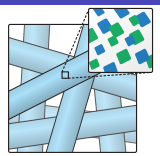

Heterogeneous media: Case studies in non-periodic averaging and perspectives in designing packaging materials

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Outline of the Talk

Microstructure models of heterogeneous media
- Distributed microstructures
- “Structured” transport
- Generic microscopic model
- Derivation via formal homogenization of a *micro-macro* model

Analysis of the micro-macro model
- Weak formulation. Basic estimates
- Global existence and uniqueness of weak solutions

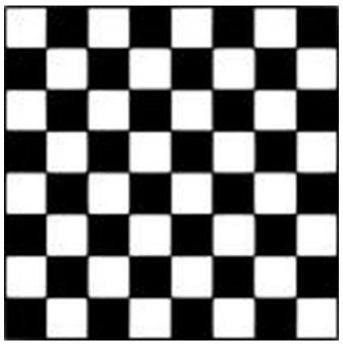
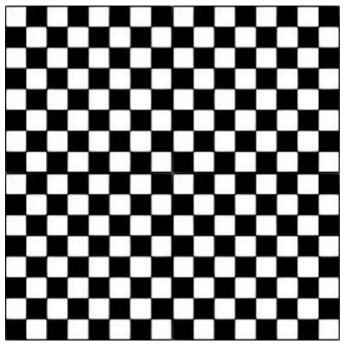
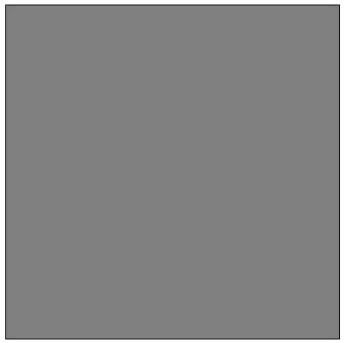
Numerical illustration

Justification of the formal homogenization
- Outline of the proof for the corrector estimate

Open issues

Heterogeneous media: Diffusion in a chessboard domain

Heterogeneous media and their homogeneous representation

Is an equivalent formulation posed in an homogeneous domain possible?

Asymptotic homogenization for chessboard-type microstructures

$$\partial_t u_\epsilon - \mathrm{div}(A_\epsilon(x)\nabla u_\epsilon) = f_\epsilon \text{ in } \Omega_\epsilon$$
$$u_\epsilon = g_\epsilon \text{ at black/white inner boundaries}$$
$$-n \cdot A_\epsilon \nabla u_\epsilon = 0 \text{ at the outer boundary + i.c.}$$

Here $A_\epsilon(x) = A(x, \frac{x}{\epsilon})$.
Idea 1: Use

$$u_\epsilon(t,x) = u_0(t,x) + \epsilon u_1(t,x,\frac{x}{\epsilon}) + \epsilon^2 u_2(t,x,\frac{x}{\epsilon}) + \mathcal{O}(\epsilon^3)$$

to get PDEs for u_0.
Idea 2: Along the same line: show the corrector estimate

$$||u_\epsilon - u_0|| \leq c(u_1, \dots)\epsilon^\alpha, \ \alpha > 0.$$

Macroscopic equation for chessboard diffusion. Range of validity?

$$\partial_t(\phi u_0) - \mathrm{div}(\phi D(x, w(x))\nabla u_0) = \phi f_0 \text{ in } \Omega$$
$$-n \cdot \phi D(x, w(x))\nabla u_0 = 0 \text{ at the outer boundary}$$

- ϕ is the chessboard porosity, i.e. $\phi = \frac{1}{16}$
- $D(\cdot, w(\cdot))$ is an effective transport coefficient
- w is a parameter depending on the chessboard's microstructure (cell functions)

Rate of convergence (correctors):

- $||u_\epsilon - u_0||_{L^2} \leq c_1 \epsilon$
- $||\partial_t u_\epsilon - \partial_t u_0||_{L^2} \leq c_2 \epsilon$
- $||\nabla u_\epsilon - \nabla u_0 - \text{oscillations}||_{L^2} \leq c_3 \sqrt{\epsilon}$

Averaging techniques in action

Towards understanding mixed transport fluxes:

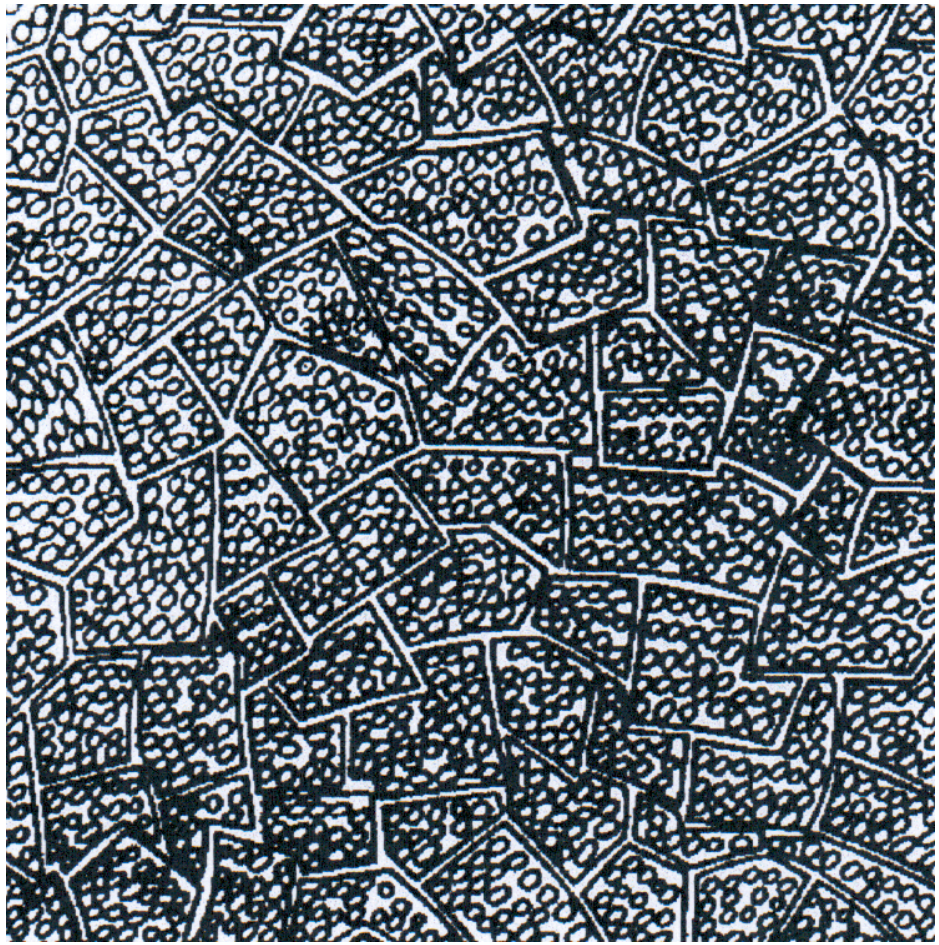
- *Estimating speeds of macroscopic corrosion fronts in concrete* [large-time behavior for free boundary problems]
- *Ionic transport in porous media* [homogenization of the Stokes-Nernst-Planck-Poisson system]
- *Multiscale combustion* [smoldering thin sheets, fast-reaction limits]
- *Cross-diffusion effects* [averaging the Becker-Döring system for hot colloids]
- *Thermo-diffusion effects* [estimating permeability tensors for mass and heat transport through porous membranes]

Bridging length scales in heterogeneous media

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

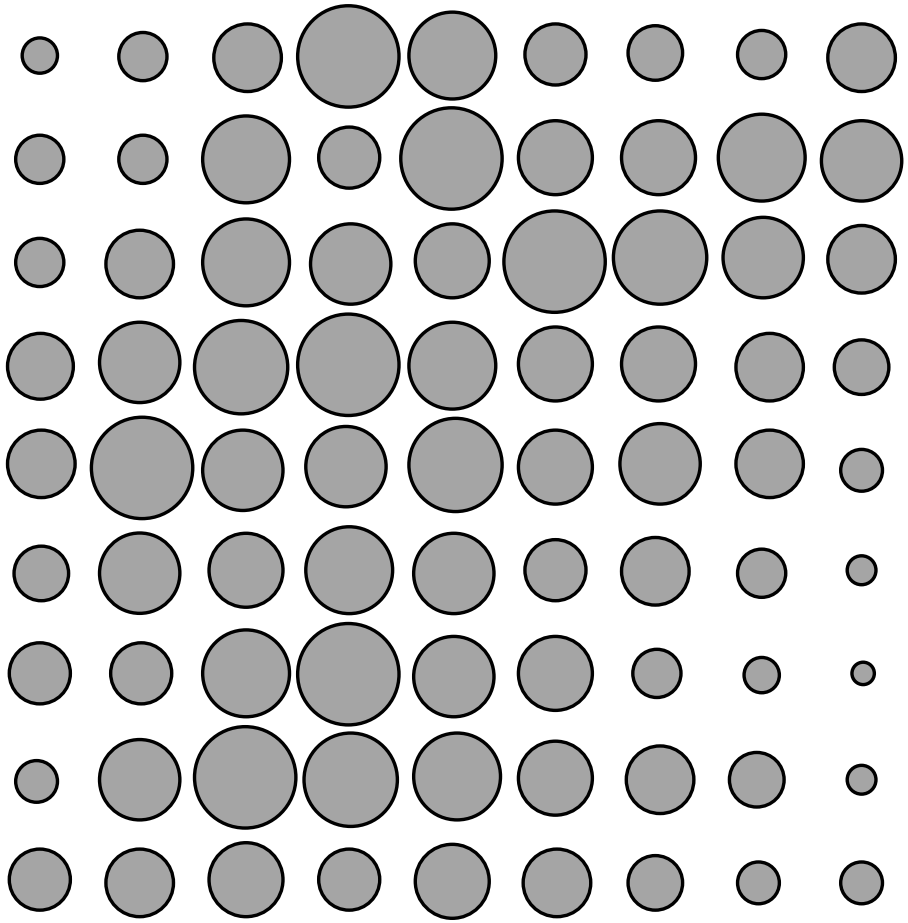
1. two-scale models – A. Friedman, A. Tzavaras, P. Knabner
2. distributed-microstructure models – R. E. Showalter and co-workers (Walkington, Cook, Clark, Visarraga, ...) + M. Böhm, S. Meier, D. Treutler, J. Esher
3. dual- or double-porosity models – U. Hornung, W. Jäger, T. Arbogast, ...
4. two-scale 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)*
5. coupling multi-physics/discrete-to-continuum etc.

Double-porosity structure of materials



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

Locally-periodic distributions of perforations



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) two-scale homogenisation asymptotics

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

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

Micro-macro model

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

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

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

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

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

and

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

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

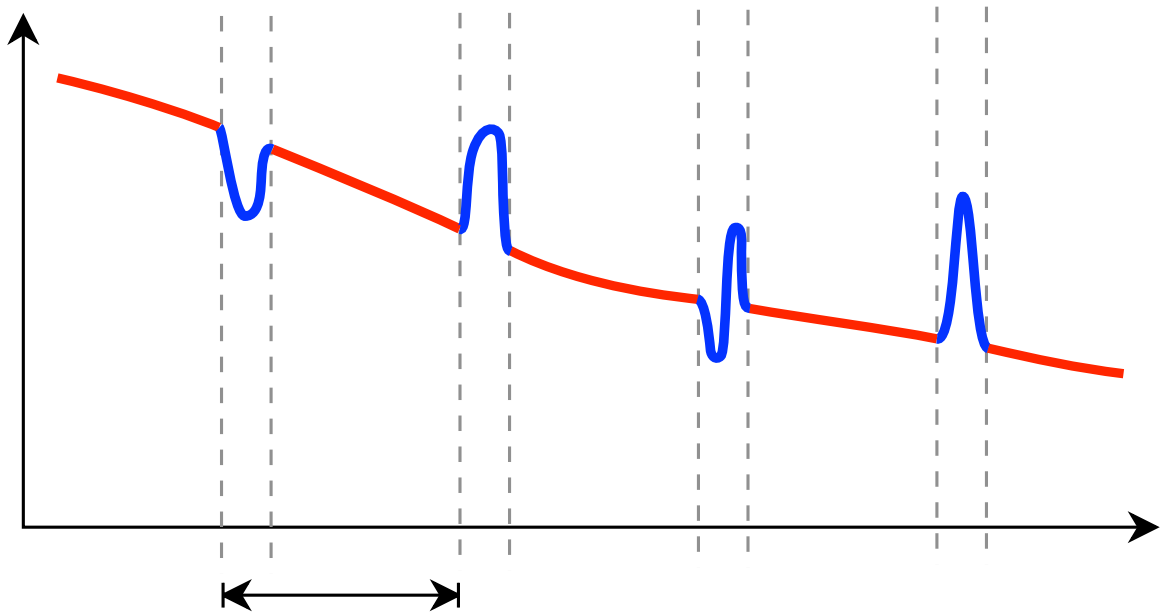
$$\begin{cases} V_j(x,y) = \nabla_y \pi_j(x,y) + e_j & \text{for all } x \in \Omega,\ y \in Y,\ |y| > r(x), \\ \nabla_y \cdot V_j(x,y) = 0 & \text{for all } x \in \Omega,\ y \in Y,\ |y| > r(x), \\ V_j = 0 & \text{for all } x \in \Omega,\ |y| = r(x), \\ V_j(x,y) \text{ and } \pi_j(x,y)\ y\text{-periodic},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

for $j = 1, 2$.

Reduced micro – macro model

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

Memory effects?



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)

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

Functional setting

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

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

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

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

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

$T : X_1 \to X_1$ 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

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

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 (in y)

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

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

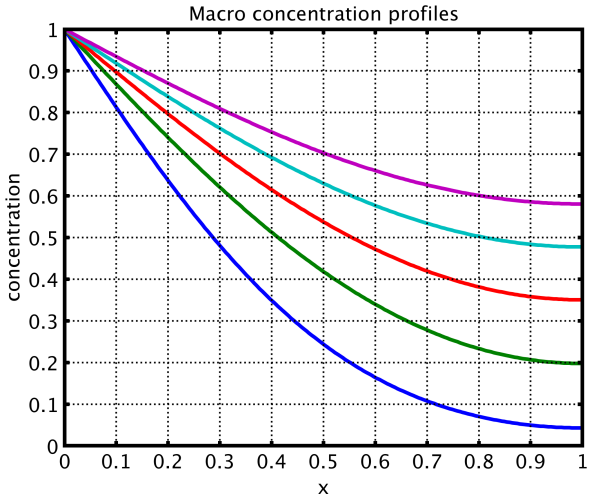
Step 3. Additional two-scale regularity (in y)

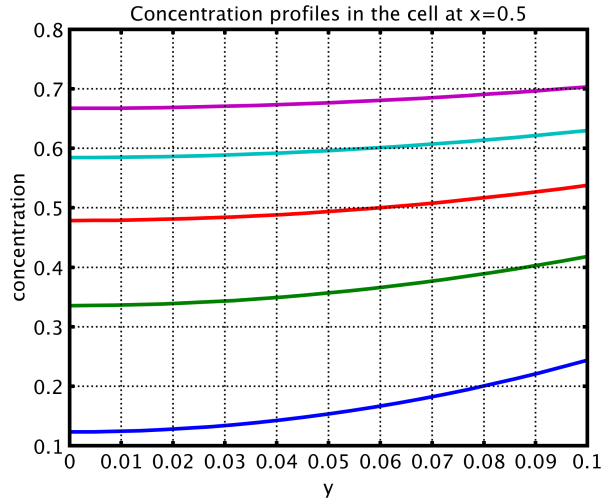
Assume (A1) and (A2). Then

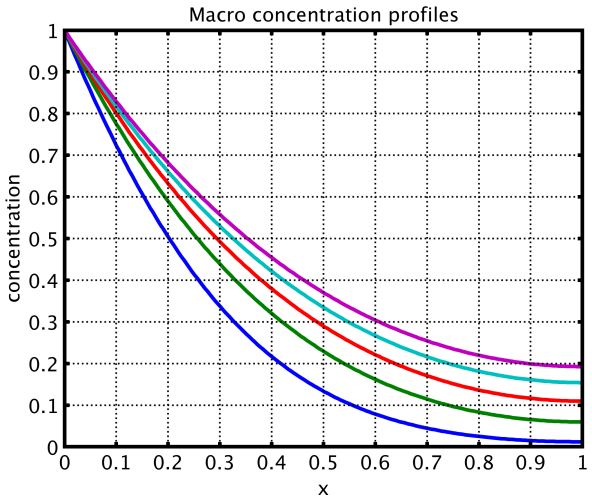
$$\hat{V} \in L^2(S; H^1(\Omega; H^2(B(0)) \cap H_0^1(B(0)))).$$

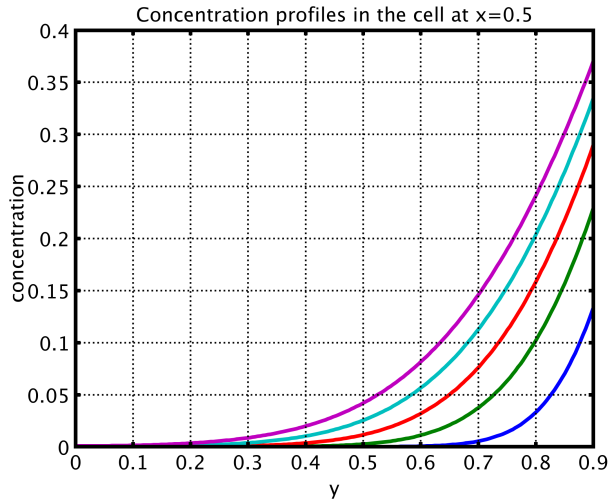
Step 4. Apply Lions-Aubin Lemma

Concentration profiles of the two-scale model









Solution profiles of the two-scale model at different times: Up: $R = 0.1$; Bottom: $R = 0.9$.

Numerical approximation of RD systems on two scales

- Convergent two-scale Galerkin approximations

  A. Muntean, M. Neuss-Radu: *A multiscale Galerkin approach for a class of nonlinear coupled reaction-diffusion systems in complex media*. JMAA 371 (2010), (2), 705-718.

- Convergence rates (*a priori*)

  A. Muntean, O. Lakkis (2010). *Rate of convergence for a Galerkin scheme approximating a two-scale reaction-diffusion system with nonlinear transmission condition*. RIMS Kokyuroku (Kyoto), 1693, pp. 85-98.

- Numerical example in $1\mathrm{D} \times 1\mathrm{D}$

Corrector estimates – How goed is the averaging method?

- (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

$$\begin{aligned} \varphi &:= u_\epsilon - u_0^\epsilon(x,t) + \epsilon U(t,x,x/\epsilon)\nabla u_0^\epsilon(x,t) \\ \psi &:= v_\epsilon - v_0^\epsilon \end{aligned}$$

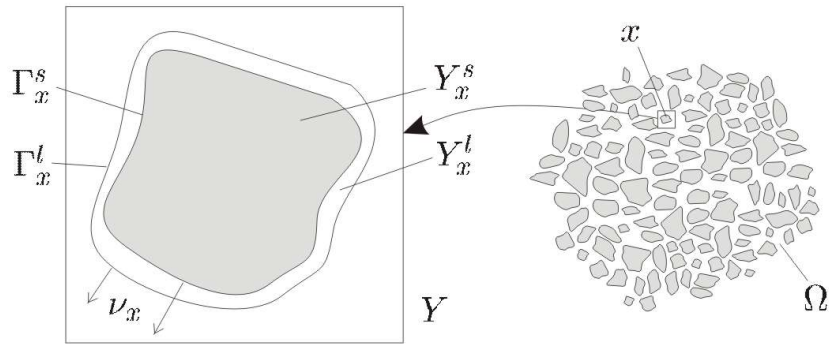
Step 3. A technical lemma:
Prove that

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

Step 4. Bookkeeping of ϵ

Open issues

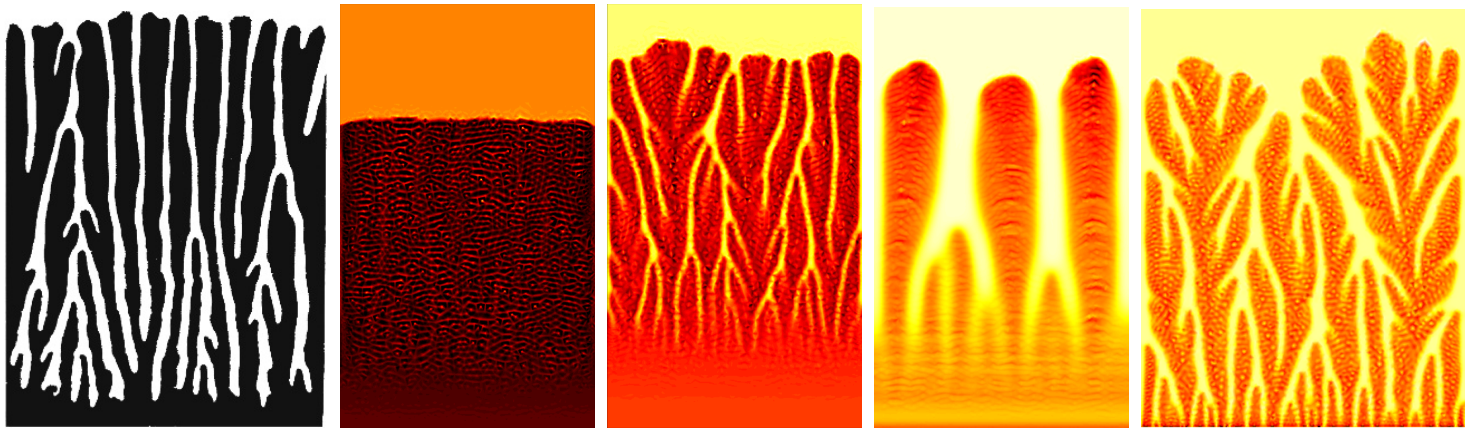
1. Computability in 2*D* (including *a priori / a posteriori* error estimates)
2. Free micro interfaces?



3. Two-scale coupling between macro PDEs and micro phase transitions [deterministic/stochastic ODEs]. Analysis + computability issues + PDEs in measures(?)
4. Applications to harvesting geothermal energy – NWO-MPE project (ongoing)
5. Applications to design of smart packaging – Preparation phase

Intermezzo: Multiscale smoldering combustion of thin sheets

- O. Zik, Z. Olami, and E. Moses (1998) *Fingering instability in combustion*, Phys. Rev. Lett. 81, 3868-3871.



- E. Ijioma, T. Ogawa, A. Muntean (2013). *Pattern formation in reverse smoldering combustion : a homogenization approach*. Combustion Theory and Modelling, 17(2), 185-223
- Ijioma, E.R., Muntean, A. Ogawa, T. (2015). *Effect of material anisotropy on the fingering instability in reverse smouldering combustion.* International Journal of Heat and Mass Transfer, 81, 924-938.
- Fatima, T., Ijioma, E.R., Ogawa, T. Muntean, A. (2014). *Homogenization and dimension reduction of filtration combustion in heterogeneous thin layers.*. Networks and Heterogeneous Media, 9(4), 709-737.

Background of this work:

- A. Muntean, T. van Noorden: *Corrector estimates for the homogenization of a locally-periodic medium with areas of low and high diffusivity*. Eur. J. Appl. Math. 24 (2013), (5), 657-677.
- T. van Noorden, A. Muntean: *Homogenization of a locally-periodic medium with areas of low and high diffusivity*. Eur. J. Appl. Math. 22 (2011), (5), 493-516.
- A. Muntean, M. Neuss-Radu: *A multiscale Galerkin approach for a class of nonlinear coupled reaction-diffusion systems in complex media*. JMAA 371 (2010), (2), 705-718.
- 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. 69(2011), (2), 261-276.
- V. Chalupecky, T. Fatima, A. Muntean: *Multiscale sulfate attack on sewer pipes: Numerical study of a fast micro-macro mass transfer limit*. J. Math-for-Industry, 2(2010) (B-7), 171-181.
- A. Muntean, O. Lakkis (2010). *Rate of convergence for a Galerkin scheme approximating a two-scale reaction-diffusion system with nonlinear transmission condition*. RIMS Kokyuroku (Kyoto), 1693, pp. 85-98.
- S. Meier, M. Peter, A. Muntean, M. Böhm, J. Kropp: *A two-scale approach to concrete carbonation* in Proc. Int. RILEM Workshop on Integral Service Life Modeling of Concrete Structures, Guimares, Portugal, 2007, 3–10.