Computational simulation of complex fine-scale heterogeneous flows using homogenization and coarse-graining approaches

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- Fine-scale diffusion model:

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

- If the scale at which the diffusivity $D(\mathbf{x})$ changes is small compared to the size of the domain Ω, then the amount of computation required to solve this model is prohibitive due to the very fine mesh required to capture the heterogeneity.

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

- Homogenized diffusion model:

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

where $U(\mathbf{x}, t)$ is a smoothed/coarse-scale approximation to the fine-scale solution $u(\mathbf{x}, t)$.

- Cell problem for first column of $\mathbf{D}_{\text{eff}}$:

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

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

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

- Cell problem for second column of $\mathbf{D}_{\text{eff}}$:

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

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

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

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

Effective Diffusivity
Solution of cell problems

- For a layered medium, the cell problems can be solved exactly yielding the following effective diffusivity:

$$D(\boldsymbol{x}) = \begin{cases} D_A & \text{if } 0 < y < \frac{L}{2}, \\ D_B & \text{if } \frac{L}{2} < y > L, \end{cases} \quad \Longrightarrow \quad \mathbf{D}_{\text{eff}} = \begin{bmatrix} D_{\text{a}} & 0 \\ 0 & D_{\text{h}} \end{bmatrix},$$

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

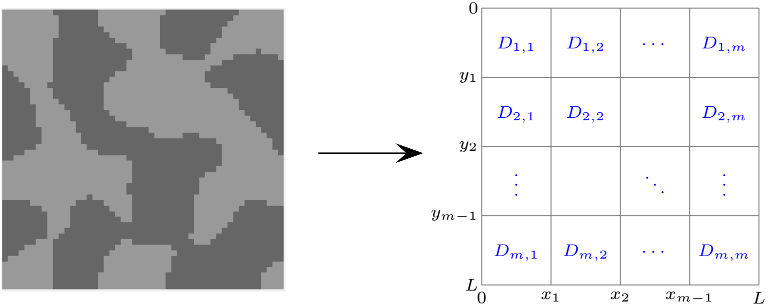
$$D_{\text{a}} = \frac{D_A + D_B}{2}, \quad D_{\text{h}} = \frac{2D_A D_B}{D_A + D_B}.$$

- 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 $\mathbf{D}_{\text{eff}}$.

Semi-analytical solution
Block heterogeneous medium

- 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 cell problem for $\mathbf{D}_{\text{eff}}(:, 1)$ (second column follows similarly).

Semi-analytical solution
Homogenization problem

- On each block domain, the cell problem is expressed as

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

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

- For a block heterogeneous domain (discontinuous diffusivity) we also require boundary conditions at the interfaces between adjacent blocks.
- 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:

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

- Change of variable:

$$v_{i,j} = \psi_{i,j} + x.$$

- On each block domain, the cell problem is now expressed as

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

- 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:

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

Semi-analytical solution
Reformulation

- Introduce unknown functions for the diffusive fluxes at interfaces between adjacent blocks, e.g.,

$$D_{i,j}\frac{\partial v_{i,j}}{\partial x} = D_{i,j+1}\frac{\partial v_{i,j+1}}{\partial x} =: g_{(j-1)m+i+1}(y), \quad \text{(vertical interfaces)}.$$
$$D_{i,j}\frac{\partial v_{i,j}}{\partial y} = D_{i+1,j}\frac{\partial v_{i+1,j}}{\partial y} =: q_{(j-1)m+i+1}(x), \quad \text{(horizontal interfaces)}.$$

- This allows us to consider the following general block problem:

$$\nabla^2 v_{i,j} = 0,$$
$$D_{i,j}\frac{\partial v_{i,j}}{\partial x} = g_{(i-1)n+j}(y), \quad \text{at } x = x_{j-1}, \qquad D_{i,j}\frac{\partial v_{i,j}}{\partial x} = g_{(i-1)n+j+1}(y), \quad \text{at } x = x_j,$$
$$D_{i,j}\frac{\partial v_{i,j}}{\partial y} = q_{(j-1)m+i}(x), \quad \text{at } y = y_{i-1}, \qquad D_{i,j}\frac{\partial v_{i,j}}{\partial y} = q_{(j-1)m+i+1}(x), \quad \text{at } y = y_i.$$

Solution on individual block (Polyanin, 2002)

- Solution on each block:

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

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.

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

- 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.

Semi-analytical solution

Determining evaluations of the unknown interface functions

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

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

- 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 $\mathbf{x}$: $m^2(2N+1)$.

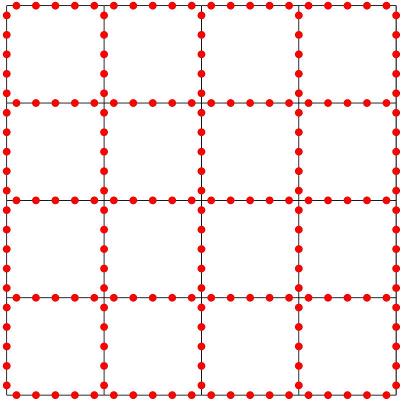


Figure 1: Abscissas (4×4 array of blocks).

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 $\mathbf{x}$: $m^2(2N+1)$.

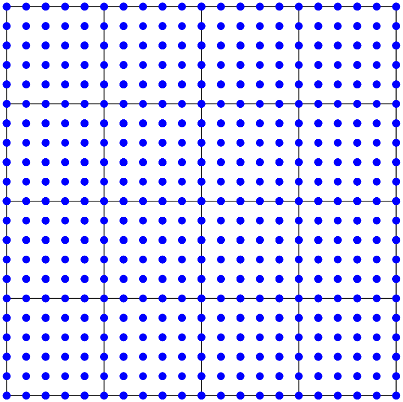


Figure 2: Nodes (4×4 array of blocks).

Semi-analytical method
Comparison to standard numerical method

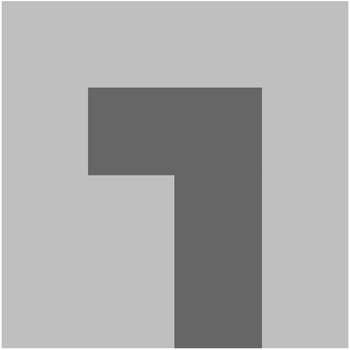


Figure 3: Standard test case (Szymkiewicz, 2013): 4×4 array of blocks (Diffusivity: dark = 0.1, light = 1).

Semi-analytical method

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.

Semi-analytical method
Application to complex geometries

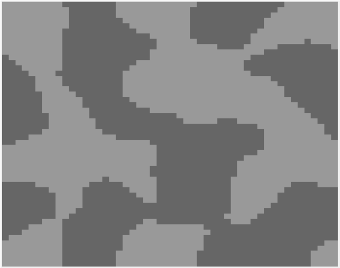
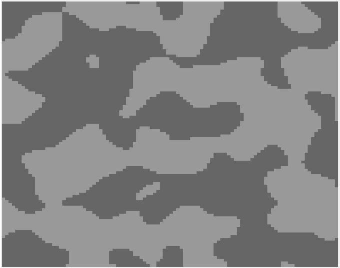
	50×50	100×100
		
$\mathbf{D}_{\text{eff}}$	$\begin{pmatrix} 0.310 & 0.0177 \\ 0.0177 & 0.342 \end{pmatrix}$	$\begin{pmatrix} 0.340 & 0.000954 \\ 0.000954 & 0.304 \end{pmatrix}$

Table 1: Diffusivity: dark = 0.1, light = 1.

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

A fast semi-analytical homogenization method for block 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 $\mathbf{D}_{\text{eff}}$.
- While achieving equivalent accuracy, semi-analytical method is faster than a standard finite volume method for the test problems we considered.
- Improved efficiency is mainly due to the much smaller linear system size required.

References

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