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Using volume averaging to correct the boundary conditions in macroscale models of multilayer diffusion

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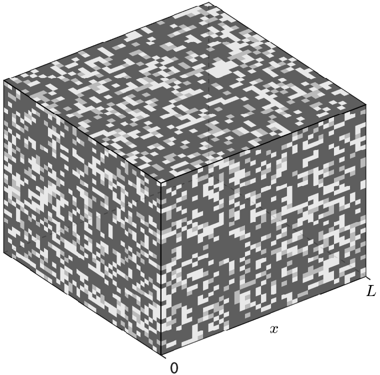
Motivation: Transport Processes in Heterogeneous Media

- Example - Linear Parabolic Transport Equation:

$$\frac{\partial u}{\partial t} = \boldsymbol{\nabla} \cdot (\boldsymbol{K}(\boldsymbol{x}) \boldsymbol{\nabla} u)\,,$$
$$\boldsymbol{x} \in \Omega \subset \mathbb{R}^d.$$

- $\boldsymbol{K}(\boldsymbol{x})$ varies with position $\boldsymbol{x}$ on a small length scale

- Computational cost of direct numerical simulation is prohibitively expensive



- Strategies to alleviate problem: Two-scale[1] or Macroscale[2] Modelling

[1] Abdulle and E (2003); Carr et al. (2016); Szymkiewicz and Lewandowska (2008)
[2] Auriault (1994); Chen et al. (2015); Whitaker (1998)

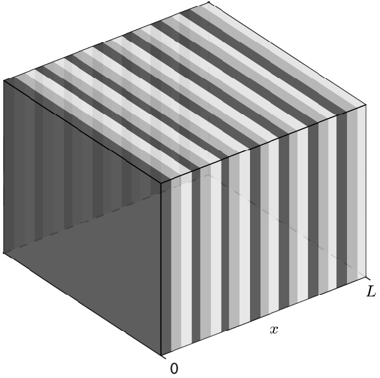
1D Prototype Problem: Layered Diffusion

- Linear diffusion in each layer:

$$\frac{\partial u_i}{\partial t} = \kappa_i \frac{\partial^2 u_i}{\partial x^2}, \quad u_i(x,0) = u_0,$$
$$i = 1, \ldots, m.$$

- External boundary conditions:

$$a_L u_1(0,t) + b_L \frac{\partial u_1}{\partial x}(0,t) = c_L,$$
$$a_R u_m(L,t) + b_R \frac{\partial u_m}{\partial x}(L,t) = c_R.$$



- Internal boundary conditions at the interfaces:

$$u_i(l_i,t) = u_{i+1}(l_i,t), \quad \kappa_i \frac{\partial u_i}{\partial x}(l_i,t) = \kappa_{i+1} \frac{\partial u_{i+1}}{\partial x}(l_i,t), \quad i = 1, \ldots, m-1.$$

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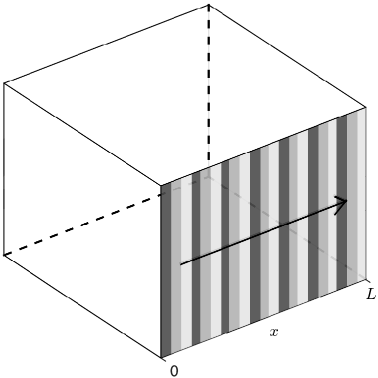

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Macroscopic modelling

- Replace heterogeneous medium with an effective homogeneous medium

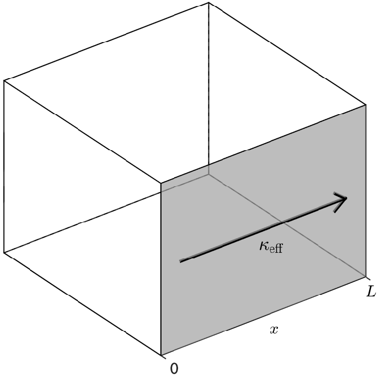
- Macroscopic equation:

$$\frac{\partial U}{\partial t} = \kappa_{\text{eff}} \frac{\partial^2 U}{\partial x^2}, \quad 0 < x < L.$$

  where $u_i(x,t) \simeq U(x,t)$ in some average sense.

- Effective diffusivity:

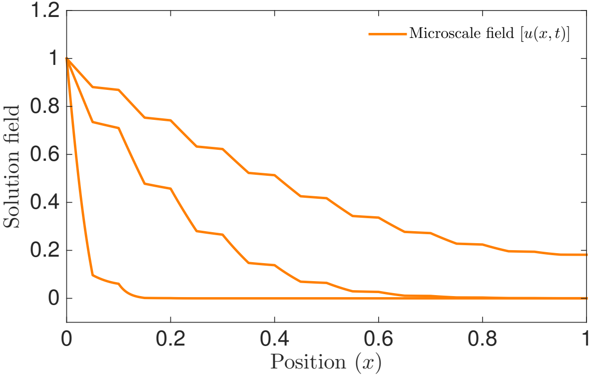
$$\kappa_{\text{eff}} = \left(\frac{1}{l_m - l_0} \sum_{i=1}^{m} \frac{l_i - l_{i-1}}{\kappa_i} \right)^{-1}$$



- *Question*: What BCs should be imposed on macroscale field?

What form should the macroscale BCs take?

$$u_1(0,t) = 1 \text{ and } \frac{\partial u_m}{\partial x}(1,t) = 0.$$



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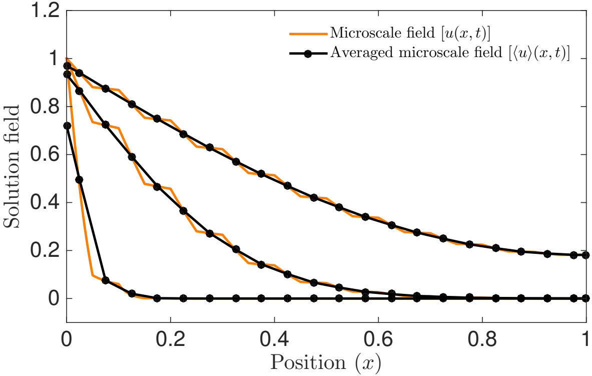
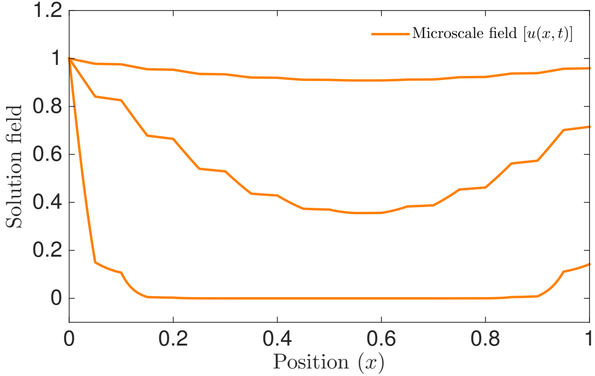


- *Observation*: Averaged microscale field does not satisfy Dirichlet BC at $x = 0$.

What form should the macroscale BCs take?

$$u_1(0,t) = 1 \text{ and } u_m(1,t) + \frac{\partial u_m}{\partial x}(1,t) = 1.$$



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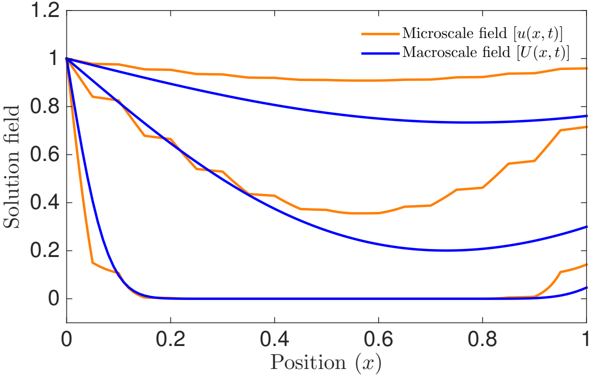

- *Observation*: Applying same Robin BC on macroscale leads to a poor match.

Volume averaging

- Averaging operator:

$$\langle \phi \rangle = \frac{1}{2\delta} \int_{-\delta}^{\delta} \phi(x+\xi,t)\, d\xi$$

- *Average plus perturbation* decomposition:

$$u_i = \langle u \rangle + \widetilde{u}_i, \quad i = 1,\ldots,m.$$

- Averaging and making some assumptions:

$$\left\langle \frac{\partial u}{\partial x} \right\rangle = \left\langle \frac{\partial}{\partial x}\left(\kappa(x)\frac{\partial u}{\partial x}\right)\right\rangle \quad \rightarrow \quad \frac{\partial \langle u \rangle}{\partial t} \simeq \frac{\partial}{\partial x}\left(\kappa_{\text{eff}}\frac{\partial \langle u \rangle}{\partial x}\right)$$

with

$$\kappa_{\text{eff}} = \frac{1}{l_p - l_0}\sum_{k=1}^{p}\int_{l_{k-1}}^{l_k} \kappa_k \left(\psi_k'(x) + 1\right)\, dx.$$

where $\psi_k(x)$ $(k = 1,\ldots,m)$ satisfy a suitable steady-state microscale problem.

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  where $\psi_k(x)$ $(k=1,\ldots,m)$ satisfy a suitable steady-state microscale problem.

Deriving the Macroscale BCs

Boundary condition at $x = 0$:

- Insert *average plus perturbation* decomposition:

$$a_L u_1 - b_L \frac{\partial u_1}{\partial x} = c_L \quad \rightarrow \quad a_L \left[\langle u\rangle + \widetilde{u}_1\right] - b_L \frac{\partial}{\partial x}\left[\langle u\rangle + \widetilde{u}_1\right] = c_L$$

- Volume averaging assumptions[3]:

$$A1\text{:}\ \widetilde{u}_1 \simeq \psi_1(x)\frac{\partial\langle u\rangle}{\partial x} \qquad A2\text{:}\ \frac{\partial \widetilde{u}_1}{\partial x} \simeq \psi_1'(x)\frac{\partial\langle u\rangle}{\partial x}$$

$$a_L\langle u\rangle - \left[b_L(1+\psi_1'(0)) - a_L\psi_1(0)\right]\frac{\partial\langle u\rangle}{\partial x} \simeq c_L.$$

- *Corrected* Macroscale BC:

$$a_L U - \left[b_L(1+\psi_1'(0)) - a_L\psi_1(0)\right]\frac{\partial U}{\partial x} = c_L$$

[3] Davit et al. (2013); Whitaker (1998)

Recap

- Microscale Model:

$$\frac{\partial u_i}{\partial t} = \frac{\partial}{\partial x}\left(\kappa_i \frac{\partial u_i}{\partial x}\right), \quad u_i(x,0) = u_0, \quad i = 1,\ldots,m,$$

$$u_{i+1}(l_i,t) = u_i(l_i,t), \quad \kappa_{i+1}\frac{\partial u_{i+1}}{\partial x}(l_i,t) = \kappa_i \frac{\partial u_i}{\partial x}(l_i,t), \quad i = 1,\ldots,m,$$

$$a_L u_1(0,t) - b_L \frac{\partial u_1}{\partial x}(0,t) = c_L, \quad a_R u_m(L,t) + b_R \frac{\partial u_m}{\partial x}(L,t) = c_R,$$

- Macroscale Model:

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial x}\left(\kappa_{\text{eff}} \frac{\partial U}{\partial x}\right), \quad U(x,0) = u_0,$$

$$a_L U(0,t) - \left[b_L(1+\psi_1'(0)) - a_L\psi_1(0)\right]\frac{\partial U}{\partial x}(0,t) = c_L,$$

$$a_R U(L,t) + \left[b_R(1+\psi_p'(l_p)) + a_R\psi_p(l_p)\right]\frac{\partial U}{\partial x}(L,t) = c_R.$$

- *Question*: What happens for a homogeneous medium?

Corrected Macroscale BCs

Microscale to Macroscale BC transisition ($x = 0$):

- Dirichlet BC → Robin BC[4]

$$u_1 = c_L \quad \rightarrow \quad U + \psi_1(0)\frac{\partial U}{\partial x} = c_L$$

- Neumann BC → Neumann BC

$$\frac{\partial u_1}{\partial x} = c_L \quad \rightarrow \quad \frac{\kappa_{\text{eff}}}{\kappa_1}\frac{\partial U}{\partial x} = c_L$$

- Flux specified BC → Flux specified BC

$$\kappa_1\frac{\partial u_1}{\partial x} = c_L \quad \rightarrow \quad \kappa_{\text{eff}}\frac{\partial U}{\partial x} = c_L$$

- Newton-type BC → Newton-type BC

$$\kappa_1\frac{\partial u_1}{\partial x} = \sigma(u_1 - u_\infty) \quad \rightarrow \quad \left[\kappa_{\text{eff}} - \sigma\psi_1(0)\right]\frac{\partial U}{\partial x} = \sigma(U - u_\infty)$$

[4] As in Allaire and Amar (1999).

Simplest case: Biperiodic Layers of equal width

Corrected Macroscale BCs at $x = 0$:

- Dirichlet BC $\rightarrow$ Robin BC[5]

$$u_1 = c_L \quad \rightarrow \quad U - \frac{h}{2}\frac{\kappa_2 - \kappa_1}{\kappa_1 + \kappa_2}\frac{\partial U}{\partial x} = c_L$$

- Neumann BC $\rightarrow$ Neumann BC

$$\frac{\partial u_1}{\partial x} = c_L \quad \rightarrow \quad \frac{\kappa_{\text{eff}}}{\kappa_1}\frac{\partial U}{\partial x} = c_L$$

- Flux specified BC $\rightarrow$ Flux specified BC

$$\kappa_1 \frac{\partial u_1}{\partial x} = c_L \quad \rightarrow \quad \kappa_{\text{eff}}\frac{\partial U}{\partial x} = c_L$$

- Newton-type BC $\rightarrow$ Newton-type BC

$$\kappa_1 \frac{\partial u_1}{\partial x} = \sigma(u_1 - u_\infty) \quad \rightarrow \quad \left[\kappa_{\text{eff}} - \sigma\frac{h}{2}\frac{\kappa_1 - \kappa_2}{\kappa_1 + \kappa_2}\right]\frac{\partial U}{\partial x} = \sigma(U - u_\infty)$$

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[5] As in Chen (2015).

Simplest case: Biperiodic Layers of equal width

Standard Macroscale BCs ($h \to 0$) at $x = 0$:

- Dirichlet BC $\to$ Dirichlet BC

$$u_1 = c_L \quad \to \quad U = c_L$$

- Neumann BC $\to$ Neumann BC

$$\frac{\partial u_1}{\partial x} = c_L \quad \to \quad \frac{\kappa_{\text{eff}}}{\kappa_1}\frac{\partial U}{\partial x} = c_L$$

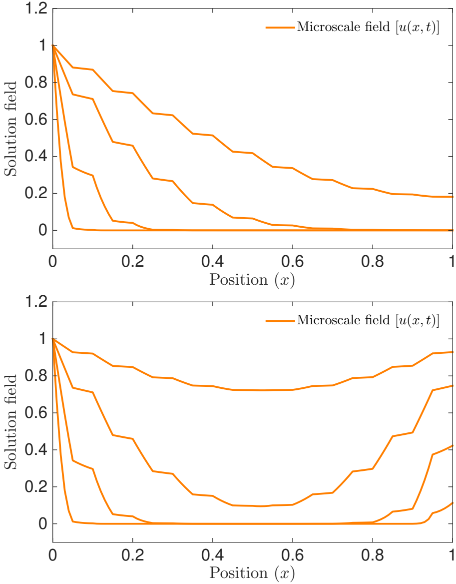
- Flux specified BC $\to$ Flux specified BC

$$\kappa_1 \frac{\partial u_1}{\partial x} = c_L \quad \to \quad \kappa_{\text{eff}}\frac{\partial U}{\partial x} = c_L$$

- Newton-type BC $\to$ Newton-type BC

$$\kappa_1 \frac{\partial u_1}{\partial x} = \sigma(u_1 - u_\infty) \quad \to \quad \kappa_{\text{eff}}\frac{\partial U}{\partial x} = \sigma(U - u_\infty)$$

Results: Dirichlet-Neumann and Dirichlet-Robin



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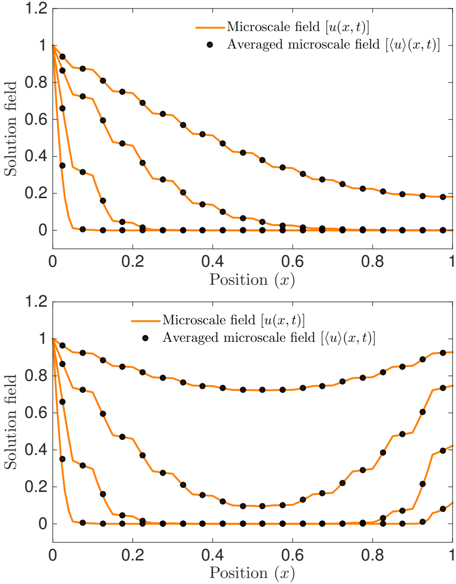

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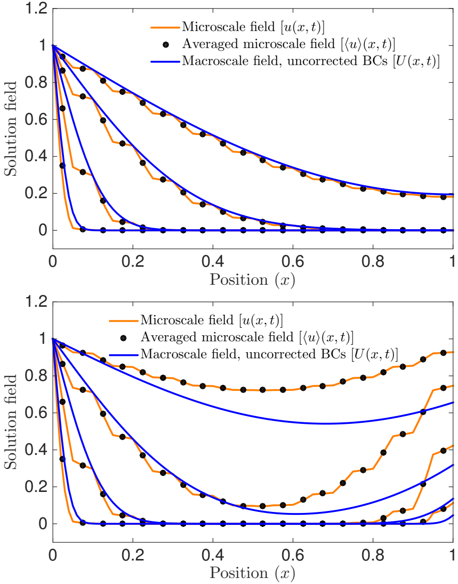

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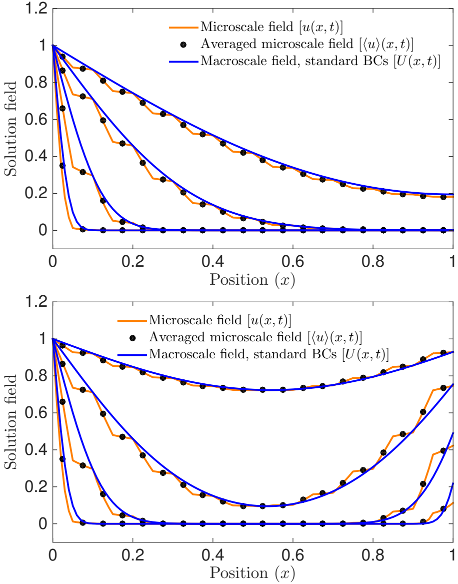

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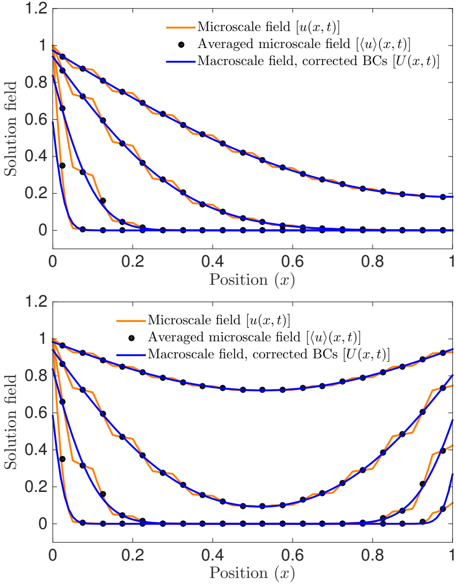

Something funny going on...

- Consider the Macroscale Model:

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial x}\left(\kappa_{\text{eff}}\frac{\partial U}{\partial x}\right), \quad U(x,0) = u_0,$$

$$U(0,t) - \underbrace{\frac{h}{2}\frac{\kappa_2 - \kappa_1}{\kappa_1 + \kappa_2}}_{\widetilde{b}_L}\frac{\partial U}{\partial x}(0,t) = c_L, \quad \frac{\partial U}{\partial x}(L,t) = 0.$$

- Macroscale field:

$$U(x,t) = U_\infty(x) + \sum_{n=1}^{\infty} c_n e^{-t\lambda_n\kappa_{\text{eff}}}\phi_n(x)\,,$$

- Eigenvalue problem:

$$\mathcal{L}\phi_n = \lambda_n\phi_n\,, \qquad \mathcal{L} = -\frac{\partial^2}{\partial x^2}\,,$$

$$\phi_n(l_0) - \widetilde{b}_L\phi_n'(l_0) = 0\,, \qquad \phi_n'(l_m) = 0\,.$$

- If $\kappa_1 > \kappa_2$ then $\widetilde{b}_L < 0$ which means there is one negative eigenvalue.

Summary, Conclusions & Future Work

- Investigated the form of the BCs in a macroscale model of layered diffusion
- Using the method of volume averaging and an "average plus perturbation" decomposition of the microscale field, we derived a set of *corrected* BCs for the macroscale field.
- *Corrected* BCs improves approximation of the averaged microscale field
- Reconstructed field that is in excellent agreement with the true microscale field
- Problems in higher-dimensional space? 2D? 3D?
- Other transport equations: Advection-Diffusion?

Thank you!

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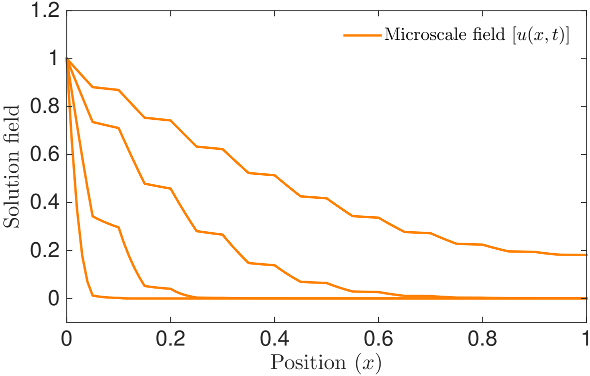
Results: Dirichlet-Neumann

Reconstructed microscale field:

$$u_i = \langle u \rangle + \widetilde{u}_i \quad \rightarrow \quad \widehat{u}_i = U + \psi_i(x)\frac{\partial U}{\partial x} \quad (i = 1, \ldots, m).$$

$$u_1(0,t) = 1 \text{ and } \frac{\partial u_m}{\partial x}(1,t) = 0.$$



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