Multiscale computational modelling of gradient-driven transport in heterogeneous media

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Groundwater Flow

Aquifer scale (Macroscopic scale)

Continuum scale (Microscopic scale)

Richards’ Equation

\[ \frac{\partial \theta}{\partial t} + \nabla \cdot [ -K \left( \nabla h + \nabla z \right) ] = Q \]

Conductivity \((K)\) varies across soil types.
**Fine-scale model**

- Gradient-driven transport:

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

where \( \psi \) and \( K \) are functions of \( u(x, t) \).

- Domain \( \Omega \) comprised of two sub-domains \( \Omega_a \) (connected) and \( \Omega_b \) (inclusions):

\[
K(u) = \begin{cases} 
K_a(u) & \text{in } \Omega_a \\
K_b(u) & \text{in } \Omega_b 
\end{cases}
\]

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

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

- Computational cost of direct numerical simulation is prohibitively expensive
**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 \( C_x \).
Macroscopic averaging
Whitaker (1998); Davit et al. (2013)

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

- Temporal averaging theorem:
  \[
  \frac{1}{|C_x|} \int_{C_{x,a}} \frac{\partial \psi_a}{\partial t} dV = \frac{|C_{x,a}|}{|C_x|} \frac{\partial}{\partial t} \left( \frac{1}{|C_{x,a}|} \int_{C_{x,a}} \psi_a dV \right)
  \]

- 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:
  \[
  \varepsilon_a \frac{\partial \psi_a}{\partial t} + \nabla_x \cdot Q_a = S \quad \varepsilon_b \frac{\partial \psi_b}{\partial t} = -S
  \]
Classical Macroscopic Model
Renard and de Marsily (1997); Szymkiewicz and Lewandowska (2006); Davit et al. (2013)

Macroscopic Model:

\[
\frac{\partial}{\partial t} \left[ \varepsilon_a \Psi_a + \varepsilon_b \Psi_b \right] + \nabla_x \cdot (-K_{\text{eff}} \nabla_x U) = 0
\]

where \( \Psi_a := \psi_a(U) \) and \( \Psi_b := \psi_b(U) \) and \( U \) is the macroscopic primary variable.

Effective conductivity:

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

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

\[
\nabla_y \cdot (K \nabla_y (\chi_j + y_j)) = 0, \quad \text{on } C_x, \quad \text{subject to } \frac{1}{|C_x|} \int_{C_x} \chi_j \, dV = 0.
\]
Two-scale Model (Model 1)

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

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

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

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. (2016)

Microscopic scale

Macroscopic scale

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

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

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. (2016)
Spatial Discretisation (Model 2)
Carr et al. (2016)
Time discretisation (Model 1 and Model 2)
Carr et al. (2011, 2016); 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 \( J_n \):
  \[
  J_n v \approx \frac{g(u_n + \varepsilon v) - g(u_n)}{\varepsilon}, \quad \varepsilon \approx \sqrt{\varepsilon M} \| u_n \|_2
  \]
Test Case: Richards’ Equation
Carr et al. (2016)

\[ q_a \cdot n = q \]

\[ \frac{\partial \theta_a}{\partial t} + \nabla \cdot \left[ -K_a(h_a) \left( \nabla h_a + \nabla z \right) \right] = 0 \quad \text{in } \Omega_a \]

\[ \frac{\partial \theta_b}{\partial t} + \nabla \cdot \left[ -K_b(h_b) \left( \nabla h_b + \nabla z \right) \right] = 0 \quad \text{in } \Omega_b \]

\[ K_b/K_a = 10^{-3} \]
Test Case: Richards’ Equation
Carr et al. (2016)

$t = 25 \text{ hrs}$

Fine-scale

Macroscopic

Two-scale (Model 1)

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

Carr et al. (2016)

$t = 100$ hrs

Fine-scale

Macroscopic

Two-scale (Model 1)

Two-scale (Model 2)

[Runtime: 6 hrs]

[Runtime: 2 sec]

[Runtime: 14 sec]

[Runtime: 4 min]
Test Case: Richards’ Equation
Carr et al. (2016)

$t = 400 \text{ hrs}$

Fine-scale

Macroscopic

Two-scale (Model 1) [Runtime: 6 hrs]

Two-scale (Model 2) [Runtime: 2 sec]

[Runtime: 14 sec]

[Runtime: 4 min]
Test Case: Richards’ Equation
Carr et al. (2016)

\[ t = 400 \text{ hrs} \]

Fine-scale

Macroscopic

Two-scale (Model 1)

Two-scale (Model 2)

[Runtime: 6 hrs]
[Runtime: 2 sec]
[Runtime: 14 sec]
[Runtime: 4 min]
Summary and Conclusions

- Presented a modified 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.
The extended distributed microstructure model for gradient-driven transport: A two-scale model for bypassing effective parameters

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\textbf{ARTICLE INFO}

\textbf{ABSTRACT}

Numerous problems involving gradient-driven transport processes—e.g., Fourier’s and Darcy’s law—in heterogeneous materials concern a physical domain that is much larger than the scale at which the coefficients vary spatially. To overcome the prohibitive computational cost associated with such problems, the well-established Distributed Microstructure Model (DMM) provides a two-scale description of the transport process that produces a computationally cheap approximation to the fine-scale solution. This is achieved via the introduction of sparsely distributed micro-cells that together resolve small patches of the fine-scale structure; a macroscopic equation with an effective coefficient describes the global transport and a microscopic equation governs the local transport within each micro-cell. In this paper, we propose a new formulation, the Extended Distributed Microstructure Model (EDMM), where the macroscopic flux is instead defined as the average of the microscopic fluxes within the micro-cells. This avoids the need for any effective parameters and more accurately accounts for a non-equilibrium field in the micro-cells. Another important contribution of the work is the presentation of a new and improved numerical scheme for performing the two-scale computations using control volume, Krylov subspace and parallel computing techniques. Numerical tests are carried out on two challenging test problems: heat conduction in a composite medium and unsaturated water flow in heterogeneous soils. The results indicate that while DMM is more efficient, EDMM is more accurate and is able to capture additional fine-scale features in the solution.

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Thank you!
References


