Forum “Math-for-Industry” 2016
Queensland University of Technology, 21–23 November 2016

Multiscale Modelling of Groundwater Flow

Dr Elliot Carr
(elliot.carr@qut.edu.au)

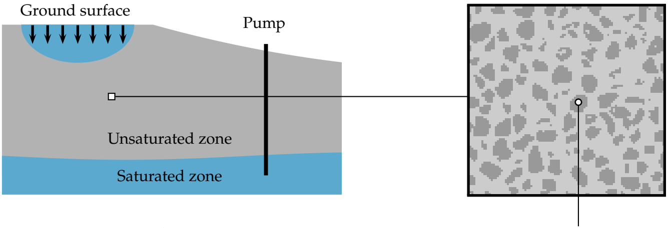
School of Mathematical Sciences
Queensland University of Technology

Joint work with...

Prof. Ian Turner
(Mathematical Sciences, QUT)

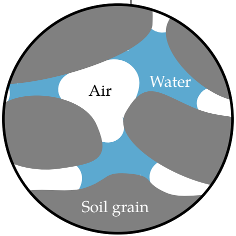
Prof. Patrick Perré
(CentraleSupélec, France)

Groundwater Flow



Aquifer scale
(Macroscopic scale)

Continuum scale
(Microscopic scale)



Pore scale

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:

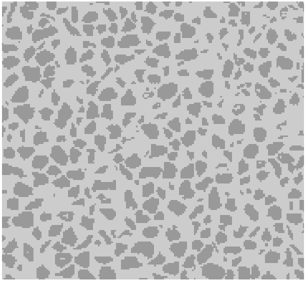
$$\frac{\partial \psi}{\partial t} + \nabla \cdot (-K\nabla u) = 0 \quad \text{in } \Omega$$

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):

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

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

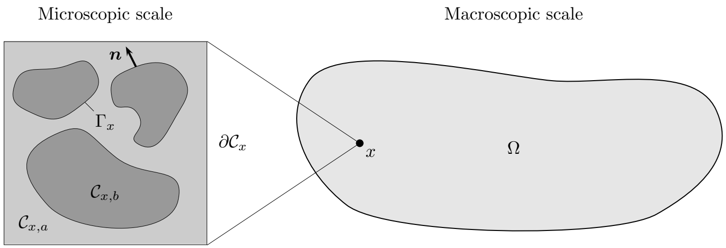


Heterogeneous domain

Ω_a ■ Ω_b ■

- Computational cost of direct numerical simulation is prohibitively expensive

Macroscopic averaging



Assumptions:

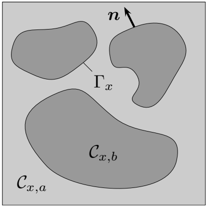
1. At each point $x \in \Omega$, there exists a micro-cell $\mathcal{C}_x$.
2. We assume that $\mathcal{C}_{x,b}$ is entirely located in the interior of the micro-cell $\mathcal{C}_x$

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:

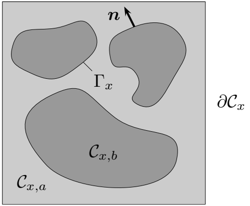
$$\frac{\partial}{\partial t}\left[\varepsilon_a \Psi_a + \varepsilon_b \Psi_b\right] + \nabla_x \cdot \left(-\boldsymbol{K}_{\text{eff}} \nabla_x U\right) = 0$$

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

- Effective conductivity:

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

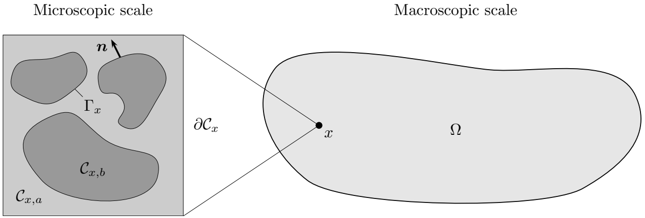
where χ_j is the solution of the periodic cell-problem on $\mathcal{C}_x$:



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

Two-scale Model (Model 1)

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



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

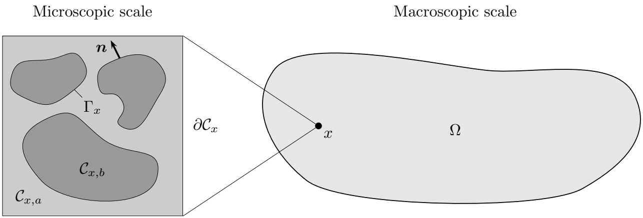
Microscopic equation: $$\frac{\partial \psi_b}{\partial t} + \nabla \cdot (-K_b \nabla u_b) = 0\,, \quad y \in \mathcal{C}_{x,b}$$

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

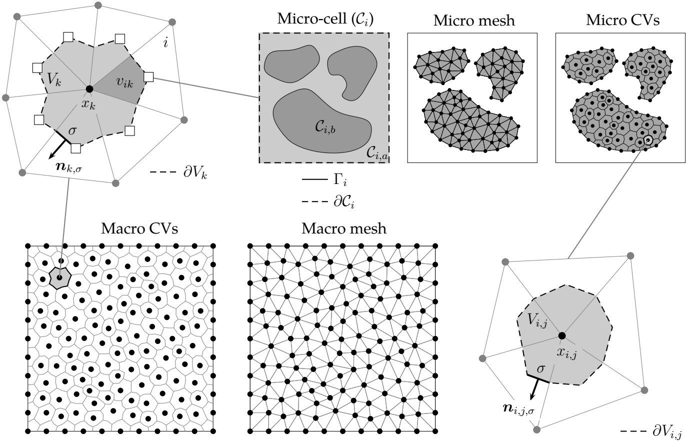
Macroscopic flux: $$\boldsymbol{Q}_a = \frac{1}{|\mathcal{C}_x|}\int_{C_x} \boldsymbol{q}\,dV$$

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

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

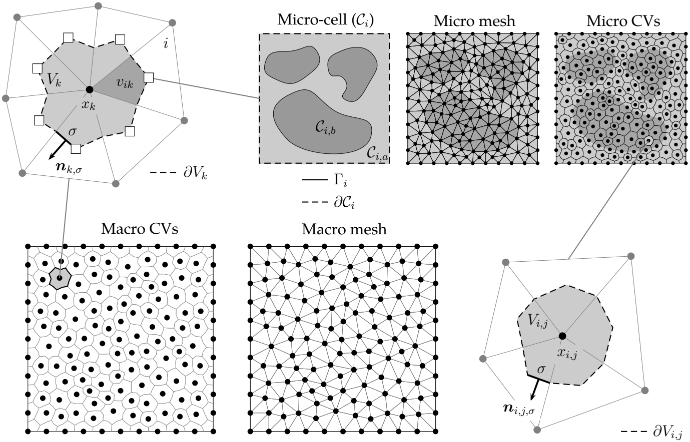
Spatial Discretisation (Model 1)

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:

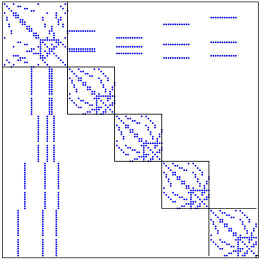
$$\frac{d\boldsymbol{u}}{dt} = \boldsymbol{g}(\boldsymbol{u}), \quad \boldsymbol{u}(0) = \boldsymbol{u}_0$$

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



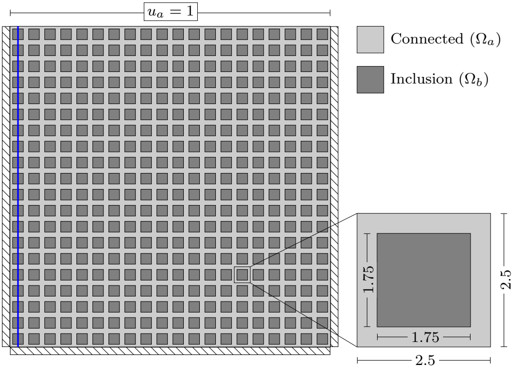
Jacobian structure $\boldsymbol{J}_n$ (Zoomed in)

- 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 A: Linear Diffusion

Carr et al. (2016)



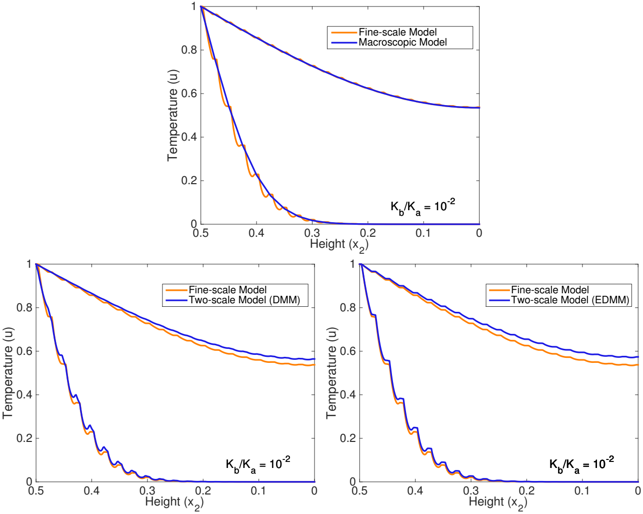
$$\frac{\partial u_a}{\partial t} + \nabla \cdot (-K_a \nabla u_a) = 0 \quad \text{in } \Omega_a$$
$$\frac{\partial u_b}{\partial t} + \nabla \cdot (-K_b \nabla u_b) = 0 \quad \text{in } \Omega_b$$

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

Test Case A: Linear Diffusion

Carr et al. (2016)

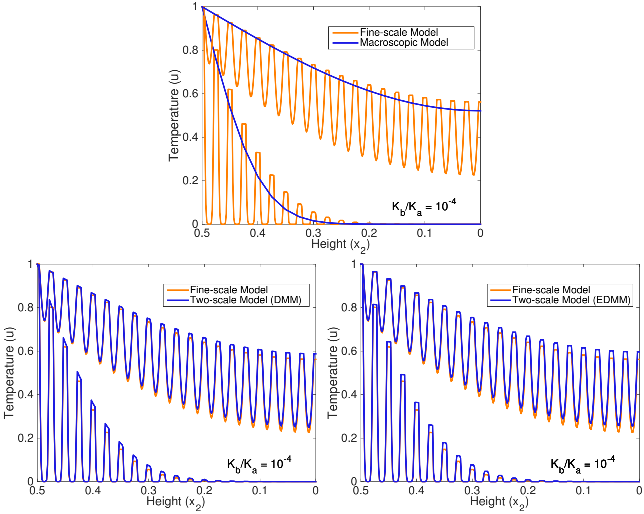
$$K_b/K_a = 10^{-2}$$



Test Case A: Linear Diffusion

Carr et al. (2016)

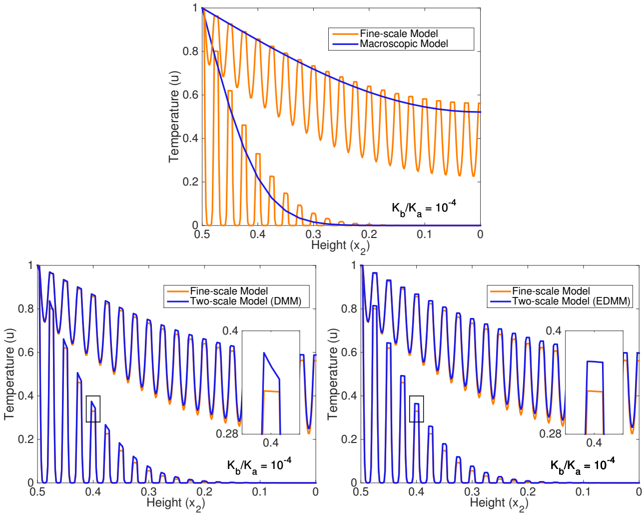
$$K_b/K_a = 10^{-4}$$



Test Case A: Linear Diffusion

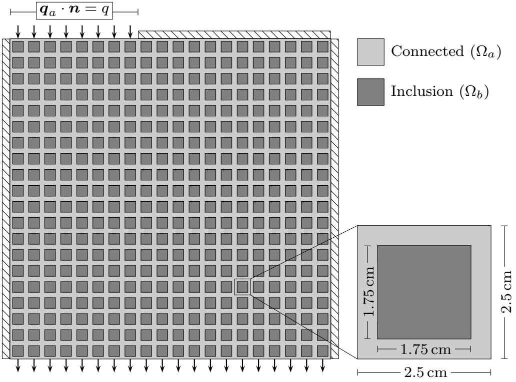
Carr et al. (2016)

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



Test Case B: Richards' Equation

Carr et al. (2016)



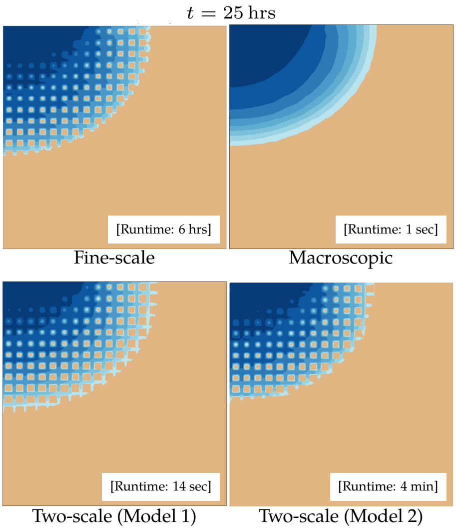
$$\frac{\partial \theta_a}{\partial t} + \nabla \cdot \left[-K_a \left(\nabla h_a + \nabla z\right)\right] = 0 \quad \text{in } \Omega_a$$

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

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

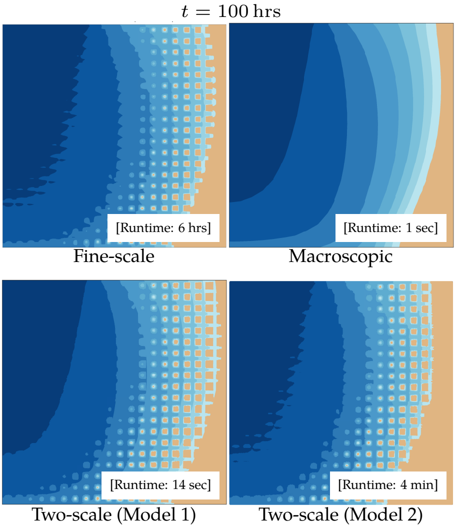
Test Case B: Richards' Equation

Carr et al. (2016)



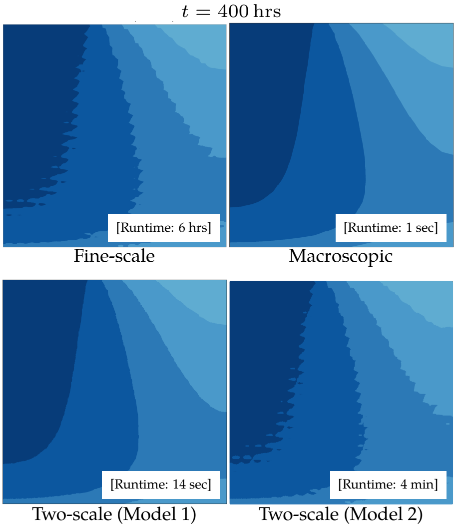
Test Case B: Richards' Equation

Carr et al. (2016)



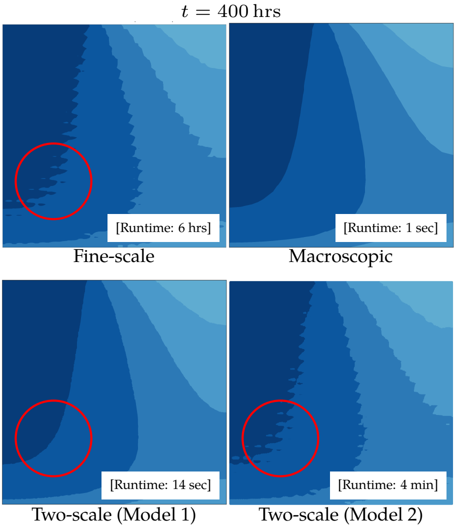
Test Case B: Richards' Equation

Carr et al. (2016)



Test Case B: 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:

Journal of Computational Physics 327 (2016) 810–829

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

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

CrossMark

E.J. Carr [a,b,*], P. Perré [b], I.W. Turner [a,c]

[a] School of Mathematical Sciences, Queensland University of Technology (QUT), Brisbane, Australia
[b] LGPM, CentraleSupelec, Université Paris-Saclay, Chatenay-Malabry, France
[c] Australian Research Council Centre of Excellence for Mathematical and Statistical Frontiers (ACEMS), Queensland University of Technology (QUT), Brisbane, Australia

A R T I C L E   I N F O

Article history:
Received 10 December 2015
Received in revised form 31 May 2016
Accepted 2 October 2016
Available online 4 October 2016

Keywords:
Two-scale
Multiscale
Microstructure
Dual-scale
Heterogeneous
Homogenization

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.

© 2016 Elsevier Inc. All rights reserved.

Thank you!

References

Carr, E. J., Moroney, T. J., and Turner, I. W. (2011). Efficient simulation of unsaturated flow using exponential time integration. *Appl. Math. Comput.*, 217(14):6587–6596.

Carr, E. J., Perré, P., and Turner, I. W. (2016). The extended distributed microstructure model for gradient-driven transport: A two-scale model for bypassing effective parameters. *J. Comput. Phys.*, 327:810–829.

Carr, E. J. and Turner, I. W. (2014). Two-scale computational modelling of water flow in unsaturated soils containing irregular-shaped inclusions. *Int. J. Numer. Meth. Eng.*, 98(3):157–173.

Davit, Y., Bell, C. G., Byrne, H. M., Chapman, L. A. C., and many others (2013). Homogenization via formal multiscale asymptotics and volume averaging: How do the two techniques compare? *Adv. Water Resour.*, 62:178–206.

Hochbruck, M., Lubich, C., and Selhofer, H. (1998). Exponential integrators for large systems of differential equations. *SIAM. J. Sci. Comput.*, 19(5):1552–1574.

Renard, P. and de Marsily, G. (1997). Calculating equivalent permeability: a review. *Advances in Water Resources*, 20(5–6):253–278.

Showalter, R. E. (1997). Microstructure models of porous media. In Hornung, U., editor, *Homogenization and Porous Media*, pages 183–202. Springer–Verlag, New York.

Szymkiewicz, A. and Lewandowska, J. (2006). Unified macroscopic model for unsaturated water flow in soils of bimodal porosity. *Hydrolog. Sci. J.*, 51(6):1106–1124.

Szymkiewicz, A. and Lewandowska, J. (2008). Micromechanical approach to unsaturated water flow in structured geomaterials by two-scale computations. *Acta Geotech.*, 3:37–47.

Whitaker, S. (1998). Coupled transport in multiphase systems: a theory of drying. In J. P. Hartnett, T. F. Irvine, Y. I. C. and Greene, G. A., editors, *Advances in Heat Transfer*, volume 31, pages 1–104. Elsevier.