HOMOGENIZATION APPROACH FOR MODELING OF REACTIVE TRANSPORT IN POROUS MEDIA

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1. **Introduction on homogenization**
2. **Reactive transport: Taylor dispersion**
3. **Numerical results**
4. **Non-equilibrium model**
5. **Generalizations and conclusion**

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-I- INTRODUCTION

DEFINITION OF HOMOGENIZATION

- ☞ Rigorous version of averaging, or upscaling
- ☞ Process of asymptotic analysis when a scale parameter $\epsilon \to 0$

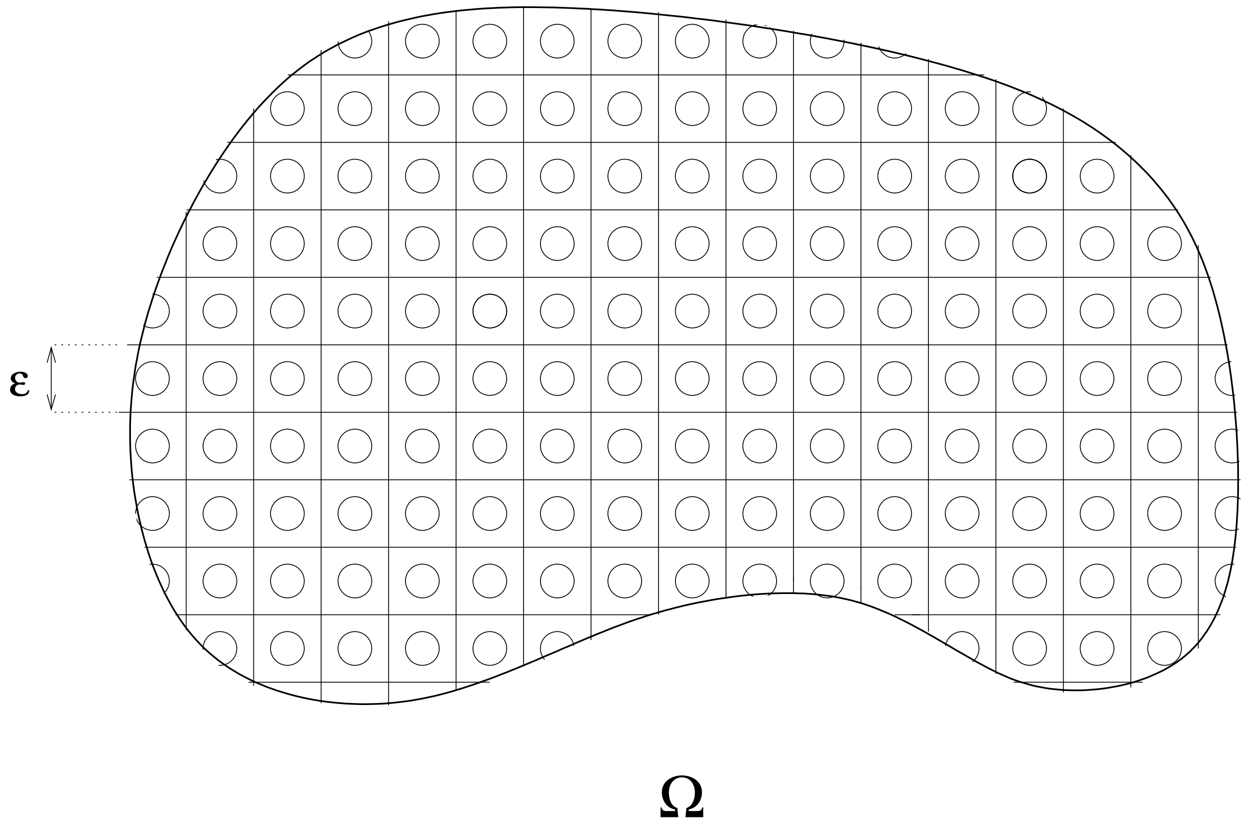
GOAL OF HOMOGENIZATION

- ☞ Extract effective or homogenized parameters for heterogeneous media
- ☞ Derive simpler macroscopic models from complicated microscopic models
- ☞ Basis for multiscale numerical methods

Various methods of homogenization (rigorous or not):

for simplicity, I focus on two-scale asymptotic expansions for periodic media.

PERIODIC HOMOGENIZATION



Main assumption: the heterogeneous medium is periodic. The small parameter ϵ is the ratio between the period and a characteristic size of the domain.

Model problem

Stationary diffusion equation

$$\begin{cases} -\operatorname{div}\left(A\left(\frac{x}{\epsilon}\right)\nabla u_\epsilon\right) = f(x) & \text{in } \Omega \\ u_\epsilon = 0 & \text{on } \partial\Omega \end{cases}$$

with a coefficient tensor $A(y)$ which is periodic in the unit cell $Y = (0,1)^N$, uniformly coercive and bounded (not necessarily symmetric)

$$\alpha|\xi|^2 \leq \sum_{i,j=1}^{N} A_{ij}(y)\xi_i\xi_j \leq \beta|\xi|^2, \quad \forall\, \xi \in \mathbb{R}^N, \forall\, y \in Y \quad (\beta \geq \alpha > 0).$$

$y \to A(y)$ 1-periodic $\Rightarrow$ $x \to A\left(\frac{x}{\epsilon}\right)$ ϵ-periodic

Reference books

BAKHVALOV N., PANASENKO G., *Homogenization : averaging processes in periodic media,* Mathematics and its applications, vol.36, Kluwer (1990).

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HORNUNG U., Ed., *Homogenization and porous media,* Springer Verlag (1996).

JIKOV V., KOZLOV S., OLEINIK O., *Homogenization of differential operators and integral functionals,* Springer, Berlin, (1995).

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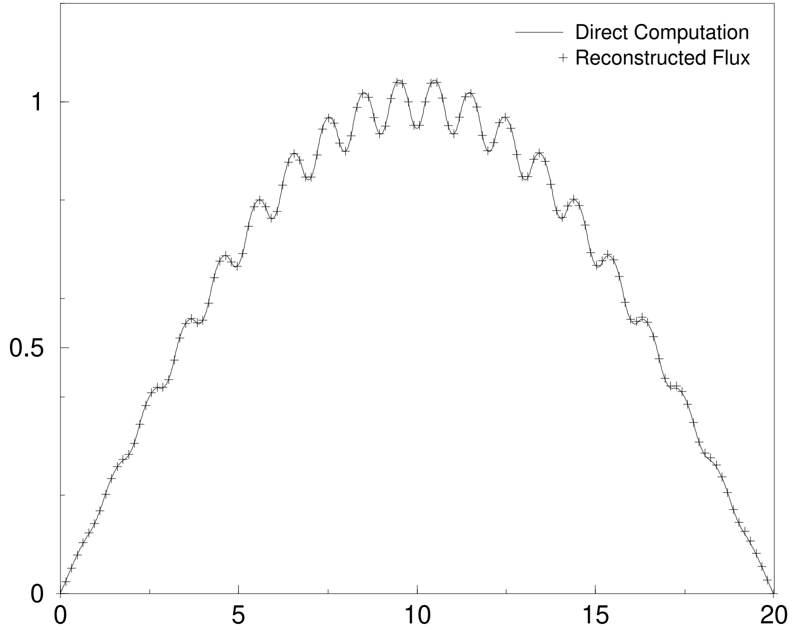
TWO-SCALE ASYMPTOTIC EXPANSIONS



Ansatz for the solution
$$u_\epsilon(x) = \sum_{i=0}^{+\infty} \epsilon^i u_i\left(x, \frac{x}{\epsilon}\right)$$

with $u_i(x, y)$ function of both variables x and y, periodic in y (see figure above).

Derivation rule
$$\nabla\left(u_i\left(x, \frac{x}{\epsilon}\right)\right) = \left(\epsilon^{-1}\nabla_y u_i + \nabla_x u_i\right)\left(x, \frac{x}{\epsilon}\right)$$

CASCADE OF EQUATIONS

$$-\epsilon^{-2}\left[\,\mathrm{div_y} A\nabla_y u_0\right]\left(x,\frac{x}{\epsilon}\right)$$

$$-\epsilon^{-1}\left[\,\mathrm{div_y} A(\nabla_x u_0+\nabla_y u_1)+\ \mathrm{div_x} A\nabla_y u_0\right]\left(x,\frac{x}{\epsilon}\right)$$

$$-\epsilon^{0}\left[\,\mathrm{div_x} A(\nabla_x u_0+\nabla_y u_1)+\ \mathrm{div_y} A(\nabla_x u_1+\nabla_y u_2)\right]\left(x,\frac{x}{\epsilon}\right)$$

$$-\sum_{i=1}^{+\infty}\epsilon^{i}\left[\,\mathrm{div_x} A(\nabla_x u_i+\nabla_y u_{i+1})+\ \mathrm{div_y} A(\nabla_x u_{i+1}+\nabla_y u_{i+2})\right]\left(x,\frac{x}{\epsilon}\right)$$

$$=f(x).$$

Interpretation of the cascade of equations

In this series, each power ϵ^i is identified to zero:

$$- \operatorname{div}_{\mathrm{y}}\Big(A(y)\nabla_y u_{i+2}(x,y)\Big) = F\left(u_i, u_{i+1}\right)(x,y) \quad \text{in} \quad Y$$

- This is a partial differential equation in the variable y for the unknown u_{i+2}.
- We supplement it with periodic boundary conditions.
- The macroscopic variable x is just a parameter.
- Only the 3 first equations are necessary.

ϵ^{-2} equation

$$u_0(x,y) \equiv u(x)$$

ϵ^{-1} equation

$$u_1(x,y) = \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x) w_i(y).$$

where the w_i's are the solutions of the cell problems

$$\begin{cases} -\operatorname{div}_{\mathrm{y}}\Big(A(y)\left(e_i + \nabla_y w_i(y)\right)\Big) = 0 & \text{in } Y \\ y \to w_i(y) & Y\text{-periodic}, \end{cases}$$

ϵ^{0} equation $\Rightarrow$ homogenized equation

$$\begin{cases} -\operatorname{div}_{\mathrm{x}}\Big(A^* \nabla_x u(x)\Big) = f(x) & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

Homogenized or effective tensor:

$$A^*_{ji} = \int_Y A(y) \left(e_i + \nabla_y w_i(y)\right) \cdot \left(e_j + \nabla_y w_j(y)\right) dy.$$

- ➯ Explicit formula for A^* (depending on the cell problems).
- ➯ A^* does not depend on ϵ, f, u or the boundary conditions.
- ➯ A^* is positive definite (not necessarily isotropic even if $A(y)$ was so).

Theorem.

$$u_\epsilon(x) = u(x) + \epsilon\, u_1\left(x, \frac{x}{\epsilon}\right) + r_\epsilon \quad \text{with} \quad \|r_\epsilon\|_{H^1(\Omega)} \leq C\epsilon^{1/2}$$

In particular $\|u_\epsilon - u\|_{L^2(\Omega)} \leq C\epsilon^{1/2}$.

Remark. The first-order corrector is not negligible for the gradient

$$\nabla u_\epsilon(x) = \nabla_x u(x) + (\nabla_y u_1)\left(x, \frac{x}{\epsilon}\right) + t_\epsilon \quad \text{with} \quad \|t_\epsilon\|_{L^2(\Omega)} \leq C\epsilon^{1/2}$$

The error estimate is limited by boundary layers.

TWO-SCALE CONVERGENCE METHOD

One way of making periodic homogenization rigorous.

Definition. A sequence of functions u_ϵ in $L^2(\Omega)$ is said to two-scale converge to a limit $u_0(x,y)$ belonging to $L^2(\Omega \times Y)$ if, for any Y-periodic smooth function $\varphi(x,y)$, it satisfies

$$\lim_{\epsilon \to 0} \int_\Omega u_\epsilon(x) \varphi\left(x, \frac{x}{\epsilon}\right) dx = \int_\Omega \int_Y u_0(x,y) \varphi(x,y) dx dy.$$

Theorem (Nguetseng, Allaire). From each bounded sequence u_ϵ in $L^2(\Omega)$ one can extract a subsequence, and there exists a limit $u_0(x,y) \in L^2(\Omega \times Y)$ such that this subsequence two-scale converges to u_0.

My goal in this lecture

- ☞ To go beyond the previous simple and "text-book" example !
- ☞ To emphasize the role of scaling in modeling issues.
- ☞ To work out the details without too much mathematics...
- ☞ I made the choice not to discuss the applications: too bad...
- ☞ My motivation was nuclear waste underground storage.

I start with the simplest of the complex models I want to address.

In the end, I will say a few words on more complex models...

-II- REACTIVE TRANSPORT

Microscopic model

- Infinite porous medium: (connected) fluid part $\Omega_f \subset \mathbb{R}^N$.
- Saturated incompressible single phase flow in Ω_f and a single solute.
- Linear reaction rates (adsorption/desorption process).
- Concentrations u in the fluid and v on the solid boundary.

convection diffusion in the bulk:

$$\frac{\partial u}{\partial \tau} + b \cdot \nabla_y u - \operatorname{div}_y(D \nabla_y u) = 0 \quad \text{in } \Omega_f \times (0, \mathcal{T}),$$

linear adsorption process on the pore boundaries:

$$\frac{\partial v}{\partial \tau} = k(u - \frac{v}{K}) = -D \nabla_y u \cdot n \quad \text{on } \partial \Omega_f \times (0, \mathcal{T}),$$

Assumptions and scaling

Incompressible fluid:

$$\operatorname{div} b = 0 \text{ in } \Omega_f \quad \text{and} \quad b \cdot n = 0 \text{ on } \partial\Omega_f .$$

At the microscopic scale (with characteristic lengthscale ℓ) the Péclet and Damkohler numbers are assumed of order 1

$$\mathbf{Pe} = \frac{\ell b}{D} \quad \text{and} \quad \mathbf{Da} = \frac{\ell k}{D}$$

To upscale this model, we define a large **macroscopic scale** ϵ^{-1} and a **long time scale** of order ϵ^{-2} (parabolic or diffusion scaling)

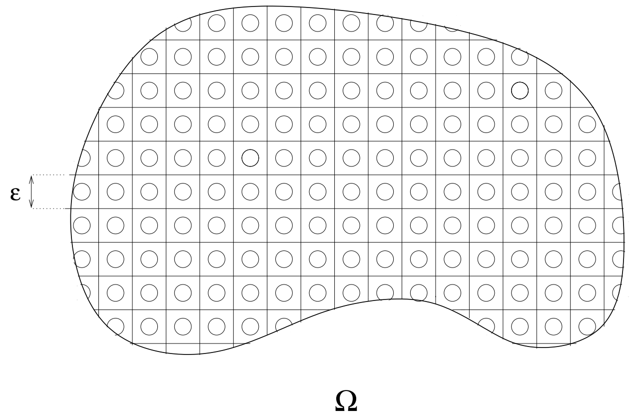
$$x = \epsilon y \quad \text{and} \quad t = \epsilon^2 \tau.$$

We define

$$u_\epsilon(t,x) = u(\tau, y) \quad \text{and } v_\epsilon(t,x) = v(\tau, y).$$

Remark: another possibily is the hyperbolic scaling $x = \epsilon y$ and $t = \epsilon \tau$.

Periodicity assumption



- ✗ Periodic unit cell $Y = (0,1)^N = Y^* \cup \mathcal{O}$ with fluid part Y^*
- ✗ Periodic (infinite) porous media $x \in \Omega_\epsilon \Leftrightarrow y \in Y^*$
- ✗ Incompressible periodic flow $b_\epsilon(x) = b\left(\frac{x}{\epsilon}\right)$ with $\text{div}_y b = 0$ in Y^* and $b \cdot n = 0$ on $\partial\mathcal{O}$
- ✗ Periodic symmetric coercive diffusion $D_\epsilon(x) = D\left(\frac{x}{\epsilon}\right)$

Rescaled model

In these rescaled variables (with $T = \epsilon^2 \mathcal{T}$) the reactive transport system is

$$\begin{cases} \dfrac{\partial u_\epsilon}{\partial t} + \dfrac{1}{\epsilon} b_\epsilon \cdot \nabla_x u_\epsilon - \operatorname{div}_x (D_\epsilon \nabla_x u_\epsilon) = 0 & \text{in } \Omega_\epsilon \times (0,T) \\ \dfrac{\partial v_\epsilon}{\partial t} = \dfrac{k}{\epsilon^2}(u_\epsilon - \dfrac{v_\epsilon}{K}) = \dfrac{-1}{\epsilon} D_\epsilon \nabla_x u_\epsilon \cdot n & \text{on } \partial\Omega_\epsilon \times (0,T) \\ u_\epsilon(x,0) = u_{init}(x) \text{ and } v_\epsilon(x,0) = v_{init}(x). \end{cases}$$

At the macroscopic scale (with characteristic lengthscale L) the Péclet and Damkohler numbers are **large**

$$\mathbf{Pe} = \frac{Lb}{D\epsilon} = \mathcal{O}(\epsilon^{-1}) \quad \mathbf{Da} = \frac{Lk}{D\epsilon} = \mathcal{O}(\epsilon^{-1})$$

Goal of homogenization

Find the effective diffusion tensor.

This is the so-called problem of **Taylor dispersion** (1953).

Many previous works, including Adler, Auriault, Choquet, van Duijn, Knabner, Mauri, Mikelic, Pop, Quintard, Rosier, Rubinstein, etc.

Theorem. The solution (u_ϵ, v_ϵ) satisfies

$$u_\epsilon(t,x) \approx u_0\left(t, x - \frac{b^*}{\epsilon}t\right) \quad \text{and} \quad v_\epsilon(t,x) \approx K u_0\left(t, x - \frac{b^*}{\epsilon}t\right)$$

with the effective drift

$$b^* = \frac{\displaystyle\int_{Y^*} b(y)dy}{|Y^*| + K|\partial\mathcal{O}|_{N-1}}$$

and u_0 the solution of the homogenized problem

$$\begin{cases} \dfrac{\partial u_0}{\partial t} - \operatorname{div}\left(A^* \nabla u_0\right) = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ u_0(t=0,x) = \dfrac{|Y^*| u_{init}(x) + |\partial\mathcal{O}|_{N-1} v_{init}(x)}{|Y^*| + K|\partial\mathcal{O}|_{N-1}} & \text{in } \mathbb{R}^N \end{cases}$$

Remark. Transport and chemistry cannot be decoupled for computing effective coefficients.

Remarks

1) Precise convergence:

$$u_\epsilon(t,x) = u_0\left(t, x - \frac{b^*}{\epsilon}t\right) + r_\epsilon^u(t,x) \quad \text{and} \quad v_\epsilon(t,x) = K u_0\left(t, x - \frac{b^*}{\epsilon}t\right) + r_\epsilon^v(t,x)$$

with

$$\lim_{\epsilon \to 0} \int_0^T \int_{\mathbb{R}^N} \left| r_\epsilon^{u,v}(t,x) \right|^2 dt\, dx = 0,$$

2) Equivalent homogenized equation with convection: change coordinates !

Define $\tilde{u}_0(t,x) = u_0\left(t, x - \frac{b^*}{\epsilon}t\right)$. Then, it is solution of

$$\begin{cases} \dfrac{\partial \tilde{u}_0}{\partial t} + \dfrac{1}{\epsilon} b^* \cdot \nabla \tilde{u}_0 - \operatorname{div}\left(A^* \nabla \tilde{u}_0\right) = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ \tilde{u}_0(t=0,x) = \dfrac{|Y^*| u_{init}(x) + |\partial \mathcal{O}|_{N-1} v_{init}(x)}{|Y^*| + K |\partial \mathcal{O}|_{N-1}} & \text{in } \mathbb{R}^N \end{cases}$$

Homogenized diffusion tensor

The homogenized diffusion tensor is

$$A^* = (|Y^*| + K|\partial\mathcal{O}|_{N-1})^{-1}\left(A_1^* + A_2^*\right)$$

with $A_1^* = \dfrac{K^2}{k}|\partial\mathcal{O}|_{N-1} b^* \otimes b^*$ and $A_2^* = \displaystyle\int_{Y^*} D(\mathbf{I} + \nabla_y w(y))(\mathbf{I} + \nabla_y w(y))^T dy$

where the components $w_i(y)$, $1 \leq i \leq N$, of $w(y)$ are solutions of the cell problem

$$\begin{cases} b(y) \cdot \nabla_y w_i - \operatorname{div_y}\left(D(y)\left(\nabla_y w_i + e_i\right)\right) = \left(b^* - b(y)\right) \cdot e_i \text{ in } Y^* \\ D(y)\left(\nabla_y w_i + e_i\right) \cdot n = K b^* \cdot e_i \text{ on } \partial\mathcal{O} \\ y \to w_i(y) \ Y\text{-periodic} \end{cases}$$

Remark that the value of b^* is exactly the compatibility condition for the existence of w_i.

TWO-SCALE ANSATZ WITH DRIFT

Formal proof of this homogenization result.

Standard two-scale asymptotic expansions must be modified to introduce an **unknown large drift** $b^* \in \mathbb{R}^N$

$$u_\epsilon(t,x) = \sum_{i=0}^{+\infty} \epsilon^i u_i\left(t, x - \frac{b^* t}{\epsilon}, \frac{x}{\epsilon}\right),$$

with $u_i(t,x,y)$ a function of the macroscopic variable x and of the periodic microscopic variable $y \in Y = (0,1)^N$.

Similarly

$$v_\epsilon(t,x) = \sum_{i=0}^{+\infty} \epsilon^i v_i\left(t, x - \frac{b^* t}{\epsilon}, \frac{x}{\epsilon}\right)$$

We plug these ansatz in the system of equations and use the usual chain rule derivation

$$\nabla\left(u_i\left(t,x-\frac{b^*t}{\epsilon},\frac{x}{\epsilon}\right)\right)=\left(\epsilon^{-1}\nabla_y u_i+\nabla_x u_i\right)\left(t,x-\frac{b^*t}{\epsilon},\frac{x}{\epsilon}\right),$$

plus a **new** contribution

$$\frac{\partial}{\partial t}\left(u_i\left(t,x-\frac{b^*t}{\epsilon},\frac{x}{\epsilon}\right)\right)=\left(\frac{\partial u_i}{\partial t}-\underbrace{\epsilon^{-1}b^*\cdot\nabla_x u_i}_{new\,term}\right)\left(t,x-\frac{b^*t}{\epsilon},\frac{x}{\epsilon}\right)$$

$$
\begin{cases}
\dfrac{\partial u_\epsilon}{\partial t} + \dfrac{1}{\epsilon} b_\epsilon \cdot \nabla_x u_\epsilon - \operatorname{div}_x (D_\epsilon \nabla_x u_\epsilon) = 0 \quad \text{in} \;\; \Omega_\epsilon \times (0,T) \\
u_\epsilon(x,0) = u_{init}(x), \quad x \in \Omega_\epsilon, \\
\dfrac{\partial v_\epsilon}{\partial t} = \dfrac{k}{\epsilon^2} (u_\epsilon - \dfrac{v_\epsilon}{K}) = -\dfrac{1}{\epsilon} D_\epsilon \nabla_x u_\epsilon \cdot n \quad \text{on} \;\; \partial\Omega_\epsilon \times (0,T) \\
v_\epsilon(x,0) = v_{init}(x), \quad x \in \partial\Omega_\epsilon
\end{cases}
$$

Fredholm alternative in the unit cell

Lemma. The boundary value problem

$$\begin{cases} b(y) \cdot \nabla_y v(y) - \operatorname{div_y} \left(D(y) \nabla_y v(y) \right) = g(y) \text{ in } Y^* \\ D(y) \nabla_y v(y) \cdot n = h(y) \text{ on } \partial\mathcal{O} \\ y \to v(y) \ Y\text{-periodic} \end{cases}$$

admits a unique solution in $H^1(Y^*)$, up to an additive constant, **if and only if**

$$\int_{Y^*} g(y)\, dy + \int_{\partial\mathcal{O}} h(y)\, ds = 0.$$

Cascade of equations

Equation of order ϵ^{-2}:

$$\begin{cases} b(y) \cdot \nabla_y u_0 - \operatorname{div}_y \left(D(y) \nabla_y u_0 \right) = 0 \text{ in } Y^* \\ D(y) \nabla_y u_0 \cdot n = 0 = k \Big(u_0 - \frac{v_0}{K} \Big) \text{ on } \partial \mathcal{O} \\ y \to u_0, v_0(t,x,y) \ Y\text{-periodic} \end{cases}$$

We deduce

$$\boxed{u_0(t,x,y) \equiv u_0(t,x) \text{ and } v_0(t,x,y) \equiv K u_0(t,x)}$$

Equation of order ϵ^{-1}:

$$\begin{cases} -b^* \cdot \nabla_x u_0 + b(y) \cdot (\nabla_x u_0 + \nabla_y u_1) - \operatorname{div_y}\left(D(y)\left(\nabla_x u_0 + \nabla_y u_1\right)\right) = 0 \text{ in } Y^* \\ -D(y)\left(\nabla_x u_0 + \nabla_y u_1\right) \cdot n = -b^* \cdot \nabla_x v_0 \cdot n = k\Big(u_1 - \frac{v_1}{K}\Big) \text{ on } \partial\mathcal{O} \\ y \to u_1, v_1(t,x,y) \; Y\text{-periodic} \end{cases}$$

We deduce

$$\boxed{u_1(t,x,y) = \sum_{i=1}^{n} \frac{\partial u_0}{\partial x_i}(t,x) w_i(y) \quad \text{and} \quad v_1 = K u_1 + \frac{K^2}{k} b^* \cdot \nabla_x u_0}$$

Cell problem

$$\begin{cases} b(y)\cdot\nabla_y w_i - \operatorname{div_y}\left(D(y)\left(\nabla_y w_i + e_i\right)\right) = \left(b^* - b(y)\right)\cdot e_i \text{ in } Y^* \\ D(y)\left(\nabla_y w_i + e_i\right)\cdot n = K b^*\cdot e_i \text{ on } \partial\mathcal{O} \\ y \to w_i(y)\ Y\text{-periodic} \end{cases}$$

The compatibility condition (Fredholm alternative) for the existence of w_i gives the value of the drift velocity:

$$b^* = \left(|Y^*| + |\partial\mathcal{O}|_{N-1}K\right)^{-1}\int_{Y^*} b(y)dy.$$

Equation of order ϵ^0:

$$\begin{cases} b\cdot\nabla_y u_2 - \operatorname{div}_y\left(D\nabla_y u_2\right) = b^*\cdot\nabla_x u_1 - b\cdot\nabla_x u_1 \\ + \operatorname{div}_y\left(D\nabla_x u_1\right) + \operatorname{div}_x\left(D(\nabla_y u_1 + \nabla_x u_0)\right) - \frac{\partial u_0}{\partial t} \quad \text{in } Y^* \\ -D(y)\left(\nabla_y u_2 + \nabla_x u_1\right)\cdot n = \frac{\partial v_0}{\partial t} - b^*\cdot\nabla_x v_1 = k\Big(u_2 - \frac{v_2}{K}\Big) \text{ on } \partial\mathcal{O} \\ y \to u_2, v_2(t,x,y) \; Y\text{-periodic} \end{cases}$$

Compatibility condition for the existence of u_2:

$$\int_{Y^*}\Big(b^*\cdot\nabla_x u_1 - b\cdot\nabla_x u_1 + \operatorname{div}_y\big(D\nabla_x u_1\big) + \operatorname{div}_x\big(D(\nabla_y u_1 + \nabla_x u_0)\big) - \frac{\partial u_0}{\partial t}\Big)dy - \int_{\partial\mathcal{O}}\big(D\nabla_x u_1\cdot n + \frac{\partial v_0}{\partial t} - b^*\cdot\nabla_x v_1\big)ds = 0$$

Replacing u_1 by its previous value in terms of $\nabla_x u_0$ we obtain the **homogenized problem**.

Homogenized equation

$$\left\{ \begin{array}{ll} \dfrac{\partial u_0}{\partial t} - \operatorname{div}\left(A^* \nabla u_0\right) = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ u_0(t=0,x) = \dfrac{|Y^*| u^0(x) + |\partial \mathcal{O}|_{N-1} v^0(x)}{|Y^*| + K |\partial \mathcal{O}|_{N-1}} & \text{in } \mathbb{R}^N, \end{array} \right.$$

The initial condition is an average of

$$u_0(t=0,x) \approx u_\epsilon(t=0,x) = u^0(x) \text{ in } Y^*$$

and

$$v_0(t=0,x) = K u_0(t=0,x) \approx v_\epsilon(t=0,x) = v^0(x) \text{ on } \partial \mathcal{O}$$

How to make a rigorous proof

The proof is made of 3 steps

1. A priori estimates.
2. Passing to the limit by two-scale convergence with drift.
3. Strong convergence.

A priori estimate

The model is well-posed: it is a standard parabolic system of equations.

Energy estimate: multiply the bulk equation by u_ϵ and the surface equation by $\epsilon v_\epsilon / K$, integrate by parts to get

$$\frac{1}{2}\frac{d}{dt}\left(\int_{\Omega_\epsilon}|u_\epsilon|^2 dx + \frac{\epsilon}{K}\int_{\partial\Omega_\epsilon}|v_\epsilon|^2 ds\right)$$

$$+\int_{\Omega_\epsilon} D_\epsilon \nabla u_\epsilon \cdot \nabla u_\epsilon dx + \frac{k}{\epsilon}\int_{\partial\Omega_\epsilon}\left(u_\epsilon - \frac{v_\epsilon}{K}\right)^2 ds = 0$$

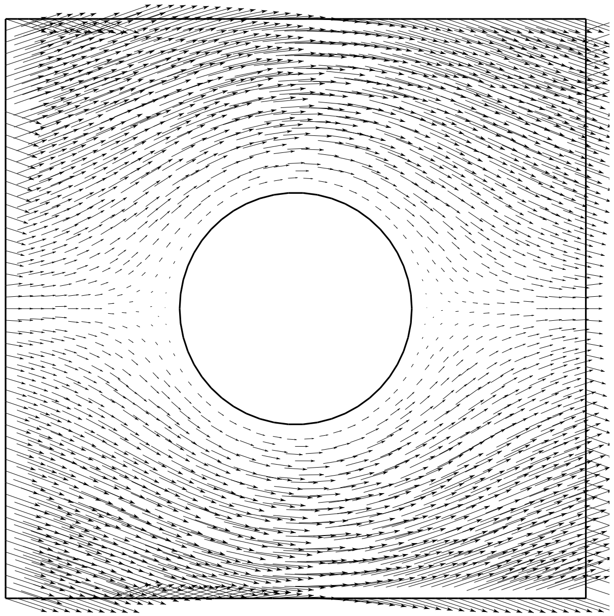
Two-scale convergence with drift

Proposition (Marusic-Paloka, Piatnitski). Let $b^* \in \mathbb{R}^N$ be a given drift velocity. Let w_ϵ be a bounded sequence in $L^2((0,T) \times \mathbb{R}^N)$. Up to a subsequence, there exist a limit $w_0(t,x,y) \in L^2((0,T) \times \mathbb{R}^N \times \mathbb{T}^N)$ such that w_ϵ two-scale converges with drift weakly to w_0 in the sense that

$$\lim_{\epsilon \to 0} \int_0^T \int_{\mathbb{R}^N} w_\epsilon(t,x) \phi \left(t, x - \frac{b^*}{\epsilon} t, \frac{x}{\epsilon} \right) dt\, dx = \int_0^T \int_{\mathbb{R}^N} \int_{\mathbb{T}^N} w_0(t,x,y) \phi(t,x,y)\, dt\, dx\, dy$$

for all functions $\phi(t,x,y) \in L^2 \left((0,T) \times \mathbb{R}^N ; C(\mathbb{T}^N) \right)$.

-III- NUMERICAL RESULTS



Academic geometry for qualitative study. For real applications go for a Representative Volume Element.

Numerical computations with FreeFem++ in 2-d for circular obstacles.

The incompressible velocity $b(y)$ is a Stokes solution in the unit cell Y.

Cell problem

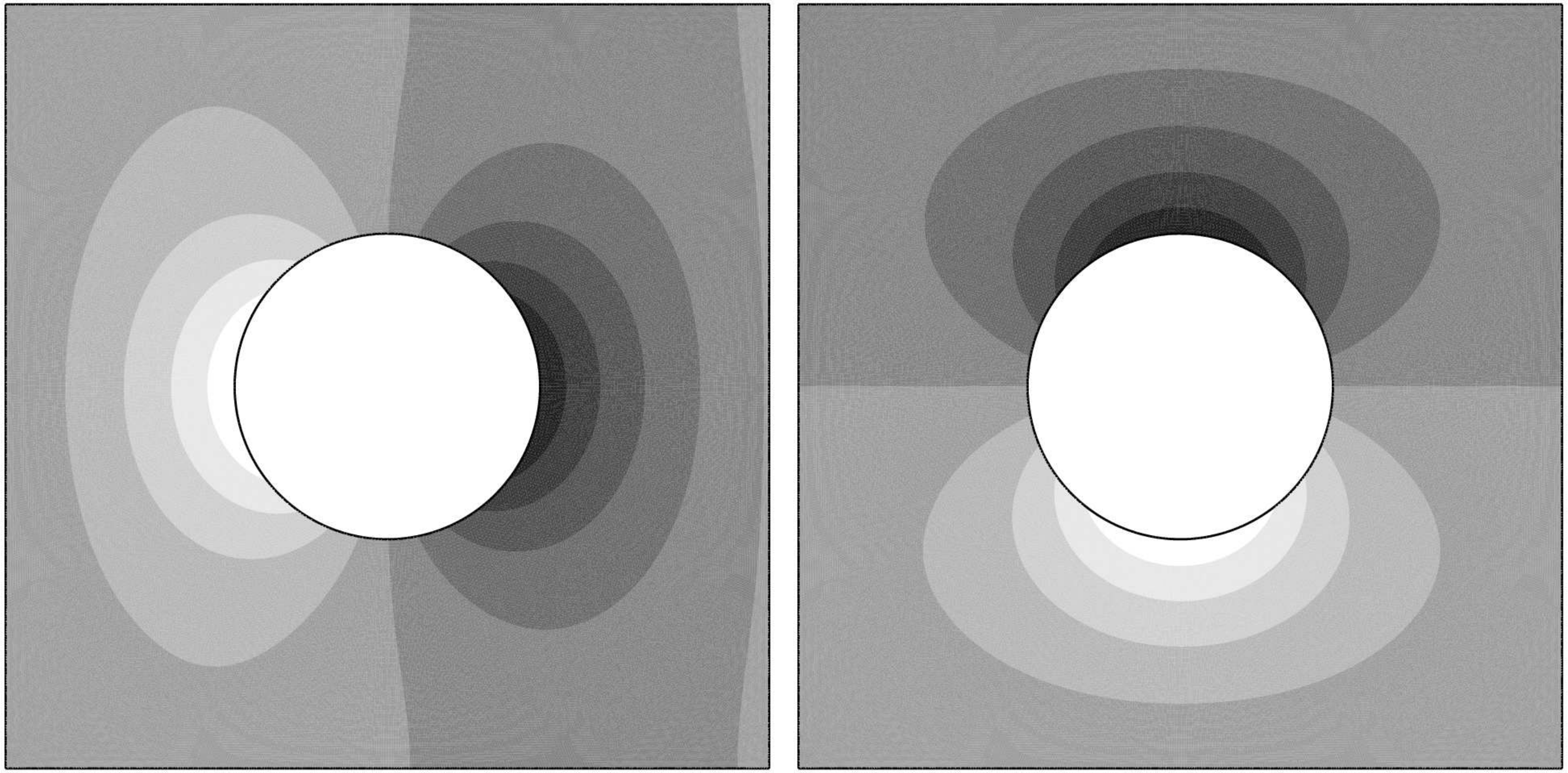
$$
\begin{cases}
b(y) \cdot \nabla_y \chi_i - D \Delta_y \chi_i = (b^* - b(y)) \cdot e_i \text{ in } Y^* \\
D \left(\nabla_y \chi_i + e_i \right) \cdot n = K b^* \cdot e_i \text{ on } \partial \mathcal{O} \\
y \to \chi_i(y) \ Y\text{-periodic}
\end{cases}
$$

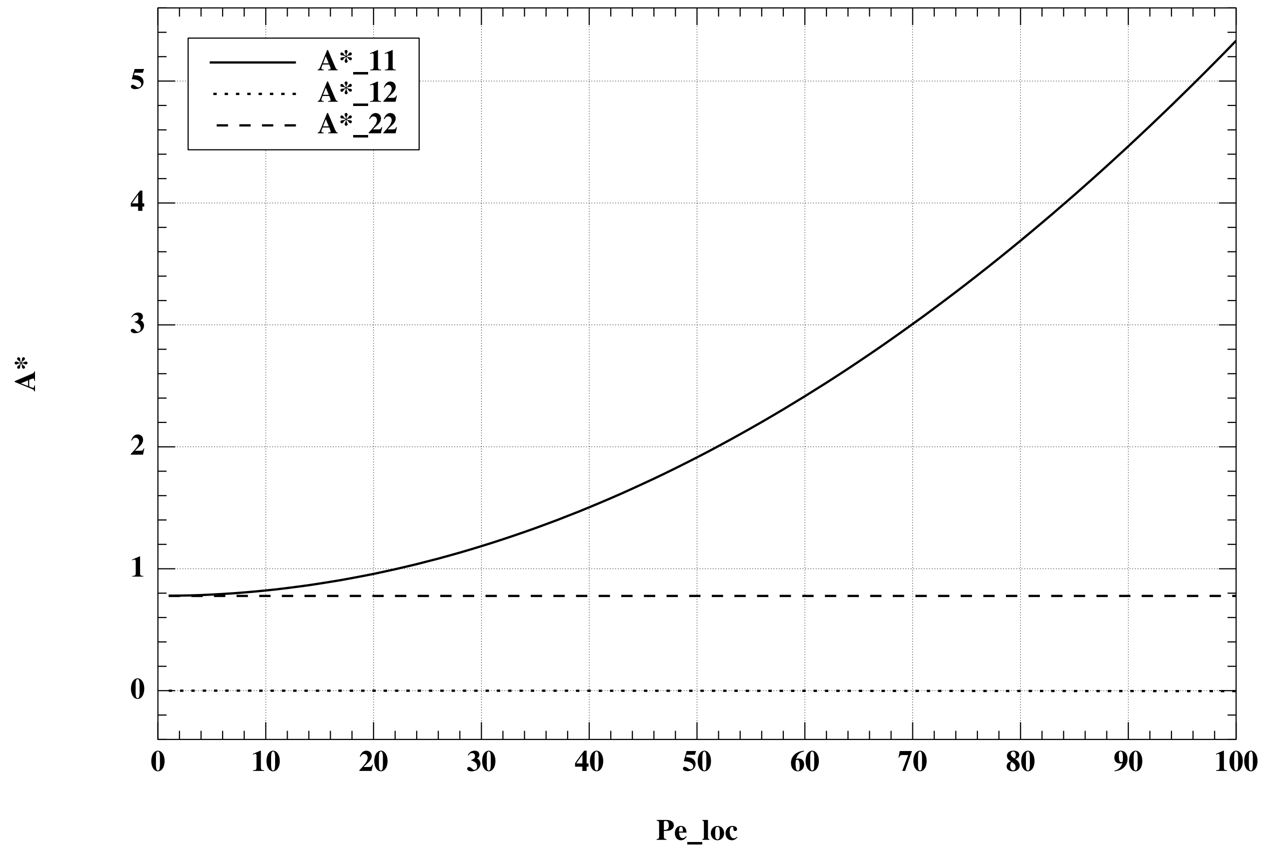
The homogenized velocity is

$$
\mathbf{b}^* = \begin{pmatrix} 0.01808 \\ -6.759 \cdot 10^{-6} \end{pmatrix}
$$

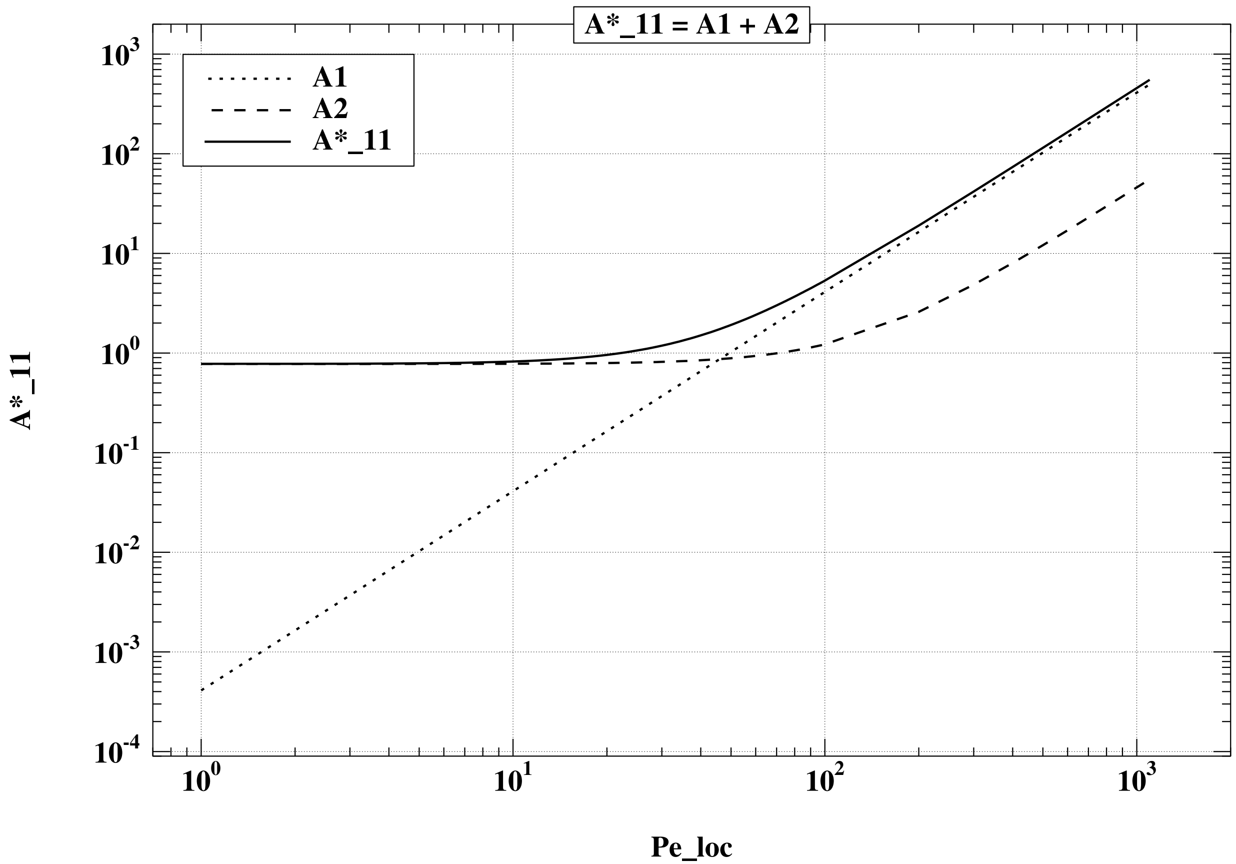
We plot the dispersion tensor A^* for increasing values of the Péclet number (multiplying the velocity field $b(y)$ by $\mathbf{Pe}$).

χ_1, χ_2

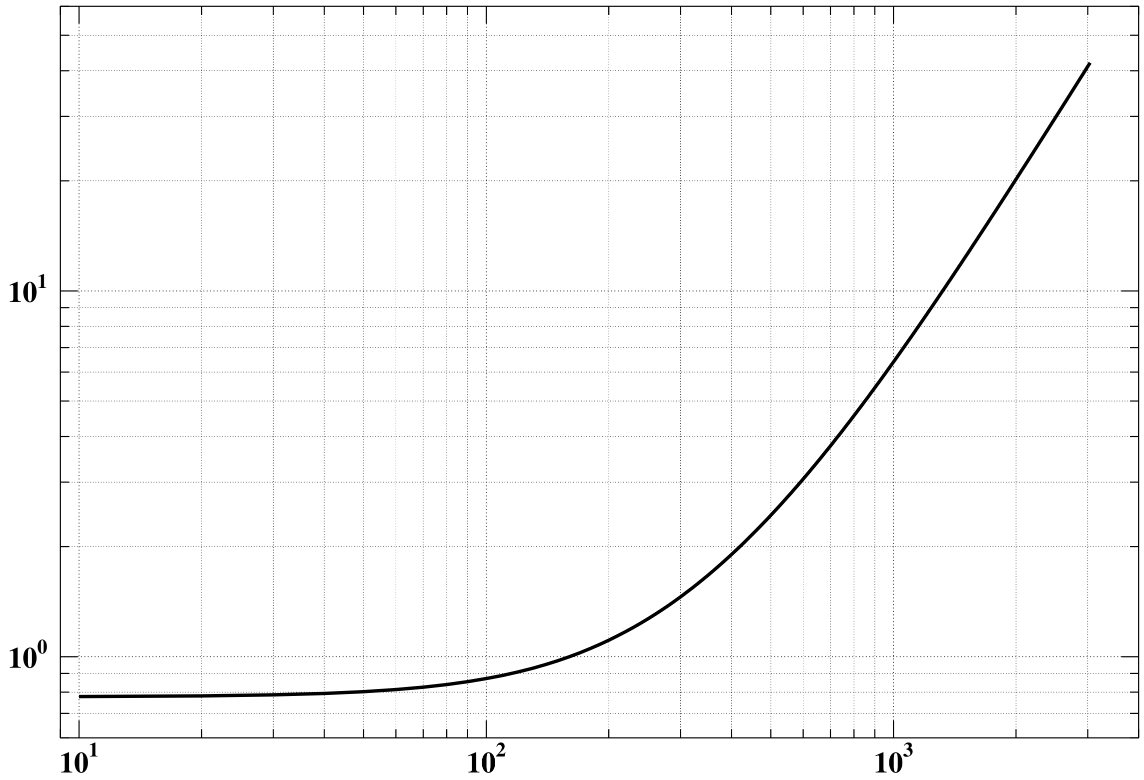




Entries A^*_{11}, A^*_{12} and A^*_{22} of the dispersion matrix A^* as a function of the local Péclet number, for $\mathrm{Da}_{loc} = 1$.

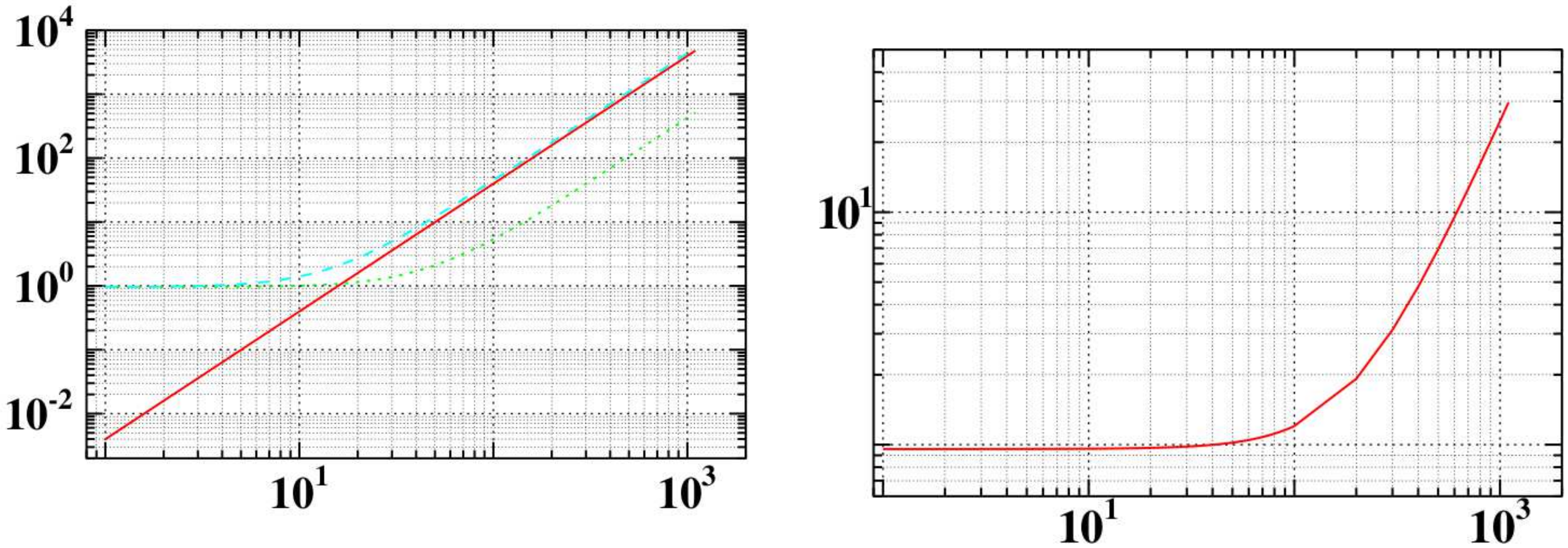


Log-log plot of the (1,1) entry of the dispersion matrix $A^* = A_1 + A_2$, together with its 2 components A_1 and A_2, as a function of the local Péclet number, for $\mathrm{Da}_{loc} = 1$.



Log-log plot of the longitudinal dispersion A_{11}^* as a function of the local Péclet number, in the **absence** of chemical reactions, $K = 0$ (asymptotic slope ≈ 1.7).

3-d case: obstacles are balls



Same log-log plot of the longitudinal dispersion A_{11}^* with (left) and without (right) chemical reactions in 3-d for a ball (asymptotic slope ≈ 1.9).

-IV- A NON-EQUILIBRIUM MODEL

✗ What if the velocity is not divergence-free ?

✗ What if reactions take place in the bulk ?

✗ For simplicity we address these issues on a simpler model **without surface concentration**.

convection diffusion reaction in the bulk:

$$\frac{\partial u}{\partial \tau} + b \cdot \nabla_y u - \operatorname{div}_y(D \nabla_y u) + r\, u = 0 \quad \text{in } \Omega_f \times (0, \mathcal{T}),$$

boundary condition:

$$-D \nabla_y u \cdot n = k\, u \quad \text{on } \partial\Omega_f \times (0, \mathcal{T}),$$

No assumption on the velocity $b(y)$ **and on the reaction coefficient** $r(y)$ **!**

Scaling

To upscale this model, we define a large **macroscopic scale** ϵ^{-1} and a **long time scale** of order ϵ^{-2} (parabolic or diffusion scaling) $x = \epsilon y$ and $t = \epsilon^2 \tau$. We define $u_\epsilon(t,x) = u(\tau, y)$ which is a solution of

$$\begin{cases} \dfrac{\partial u_\epsilon}{\partial t} + \dfrac{1}{\epsilon} b_\epsilon \cdot \nabla_x u_\epsilon - \operatorname{div}_x(D_\epsilon \nabla_x u_\epsilon) + \dfrac{1}{\epsilon^2} r_\epsilon \, u_\epsilon = 0 \quad \text{in} \;\; \Omega_\epsilon \times (0,T) \\ u_\epsilon(x,0) = u_{init}(x), \quad x \in \Omega_\epsilon, \\ -D_\epsilon \nabla_x u_\epsilon \cdot n = \dfrac{k}{\epsilon} u_\epsilon \quad \text{on} \;\; \partial\Omega_\epsilon \times (0,T). \end{cases}$$

New ansatz: (unknown) drift $b^* \in \mathbb{R}^N$ and (unknown) reaction rate $r^* \in \mathbb{R}$

$$u_\epsilon(t,x) = e^{-r^* \epsilon^{-2} t} \sum_{i=0}^{+\infty} \epsilon^i u_i \left(t, x - \frac{b^* t}{\epsilon}, \frac{x}{\epsilon} \right),$$

with $u_i(t,x,y)$ Y-periodic with respect to y.

New ϵ^{-2} equation:

$$\begin{cases} b(y)\cdot\nabla_y u_0 - \operatorname{div}_y\left(D(y)\nabla_y u_0\right) + r(y)u_0 = r^* u_0 \text{ in } Y^* \\ D(y)\nabla_y u_0\cdot n + k u_0 = 0 \text{ on } \partial\mathcal{O} \\ y\to u_0(x,y)\ Y\text{-periodic} \end{cases}$$

It is a spectral problem ! The parameter r^* is the first eigenvalue:

$$\begin{cases} b\cdot\nabla_y\psi - \operatorname{div}_y\left(D\nabla_y\psi\right) + r\psi = r^*\psi & \text{in } Y^* \\ D\nabla_y\psi\cdot n + k\psi = 0 & \text{on } \partial\mathcal{O} \\ y\to\psi(y) & Y-\text{periodic} \end{cases}$$

By uniqueness of the first cell eigenfunction ψ (Krein-Rutman), we deduce

$$\boxed{u_0(x,y)\equiv u(x)\,\psi(y)}$$

Only the first eigenfunction is positive and can be interpreted as a local equilibrium concentration.

New ϵ^{-1} equation: (cell problem)

$$\left\{ \begin{array}{l} b(y)\cdot\nabla_y u_1 - \operatorname{div_y}\left(D(y)\nabla_y u_1\right) + r(y)u_1 - r^* u_1 = \\ \qquad\qquad b^*\cdot\nabla_x u_0 - b(y)\cdot\nabla_x u_0 + \operatorname{div_y}\left(D(y)\nabla_x u_0\right) \text{ in } Y^* \\ D(y)\nabla_y u_1(x,y)\cdot n + k u_1 = -D(y)\nabla_x u_0\cdot n \text{ on } \partial\mathcal{O} \\ y \to u_1(x,y) \ Y\text{-periodic} \end{array} \right.$$

We define b^* such that the Fredholm alternative holds true, i.e. the right hand side is orthogonal to ψ^* the first adjoint eigenfunction.

We deduce that u_1 depends linearly on $\nabla_x u_0(x,y) = \psi(y)\nabla_x u(x)$:

$$\boxed{u_1(x,y) = \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x)\psi(y)w_i(y)}$$

New ϵ^0 equation:

$$\begin{cases} b \cdot \nabla_y u_2 - \operatorname{div_y}(D\nabla_y u_2) + r u_2 - r^* u_2 = b^* \cdot \nabla_x u_1 - b \cdot \nabla_x u_1 \\ \qquad + \operatorname{div_y}(D\nabla_x u_1) + \operatorname{div_x}(D(\nabla_y u_1 + \nabla_x u_0)) - \frac{\partial u_0}{\partial t} + f \text{ in } Y^* \\ D(y)\nabla_y u_2 \cdot n + k u_2 = -D(y)\nabla_x u_1 \cdot n \text{ on } \partial\mathcal{O} \\ y \to u_2(x,y) \ Y\text{-periodic} \end{cases}$$

Fredholm condition for the existence of u_2:

$$\int_{Y^*} \Big(b^* \cdot \nabla_x u_1 - b \cdot \nabla_x u_1 + \operatorname{div_y}\big(D\nabla_x u_1\big) + \operatorname{div_x}\big(D(\nabla_y u_1 + \nabla_x u_0)\big) \\ - \frac{\partial u_0}{\partial t} + f \Big) \psi^* dy - \int_{\partial\mathcal{O}} \psi^* D\nabla_x u_1 \cdot n \, ds = 0$$

We replace u_1 by its value in terms of $\nabla_x u$ and we find the **homogenized problem**.

Theorem.

$$u_\epsilon(t,x) \approx e^{-r^*\epsilon^{-2}t}\,\psi\left(\frac{x}{\epsilon}\right) u\left(t, x - \frac{b^* t}{\epsilon}\right)$$

Homogenized problem:

$$\begin{cases} \frac{\partial u}{\partial t} - \operatorname{div}(D^*\nabla u) = 0 & \text{in } \mathbb{R}^N \\ u(0) = u_{init} & \text{in } \mathbb{R}^N \end{cases}$$

with a new formula for D^*, and the effective velocity

$$b^* = \int_{Y^*} \left[\psi\psi^* b + \psi D\nabla\psi^* - \psi^* D\nabla\psi\right](y)\,dy$$

Equivalent statement of the same theorem

$$\boxed{u_\epsilon(t,x) \approx \psi\left(\frac{x}{\epsilon}\right) \tilde{u}(t,x)}$$

with $\tilde{u}(t,x) = e^{-r^*\epsilon^{-2}t} u\left(t, x - \dfrac{b^* t}{\epsilon}\right)$

Modified homogenized problem:

$$\begin{cases} \dfrac{\partial \tilde{u}}{\partial t} + \epsilon^{-1} b^* \cdot \nabla \tilde{u} - \operatorname{div}(D^* \nabla \tilde{u}) + \epsilon^{-2} r^* \tilde{u} = 0 & \text{in } \mathbb{R}^N \\ \tilde{u}(0) = u_{init} & \text{in } \mathbb{R}^N \end{cases}$$

Remark. Cf. H. Brenner - P. Adler (1982), R. Mauri (1991), P. Donato - A. Piatnitski (2006), G. Allaire - A.-L. Raphael (2007).

-V- GENERALIZATIONS AND CONCLUSION

Known generalizations:

- ✩ Nonlinear effects: Langmuir isotherm for adsorption
- ✩ Multiphase or multicomponents transport
- ✩ Electrokinetics

Open problems:

- ✩ Nonlinear effects with spatially varying drift
- ✩ Multicomponent transport with non-linear reactions (law of mass action)
- ✩ Stochastic setting rather than periodic (still with separation of scales)

G. Allaire, A.-L. Raphael, *Homogenization of a convection-diffusion model with reaction in a porous medium,* C. R. Acad. Sci. Paris, Série I, 344, 523-528 (2007).

G. Allaire, A. Mikelic, A. Piatnitski, *Homogenization approach to the dispersion theory for reactive transport through porous media,* SIAM J. Math. Anal. 42, 125-144 (2010).

G. Allaire, R. Brizzi, A. Mikelic, A. Piatnitski, *Two-scale expansion with drift approach to the Taylor dispersion for reactive transport through porous media*, Chemical Engineering Science, 65, pp.2292-2300 (2010).

G. Allaire, H. Hutridurga, *Homogenization of reactive flows in porous media and competition between bulk and surface diffusion,* IMA J. Appl. Math., 77, 788-815 (2012).

G. Allaire, A. Mikelic, A. Piatnitski, *Homogenization of The Linearized Ionic Transport Equations in Rigid Periodic Porous Media,* J. of Math. Physics, 51, 123103 (2010).

G. Allaire, R. Brizzi, J.-F. Dufrêche, A. Mikelic, A. Piatnitski, *Role of non-ideality for the ion transport in porous media: derivation of the macroscopic equations using upscaling,* Physica D, 282, pp.39-60 (2014).

Cell problem for computing D^* and $u_1(x,y) = \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x)\psi(y)w_i(y)$:

$$\begin{cases} \tilde{b}\cdot(e_i+\nabla_y w_i) - \operatorname{div}_y\left(\tilde{D}\,(e_i+\nabla_y w_i)\right) = b^*\cdot e_i & \text{in } Y^* \\ \tilde{D}\,(e_i+\nabla_y w_i)\cdot n = 0 & \text{on } \partial\mathcal{O} \\ y \to w_i(y) & Y\text{-periodic} \end{cases}$$

with $\tilde{D} = D\psi\psi^*$ and $\tilde{b} = [\psi\psi^* b + \psi D\nabla\psi^* - \psi^* D\nabla\psi)]$ which satisfies

$$\operatorname{div}_y \tilde{b} = 0 \text{ in } Y^*, \quad \tilde{b}\cdot n = 0 \text{ on } \partial\mathcal{O}, \quad b^* = \frac{1}{|Y^*|}\int_{Y^*} \tilde{b}(y)\,dy.$$

Therefore the Fredholm condition is satisfied for w_i !

Homogenized diffusion tensor:

$$D^*_{ij} = \frac{1}{|Y^*|}\int_{Y^*} \tilde{D}\,(e_i+\nabla_y w_i)\cdot(e_j+\nabla_y w_j)\,dy.$$