Coarse-scale simulation of heterogeneous flows: application to groundwater modelling

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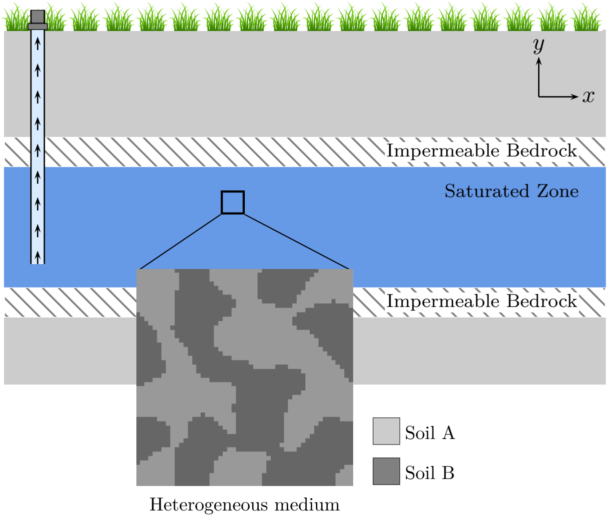
- Groundwater refers to water present in the pore space of soils in aquifers located below the Earth's surface.
- Groundwater is a major source of the world's freshwater supply and in many regional areas of Australia constitutes the only available supply of freshwater.
- Groundwater supplies are susceptible to problems such as over-withdrawal causing the water levels to dip below the reach of existing wells and contamination from pollutants emanating from the ground surface (e.g. hazardous industrial waste, garbage landfills, pesticides applied to crops).
- Mathematical and computational modelling provides valuable insight to inform decisions regarding the management of groundwater resources.
- Mathematical and computational challenges of groundwater modelling include having to deal with a highly heterogeneous geological structure.

Groundwater modelling

Aquifer system



- I will focus on flow in the saturated zone.
- Groundwater flow equation (MODFLOW, Harbaugh (2005)):

$$S_s \frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(K_x(\mathbf{x})\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y(\mathbf{x})\frac{\partial h}{\partial y}\right),$$

  where h is the dependent variable, $\mathbf{x}$ and t are independent variables, K_x and K_y are hydraulic conductivities and S_s is the specific storage.
- Variable of interest: hydraulic head field $h(\mathbf{x}, t)$, which determines where groundwater will flow.
- In this talk, I will make the simplifying assumption that the heterogeneous medium is locally isotropic:

$$K_x(\mathbf{x}) = K_y(\mathbf{x}) = K(\mathbf{x}).$$

- Fine-scale equation:

$$\frac{\partial h}{\partial t} + \boldsymbol{\nabla} \cdot (-D(\mathbf{x})\nabla h) = 0, \quad x \in \Omega \subset \mathbb{R}^2.$$

- If the scale at which $D(\mathbf{x}) = K(\mathbf{x})/S_s$ changes is small compared to the size of the domain Ω, then computational resources required to resolve the fine-scale are prohibitive due to the very fine mesh required to capture the heterogeneity.

- This can be overcome by homogenizing or partially-homogenizing the heterogeneous medium.

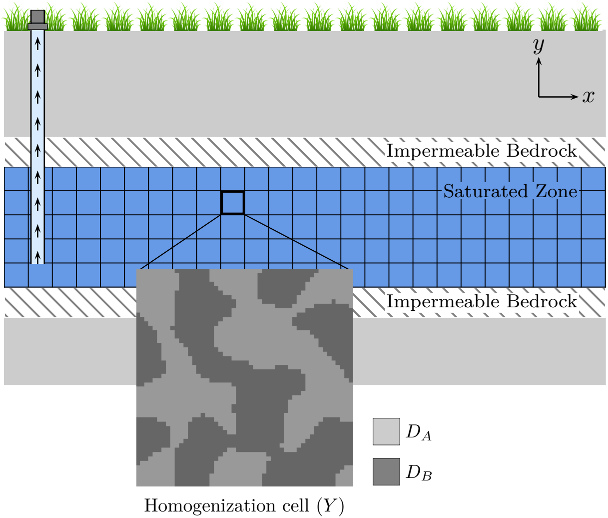
- Coarse-scale equation:

$$\frac{\partial H}{\partial t} + \boldsymbol{\nabla} \cdot (-\mathbf{D}_{\text{eff}}(\mathbf{x})\nabla H) = 0, \quad x \in \Omega \subset \mathbb{R}^2,$$

  where $H(\mathbf{x}, t)$ is a smoothed/coarse-scale approximation to the fine-scale field $h(\mathbf{x}, t)$ and $\mathbf{D}_{\text{eff}}(\mathbf{x})$ is a slowly varying effective diffusivity.

Groundwater modelling

Aquifer system



Effective Diffusivity

Homogenization of a cell $Y = [0, L]^2$

- Cell problem for first column of $\mathbf{D}_{\text{eff}}$ (Hornung, 1997):

$$\nabla \cdot (D(\boldsymbol{x})\nabla(\psi + x)) = 0, \quad \boldsymbol{x} = (x, y) \in Y = [0, L]^2,$$

$$\psi(\boldsymbol{x}) \text{ is periodic with period } Y, \quad \frac{1}{L^2}\int_Y \psi \, \mathrm{d}V = 0,$$

$$\mathbf{D}_{\text{eff}}(:, 1) = \frac{1}{L^2}\int_Y D(\boldsymbol{x})\nabla(\psi + x) \, \mathrm{d}V.$$

- Cell problem for second column of $\mathbf{D}_{\text{eff}}$ (Hornung, 1997):

$$\nabla \cdot (D(\boldsymbol{x})\nabla(\psi + y)) = 0, \quad \boldsymbol{x} = (x, y) \in Y = [0, L]^2,$$

$$\psi(\boldsymbol{x}) \text{ is periodic with period } Y, \quad \frac{1}{L^2}\int_Y \psi \, \mathrm{d}V = 0,$$

$$\mathbf{D}_{\text{eff}}(:, 2) = \frac{1}{L^2}\int_Y D(\boldsymbol{x})\nabla(\psi + y) \, \mathrm{d}V.$$

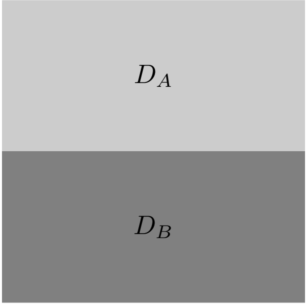
- Definitions involving non-periodic boundary conditions also exist (e.g. confined or uniform boundary conditions).

- For a layered medium, the cell problems can be solved exactly:

$$\mathbf{D}_{\mathrm{eff}} = \begin{bmatrix} D_{\mathrm{a}} & 0 \\ 0 & D_{\mathrm{h}} \end{bmatrix},$$

where D_{a} and D_{h} are the arithmetic and harmonic means:

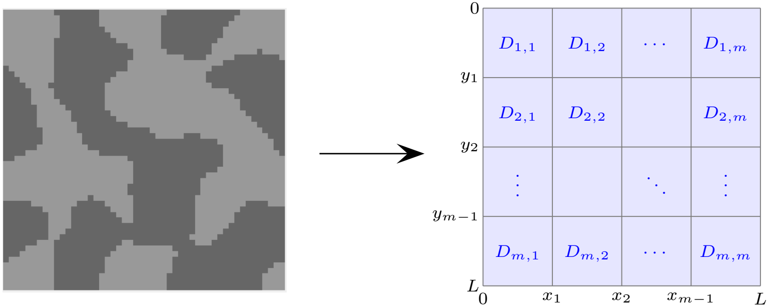
$$D_{\mathrm{a}} = \frac{D_A + D_B}{2}, \quad D_{\mathrm{h}} = \frac{2D_AD_B}{D_A + D_B}.$$



- For complex geometries, numerical methods are required (Carr and Turner, 2014; Rupp et al., 2018; Szymkiewicz and Lewandowska, 2006).

- The goal of this work is to develop a semi-analytical method for solving the cell problems and computing $\mathbf{D}_{\mathrm{eff}}$.

- Complex heterogenous geometries can be represented as an array of blocks.
- Consider the $Y = [0, L]^2$ consisting of an m^2 grid of rectangular blocks:



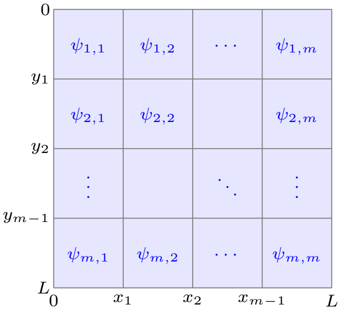
- Each block is isotropic with its own diffusivity value.
- Consider the cell problem for $\mathbf{D}_{\text{eff}}(:,1)$ (second column follows similarly)...

Semi-analytical solution
Homogenization problem

- Cell problem becomes:

$$0 = \nabla \cdot (D_{i,j} \nabla(\psi_{i,j} + x)),$$

  where $D_{i,j}$ is the diffusivity in the (i,j)th block (row i, column j).



- Solution and the flux are continuous at each interface:
  - Horizontal interfaces:

$$\psi_{i,j} = \psi_{i+1,j}, \quad D_{i,j}\frac{\partial \psi_{i,j}}{\partial y} = D_{i+1,j}\frac{\partial \psi_{i+1,j}}{\partial y}.$$

  - Vertical interfaces:

$$\psi_{i,j} = \psi_{i,j+1}, \quad D_{i,j}\left(\frac{\partial \psi_{i,j}}{\partial x} + 1\right) = D_{i,j+1}\left(\frac{\partial \psi_{i,j+1}}{\partial x} + 1\right).$$

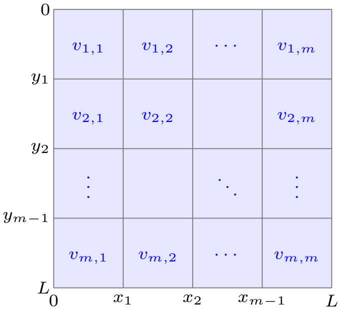
Semi-analytical solution

Change of variable: $v_{i,j} = \psi_{i,j} + x$

- Cell problem becomes:

$$\nabla^2 v_{i,j} = 0,$$

where $D_{i,j}$ is the diffusivity in the (i,j)th block (row i, column j).



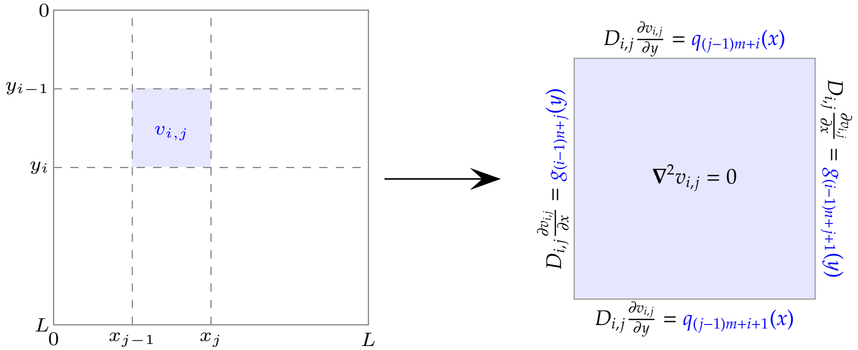
- Solution and the flux are continuous at each interface:
  - Horizontal interfaces:

$$v_{i,j} = v_{i+1,j}, \qquad D_{i,j}\frac{\partial v_{i,j}}{\partial y} = D_{i+1,j}\frac{\partial v_{i+1,j}}{\partial y}.$$

  - Vertical interfaces:

$$v_{i,j} = v_{i,j+1}, \qquad D_{i,j}\frac{\partial v_{i,j}}{\partial x} = D_{i+1,j}\frac{\partial v_{i,j+1}}{\partial x}.$$

- Introduce unknown functions for the diffusive fluxes at interfaces between adjacent blocks:



Semi-analytical solution
Solution on individual block (Polyanin, 2002)

- Solution on each block:

$$v_{i,j}(x,y) = -\frac{a_{i,j,0}}{4l_j}(x-x_j)^2 + \frac{b_{i,j,0}}{4l_j}(x-x_{j-1})^2 - \frac{c_{i,j,0}}{4h_i}(y-y_i)^2 + \frac{d_{i,j,0}}{4h_i}(y-y_{i-1})^2$$
$$- h_i \sum_{k=1}^{\infty} \frac{a_{i,j,k}}{\gamma_{i,j,k}} \cosh\left[\frac{k\pi(x-x_j)}{h_i}\right] \cos\left[\frac{k\pi(y-y_{i-1})}{h_i}\right]$$
$$+ h_i \sum_{k=1}^{\infty} \frac{b_{i,j,k}}{\gamma_{i,j,k}} \cosh\left[\frac{k\pi(x-x_{j-1})}{h_i}\right] \cos\left[\frac{k\pi(y-y_{i-1})}{h_i}\right]$$
$$- l_j \sum_{k=1}^{\infty} \frac{c_{i,j,k}}{\mu_{i,j,k}} \cosh\left[\frac{k\pi(y-y_i)}{l_j}\right] \cos\left[\frac{k\pi(x-x_{j-1})}{l_j}\right]$$
$$+ l_j \sum_{k=1}^{\infty} \frac{d_{i,j,k}}{\mu_{i,j,k}} \cosh\left[\frac{k\pi(y-y_{i-1})}{l_j}\right] \cos\left[\frac{k\pi(x-x_{j-1})}{l_j}\right] + K_{i,j},$$

where $\gamma_{i,j,k} = k\pi \sinh \frac{k\pi l_j}{h_i}$ and $\mu_{i,j,k} = k\pi \sinh \frac{k\pi h_i}{l_j}$, $h_i = y_i - y_{i-1}$ and $l_j = x_j - x_{j-1}$.

Semi-analytical solution
Coefficients

- Coefficients are integrals of unknown flux functions, e.g.

$$a_{i,j,k} = \frac{2}{h_i} \int_{y_{i-1}}^{y_i} \frac{g_{(i-1)n+j}(y)}{D_{i,j}} \cos\left(\frac{k\pi(y - y_{i-1})}{h_i}\right) \mathrm{d}y.$$

- We approximate these integrals numerically using a midpoint rule, e.g.

$$a_{i,j,k} \approx \frac{2}{D_{i,j}h_i} \sum_{p=1}^{N} \omega_p g_{(i-1)n+j}(y_p) \cos\left(\frac{k\pi(y_p - y_{i-1})}{h_i}\right),$$

  where N is the number of abscissas per interface and ω_p and y_p are the appropriate weights and abscissas.

- Quadrature approximation requires the evaluations of the unknown interface functions at the abscissas, e.g. $g_{(i-1)n+j}(y_p)$.

- By determining these evaluations, we can compute the coefficients (e.g. $a_{i,j,k}$) and thus compute the effective diffusivity.

- Enforce continuity of the solution at the abscissas along each interface, e.g.

$$v_{i+1,j}(x_p, y_i) - v_{i,j}(x_p, y_i) = 0 \quad \text{(horizontal interface).}$$

- This yields a system of linear equations that can be solved for the evaluations of the unknown interface functions:

$$\mathbf{A}\mathbf{x} = \mathbf{b},$$

where $\mathbf{x}$ is a vector of dimension $m^2(N+1)$ containing the required evaluations.

- As we have an analytical expression for the solution of the interface functions, the entries of $\mathbf{D}_{\text{eff}}$ can be expressed in terms of the coefficients, e.g.

$$\mathbf{D}_{\text{eff}}(1,1) = \frac{1}{L^2}\sum_{i=1}^{m}\sum_{j=1}^{n}\left[\frac{D_{i,j}A_{i,j}(a_{i,j,0} + b_{i,j,0})}{4} + l_j^2\sum_{k=1}^{\infty}\frac{(c_{i,j,k} - d_{i,j,k})[1-(-1)^k]}{k\pi}\right],$$

where $A_{i,j} = l_j h_i$ is the area of the (i,j)th block.

Linear system dimension
Comparison to a standard numerical method

- m by m array of square blocks.
- N abscissas per interface.
- Assume spacing between abscissas and nodes is equal.
- Linear system:

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

- Finite volume method:
  Dimension of $\mathbf{x}$: m^2N^2.
- Semi-analytical method:
  Dimension of $\mathbf{x}$: $m^2(2N+1)$.

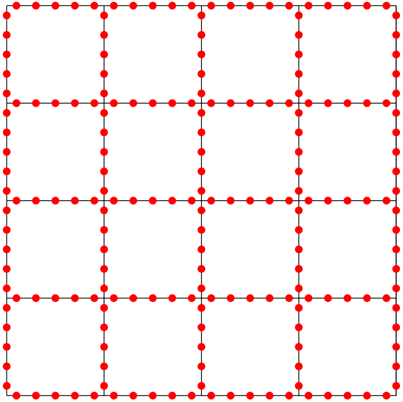


Figure 1: Abscissas (4×4 array of blocks).

- m by m array of square blocks.
- N abscissas per interface.
- Assume spacing between abscissas and nodes is equal.
- Linear system:

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

- Finite volume method:
  Dimension of $\mathbf{x}$: m^2N^2.
- Semi-analytical method:
  Dimension of $\mathbf{x}$: $m^2(2N+1)$.

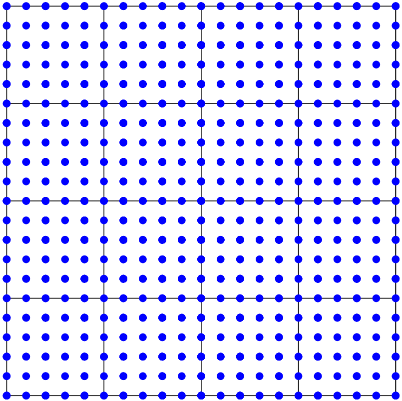
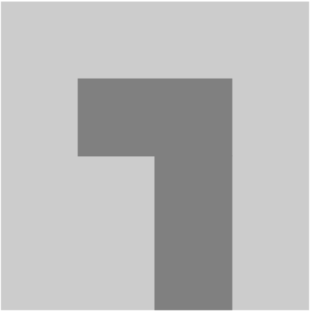


Figure 2: Nodes (4×4 array of blocks).



Standard test case (Szymkiewicz, 2013): 4×4 array of blocks.

Diffusivity: 1.0 0.1.

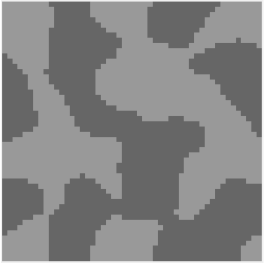
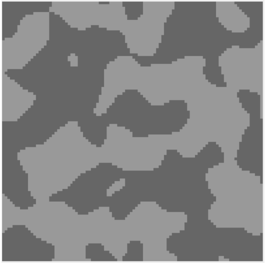
Results

Comparison to standard numerical method

	Semi-Analytical		Finite Volume	
N	$\lvert(\mathbf{D}_{\text{eff}} - \widetilde{\mathbf{D}}_{\text{eff}})./\mathbf{D}_{\text{eff}}\rvert$	Runtime (s)	$\lvert(\mathbf{D}_{\text{eff}} - \widetilde{\mathbf{D}}_{\text{eff}})./\mathbf{D}_{\text{eff}}\rvert$	Runtime (s)
4	$\begin{pmatrix} 6.84\text{e-}3 & 5.04\text{e-}3 \\ 5.04\text{e-}3 & 4.47\text{e-}3 \end{pmatrix}$	0.00747	$\begin{pmatrix} 1.30\text{e-}2 & 2.44\text{e-}3 \\ 2.44\text{e-}3 & 8.47\text{e-}3 \end{pmatrix}$	0.00923
8	$\begin{pmatrix} 3.01\text{e-}3 & 2.21\text{e-}3 \\ 2.21\text{e-}3 & 1.98\text{e-}3 \end{pmatrix}$	0.0109	$\begin{pmatrix} 4.82\text{e-}3 & 1.88\text{e-}3 \\ 1.88\text{e-}3 & 3.14\text{e-}3 \end{pmatrix}$	0.0277
16	$\begin{pmatrix} 1.40\text{e-}3 & 1.02\text{e-}3 \\ 1.02\text{e-}3 & 9.23\text{e-}4 \end{pmatrix}$	0.0331	$\begin{pmatrix} 1.75\text{e-}3 & 9.12\text{e-}4 \\ 9.12\text{e-}4 & 1.14\text{e-}3 \end{pmatrix}$	0.115
32	$\begin{pmatrix} 6.77\text{e-}4 & 4.94\text{e-}4 \\ 4.94\text{e-}4 & 4.48\text{e-}4 \end{pmatrix}$	0.0629	$\begin{pmatrix} 6.17\text{e-}4 & 3.76\text{e-}4 \\ 3.76\text{e-}4 & 4.02\text{e-}4 \end{pmatrix}$	0.530
64	$\begin{pmatrix} 3.42\text{e-}4 & 2.50\text{e-}4 \\ 2.50\text{e-}4 & 2.27\text{e-}4 \end{pmatrix}$	0.270	$\begin{pmatrix} 2.05\text{e-}4 & 1.36\text{e-}4 \\ 1.36\text{e-}4 & 1.33\text{e-}4 \end{pmatrix}$	2.92

$\widetilde{\mathbf{D}}_{\text{eff}}$: Approximate $\mathbf{D}_{\text{eff}}$ (semi-analytical or finite volume method)
$\mathbf{D}_{\text{eff}}$: Benchmark $\mathbf{D}_{\text{eff}}$ using finite volume method with a very fine grid.

Results
Application to complex geometries

50×50	100×100
	
$\mathbf{D}_{\text{eff}} = \begin{pmatrix} 0.310 & 0.0177 \\ 0.0177 & 0.342 \end{pmatrix}$	$\mathbf{D}_{\text{eff}} = \begin{pmatrix} 0.340 & 0.000954 \\ 0.000954 & 0.304 \end{pmatrix}$

Diffusivity: 1.0 0.1.

Actual geometry	Pixellated (128×128)
	
$\mathbf{D}_{\text{eff}} = \begin{pmatrix} 0.4796 & -0.0172 \\ -0.0172 & 0.4370 \end{pmatrix}$	Runtime $= 311$ secs $\left\lVert \mathbf{D}_{\text{eff}} - \mathbf{D}_{\text{eff}}^{(approx)} \right\rVert_{\max} = 9.0\times 10^{-4}$

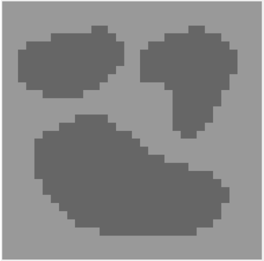
Diffusivity: 1.0 0.1.

Actual geometry	Pixellated (64×64)
	
$\mathbf{D}_{\text{eff}} = \begin{pmatrix} 0.4796 & -0.0172 \\ -0.0172 & 0.4370 \end{pmatrix}$	Runtime = 12 secs $\left\|\mathbf{D}_{\text{eff}} - \mathbf{D}_{\text{eff}}^{(approx)}\right\|_{\max} = 2.9\times 10^{-3}$

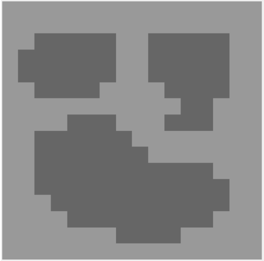
Diffusivity: 1.0 0.1.

Results

Application to pixellated irregular geometries

Actual geometry	Pixellated (32×32)
	
$\mathbf{D}_{\text{eff}} = \begin{pmatrix} 0.4796 & -0.0172 \\ -0.0172 & 0.4370 \end{pmatrix}$	Runtime $= 1$ sec $\left\lVert \mathbf{D}_{\text{eff}} - \mathbf{D}_{\text{eff}}^{(approx)} \right\rVert_{\max} = 5.3\times10^{-3}$

Diffusivity: 1.0 0.1.

Actual geometry	Pixellated (16×16)
	
$\mathbf{D}_{\text{eff}} = \begin{pmatrix} 0.4796 & -0.0172 \\ -0.0172 & 0.4370 \end{pmatrix}$	Runtime $= 0.1$ sec $\left\lVert \mathbf{D}_{\text{eff}} - \mathbf{D}_{\text{eff}}^{(approx)} \right\rVert_{\max} = 1.0 \times 10^{-2}$

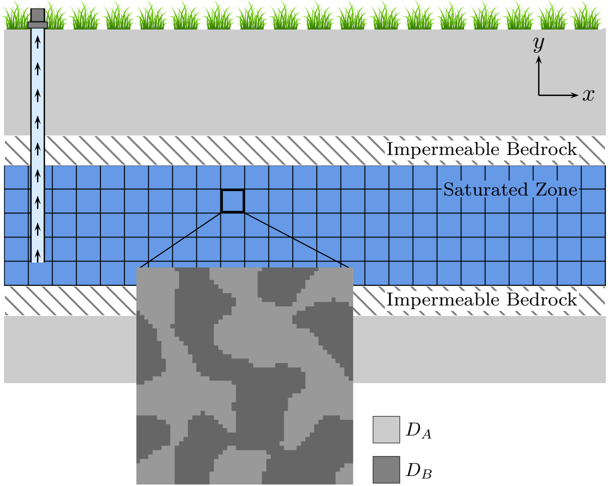
Diffusivity: 1.0 0.1.

Results

Application to pixellated irregular geometries

Actual geometry	Pixellated (8×8)
	
$\mathbf{D}_{\text{eff}} = \begin{pmatrix} 0.4796 & -0.0172 \\ -0.0172 & 0.4370 \end{pmatrix}$	Runtime $= 0.01$ sec $\left\lVert \mathbf{D}_{\text{eff}} - \mathbf{D}_{\text{eff}}^{(approx)} \right\rVert_{\max} = 4.4 \times 10^{-2}$

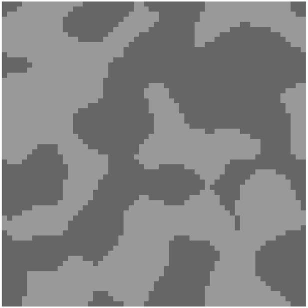
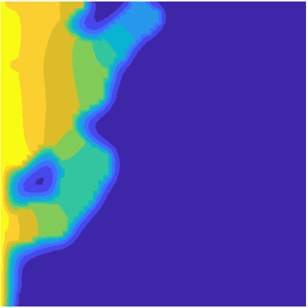
Diffusivity: 1.0 0.1.



Homogenization cell (Y)

Coarse-scale simulations
Preliminary results

Preliminary investigation into effect of coarse-graining on hydraulic head fields

Diffusivity field	Solution at $t = 0.1$
	

Benchmark/Target solution field.

Diffusivity: 1.0 0.1

Fine-scale equation: $\dfrac{\partial h}{\partial t} + \boldsymbol{\nabla} \cdot (-D(\mathbf{x})\nabla h) = 0.$

Coarse-scale simulations
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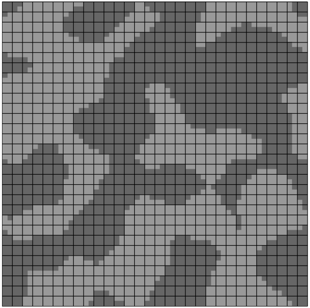
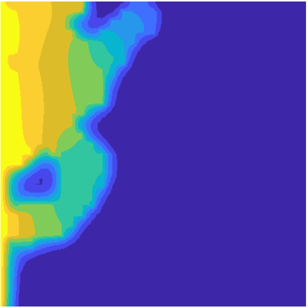
Diffusivity field	Solution at $t = 0.1$
	

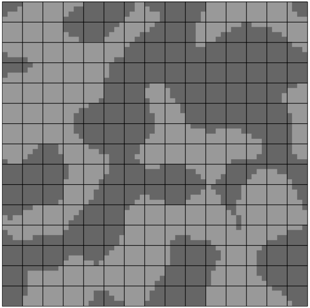
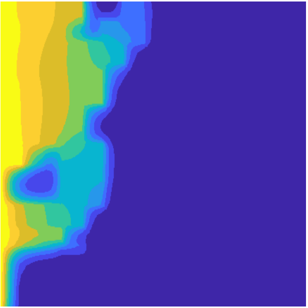
Homogenization blocks of size 2×2. Diffusivity: 1.0 0.1

Coarse-scale equation: $\dfrac{\partial H}{\partial t} + \boldsymbol{\nabla} \cdot (-\mathbf{D}_{\mathrm{eff}}(\mathbf{x})\nabla H) = 0.$

Coarse-scale simulations

Preliminary results

Preliminary investigation into effect of coarse-graining on hydraulic head fields

Diffusivity field	Solution at $t = 0.1$
	

Homogenization blocks of size 4×4.

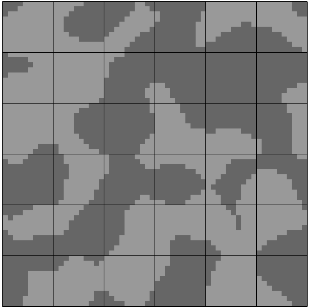
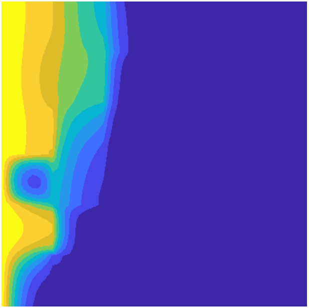
Diffusivity: 1.0 0.1

Coarse-scale equation: $\dfrac{\partial H}{\partial t} + \boldsymbol{\nabla} \cdot (-\mathbf{D}_{\mathrm{eff}}(\mathbf{x})\nabla H) = 0.$

Coarse-scale simulations

Preliminary results

Preliminary investigation into effect of coarse-graining on hydraulic head fields

Diffusivity field	Solution at $t = 0.1$
	

Homogenization blocks of size 10×10.

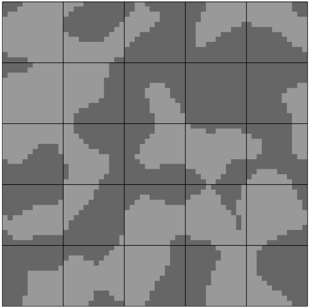
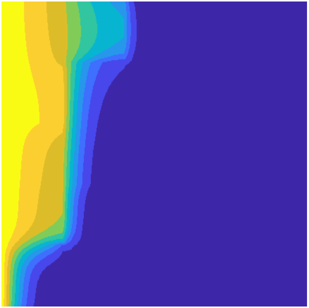
Diffusivity: 1.0 0.1

Coarse-scale equation: $\dfrac{\partial H}{\partial t} + \boldsymbol{\nabla} \cdot (-\mathbf{D}_{\text{eff}}(\mathbf{x})\nabla H) = 0.$

Coarse-scale simulations

Preliminary results

Preliminary investigation into effect of coarse-graining on hydraulic head fields

Diffusivity field	Solution at $t = 0.1$
	

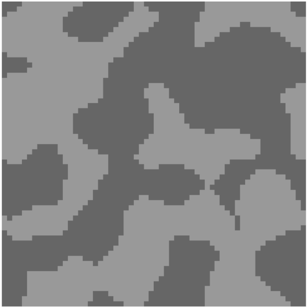
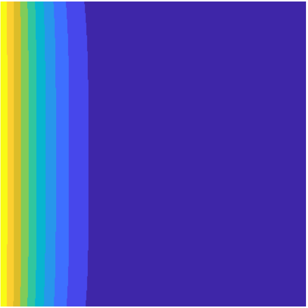
Homogenization blocks of size 12×12.

Diffusivity: 1.0 0.1

Coarse-scale equation: $\dfrac{\partial H}{\partial t} + \boldsymbol{\nabla} \cdot (-\mathbf{D}_{\mathrm{eff}}(\mathbf{x})\nabla H) = 0.$

Coarse-scale simulations
Preliminary results

Preliminary investigation into effect of coarse-graining on hydraulic head fields

Diffusivity field	Solution at $t = 0.1$
	

Completely homogenized.

Diffusivity: 1.0 0.1

Coarse-scale equation: $\dfrac{\partial H}{\partial t} + \boldsymbol{\nabla} \cdot (-\mathbf{D}_{\text{eff}} \nabla H) = 0.$

Full details

March, Carr and Turner (2019)

Preprint available on the arXiv repository:
https://arxiv.org/abs/1812.06680.

Semi-analytical solution of the homogenization boundary value problem for block locally-isotropic heterogeneous media

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Summary and Future work

March, Carr and Turner (2019)

- New semi-analytical method for solving boundary value problems on block locally-isotropic heterogenous media.
- Method provides explicit formula for effective diffusivity $\mathbf{D}_{\text{eff}}$ for highly complex heterogeneous media.
- While achieving equivalent accuracy, semi-analytical method is faster than a standard finite volume method for the test problems we considered.
- Improved efficiency due to the much smaller linear system.
- Potential to significantly speed up coarse-scale simulations of heterogeneous flows (e.g. groundwater flow, heat conduction in composite materials, etc).

References

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.

Harbaugh, A. W. (2005). Modflow-2005, the u.s. geological survey modular groundwater model – the ground-water flow process: U.s. geological survey techniques and methods, 6–a16. (6–A16).

Hornung, U. (1997). *Homogenization and Porous Media*. Springer-Verlag New York.

Rupp, A., Knabner, P., and Dawson, C. (2018). A local discontinuous Galerkin scheme for Darcy flow with internal jumps. *Computat Geosci*, 22(4):1149–1159.

Szymkiewicz, A. (2013). *Modelling Water Flow in Unsaturated Porous Media*. Springer.

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