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Semi-analytical solutions for transport PDEs in heterogeneous media

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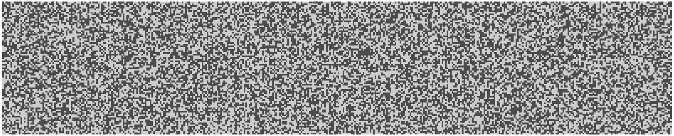
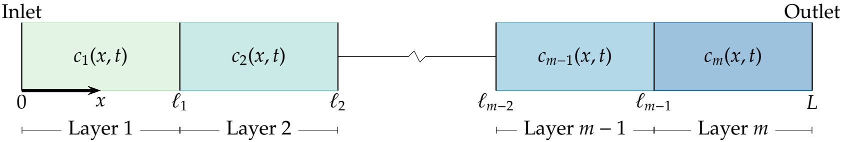
- Generic scalar transport equation:

$$R(\mathbf{x})\frac{\partial c}{\partial t} = \nabla \cdot (\mathbf{D}(\mathbf{x})\nabla c - \mathbf{v}(\mathbf{x})c) + S(c,\mathbf{x}), \qquad \Omega \subset \mathbb{R}^d.$$

- Heterogeneous media: coefficients vary spatially.



- This talk is comprised of two parts:
  - Part 1:
    Semi-analytical solutions to the advection-diffusion-reaction equation in heterogeneous (layered) media.
  - Part 2:
    Semi-analytical solutions to the homogenization boundary value problem for diffusion in 2D heterogeneous media.



$$R(x)\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D(x)\frac{\partial c}{\partial x} - v(x)c\right) - \mu(x)c + \gamma(x).$$

$$R(x), D(x), v(x), \mu(x), \gamma(x) = \begin{cases} R_1, D_1, v_1, \mu_1, \gamma_1, & 0 < x < \ell_1, \\ R_2, D_2, v_2, \mu_2, \gamma_2, & \ell_1 < x < \ell_2, \\ \quad\vdots & \quad\vdots \\ R_m, D_m, v_m, \mu_m, \gamma_m, & \ell_{m-1} < x < L. \end{cases}$$

Advection-diffusion-reaction in layered media

Governing equations

- Governing equations (Guerrero et al., 2013; van Genuchten and Alves, 1982):

$$R_i\frac{\partial c_i}{\partial t} = D_i\frac{\partial^2 c_i}{\partial x^2} - v_i\frac{\partial c_i}{\partial x} - \mu_i c_i + \gamma_i, \qquad i = 1,\ldots,m,$$
$$c_i(x,0) = f_i,$$
$$c_i(\ell_i,t) = c_{i+1}(\ell_i,t),$$
$$\theta_i D_i\frac{\partial c_i}{\partial x}(\ell_i,t) = \theta_{i+1}D_{i+1}\frac{\partial c_{i+1}}{\partial x}(\ell_i,t),$$

where $v_i\theta_i = v_{i+1}\theta_{i+1}$.

- Nomenclature:
  - $c_i(x,t)$: solute concentration [ML^{-3}] in the ith layer
  - R_i: retardation factor [$-$]
  - D_i: dispersion coefficient [L^2T^{-1}]
  - v_i: pore-water velocity [LT^{-1}]
  - μ_i: rate constant for first-order decay [T^{-1}]
  - γ_i: rate constant for zero-order production [T^{-1}]
  - θ_i: volumetric water content [L^3L^{-3}] in the ith layer

- Inlet boundary condition ($x = 0$):
  - Concentration-type:

$$c_1(0,t) = c_0(t),$$

  - Flux-type:

$$v_1 c_1(0,t) - D_1 \frac{\partial c_1}{\partial x}(0,t) = v_1 c_0(t),$$

- Outlet boundary condition ($x = L$):

$$\frac{\partial c_m}{\partial x}(L,t) = 0.$$

- General boundary conditions:

$$\text{Inlet:} \qquad a_0 c_1(0,t) - b_0 \frac{\partial c_1}{\partial x}(0,t) = g_0(t),$$

$$\text{Outlet:} \qquad a_L c_m(L,t) + b_L \frac{\partial c_m}{\partial x}(L,t) = g_L(t).$$

- Eigenfunction expansion solution:

$$c_i(x,t) = \sum_{n=1}^{\infty} a_n T_n(\lambda_n;t) X_n(\lambda_n;x).$$

- Eigenvalues ($\lambda_n, n \in \mathbb{N}^+$) are identified by substituting eigenfunctions into the boundary and interface conditions and enforcing a non-trivial solution.

- This yields a nonlinear transcendental equation for the eigenvalues arising from the evaluation of a $2m \times 2m$ determinant

$$f(\lambda) = 0,$$

$$\text{where} \quad f(\lambda) := \det(\mathbf{A}(\lambda)), \qquad \mathbf{A} \in \mathbb{R}^{2m\times 2m}.$$

- For many layers (large m) evaluating $f(\lambda)$ is numerically unstable.

- Solutions tend to breakdown for $m > 10$ layers (Carr and Turner, 2016).

- Solutions for maximum of seven layers given by Liu et al. (1998) (advection-diffusion only with $\mu_i = \gamma_i = 0$) and Guerrero et al. (2013) (advection-diffusion-reaction with $\gamma_i = 0$).

Advection-diffusion-reaction in layered media

Analytical solution via Laplace transform

- Idea: reformulate the model into m isolated single layer problems (Carr and Turner, 2016; Rodrigo and Worthy, 2016; Zimmerman et al., 2016).

- Introduce unknown functions of time, $g_i(t)$ ($i = 1, \ldots, m-1$), at the layer interfaces (Carr and Turner, 2016; Rodrigo and Worthy, 2016):

$$g_i(t) := \theta_i D_i \frac{\partial c_i}{\partial x}(\ell_i, t).$$

- Yields isolated single layer problems e.g. in the first layer:

$$R_1 \frac{\partial c_1}{\partial t} = D_1 \frac{\partial^2 c_1}{\partial x^2} - v_1 \frac{\partial c_1}{\partial x} - \mu_1 c_1 + \gamma_1,$$

$$c_1(x,0) = f_1,$$

$$a_0 c_1(0,t) - b_0 \frac{\partial c_1}{\partial t}(0,t) = g_0(t),$$

$$\theta_1 D_1 \frac{\partial c_1}{\partial x}(\ell_1, t) = g_1(t).$$

- Each problem coupled together by imposing continuity of concentration at the interfaces.

Advection-diffusion-reaction in layered media

Analytical solution via Laplace transform

- Solve each layer problem expressing the solution in terms of the unknown interface functions.

- Taking Laplace transforms yields boundary value problems e.g. in the first layer:

$$D_1 \frac{\mathrm{d}^2 C_1}{\mathrm{d}x^2} - v_1 \frac{\mathrm{d}C_1}{\mathrm{d}x} - (\mu_1 + R_1 s) C_1 = -R_1 f_1 - \frac{\gamma_1}{s},$$

$$a_0 C_1(0,s) - b_0 \frac{\mathrm{d}C_1}{\mathrm{d}x}(0,s) = G_0(s),$$

$$\theta_1 D_1 \frac{\mathrm{d}C_1}{\mathrm{d}x}(\ell_1, s) = G_1(s),$$

where $C_i(x,s) = \mathcal{L}\{c_i(x,t)\}$ denotes the Laplace transform of $c_i(x,t)$ with transformation variable $s \in \mathbb{C}$ and $G_i(s) = \mathcal{L}\{g_i(t)\}$ for $i = 1, \ldots, m-1$.

- Laplace transforms of the boundary functions:

$$G_0(s) = \mathcal{L}\{g_0(t)\}$$

$$G_L(s) = \mathcal{L}\{g_L(t)\}$$

are assumed to be able to be found analytically.

- The boundary value problems all involve second-order constant-coefficient differential equations

- Solving using standard techniques defines the concentration in the Laplace domain:

$$\begin{aligned} C_1(x,s) &= A_1(x,s)G_0(s) + B_1(x,s)G_1(s) + P_1(x,s), \\ C_i(x,s) &= A_i(x,s)G_{i-1}(s) + B_i(x,s)G_i(s) + P_i(x,s), \quad i = 2,\ldots,m-1, \\ C_m(x,s) &= A_m(x,s)G_{m-1}(s) + B_m(x,s)G_L(s) + P_m(x,s), \end{aligned}$$

  where the functions P_i, A_i and B_i ($i = 1,\ldots,m$) are known functions.

- To determine $G_1(s),\ldots,G_{m-1}(s)$, the Laplace transformations of the unknown interface functions $g_1(t),\ldots,g_{m-1}(t)$, we enforce continuity of concentration at each interface in the Laplace domain:

$$C_i(\ell_i,s) = C_{i+1}(\ell_i,s), \quad i = 1,\ldots,m-1. \tag{1}$$

- This yields a tridiagonal system of linear equations $\mathbf{A}\mathbf{x} = \mathbf{b}$, where $\mathbf{x} = (G_1(s),\ldots,G_{m-1}(s))^T$.

- Summary: Concentration can be evaluated at any x and s in the Laplace domain.

- Inversion of the Laplace transform is carried out numerically.
- Hence, our solution method is *semi*-analytical.
- Trefethen et al. (2006) defines the following approximation:

$$c_i(x,t) = \mathcal{L}^{-1}\left\{C_i(x,s)\right\} \approx -\frac{2}{t}\Re\left\{\sum_{\substack{k=1\\ k\text{ odd}}}^{N} w_k C_i\left(x,s_k\right)\right\},$$

  where N is even, $s_k = z_k/t$ and $w_k, z_k \in \mathbb{C}$ are the residues and poles of the best (N,N) rational approximation to e^z on the negative real line.

- Summary: Concentration can be evaluated at any x and t in the time domain.
- Attractiveness is that the solution is completely explicit. Unlike eigenfunction expansion solutions that require a nonlinear algebraic equation to be solved for the eigenvalues:

$$f(\lambda) = 0,$$

$$\text{where} \quad f(\lambda) := \det(\mathbf{A}(\lambda)), \qquad \mathbf{A} \in \mathbb{R}^{2m\times 2m}.$$

Advection-diffusion-reaction in layered media
Heaviside inlet boundary condition

- In solute transport problems, it is common to apply a Heaviside step function at the inlet:

$$c_0(t) = c_0 H(t_0 - t) = \begin{cases} c_0, & 0 < t < t_0, \\ 0, & t > t_0, \end{cases}$$

  where c_0 is a constant and $t_0 > 0$ is the duration.

- Yields $G_0(s) = \exp(-t_0 s)/s$ and $G_0(s) = v_1 \exp(-t_0 s)/s$ for the concentration-type and flux-type boundary condition, respectively.

- Such exponential functions are well known to cause numerical problems in algorithms for inverting Laplace transforms (Kuhlman, 2013).

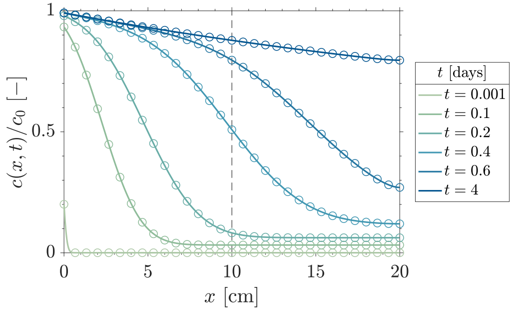
- To overcome this problem, we use superposition of solutions

$$c_i(x,t) = \begin{cases} \widetilde{c_i}(x,t), & 0 < t < t_0, \\ \widetilde{c_i}(x,t) - \widehat{c_i}(x,t-t_0), & t > t_0, \end{cases}$$

  where $\widetilde{c_i}(x,t)$ is the solution with $g_0(t) = c_0$ and $\widehat{c_i}(x,t)$ is the solution with $g_0(t) = c_0$, $f_i = 0$ and $\gamma_i = 0$.

Advection-diffusion-reaction in layered media

One layer test case

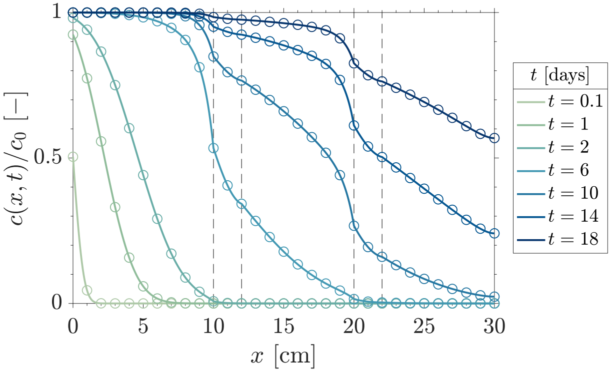


$$\text{BCs}: \quad v_1 c_1(0,t) - D_1 \frac{\partial c_1}{\partial x}(0,t) = v_1 c_0, \qquad \frac{\partial c_2}{\partial t}(20,t) = 0.$$

Benchmarked against single-layer analytical solutions (van Genuchten and Alves, 1982).

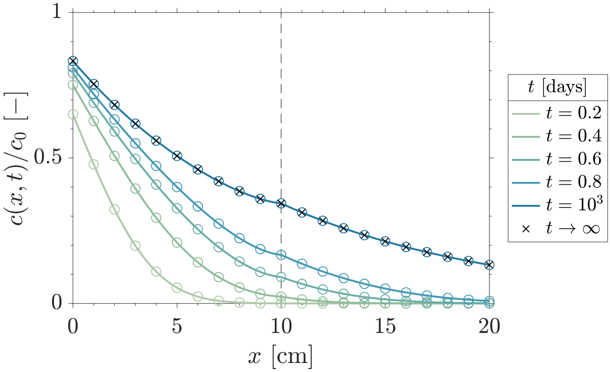
Absolute errors

$t = 10^{-3}$	$t = 0.1$	$t = 0.2$	$t = 0.4$	$t = 0.6$	$t = 4$
4.11×10^{-14}	5.53×10^{-10}	8.69×10^{-9}	1.24×10^{-9}	5.84×10^{-8}	6.10×10^{-10}



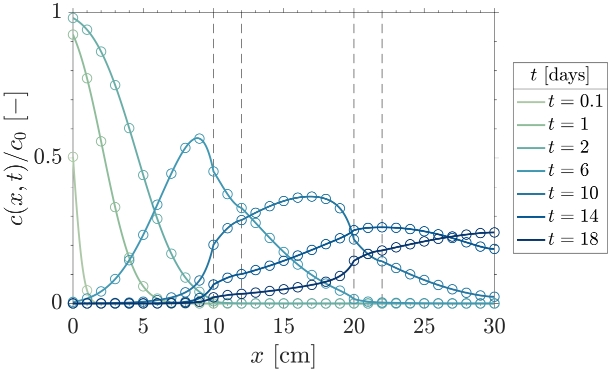
$$\text{BCs}: \qquad v_1 c_1(0,t) - D_1 \frac{\partial c_1}{\partial x}(0,t) = v_1 c_0, \qquad \frac{\partial c_5}{\partial t}(30,t) = 0.$$

Agrees with Liu et al. (1998) and Guerrero et al. (2013) solutions.



$$\text{BCs}: \quad v_1 c_1(0,t) - D_1 \frac{\partial c_1}{\partial x}(0,t) = v_1 c_0, \qquad \frac{\partial c_2}{\partial t}(30,t) = 0.$$

Indicates a problem with Guerrero et al. (2013) solution for $\mu_i \neq 0$.



$$\text{BCs}: \quad v_1 c_1(0,t) - D_1 \frac{\partial c_1}{\partial x}(0,t) = v_1 c_0 H(t_0 - t), \qquad \frac{\partial c_5}{\partial t}(30,t) = 0.$$

Agrees with standard numerical solution (finite volume).

- Summary:
  - Developed a semi-analytical Laplace-transform based method solution to the one-dimensional linear advection-dispersion-reaction equation in a layered medium.
  - Novelty: introduce unknown functions at the interfaces between adjacent layers, which allows the multilayer problem to be solved separately on each layer.
  - Solution is quite general. Accommodates arbitrary number of layers and arbitrary time-varying boundary conditions at the inlet and outlet.
  - Solutions generalise recent work on diffusion (Carr and Turner, 2016; Rodrigo and Worthy, 2016) and reaction-diffusion (Zimmerman et al., 2016) in layered media.
- Limitations:
  - Specific initial and interface conditions.

https://arxiv.org/abs/2001.08387 https://github.com/elliotcarr/Carr2020a

Solving advection-diffusion-reaction problems in layered media using the Laplace transform

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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 $u(\mathbf{x}, t)$.

Homogenization of 2D heterogeneous media

Effective diffusivity for a cell $\Upsilon = [0, L]^2$

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

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

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

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

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

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

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

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

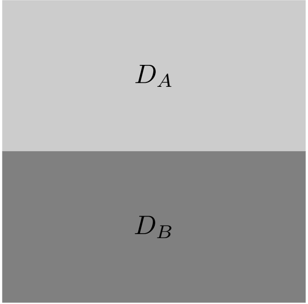
Homogenization of 2D heterogeneous media
Solution of cell problems

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

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

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

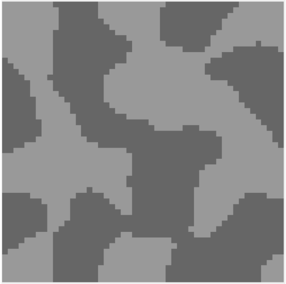
$$D_{\text{a}} = \frac{D_A + D_B}{2}, \quad D_{\text{h}} = \frac{2D_A D_B}{D_A + D_B}.$$

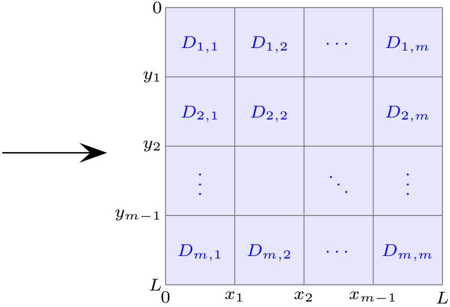


- For complex geometries, numerical methods are required (Carr and Turner, 2014; Rupp et al., 2018; Szymkiewicz and Lewandowska, 2006).

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

- 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:

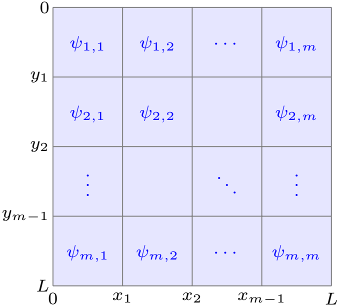




- Each block is isotropic with its own diffusivity value.
- Consider the cell problem for $\mathbf{D}_{\text{eff}}(:,1)$ (second column follows similarly)...

Homogenization of 2D heterogeneous media

Block heterogeneous medium



- 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:

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

Homogenization of 2D heterogeneous media

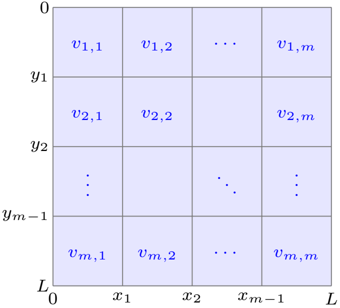
Change of variable: $v_{i,j} = \psi_{i,j} + x$

- 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:

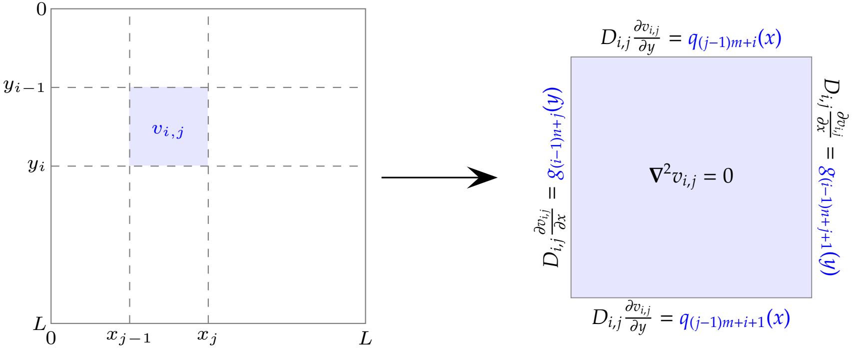
$$v_{i,j} = v_{i+1,j}, \qquad D_{i,j}\frac{\partial v_{i,j}}{\partial y} = D_{i+1,j}\frac{\partial v_{i+1,j}}{\partial y}.$$

  - Vertical interfaces:

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

Homogenization of 2D heterogeneous media
Reformulation

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



- 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.

Homogenization of 2D heterogeneous media

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.

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

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

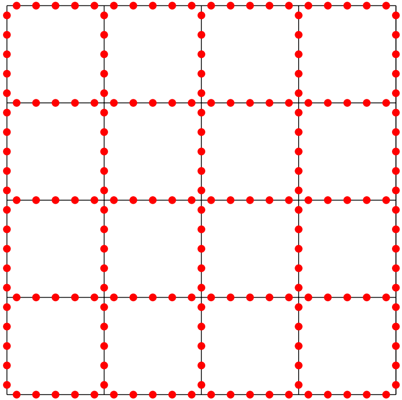


Figure 1: Abscissas (4×4 array of blocks).

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

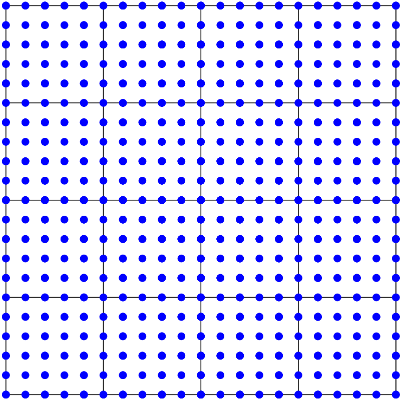


Figure 2: Nodes (4×4 array of blocks).

Results

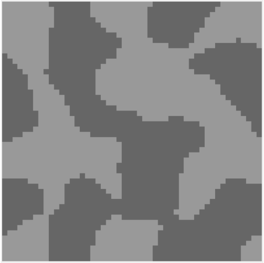
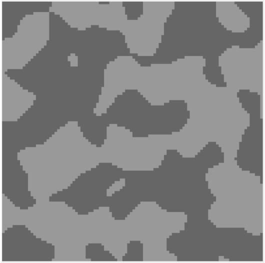
Comparison to standard numerical method

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

Diffusivity: 1.0 0.1.

	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.

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.

- 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 diffusion (e.g. groundwater flow, heat conduction in composite materials, etc).

https://arxiv.org/abs/1812.06680 https://github.com/NathanMarch/Homogenization

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

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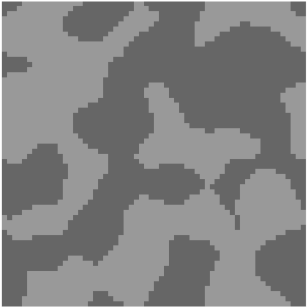
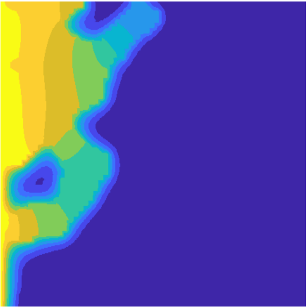
Coarse-scale simulations
Preliminary results

Preliminary investigation into effect of coarse-graining.

Diffusivity field	Solution at $t = 0.1$
	

Benchmark/Target solution field.

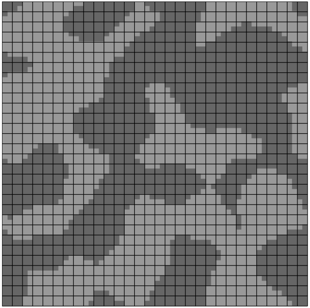
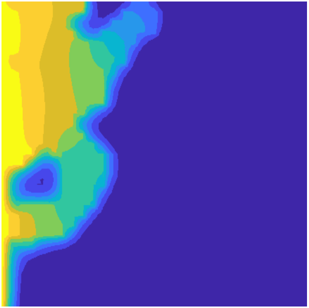
Diffusivity: 1.0 0.1

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

Coarse-scale simulations

Preliminary results

Preliminary investigation into effect of coarse-graining.

Diffusivity field	Solution at $t = 0.1$
	

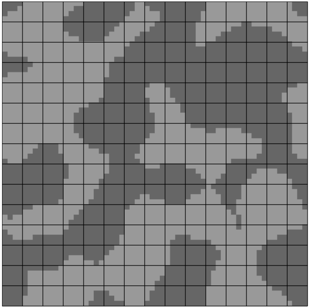
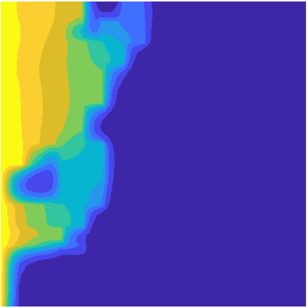
Homogenization blocks of size 2×2.

Diffusivity: 1.0 0.1

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

Coarse-scale simulations
Preliminary results

Preliminary investigation into effect of coarse-graining.

Diffusivity field	Solution at $t = 0.1$
	

Homogenization blocks of size 4×4.

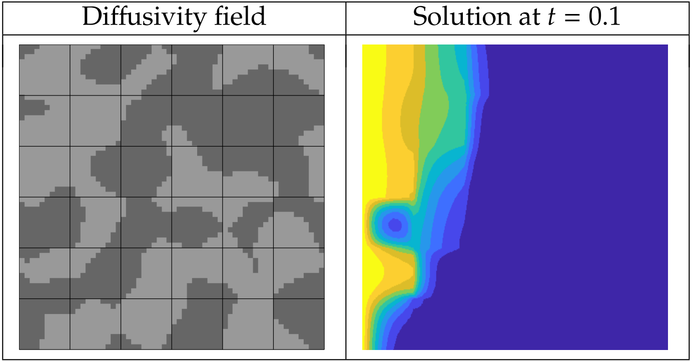
Diffusivity: 1.0 0.1

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

Coarse-scale simulations

Preliminary results

Preliminary investigation into effect of coarse-graining.



Homogenization blocks of size 10×10.

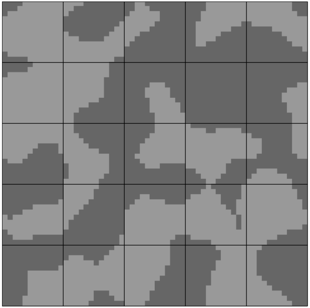
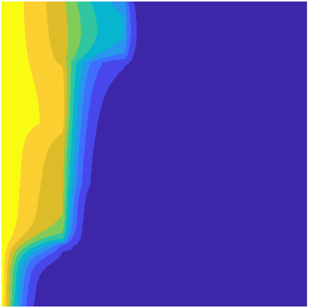
Diffusivity: 1.0 0.1

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

Coarse-scale simulations

Preliminary results

Preliminary investigation into effect of coarse-graining.

Diffusivity field	Solution at $t = 0.1$
	

Homogenization blocks of size 12×12.

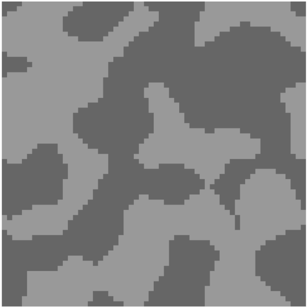
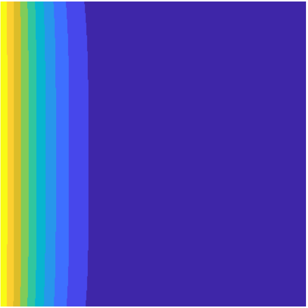
Diffusivity: 1.0 0.1

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

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