Multiscale Modelling of Groundwater Flow

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Joint work with...

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Groundwater Flow

Aquifer scale  
(Macroscopic scale)

Water
Soil grain
Air

Pore scale
Unsaturated zone
Saturated zone

Continuum scale  
(Microscopic scale)

Pump

Richards’ Equation

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

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:
  \[
  \frac{1}{|C_x|} \int_{C_{x,a}} \frac{\partial \psi_a}{\partial t} dV = \frac{|C_{x,a}|}{|C_x|} \frac{\partial}{\partial t} \int_{C_{x,a}} \psi_a dV
  \]

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

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

Macroscopic Model:

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

where \( \Psi_a := \psi_a(U) \) and \( \Psi_b := \psi_b(U) \) and \( U \)

is the macroscopic primary variable.

Effective conductivity:

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

where \( \chi_j \) is the solution of the periodic cell-

problem on \( C_x \):

\[ \nabla_y \cdot \left( K \nabla y (\chi_j + y_j) \right) = 0, \quad \text{on } C_x, \quad \text{subject to } \frac{1}{|C_x|} \int_{C_x} \chi_j \, dV = 0. \]
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)

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)

\begin{itemize}
\item Micro-cell \( (C_i) \)
\item Micro mesh
\item Micro CVs
\end{itemize}

\begin{itemize}
\item Macro mesh
\item Macro CVs
\end{itemize}

\begin{itemize}
\item \( \Gamma_i \)
\item \( \partial C_i \)
\end{itemize}
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:

\[
u_{n+1} = u_n + \tau_n J^{-1}_n (e^{\tau_n J_n} - I) g_n
\]

▶ Explicit scheme

▶ Krylov subspace methods for computing \( J^{-1}_n (e^{\tau_n J_n} - I) g_n \) 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 A: Linear Diffusion

Carr et al. (2016)

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

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

\[ K_b / K_a = 10^{-p} \]
Test Case A: Linear Diffusion
Carr et al. (2016)

\[ \frac{K_b}{K_a} = 10^{-2} \]
Test Case A: Linear Diffusion
Carr et al. (2016)

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

![Temperature profile for different models and conditions](chart.png)

- Fine-scale Model
- Macroscopic Model
- Two-scale Model (DMM)
- Two-scale Model (EDMM)

Kb/Ka = 10^{-4}
Test Case A: Linear Diffusion

Carr et al. (2016)

\[ K_b/K_a = 10^{-4} \]
Test Case B: Richards’ Equation
Carr et al. (2016)

\[ q_a \cdot n = q \]

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

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

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

$t = 25$ hrs

Fine-scale

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

Macroscopic

[Runtime: 1 sec] Two-scale (Model 2)

[Runtime: 14 sec]
Test Case B: Richards’ Equation
Carr et al. (2016)

\[ t = 100 \text{ hrs} \]

Fine-scale

Macroscopic

Two-scale (Model 1)

Two-scale (Model 2)

[Runtime: 6 hrs]

[Runtime: 1 sec]

[Runtime: 14 sec]

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

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

Fine-scale

[Runtime: 6 hrs]

Macroscopic

[Runtime: 1 sec]

Two-scale (Model 1)

[Runtime: 14 sec]

Two-scale (Model 2)

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

$t = 400$ hrs

Fine-scale

[Runtime: 6 hrs]

Macroscopic

[Runtime: 1 sec]

Two-scale (Model 1)

[Runtime: 14 sec]

Two-scale (Model 2)

[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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A B S T R A C T

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


