{Bounded}: \quad 0 < m \leq A(x_1, x_2, y_1, y_2) \leq M < \infty,$$

$$\begin{aligned}\text{Periodic}: \quad & A(x_1, x_2, y_1, y_2) = A(x_1, x_2, y_1 + 1, y_2) \\ &= A(x_1, x_2, y_1, y_2 + 1) = A(x_1, x_2, y_1 + 1, y_2 + 1) = \ldots .\end{aligned}$$

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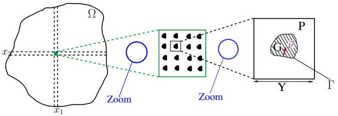
Periodicity and micro-scale model



Let $A^\varepsilon : \mathbb{R}^2 \to \mathbb{R}$ - rapidly oscillating scalar function (can be extended to matrices) - defined by $A^\varepsilon(x) = A\left(x, \frac{x}{\varepsilon}\right)$ for all $x = (x_1, x_2)^T \in \mathbb{R}^2$, where $A : \mathbb{R}^4 \to \mathbb{R}$ satisfies for all $x = (x_1, x_2)^T$ and $y = (y_1, y_2)^T$

$$\text{Bounded :} \qquad 0 < m \leq A(x_1, x_2, y_1, y_2) \leq M < \infty,$$

$$\begin{aligned}\text{Periodic :} \qquad & A(x_1, x_2, y_1, y_2) = A(x_1, x_2, y_1 + 1, y_2) \\ & = A(x_1, x_2, y_1, y_2 + 1) = A(x_1, x_2, y_1 + 1, y_2 + 1) = \ldots.\end{aligned}$$

Consider the diffusion problem in the perforated domain (porous medium)

$$(P^\varepsilon) \quad \begin{cases} -\nabla \cdot (A^\varepsilon(\mathrm{x}) \nabla u^\varepsilon) &= f, & \text{for all } x \in \Omega^\varepsilon (\text{pore space}), \\ -\nu \cdot (A^\varepsilon(\mathrm{x}) \nabla u^\varepsilon) &= 0, & \text{at } \Gamma^\varepsilon (\text{pore walls}), \\ u^\varepsilon &= 0, & \text{at } \partial\Omega (\text{outer boundary}). \end{cases}$$

Note: The equation is defined only in the pore space Ω^ε, not in the grain space $\Omega \backslash \bar{\Omega}^\varepsilon$!

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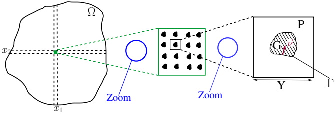
Asymptotic expansions

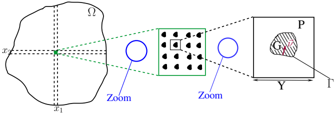


As before, take $y = \frac{x}{\varepsilon}$ and use

$$u^\varepsilon(x) = u_0(x,y) + \varepsilon u_1(x,y) + \varepsilon^2 u_2(x,y) + \dots, \text{ with } u_k \text{ being } Y\text{-periodic;}$$

$$A^\varepsilon(x) = A(x,y) \qquad \text{and} \qquad \nabla \longrightarrow \nabla_x + \frac{1}{\varepsilon}\nabla_y$$

Asymptotic expansions



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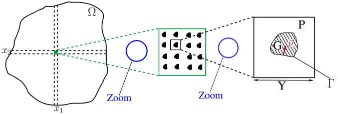
$$A^\varepsilon(x) = A(x,y) \qquad \text{and} \qquad \nabla \longrightarrow \nabla_x + \frac{1}{\varepsilon}\nabla_y$$

Equation (in Ω^ε)

$$\begin{aligned} & -\tfrac{1}{\varepsilon^2}\ \nabla_y \cdot (A(x,y)\nabla_y u_0(x,y)) \\ & -\tfrac{1}{\varepsilon}\ \{\nabla_x \cdot [A(x,y)\nabla_y u_0(x,y)] + \nabla_y \cdot [A(x,y)(\nabla_x u_0(x,y) + \nabla_y u_1(x,y))]\} \\ & - \{\nabla_x \cdot [A(x,y)(\nabla_x u_0(x,y) + \nabla_y u_1(x,y))] + \nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))]\} \\ & = f + O(\varepsilon), \qquad \text{in } \Omega^\varepsilon. \end{aligned}$$

Asymptotic expansions



As before, take $y = \frac{x}{\varepsilon}$ and use

$$u^\varepsilon(x) = u_0(x,y) + \varepsilon u_1(x,y) + \varepsilon^2 u_2(x,y) + \ldots, \text{ with } u_k \text{ being } Y\text{-periodic;}$$

$$A^\varepsilon(x) = A(x,y) \qquad \text{and} \qquad \nabla \longrightarrow \nabla_x + \frac{1}{\varepsilon}\nabla_y$$

Equation (in Ω^ε)

$$\begin{aligned} &-\tfrac{1}{\varepsilon^2}\ \nabla_y \cdot (A(x,y)\nabla_y u_0(x,y)) \\ &-\tfrac{1}{\varepsilon}\ \{\nabla_x \cdot [A(x,y)\nabla_y u_0(x,y)] + \nabla_y \cdot [A(x,y)(\nabla_x u_0(x,y) + \nabla_y u_1(x,y))]\} \\ &-\{\nabla_x \cdot [A(x,y)(\nabla_x u_0(x,y) + \nabla_y u_1(x,y))] + \nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))]\} \\ &= f + O(\varepsilon), \qquad \text{in } \Omega^\varepsilon. \end{aligned}$$

Boundary condition (at Γ^ε)

$$\begin{aligned} 0 = &-\tfrac{1}{\varepsilon}\left\{\nu \cdot \left(A(x,y)\nabla_y u_0(x,y)\right)\right\} - \left\{\nu \cdot \left(A(x,y)(\nabla_x u_0(x,y) + \nabla_y u_1(x,y)\right)\right\} \\ &-\varepsilon\left\{\nu \cdot \left(A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y)\right)\right\} + O(\varepsilon^2), \qquad \text{on } \Gamma^\varepsilon. \end{aligned}$$

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Lowest order terms

$$
\begin{aligned}
& -\frac{1}{\varepsilon^2}\ \nabla_y \cdot (A(x,y)\nabla_y u_0(x,y)) \\
& -\frac{1}{\varepsilon}\left\{\nabla_x \cdot [A(x,y)\nabla_y u_0(x,y)] + \nabla_y \cdot [A(x,y)(\nabla_x u_0(x,y) + \nabla_y u_1(x,y))]\right\} \\
& -\left\{\nabla_x \cdot [A(x,y)(\nabla_x u_0(x,y) + \nabla_y u_1(x,y))] + \nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))]\right\} \\
= \quad & f + O(\varepsilon), \qquad \text{in } \Omega^\varepsilon. \\
0 = \quad & -\frac{1}{\varepsilon}\left\{\nu \cdot \left(A(x,y)\nabla_y u_0(x,y)\right)\right\} - \left\{\nu \cdot \left(A(x,y)(\nabla_x u_0(x,y) + \nabla_y u_1(x,y)\right)\right\} \\
& \qquad -\varepsilon\left\{\nu \cdot \left(A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y)\right)\right\} + O(\varepsilon^2), \qquad \text{on } \Gamma^\varepsilon.
\end{aligned}
$$

Lowest order terms

$$
\begin{aligned}
& -\frac{1}{\varepsilon^2}\,\nabla_y \cdot (A(x,y)\nabla_y u_0(x,y)) \\
& -\frac{1}{\varepsilon}\left\{\nabla_x \cdot [A(x,y)\nabla_y u_0(x,y)] + \nabla_y \cdot [A(x,y)(\nabla_x u_0(x,y) + \nabla_y u_1(x,y))]\right\} \\
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= \;& f + O(\varepsilon), \quad \text{in } \Omega^\varepsilon. \\
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& -\varepsilon\left\{\nu \cdot \big(A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))\big)\right\} + O(\varepsilon^2), \quad \text{on } \Gamma^\varepsilon.
\end{aligned}
$$

(*Problem* P^{-2})

$$
\begin{cases}
-\nabla_y \cdot (A(x,y)\nabla_y u_0(x,y)) = 0, & \text{for all } y \in \mathcal{P}, \\
-\nu \cdot \big(A(x,y)\nabla_y u_0(x,y)\big) = 0, & \text{for all } y \in \Gamma, \\
u_0(x,y) \text{ is } Y - \text{periodic.} &
\end{cases}
$$

Lowest order terms

$$
\begin{aligned}
& -\frac{1}{\varepsilon^2}\nabla_y \cdot (A(x,y)\nabla_y u_0(x,y)) \\
& -\frac{1}{\varepsilon}\left\{\nabla_x \cdot [A(x,y)\nabla_y u_0(x,y)] + \nabla_y \cdot [A(x,y)(\nabla_x u_0(x,y) + \nabla_y u_1(x,y))]\right\} \\
& -\left\{\nabla_x \cdot [A(x,y)(\nabla_x u_0(x,y) + \nabla_y u_1(x,y))] + \nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))]\right\} \\
= \quad & f + O(\varepsilon), \quad \text{in } \Omega^\varepsilon.
\end{aligned}
$$

$$
\begin{aligned}
0 = \quad & -\frac{1}{\varepsilon}\left\{\nu \cdot \left(A(x,y)\nabla_y u_0(x,y)\right)\right\} - \left\{\nu \cdot \left(A(x,y)(\nabla_x u_0(x,y) + \nabla_y u_1(x,y))\right)\right\} \\
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$$
(\textit{Problem } P^{-2}) \quad \left\{
\begin{array}{rcll}
-\nabla_y \cdot (A(x,y)\nabla_y u_0(x,y)) & = & 0, & \text{for all } y \in \mathcal{P}, \\
-\nu \cdot \left(A(x,y)\nabla_y u_0(x,y)\right) & = & 0, & \text{for all } y \in \Gamma, \\
u_0(x,y) & \text{is} & Y-\text{periodic.} &
\end{array}
\right.
$$

Note: The only possible solution is y-independent, $u_0(x,y) = u_0(x)$, so $\nabla_y u_0(x,y) = 0$ for all $y \in \mathcal{P}$. Again, x plays the role of a parameter.

Q: $u_0(x) = ?$

Correctors

$$
\begin{aligned}
& -\frac{1}{\varepsilon^2}\ \nabla_y \cdot (A(x,y)\nabla_y u_0(x)) \\
& -\frac{1}{\varepsilon}\left\{\nabla_x \cdot [A(x,y)\nabla_y u_0(x)] + \nabla_y \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))]\right\} \\
& -\left\{\nabla_x \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] + \nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))]\right\} \\
= \quad & f + O(\varepsilon), \qquad \text{in } \Omega^\varepsilon. \\
0 = \quad & -\frac{1}{\varepsilon}\left\{\nu \cdot \big(A(x,y)\nabla_y u_0(x)\big)\right\} - \left\{\nu \cdot \big(A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))\big)\right\} \\
& \qquad -\varepsilon\left\{\nu \cdot \big(A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))\big)\right\} + O(\varepsilon^2), \qquad \text{on } \Gamma^\varepsilon.
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\begin{aligned}
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& -\frac{1}{\varepsilon}\left\{\nabla_x \cdot [A(x,y)\nabla_y u_0(x)] + \nabla_y \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))]\right\} \\
& -\left\{\nabla_x \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] + \nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))]\right\} \\
= \quad & f + O(\varepsilon), \qquad \text{in } \Omega^\varepsilon. \\
0 = \quad & -\frac{1}{\varepsilon}\left\{\nu \cdot \big(A(x,y)\nabla_y u_0(x)\big)\right\} - \left\{\nu \cdot \big(A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))\big)\right\} \\
& \qquad -\varepsilon\left\{\nu \cdot \big(A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))\big)\right\} + O(\varepsilon^2), \qquad \text{on } \Gamma^\varepsilon.
\end{aligned}
$$

$$
(\textit{Problem } P^{-1}) \quad \left\{
\begin{aligned}
-\nabla_y \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] \quad &= \quad 0, \qquad \text{for all } y \in \mathcal{P}, \\
-\nu \cdot \big(A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))\big) \quad &= \quad 0, \qquad \text{for all } y \in \Gamma, \\
u_1(x,y) \quad & \text{is} \quad Y - \text{periodic.}
\end{aligned}
\right.
$$

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Correctors

$$
\begin{aligned}
& -\frac{1}{\varepsilon^2}\, \nabla_y \cdot (A(x,y)\nabla_y u_0(x)) \\
& -\frac{1}{\varepsilon}\, \{\nabla_x \cdot [A(x,y)\nabla_y u_0(x)] + \nabla_y \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))]\} \\
& - \{\nabla_x \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] + \nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))]\} \\
= \quad & f + O(\varepsilon), \quad \text{in } \Omega^\varepsilon. \\
0 = \quad & -\frac{1}{\varepsilon}\left\{\nu \cdot \left(A(x,y)\nabla_y u_0(x)\right)\right\} - \left\{\nu \cdot \left(A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))\right)\right\} \\
& \qquad -\varepsilon \left\{\nu \cdot \left(A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))\right)\right\} + O(\varepsilon^2), \quad \text{on } \Gamma^\varepsilon.
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-\nabla_y \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] & = & 0, & \text{for all } y \in \mathcal{P}, \\
-\nu \cdot \left(A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))\right) & = & 0, & \text{for all } y \in \Gamma, \\
u_1(x,y) & \text{is} & Y - \text{periodic.} &
\end{array} \right.
$$

Since $\nabla_x u_0(x) = \sum_{j=1}^{2} \mathrm{e}_j\ \partial_{x_j} u_0(x)$, replace $\nabla_x u_0(x)$ by e_j and consider again the *cell problems*

$$
(P_j^{-1})(x) \quad \left\{ \begin{array}{rcll}
-\nabla_y \cdot \left(A(x,y)\nabla_y w^j(x,y)\right) & = & \nabla_y \cdot \left(A(x,y)\ \mathrm{e}_j\right), & \text{for all } y \in \mathcal{P}, \\
-\nu \cdot \left(A(x,y)\nabla_y w^j(x,y)\right) & = & \nu \cdot \left(A(x,y)\mathrm{e}_j\right), & \text{for all } y \in \Gamma, \\
w^j(x,y) & \text{is} & Y - \text{periodic}, & \int_{\mathcal{P}} w^j(x,y)dy = 0.
\end{array} \right.
$$

Correctors

$$
\begin{aligned}
& -\frac{1}{\varepsilon^2}\ \nabla_y \cdot (A(x,y)\nabla_y u_0(x)) \\
& -\frac{1}{\varepsilon}\left\{\nabla_x \cdot [A(x,y)\nabla_y u_0(x)] + \nabla_y \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))]\right\} \\
& -\left\{\nabla_x \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] + \nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))]\right\} \\
= \quad & f + O(\varepsilon), \qquad \text{in } \Omega^\varepsilon. \\
0 = \quad & -\frac{1}{\varepsilon}\left\{\nu \cdot \left(A(x,y)\nabla_y u_0(x)\right)\right\} - \left\{\nu \cdot \left(A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))\right)\right\} \\
& \qquad -\varepsilon\left\{\nu \cdot \left(A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))\right)\right\} + O(\varepsilon^2), \qquad \text{on } \Gamma^\varepsilon.
\end{aligned}
$$

(*Problem* P^{-1})
$$
\left\{
\begin{aligned}
-\nabla_y \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] &= 0, && \text{for all } y \in \mathcal{P}, \\
-\nu \cdot \left(A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))\right) &= 0, && \text{for all } y \in \Gamma, \\
u_1(x,y) &\ \text{is} && Y - \text{periodic.}
\end{aligned}
\right.
$$

As before, this gives

$$
u_1(x,y) = \tilde{u}_1(x) + \sum_{j=1}^{2} w^j(x,y)\ \partial_{x_j} u_0(x),
$$

Note: Now w^j depends explicitly on x!

Perforated domains: 0-order terms

$$
\begin{aligned}
& -\frac{1}{\varepsilon^2}\ \nabla_y \cdot (A(x,y)\nabla_y u_0(x)) \\
& -\frac{1}{\varepsilon}\left\{\nabla_x \cdot [A(x,y)\nabla_y u_0(x)] + \nabla_y \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))]\right\} \\
& -\left\{\nabla_x \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] + \nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))]\right\} \\
= \quad & f + O(\varepsilon), \qquad \text{in } \Omega^\varepsilon. \\
0 = \quad & -\frac{1}{\varepsilon}\left\{\nu \cdot \left(A(x,y)\nabla_y u_0(x)\right)\right\} - \left\{\nu \cdot \left(A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))\right)\right\} \\
& \qquad -\varepsilon\left\{\nu \cdot \left(A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))\right)\right\} + O(\varepsilon^2), \qquad \text{on } \Gamma^\varepsilon.
\end{aligned}
$$

Perforated domains: 0-order terms

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\begin{aligned}
& -\frac{1}{\varepsilon^2}\ \nabla_y \cdot (A(x,y)\nabla_y u_0(x)) \\
& -\frac{1}{\varepsilon}\{\nabla_x \cdot [A(x,y)\nabla_y u_0(x)] + \nabla_y \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))]\} \\
& -\{\nabla_x \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] + \nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))]\} \\
= \quad & f + O(\varepsilon), \qquad \text{in } \Omega^\varepsilon. \\
0 = \quad & -\frac{1}{\varepsilon}\left\{\nu \cdot \left(A(x,y)\nabla_y u_0(x)\right)\right\} - \left\{\nu \cdot \left(A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))\right)\right\} \\
& \qquad -\varepsilon\left\{\nu \cdot \left(A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))\right)\right\} + O(\varepsilon^2), \qquad \text{on } \Gamma^\varepsilon.
\end{aligned}
$$

$$
(P^0)(x) \quad \left\{
\begin{aligned}
& -\nabla_x \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] \\
& \qquad -\nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))] \quad = \quad f,\ \text{for all } y \in \mathcal{P}, \\
& \qquad -\nu \cdot \left(A(x,y)(\nabla_y u_2(x,y) + \nabla_x u_1(x,y))\right) \quad = \quad 0 \text{ for all } y \in \Gamma, \\
& \qquad u_2(x,y) \quad \text{is} \quad Y - \text{periodic}.
\end{aligned}
\right.
$$

Perforated domains: 0-order terms

$$
\begin{aligned}
&-\frac{1}{\varepsilon^2}\,\nabla_y\cdot(A(x,y)\nabla_y u_0(x))\\
&-\frac{1}{\varepsilon}\,\{\nabla_x\cdot[A(x,y)\nabla_y u_0(x)]+\nabla_y\cdot[A(x,y)(\nabla_x u_0(x)+\nabla_y u_1(x,y))]\}\\
&-\{\nabla_x\cdot[A(x,y)(\nabla_x u_0(x)+\nabla_y u_1(x,y))]+\nabla_y\cdot[A(x,y)(\nabla_x u_1(x,y)+\nabla_y u_2(x,y))]\}\\
=\;& f+O(\varepsilon),\qquad \text{in } \Omega^\varepsilon.\\
0=\;& -\frac{1}{\varepsilon}\left\{\nu\cdot\left(A(x,y)\nabla_y u_0(x)\right)\right\}-\left\{\nu\cdot\left(A(x,y)(\nabla_x u_0(x)+\nabla_y u_1(x,y))\right)\right\}\\
&\qquad -\varepsilon\left\{\nu\cdot\left(A(x,y)(\nabla_x u_1(x,y)+\nabla_y u_2(x,y))\right)\right\}+O(\varepsilon^2),\qquad \text{on } \Gamma^\varepsilon.
\end{aligned}
$$

$$
(P^0)(x)\quad
\begin{cases}
-\nabla_x\cdot[A(x,y)(\nabla_x u_0(x)+\nabla_y u_1(x,y))] & \\
\quad -\nabla_y\cdot[A(x,y)(\nabla_x u_1(x,y)+\nabla_y u_2(x,y))] = f, & \text{for all } y\in\mathcal{P},\\
-\nu\cdot\left(A(x,y)(\nabla_y u_2(x,y)+\nabla_x u_1(x,y))\right) = 0 & \text{for all } y\in\Gamma,\\
u_2(x,y) \text{ is } Y-\text{periodic.} &
\end{cases}
$$

Note: Again, we have three unknown functions u_0, u_1 and u_2. We know how the first two are related, but nothing about u_2.

Perforated domains: 0-order terms

$$(P^0)(x) \quad \begin{cases} -\nabla_x \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] & & \\ \quad -\nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))] & = & f, \text{ for all } y \in \mathcal{P}, \\ -\nu \cdot \left(A(x,y)(\nabla_y u_2(x,y) + \nabla_x u_1(x,y))\right) & = & 0 \text{ for all } y \in \Gamma, \\ u_2(x,y) & \text{is} & Y - \text{periodic.} \end{cases}$$

Idea: Eliminate u_2 by integration!

Perforated domains: 0-order terms

$$(P^0)(x) \quad \begin{cases} -\nabla_x \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] & \\ \quad -\nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))] & = \quad f, \text{ for all } y \in \mathcal{P}, \\ -\nu \cdot \left(A(x,y)(\nabla_y u_2(x,y) + \nabla_x u_1(x,y))\right) & = \quad 0 \text{ for all } y \in \Gamma, \\ u_2(x,y) & \text{is} \quad Y - \text{periodic.} \end{cases}$$

Idea: Eliminate u_2 by integration!

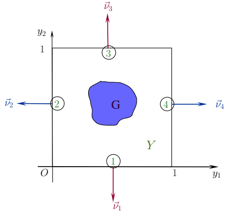
For all $x \in \Omega$, with $|\mathcal{P}| = \int_{\mathcal{P}} dy$ (the volume of the void space in a reference cell, the *porosity*) one has

$$-\nabla_x \cdot \left[\int_{\mathcal{P}} A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))dy\right]$$
$$- \int_{\mathcal{P}} \nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))]dy = |\mathcal{P}| f(x).$$

Perforated domains: 0-order terms

$$(P^0)(x) \quad \begin{cases} -\nabla_x \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] & \\ \quad -\nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))] = f, & \text{for all } y \in \mathcal{P}, \\ -\nu \cdot \left(A(x,y)(\nabla_y u_2(x,y) + \nabla_x u_1(x,y))\right) = 0 & \text{for all } y \in \Gamma, \\ u_2(x,y) \text{ is } Y - \text{periodic.} & \end{cases}$$

<u>Idea</u>: Eliminate u_2 by integration!



For all $x \in \Omega$, with $|\mathcal{P}| = \int_{\mathcal{P}} dy$ (the volume of the void space in a reference cell, the *porosity*) one has

$$-\nabla_x \cdot \left[\int_{\mathcal{P}} A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))dy\right]$$
$$\quad - \int_{\mathcal{P}} \nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))]dy = |\mathcal{P}| f(x).$$

Note:

$$\int_{\mathcal{P}} \nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))]dy$$
$$= \int_{\partial\mathcal{P}} \nu \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))]d\sigma_y = 0.$$

Perforated domains: upscaled/homogenized equation

$$
(P^0)(x) \quad \begin{cases} -\nabla_x \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] & \\ \qquad -\nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))] = f, \text{ for all } y \in \mathcal{P}, & \\ -\nu \cdot \big(A(x,y)(\nabla_y u_2(x,y) + \nabla_x u_1(x,y))\big) = 0 \text{ for all } y \in \Gamma, & \\ u_2(x,y) \text{ is } Y - \text{periodic.} & \end{cases}
$$

Perforated domains: upscaled/homogenized equation

$$(P^0)(x) \quad \begin{cases} -\nabla_x \cdot [A(x,y)(\nabla_x u_0(x) + \nabla_y u_1(x,y))] & & \\ \qquad -\nabla_y \cdot [A(x,y)(\nabla_x u_1(x,y) + \nabla_y u_2(x,y))] & = & f, \text{ for all } y \in \mathcal{P}, \\ -\nu \cdot (A(x,y)(\nabla_y u_2(x,y) + \nabla_x u_1(x,y))) & = & 0 \text{ for all } y \in \Gamma, \\ u_2(x,y) & \text{is} & Y - \text{periodic.} \end{cases}$$

With $u_1(x,y) = \tilde{u}_1(x) + \sum_{j=1}^{2} w^j(x,y)\, \partial_{x_j} u_0(x)$, this gives

$$-\nabla_x \cdot \left[\int_{\mathcal{P}} A(x,y) \left(\nabla_x u_0(x) + \sum_{j=1}^{d} \partial_{x_j} u_0(x)\; \nabla_y w^j(x,y) \right) dy \right] = |\mathcal{P}| f(x).$$

Perforated domains: upscaled/homogenized equation

$$(P^0)(x)\quad \begin{cases} -\nabla_x\cdot[A(x,y)(\nabla_x u_0(x)+\nabla_y u_1(x,y))] & \\ \quad -\nabla_y\cdot[A(x,y)(\nabla_x u_1(x,y)+\nabla_y u_2(x,y))] &= f,\ \text{for all } y\in\mathcal{P},\\ -\nu\cdot\left(A(x,y)(\nabla_y u_2(x,y)+\nabla_x u_1(x,y))\right) &= 0 \text{ for all } y\in\Gamma,\\ u_2(x,y) & \text{is}\quad Y-\text{periodic.}\end{cases}$$

With $u_1(x,y)=\tilde{u}_1(x)+\sum_{j=1}^{2} w^j(x,y)\ \partial_{x_j}u_0(x)$, this gives

$$-\nabla_x\cdot\left[\int_{\mathcal{P}} A(x,y)\left(\nabla_x u_0(x)+\sum_{j=1}^{d}\partial_{x_j}u_0(x)\ \nabla_y w^j(x,y)\right)dy\right]=|\mathcal{P}|f(x).$$

Upscaled model (after dividing by $|\mathcal{P}|$, and with $U=u_0(x)$):

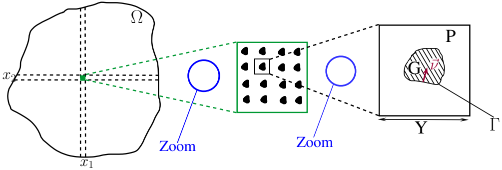
$$(P)\quad\begin{cases}-\nabla\cdot(A^*(x)\nabla U) &= f, \quad \text{for all } x\in\Omega,\\ U &= 0,\quad \text{on } \partial\Omega,\end{cases}$$

with $A^*:\Omega\to\mathbb{R}^{d\times d}$ having the elements $a^*_{ij}:\Omega\to\mathbb{R}$, $(i,j\in\{1,2\})$

$$a^*_{ij}:\Omega\to\mathbb{R},\quad (i,j\in\{1,2\})a^*_{ij}(x)=\frac{1}{|\mathcal{P}|}\int_{\mathcal{P}}\left(A(x,y)(\mathrm{e}_j+\nabla_y w^j(x,y))\right)\cdot\mathrm{e}_i\,dy.$$

Note: A^* is symmetric and positive definite.

The derivation of the Darcy law



Porous medium (macro-scale, Darcy): $\Omega \subset \mathbb{R}^2$, (or $\Omega \subset \mathbb{R}^d, d \geq 1$)

Pore space (micro-scale, pores): $\Omega^\varepsilon \subset \Omega$ ($0 < \varepsilon << 1$)

With $Y = [0,1]^2$ (unit cell), decompose $Y = \mathcal{P} \cup \mathcal{G} \cup \Gamma$ (*pore, grain, wall*);

For $\mathrm{k} = (k_1, k_2)^T \in \mathbb{Z}^2$, define $\Theta_\mathrm{k} = \{x + \mathrm{k}/x \in \Theta\}$, and

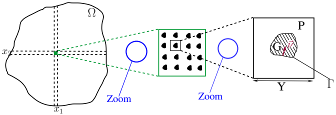
$$\varepsilon\Theta = \{\varepsilon x / x \in \Theta\} \text{ (with } \Theta \in \{\mathcal{P}, \mathcal{G}, \Gamma\})$$

Assume $\bar{\Omega} = \cup \left\{\varepsilon(\mathrm{k} + \bar{Y})/\mathrm{k} \in \mathcal{K}_\varepsilon\right\}$, with $\mathcal{K}_\varepsilon$ - set of indices;

Define

$$\Omega^\varepsilon = \cup \{\varepsilon(\mathrm{k} + \mathcal{P})/\mathrm{k} \in \mathcal{K}_\varepsilon\} \text{ (the total pore/void space)}$$
$$\Gamma^\varepsilon = \cup \{\varepsilon(\mathrm{k} + \Gamma)/\mathrm{k} \in \mathcal{K}_\varepsilon\} \text{ (the grain boundaries/pore walls)}$$

The micro-scale flow model

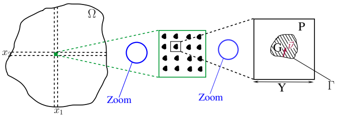


Stokes flow at the scale of pores:

$$\begin{cases} \varepsilon^2 \mu \Delta \mathrm{q}^{\ \varepsilon} = \nabla p^\varepsilon(x), & \text{in } \Omega^\varepsilon \\ \nabla \cdot \mathrm{q}^\varepsilon(x) = 0, & \text{in } \Omega^\varepsilon \\ \mathrm{q}^\varepsilon(x) = 0, & \text{on } \Gamma^\varepsilon, \end{cases}$$

Note: Small viscosity, $O(\varepsilon^2)$, or large pressure gradients

Asymptotic expansion



Stokes flow at the scale of pores:

$$\begin{cases} \varepsilon^2 \mu \Delta \mathrm{q}^{\varepsilon} = \nabla p^{\varepsilon}(x), & \text{in } \Omega^{\varepsilon} \\ \nabla \cdot \mathrm{q}^{\varepsilon}(x) = 0, & \text{in } \Omega^{\varepsilon} \\ \mathrm{q}^{\varepsilon}(x) = 0, & \text{on } \Gamma^{\varepsilon}, \end{cases}$$

Note: Small viscosity, $O(\varepsilon^2)$, or large pressure gradients

Homogenization ansatz: with x replaced by $(x, y = x/\varepsilon)$

$$\mathrm{q}^{\varepsilon} = \mathrm{q}_0(x,y) + \varepsilon \mathrm{q}_1(x,y) + \varepsilon^2 \mathrm{q}_2(x,y) + \dots$$

$$p^{\varepsilon} = p_0(x,y) + \varepsilon p_1(x,y) + \varepsilon^2 p_2(x,y) + \dots$$

$$\nabla \to \nabla_x + \frac{1}{\varepsilon}\nabla y, \qquad \Delta \to \Delta_x + \frac{1}{\varepsilon}\nabla_x \cdot \nabla_y + \frac{1}{\varepsilon}\nabla_y \cdot \nabla_x + \frac{1}{\varepsilon^2}\Delta y$$

with q_k, p_k - Y-periodic.

UHASSELT

Asymptotic expansion

Homogenization ansatz: with x replaced by $(x, y = x/\varepsilon)$

$$\begin{aligned} \mathrm{q}^{\,\varepsilon} &= \mathrm{q}_0(x,y) + \varepsilon \mathrm{q}_1(x,y) + \varepsilon^2 \mathrm{q}_2(x,y) + \dots \\ p^\varepsilon &= p_0(x,y) + \varepsilon p_1(x,y) + \varepsilon^2 p_2(x,y) + \dots \end{aligned}$$

$$\nabla \to \nabla_x + \frac{1}{\varepsilon}\nabla y, \qquad \Delta \to \Delta_x + \frac{1}{\varepsilon}\nabla_x \cdot \nabla_y + \frac{1}{\varepsilon}\nabla_y \cdot \nabla_x + \frac{1}{\varepsilon^2}\Delta y$$

with q_k, p_k - Y-periodic.

$$\begin{cases} \mu \Delta_y \mathrm{q}_0(x,y) + \varepsilon \mu \left[(\nabla_x \cdot \nabla_y + \nabla_y \cdot \nabla_x)\mathrm{q}_0 + \Delta_y \mathrm{q}_1 \right] + O(\varepsilon^2) \\ \quad = \frac{1}{\varepsilon}\nabla_y p_0 + (\nabla_x p_0 + \nabla_y p_1) + \varepsilon(\nabla_x p_1 + \nabla_y p_2) + O(\varepsilon^2), \quad \text{in } \Omega^\varepsilon \\ \frac{1}{\varepsilon}\nabla_y \cdot \mathrm{q}_0 + (\nabla_x \cdot \mathrm{q}_0 + \nabla_y \cdot \mathrm{q}_1) + \varepsilon(\nabla_x \cdot \mathrm{q}_1 + \nabla_y \cdot \mathrm{q}_2) + O(\varepsilon^2) = 0, \quad \text{in } \Omega^\varepsilon \\ \mathrm{q}_0 + \varepsilon \mathrm{q}_1 + \varepsilon^2 \mathrm{q}_2 + O(\varepsilon^2) = 0, \quad \text{on } \Gamma^\varepsilon. \end{cases}$$

The derivation of the Darcy law: y-independent pressure

$$\begin{cases} \mu\Delta_y \mathrm{q}_0(x,y) + \varepsilon\mu\left[(\nabla_x\cdot\nabla_y + \nabla_y\cdot\nabla_x)\mathrm{q}_0 + \Delta_y \mathrm{q}_1\right] + O(\varepsilon^2) \\ \quad = \frac{1}{\varepsilon}\nabla_y p_0 + (\nabla_x p_0 + \nabla_y p_1) + \varepsilon(\nabla_x p_1 + \nabla_y p_2) + O(\varepsilon^2), \quad \text{in } \Omega^\varepsilon \\ \frac{1}{\varepsilon}\nabla_y\cdot \mathrm{q}_0 + (\nabla_x\cdot \mathrm{q}_0 + \nabla_y\cdot \mathrm{q}_1) + \varepsilon(\nabla_x\cdot \mathrm{q}_1 + \nabla_y\cdot \mathrm{q}_2) + O(\varepsilon^2) = 0, \quad \text{in } \Omega^\varepsilon \\ \mathrm{q}_0 + \varepsilon \mathrm{q}_1 + \varepsilon^2 \mathrm{q}_2 + O(\varepsilon^2) = 0, \quad \text{on } \Gamma^\varepsilon. \end{cases}$$

Lowest order term:

Problem P^{-1} $\nabla_y p_0 = 0$, for all $y \in \mathcal{P}$

gives $p_0 = p_0(x)$.

The derivation of the Darcy law: 0-order velocity

$$\begin{cases} \mu\Delta_y \mathrm{q}_0(x,y) + \varepsilon\mu\left[(\nabla_x\cdot\nabla_y + \nabla_y\cdot\nabla_x)\mathrm{q}_0 + \Delta_y \mathrm{q}_1\right] + O(\varepsilon^2) \\ \quad = \frac{1}{\varepsilon}\nabla_y p_0 + (\nabla_x p_0 + \nabla_y p_1) + \varepsilon(\nabla_x p_1 + \nabla_y p_2) + O(\varepsilon^2), \quad \text{in } \Omega^\varepsilon \\ \frac{1}{\varepsilon}\nabla_y\cdot \mathrm{q}_0 + (\nabla_x\cdot \mathrm{q}_0 + \nabla_y\cdot \mathrm{q}_1) + \varepsilon(\nabla_x\cdot \mathrm{q}_1 + \nabla_y\cdot \mathrm{q}_2) + O(\varepsilon^2) = 0, \quad \text{in } \Omega^\varepsilon \\ \mathrm{q}_0 + \varepsilon \mathrm{q}_1 + \varepsilon^2 \mathrm{q}_2 + O(\varepsilon^2) = 0, \quad \text{on } \Gamma^\varepsilon. \end{cases}$$

Next terms (w.r.t. y):

Problem P^0

$$\begin{cases} \mu\Delta_y \mathrm{q}_0(x,y) = \nabla_x p_0(x) + \nabla_y p_1(x,y), & \text{in } \mathcal{P} \\ \nabla_y\cdot \mathrm{q}_0(x,y) = 0, & \text{in } \mathcal{P} \\ \mathrm{q}_0(x,y) = 0, & \text{on } \Gamma \\ \mathrm{q}_0, p_1 \;-\; Y\text{-periodic.} \end{cases}$$

The derivation of the Darcy law: cell problems

Problem P^0

$$\begin{cases} \mu\Delta_y q_0(x,y) &= \nabla_x p_0(x) + \nabla_y p_1(x,y), & \text{in } \mathcal{P} \\ \nabla_y \cdot q_0(x,y) &= 0, & \text{in } \mathcal{P} \\ q_0(x,y) &= 0, & \text{on } \Gamma \\ q_0, p_1 &- \ Y\text{-periodic.} & \end{cases}$$

Idea: Express the p_0-dependence of q_0 through "cell problems".

Since $\nabla_x p_0(x) = \sum_{j=1}^d e_j \partial_{x_j} p_0(x)$, solve

$$(P_j) \begin{cases} -\Delta_y \chi^j(y) &= \nabla_y \Pi^j(y) + e_j, & \text{in } \mathcal{P} \\ \nabla_y \cdot \chi^j(y) &= 0, & \text{in } \mathcal{P} \\ \chi^j(y) &= 0, & \text{on } \Gamma \\ \chi^j, \Pi^j &- \ Y - \text{periodic,} & \end{cases}$$

and identify

$$q_0(x,y) = -\frac{1}{\mu}\sum_{j=1}^d \partial_{x_j} p_0(x) \cdot \chi^j(y), \quad p_1(x,y) = \sum_{j=1}^d \partial_{x_j} p_0(x) \cdot \Pi^j(y).$$

The Darcy law (upscaled model)

The *averaged velocity*

$$\mathrm{q}(x) = \frac{1}{|\mathcal{P}|}\int_{\mathcal{P}} \mathrm{q}_0(x,y)dy,$$

satisfies the Darcy law

$$\mathrm{q}(x) = -\frac{1}{\mu}\underline{\mathrm{K}}\,\nabla p_0(x) \qquad \text{(for all } x \text{ in } \Omega),$$

where the *permeability* tensor $\underline{\mathrm{K}}$ is defined by $(\chi^j = (\chi_1^j, \cdots, \chi_d^j)^T)$

$$k_{ij} = \frac{1}{|\mathcal{P}|}\int_{\mathcal{P}} \chi_i^j(y)dy, \quad \text{for all } i,j = 1,\ldots,d.$$

The Darcy law: properties

The *averaged velocity*

$$\mathrm{q}(x) = \frac{1}{|\mathcal{P}|}\int_{\mathcal{P}} \mathrm{q}_0(x,y)dy,$$

satisfies the Darcy law

$$\mathrm{q}(x) = -\frac{1}{\mu}\underline{\mathrm{K}}\ \nabla p_0(x) \qquad \text{(for all } x \text{ in } \Omega\text{)},$$

where the *permeability* tensor $\underline{\mathrm{K}}$ is defined by $(\chi^j = (\chi_1^j, \cdots, \chi_d^j)^T)$

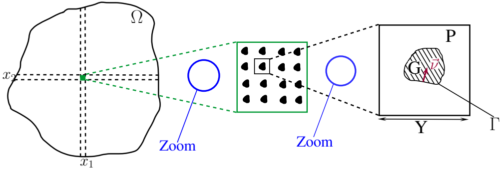
$$k_{ij} = \frac{1}{|\mathcal{P}|}\int_{\mathcal{P}} \chi_i^j(y)dy, \qquad \text{for all } i,j = 1,\ldots,d.$$

<u>Note</u>: Since $\nabla_x \cdot \mathrm{q}_0 + \nabla_y \cdot \mathrm{q}_1 = 0$, q is divergence-free!

$$\begin{aligned}
\nabla_x \cdot \mathrm{q}(x) &= \tfrac{1}{|\mathcal{P}|}\int_{\mathcal{P}} \nabla_x \cdot \mathrm{q}_0(x,y)dy \\
&= -\tfrac{1}{|\mathcal{P}|}\int_{\mathcal{P}} \nabla_y \cdot \mathrm{q}_1(x,y)dy \\
&= -\tfrac{1}{|\mathcal{P}|}\int_{\partial\mathcal{P}} \nu \cdot \mathrm{q}_1(x,y)d\sigma_y \\
&= -\tfrac{1}{|\mathcal{P}|}\int_{\partial Y} \nu \cdot \mathrm{q}_1(x,y)d\sigma_y - \tfrac{1}{|\mathcal{P}|}\int_{\Gamma} \nu \cdot \mathrm{q}_1(x,y)d\sigma_y = 0.
\end{aligned}$$

Lemma. The tensor $\underline{\mathrm{K}}$ is symmetric and positive definite.

The pore-scale reactive flow model



In Ω_P^ε:

$$\begin{cases} \varepsilon^2 \mu \, \Delta \mathrm{q} &= \nabla p, \\ \nabla \cdot \mathrm{q} &= 0, \\ \partial_t u &= D \Delta u - \nabla \cdot (\mathrm{q} u). \end{cases}$$

At Γ_G^ε:

$$\begin{cases} \mathrm{q} &= \bar{0}, \\ -D\nu \cdot \nabla u &= \varepsilon \partial_t v, \\ \partial_t v &= D_a (r_S - r_I). \end{cases}$$

Rem: Non-equilibrium kinetics, $Da = O(1)$.

Pb: Find an upscaled model!

Asymptotic expansion

In Ω_P^ε:

$$\begin{cases} \varepsilon^2 \mu \, \Delta \mathrm{q} & = & \nabla p, \\ \nabla \cdot \mathrm{q} & = & 0, \\ \partial_t u & = & D\Delta u - \nabla \cdot (\mathrm{q} u). \end{cases}$$

At Γ_G^ε:

$$\begin{cases} \mathrm{q} & = & \bar{0}, \\ -D\nu \cdot \nabla u & = & \varepsilon \partial_t v, \\ \partial_t v & = & D_a(r_S - r_I). \end{cases}$$

Asymptotic expansion

In Ω_P^ε:

$$\begin{cases} \varepsilon^2 \mu \, \Delta \mathrm{q} &= \nabla p, \\ \nabla \cdot \mathrm{q} &= 0, \\ \partial_t u &= D\Delta u - \nabla \cdot (\mathrm{q} u). \end{cases}$$

At Γ_G^ε:

$$\begin{cases} \mathrm{q} &= \bar{0}, \\ -D\nu \cdot \nabla u &= \varepsilon \partial_t v, \\ \partial_t v &= D_a(r_S - r_I). \end{cases}$$

Fast/slow variable:

$$x \longrightarrow (x, y), \text{ with } \boxed{y = \frac{x}{\varepsilon}}, \quad \text{giving} \quad \frac{\partial u}{\partial x_i}(x) \longrightarrow \frac{\partial u}{\partial x_i}(x, y) + \frac{1}{\varepsilon} \frac{\partial u}{\partial y_i}(x, y)$$

Homogenization ansatz:

$$u^\varepsilon(t, x) = u_0(t, x, y) + \varepsilon u_1(t, x, y) + \varepsilon^2 u_2(t, x, y) + \dots,$$

$$v^\varepsilon(t, x) = v_0(t, x, y) + \varepsilon v_1(t, x, y) + \varepsilon^2 v_2(t, x, y) + \dots,$$

$$r_\alpha(u^\varepsilon, v^\varepsilon) = r_\alpha(u_0, v_0) + \varepsilon u_1 \partial_u r_\alpha(u_0, v_0) + \varepsilon u_1 \partial_u r_\alpha(u_0, v_0) + \dots, (\alpha = S, I)$$

$$\mathrm{q}^{\,\varepsilon}(x) = \mathrm{q}_0(x) + \varepsilon \mathrm{q}_1(x, y) + \varepsilon^2 \mathrm{q}_2(x, y) + \dots$$

with u_k and q_k being Y-periodic.

The reactive transport component of the model

$$\text{In } \Omega_P^\varepsilon: \quad \partial_t u_0 + \left(\nabla_x + \tfrac{1}{\varepsilon}\nabla_y\right)\cdot\left((\mathbf{q}_0 + \varepsilon \mathbf{q}_1)(u_0 + \varepsilon u_1)\right) = \left(\nabla_x + \tfrac{1}{\varepsilon}\nabla_y\right)\cdot\left[D\left(\nabla_x + \tfrac{1}{\varepsilon}\nabla_y\right)(u_0 + \varepsilon u_1 + \varepsilon^2 u_2)\right] + O(\varepsilon)$$

$$\text{At } \Gamma_G^\varepsilon: \quad -\nu\cdot D\left(\tfrac{1}{\varepsilon}\nabla_y u_0 + (\nabla_x u_0 + \nabla_y u_1) + \varepsilon(\nabla_x u_1 + \nabla_y u_2)\right) = \varepsilon\partial_t v_0 + O(\varepsilon^2)$$

$$\partial_t v_0 = Da(r_S(u_0, v_0) - r_I(u_0, v_0)) + O(\varepsilon)$$

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As before

$$\mathrm{q}(x) = \frac{1}{|\mathcal{P}|}\int_{\mathcal{P}} \mathrm{q}_0(x,y)dy = -\frac{1}{\mu}\mathrm{K}\,\nabla p_0(x) \quad \text{(Darcy law)}$$
$$\nabla_x\cdot\mathrm{q}(x) = \nabla_x\cdot\mathrm{q}_0(x,y) + \nabla_y\cdot\mathrm{q}_1(x,y) = 0 \quad \text{(divergence free)}$$

$$u_0(x,y) = u_0(x) \quad \text{(no } y\text{-dependence), and}$$
$$u_1(x,y) = \tilde{u}_1(x) + \sum_{j=1}^d w^j(x,y)\,\partial_{x_j}u_0(x),$$

with w^j solving the cell problems (use $\nabla_y\cdot\mathrm{q}_0 = 0$)

$$(P_j^{-1})(x)\begin{cases} -\nabla_y\cdot\left(D\nabla_y w^j(y)\right) = 0, & \text{in } \mathcal{P},\\ -\nu\cdot\left(D\nabla_y w^j(y)\right) = \nu\cdot\left(D\mathrm{e}_j\right), & \text{on } \Gamma,\\ w^j(y) \text{ is } Y-\text{periodic}, & \int_{\mathcal{P}} w^j(y)dy = 0.\end{cases}$$

The reactive transport component: 0-order terms

The problems

$$
\begin{cases}
\partial_t u_0 + & \nabla_x \cdot (\mathrm{q}_0 u_0) + \nabla_y \cdot (\mathrm{q}_0 u_1 + \mathrm{q}_1 u_0) \\
& = \{\nabla_x \cdot (D\,(\nabla_x u_0 + \nabla_y u_1)) + \nabla_y \cdot (D(\nabla_x u_1 + \nabla_y u_2))\}\,, \qquad \text{in } \mathcal{P} \\
\partial_t v_0 & = -\nu \cdot \{D\,(\nabla_x u_1 + \nabla_y u_2)\}\,, \qquad \text{at } \Gamma \\
\partial_t v_0 & = Da(r_S(u_0, v_0) - r_I(u_0, v_0)), \qquad \text{at } \Gamma
\end{cases}
$$

The reactive transport component: 0-order terms

The problems

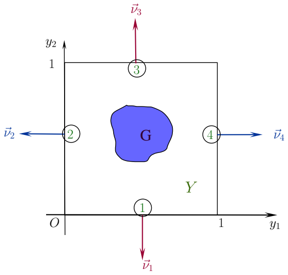
$$\begin{cases} \partial_t u_0 + & \nabla_x \cdot (q_0 u_0) + \nabla_y \cdot (q_0 u_1 + q_1 u_0) \\ & = \{\nabla_x \cdot (D(\nabla_x u_0 + \nabla_y u_1)) + \nabla_y \cdot (D(\nabla_x u_1 + \nabla_y u_2))\}, \quad \text{in } \mathcal{P} \\ \partial_t v_0 & = -\nu \cdot \{D(\nabla_x u_1 + \nabla_y u_2)\}, \quad \text{at } \Gamma \\ \partial_t v_0 & = Da(r_S(u_0, v_0) - r_I(u_0, v_0)), \quad \text{at } \Gamma \end{cases}$$

Integrate over $\mathcal{P}$ (and divide by $|\mathcal{P}|$)

$$\partial_t u_0 + \nabla_x \cdot (q u_0) + \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} \nabla_y \cdot (q_0 u_1 + q_1 u_0) dy$$

$$= \nabla_x \cdot (D \cdot \nabla_x u_0) + \frac{1}{|\mathcal{P}|} \nabla_x \cdot \left(\int_{\mathcal{P}} D \nabla_y u_1 dy \right) + \frac{1}{|\mathcal{P}|} \int_{\mathcal{P}} \nabla_y \cdot \{D(\nabla_x u_1 + \nabla_y u_2)\} \, dy$$

Incorporating adsorption/desorption effects



Note: $$\int_{\mathcal{P}} \nabla_y \cdot (\mathsf{q}_0 u_1 + \mathsf{q}_1 u_0) dy = \int_{\partial P} \nu \cdot (\mathsf{q}_0 u_1 + \mathsf{q}_1 u_0) d\sigma_y$$
$$= \int_{\partial Y} \nu \cdot (\mathsf{q}_0 u_1 + \mathsf{q}_1 u_0) d\sigma_y + \int_{\Gamma} \nu \cdot (\mathsf{q}_0 u_1 + \mathsf{q}_1 u_0) d\sigma_y = 0,$$

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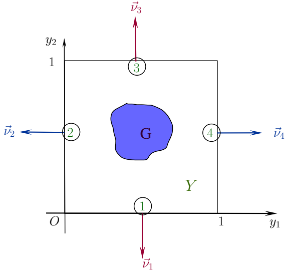

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$$= \int_{\partial Y} \nu \cdot (\mathsf{q}_0 u_1 + \mathsf{q}_1 u_0) d\sigma_y + \int_{\Gamma} \nu \cdot (\mathsf{q}_0 u_1 + \mathsf{q}_1 u_0) d\sigma_y = 0,$$

and $\int_{\mathcal{P}} \nabla_y \cdot \{D(\nabla_x u_1 + \nabla_y u_2)\}\, dy$

$$= \int_{\partial Y} D\nu \cdot (\nabla_x u_1 + \nabla_y u_2) d\sigma_y + \int_{\Gamma} D\nu \cdot (\nabla_x u_1 + \nabla_y u_2) d\sigma_y$$

$$= 0 - \int_{\Gamma} \partial_t v_0 d\sigma_y = -\int_{\Gamma} Da(r_S - r_I) d\sigma_y = -|\Gamma| Da(r_S - r_I).$$

Rem: For simplicity, here we assumed that the initial conditions for u and v are ε-independent; this implies the same for u_0 and v_0.

The Darcy-scale model, non-equilibrium kinetics

Using the cell problems, $U := u_0$, $V := v_0$, q and p solve the effective model

$$\begin{cases} \mathrm{q} = -\frac{1}{\mu}\mathrm{K}\,\nabla p & \text{in } \Omega, \\ \nabla\cdot\mathrm{q} = 0 & \text{in } \Omega, \\ \partial_t U + \frac{|\Gamma|}{|\mathcal{P}|} Da(r_S(U,V) - r_I(U,V)) & \\ \quad = \nabla\cdot(A^*\nabla U) - \nabla\cdot(\mathrm{q}U), & \text{in } (0,T]\times\Omega, \\ \partial_t V = Da(r_S(U,V) - r_I(U,V)), & \text{in } (0,T]\times\Omega, \end{cases}$$

with $A^* \in \mathbb{R}^{d\times d}$, $a^*_{ij} = \int_Y D\big(\delta_{ij} + \sum_{j=1}^{d} \partial_{y_i} w^j(y)\big)dy$

Note: Assuming that the initial data for v is ε dependent, or the grain boundary is heterogeneous ($r = r_\alpha(\frac{x}{\varepsilon}, u, v)$ for $x \in \Gamma^\varepsilon$), then the last equation is y-dependent,

$$\partial_t V = Da(r_S(U,V) - r_I(U,V)), \text{ on } (0,T]\times\Omega\times\Gamma,$$

and

$$\frac{|\Gamma|}{|\mathcal{P}|} Da(r_S(U,V) - r_I(U,V)) \text{ is replaced by } \frac{Da}{|\mathcal{P}|}\int_\Gamma (r_S(U,V) - r_I(U,V))d\sigma_y.$$

Last remarks

- Homogenization method for deriving upscaled equations approximating problems involving rapid oscillations (parameters, or complex domains).
- Lecture notes (will be updated), slides
- Questions?

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- Many thanks, hope to see you next week, have a haelthy week and a nice weekend!