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Multiscale computational modelling of gradient-driven transport in heterogeneous media

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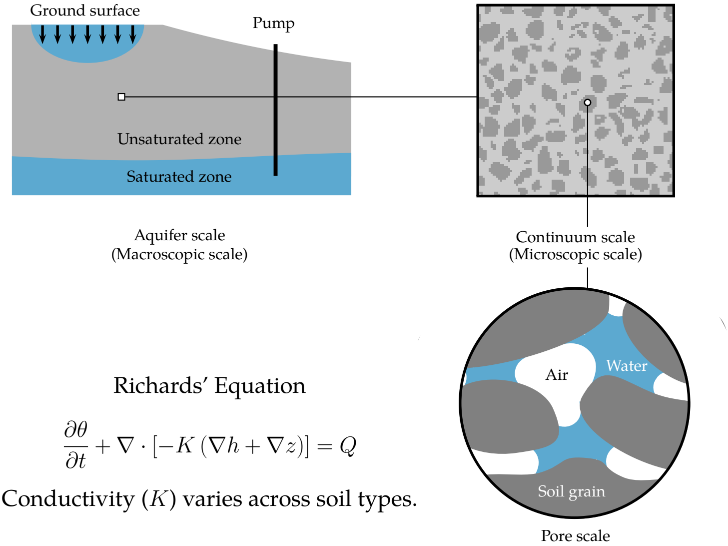
Groundwater Flow



Richards' Equation

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

Conductivity (K) varies across soil types.

Fine-scale model

- Gradient-driven transport:

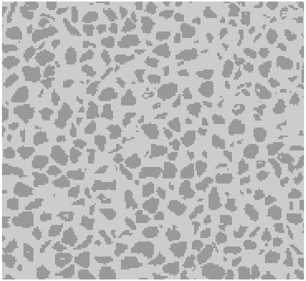
$$\frac{\partial \psi}{\partial t} + \nabla \cdot (-K\nabla u) = 0 \quad \text{in } \Omega$$

where ψ and K are functions of $u(\mathbf{x}, t)$.

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

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

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

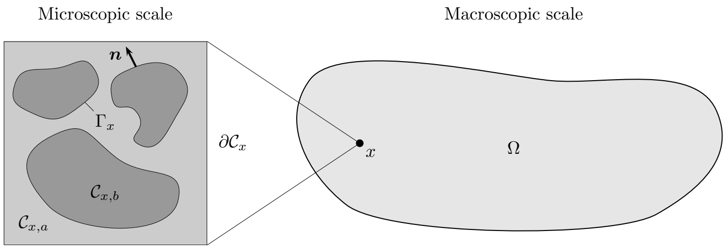


Heterogeneous domain

Ω_a Ω_b

- Computational cost of direct numerical simulation is prohibitively expensive

Macroscopic averaging

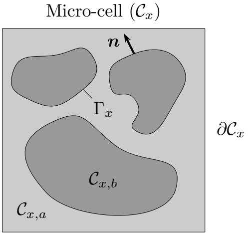


Assumptions:

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

Macroscopic averaging

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



- Average over the micro-cell:

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

- Temporal averaging theorem:

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

- 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:

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

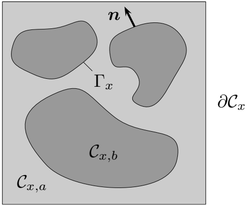
Classical Macroscopic Model

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

- Macroscopic Model:

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

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



- Effective conductivity:

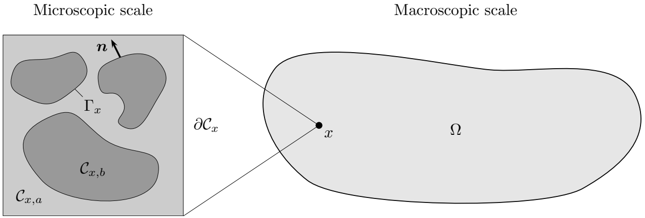
$$(\boldsymbol{K}_{\text{eff}})_{:,j} = \frac{1}{|\mathcal{C}_x|}\int_{\mathcal{C}_x} K e_j \, dV + \frac{1}{|\mathcal{C}_x|}\int_{\mathcal{C}_x} K \nabla_y \chi_j \, dV$$

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

$$\nabla_y \cdot \left(K \, \nabla_y(\chi_j + y_j)\right) = 0, \quad \text{on } \mathcal{C}_x, \quad \text{subject to} \quad \frac{1}{|\mathcal{C}_x|}\int_{\mathcal{C}_x} \chi_j \, dV = 0.$$

Two-scale Model (Model 1)

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



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

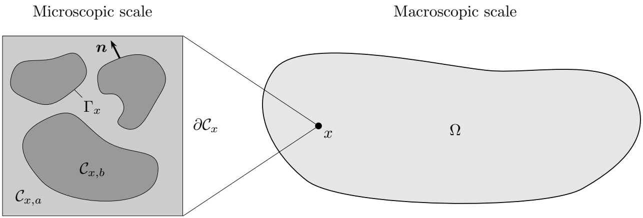
Microscopic equation: $$\frac{\partial \psi_b}{\partial t} + \nabla \cdot (-K_b \nabla u_b) = 0\,, \quad y \in \mathcal{C}_{x,b}$$

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. (2016)



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

Microscopic equation: $$\frac{\partial \psi}{\partial t} + \nabla \cdot (-K\nabla u) = 0\,, \quad y \in \mathcal{C}_x$$

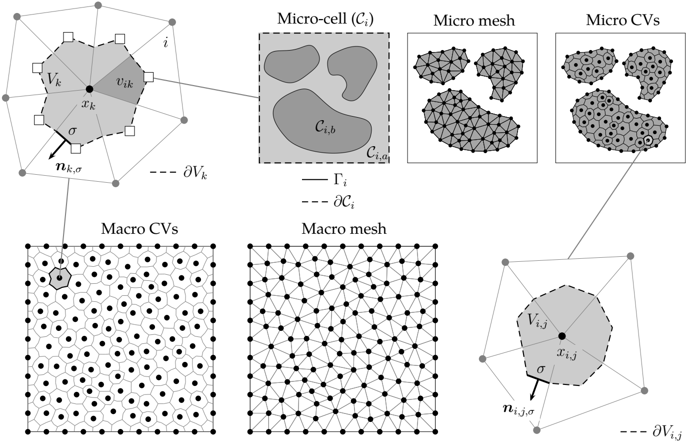
Macroscopic flux: $$\boldsymbol{Q}_a = \frac{1}{|\mathcal{C}_x|} \int_{C_x} \boldsymbol{q}\, dV$$

Microscopic BC: $$u = U_a\,, \quad y \in \partial\mathcal{C}_x$$

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

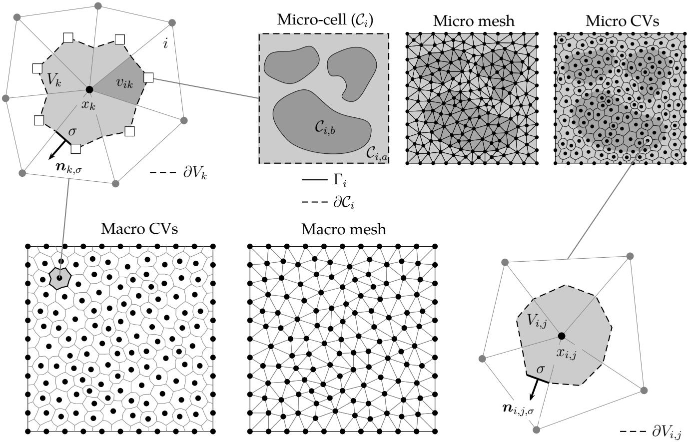
Spatial Discretisation (Model 1)

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:

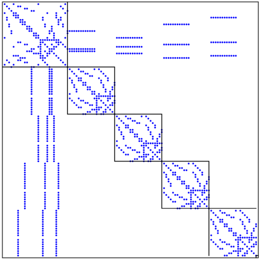
$$\frac{d\boldsymbol{u}}{dt} = \boldsymbol{g}(\boldsymbol{u}), \quad \boldsymbol{u}(0) = \boldsymbol{u}_0$$

  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



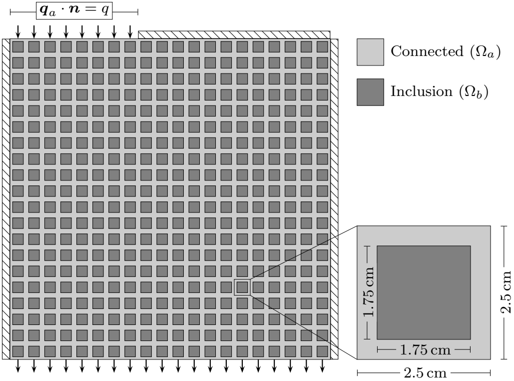
Jacobian structure $\boldsymbol{J}_n$
(Zoomed in)

- 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 $\boldsymbol{J}_n$:

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

Test Case: Richards' Equation

Carr et al. (2016)



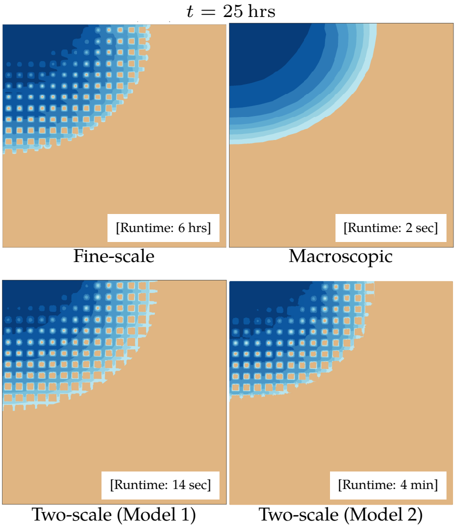
$$\frac{\partial \theta_a}{\partial t} + \nabla \cdot [-K_a(h_a)\,(\nabla h_a + \nabla z)] = 0 \quad \text{in } \Omega_a$$

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

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

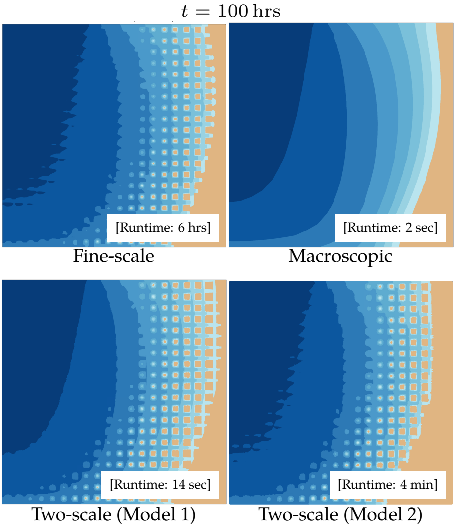
Test Case: Richards' Equation

Carr et al. (2016)



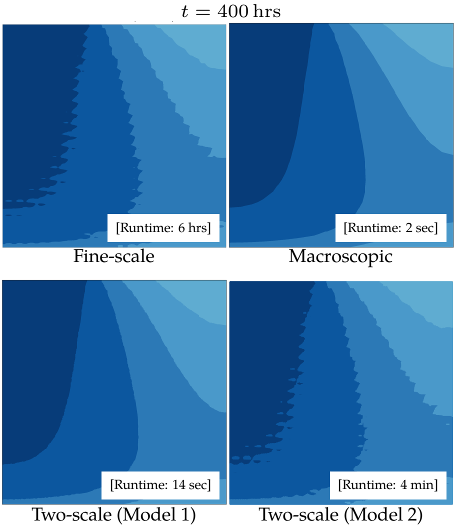
Test Case: Richards' Equation

Carr et al. (2016)



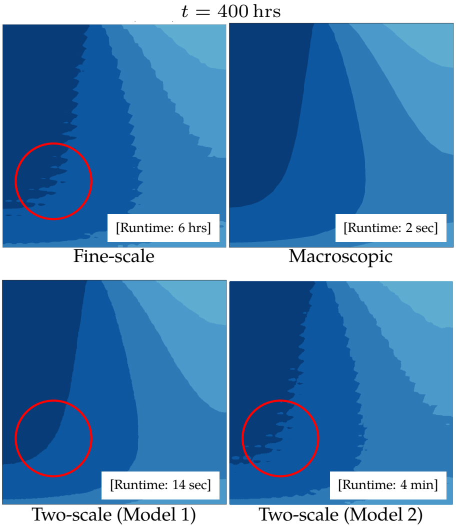
Test Case: Richards' Equation

Carr et al. (2016)



Test Case: Richards' Equation

Carr et al. (2016)



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.

For more details see:

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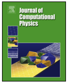

The extended distributed microstructure model for gradient-driven transport: A two-scale model for bypassing effective parameters

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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.

Thank you!

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