Two-scale PDE-based numerical modelling of gradient-driven transport in heterogeneous materials

EMAC, University of South Australia, 6–9 December 2015

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Fine-scale model

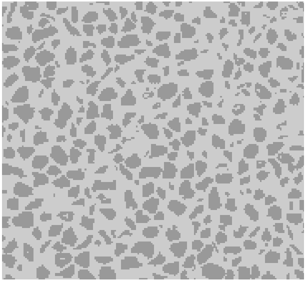
- Gradient-driven transport:

$$\frac{\partial u}{\partial t} + \nabla \cdot (-K \nabla u) = 0 \quad \text{in } \Omega$$

- Ω comprised of two sub-domains Ω_a (connected) and Ω_b (inclusions):

$$K = \begin{cases} K_a & \text{in } \Omega_a \\ K_b & \text{in } \Omega_b \end{cases}$$

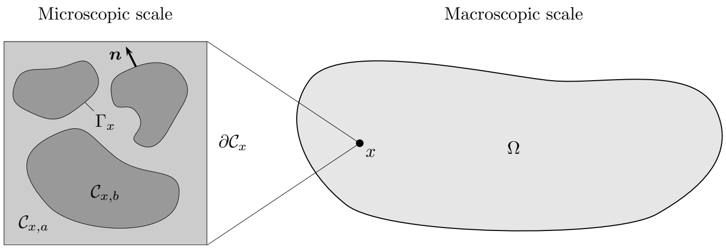
$$\frac{\partial u_a}{\partial t} + \nabla \cdot (-K_a \nabla u_a) = 0 \quad \text{in } \Omega_a$$
$$\frac{\partial u_b}{\partial t} + \nabla \cdot (-K_b \nabla u_b) = 0 \quad \text{in } \Omega_b$$



Heterogeneous domain
Ω_a Ω_b

- Computational cost of direct numerical simulation is prohibitively expensive when the medium exhibits small-scale heterogeneity.

Macroscopic averaging



Assumptions:

1. At each point $x \in \Omega$, there exists a micro-cell $\mathcal{C}_x$.
2. We assume that $\mathcal{C}_{x,b}$ is entirely located in the interior of the micro-cell $\mathcal{C}_x$

Classical Macroscopic Model

Rendard and de Marsily (1997); Szymkiewicz and Lewandowska (2006); Davit et al. (2013)

- Macroscopic Model:

$$\frac{\partial U}{\partial t} + \nabla_x \cdot (-\boldsymbol{K}_{\text{eff}} \nabla_x U) = 0; \quad U = \frac{1}{|\mathcal{C}_x|} \int_{\mathcal{C}_x} u \, dV$$

- Effective conductivity:

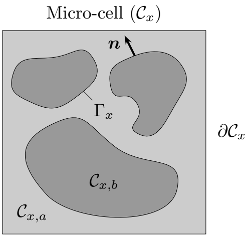
$$(\boldsymbol{K}_{\text{eff}})_{:,j} = \frac{1}{|\mathcal{C}_x|} \int_{\mathcal{C}_x} K e_j \, dV + \frac{1}{|\mathcal{C}_x|} \int_{\mathcal{C}_x} \nabla_y \chi_j \, dV$$

where χ_j is the solution of the periodic cell-problem on $\mathcal{C}_x$:

$$\nabla_y \cdot (K \, \nabla_y (\chi_j + y_j)) = 0 \quad y \in \mathcal{C}_x$$

subject to:

$$\frac{1}{|\mathcal{C}_x|} \int_{\mathcal{C}_x} \chi_j \, dV = 0$$



Macroscopic averaging

Whitaker (1998); Davit et al. (2013)

- Average over the micro-cell:

$$\frac{1}{|\mathcal{C}_x|}\int_{\mathcal{C}_{x,a}} \frac{\partial u_a}{\partial t}\, dV + \frac{1}{|\mathcal{C}_x|}\int_{\mathcal{C}_{x,a}} (\nabla\cdot\boldsymbol{q}_a)\, dV = 0$$

- Temporal averaging theorem:

$$\frac{1}{|\mathcal{C}_x|}\int_{\mathcal{C}_{x,a}} \frac{\partial u_a}{\partial t}\, dV = \underbrace{\frac{|C_{x,a}|}{|\mathcal{C}_x|}}_{\varepsilon_a} \frac{\partial}{\partial t} \underbrace{\frac{1}{|\mathcal{C}_{x,a}|}\int_{\mathcal{C}_{x,a}} u_a\, dV}_{U_a}$$

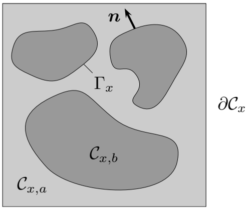
- Spatial averaging theorem:

$$\frac{1}{|\mathcal{C}_x|}\int_{\mathcal{C}_{x,a}} (\nabla\cdot\boldsymbol{q}_a)\, dV = \nabla_x\cdot \underbrace{\frac{1}{|\mathcal{C}_x|}\int_{\mathcal{C}_{x,a}} \boldsymbol{q}_a\, dV}_{\boldsymbol{Q}_a} - \underbrace{\frac{1}{|\mathcal{C}_x|}\int_{\Gamma_x} \boldsymbol{q}_a\cdot\boldsymbol{n}\, ds}_{S}$$

- Macroscopic (averaged) equations:

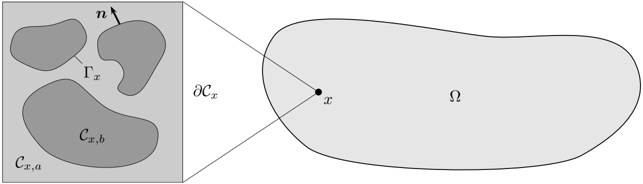
$$\varepsilon_a\frac{\partial U_a}{\partial t} + \nabla_x\cdot\boldsymbol{Q}_a = S \qquad \varepsilon_b\frac{\partial U_b}{\partial t} = -S$$

Micro-cell $(\mathcal{C}_x)$



Two-scale Model (Model 1)

Showalter (1997); Szymkiewicz and Lewandowska (2008); Carr and Turner (2014)



Macroscopic equation: $$\varepsilon_a \frac{\partial U_a}{\partial t} + \nabla_x \cdot (-\mathbf{K}_{\text{eff}} \nabla_x U_a) = S\,, \quad x \in \Omega$$

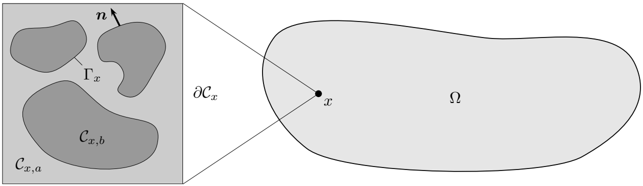
Microscopic equation: $$\frac{\partial u_b}{\partial t} + \nabla \cdot (-K_b \nabla u_b) = 0\,, \quad y \in \mathcal{C}_{x,b}$$

Microscopic BC: $$u_b = U_a\,, \quad y \in \Gamma_x$$

Source term: $$S = -\frac{1}{|\mathcal{C}_x|} \int_{\Gamma_x} \boldsymbol{q}_b \cdot \boldsymbol{n}\, ds$$

Two-scale Model (Model 2)

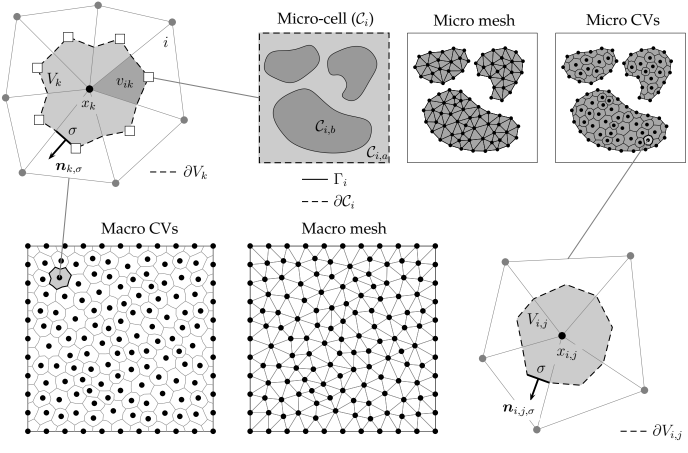
Carr et al. (2015)



Macroscopic equation:	$\varepsilon_a \dfrac{\partial U_a}{\partial t} + \nabla_x \cdot \boldsymbol{Q}_a = S\,, \quad x \in \Omega$
Microscopic equation:	$\dfrac{\partial u}{\partial t} + \nabla \cdot (-K\nabla u) = 0\,, \quad y \in \mathcal{C}_x$
Macroscopic flux:	$\boldsymbol{Q}_a = \dfrac{1}{\lvert\mathcal{C}_x\rvert} \displaystyle\int_{C_x} \boldsymbol{q}\, dV$
Microscopic BC:	$u = U_a\,, \quad y \in \partial\mathcal{C}_x$
Source term:	$S = -\dfrac{1}{\lvert\mathcal{C}_x\rvert} \displaystyle\int_{\Gamma_x} \boldsymbol{q}_b \cdot \boldsymbol{n}\, ds$

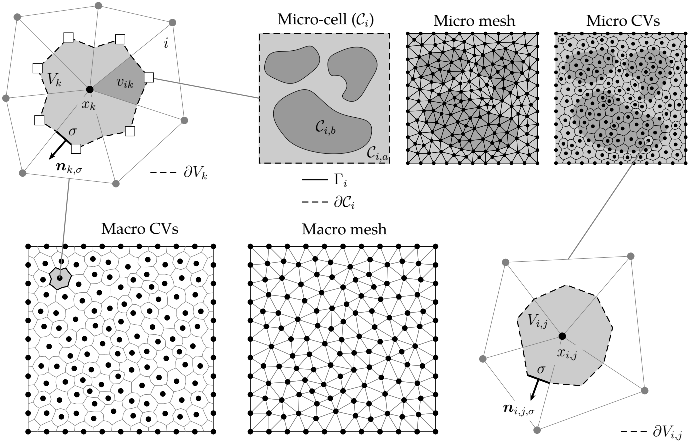
Spatial Discretisation (Model 1)

Carr and Turner (2014); Carr et al. (2015)



Spatial Discretisation (Model 2)

Carr et al. (2015)



Time discretisation (Model 1 and Model 2)

Carr et al. (2011, 2015); Carr and Turner (2014); Hochbruck et al. (1998)

- Spatial discretisation can be expressed in the form:

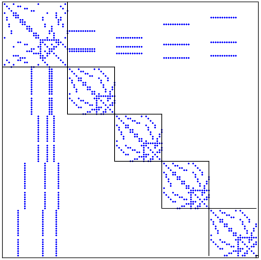
$$\frac{d\boldsymbol{u}}{dt} = \boldsymbol{g}(\boldsymbol{u}), \quad \boldsymbol{u}(0) = \boldsymbol{u}_0$$

where number of unknowns is *very* large.

- Exponential Euler method:

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + \tau_n \boldsymbol{J}_n^{-1}\left(e^{\tau_n \boldsymbol{J}_n} - \boldsymbol{I}\right)\boldsymbol{g}_n$$

- Explicit scheme



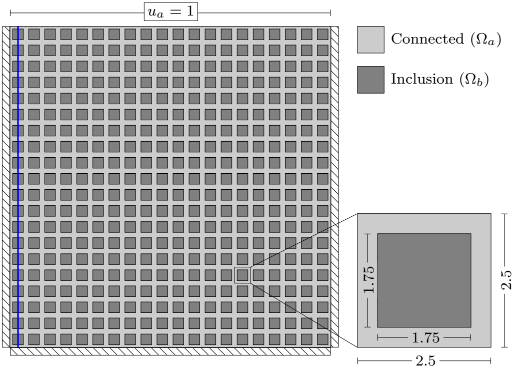
Jacobian structure $\boldsymbol{J}_n$ (Zoomed in)

- Krylov subspace methods for computing $\boldsymbol{J}_n^{-1}\left(e^{\tau_n \boldsymbol{J}_n} - \boldsymbol{I}\right)\boldsymbol{g}_n$ converge rapidly without preconditioning, and require only matrix-vector products with $\boldsymbol{J}_n$:

$$\boldsymbol{J}_n\boldsymbol{v} \approx \frac{\boldsymbol{g}(\boldsymbol{u}_n + \varepsilon\|\boldsymbol{v}\|_2\boldsymbol{v}) - \boldsymbol{g}(\boldsymbol{u}_n)}{\varepsilon\|\boldsymbol{v}\|_2}, \quad \varepsilon \approx 10^{-8}$$

Test Case A: Diffusion Equation

Carr et al. (2015)



$$\frac{\partial u_a}{\partial t} + \nabla \cdot (-K_a \nabla u_a) = 0 \quad \text{in } \Omega_a$$

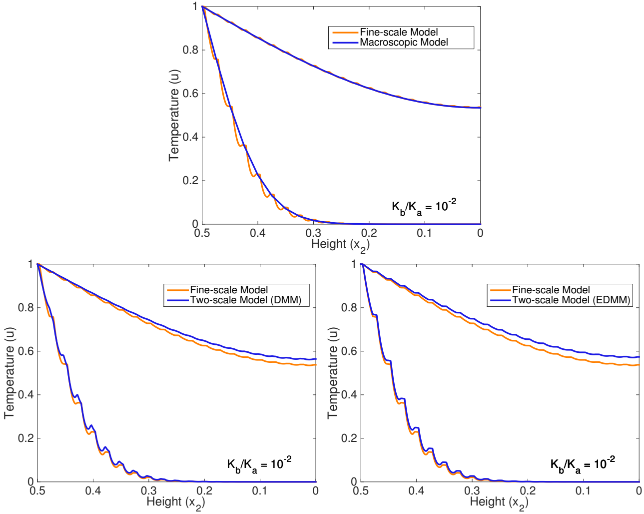
$$\frac{\partial u_b}{\partial t} + \nabla \cdot (-K_b \nabla u_b) = 0 \quad \text{in } \Omega_b$$

$$K_b/K_a = 10^{-p}$$

Test Case A: Diffusion Equation

Carr et al. (2015)

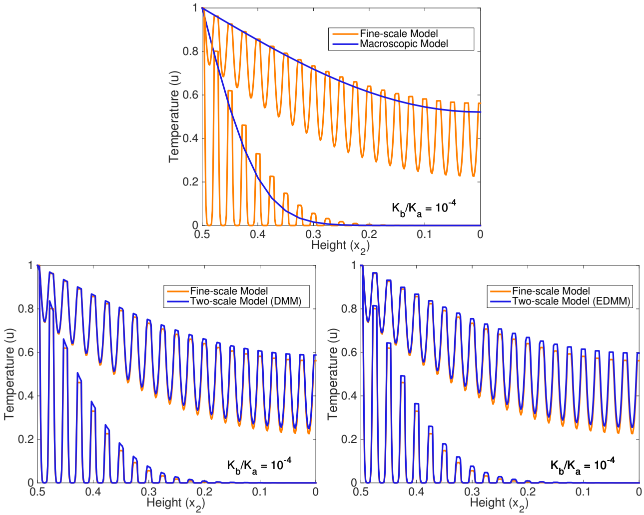
$$K_b/K_a = 10^{-2}$$



Test Case A: Diffusion Equation

Carr et al. (2015)

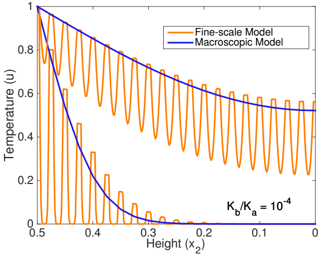
$$K_b/K_a = 10^{-4}$$

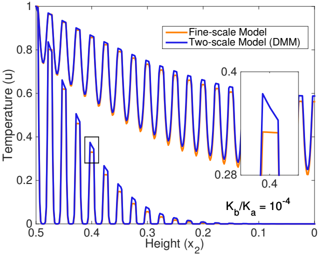


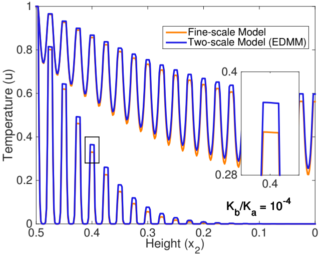
Test Case A: Diffusion Equation

Carr et al. (2015)

$$K_b/K_a = 10^{-4}$$

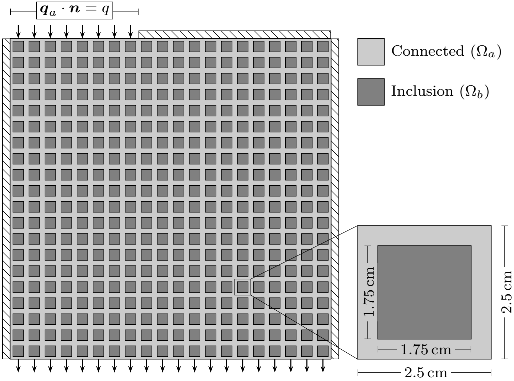






Test Case B: Richards' Equation

Carr et al. (2015)



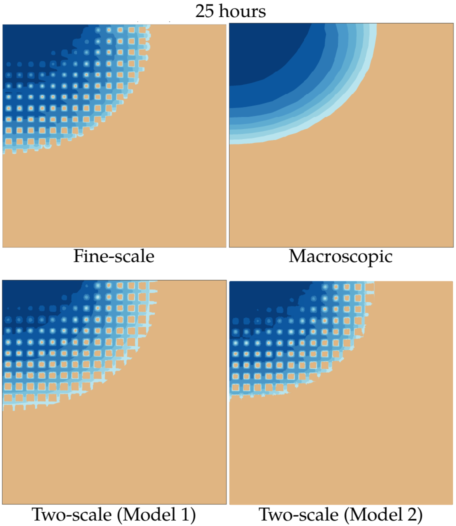
$$\frac{\partial \theta_a}{\partial t} + \nabla \cdot (-K_a \nabla \psi_a - K_a \mathbf{e}_2) = 0 \quad \text{in } \Omega_a$$

$$\frac{\partial \theta_b}{\partial t} + \nabla \cdot (-K_b \nabla \psi_b - K_b \mathbf{e}_2) = 0 \quad \text{in } \Omega_b$$

$$K_b / K_a = 10^{-3}$$

Test Case B: Richards' Equation

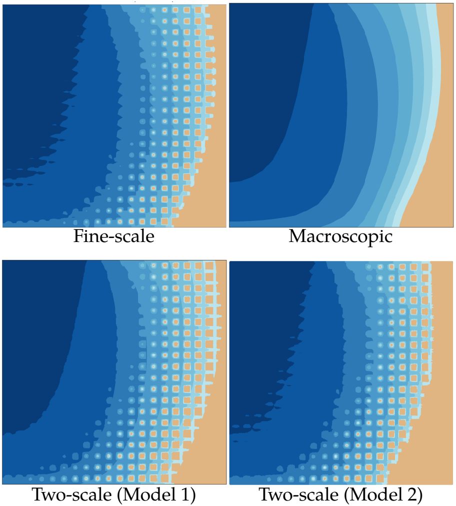
Carr et al. (2015)



Test Case B: Richards' Equation

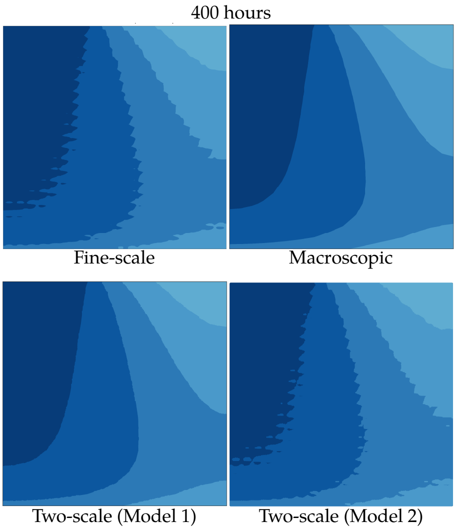
Carr et al. (2015)

100 hours



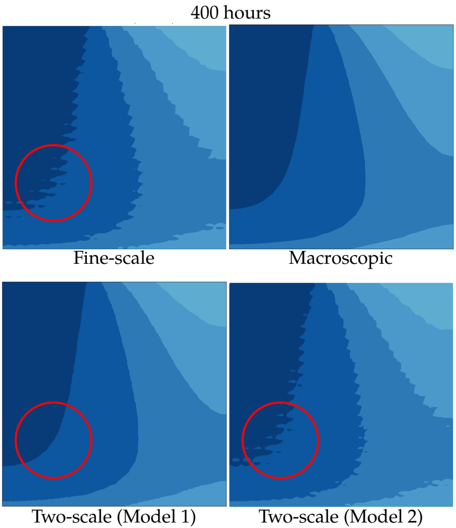
Test Case B: Richards' Equation

Carr et al. (2015)



Test Case B: Richards' Equation

Carr et al. (2015)



Summary and Conclusions

- Presented a new two-scale model for gradient-driven transport/flow problems in heterogeneous materials (Model 2)
- The novel approach avoids the need for an effective parameter in the macroscopic equation by computing the macroscopic flux as the average of the microscopic fluxes over the micro-cell.
- Numerical experiments demonstrated that both two-scale models (Model 1 and Model 2) produce numerical solutions that are in excellent agreement with the fine-scale model at a reduced computational cost.
- Model 1 requires less computational time
- Model 2 is more accurate and able to capture additional fine-scale features in the solution.

Thank you!

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