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

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Fine-scale model

- Gradient-driven transport:
  \[
  \frac{\partial u}{\partial t} + \nabla \cdot (-K \nabla u) = 0 \quad \text{in } \Omega
  \]

- \(\Omega\) comprised of two sub-domains \(\Omega_a\) (connected) and \(\Omega_b\) (inclusions):
  \[
  K = \begin{cases} 
  K_a & \text{in } \Omega_a \\
  K_b & \text{in } \Omega_b 
  \end{cases}
  \]
  \[
  \frac{\partial u_a}{\partial t} + \nabla \cdot (-K_a \nabla u_a) = 0 \quad \text{in } \Omega_a
  \]
  \[
  \frac{\partial u_b}{\partial t} + \nabla \cdot (-K_b \nabla u_b) = 0 \quad \text{in } \Omega_b
  \]

- 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 \( C_x \).
2. We assume that \( C_{x,b} \) is entirely located in the interior of the micro-cell \( C_x \)
Classical Macroscopic Model

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

- Macroscopic Model:

\[
\frac{\partial U}{\partial t} + \nabla_x \cdot (-K_{\text{eff}} \nabla_x U) = 0; \quad U = \frac{1}{|C_x|} \int_{C_x} u \, dV
\]

- Effective conductivity:

\[
(K_{\text{eff}}):_{i,j} = \frac{1}{|C_x|} \int_{C_x} K_{e,j} \, dV + \frac{1}{|C_x|} \int_{C_x} \nabla_y \chi_j \, dV
\]

where \( \chi_j \) is the solution of the periodic cell-problem on \( C_x \):

\[
\nabla_y \cdot (K \nabla_y (\chi_j + y_j)) = 0 \quad y \in C_x
\]

subject to:

\[
\frac{1}{|C_x|} \int_{C_x} \chi_j \, dV = 0
\]
Macroscopic averaging
Whitaker (1998); Davit et al. (2013)

- Average over the micro-cell:
  \[
  \frac{1}{|C_x|} \int_{C_{x,a}} \frac{\partial u_a}{\partial t} \, dV + \frac{1}{|C_x|} \int_{C_{x,a}} (\nabla \cdot q_a) \, dV = 0
  \]

- Temporal averaging theorem:
  \[
  \frac{1}{|C_x|} \int_{C_{x,a}} \frac{\partial u_a}{\partial t} \, dV = \frac{|C_{x,a}|}{|C_x|} \frac{\partial}{\partial t} \frac{1}{|C_{x,a}|} \int_{C_{x,a}} u_a \, dV
  \]

- Spatial averaging theorem:
  \[
  \frac{1}{|C_x|} \int_{C_{x,a}} (\nabla \cdot q_a) \, dV = \nabla_x \cdot \left( \frac{1}{|C_x|} \int_{C_{x,a}} q_a \, dV \right) - \frac{1}{|C_x|} \int_{\Gamma_x} q_a \cdot n \, ds
  \]

- Macroscopic (averaged) equations:
  \[
  \varepsilon_a \frac{\partial U_a}{\partial t} + \nabla_x \cdot Q_a = S \quad \varepsilon_b \frac{\partial U_b}{\partial t} = -S
  \]
Two-scale Model (Model 1)
Showalter (1997); Szymkiewicz and Lewandowska (2008); Carr and Turner (2014)

Macroscopic equation:
\[ \varepsilon_a \frac{\partial U_a}{\partial t} + \nabla_x \cdot (-K_{\text{eff}} \nabla_x U_a) = S, \quad x \in \Omega \]

Microscopic equation:
\[ \frac{\partial u_b}{\partial t} + \nabla \cdot (-K_b \nabla u_b) = 0, \quad y \in C_{x,b} \]

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

Source term:
\[ S = -\frac{1}{|C_x|} \int_{\Gamma_x} q_b \cdot n \, ds \]
Two-scale Model (Model 2)
Carr et al. (2015)

Microscopic scale

Macroscopic scale

Macroscopic equation:
\[ \varepsilon_a \frac{\partial U_a}{\partial t} + \nabla_x \cdot \mathbf{Q}_a = S, \quad x \in \Omega \]

Microscopic equation:
\[ \frac{\partial u}{\partial t} + \nabla \cdot (-K \nabla u) = 0, \quad y \in C_x \]

Macroscopic flux:
\[ \mathbf{Q}_a = \frac{1}{|C_x|} \int_{C_x} \mathbf{q} \, dV \]

Microscopic BC:
\[ u = U_a, \quad y \in \partial C_x \]

Source term:
\[ S = -\frac{1}{|C_x|} \int_{\Gamma_x} \mathbf{q}_b \cdot \mathbf{n} \, ds \]
Spatial Discretisation (Model 1)
Carr and Turner (2014); Carr et al. (2015)

![Diagram of spatial discretisation model]

- Macro mesh
- Micro mesh
- Micro-cell
- Macro CVs
- Micro CVs

\[ V_{i,j}, \sigma \]
\[ x_{i,j} \]
\[ n_{i,j,\sigma} \]
\[ \partial V_{i,j} \]
\[ \Gamma_i \]
\[ \partial C_i \]
Spatial Discretisation (Model 2)
Carr et al. (2015)

\[ V_k \]

\[ v_{ik} \]

\[ x_k \]

\[ n_{k,\sigma} \]

\[ \partial V_k \]

\[ \Gamma_i \]

\[ \partial C_i \]

\[ C_{i,b} \]

\[ C_{i,\alpha} \]

Micro mesh

Macro mesh

Micro CVs

Macro CVs
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:
  \[ \frac{du}{dt} = g(u), \quad u(0) = u_0 \]
  where number of unknowns is very large.

- Exponential Euler method:
  \[ u_{n+1} = u_n + \tau_n J_n^{-1} (e^{\tau_n J_n} - I) g_n \]

- Explicit scheme

- Krylov subspace methods for computing \( J_n^{-1} (e^{\tau_n J_n} - I) g_n \) converge rapidly without preconditioning, and require only matrix-vector products with \( J_n \):
  \[ J_n v \approx \frac{g(u_n + \varepsilon \|v\|_2 v) - g(u_n)}{\varepsilon \|v\|_2}, \quad \varepsilon \approx 10^{-8} \]
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)

\[ \frac{K_b}{K_a} = 10^{-2} \]

![Diagram showing temperature profiles for fine-scale model and two-scale models (DMM and EDMM)]
Test Case A: Diffusion Equation

Carr et al. (2015)

\[ \frac{K_b}{K_a} = 10^{-4} \]

\[ \frac{K_b}{K_a} = 10^{-4} \]
Test Case A: Diffusion Equation
Carr et al. (2015)

\[ \frac{K_b}{K_a} = 10^{-4} \]
Test Case B: Richards’ Equation
Carr et al. (2015)

\[ q_a \cdot n = q \]

\[ \frac{\partial \theta_a}{\partial t} + \nabla \cdot (-K_a \nabla \psi_a - K_a e_2) = 0 \quad \text{in} \quad \Omega_a \]

\[ \frac{\partial \theta_b}{\partial t} + \nabla \cdot (-K_b \nabla \psi_b - K_b e_2) = 0 \quad \text{in} \quad \Omega_b \]

\[ \frac{K_b}{K_a} = 10^{-3} \]
Test Case B: Richards’ Equation
Carr et al. (2015)

25 hours

Fine-scale

Macroscopic

Two-scale (Model 1)

Two-scale (Model 2)
Test Case B: Richards’ Equation
Carr et al. (2015)

100 hours

Fine-scale

Macroscopic

Two-scale (Model 1)

Two-scale (Model 2)
Test Case B: Richards’ Equation
Carr et al. (2015)

400 hours

Fine-scale
Macroscopic

Two-scale (Model 1)
Two-scale (Model 2)
Test Case B: Richards’ Equation

Carr et al. (2015)

400 hours

Fine-scale

Macroscopic

Two-scale (Model 1)

Two-scale (Model 2)
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!
References


