Locally-periodic media with areas of low and high diffusivity. How can we average them?

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Outline of the Talk

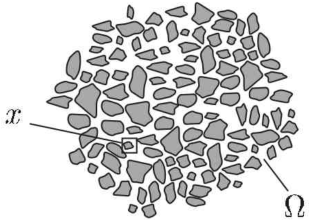
Length scales in heterogeneous media

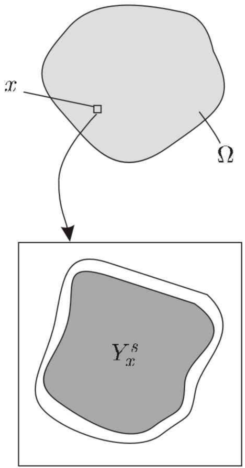
Bridging length scales in heterogeneous media

- Averaging techniques (periodic homogenization, ...)
- PDE models with distributed microstructure

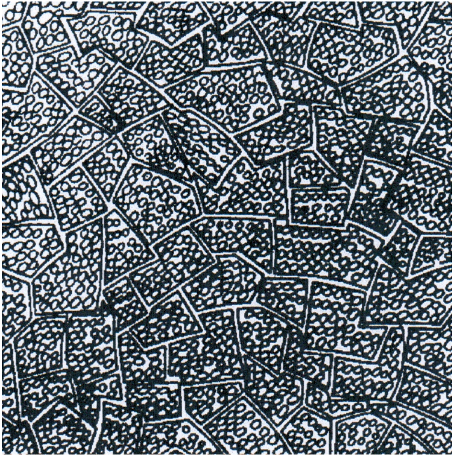
1. two-scale models – A. Friedman, A. Tzavaras, P. Knabner
2. distributed-microstructure models – R. E. Showalter and co-workers (Walkington, Cook, Clark, Visarraga, ...) + M. Böhm, S. Meier
3. dual- or double-porosity models – U. Hornung, W. Jäger, T. Arbogast, ...
4. two-scale models with freely evolving micro-interfaces – C. Eck., H. Emmerich, P. Knabner, A. Muntean (2 scale phase-field models), *S. Meier, A. Muntean (2 scale fast-reaction asymptotics)*

Typical two-scale geometry



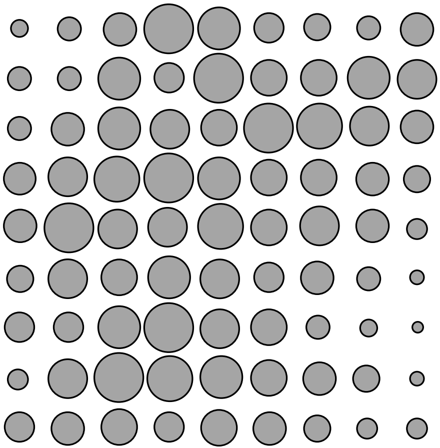


Double-porosity structure of materials



Barenblatt, Zheltov, Kochina, *PMM*, 24(1960), 5, pp. 852–864

Locally-periodic distributions of perforations



T. van Noorden, A. Muntean , *European J. Appl. Math.* (2011)

Generic micro-model

$$\begin{cases} u_t^\epsilon = \nabla\cdot(D_h\nabla u^\epsilon - q^\epsilon u^\epsilon) \\ q^\epsilon = -\kappa\nabla p^\epsilon \\ \nabla\cdot q^\epsilon = 0 \end{cases} \quad \text{in } \Omega_h^\epsilon,$$

$$\begin{cases} v_t^\epsilon = \epsilon^2\nabla\cdot(D_l\nabla v^\epsilon) \end{cases} \quad \text{in } \Omega_l^\epsilon,$$

$$\begin{cases} \nu^\epsilon\cdot(D_h\nabla u^\epsilon) = \epsilon^2\nu^\epsilon\cdot(D_l\nabla v^\epsilon) \\ u^\epsilon = v^\epsilon \\ q^\epsilon = 0 \end{cases} \quad \text{on } \Gamma^\epsilon,$$

$$\begin{cases} u^\epsilon(x,t) = u_b(x,t) \\ q^\epsilon(x,t) = q_b(x,t) \end{cases} \quad \text{on } \Gamma,$$

$$\begin{cases} u^\epsilon(x,0) = u_I^\epsilon(x) & \text{in } \Omega_h^\epsilon, \\ v^\epsilon(x,0) = v_I^\epsilon(x) & \text{in } \Omega_l^\epsilon, \end{cases}$$

Basic ideas of the formal asymptotics

$$\begin{aligned}
u^\epsilon(x,t) &= u_0(x,x/\epsilon,t) + \epsilon u_1(x,x/\epsilon,t) + \epsilon^2 u_2(x,x/\epsilon,t) + \ldots \\
v^\epsilon(x,t) &= v_0(x,x/\epsilon,t) + \epsilon v_1(x,x/\epsilon,t) + \epsilon^2 v_2(x,x/\epsilon,t) + \ldots \\
q^\epsilon(x,t) &= q_0(x,x/\epsilon,t) + \epsilon q_1(x,x/\epsilon,t) + \epsilon^2 q_2(x,x/\epsilon,t) + \ldots \\
p^\epsilon(x,t) &= p_0(x,x/\epsilon,t) + \epsilon p_1(x,x/\epsilon,t) + \epsilon^2 p_2(x,x/\epsilon,t) + \ldots
\end{aligned}$$

$$\begin{aligned}
|\nabla S^\epsilon| &= \frac{1}{\epsilon}|\nabla_y S| + O(\epsilon^0) \\
\nu^\epsilon &= \nu_0 + \epsilon\nu_1 + O(\epsilon^2), \\
\Omega_\ell^\epsilon &= \{S(x,x/\epsilon) < 0 : x \in \Omega\}, \\
\Omega_h^\epsilon &= \{S(x,x/\epsilon) > 0 : x \in \Omega\}
\end{aligned}$$

Micro-macro model

$$\begin{cases} \partial_t v_0(x,y,t) = D_l \Delta_y v_0(x,y,t) & |y| < r(x),\ x \in \Omega, \\ \partial_t \left(\theta(x) u_0 + \int_{|y|<r(x)} v_0 \, dy \right) = & \\ \qquad \operatorname{div}_x (D_h \mathcal{A}(x) \nabla_x u_0 - \bar{q} u_0) & \text{for } x \in \Omega, \\ \bar{q} = -\mathcal{K}(x) \nabla_x p_0 & \text{for } x \in \Omega, \\ \nabla_x \cdot \bar{q} = 0 & \text{for } x \in \Omega, \end{cases}$$

$$\begin{cases} v_0(x,y,t) = u_0(x,t) & \text{for } |y| = r(x), \\ u_0(x,t) = u_b(x,t) & \text{for } x \in \Gamma, \\ \bar{q}(x,t) = q_b(x,t) & \text{for } x \in \Gamma, \end{cases}$$

$$\begin{cases} u_0(x,0) = u_I(x) & \text{for } x \in \Omega, \\ v_0(x,y,0) = v_I(x,y) & \text{for } |y| < r(x),\ x \in \Omega. \end{cases}$$

The porosity $\theta(x)$ of the medium is given by

$$\theta(x) := 1 - \pi r^2(x),$$

while the effective diffusivity $\mathcal{D}(x) := (a_{ij}(x))_{i,j}$ and the effective permeability $\mathcal{K}(x) := (k_{ij}(x))_{i,j}$ are defined by

$$a_{ij}(x) := D_h \int_{\{y \in U \mid |y| > r(x)\}} \delta_{ij} + \partial_{y_i} U_j(x, y, t)\, dy,$$

and

$$k_{ij}(x) := \int_{\{y \in U \mid |y| > r(x)\}} V_{ji}(x, y, t)\, dy.$$

x-dependent cell problems

$$
\begin{cases}
\Delta_y U_j(x,y) = 0 & \text{for all } x \in \Omega,\ y \in Y,\ |y| > r(x), \\
\nu_0 \cdot \nabla_y U_j(x,y) = -\nu_0 \cdot e_j & \text{for all } x \in \Omega,\ |y| = r(x), \\
U_j(x,y)\ y\text{-periodic},
\end{cases}
$$

and

$$
\begin{cases}
V_j(x,y) = \nabla_y \pi_j(x,y) + e_j & \text{for all } x \in \Omega,\ y \in Y,\ |y| > r(x), \\
\nabla_y \cdot V_j(x,y) = 0 & \text{for all } x \in \Omega,\ y \in Y,\ |y| > r(x), \\
V_j = 0 & \text{for all } x \in \Omega,\ |y| = r(x), \\
V_j(x,y) \text{ and } \pi_j(x,y)\ y\text{-periodic},
\end{cases}
$$

for $j = 1, 2$.

Micro-macro model

$$
\begin{cases}
\partial_t v_0(x,y,t) = D_l \Delta_y v_0(x,y,t) & |y| < r(x),\ x \in \Omega,\\
\partial_t \left(\theta(x) u_0 + \int_{|y|<r(x)} v_0\, dy \right) = & \\
\qquad \mathrm{div}_x (D_h \mathcal{A}(x) \nabla_x u_0 - \bar{q} u_0) & \text{for } x \in \Omega,\\
\bar{q} = -\mathcal{K}(x) \nabla_x p_0 & \text{for } x \in \Omega,\\
\nabla_x \cdot \bar{q} = 0 & \text{for } x \in \Omega,
\end{cases}
$$

$$
\begin{cases}
v_0(x,y,t) = u_0(x,t) & \text{for } |y| = r(x),\\
u_0(x,t) = u_b(x,t) & \text{for } x \in \Gamma,\\
\bar{q}(x,t) = q_b(x,t) & \text{for } x \in \Gamma,
\end{cases}
$$

$$
\begin{cases}
u_0(x,0) = u_I(x) & \text{for } x \in \Omega,\\
v_0(x,y,0) = v_I(x,y) & \text{for } |y| < r(x),\ x \in \Omega.
\end{cases}
$$

Reduced micro – macro model

$$\begin{cases} \theta(x)\partial_t u - \nabla_x \cdot (D(x)\nabla_x u - qu) = -\int_{\partial B(x)} \nu_y \cdot (D_l \nabla_y v)\, d\sigma & \text{in } \Omega, \\ \partial_t v - D_l \Delta_y v = 0 & \text{in } B(x), \\ u(x,t) = v(x,y,t) & \text{at } (x,y) \in \Omega \times \partial B(x) \\ u(x,t) = u_b(x,t) & \text{at } x \in \partial\Omega, \\ u(x,0) = u_I(x) & \text{in } \overline{\Omega}, \\ v(x,y,0) = v_I(x,y) & \text{at } (x,y) \in \overline{\Omega} \times \overline{B(x)} \end{cases}$$

Assumptions on data and parameters

(A1) $S_0 : \Omega \times U \to \mathbb{R}$, which defines $B(x)$ and also the 1-dimensional boundary $\Omega \times \partial B(x)$ of $\Omega \times B(x)$ as

$$(x, y) \in \Omega \times \partial B(x) \text{ if and only if } S_0(x, y) = 0,$$

is an element of $C^2(\overline{\Omega \times U})$. Additionally, the Clarke gradient $\partial_y S_0(x, y)$ is regular for all choices of $(x, y) \in \overline{\Omega \times U}$.

(A2)

$$\begin{cases} \theta,\ D \in L^\infty_+(\Omega), \\ q \in L^\infty(\Omega; \mathbb{R}^d) \text{ with } \nabla \cdot q = 0, \\ u_b \in L^\infty_+(\Omega \times S) \cap H^1(S; L^2(\Omega)), \\ \partial_t u_b \leq 0 \text{ a.e. } (x, t) \in \Omega \times S, \\ u_I \in L^\infty_+(\overline{\Omega}) \cap H_1, \\ v_I(x, \cdot) \in L^\infty_+(B(x)) \cap H_2 \text{ for a.e. } x \in \overline{\Omega}. \end{cases}$$

Functional setting

$$
\begin{aligned}
V_1 &:= H_0^1(\Omega),\\
V_2 &:= L^2(\Omega; H^2(B(x))),\\
H_1 &:= L^2_\theta(\Omega),\\
H_2 &:= L^2(\Omega; L^2(B(x))).
\end{aligned}
$$

If $0 < |B(x)|, |\partial B(x)| < \infty$, then the direct Hilbert integrals

$$
\begin{aligned}
L^2(\Omega; H^1(B(x))) &:= \{u \in L^2(\Omega; L^2(B(x))) : \nabla_y u \in L^2(\Omega; L^2(B(x)))\}\\
L^2(\Omega; H^1(\partial B(x))) &:= \{u : \Omega \times \partial B(x) \to \mathbb{R} \text{ meas. s. t. } \int_\Omega ||u(x)||^2_{L^2(\partial B(x))} < \infty\}
\end{aligned}
$$

are separable Hilbert spaces with *distributed trace*:

$$\gamma : L^2(\Omega; H^1(B(x))) \to L^2(\Omega, L^2(\partial B(x)))$$

given by

$$\gamma u(x,s) := (\gamma_x U(x))(s), \; x \in \Omega, s \in \partial B(x), u \in L^2(\Omega; H^1(B(x)))$$

Definition (Weak formulation)

Assume (A1) and (A2). The pair (u, v), with $u = U + u_b$ and where $(U, v) \in \mathbb{V}$, is a weak solution if the following identities hold

$$\int_\Omega \theta \partial_t (U + u_b)\phi \, dx + \int_\Omega (D\nabla_x (U + u_b) - q(U + u_b)) \cdot \nabla_x \phi \, dx = - \int_\Omega \int_{\partial B(x)} \nu_y \cdot (D_l \nabla_y v)\phi \, d$$

$$\int_\Omega \int_{B(x)} \partial_t v \psi \, dydx + \int_\Omega \int_{B(x)} D_l \nabla_y \cdot \nabla_y \psi \, dydx = \int_\Omega \int_{\partial B(x)} \nu_y \cdot (D_l \nabla_y v)\phi \, d\sigma dx,$$

for all $(\phi, \psi) \in \mathbb{V}$ and $t \in S$.

Basic estimates

Lemma

Let (A1) and (A2) be satisfied. Then any weak solution (u, v) *of problem* (P) *has the following properties:*

(i) $u \geq 0$ *for a.e.* $x \in \Omega$ *and for all* $t \in S$*;*

(ii) $v \geq 0$ *for a.e.* $(x, y) \in \Omega \times B(x)$ *and for all* $t \in S$*;*

(iii) $u \leq M_1$ *for a.e.* $x \in \Omega$ *and for all* $t \in S$*;*

(iv) $v \leq M_2$ *for a.e.* $(x, y) \in \Omega \times B(x)$ *and for all* $t \in S$*;*

(v) *The following energy inequality holds:*

$$\begin{aligned} \|u\|^2_{L^2(S;V_1)\cap L^\infty(S;H_1)} &+ \|v\|^2_{L^2(S;L^2(\Omega,V_2))\cap L^\infty(S;H_2)} \\ &+ \|\nabla_x u\|^2_{L^2(S;H_1)} + \|\nabla_y v\|^2_{L^2(S\times\Omega\times B(x))} \leq c_1. \end{aligned}$$

N.B. Assume (A1), (A2). Then uniqueness of weak solutions holds.

Global existence

Theorem

There exists at least a weak solution of the micro-macro model.

Proof. (Sketch)
Schauder fixed-point argument in $L^2(S; L^2(\Omega))$ framework

$$
\begin{aligned}
X_1 &:= L^2(S; L^2(\Omega)), \\
X_2 &:= L^2(S; H_0^1(\Omega)) \cap H^1(S; L^2(\Omega)), \\
X_3 &:= L^2(S; V_2) \cap H^1(S; L^2(\Omega; L^2(B(x)))).
\end{aligned}
$$

$T : X_1 \to X_1$ with $T := T_3 \circ T_2 \circ T_1$.

T_1 maps a $f \in X_1$ to the solution $w \in X_2$ of

$$\int_\Omega \theta \partial_t (U + u_b) \phi \, dx + \int_\Omega (D \nabla_x (U + u_b) - q(U + u_b)) \cdot \nabla_x \phi \, dx = - \int_\Omega f \phi \, dx,$$

for all $\phi \in H_0^1(\Omega)$.
T_2 maps a $w \in X_2$ to a solution $v \in X_3$ of

$$\int_\Omega \int_{B(x)} \partial_t (V + w) \psi \, dydx + \int_\Omega \int_{B(x)} D_l \nabla_y (V + w) \cdot \nabla_y \psi \, dydx = \int_\Omega \int_{\partial B(x)} \nu_y \cdot (D_l \nabla_y (V + w)) \psi \, d\sigma dx,$$

for all $\psi \in V_2$ and $t \in S$.
T_3 maps a $v \in X_3$ to $f \in X_1$ by

$$f = \int_{\partial B(x)} \nu_y \cdot \nabla_y v \, d\sigma.$$

Lemma

T is well defined.

Compactness step

Lemma

The operator T is compact.

Step 1. Use $\Psi : \Omega \times B(0) \to \Omega \times B(x)$.

We call Ψ a *regular C^2-motion* if $\Psi \in C^2(\Omega \times B(0))$ with the property that for each $x \in \Omega$

$$\Psi(x, \cdot) : B(0) \to B(x) := \Psi(x, B(0))$$

is bijective, and if there exist constants $c, C > 0$ such that

$$c \leq \det \nabla_y \Psi(x, y) \leq C,$$

for all $(x, y) \in \Omega \times B(0)$. The existence of such a mapping is ensured by the fact that $S_0 \in C^2(\overline{\Omega \times U})$, by (A1). If Ψ is a regular C^2-motion, then

$$F := \nabla_y \Psi \text{ and } J := \det F$$

are continuous functions of x and y.

$$\nabla_y v = F^{-T} \nabla_{\hat{y}} \hat{v}, \partial_t v = \partial_t \hat{v},$$

$$\int_{\partial B(x)} \nu_y \cdot j \, d\sigma = \int_{\Gamma_0} J F^{-T} \hat{\nu}_{\hat{y}} \cdot \hat{j} \, d\sigma.$$

The transformed equation can be now written as:
Let $w \in X_2$ be given.
Find $\hat{V} \in L^2(S; L^2(\Omega; H_0^1(B(0)))) \cap H^1(S; L^2(\Omega; L^2(B(0))))$ such that

$$\int_\Omega \int_{B(0)} \partial_t(\hat{V} + w)\psi J \, dydx + \int_\Omega \int_{B(0)} JF_{-1} D_l F^{-T} \nabla_y(\hat{V} + w) \cdot \nabla_y \psi \, dydx = \int_\Omega \int_{\Gamma_0} \hat{\nu}_y \cdot (JF^{-1} D_l F^{-T} \nabla_y(\hat{V} + w))\psi \, d\sigma dx,$$

for all $\psi \in L^2(\Omega; H_0^1(B(0)))$ and $t \in S$.

Denote by Γ_0 the boundary of $B(0)$.

Step 2. Interior and boundary regularity

Assume (A1) and (A2). Then Γ_0 is C^2 and

$$\hat{V} \in L^2(S; L^2(\Omega; H^2(B(0)) \cap H_0^1(B(0)))).$$

Step 3. Additional two-scale regularity

Assume (A1) and (A2). Then

$$\hat{V} \in L^2(S; H^1(\Omega; H^2(B(0)) \cap H_0^1(B(0)))).$$

Step 4. Apply Lions-Aubin Lemma

Getting correctors: Basic idea

- (u_ϵ, v_ϵ) solution vector for the micro problem
- (u_0, v_0) solution vector for the macro problem
- $u_0^\epsilon, v_0^\epsilon, u_1^\epsilon$ macroscopic reconstructions

$$
\begin{aligned}
u_0^\epsilon(x,t) &:= u_0(x,t)\\
v_0^\epsilon(x,t) &:= v_0(x,x/\epsilon,t)\\
u_1^\epsilon(x,t) &:= u_0^\epsilon(x,t) + \epsilon U(t,x,x/\epsilon)\nabla u_0^\epsilon(x,t)
\end{aligned}
$$

Justification of the formal asymptotics

Theorem

Assume (A1) and (A2). Then the following convergence rate holds

$$||u_\epsilon - u_0^\epsilon||_{L^\infty(S,L^2(\Omega_\epsilon))} + ||v_\epsilon - v_0^\epsilon||_{L^\infty(S,L^2(\Omega-\Omega_\epsilon))} +$$
$$||u_\epsilon - u_1^\epsilon||_{L^\infty(S,H^1(\Omega_\epsilon))} + \epsilon||v_\epsilon - v_0^\epsilon||_{L^\infty(S,H^1(\Omega-\Omega_\epsilon))} \leq c\sqrt{\epsilon}$$

Outline of the proof for the corrector estimate

Step 1.
Write weak formulations for both *micro* and *macro* pbs. (the later in terms of macro reconstructions)
Step 2.
Subtract the 2 weak formulations and choose suitable test functions

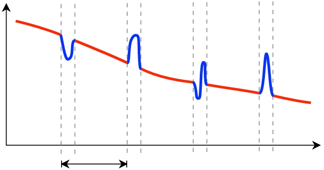
$$\varphi := u_\epsilon - u_0^\epsilon(x,t) + \epsilon U(t,x,x/\epsilon)\nabla u_0^\epsilon(x,t)$$
$$\psi := v_\epsilon - v_0^\epsilon$$

Step 3. A technical lemma:
Prove that

$$|\epsilon \int_{S_\epsilon} \epsilon D_\ell \nabla v_\epsilon \cdot \nu_\epsilon \psi d\sigma - \frac{1}{|Y - B(x)|} \int_{\partial B(x)} \nu_y \cdot D_\ell \nabla_y v_0^\epsilon \psi d\sigma| \leq c\epsilon ||\psi||_{H^1(\Omega_\epsilon)}.$$

Step 4. Bookkeeping of ϵ

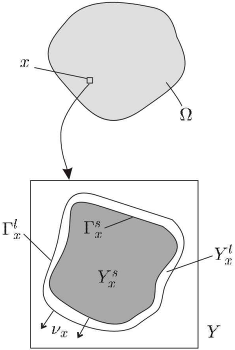
Open issues



0. Large-time behavior
1. Analysis without fixing the *x*-domains
2. Computability in *x*-domains
3. *A posteriori* estimates (Is the *lazy-man solution* applicable?)
4. Strong scale separation vs. weak scale separation

Open issues

5. Rigorous homogenization asymptotics for *t*-dependent microstructures
6. Free micro interfaces? (and again: analysis, computability, scale separation issues, boundary layers effects)



Related work

- T. van Noorden, A. Muntean: *Homogenization of a locally-periodic medium with areas of low and high diffusivity*. European J. Appl. Math. (2011).
- A. Muntean, T. van Noorden: *Corrector estimates for the homogenization of a locally-periodic medium with areas of low and high diffusivity* CASA Report, No. 11-29, Technische Universiteit Eindhoven (2011).
- A. Muntean, M. Neuss-Radu: *A multiscale Galerkin approach for a class of nonlinear coupled reaction-diffusion systems in complex media*. J. Math. Appl. Anal. (2010).
- T. Fatima, N. Arab, E. Zemskov, A. Muntean: *Homogenization of a reaction-diffusion system modeling sulfate corrosion in locally-periodic perforated domains*. J. Engng. Math. (2010).
- V. Chalupecky, T. Fatima, A. Muntean: *Multiscale sulfate attack on sewer pipes: Numerical study of a fast micro-macro mass transfer limit*. Journal of Math-for-Industry, (2010).