Scaling effects and homogenization of reaction-diffusion problems with nonlinear drift

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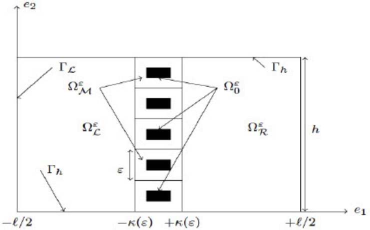
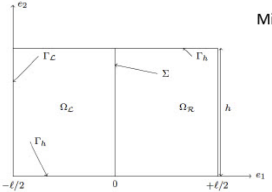
Outline

- Homogenization of reaction-diffusion-drift problem with variable scaling defined in a thin layer
- Homogenization of large drift problem in an unbounded domain using asymptotic expansion with drift
- Rigorous homogenization of large drift problem with nonlinear boundary condition
- Iterative scheme to study the solvability and numerical simulation for strongly coupled nonlinear dispersion problem.

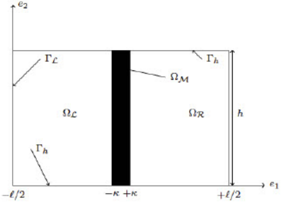
Model Geometry



Microscopic domain



$\varepsilon \to 0$ with $\kappa(\varepsilon) = \varepsilon$



$\varepsilon \to 0$ with $\kappa(\varepsilon)$ =constant

Microscopic equations

$$
\begin{aligned}
\frac{\partial u_l^\varepsilon}{\partial t} + \mathrm{div}(-D_L \nabla u_l^\varepsilon + B_L P_\delta(u_l^\varepsilon)) = f_l \quad \text{on } (0,T)\times\Omega_{\mathcal{L}}^\varepsilon,\\
\frac{\partial u_r^\varepsilon}{\partial t} + \mathrm{div}(-D_R \nabla u_r^\varepsilon + B_R P_\delta(u_r^\varepsilon)) = f_r \quad \text{on } (0,T)\times\Omega_{\mathcal{R}}^\varepsilon,\\
\varepsilon^\alpha \frac{\partial u_m^\varepsilon}{\partial t} + \mathrm{div}(-\varepsilon^\beta D_M^\varepsilon \nabla u_m^\varepsilon + \varepsilon^\gamma B_M^\varepsilon P_\delta(u_m^\varepsilon)) = \varepsilon^\alpha f_m^\varepsilon \quad \text{on } (0,T)\times\Omega_{\mathcal{M}}^\varepsilon,
\end{aligned}
$$

$$
P_\delta(r) := \rho_\delta * P(r),
$$

$$
P(r) := \begin{cases} a_0 + a_1 r + \cdots + a_m r^m & \text{for } r \in [0,1],\\ 0 & \text{otherwise.}\end{cases}
$$

A special structure of the drift $P(r) = r(1-r)$ was obtained from the mean-field limit of a totally asymmetric simple exclusion process for a population of interacting particles crossing a domain with obstacles [E. N. M. Cirillo, O. Krehel, A. Muntean, R. van Santen, and A. Sengar (2016)] .

Boundary and Transmission Conditions

$$u_l^\varepsilon = U_L \text{ on } (0,T)\times\Gamma_{\mathcal{L}},$$
$$u_r^\varepsilon = U_R \text{ on } (0,T)\times\Gamma_{\mathcal{R}},$$

$$(-\varepsilon^\beta D_M^\varepsilon \nabla u_m^\varepsilon + \varepsilon^\gamma B_M^\varepsilon P_\delta(u_m^\varepsilon))\cdot n_m^\varepsilon = \varepsilon^\xi g_0^\varepsilon \text{ on } (0,T)\times\Gamma_0^\varepsilon,$$
$$(-D_L\nabla u_l^\varepsilon + B_L P_\delta(u_l^\varepsilon))\cdot n_l = g_l \text{ on } (0,T)\times(\Gamma_h\cap\partial\Omega_{\mathcal{L}}^\varepsilon),$$
$$(-D_R\nabla u_r^\varepsilon + B_R P_\delta(u_r^\varepsilon))\cdot n_r = g_r \text{ on } (0,T)\times(\Gamma_h\cap\partial\Omega_{\mathcal{R}}^\varepsilon),$$

$$u_l^\varepsilon(0,x) = h_l^\varepsilon(x) \text{ for all } x\in\overline{\Omega}_{\mathcal{L}}^\varepsilon,$$
$$u_r^\varepsilon(0,x) = h_r^\varepsilon(x) \text{ for all } x\in\overline{\Omega}_{\mathcal{R}}^\varepsilon,$$
$$u_m^\varepsilon(0,x) = h_m^\varepsilon(x) \text{ for all } x\in\overline{\Omega}_{\mathcal{M}}^\varepsilon,$$

$$u_l^\varepsilon = u_M^\varepsilon \text{ on } \mathcal{B}_{\mathcal{L}}^\varepsilon,$$
$$u_r^\varepsilon = u_M^\varepsilon \text{ on } \mathcal{B}_{\mathcal{R}}^\varepsilon,$$
$$(-\varepsilon^\beta D_M^\varepsilon\nabla u_m^\varepsilon + \varepsilon^\gamma B_M^\varepsilon P_\delta(u_m^\varepsilon))\cdot n_m^\varepsilon = (-D_L\nabla u_l^\varepsilon + B_L P_\delta(u_l^\varepsilon))\cdot n_l \text{ on } \mathcal{B}_{\mathcal{L}}^\varepsilon,$$
$$(-\varepsilon^\beta D_M^\varepsilon\nabla u_m^\varepsilon + \varepsilon^\gamma B_M^\varepsilon P_\delta(u_m^\varepsilon))\cdot n_m^\varepsilon = (-D_R\nabla u_r^\varepsilon + B_R P_\delta(u_r^\varepsilon))\cdot n_r \text{ on } \mathcal{B}_{\mathcal{R}}^\varepsilon.$$

Choices of Scalings and Transformation of Problem

Table 1: List of discussed scalings.

Scaling options for infinitely thin layer	
Choice S1	Choice S2
$\alpha = -1$	$\alpha = -1$
$\beta = 1$	$\beta \in (0, 1)$
$\gamma \geq 1$	$\gamma \geq \beta$
$\xi \geq \frac{1}{2}$	$\xi \geq \min\{\beta - \frac{1}{2}, 0\}$

Scaling options for finitely thin layer	
Choice S3	Choice S4
$\alpha \in (-1, \infty)$	$\alpha \in (-1, \infty)$
$\beta - \alpha = 0$	$\beta - \alpha \in (0, \infty)$
$\gamma - \alpha \geq 0$	$\gamma - \alpha \geq 0$
$\xi - \alpha > 1$	$\xi - \alpha > 1$

Choices of Scalings and Transformation of Problem

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$\alpha \in (-1, \infty)$	$\alpha \in (-1, \infty)$
$\beta - \alpha = 0$	$\beta - \alpha \in (0, \infty)$
$\gamma - \alpha \geq 0$	$\gamma - \alpha \geq 0$
$\xi - \alpha > 1$	$\xi - \alpha > 1$

$$v_i^\varepsilon := u_i^\varepsilon + \frac{1}{2}(x_1 - \frac{\ell}{2})U_L - \frac{1}{2}(x_1 + \frac{\ell}{2})U_R,$$
$$u_i^\varepsilon = v_i^\varepsilon - u_b,$$

where $i \in \{l, m, r\}$.

Two Scale Convergence for Thin Layer

Definition

We define the sequence of functions $v_\varepsilon^m \in L^2((0,T) \times \Omega_{\mathcal{M}}^\varepsilon)$ two-scale converges to $v_0(t,\bar{x},y) \in L^2((0,T) \times \mathbf{\Sigma} \times Z)$ if

$$\lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_0^T \int_{\Omega_{\mathcal{M}}^\varepsilon} v_\varepsilon^m(t,x)\psi(t,\bar{x},\frac{x}{\varepsilon})dxdt = \int_0^T \int_{\mathbf{\Sigma}} \int_Z v_0(t,\bar{x},y)\psi(t,\bar{x},y)dydxdt,$$

for all $\psi \in L^2((0,T) \times \mathbf{\Sigma}; C_\#(\bar{Z}))$, where $\mathbf{\Sigma} := \{(0,x_2) \in \mathbf{\Omega} : x_2 \in (0,h)\}$ and we denote the two-scale convergence of v_m^ε to v_m^0 as $v_m^\varepsilon \overset{2-s}{\rightharpoonup} v_m^0$.

Definition

We define the sequence of functions $v_\varepsilon^m \in L^2((0,T) \times \Gamma_0^\varepsilon)$ two-scale converges to $v_0(t,\bar{x},y) \in L^2((0,T) \times \mathbf{\Sigma} \times \partial Y_0)$ if

$$\lim_{\varepsilon \to 0} \int_0^T \int_{\Gamma_0^\varepsilon} v_\varepsilon^m(t,x)\psi(t,\bar{x},\frac{x}{\varepsilon})d\sigma_x dt = \int_0^T \int_{\mathbf{\Sigma}} \int_{\partial Y_0} v_0(t,\bar{x},y)\psi(t,\bar{x},y)d\sigma_y d\bar{x}dt$$

for all $\psi \in L^2((0,T) \times \mathbf{\Sigma}; C_\#(\overline{\partial Y_0}))$.

Compactness results

Theorem (M. Neuss-Radu and W. Jäger (2007))

For any sequence $v_\varepsilon^m \in L^2((0,T) \times \Omega_{\mathcal{M}}^\varepsilon)$ satisfying the condition

$$\frac{1}{\varepsilon} \|v_\varepsilon^m\|^2_{L^2((0,T)\times\Omega_{\mathcal{M}}^\varepsilon)} \leq C,$$

then there exists a subsequence (again denoted as v_ε^m) such that v_ε^m two-scale converges to $v_0^m \in L^2((0,T) \times \Sigma \times Z)$.

Theorem (A. Bhattacharya, M. Gahn and M. Neuss-Radu (2020))

For any sequence $v_\varepsilon^m \in L^2((0,T) \times \Gamma_0^\varepsilon)$ satisfying the condition

$$\|v_\varepsilon^m\|^2_{L^2((0,T)\times\Gamma_0^\varepsilon)} \leq C,$$

then there exists a subsequence (again denoted as v_ε^m) such that v_ε^m two-scale converges to $v_0^m \in L^2((0,T) \times \Sigma \times \partial Y_0)$.

Macroscopic model

Theorem (V.R., E. N. M. Cirillo, I. de Bonis and A. Muntean (2022))

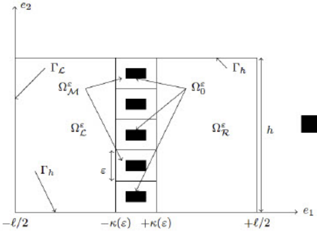
The upscaled model for the scaling choice S1 is: Find

$$v_l^0 \in L^2((0,T); H^1(\Omega_{\mathcal{L}})) \cap H^1((0,T); L^2(\Omega_{\mathcal{L}})),$$
$$v_m^0 \in L^2((0,T) \times \mathbf{\Sigma}; H^1(Z)) \cap H^1((0,T) \times \mathbf{\Sigma}; L^2(Z)),$$
$$v_r^0 \in L^2((0,T); H^1(\Omega_{\mathcal{R}})) \cap H^1((0,T); L^2(\Omega_{\mathcal{R}})),$$

satisfying

$$\frac{\partial v_l^0}{\partial t} + \mathrm{div}(-D_L \nabla v_l^0 + B_L P_\delta(v_l^0 - u_b)) = f_{b_l} \quad \text{on } (0,T) \times \Omega_{\mathcal{L}},$$
$$\frac{\partial v_r^0}{\partial t} + \mathrm{div}(-D_R \nabla v_r^0 + B_R P_\delta(v_r^0 - u_b)) = f_{b_r} \quad \text{on } (0,T) \times \Omega_{\mathcal{R}},$$
$$v_l^0 = 0 \text{ on } (0,T) \times \Gamma_{\mathcal{L}},$$
$$v_r^0 = 0 \text{ on } (0,T) \times \Gamma_{\mathcal{R}},$$

$$v_l^0(t,\bar{x}) = v_m^0(t,\bar{x},y) \text{ for a.e. } (t,\bar{x},y) \in (0,T) \times \mathbf{\Sigma} \times Z_L,$$
$$v_r^0(t,\bar{x}) = v_m^0(t,\bar{x},y) \text{ for a.e. } (t,\bar{x},y) \in (0,T) \times \mathbf{\Sigma} \times Z_R,$$


e_2
$\Gamma_{\mathcal{L}}$
Γ_h
$\Omega^{\varepsilon}_{\mathcal{M}}$
Ω^{ε}_0
$\Omega^{\varepsilon}_{\mathcal{L}}$
$\Omega^{\varepsilon}_{\mathcal{R}}$
h
ε
Γ_h
e_1
$-\ell/2$
$-\kappa(\varepsilon)$
$+\kappa(\varepsilon)$
$+\ell/2$
$\varepsilon \to 0$
e_2
$\Gamma_{\mathcal{L}}$
Γ_h
Σ
$\Omega_{\mathcal{L}}$
$\Omega_{\mathcal{R}}$
h
Γ_h
e_1
$-\ell/2$
0
$+\ell/2$

Theorem (cont.)

$$(-D_L\nabla v_l^0 + B_L P_\delta(v_l^0 - u_b))\cdot n_l = g_{b_l} \text{ on } (\Gamma_h \cap \partial\Omega_{\mathcal{L}}) \times (0,T),$$
$$(-D_R\nabla v_r^0 + B_R P_\delta(v_r^0 - u_b))\cdot n_r = g_{b_r} \text{ on } (\Gamma_h \cap \partial\Omega_{\mathcal{R}}) \times (0,T),$$
$$v_l^0(0,x) = h_{b_l}^0 \text{ on } \overline{\Omega}_{\mathcal{L}},$$
$$v_r^0(0,x) = h_{b_r}^0 \text{ on } \overline{\Omega}_{\mathcal{R}},$$

$$\begin{aligned}(-D_L\nabla v_l^0 + B_L P_\delta(v_l^0 - u_b) + D_R\nabla v_r^0 - B_R P_\delta(v_r^0 - u_b))\cdot n_l \\ = \int_{Z_L} D_M \nabla_y v_m^0 \cdot n_l d\sigma + D_L \nabla_x u_b(t,\bar{x})\cdot n_l \\ - \int_{Z_R} D_M \nabla_y v_m^0 \cdot n_l d\sigma + D_R \nabla_x u_b(t,\bar{x})\cdot n_l \quad \text{on } (0,T)\times\boldsymbol{\Sigma},\end{aligned}$$

and v_0^m solves the following cell problem

$$\frac{\partial v_m^0}{\partial t} + \mathrm{div}_y(-D_M\nabla_y v_m^0) = f_{a_0} \qquad \text{on } (0,T)\times\boldsymbol{\Sigma}\times Z,$$
$$(-D_M\nabla_y v_m^0)\cdot n = 0 \qquad \text{on } (0,T)\times\boldsymbol{\Sigma}\times(\partial Z\setminus(Z_L\cup Z_R)),$$
$$v_l^0(0,x) = h_{b_l}^0 \qquad \text{on } \boldsymbol{\Sigma}\times Z.$$

Microscopic Problem: Reaction-Diffusion Equation with Large Drift

We consider the following reaction-diffusion-drift problem

$$\begin{aligned}
\frac{\partial u^\varepsilon}{\partial t} + \mathrm{div}(-D^\varepsilon \nabla u^\varepsilon + \frac{1}{\varepsilon} B^\varepsilon P(u^\varepsilon)) &= f^\varepsilon && \text{on} && (0,T)\times\Omega_\varepsilon,\\
(-D^\varepsilon \nabla u^\varepsilon + \frac{1}{\varepsilon} B^\varepsilon P(u^\varepsilon))\cdot n_\varepsilon &= \varepsilon g_N^\varepsilon && \text{on} && (0,T)\times\Gamma_N^\varepsilon,\\
u^\varepsilon &= \varepsilon^\gamma g_D^\varepsilon && \text{on} && (0,T)\times\Gamma_D^\varepsilon,\\
u^\varepsilon(0) &= g && \text{in} && \overline{\Omega}_\varepsilon,
\end{aligned}$$

where Ω_ε is periodic replication of ε scaled standard cell Z in $\mathbb{R}^2$ and

$$P(r) := a_0(\frac{x}{\varepsilon}) + a_1(\frac{x}{\varepsilon})r + \cdots + a_m(\frac{x}{\varepsilon})r^m.$$

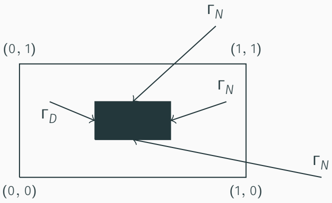


Figure 1: Standard cell Z exhibiting a rectangular obstacle Y_0 placed in the center.

Assumptions

(D1) D is uniformly elliptic.

(D2) $B : C^1_{\#}(Z) \to \mathbb{R}^2$ satisfies

$$\begin{cases} \mathrm{div}_y B & = 0 \quad \text{in} \quad Z, \\ B \cdot n_y & = 0 \quad \text{on} \quad \Gamma_N, \\ \mathrm{div}_y(Ba_i) & = 0 \quad \text{for} \quad i \in \{0,1,2,3,\cdots,m\}, \\ \int_Z (Ba_i)dy & = 0 \quad \text{for} \quad i \in \{2,3,\cdots,m\}. \end{cases}$$

(D3) $f^\varepsilon(t,x) := f(t,x,\frac{x}{\varepsilon})$, $g_N^\varepsilon(t,x) := g_N(t,x,\frac{x}{\varepsilon})$, $g_D^\varepsilon(t,x) := g_D(t,\frac{x}{\varepsilon})$ such that $f \in L^\infty(0,T;C_c(\mathbb{R}^2) \times L^2_{\#}(Z))$, $g_N \in L^\infty(0,T;C_c(\mathbb{R}^2) \times L^2_{\#}(\Gamma_N))$ and $g_D \in L^2(0,T;L^2_{\#}(\Gamma_D))$.

(D4) $g : \mathbb{R}^2 \to \mathbb{R}^+ \cup \{0\}$ such that $g \in L^\infty(\mathbb{R}^2) \cap L^2(\mathbb{R}^2)$.

(D5) The inequality $\int_Z f\,dy - \int_{\Gamma_N} g_N d\sigma_y \geq 0$ hold.

Assumptions and Technique

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(D4) $g : \mathbb{R}^2 \to \mathbb{R}^+ \cup \{0\}$ such that $g \in L^\infty(\mathbb{R}^2) \cap L^2(\mathbb{R}^2)$.

(D5) The inequality $\int_Z f\, dy - \int_{\Gamma_N} g_N d\sigma_y \geq 0$ hold.

Homogenization tool

Two scale expansion with drift [G. Allaire, R. Brizzi, A. Mikelić and A. Piatnitski, *Chem. Eng. Sci.* (2010)]

$$u^\varepsilon(t,x) = \sum_{k=0}^{\infty} \varepsilon^k u_k\left(t, x - \frac{B^* t}{\varepsilon}, \frac{x}{\varepsilon}\right).$$

Assumptions and Technique

Assumptions

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(D4) $g : \mathbb{R}^2 \to \mathbb{R}^+ \cup \{0\}$ such that $g \in L^\infty(\mathbb{R}^2) \cap L^2(\mathbb{R}^2)$.

(D5) The inequality $\int_Z f dy - \int_{\Gamma_N} g_N d\sigma_y \geq 0$ hold.

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$$u^\varepsilon(t,x) = \sum_{k=0}^{\infty} \varepsilon^k u_k \left(t, x - \frac{B^* t}{\varepsilon}, \frac{x}{\varepsilon} \right).$$

Note: If $|\Gamma_D| > 0$, then $u^0 \equiv 0$.

Upscaled Model[1]

Find the pair (u_0, W) satisfying the following system of equations:

$$\begin{aligned} \partial_t u_0 + \mathrm{div}(-D^*(u_0, W)\nabla_x u_0) &= \frac{1}{|Z|}\int_Z f\,dy + \frac{-1}{|Z|}\int_{\Gamma_N} g_N\,d\sigma_y \quad &\text{on} \quad (0,T)\times\mathbb{R}^2,\\ u_0(0) &= g \quad &\text{on} \quad \mathbb{R}^2, \end{aligned}$$

$$\begin{aligned} -\nabla_y \cdot D(y)\nabla_y w_i + P'(u_0)\nabla_y \cdot (B(y)w_i) &= \nabla_y \cdot D(y)e_i + B^* \cdot e_i - P'(u_0)B(y)\cdot e_i \quad &\text{on} \quad Z,\\ \big(-D(y)\nabla_y w_i + BP'(u_0)w_i\big)\cdot n_y &= (-D(y)e_i)\cdot n_y \quad &\text{on} \quad \Gamma_N,\\ w_i \ \text{is } Z\text{-periodic}, & \end{aligned}$$

where $W = (w_1, w_2)$ and $i \in \{1, 2\}$.

[1] V.R., E. N. M. Cirillo and A. Muntean, *Quart. Appl. Math.* (2022)

Effective Dispersion Tensor

The effective dispersion tensor D^* is defined as

$$D^*(u_0, W) = \frac{1}{|Z|} \int_Z D(y) \left(I + \begin{bmatrix} \frac{\partial w_1}{\partial y_1} & \frac{\partial w_2}{\partial y_1} \\ \frac{\partial w_1}{\partial y_2} & \frac{\partial w_2}{\partial y_2} \end{bmatrix} \right) dy + \frac{1}{|Z|} \int_Z B^* W(y)^t \, dy - \frac{1}{|Z|} \int_Z P'(u_0) B(y) W(y)^t \, dy,$$

and the effective drift is defined as

$$B^* \cdot e_i = \frac{\int_Z a_1(y) B(y) \cdot e_i dy}{|Z|}.$$

We consider the following reaction-diffusion-drift problem

$$\begin{aligned} \frac{\partial u^\varepsilon}{\partial t} + \mathrm{div}(-D^\varepsilon \nabla u^\varepsilon + \frac{1}{\varepsilon} B^\varepsilon P(u^\varepsilon)) = f^\varepsilon \quad & \text{on} \quad (0,T)\times\Omega^\varepsilon, \\ (-D^\varepsilon \nabla u^\varepsilon + \frac{1}{\varepsilon} B^\varepsilon P(u^\varepsilon)) \cdot n_\varepsilon = \varepsilon g_N(u^\varepsilon) \quad & \text{on} \quad (0,T)\times\Gamma_N^\varepsilon, \\ u^\varepsilon(0) = g \quad & \text{in} \quad \overline{\Omega}^\varepsilon, \end{aligned}$$

where the nonlinearity $P(\cdot)$ defined as

$$P(u^\varepsilon) = u^\varepsilon(1 - C^\varepsilon u^\varepsilon),$$

with

$$\int_Z BC dy = 0.$$

Assumptions on the data

Assumptions

(D1) D^ε is uniformly elliptic and $D^\varepsilon \in C_{\#}^{2,\beta}(Z)^{2\times 2}$ for some $0 < \beta < 1$.

(D2) $B \in C_{\#}^{1,\beta}(Z)^2$, $C \in C_{\#}^{1,\beta}(Z)$ satisfies

$$\begin{cases} \mathrm{div} B = 0 \quad \text{in} \quad Z, \\ \mathrm{div}(BC) = 0 \quad \text{in} \quad Z, \\ B \cdot n_y = 0 \quad \text{on} \quad \Gamma_N. \end{cases}$$

.

(D3) $f^\varepsilon \in C_c^2(\mathbb{R}^2)$ such that $f^\varepsilon \xrightarrow{2-drift(B^*)} f$.

(D4) $g_N \in C^1(\mathbb{R})$ satisfies

$$-g_N(x)x < 0 \ \text{ for all } \ x \neq 0,$$
$$g_N(x) \leq g_N(y) \ \text{ if } \ x \leq y.$$

(D5) $g : \mathbb{R}^2 \to \mathbb{R}^+$ such that

$$g \in C_c^\infty(\mathbb{R}^2).$$

Weak formulation for the microscopic problem

Definition

A weak solution to the microscopic problem is a function $u^\varepsilon \in L^2(0,T;H^1(\Omega^\varepsilon)) \cap H^1(0,T;L^2(\Omega^\varepsilon))$ satisfying

$$\int_{\Omega^\varepsilon} \partial_t u^\varepsilon \phi dx + \int_{\Omega^\varepsilon} D^\varepsilon \nabla u^\varepsilon \nabla \phi dx - \frac{1}{\varepsilon}\int_{\Omega^\varepsilon} B^\varepsilon u^\varepsilon (1 - C^\varepsilon u^\varepsilon) \nabla \phi dx$$
$$= \int_{\Omega^\varepsilon} f^\varepsilon \phi dx - \varepsilon \int_{\Gamma_N^\varepsilon} g_N(u^\varepsilon) \phi d\sigma,$$

for all $\phi \in H^1(\Omega^\varepsilon)$ and a.e. $t \in (0,T)$ with the initial condition $u(0) = g$.

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$$\int_{\Omega^\varepsilon} \partial_t u^\varepsilon \phi dx + \int_{\Omega^\varepsilon} D^\varepsilon \nabla u^\varepsilon \nabla \phi dx - \frac{1}{\varepsilon}\int_{\Omega^\varepsilon} B^\varepsilon u^\varepsilon (1 - C^\varepsilon u^\varepsilon)\nabla \phi dx = \int_{\Omega^\varepsilon} f^\varepsilon \phi dx - \varepsilon \int_{\Gamma_N^\varepsilon} g_N(u^\varepsilon)\phi d\sigma,$$

for all $\phi \in H^1(\Omega^\varepsilon)$ and a.e. $t \in (0,T)$ with the initial condition $u(0) = g$.

Theorem

For every fixed $\varepsilon > 0$, there exists a unique weak solution $u^\varepsilon \in L^2(0,T;H^1(\Omega^\varepsilon)) \cap H^1(0,T;L^2(\Omega^\varepsilon))$ to the microscopic problem.

Upscaling of microscopic problem- Two scale convergence with drift

Definition (Two scale convergence with drift)

Let $r \in \mathbb{R}^2$ and $u^\varepsilon \in L^2(0,T;L^2(\Omega^\varepsilon))$, we say u^ε two-scale converges with drift r to u_0 (denote as $u^\varepsilon \xrightarrow{2-drift} u_0$), if for all $\phi \in C_c^\infty((0,T)\times\mathbb{R}^2; C_\#^\infty(Z))$ the following identity hold

$$\lim_{\varepsilon\to 0}\int_0^T\int_{\Omega^\varepsilon} u^\varepsilon(t,x)\phi(t,x-\frac{rt}{\varepsilon},\frac{x}{\varepsilon})dxdt = \int_0^T\int_{\mathbb{R}^2}\int_Z u_0(t,x,y)\phi(t,x,y)dydxdt.$$

Upscaling of the microscopic problem- Compactness result

Theorem (E. Marušić-Paloka and A. Piatnitski (2005))

Let $u^\varepsilon \in L^2(0,T;H^1(\Omega^\varepsilon))$ *and there exist a constant* $C > 0$, *such that*

$$\|u^\varepsilon\|_{L^2(0,T;H^1(\Omega^\varepsilon))} \leq C,$$

then there exist $u_0 \in L^2(0,T;H^1(\mathbb{R}^2))$ *and* $u_1 \in L^2((0,T) \times H^1(\mathbb{R}^2); H^1_\#(Z))$ *such that*

$$u^\varepsilon \xrightarrow{2-drift} u_0,$$

$$\nabla u^\varepsilon \xrightarrow{2-drift} \nabla_x u_0 + \nabla_y u_1.$$

Theorem (G. Allaire and H. Hutridurga (2012))

Let $u^\varepsilon \in L^2(0,T;L^2(\Gamma_N^\varepsilon))$ *and there exists a constant* $C > 0$ *independent of* ε *such that*

$$\varepsilon\|u^\varepsilon\|_{L^2(0,T;L^2(\Gamma_N^\varepsilon))} \leq C,$$

then there exists $u_0 \in L^2(0,T;L^2(\mathbb{R}^2 \times \Gamma_N))$ *such that*

$$\lim_{\varepsilon\to 0} \varepsilon \int_0^T \int_{\Gamma_N^\varepsilon} u^\varepsilon(t,x)\phi(t,x-\frac{rt}{\varepsilon},\frac{x}{\varepsilon})dxdt = \int_0^T \int_{\mathbb{R}^2} \int_{\Gamma_N} u_0(t,x,y)\phi(t,x,y)dydxdt.$$

Strong convergence in moving coordinate

Theorem

Assume (D1)–(D5) hold. Then there exist $u_0 \in L^2(0,T;H^1(\mathbb{R}^2))$ *such that*

$$\lim_{\varepsilon\to 0}\int_0^T\int_{\Omega^\varepsilon}\left|u^\varepsilon(t,x)-u_0\left(t,x-\frac{B^*t}{\varepsilon}\right)\right|^2 dxdt = 0,$$

$$\lim_{\varepsilon\to 0}\varepsilon\int_0^T\int_{\Gamma_N^\varepsilon}\left|u^\varepsilon(t,x)-u_0\left(t,x-\frac{B^*t}{\varepsilon}\right)\right|^2 d\sigma dt = 0.$$

where

$$B^*\cdot e_i := \frac{\int_Z B(y)\cdot e_i dy}{|Z|}.$$

Macroscopic Equation[2]

The weak solution u^ε of the microscopic problem converges to $u^0(t,x)$ in the sense of two-scale with drift B^* as $\varepsilon \to 0$, where $u^0(t,x)$ is the weak solution of the homogenized reaction-dispersion problem

$$\begin{aligned} \partial_t u_0 + \operatorname{div}(-D^*(u_0, W)\nabla_x u_0) &= \frac{1}{|Z|}\int_Z f\,dy - \frac{|\Gamma_N|}{|Z|} g_N(u_0) && \text{in} \quad (0,T)\times\mathbb{R}^2, \\ u_0(0) &= g && \text{in} \quad \mathbb{R}^2, \end{aligned}$$

$$\begin{aligned} &-\nabla_y \cdot D(y)\nabla_y w_i + B(y)(1-2C(y)u_0)\cdot\nabla_y w_i \\ &\qquad = \nabla_y \cdot D(y)e_i + B^*\cdot e_i - B(y)(1-2C(y)u_0)\cdot e_i \quad \text{in} \quad (0,T)\times\mathbb{R}^2\times Z, \\ &(-D(y)\nabla_y w_i + B(y)(1-2C(y)u_0)w_i)\cdot n_y = (-D(y)e_i)\cdot n_y \quad \text{on} \quad (0,T)\times\mathbb{R}^2\times\Gamma_N, \\ &w_i(t,x,\cdot) \ \text{ is } Z\text{–periodic}, \end{aligned}$$

where $i \in \{1,2\}$.

[2] V.R., I. de Bonis, E. N. M. Cirillo and A. Muntean, *Quart. Appl. Math.* (2024)

Effective Drift and Dispersion Tensor

The effective drift B^* is defined as

$$B^* \cdot e_i := \frac{\int_Z B(y) \cdot e_i dy}{|Z|},$$

and the effective dispersion tensor D^* is defined as

$$D^*(u_0, W) := \frac{1}{|Z|} \int_Z D(y) \left(I + \begin{bmatrix} \frac{\partial w_1}{\partial y_1} & \frac{\partial w_2}{\partial y_1} \\ \frac{\partial w_1}{\partial y_2} & \frac{\partial w_2}{\partial y_2} \end{bmatrix} \right) dy$$
$$+ \frac{1}{|Z|} \int_Z B^* W(y)^t \, dy - \frac{1}{|Z|} \int_Z B(y)(1 - 2C(y)u_0) W(y)^t \, dy.$$

Corrector result

Theorem (V.R., I. de Bonis E. N. M. Cirillo and A. Muntean (2024))

Assume $g_N(r) = r$ *for all* $r \in \mathbb{R}$*. Then*

$$\lim_{\varepsilon \to 0} \left\| \nabla \left(u^\varepsilon(t,x) - u_0(t, x - \frac{B^* t}{\varepsilon}) - \varepsilon u_1(t, x - \frac{B^* t}{\varepsilon}, \frac{x}{\varepsilon}) \right) \right\|_{L^2(0,T;L^2(\Omega^\varepsilon))} = 0,$$

where $u_1 = \sum w_i \partial_{x_i} u_0$, u^ε *solves the microscopic problem,* u_0, w_1, w_2 *solves the upscaled problem and the cell problem respectively.*

Strongly coupled parabolic-elliptic system

$$
\begin{aligned}
\partial_t u + \mathrm{div}(-D^*(u,W)\nabla u) &= f && \text{in } (0,T)\times\Omega,\\
u &= 0 && \text{on } (0,T)\times\partial\Omega,\\
u(0) &= g && \text{in } \overline{\Omega},\\
\mathrm{div}_y\left(-D\nabla_y w_i + G_i(u)Bw_i\right) &= \mathrm{div}_y(De_i) && \text{in } Y,\\
(-D\nabla_y w_i + G_i(u)Bw_i)\cdot n_y &= (De_i)\cdot n_y && \text{on } \Gamma_N,\\
w_i &\text{ is Y–periodic,}
\end{aligned}
$$

where

$$D^*(u,W) := \frac{1}{|Y|}\int_Y D(y)\left(I + \begin{bmatrix} \frac{\partial w_1}{\partial y_1} & \frac{\partial w_2}{\partial y_1} \\ \frac{\partial w_1}{\partial y_2} & \frac{\partial w_2}{\partial y_2}\end{bmatrix}\right) dy.$$

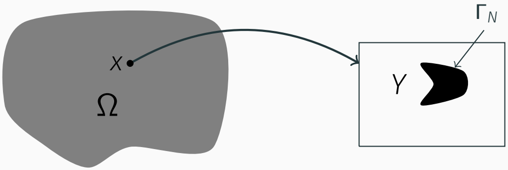

Figure 2: Schematic representation of the macroscopic domain Ω and the cell Y with internal boundary Γ_N.

Assumptions

Assumptions on the data

- The microscopic diffusion matrix satisfies $D \in (L^\infty(Y))^{2\times 2}$ and there exists $\theta > 0$ such that

$$\theta|\eta|^2 \le D\eta \cdot \eta \quad \text{for all } \eta \in \mathbb{R}^2 \text{ and almost all } y \in Y.$$

- $G_1, G_2 : \mathbb{R} \to \mathbb{R}$ are locally Lipschitz functions.
- The microscopic drift velocity $B \in (H^1_\#(Y) \cap L^\infty(Y))^2$ satisfies

$$\begin{cases} \mathrm{div}_y B = 0 & \text{in} \quad Y, \\ B \cdot n_y = 0 & \text{on} \quad \Gamma_N. \end{cases}$$

- The reaction rate satisfies $f \in C^{\alpha, \frac{\alpha}{2}}((0,T) \times \Omega)$ and the initial condition $g \in C^{2+\alpha}(\Omega)$, for some $0 < \alpha < 1$.

Iterative scheme

Set $u^0 = g$, for any $k \in \mathbb{N} \cup \{0\}$, u^{k+1}, w_1^k, and w_2^k satisfy:

$$\begin{aligned} \mathrm{div}_y \left(-D\nabla_y w_i^k + G_i(u^k) B w_i^k \right) &= \mathrm{div}_y (De_i) && \text{in } \; Y, \\ \left(-D\nabla_y w_i^k + BG_i(u^k) w_i^k \right) \cdot n_y &= (De_i) \cdot n_y && \text{on } \; \Gamma_N, \\ w_i^k \; \text{ is } Y\text{–periodic} & && i \in \{1,2\}, \end{aligned}$$

$$\begin{aligned} \partial_t u^{k+1} + \mathrm{div}(-D^*(u^k, W^k) \nabla_x u^{k+1}) &= f && \text{in } \; (0,T) \times \Omega, \\ u^{k+1}(0) &= g && \text{in } \; \overline{\Omega}, \\ u^{k+1} &= 0 && \text{on } \; (0,T) \times \partial\Omega, \end{aligned}$$

where the dispersion matrix $D^*(u^k, W^k)$ is given by

$$D^*(u^k, W^k) := \frac{1}{|Y|} \int_Y D(y) \left(I + \begin{bmatrix} \frac{\partial w_1^k}{\partial y_1} & \frac{\partial w_2^k}{\partial y_1} \\ \frac{\partial w_1^k}{\partial y_2} & \frac{\partial w_2^k}{\partial y_2} \end{bmatrix} \right) dy.$$

Lemma

The macroscopic dispersion matrix $D^*(u^k, W^k)$ satisfies the following properties:

- *There exists $\lambda > 0$ independent of k such that*

$$\lambda|\eta|^2 \leq D^*(u^k, W^k)\eta \cdot \eta \quad \textit{for all } \eta \in \mathbb{R}^2.$$

- *There exist a constant $C > 0$ independent of k such that*

$$|[D^*(u^k, W^k)]_{i,j}| \leq C, \quad (i, j \in \{1, 2\}).$$

- *There exist $C > 0$ independ of m and n, such that*

$$|D^*(u^m, W^m) - D^*(u^n, W^n)| \leq C|u^m - u^n|.$$

Convergence of the iterative scheme

Theorem (V.R., S. Nepal, R. Lyons, M. Eden and A. Muntean (2023))

There exists a $u \in L^2((0,T); H^1(\Omega))$ *and a* $W \in L^\infty((0,T) \times \Omega; \mathcal{W}^2)$ *such that,*

$$
\begin{aligned}
u^k &\to u && \textit{strongly in} && L^2((0,T) \times \Omega),\\
D^*(u^k, W^k) &\to D^*(u, W) && \textit{strongly in} && L^2((0,T) \times \Omega),\\
\nabla u^k &\rightharpoonup \nabla u && \textit{weakly in} && L^2((0,T) \times \Omega),\\
\partial_t u^k &\rightharpoonup \partial_t u && \textit{weakly in} && L^2((0,T); H^{-1}(\Omega)).
\end{aligned}
$$

Moreover, (u, W) *is a solution to the nonlinear parabolic-elliptic system.*

Summary

- ➤ We studied the effect of different scaling on the upscaling of the reaction-diffusion-drift problem posed on a homogeneous domain separated by a thin layer
- ➤ We derived a nonlinear reaction-dispersion model as the upscaled model for the reaction-diffusion problem with large non-linear drift in an unbounded perforated domain.
- ➤ We proposed an iterative scheme that helps to show the existence and numerical scheme for a strongly coupled reaction dispersion problem.

Potential future works

- ➢ Derive a corrector estimate for every upscaled model that is presented in the thesis.
- ➢ Derive the effective model for the evolution of two (or more) populations of interacting particles moving with drift in a composite material.
- ➢ Derive macroscopic equation and effective transmission condition for large nonlinear drift problem for bounded thin domain
- ➢ Find efficient numerical scheme and order of convergent for the coupled nonlinear-dispersion problem

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