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

Elliot Carr

Joint work with Nathan March (QUT) and Ian Turner (QUT)

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Groundwater modelling
Significance and motivation

▶ 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

Heterogeneous medium

Soil A

Soil B
I will focus on flow in the saturated zone.

Groundwater flow equation (MODFLOW, Harbaugh (2005)):

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

where \( h \) is the dependent variable, \( x \) 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 \( h(x,t) \), which determines where groundwater will flow.

In this talk, I will make the simplifying assumption that the heterogeneous medium is locally isotropic:

\[ K_x(x) = K_y(x) = K(x). \]
Homogenization

Introduction

- Fine-scale equation:
  \[ \frac{\partial h}{\partial t} + \nabla \cdot (-D(x)\nabla h) = 0, \quad x \in \Omega \subset \mathbb{R}^2. \]

- If the scale at which \( D(x) = K(x)/S_s \) changes is small compared to the size of the domain \( \Omega \), 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:
  \[ \frac{\partial H}{\partial t} + \nabla \cdot (-D_{\text{eff}}(x)\nabla H) = 0, \quad x \in \Omega \subset \mathbb{R}^2, \]

  where \( H(x, t) \) is a smoothed/coarse-scale approximation to the fine-scale field \( h(x, t) \) and \( D_{\text{eff}}(x) \) is a slowly varying effective diffusivity.
Effective Diffusivity
Homogenization of a cell $Y = [0, L]^2$

- Cell problem for first column of $D_{\text{eff}}$ (Hornung, 1997):
  \[
  \nabla \cdot \left( D(x) \nabla (\psi + x) \right) = 0, \quad x = (x, y) \in Y = [0, L]^2,
  \]
  \[
  \psi(x) \text{ is periodic with period } Y, \quad \frac{1}{L^2} \int_Y \psi \, dV = 0,
  \]
  \[
  D_{\text{eff}}(:, 1) = \frac{1}{L^2} \int_Y D(x) \nabla (\psi + x) \, dV.
  \]

- Cell problem for second column of $D_{\text{eff}}$ (Hornung, 1997):
  \[
  \nabla \cdot \left( D(x) \nabla (\psi + y) \right) = 0, \quad x = (x, y) \in Y = [0, L]^2,
  \]
  \[
  \psi(x) \text{ is periodic with period } Y, \quad \frac{1}{L^2} \int_Y \psi \, dV = 0,
  \]
  \[
  D_{\text{eff}}(:, 2) = \frac{1}{L^2} \int_Y D(x) \nabla (\psi + y) \, dV.
  \]

- 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:

\[
\mathbf{D}_{\text{eff}} = \begin{bmatrix} D_a & 0 \\ 0 & D_h \end{bmatrix},
\]

where \(D_a\) and \(D_h\) are the arithmetic and harmonic means:

\[
D_a = \frac{D_A + D_B}{2}, \quad D_h = \frac{2D_A D_B}{D_A + D_B}.
\]

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 \(\mathbf{D}_{\text{eff}}\).
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 $D_{\text{eff}}(:, 1)$ (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:
    \[
    v_{i,j} = v_{i+1,j},
    \quad D_{i,j} \frac{\partial v_{i,j}}{\partial y} = D_{i+1,j} \frac{\partial v_{i+1,j}}{\partial y}.
    \]
  
  - Vertical interfaces:
    \[
    v_{i,j} = v_{i,j+1},
    \quad D_{i,j} \frac{\partial v_{i,j}}{\partial x} = D_{i+1,j} \frac{\partial v_{i,j+1}}{\partial x}.
    \]
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 \(l_j = x_{j} - x_{j-1}\).
Coefficients are integrals of unknown flux functions, e.g.

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

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 \( \omega_p \) 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.
Semi-analytical solution
Determining evaluations of the unknown interface functions

- Enforce continuity of the solution at the abscissas along each interface, e.g.
  \[ v_{i+1,j}(x_p, y_i) - v_{i,j}(x_p, y_i) = 0 \] (horizontal interface).

- This yields a system of linear equations that can be solved for the evaluations of the unknown interface functions:
  \[ Ax = b, \]
  where \( x \) 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 \( D_{\text{eff}} \) can be expressed in terms of the coefficients, e.g.
  \[ D_{\text{eff}}(1, 1) = \frac{1}{L^2} \sum_{i=1}^{m} \sum_{j=1}^{n} \left[ \frac{D_{i,j}A_{i,j}(a_{i,j,0} + b_{i,j,0})}{4} + l_j^2 \sum_{k=1}^{\infty} \frac{(c_{i,j,k} - d_{i,j,k})[1 - (-1)^k]}{k\pi} \right], \]
  where \( A_{i,j} = l_jh_i \) 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:

\[
Ax = b
\]

Finite volume method:
Dimension of \( x \): \( m^2N^2 \).

Semi-analytical method:
Dimension of \( x \): \( m^2(2N + 1) \).

Figure 1: Abscissas (4 \( \times \) 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:
  
  $Ax = b$

- Finite volume method:
  
  Dimension of $x$: $m^2N^2$.

- Semi-analytical method:
  
  Dimension of $x$: $m^2(2N + 1)$.

Figure 2: Nodes (4 × 4 array of blocks).
Results
Comparison to standard numerical method

Standard test case (Szymkiewicz, 2013): $4 \times 4$ array of blocks.

Diffusivity: 
- Gray: 1.0
- Dark gray: 0.1.
# Results

## Comparison to standard numerical method

<table>
<thead>
<tr>
<th>$N$</th>
<th>Semi-Analytical</th>
<th>Finite Volume</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$(D_{\text{eff}} - \tilde{D}<em>{\text{eff}})/D</em>{\text{eff}}$</td>
<td>Runtime (s)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>(6.84e-3  5.04e-3)</td>
<td>0.00747</td>
</tr>
<tr>
<td></td>
<td>(5.04e-3  4.47e-3)</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>(3.01e-3  2.21e-3)</td>
<td>0.0109</td>
</tr>
<tr>
<td></td>
<td>(2.21e-3  1.98e-3)</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>(1.40e-3  1.02e-3)</td>
<td>0.0331</td>
</tr>
<tr>
<td></td>
<td>(1.02e-3  9.23e-4)</td>
<td></td>
</tr>
<tr>
<td>32</td>
<td>(6.77e-4  4.94e-4)</td>
<td>0.0629</td>
</tr>
<tr>
<td></td>
<td>(4.94e-4  4.48e-4)</td>
<td></td>
</tr>
<tr>
<td>64</td>
<td>(3.42e-4  2.50e-4)</td>
<td>0.270</td>
</tr>
<tr>
<td></td>
<td>(2.50e-4  2.27e-4)</td>
<td></td>
</tr>
</tbody>
</table>

$\tilde{D}_{\text{eff}}$: Approximate $D_{\text{eff}}$ (semi-analytical or finite volume method)

$D_{\text{eff}}$: Benchmark $D_{\text{eff}}$ using finite volume method with a very fine grid.
Results
Application to complex geometries

<table>
<thead>
<tr>
<th>50 × 50</th>
<th>100 × 100</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Image 1" /></td>
<td><img src="image2.png" alt="Image 2" /></td>
</tr>
</tbody>
</table>

\[
D_{\text{eff}} = \begin{pmatrix}
0.310 & 0.0177 \\
0.0177 & 0.342 \\
\end{pmatrix}
\]

\[
D_{\text{eff}} = \begin{pmatrix}
0.340 & 0.000954 \\
0.000954 & 0.304 \\
\end{pmatrix}
\]

Diffusivity: 1.0 0.1.
Results
Application to pixellated irregular geometries

<table>
<thead>
<tr>
<th>Actual geometry</th>
<th>Pixellated (128 × 128)</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Actual geometry" /></td>
<td><img src="image2.png" alt="Pixellated (128 × 128)" /></td>
</tr>
</tbody>
</table>

\[
\mathbf{D}_{\text{eff}} = \begin{pmatrix}
0.4796 & -0.0172 \\
-0.0172 & 0.4370
\end{pmatrix}
\]

\[
\|\mathbf{D}_{\text{eff}} - \mathbf{D}^{(\text{approx})}_{\text{eff}}\|_{\text{max}} = 9.0 \times 10^{-4}
\]

Diffusivity: 
- Gray: 1.0
- Black: 0.1

Runtime = 311 secs

[Dr Elliot Carr](https://elliotcarr.github.io)
### Results

**Application to pixellated irregular geometries**

<table>
<thead>
<tr>
<th>Actual geometry</th>
<th>Pixellated (64 × 64)</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Actual geometry" /></td>
<td><img src="image2.png" alt="Pixellated geometry" /></td>
</tr>
</tbody>
</table>

\[
\mathbf{D}_{\text{eff}} = \begin{pmatrix}
0.4796 & -0.0172 \\
-0.0172 & 0.4370
\end{pmatrix}
\]

\[
\|\mathbf{D}_{\text{eff}} - \mathbf{D}^{(\text{approx})}_{\text{eff}}\|_{\max} = 2.9 \times 10^{-3}
\]

Runtime = 12 secs

Diffusivity: 
- Light gray: 1.0
- Dark gray: 0.1
# Results

**Application to pixellated irregular geometries**

<table>
<thead>
<tr>
<th>Actual geometry</th>
<th>Pixellated (32 × 32)</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Actual geometry image" /></td>
<td><img src="image2.png" alt="Pixellated image" /></td>
</tr>
</tbody>
</table>

\[
D_{\text{eff}} = \begin{pmatrix} 0.4796 & -0.0172 \\ -0.0172 & 0.4370 \end{pmatrix}
\]

\[
\|D_{\text{eff}} - D_{\text{eff}}^{(\text{approx})}\|_{\text{max}} = 5.3 \times 10^{-3}
\]

**Runtime** = 1 sec

Diffusivity: 
- Gray: 1.0
- Gray: 0.1
Results
Application to pixellated irregular geometries

Actual geometry

Pixellated (16 × 16)

\[
D_{\text{eff}} = \begin{pmatrix}
0.4796 & -0.0172 \\
-0.0172 & 0.4370
\end{pmatrix}
\]

\[
\|D_{\text{eff}} - D_{\text{eff}}^{(\text{approx})}\|_{\text{max}} = 1.0 \times 10^{-2}
\]

Runtime = 0.1 sec

Diffusivity: 

\[
\begin{array}{c}
\text{Gray} & \text{1.0} \\
\text{Gray} & \text{0.1}
\end{array}
\]
## Results

Application to pixellated irregular geometries

<table>
<thead>
<tr>
<th>Actual geometry</th>
<th>Pixellated (8 × 8)</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Actual geometry" /></td>
<td><img src="image2.png" alt="Pixellated (8 × 8)" /></td>
</tr>
</tbody>
</table>

\[
D_{\text{eff}} = \begin{pmatrix}
0.4796 & -0.0172 \\
-0.0172 & 0.4370
\end{pmatrix}
\]

Runtime = 0.01 sec

\[
\left\| D_{\text{eff}} - D^{(\text{approx})}_{\text{eff}} \right\|_{\text{max}} = 4.4 \times 10^{-2}
\]

Diffusivity: 
- Light grey: 1.0
- Dark grey: 0.1
Groundwater modelling
Coarse-scale modelling

Impermeable Bedrock
Saturated Zone

Homogenization cell ($Y$)

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

<table>
<thead>
<tr>
<th>Diffusivity field</th>
<th>Solution at $t = 0.1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>![Diffusivity field image]</td>
<td>![Solution image]</td>
</tr>
</tbody>
</table>

Benchmark/Target solution field.

Fine-scale equation: \( \frac{\partial h}{\partial t} + \nabla \cdot (-D(x)\nabla h) = 0. \)
Preliminary investigation into effect of coarse-graining on hydraulic head fields

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Homogenization blocks of size $2 \times 2$. Diffusivity: 

\[
\frac{\partial H}{\partial t} + \nabla \cdot (-D_{\text{eff}}(x) \nabla H) = 0.
\]
Preliminary investigation into effect of coarse-graining on hydraulic head fields

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</tr>
</tbody>
</table>

Homogenization blocks of size $4 \times 4$.  

Coarse-scale equation:  

$$\frac{\partial H}{\partial t} + \nabla \cdot (-D_{\text{eff}}(x)\nabla H) = 0.$$  

Diffusivity:  

- Light grey: 1.0
- Dark grey: 0.1
Preliminary investigation into effect of coarse-graining on hydraulic head fields

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</tr>
</tbody>
</table>

Homogenization blocks of size $10 \times 10$. Diffusivity: 

| Diffusivity: | 1.0 | 0.1 |

Coarse-scale equation: 

$$\frac{\partial H}{\partial t} + \nabla \cdot (-D_{\text{eff}}(x)\nabla H) = 0.$$
Preliminary investigation into effect of coarse-graining on hydraulic head fields

<table>
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</table>

Homogenization blocks of size $12 \times 12$. Diffusivity: 1.0, 0.1

Coarse-scale equation: \[ \frac{\partial H}{\partial t} + \nabla \cdot (-D_{\text{eff}}(x)\nabla H) = 0. \]
Preliminary investigation into effect of coarse-graining on hydraulic head fields

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</thead>
<tbody>
<tr>
<td>![Diffusivity field image]</td>
<td>![Solution at $t = 0.1$ image]</td>
</tr>
</tbody>
</table>

Completely homogenized.

Coarse-scale equation: \( \frac{\partial H}{\partial t} + \nabla \cdot ( - \mathbf{D}_{\text{eff}} \nabla H ) = 0. \)
Semi-analytical solution of the homogenization boundary value problem for block locally-isotropic heterogeneous media

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\textsuperscript{b}ARC Centre of Excellence for Mathematical and Statistical Frontiers (ACEMS), Queensland University of Technology (QUT), Brisbane, Australia.

Preprint available on the arXiv repository:
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 $D_{\text{eff}}$ 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).


