A fast semi-analytical homogenization method for block heterogeneous media

Nathan G. March\textsuperscript{a}, Elliot J. Carr\textsuperscript{*a}, and Ian W. Turner\textsuperscript{a,b}

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

Abstract

Direct numerical simulation of flow through heterogeneous media can be difficult due to the computational cost of resolving fine-scale heterogeneities. One method to overcome this difficulty is to coarse-grain the model by decomposing the domain into a number of smaller sub-domains and homogenizing the heterogeneous medium within each sub-domain. In the resulting coarse-grained model, the fine-scale diffusivity on each sub-domain is replaced by an effective diffusivity, calculated from the solution of an appropriate boundary value problem over the sub-domain. However, in simulations in which the heterogeneous sub-domain geometries evolve over time, the effective diffusivities need to be repeatedly recomputed and may bottleneck a simulation. In this paper, we present a new semi-analytical method for solving the boundary value problem and computing the effective diffusivity for block heterogeneous media. We compare the new method to a standard finite volume method and show that the equivalent accuracy can be achieved in less computational time for several standard test cases. We also demonstrate how the new method can be used to homogenize complex heterogeneous geometries represented by a grid of blocks. These results indicate that our new semi-analytical method has the potential to significantly speed up coarse-grain simulations of flow in heterogeneous media.

Keywords: effective diffusivity; homogenization; coarse-grained modelling; heterogeneous media.

1 Introduction

Consider the diffusion equation:

\[
\frac{\partial}{\partial t} u(x,t) + \nabla \cdot (-D(x)\nabla u(x,t)) = 0, \quad x \in \Omega,
\]

where \(D(x)\) is a spatially dependent, isotropic diffusivity. This equation is infeasible to solve numerically if the scale at which the diffusivity \(D(x)\) changes is small compared to the size of the domain \(\Omega\), due to the prohibitively fine mesh required to capture the fine-scale heterogeneity [1, 5, 9, 10, 13]. One method of overcoming this problem is to coarse-grain the model by decomposing the domain into a number of smaller sub-domains and homogenizing the heterogeneous medium within each sub-domain [25] (see Figure 1). In this case, the diffusivity \(D(x)\) on each sub-domain is replaced by an equivalent or effective diffusivity \(D_{\text{eff}}\), yielding the coarse-grained equation:

\[
\frac{\partial}{\partial t} U(x,t) + \nabla \cdot (-D_{\text{eff}}(x)\nabla U(x,t)) = 0, \quad x \in \Omega,
\]

where \(U(x,t)\) provides a coarse-scale approximation to \(u(x,t)\) and \(D_{\text{eff}}\) is spatially dependent because it varies between sub-domains. The attraction of the coarse-grained equation (2) over the fine-scale equation (1) is that \(D_{\text{eff}}\) varies on a much coarser scale than \(D(x)\). This means a coarser mesh can be used to solve the coarse-grained equation (2) leading to more computationally efficient simulations. The efficiency of the coarse-grained model, however, is negated to some extent if the overhead of computing the effective diffusivities on each sub-domain is high. This computational overhead is further increased if the heterogeneous medium within each sub-domain evolves over time (see Figure 1) as the effective diffusivities would need now be updated repeatedly throughout the simulation. The aim of this paper is to develop an accurate and efficient method for calculating \(D_{\text{eff}}\) to alleviate this bottleneck in simulations.

\*Corresponding Author: elliot.carr@qut.edu.au
According to the homogenization literature [4, 6–8, 10, 14, 26], for a diffusivity \( D(x, y) \) defined on a rectangular domain \([x_0, x_n] \times [y_0, y_m]\) the first and second columns of the corresponding effective diffusivity can be computed using the following formulae:

\[
[D_{\text{eff}}]_{(:,1)} = \frac{1}{A} \int_{y_0}^{y_m} \int_{x_0}^{x_n} D(x, y) \nabla (\psi^{(x)}(x, y) + x) \, dx \, dy, \quad [D_{\text{eff}}]_{(:,2)} = \frac{1}{A} \int_{y_0}^{y_m} \int_{x_0}^{x_n} D(x, y) \nabla (\psi^{(y)}(x, y) + y) \, dx \, dy,
\]

(3)

where \( A = (x_n - x_0)(y_m - y_0) \) and \( \psi^{(\xi)}(x, y) \) is the solution of a boundary value problem involving the PDE:

\[
0 = \nabla \cdot (D(x, y) \nabla (\psi^{(\xi)} + \xi)), \quad x_0 < x < x_n, \quad y_0 < y < y_m.
\]

(4)

For a layered heterogeneous medium [8, 26], this boundary value problem has an exact solution yielding an effective diffusivity consisting of area-weighted arithmetic and harmonic averages of the layer diffusivities in the directions parallel and perpendicular to the layers, respectively [26]. In general, however, the boundary value problem cannot be solved analytically and one must turn to numerical techniques. In previous work by two of the authors of the current paper [4], an unstructured vertex-centered control volume finite element method was implemented to solve the boundary value problem on a two-dimensional irregular heterogeneous domain. The computed effective conductivities were then utilised within a two-scale model of unsaturated groundwater flow presented by Szymkiewicz and Lewandowska [28]. Szymkiewicz [26] implemented a finite volume method in three dimensions using cuboid finite volumes, each of which has a scalar conductivity. His formulation resulted in a system of linear equations with a sparse and banded coefficient matrix, which was solved using a conjugate gradient method. Recently, Ray et al. [21] implemented a local discontinuous Galerkin method in both two and three dimensions. This method is detailed further by Rupp et al. [23] and uses a formulation in which auxiliary flux variables are used to replace the higher order equations with a system of first-order equations.
If the heterogeneous medium within each sub-domain evolves over time (as in Figure 1), applying a numerical method to solve the PDE \( (4) \) may require re-meshing of the geometry. To address this issue, which could potentially bottleneck the simulation, we develop a new semi-analytical method for solving the boundary value problem. Our method assumes the heterogeneous medium takes the form of an arbitrarily-sized rectangular array of blocks, where the diffusivity is isotropic and constant within each individual block. Our novel strategy is to first reformulate the heterogeneous boundary value problem into a family of homogeneous boundary value problems on the individual blocks. This is achieved by introducing unknown functions representing the flux at the interfaces between adjacent blocks as utilised previously in one spatial dimension by several authors [3, 5, 22]. Solving each homogeneous boundary value problem using standard techniques yields analytical solution expressions that depend on integrals involving the unknown interface functions. By applying an appropriate numerical quadrature rule to these integrals and enforcing continuity of the solution across each interface, we show how the solution can be computed in each block. The net result is a semi-analytical method for solving the boundary value problem and calculating the effective diffusivity for a block heterogeneous domain.

Our new semi-analytical method has several desirable properties:

- it is able to compute, in less computational time, an effective diffusivity to the same level of accuracy as a standard finite volume method;
- it can capture highly complex heterogeneous geometries (see Figure 1); and
- it allows the heterogeneous geometry to be evolved over time in a straightforward manner by simply modifying the diffusivities in the individual blocks to conform to the change in heterogeneous structure.

Together, these properties suggest that our semi-analytical method has the potential to significantly speed up simulations of the coarse-grained equation (2).

The remaining sections of this paper are organised as follows. In section 2 we define the boundary value problem and effective diffusivity for a block heterogeneous medium. In section 3, we develop the new semi-analytical method for solving the boundary value problem and computing the effective diffusivity, describe its implementation and discuss the conditions required to ensure that it provides an accurate solution. In section 4, we discuss a standard finite volume method for solving the boundary value problem, which we use to assess the accuracy of our semi-analytical method. In section 5, we compare the semi-analytical and finite volume methods in terms of accuracy and efficiency for a variety of test cases from the literature and demonstrate how the semi-analytical method can be used to homogenize complex heterogeneous geometries. We conclude the paper in section 6 with a summary of the key findings of the work.

## 2 Definition of effective diffusivity

Consider a rectangular heterogeneous domain \([x_0, x_n] \times [y_0, y_m]\) consisting of an \(m\) by \(n\) array of blocks. Let the \((i,j)\)th block have domain \([x_{i-1}, x_i] \times [y_{j-1}, y_j]\) and diffusivity \(D_{i,j}\) with vertical interfaces between blocks at \(x = x_j\) \((j = 1, \ldots, n - 1)\) and horizontal interfaces between blocks at \(y = y_i\) \((i = 1, \ldots, m - 1)\) (see Figure 2). For this domain the first and second columns of the effective diffusivity \(D_{\text{eff}}\) are given by:

\[
[D_{\text{eff}}]_{(:,1)} = \frac{1}{A} \sum_{i=1}^{m} \sum_{j=1}^{n} \int_{y_{i-1}}^{y_i} \int_{x_{j-1}}^{x_j} D_{i,j} \nabla (\psi_{i,j}^{(x)}(x, y) + x) \, dx \, dy,
\]

\[
[D_{\text{eff}}]_{(:,2)} = \frac{1}{A} \sum_{i=1}^{m} \sum_{j=1}^{n} \int_{y_{i-1}}^{y_i} \int_{x_{j-1}}^{x_j} D_{i,j} \nabla (\psi_{i,j}^{(y)}(x, y) + y) \, dx \, dy,
\]

where \(A = (x_n - x_0)(y_m - y_0)\) and \(\psi_{i,j}^{(\xi)}\) satisfies the following PDE on the \((i,j)\)th block:

\[
0 = \nabla \cdot (D_{i,j} \nabla (\psi_{i,j}^{(\xi)}(x, y) + \xi)), \quad x_{j-1} < x < x_j, \quad y_{i-1} < y < y_i.
\]

At the interfaces between adjacent blocks both the solution and flux are continuous \([4, 26, 27]\), leading to the following interface conditions:

\[
\psi_{i,j}^{(\xi)}(x, y_i) = \psi_{i+1,j}^{(\xi)}(x, y_i), \quad x_{j-1} < x < x_j, \quad i = 1, \ldots, m - 1, \quad j = 1, \ldots, n,
\]

\[
\psi_{i,j}^{(\xi)}(x_j, y) = \psi_{i,j+1}^{(\xi)}(x_j, y), \quad y_{i-1} < y < y_i, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n - 1,
\]

\[
D_{i,j} \frac{\partial}{\partial y} \left( \psi_{i,j}^{(\xi)} + \xi \right)_{y=y_i} = D_{i+1,j} \frac{\partial}{\partial y} \left( \psi_{i+1,j}^{(\xi)} + \xi \right)_{y=y_i}, \quad x_{j-1} < x < x_j, \quad i = 1, \ldots, m - 1, \quad j = 1, \ldots, n,
\]

\[
D_{i,j} \frac{\partial}{\partial x} \left( \psi_{i,j}^{(\xi)} + \xi \right)_{x=x_j} = D_{i,j+1} \frac{\partial}{\partial x} \left( \psi_{i,j+1}^{(\xi)} + \xi \right)_{x=x_j}, \quad y_{i-1} < y < y_i, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n - 1.
\]
where periodic conditions hold at the external boundaries of the domain:

\[
\psi_{i,j}^{(\xi)}(x, y) = \psi_{i,m,j}^{(\xi)}(x, y_m), \quad x_{j-1} < x < x_j, \quad j = 1, \ldots, n, \quad i = 1, \ldots, m,
\]

\[
\psi_{i,1}^{(\xi)}(x, y) = \psi_{i,n,j}^{(\xi)}(x, y), \quad y_{i-1} < y < y_i, \quad i = 1, \ldots, m,
\]

\[
D_{i,j} \frac{\partial}{\partial x} \left( \psi_{i,j}^{(\xi)} + \xi \right) \bigg|_{x=x_{j-1}} = D_{m,j} \frac{\partial}{\partial y} \left( \psi_{m,j}^{(\xi)} + \xi \right) \bigg|_{y=y_{m-1}}, \quad x_{j-1} < x < x_j, \quad j = 1, \ldots, n,
\]

\[
D_{i,1} \frac{\partial}{\partial x} \left( \psi_{i,1}^{(\xi)} + \xi \right) \bigg|_{x=x_{i-1}} = D_{i,n} \frac{\partial}{\partial y} \left( \psi_{i,n}^{(\xi)} + \xi \right) \bigg|_{y=y_{i-1}}, \quad y_{i-1} < y < y_i, \quad i = 1, \ldots, m.
\]

The boundary value problem (7)–(15) has an infinite number of solutions [4, 26, 27] as any arbitrary constant may be added to the solution \(\psi_{i,j}^{(\xi)}\) and it will still satisfy the PDE (7) as well as the boundary conditions (8)–(15). To ensure a unique solution, we follow standard practice [4, 10, 25, 26] and impose a zero mean condition on the solution:

\[
\frac{1}{A} \sum_{i=1}^{m} \sum_{j=1}^{n} \int_{y_{i-1}}^{y_i} \int_{x_{j-1}}^{x_j} \psi_{i,j}^{(\xi)}(x, y) \, dx \, dy = 0.
\]

With \(\psi_{i,j}(x, y)\) known for \(\xi = x, y\), the effective diffusivity, \(D_{\text{eff}}\), can be computed from equations (5)–(6). Interpretation of the entries of the symmetric positive definite matrix \(D_{\text{eff}}\) comes from its diagonalization, \(D_{\text{eff}} = P\Lambda P^T\). Here, \(P \in \mathbb{R}^{2 \times 2}\) is an orthonormal matrix whose columns define the principal directions of diffusion and \(\Lambda \in \mathbb{R}^{2 \times 2}\) is a diagonal matrix whose entries represent the apparent diffusivities in these directions [17].

### 3 Semi-analytical method

#### 3.1 Solution approach

We now describe our new semi-analytical solution approach for solving the boundary value problem (7)–(16) which enables the effective diffusivity (5)-(6) to be determined. We first transform equation (7) into Laplace’s equation via the transformation:

\[
\psi_{i,j}^{(\xi)}(x, y) = \psi_{i,j}(x, y) + \xi,
\]

for \(i = 1, \ldots, m\) and \(j = 1, \ldots, n\). Substituting equation (17) into equations (7)–(15) yields:

\[
D_{i,j} \left( \frac{\partial^2 \psi_{i,j}^{(\xi)}}{\partial x^2} + \frac{\partial^2 \psi_{i,j}^{(\xi)}}{\partial y^2} \right) = 0, \quad x_{j-1} < x < x_j, \quad y_{i-1} < y < y_i.
\]
with the following conditions on the solution \( v_{i,j}^{(\xi)} \) at the interfaces and boundaries:

\[
\begin{align*}
    v_{i,j}^{(\xi)}(x, y_i) &= v_{i+1,j}^{(\xi)}(x, y_i), & x_{j-1} < x < x_j, & i = 1, \ldots, m-1, & j = 1, \ldots, n, \\
    v_{i,j}^{(\xi)}(x, y) &= v_{i+1,j}^{(\xi)}(x, y), & y_{i-1} < y < y_i, & i = 1, \ldots, m, & j = 1, \ldots, n-1, \\
    v_{i,j}^{(\xi)}(x_0, y) &= \begin{cases} v_{i,n}^{(\xi)}(x_0, y) + x_0 - x_n, & \text{if } \xi = x, \\
        v_{i,j}^{(\xi)}(x_0, y), & \text{if } \xi = y, \end{cases} & y_{i-1} < y < y_i, & i = 1, \ldots, m, \\
    v_{i,j}^{(\xi)}(x, y_0) &= \begin{cases} v_{m,j}^{(\xi)}(x, y_m), & \text{if } \xi = x, \\
        v_{i,j}^{(\xi)}(x, y_0) + y_0 - y_m, & \text{if } \xi = y, \end{cases} & x_{j-1} < x < x_j, & j = 1, \ldots, n,
\end{align*}
\]

and the following conditions on the flux at the interfaces and boundaries:

\[
\begin{align*}
    D_{i,1} \frac{\partial v_{i,j}^{(\xi)}}{\partial x}(x_0, y) &= D_{i,n} \frac{\partial v_{i,n}^{(\xi)}}{\partial y}(x_n, y), & y_{i-1} < y < y_i, & i = 1, \ldots, m, \\
    D_{j,1} \frac{\partial v_{i,j}^{(\xi)}}{\partial y}(x, y_0) &= D_{m,j} \frac{\partial v_{m,j}^{(\xi)}}{\partial x}(x, y_m), & x_{j-1} < x < x_j, & j = 1, \ldots, n, \\
    D_{i,j} \frac{\partial v_{i,j}^{(\xi)}}{\partial y}(x, y_1) &= D_{i+1,j} \frac{\partial v_{i+1,j}^{(\xi)}}{\partial y}(x, y_1), & x_{j-1} < x < x_j, & i = 1, \ldots, m-1, & j = 1, \ldots, n, \\
    D_{i,j} \frac{\partial v_{i,j}^{(\xi)}}{\partial x}(x, y) &= D_{i,j+1} \frac{\partial v_{i,j+1}^{(\xi)}}{\partial x}(x, y), & y_{i-1} < y < y_i, & i = 1, \ldots, m, & j = 1, \ldots, n-1.
\end{align*}
\]

Additionally, the zero mean condition (16) now takes the form:

\[
\sum_{i=1}^{m} \sum_{j=1}^{n} \int_{y_{i-1}}^{y_i} \int_{x_{j-1}}^{x_j} v_{i,j}^{(\xi)}(x, y) \, dx \, dy = \begin{cases} \frac{x_n + x_0}{2}, & \text{if } \xi = x, \\
        \frac{y_m + y_0}{2}, & \text{if } \xi = y. \end{cases}
\]

Our semi-analytical approach for solving this transformed boundary value problem involves first setting the fluxes at the interfaces and boundaries in equations (23)–(26) to be unknown functions of space [3, 5] as follows:

\[
\begin{align*}
    D_{i,1} \frac{\partial v_{i,j}^{(\xi)}}{\partial x}(x_0, y) &= D_{i,n} \frac{\partial v_{i,n}^{(\xi)}}{\partial y}(x_n, y) := g_{(i-1)n+1}(y), & y_{i-1} < y < y_i, & i = 1, \ldots, m, \\
    D_{j,1} \frac{\partial v_{i,j}^{(\xi)}}{\partial y}(x, y_0) &= D_{m,j} \frac{\partial v_{m,j}^{(\xi)}}{\partial x}(x, y_m) := q_{(j-1)m+1}(x), & x_{j-1} < x < x_j, & j = 1, \ldots, n, \\
    D_{i,j} \frac{\partial v_{i,j}^{(\xi)}}{\partial y}(x, y_1) &= D_{i+1,j} \frac{\partial v_{i+1,j}^{(\xi)}}{\partial y}(x, y_1), & y_{i-1} < y < y_i, & i = 1, \ldots, m-1, & j = 1, \ldots, n, \\
    D_{i,j} \frac{\partial v_{i,j}^{(\xi)}}{\partial x}(x, y) &= D_{i,j+1} \frac{\partial v_{i,j+1}^{(\xi)}}{\partial x}(x, y), & x_{j-1} < x < x_j, & i = 1, \ldots, m-1, & j = 1, \ldots, n-1.
\end{align*}
\]

This allows us to reformulate the heterogeneous boundary value problem (18)–(26) into a family of boundary value problems on each of the \( mn \) blocks:

\[
D_{i,j} \left( \frac{\partial^2 v_{i,j}^{(\xi)}}{\partial x^2} + \frac{\partial^2 v_{i,j}^{(\xi)}}{\partial y^2} \right) = 0, \quad x_{j-1} < x < x_j, \quad y_{i-1} < y < y_i,
\]

\[
D_{i,j} \frac{\partial v_{i,j}^{(\xi)}}{\partial x}(x_{j-1}, y) = g_{(i-1)n+1}(y), \quad D_{i,j} \frac{\partial v_{i,j}^{(\xi)}}{\partial x}(x_{j+1}, y) = g_{(i-1)n+1}(y), \quad y_{i-1} < y < y_i,
\]

\[
D_{i,j} \frac{\partial v_{i,j}^{(\xi)}}{\partial y}(x, y_{i-1}) = q_{(j-1)m+1}(x), \quad D_{i,j} \frac{\partial v_{i,j}^{(\xi)}}{\partial y}(x, y_i) = q_{(j-1)m+1}(x), \quad x_{j-1} < x < x_j,
\]

where the unknown interface and boundary functions, introduced in equations (28)–(31), are constrained to satisfy the interface and boundary conditions (19)–(22). The boundary conditions (33)–(34) are valid for all blocks except those
in either the bottom row ($i = m$) or right column ($j = n$). The boundary conditions for these blocks are similar to equations (33)–(34) and are detailed in A.

The solution of the boundary value problem (32)–(34) is given by [18]:

$$v_{i,j}^{(ξ)}(x, y) = -\frac{a_{i,j,0}^{(ξ)}}{4l_j}(x - x_j)^2 + \frac{b_{i,j,0}^{(ξ)}}{4l_j}(x - x_{j-1})^2 - \frac{c_{i,j,0}^{(ξ)}}{4h_i}(y - y_{i-1})^2 + \frac{d_{i,j,0}^{(ξ)}}{4h_i}(y - y_i)^2 + K_{i,j},$$

$$- h_i \sum_{k=1}^{\infty} a_{i,j,k}^{(ξ)} \cosh \left[ \frac{k\pi(x - x_j)}{h_i} \right] \cos \left( \frac{k\pi(y - y_{i-1})}{h_i} \right) + h_i \sum_{k=1}^{\infty} b_{i,j,k}^{(ξ)} \cosh \left[ \frac{k\pi(x - x_{j-1})}{h_i} \right] \cos \left( \frac{k\pi(y - y_{i-1})}{h_i} \right)$$

$$- l_j \sum_{k=1}^{\infty} c_{i,j,k}^{(ξ)} \cosh \left[ \frac{k\pi(y - y_j)}{l_j} \right] \cos \left( \frac{k\pi(x - x_{j-1})}{l_j} \right) + l_j \sum_{k=1}^{\infty} d_{i,j,k}^{(ξ)} \cosh \left[ \frac{k\pi(y - y_{i-1})}{l_j} \right] \cos \left( \frac{k\pi(x - x_{j-1})}{l_j} \right),$$

(35)

where:

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

(36)

and $K_{i,j}$ is an arbitrary constant. While for the solution of the boundary value problem (32)–(34) the constant $K_{i,j}$ is arbitrary, in the context of the solution across the entire domain $[x_0, x_n] \times [y_0, y_m]$ consisting of all $mn$ boundary value problems, the constants are not arbitrary as they are required to ensure continuity of the solution across the interfaces and boundaries. Note that the coefficients $a_{i,j,k}^{(ξ)}, b_{i,j,k}^{(ξ)}, c_{i,j,k}^{(ξ)}$ and $d_{i,j,k}^{(ξ)}$ appearing in equation (35) depend on the values of $i$ and $j$. For $i = 1, \ldots, m - 1$ and $1 = j, \ldots, n - 1$:

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

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

$$c_{i,j,k}^{(ξ)} = \frac{2}{l_j} \int_{x_{j-1}}^{x_j} \frac{g_{(j-1)m+i}(x)}{D_{i,j}} \cos \left( \frac{k\pi(x - x_{j-1})}{l_j} \right) dx,$$

$$d_{i,j,k}^{(ξ)} = \frac{2}{l_j} \int_{x_{j-1}}^{x_j} \frac{g_{(j-1)m+i+1}(x)}{D_{i,j}} \cos \left( \frac{k\pi(x - x_{j-1})}{l_j} \right) dx,$$

(37)

(38)

where $k = 0, 1, \ldots, \infty$, while for the bottom row ($i = m$) and right column ($j = n$) of blocks the coefficients are similar and given in B.

Due to the boundary conditions (33)–(34), the solution (35) requires an additional solvability condition to ensure a net flux of zero is imposed on each block [18]. This condition takes the form:

$$\int_{y_{i-1}}^{y_i} \frac{g_{(i-1)n+j}(y)}{D_{i,j}} dy - \int_{y_{i-1}}^{y_i} \frac{g_{(i-1)n+j+1}(y)}{D_{i,j}} dy + \int_{x_{j-1}}^{x_j} \frac{q_{(j-1)m+i}(x)}{D_{i,j}} dx - \int_{x_{j-1}}^{x_j} \frac{q_{(j-1)m+i+1}(x)}{D_{i,j}} dx = 0,$$

(39)

for $i = 1, \ldots, m - 1$ and $j = 1, \ldots, n - 1$. The solvability conditions for the bottom row ($i = m$) and right column ($j = n$) of blocks have a similar form to equation (39) and are given in C.

Through the coefficients (37)–(38), the solution (35) in each block involves the integral of the unknown interface and boundary functions, introduced in equations (28)–(31), and the unknown constants $K_{i,j}$. By applying the as yet unused interface and boundary conditions (19)–(22), we now derive a linear system of equations whose solution allows the integrals appearing in the coefficients (37)–(38) to be approximated. This is achieved by first applying a quadrature rule to these integrals. For example using the expressions for $a_{i,j,k}^{(ξ)}$ and $c_{i,j,k}^{(ξ)}$ in equations (37)–(38), we have:

$$a_{i,j,k}^{(ξ)} = \frac{2}{h_i} \int_{y_{i-1}}^{y_i} \frac{g_{(i-1)n+j}(y)}{D_{i,j}} \cos \left( \frac{k\pi(y - y_{i-1})}{h_i} \right) dy \approx \frac{2}{D_{i,j}h_i} \sum_{p=1}^{N_x} w_x^{(p)} g_{(i-1)n+j}(y^{(i,p)}) \cos \left( \frac{k\pi(y^{(i,p)} - y_{i-1})}{h_i} \right),$$

(40)

$$c_{i,j,k}^{(ξ)} = \frac{2}{l_j} \int_{x_{j-1}}^{x_j} \frac{q_{(j-1)m+i}(x)}{D_{i,j}} \cos \left( \frac{k\pi(x - x_{j-1})}{l_j} \right) dx \approx \frac{2}{D_{i,j}l_j} \sum_{p=1}^{N_y} w_y^{(p)} g_{(j-1)m+i}(x^{(j,p)}) \cos \left( \frac{k\pi(x^{(j,p)} - x_{j-1})}{l_j} \right),$$

(41)

where $w_x^{(p)}$ and $w_y^{(p)}$ are the weights of the $p$th abscissa, $x^{(j,p)}$ and $y^{(i,p)}$, respectively and $N_x$ and $N_y$ denote the number of abscissas. The weights $w_x^{(p)}$ and $w_y^{(p)}$ and abscissas $x^{(j,p)}$ and $y^{(i,p)}$ depend on the type of quadrature rule chosen, as will be discussed in the following section. There are a total of $2mn$ unknown flux functions, $q_{(i-1)n+j+1}(x)$ and $g_{(i-1)n+j}(y)$ for $i = 1, \ldots, m$ and $j = 1, \ldots, n$, with the integrals involving these functions approximated using a quadrature rule with $N_x$ and $N_y$ function evaluations, respectively. In total, this yields $mn(N_x + N_y)$ unknown
evaluations at the abscissas: \( q_{(j-1)m+i} \) for \( i = 1, \ldots, m, j = 1, \ldots, n \) and \( p = 1, \ldots, N_x \) and \( q_{(i-1)n+j} \) for \( i = 1, \ldots, m, j = 1, \ldots, n \) and \( p = 1, \ldots, N_y \). To compute these evaluations, which appear in equations (40)–(41), we make use of the boundary and interface conditions (19)–(22) evaluated at each of the abscissas:

\[
v^{(\xi)}_{i+1,j}(x^{(j,p)}, y_i) - v^{(\xi)}_{i,j}(x^{(j,p)}, y_i) = 0, \quad x_{j-1} < x^{(j,p)} < x_j, \quad i = 1, \ldots, m - 1, \quad j = 1, \ldots, n, \quad p = 1, \ldots, N_x, \tag{42}
\]

\[
v^{(\xi)}_{i,j+1}(x_j, y^{(i,p)}) - v^{(\xi)}_{i,j}(x_j, y^{(i,p)}) = 0, \quad y_{i-1} < y^{(i,p)} < y_i, \quad i = 1, \ldots, m, \quad j = 1, \ldots, n - 1, \quad p = 1, \ldots, N_y, \tag{43}
\]

\[
v^{(\xi)}_{m,j}(x^{(j,p)}, y_m) - v^{(\xi)}_{m,j}(x^{(j,p)}, y_0) = \begin{cases} 0 & \text{if } \xi = x, \\
y_m - y_0 & \text{if } \xi = y, \end{cases} \quad x_{j-1} < x^{(j,p)} < x_j, \quad j = 1, \ldots, n, \quad p = 1, \ldots, N_x, \tag{44}
\]

\[
v^{(\xi)}_{i,n}(x_n, y^{(i,p)}) - v^{(\xi)}_{i,1}(x_0, y^{(i,p)}) = \begin{cases} x_n - x_0 & \text{if } \xi = x, \\
y_m - y_0 & \text{if } \xi = y, \end{cases} \quad y_{i-1} < y^{(i,p)} < y_i, \quad i = 1, \ldots, m, \quad p = 1, \ldots, N_y. \tag{45}
\]

Equations (42)–(45) define a system of \( mn(N_x + N_y) \) equations linear in the \( mn(N_x + N_y) \) unknown evaluations at the abscissas. In addition to these unknowns, we have an additional \( mn \) unknowns corresponding to the constants \( K_{i,j} \) appearing in equation (35). These unknowns are accounted for by imposing the solvability conditions (39), with the integrals replaced with quadrature approximations similar to those used in equations (40)–(41). The solvability conditions ensure a zero net flux on each block and as periodic conditions are imposed on the external boundaries of the domain, the solvability condition in any one of the \( mn \) blocks is redundant. To account for this redundancy, we replace the solvability conditions on block \( mn \) with the zero mean condition (16). In the solution expression (35), all terms with the exception of the constants \( K_{i,j} \) integrate to zero over their domain of integration \([x_{j-1}, x_j] \times [y_{i-1}, y_i]\). This allows for the zero mean condition (27) to be written in the following form:

\[
\sum_{i=1}^{m} \sum_{j=1}^{n} K_{i,j} = \begin{cases} \frac{x_n + x_0}{2} & \text{if } \xi = x, \\
\frac{y_m + y_0}{2} & \text{if } \xi = y. \end{cases} \tag{46}
\]

Assembling equations (42)–(46) yields a linear system:

\[
Ax = b, \tag{47}
\]

where \( A \in \mathbb{R}^{N \times N} \), \( x \in \mathbb{R}^{N} \), \( b \in \mathbb{R}^{N} \) and \( N = mn(N_x + N_y) + 1 \). The entries of \( A \) and \( b \) are determined via the solvability conditions (39), the continuity conditions (42)–(45) and the zero mean condition (46). The vector \( x \) contains the function evaluations \( q_{(j-1)m+i}(x^{(j,p)}) \) for \( i = 1, \ldots, m, j = 1, \ldots, n \) and \( p = 1, \ldots, N_x \) and \( g_{(i-1)n+j}(y^{(i,p)}) \) for \( i = 1, \ldots, m, j = 1, \ldots, n \) and \( p = 1, \ldots, N_y \) as well as the constants \( K_{i,j} \) for \( i = 1, \ldots, m \) and \( j = 1, \ldots, n \). Note that when constructing the linear system, we truncate the summations appearing in the solution expression (35) after a finite number of terms, \( k = N_x x \). Solving the linear system (47) then allows the approximations to the integrals (40) and (41) to be computed and thus the solution (35) can be evaluated. With \( v^{(\xi)}_{i,j}(x,y) \) computed, the solution of the original boundary value problem (7)–(16) can be calculated as \( \psi^{(\xi)}_{i,j}(x,y) = v^{(\xi)}_{i,j}(x,y) - \xi \).

In terms of the transformed solution \( v^{(\xi)}_{i,j}(x,y) \), the four entries of the effective diffusivity are given by:

\[
[D_{\text{eff}}]_{(1,1)} = \frac{1}{A} \sum_{i=1}^{m} \sum_{j=1}^{n} \int_{y_{i-1}}^{y_i} \int_{x_{j-1}}^{x_j} D_{i,j} \frac{\partial v^{(\xi)}_{i,j}}{\partial x} dx dy, \quad [D_{\text{eff}}]_{(2,1)} = \frac{1}{A} \sum_{i=1}^{m} \sum_{j=1}^{n} \int_{y_{i-1}}^{y_i} \int_{x_{j-1}}^{x_j} D_{i,j} \frac{\partial v^{(\xi)}_{i,j}}{\partial y} dx dy, \tag{48}
\]

\[
[D_{\text{eff}}]_{(1,2)} = \frac{1}{A} \sum_{i=1}^{m} \sum_{j=1}^{n} \int_{y_{i-1}}^{y_i} \int_{x_{j-1}}^{x_j} D_{i,j} \frac{\partial v^{(\eta)}_{i,j}}{\partial x} dx dy, \quad [D_{\text{eff}}]_{(2,2)} = \frac{1}{A} \sum_{i=1}^{m} \sum_{j=1}^{n} \int_{y_{i-1}}^{y_i} \int_{x_{j-1}}^{x_j} D_{i,j} \frac{\partial v^{(\eta)}_{i,j}}{\partial y} dx dy. \tag{49}
\]

As we have an analytical expression for \( v^{(\xi)}_{i,j}(x,y) \) (35) we can perform the differentiations and integrations appearing in
Hence, we use the regular midpoint rule as the quadrature rule in our semi-analytical method. The Filon-midpoint rule was found to be consistently less accurate than the regular midpoint rule in testing. Returned inaccurate results for both the solution of the boundary value problem (18)–(26) and the effective diffusivity were used. However, when implemented in the semi-analytical method, we found that the Gaussian quadrature methods tested were able to compute similar integrals of oscillatory functions in initial testing, provided that enough abscissas were used. Many of these quadrature rules use abscissas at the endpoints, have frequency-dependent abscissas and/or require additional information about the function, such as its derivatives and as such are not able to be implemented for our semi-analytical method. We then considered: the midpoint rule, a Filon-midpoint rule demonstrated by Potticary [19] and Levin [11, 15] type methods, which are quadrature rules well-suited to highly oscillatory functions. However, many Gaussian quadrature methods that do not use abscissas at the endpoints. As the integrals appearing in the coefficients (37)–(38) contain an oscillatory function, we investigated Filon [11, 12] and Levin [11, 15] type methods, which are quadrature rules well-suited to highly oscillatory functions. However, many of these quadrature rules use abscissas at the endpoints, have frequency-dependent abscissas and/or require additional information about the function, such as its derivatives and as such are not able to be implemented for our semi-analytical method. We then considered: the midpoint rule, a Filon-midpoint rule demonstrated by Potticary [19] and various Gaussian quadrature methods that do not use abscissas at the endpoints. The Gaussian quadrature methods tested were able to compute similar integrals of oscillatory functions in initial testing, provided that enough abscissas were used. However, when implemented in the semi-analytical method, we found that the Gaussian quadrature methods returned inaccurate results for both the solution of the boundary value problem (18)–(26) and the effective diffusivity (50)–(53). The Filon-midpoint rule was found to be consistently less accurate than the regular midpoint rule in testing. Hence, we use the regular midpoint rule as the quadrature rule in our semi-analytical method.

The midpoint rule uses evenly spaced abscissas, which leads to a restriction on the maximum number of terms, N_{eig}, taken in the summations appearing in the solution (35). The functions integrated in the definition of the coefficients

\[
[D_{\text{eff}}]_{(1,1)} = \frac{1}{A} \sum_{i=1}^{m} \sum_{j=1}^{n} D_{i,j} A_{i,j} (c_{i,j,0}^{(x)} + b_{i,j,0}^{(x)}) + \frac{N_{eig}}{k\pi} \sum_{k=1}^{N_{eig}} (c_{i,j,k}^{(x)} - d_{i,j,k}^{(x)})(1 - (-1)^k), 
\]

\[
[D_{\text{eff}}]_{(1,2)} = \frac{1}{A} \sum_{i=1}^{m} \sum_{j=1}^{n} D_{i,j} A_{i,j} (c_{i,j,0}^{(y)} + b_{i,j,0}^{(y)}) + \frac{N_{eig}}{k\pi} \sum_{k=1}^{N_{eig}} (c_{i,j,k}^{(y)} - d_{i,j,k}^{(y)})(1 - (-1)^k), 
\]

\[
[D_{\text{eff}}]_{(2,1)} = \frac{1}{A} \sum_{i=1}^{m} \sum_{j=1}^{n} D_{i,j} A_{i,j} (c_{i,j,0}^{(x)} + d_{i,j,0}^{(x)}) + h_{x}^{2} \sum_{k=1}^{N_{eig}} (c_{i,j,k}^{(x)} - b_{i,j,k}^{(x)})(1 - (-1)^k), 
\]

\[
[D_{\text{eff}}]_{(2,2)} = \frac{1}{A} \sum_{i=1}^{m} \sum_{j=1}^{n} D_{i,j} A_{i,j} (c_{i,j,0}^{(y)} + d_{i,j,0}^{(y)}) + h_{y}^{2} \sum_{k=1}^{N_{eig}} (c_{i,j,k}^{(y)} - b_{i,j,k}^{(y)})(1 - (-1)^k). 
\]

Finally, we remark that the coefficient matrix A in the linear system (47) is identical for both \(\xi = x\) and \(\xi = y\). This means that the linear system for \(\xi = x\) and the linear system for \(\xi = y\) can both be solved with only one matrix factorisation.

### 3.2 Choice of quadrature method

There are several constraints governing the choice of quadrature method utilized in the approximations of the integrals (40)–(41):

- **Abscissas cannot include the vertices of blocks**
  
  If a vertex of a block is used as an abscissa in the quadrature rules (40)–(41), then the set of four continuity conditions (42)–(45) evaluated at the vertex will be linearly dependent. If all \(mn\) vertices are used in the quadrature rules (40)–(41), then the linear system (47) is deficient in rank by \(mn\). As the vertices of the blocks are the limits of integration for all integrals appearing in the coefficients (37)–(38), to ensure linear independence we implement a quadrature rule that uses at most one of the limits of integration as an abscissa. While we could implement different quadrature rules that use endpoints for some integrals and do not use endpoints for other integrals, we take the simplest option of using no endpoints.

- **The quadrature rule must use the same abscissas for all frequencies**

  The linear system (47) is generated by evaluating the boundary and interface conditions (42)–(45) at the abscissas used in the quadrature formulae (40)-41). In order to minimise the size of the the linear system (47), the same abscissas \(x^{(i,p)}\) and \(y^{(i,p)}\) should be used for all \(k = 0, \ldots, N_{eig}\). Hence, we restrict the choice of quadrature rules to those that do not use frequency-dependent abscissas.

- **The quadrature rule cannot make use of any information about the function being integrated**

  As the evaluations, \(q_{(i-1)n+j}(x^{(i,p)})\) for \(i = 1, \ldots, m, j = 1, \ldots, n\) and \(p = 1, \ldots, N_{x}\) and \(g_{(i-1)n+j}(y^{(i,p)})\) for \(i = 1, \ldots, m, j = 1, \ldots, n\) and \(p = 1, \ldots, N_{y}\), used to approximate the integrals (37)–(38) are determined via the solution of the linear system (47), the quadrature rule must be a linear function of these evaluations and cannot use any other information about the function.

As the integrals appearing in the coefficients (37)–(38) contain an oscillatory function, we investigated Filon [11, 12] and Levin [11, 15] type methods, which are quadrature rules well-suited to highly oscillatory functions. However, many of these quadrature rules use abscissas at the endpoints, have frequency-dependent abscissas and/or require additional information about the function, such as its derivatives and as such are not able to be implemented for our semi-analytical method. We then considered: the midpoint rule, a Filon-midpoint rule demonstrated by Potticary [19] and various Gaussian quadrature methods that do not use abscissas at the endpoints. The Gaussian quadrature methods tested were able to compute similar integrals of oscillatory functions in initial testing, provided that enough abscissas were used. However, when implemented in the semi-analytical method, we found that the Gaussian quadrature methods returned inaccurate results for both the solution of the boundary value problem (18)–(26) and the effective diffusivity (50)–(53). The Filon-midpoint rule was found to be consistently less accurate than the regular midpoint rule in testing. Hence, we use the regular midpoint rule as the quadrature rule in our semi-analytical method.

The midpoint rule uses evenly spaced abscissas, which leads to a restriction on the maximum number of terms, \(N_{eig}\), taken in the summations appearing in the solution (35). The functions integrated in the definition of the coefficients
are similar to \( \tilde{f}(x) = f(x) \cos(k\pi x/L) \) with limits of integration of \( x = 0 \) and \( x = L \). The period of \( \tilde{f}(x) \) is \( 2L/k \) and with \( N_x \) evenly spaced abscissas used in the approximation of the integrals, the spacing between abscissas is \( L/(N_x - 1) \). If \( 2L/k = L/(N_x - 1) \) the abscissas align with the peaks of \( \tilde{f}(x) \), which causes each evaluation of \( \tilde{f}(x) \) to occur at an abscissa \( x = x^* \) at which \( f(x^*) = \tilde{f}(x^*) \). This has the effect of returning the value of the integral of \( f(x) \) from \( x = 0 \) to \( x = L \) instead of \( \tilde{f}(x) \). Figure 3 shows this behaviour for the example \( f(x) = x \). Hence, to ensure an accurate solution we set an upper limit on the maximum number of terms in the summations in equation (35) to ensure \( 2L/k < L/(N_x - 1) \), for all \( k = 1, \ldots, N_{\text{eig}} \), leading to the restriction \( N_{\text{eig}} \leq 2N_x - 3 \).}

\[ \sum_{s \in e_x} D(x_{\text{mid}}^{(s)}, y_{\text{mid}}^{(s)}) \left( \frac{\partial \psi^{(l)}}{\partial x} (x_{\text{mid}}^{(s)}, y_{\text{mid}}^{(s)}) + \delta_{x} \right) \frac{h_x}{2} + \sum_{s \in e_y} D(x_{\text{mid}}^{(s)}, y_{\text{mid}}^{(s)}) \left( \frac{\partial \psi^{(l)}}{\partial y} (x_{\text{mid}}^{(s)}, y_{\text{mid}}^{(s)}) + \delta_{y} \right) \frac{h_y}{2} = 0, \]

where \( e_x \) and \( e_y \) are the sets of vertical and horizontal edges of the control volume, \( (x_{\text{mid}}^{(s)}, y_{\text{mid}}^{(s)}) \) are the coordinates of the midpoint of edge \( s \) of the control volume and \( \delta_{x} \) and \( \delta_{y} \) are Kronecker deltas, taking the value of one when the subscripts are equal and zero otherwise. The equation (54) is valid for all nodes, except those located along the boundaries \( x = x_n \) and \( y = y_m \). For these nodes, the finite volume equation (54) is modified to accommodate the periodic boundary conditions, as discussed in detail by Carr et al. [6].

Approximating the spatial derivatives appearing in equation (54) using second-order central differences and assembling the resulting finite volume equations for each node yields a linear system of the form:

\[ A_{\text{FVM}} \psi_{\text{FVM}} = b_{\text{FVM}}, \]

where \( x_{\text{FVM}} \) is a vector of length \( N_{\text{FVM}}^{(x)} \times N_{\text{FVM}}^{(y)} \) containing the discrete unknown values of \( \psi^{(l)} \) at each of the nodes. After solving this linear system, we use a bilinear interpolant of \( \psi^{(l)} \) over each element to approximate the gradient within

![Figure 3: Plot of \( \tilde{f}(x) = x \cos(20\pi x) \) interpolated at abscissas with a uniform spacing of 0.1. The interpolated function, represented in black, incorrectly appears identical to \( f(x) = x \).]
each element. This allows us to approximate the integrals in equation (3), yielding the following formulae for the first and second columns of the effective diffusivity:

\[ D_{\text{eff}}[(:,1)] = \frac{1}{A} \sum_{p=1}^{N_{x,\text{FVM}}} \sum_{q=1}^{N_{y,\text{FVM}}} D(x_c^{(p)}, y_c^{(q)})(\nabla \phi^{(x)}(x_c^{(p)}, y_c^{(q)})) e_1 h_x h_y, \]

\[ D_{\text{eff}}[(:,2)] = \frac{1}{A} \sum_{p=1}^{N_{x,\text{FVM}}} \sum_{q=1}^{N_{y,\text{FVM}}} D(x_c^{(p)}, y_c^{(q)})(\nabla \phi^{(y)}(x_c^{(p)}, y_c^{(q)})) e_2 h_x h_y, \]

where \((x_c^{(p)}, y_c^{(q)})\) is the centroid of the \((p,q)\)th element, \(e_1 = [1,0]^T\) and \(e_2 = [0,1]^T\).

5 Numerical results

In this section we verify the accuracy and efficiency of our new semi-analytical method and demonstrate its applicability to problems on complex heterogeneous geometries. In all comparisons between the semi-analytical and finite volume methods, we ensure that the spacing between abscissas and the spacing between nodes are identical by setting \(N_{x,\text{FVM}} = n N_x\) and \(N_{y,\text{FVM}} = m N_y\) in the finite volume method, where \(N_x\) and \(N_y\) denote the number of abscissas per interface in the semi-analytical method. Both the semi-analytical and finite volume methods were implemented in MATLAB and the linear systems for both methods, equations (47) and (55), were stored in sparse format and solved using the backslash operator. All numerical experiments were carried out in MATLAB (version 2017A) running on an early 2015 MacBook Pro with a 2.7GHz dual-core Intel Core i5 processor and 8GB of memory on macOS Version 10.13.5.

The efficiency of the MATLAB code implementing the semi-analytical method can be improved by assuming that \(m = n\) (i.e. the same number of blocks in both the horizontal and vertical directions) and that all \(mn\) blocks are the same size. The main source of the improvement in efficiency is in being able to compute the summations appearing in the solution (35) only once, instead of once for each abscissa used in the method. All of the test cases we consider and the majority of the problems we encountered in the literature have \(m = n\) and identically sized blocks, so all calculations in this paper are computed using the more efficient version of the MATLAB code. The MATLAB codes implementing the semi-analytical method for both \(m = n\) and \(m \neq n\) are available on our GitHub repository: https://github.com/NathanMarch/Homogenization.

5.1 Accuracy and efficiency of the semi-analytical method

As a first verification of the accuracy of the semi-analytical solution we consider four geometries previously presented by Szymkiewicz [27]. These four test geometries are depicted in Table 1 and take the form of a square cell of dimension 1 by 1 comprised of an 8 by 8 array of blocks each of dimension 0.125 by 0.125. The dark grey blocks have a diffusivity of 0.1 and the light grey blocks have a diffusivity of 1. Case 1 has a square shaped inclusion of dark grey blocks in the centre of the cell, case 2 consists of one larger dark grey inclusion in the centre of the cell and four smaller dark grey inclusions at the corners, case 3 consists of three layers, of which the middle layer is dark grey and case 4 contains an L-shaped dark grey inclusion. We compute the effective diffusivity using both the semi-analytical and finite volume methods for cases 1–4 and compare the results to those presented by Szymkiewicz [27]. We set \(N_x = N_y = 16\) and \(N_{\text{eig}} = 2 N_x - 3 = 29\) for the semi-analytical method and \(N_{x,\text{FVM}} = N_{y,\text{FVM}} = 4 N_x = 4 N_y = 64\) for the finite volume method. The results in Table 1 demonstrate that both the semi-analytical and finite volume methods are in very good agreement with the results presented by Szymkiewicz [27], agreeing to at least two significant figures for all entries in each effective diffusivity.

The effective diffusivities for cases 1–3 are diagonal matrices as each geometry is invariant under a rotation of 180° [24, 25]. Additionally, the diagonal entries of the effective diffusivity for case 1 are identical as the geometry is also invariant under a rotation of 90°. As cases 1–3 have effective diffusivities that are diagonal, the principal directions of diffusion are in the horizontal \((x)\) and vertical \((y)\) directions and the diagonal elements represent the diffusivity in these directions (see Table 1). For cases 2 and 3 the diffusivity in the horizontal direction is larger than the diffusivity in the vertical direction. This is because, unlike for flow in the horizontal direction, flow in the vertical direction must pass through or around the low diffusive (dark grey) blocks. Case 3 is a layered medium, so the diffusivity in the horizontal and vertical directions are the area-weighted arithmetic and harmonic averages of the layer diffusivities, respectively. The eigenvalues of the effective diffusivity for case 4 are 0.527 and 0.682 and the corresponding normalised eigenvectors are \([0.982, 0.189]^T\) and \([0.189, -0.982]^T\), which define principal directions of diffusion for case 4 that are rotated 10.9° anti-clockwise from the standard Cartesian axes (see Table 1).
We now compare the accuracy of the semi-analytical method to the finite volume method by first computing a benchmark effective diffusivity using the finite volume method with a very fine node spacing. We consider the geometries of cases 1 and 4 as presented by Szymkiewicz [27], represented as both 4 by 4 and 16 by 16 grids of equal-sized blocks. For the 4 by 4 configuration each block is of size 0.25 by 0.25 while for the 16 by 16 configuration each block is of size 0.0625 by 0.0625. For the 4 by 4 configuration we compute the effective diffusivity using \( N_x = N_y = 4 \). For the 16 by 16 configuration we compute the effective diffusivity using \( N_x = N_y = 16 \) for the semi-analytical method and \( N_{x,FVM} = N_{y,FVM} = 16N_x = 16N_y = 16, 32, 64, 128 \) and 256 for the finite volume method. For both configurations, the benchmark effective diffusivity is computed using the finite volume method with \( N_{x,FVM} = N_{y,FVM} = 1024 \). For the semi-analytical method, \( N_{\text{eig}} \) is set as the minimum of \( 2N_x - 3 \) and 100. This is because, as mentioned in section 3.2, the value \( 2N_x - 3 \) is the upper limit on the maximum number of terms in the summations in equation (35) and in preliminary testing we found that using more than 100 terms in the summation had negligible effect on the solution. We compute our relative error \( E = |(D_{\text{eff}} - D_{\text{eff}}^*)/D_{\text{eff}}| \), where \( \otimes \) represents Hadamard/element-wise division, \( D_{\text{eff}} \) represents the effective diffusivity as calculated from the semi-analytical/finite volume solution under comparison and \( D_{\text{eff}}^* \) is the benchmark effective diffusivity. We also record the runtime for both the semi-analytical and finite volume methods, which includes the time taken to solve the boundary value problem (18)–(27) and compute the effective diffusivity via equations (50)–(53) and (56)–(57). All runtimes reported in this section were calculated by performing each calculation ten times and taking the median runtime. Results in Table 2 demonstrate that the semi-analytical method is either faster or more accurate (or both) than the finite volume method, indicating that for a specified level of accuracy the semi-analytical method is more efficient.

We now further explore the efficiency of our new semi-analytical method by comparing the size of the linear systems, equations (47) and (55), and the time taken to compute the effective diffusivity for both the semi-analytical and finite volume methods. To do this we consider a square domain with \( x_0 = y_0 = 0 \) and \( x_n = y_m = 1 \), consisting of an \( m \) by \( m \) grid of equal-sized blocks for \( m = 2, \ldots, 40 \), i.e., we consider a 2 by 2 grid, a 3 by 3 grid etc. The domain is a checkerboard structure consisting of diffusivities of 0.1 and 1 with a diffusivity of 0.1 in the top left corner. For example, the diffusivities for \( m = 3 \) are:

\[
\begin{bmatrix}
D_{1,1} & D_{1,2} & D_{1,3} \\
D_{2,1} & D_{2,2} & D_{2,3} \\
D_{3,1} & D_{3,2} & D_{3,3}
\end{bmatrix}
= \begin{bmatrix}
0.1 & 1 & 0.1 \\
1 & 0.1 & 1 \\
0.1 & 1 & 0.1
\end{bmatrix}.
\]

As usual, we specify the spacing between abscissas for the semi-analytical method to be the same as the spacing between nodes for the finite volume method. We compute the effective diffusivity using \( N_x = N_y = 16 \) and \( N_{\text{eig}} = 2N_x - 3 = 29 \) for the semi-analytical method and \( N_{x,FVM} = N_{y,FVM} = 16m \) for the finite volume method. This leads to the linear system (47) in the semi-analytical method having dimension \( m^2(2N_x + 1) = 33m^2 \) and the linear system (55) in the finite volume method having dimension \( m^2N_x^2 = 256m^2 \). Results in Figure 4 demonstrate that the efficiency advantage of

| Geometry | Case 1 | Case 2 | Case 3 | Case 4 |
|----------|--------|--------|--------|--------|
| Szymkiewicz [27] | \( \begin{bmatrix} 0.649 & 0 \\ 0 & 0.649 \end{bmatrix} \) | \( \begin{bmatrix} 0.693 & 0 \\ 0 & 0.566 \end{bmatrix} \) | \( \begin{bmatrix} 0.775 & 0 \\ 0 & 0.309 \end{bmatrix} \) | \( \begin{bmatrix} 0.533 & -0.0286 \\ -0.0286 & 0.675 \end{bmatrix} \) |
| Finite Volume | \( \begin{bmatrix} 0.648 & 0 \\ 0 & 0.648 \end{bmatrix} \) | \( \begin{bmatrix} 0.694 & 0 \\ 0 & 0.566 \end{bmatrix} \) | \( \begin{bmatrix} 0.775 & 0 \\ 0 & 0.308 \end{bmatrix} \) | \( \begin{bmatrix} 0.533 & -0.0286 \\ -0.0286 & 0.676 \end{bmatrix} \) |
| Semi-Analytical | \( \begin{bmatrix} 0.648 & 0 \\ 0 & 0.648 \end{bmatrix} \) | \( \begin{bmatrix} 0.693 & 0 \\ 0 & 0.566 \end{bmatrix} \) | \( \begin{bmatrix} 0.775 & 0 \\ 0 & 0.308 \end{bmatrix} \) | \( \begin{bmatrix} 0.533 & -0.0286 \\ -0.0286 & 0.676 \end{bmatrix} \) |

Table 1: Effective diffusivity for cases 1–4 as calculated using the semi-analytical and finite volume methods and compared to the results presented by Szymkiewicz [27]. The principal directions of diffusion are overlaid upon each geometry. All results are reported to three significant figures, consistent with Szymkiewicz [27].
the semi-analytical method over the finite volume method becomes more pronounced as \( m \) increases. This is because as the number of blocks increases, the size of the linear system increases (see Figure 4) and the time taken to solve these systems becomes the dominant computational cost of calculating the effective diffusivity. This improvement in efficiency that the semi-analytical method has over the finite volume method demonstrates the potential of the semi-analytical method to significantly speed up simulations of transport processes across block, heterogeneous media.

## 5.2 Results for complex heterogeneous geometries

We now demonstrate how the semi-analytical method can be used to homogenize complex heterogeneous geometries. For our demonstration, we consider a square cell of dimension 1 by 1 consisting of an \( m \) by \( m \) array of square blocks and generate aggregated, random geometries of two different media. We first generate \( m^2 \) uniformly distributed, random

| Case 1 (4 by 4) | Semi-Analytical | Time (s) | Relative Error (\( E \)) | Finite Volume | Time (s) | Relative Error (\( E \)) |
|----------------|-----------------|---------|--------------------------|---------------|---------|--------------------------|
| \( N_x \)     |                 |         |                          |               |         |                          |
| 4             | (4.09 \times 10^{-3}, 0) | 0.00805| (7.85 \times 10^{-3}, 0) | 0.00938       |         |                          |
| 8             | (1.80 \times 10^{-3}, 0) | 0.0112 | (2.89 \times 10^{-3}, 0) | 0.0280        |         |                          |
| 16            | (8.34 \times 10^{-4}, 0) | 0.0338 | (1.05 \times 10^{-3}, 0) | 0.113         |         |                          |
| 32            | (4.04 \times 10^{-4}, 0) | 0.0630 | (3.69 \times 10^{-4}, 0) | 0.531         |         |                          |
| 64            | (2.04 \times 10^{-4}, 0) | 0.269  | (1.22 \times 10^{-4}, 0) | 2.93          |         |                          |

| Case 4 (4 by 4) | Semi-Analytical | Time (s) | Relative Error (\( E \)) | Finite Volume | Time (s) | Relative Error (\( E \)) |
|----------------|-----------------|---------|--------------------------|---------------|---------|--------------------------|
| \( N_x \)     |                 |         |                          |               |         |                          |
| 4             | (6.84 \times 10^{-3}, 5.04 \times 10^{-3}) | 0.00747| (1.30 \times 10^{-2}, 2.44 \times 10^{-3}) | 0.00923       |         |                          |
| 8             | (3.01 \times 10^{-3}, 2.21 \times 10^{-3}) | 0.0109 | (4.82 \times 10^{-3}, 1.88 \times 10^{-3}) | 0.0277        |         |                          |
| 16            | (2.21 \times 10^{-3}, 1.98 \times 10^{-3}) | 0.0331 | (1.75 \times 10^{-3}, 9.12 \times 10^{-4}) | 0.115         |         |                          |
| 32            | (1.40 \times 10^{-3}, 1.02 \times 10^{-3}) | 0.0629 | (9.12 \times 10^{-4}, 1.14 \times 10^{-3}) | 0.530         |         |                          |
| 64            | (1.02 \times 10^{-3}, 9.23 \times 10^{-4}) | 0.270  | (3.76 \times 10^{-4}, 4.02 \times 10^{-4}) | 2.92          |         |                          |

| Case 1 (16 by 16) | Semi-Analytical | Time (s) | Relative Error (\( E \)) | Finite Volume | Time (s) | Relative Error (\( E \)) |
|-------------------|-----------------|---------|--------------------------|---------------|---------|--------------------------|
| \( N_x \)        |                 |         |                          |               |         |                          |
| 4                 | (5.60 \times 10^{-4}, 0) | 0.0702 | (1.05 \times 10^{-3}, 0) | 0.124         |         |                          |
| 8                 | (2.52 \times 10^{-4}, 5.60 \times 10^{-4}) | 0.151 | (3.69 \times 10^{-4}, 0) | 0.549         |         |                          |
| 16                | (1.25 \times 10^{-4}, 2.52 \times 10^{-4}) | 0.619 | (1.22 \times 10^{-4}, 0) | 2.98          |         |                          |

| Case 4 (16 by 16) | Semi-Analytical | Time (s) | Relative Error (\( E \)) | Finite Volume | Time (s) | Relative Error (\( E \)) |
|-------------------|-----------------|---------|--------------------------|---------------|---------|--------------------------|
| \( N_x \)        |                 |         |                          |               |         |                          |
| 4                 | (9.38 \times 10^{-4}, 7.42 \times 10^{-4}) | 0.0696 | (1.75 \times 10^{-3}, 9.12 \times 10^{-4}) | 0.0650        |         |                          |
| 8                 | (4.22 \times 10^{-4}, 3.34 \times 10^{-4}) | 0.151  | (6.17 \times 10^{-4}, 3.76 \times 10^{-4}) | 0.388         |         |                          |
| 16                | (3.34 \times 10^{-4}, 2.75 \times 10^{-4}) | 0.615  | (3.76 \times 10^{-4}, 4.02 \times 10^{-4}) | 2.43          |         |                          |

Table 2: Error and runtimes of the effective diffusivities calculated using the semi-analytical and finite volume methods.
Figure 4: Comparison of time taken to solve the linear system and size of the linear system for both the semi-analytical and finite volume methods for geometries consisting of an $m \times m$ grid, for $m = 2, \ldots, 40$. The time taken represents the time to formulate and solve the linear systems, as well as to calculate the effective diffusivity.

Table 3: Effective diffusivity for four randomly generated aggregated mediums consisting of a 10 by 10, 20 by 20, 50 by 50 and 100 by 100 array of blocks, respectively, as calculated using the semi-analytical method. In all four cases $N_x = N_y = 8$ and the number of blocks with diffusivity 0.1 (dark grey blocks) is equal to the number of blocks with diffusivity 1 (light grey blocks). The aggregated geometries were inspired by those presented by Ray et al. [20].
numbers between 0 and 1 denoted by $D_{i,j}^{(0)}$ where $i = 1, \ldots, m$ and $j = 1, \ldots, m$. We then perform the following iteration:

$$D_{i,j}^{(k+1)} = \frac{4}{9} D_{i,j}^{(k)} + \frac{1}{9} \left( D_{i-1,j}^{(k)} + D_{i+1,j}^{(k)} + D_{i,j-1}^{(k)} + D_{i,j+1}^{(k)} \right) + \frac{1}{36} \left( D_{i-1,j-1}^{(k)} + D_{i-1,j+1}^{(k)} + D_{i+1,j-1}^{(k)} + D_{i+1,j+1}^{(k)} \right),$$  \hspace{1cm} (59)

for all $i = 1, \ldots, m$ and $j = 1, \ldots, m$, where $D_{i,j}^{(k)}$ represents the diffusivity in the $(i,j)$th block of the domain (see Figure 2) at the $k$th iteration and the weightings are inspired by those used in lattice Boltzmann methods [16]. For the purposes of the algorithm in equation (59), we assume periodicity to process the blocks along the boundaries, for example, when $i = 1$, we set $i - 1$ to be equal to $m$. After performing a fixed number of iterations, we are left with an array of diffusivities (see Figure 2) containing entries between 0 and 1, where larger values are aggregated together and smaller values are aggregated together. To ensure the geometry is comprised of equal parts light grey (diffusivity of 1) and dark grey (diffusivity of 0.1), we then prescribe that the largest 0.5$m^2$ entries of the array are 1 and the remaining 0.5$m^2$ entries are 0.1.

Table 3 presents some example geometries generated using the above procedure for $m = 10, 20, 50$ and 100, which resemble realistic geometries presented by Amaziane et al. [2] and Sviercoski et al. [25]. These figures demonstrate the highly complex heterogeneous geometries that can be captured using blocks and how the semi-analytical method can be used to calculate the effective diffusivity for such geometries.

6 Conclusion

In this paper we have presented a new semi-analytical method to calculate the effective diffusivity on a two-dimensional block heterogeneous domain. Our novel approach involves reformulating the heterogeneous boundary value problem as a family of homogeneous boundary value problems on each of the blocks by introducing unknown functions representing the flux at the interfaces between adjacent blocks. We then solve each homogeneous boundary value problem via standard techniques to yield an analytical solution dependent upon the integrals of the unknown interface functions. By applying an appropriate numerical quadrature rule to these integrals and enforcing continuity of the solution across each interface, the solution of the original heterogeneous boundary value problem can be computed, which allows the effective diffusivity of the block heterogeneous domain to be calculated. Our numerical experiments demonstrated that the new semi-analytical method yields accurate results when applied to standard test problems from the literature. For all of these test problems, we found that our semi-analytical method was faster and/or more accurate than a standard finite volume method. The primary reason for this is that the linear system for the semi-analytical method is much smaller than the linear system for the finite volume method as unknowns are located only along interfaces between adjacent blocks and not in the interior of the blocks. We also demonstrated that our semi-analytical method can be applied to complex heterogeneous domains.

While all of the heterogeneous media considered in this paper consist of only two different materials, our semi-analytical method is not restricted to such media and can easily be applied to media in which the diffusivity in each block is different. Furthermore, we only considered periodic boundary conditions (12)–(15), however, our semi-analytical method can be modified to accommodate additional forms of boundary conditions used in other homogenization techniques [27]. There is also room for improvement in our semi-analytical method that may further improve its efficiency and accuracy. For example: (i) allowing for blocks of different sizes where not all interfaces are aligned would reduce the number of interface functions and thus reduce the size of the resulting linear system (47); (ii) applying a quadrature rule to approximate the integrals involving the interface functions that allows for more than $2N_a - 3$ terms to be taken in the summations appearing in the solution (35) would likely improve the accuracy. In future work we plan to use the semi-analytical method to compute the effective diffusivities required in the coarse-grained equation (2) to further investigate its potential for speeding up coarse-grained simulations.

Acknowledgments

The first author acknowledges discussions with Nadja Ray and Andreas Rupp from Friedrich-Alexander University of Erlangen-Nürnberg on randomly generating aggregated heterogeneous domains. The second and third authors acknowledge funding from the Australian Research Council (DE150101137, DP150103675).
A Boundary conditions for blocks in bottom row and right column

The boundary conditions (33)–(34) are valid for all blocks except those in either the bottom row \( (i = m) \) or right column \( (j = n) \). For the blocks in the bottom row and right column, the boundary conditions are:

\[
D_{m,j} \frac{\partial v_{m,j}^{(\xi)}}{\partial x}(x_{j-1}, y) = g_{(m-1)n+j}(y), \\
D_{m,j} \frac{\partial v_{m,j}^{(\xi)}}{\partial x}(x, y_{m-1}) = q_j(y), \\
D_{m,j} \frac{\partial v_{m,j}^{(\xi)}}{\partial y}(x, y_{m-1}) = q_{j}(y), \\
D_{m,j} \frac{\partial v_{m,j}^{(\xi)}}{\partial y}(x, y) = g_{(m-1)n+j+1}(y), \\
D_{m,j} \frac{\partial v_{m,j}^{(\xi)}}{\partial x}(x_{j-1}, y) = g_{(m-1)n+j+1}(y), \quad y_{m-1} < y < y_{m}, \\
D_{m,j} \frac{\partial v_{m,j}^{(\xi)}}{\partial y}(x, y_{m-1}) = q_j(y), \quad x_{j-1} < x < x_j,
\]

for \( j = 1, \ldots, n-1 \),

\[
D_{i,n} \frac{\partial v_{i,n}^{(\xi)}}{\partial x}(x_{n-1}, y) = g_n(y), \\
D_{i,n} \frac{\partial v_{i,n}^{(\xi)}}{\partial y}(x, y_{n-1}) = q_{n}(y), \\
D_{i,n} \frac{\partial v_{i,n}^{(\xi)}}{\partial y}(x, y) = g_{(i-1)n+1}(y), \\
D_{i,n} \frac{\partial v_{i,n}^{(\xi)}}{\partial x}(x_{n-1}, y) = g_{(i-1)n+1}(y), \quad y_{n-1} < y < y_{n},
\]

for \( i = 1, \ldots, m-1 \), and

\[
D_{m,n} \frac{\partial v_{m,n}^{(\xi)}}{\partial x}(x_{n-1}, y) = g_{mn}(y), \\
D_{m,n} \frac{\partial v_{m,n}^{(\xi)}}{\partial y}(x, y_{n-1}) = q_{n}(y), \\
D_{m,n} \frac{\partial v_{m,n}^{(\xi)}}{\partial y}(x, y) = g_{(m-1)n+1}(y), \\
D_{m,n} \frac{\partial v_{m,n}^{(\xi)}}{\partial x}(x_{n-1}, y) = g_{(m-1)n+1}(y), \quad y_{m-1} < y < y_{m},
\]

B Coefficients for blocks in bottom row and right column

The coefficients (37)–(38) are valid for all blocks except those in either the bottom row \( (i = m) \) or right column \( (j = n) \). For the blocks in the bottom row and right column, the coefficients are defined as:

\[
a_{m,j,k}^{(\xi)} = \frac{2}{h_{m}} \int_{y_{m-1}}^{y_{m}} \frac{g_{(m-1)n+j+1}(y)}{D_{m,j}} \cos \left( \frac{k\pi(y - y_{m-1})}{h_{m}} \right) \, dy, \\
b_{m,j,k}^{(\xi)} = \frac{2}{h_{m}} \int_{y_{m-1}}^{y_{m}} \frac{g_{(m-1)n+j+1}(y)}{D_{m,j}} \cos \left( \frac{k\pi(y - y_{m-1})}{h_{m}} \right) \, dy,
\]

\[
c_{m,j,k}^{(\xi)} = \frac{2}{l_{j}} \int_{x_{j-1}}^{x_{j}} q_{m}(x) \cos \left( \frac{k\pi(x - x_{j-1})}{l_{j}} \right) \, dx,
\]

\[
d_{m,j,k}^{(\xi)} = \frac{2}{l_{j}} \int_{x_{j-1}}^{x_{j}} q_{(j-1)m+1}(x) \cos \left( \frac{k\pi(x - x_{j-1})}{l_{j}} \right) \, dx,
\]

for \( j = 1, \ldots, n-1 \),

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

\[
b_{i,n,k}^{(\xi)} = \frac{2}{h_{i}} \int_{y_{i-1}}^{y_{i}} \frac{g_{(i-1)n+1}(y)}{D_{i,n}} \cos \left( \frac{k\pi(y - y_{i-1})}{h_{i}} \right) \, dy,
\]

\[
c_{i,n,k}^{(\xi)} = \frac{2}{l_{n}} \int_{x_{n-1}}^{x_{n}} q_{n}(x) \cos \left( \frac{k\pi(x - x_{n-1})}{l_{n}} \right) \, dx,
\]

\[
d_{i,n,k}^{(\xi)} = \frac{2}{l_{n}} \int_{x_{n-1}}^{x_{n}} q_{(i-1)n+1}(x) \cos \left( \frac{k\pi(x - x_{n-1})}{l_{n}} \right) \, dx,
\]
for $i = 1, \ldots, m-1$, and
\begin{align}
a^{(i)}_{m,n,k} &= \frac{2}{h_m} \int_{y_{i-1}}^{y_i} \frac{g_{m,n}(y)}{D_{m,n}} \cos \left( \frac{k\pi(y - y_{m-1})}{h_m} \right) \, dy, \
b^{(i)}_{m,n,k} &= \frac{2}{h_m} \int_{y_{i-1}}^{y_i} \frac{g_{m-1,n+1}(y)}{D_{m,n}} \cos \left( \frac{k\pi(y - y_{m-1})}{h_m} \right) \, dy, \\
c^{(i)}_{m,n,k} &= \frac{2}{l_n} \int_{x_{n-1}}^{x_n} \frac{g_{m,n}(x)}{D_{m,n}} \cos \left( \frac{k\pi(x - x_{n-1})}{l_n} \right) \, dx, \\
d^{(i)}_{m,n,k} &= \frac{2}{l_n} \int_{x_{n-1}}^{x_n} \frac{g_{n-1,m+1}(x)}{D_{m,n}} \cos \left( \frac{k\pi(x - x_{n-1})}{l_n} \right) \, dx.
\end{align}

C Solvability conditions for blocks in bottom row and right column

The solvability conditions (39) are valid for all blocks except those in either the bottom row ($i = m$) or right column ($j = n$). For the blocks in the bottom row and right column, the solvability conditions are:
\begin{align}
\int_{y_{m-1}}^{y_m} \frac{g_{(m-1)n+1}(y)}{D_{m,j}} \, dy - \int_{y_{m-1}}^{y_m} \frac{g_{(m-1)n+j+1}(y)}{D_{m,j}} \, dy + \int_{x_{j-1}}^{x_j} \frac{q_j(x)}{D_{m,j}} \, dx - \int_{x_{j-1}}^{x_j} \frac{q_{(j-1)m+1}(x)}{D_{m,j}} \, dx &= 0, \\
\text{for } j = 1, \ldots, n-1,
\end{align}
\begin{align}
\int_{x_{i-1}}^{x_i} \frac{g_{i+1}(y)}{D_{i,n}} \, dy - \int_{x_{i-1}}^{x_i} \frac{g_{i+1}(y)}{D_{i,n}} \, dy + \int_{x_{n-1}}^{x_n} \frac{q_{(n-1)m+1}(x)}{D_{i,n}} \, dx - \int_{x_{n-1}}^{x_n} \frac{q_{(n-1)m+1}(x)}{D_{i,n}} \, dx &= 0, \\
\text{for } i = 1, \ldots, m-1,
\end{align}
and
\begin{align}
\int_{y_{m-1}}^{y_m} \frac{g_{m,n}(y)}{D_{m,n}} \, dy - \int_{y_{m-1}}^{y_m} \frac{g_{m,n}(y)}{D_{m,n}} \, dy + \int_{x_{n-1}}^{x_n} \frac{q_{n+1}(x)}{D_{m,n}} \, dx - \int_{x_{n-1}}^{x_n} \frac{q_{n+1}(x)}{D_{m,n}} \, dx &= 0.
\end{align}

References

[1] A. Abdulle and W. E. Finite difference heterogeneous multi-scale method for homogenization problems. J Comput Phys, 191:18–39, 2003.
[2] B. Amaziane, T. Hontans, and J. V. Koebbe. Equivalent permeability and simulation of two-phase flow in heterogeneous porous media. Computat Geosci, 5:279–300, 2001.
[3] E. J. Carr and N. G. March. Semi-analytical solution of multilayer diffusion problems with time-varying boundary conditions and general interface conditions. Appl Math Comput, 333:286–303, 2018.
[4] E. J. Carr and I. W. Turner. Two-scale computational modelling of water flow in unsaturated soils containing irregular-shaped inclusions. Int J Numer Meth Eng, 98(3):157–173, 2014.
[5] E. J. Carr and I. W. Turner. A semi-analytical solution for multilayer diffusion in a composite medium consisting of a large number of layers. Appl Math Model, 40:7034–7050, 2016.
[6] E. J. Carr, I. W. Turner, and P. Perré. A dual-scale modelling approach for drying hygroscopic porous media. Multiscale Model Sim, 11(1):362–384, 2013.
[7] E. J. Carr, P. Perré, and I. W. Turner. The extended distributed microstructure model for gradient-driven transport: A two-scale model for bypassing effective parameters. J Comput Phys, 327:810–829, 2016.
[8] E. J. Carr, I. W. Turner, and P. Perré. Macroscale modelling of multilayer diffusion: using volume averaging to correct the boundary conditions. Appl Math Model, 47:600–618, 2017.
[9] F. Chen and L. Ren. Application of the finite difference heterogeneous multiscale method to the Richards’ equation. Water Resour Res, 44:N07413, 2008.
[10] Y. Davit, C. G. Bell, H. M. Byrne, L. A. C. Chapman, L. S. Kimpton, G. E. Lang, K. H. L. Leonard, J. M. Oliver, N. C. Pearson, R. J. Shipley, S. L. Waters, J. P. Whiteley, B. D. Wood, and M. Quintard. Homogenization via formal multiscale asymptotics and volume averaging: How do the two techniques compare? *Adv Water Resour*, 62:178–206, 2013.

[11] A. Deaño, D. Huybrechs, and A. Iserles. *Computing Highly Oscillatory Integrals*. Society for Industrial and Applied Mathematics, Philadelphia, 2018.

[12] L. N. G. Filon. On a quadrature formula for trigonometric integrals. *Proc R Soc Edin A-Ma*, 49:38–47, 1928.

[13] H. Hajibeygi and P. Jenny. Multiscale finite-volume method for parabolic problems arising from compressible multiphase flow in porous media. *J Comput Phys*, 228:5129–5147, 2009.

[14] U. Hornung. *Homogenization and Porous Media*. Springer-Verlag New York, 1997.

[15] D. Levin. Fast integration of rapidly oscillatory functions. *J Comput Math*, 67:95–101, 1996.

[16] D. A. Perumal and A. K. Dass. A review on the development of lattice Boltzmann computation of macro fluid flows and heat transfer. *Alexandria Eng J*, 54(4):955–971, 2015.

[17] J. L. Plawsky. *Transport Phenomena Fundamentals*. Chemical Industries. CRC Press, second edition, 2009.

[18] A. D. Polyanin. *Handbook of Linear Partial Differential Equations for Engineers and Scientists*. Chapman and Hall, 2002.

[19] S. Potticary. Efficient evaluation of highly oscillatory integrals. Master’s Thesis, University of Reading, 2005.

[20] N. Ray, A. Rupp, and A. Prechtel. Discrete-continuum multiscale model for transport, biomass development and solid restructuring in porous media. *Adv Water Resour*, 107:393–404, 2017.

[21] N. Ray, A. Rupp, R. Schulz, and P. Knabner. Old and new approaches predicting the diffusion in porous media. *Transport Porous Med*, 124(3):803–824, 2018.

[22] M. R. Rodrigo and A. L. Worthy. Solution of multilayer diffusion problems via the Laplace transform. *J Math Anal Appl*, 444:475–502, 2016.

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

[24] R. F. Sviercoski, C. L. Winter, and A. Warrick. Analytical approximation for the generalized Laplace equation with step function coefficient. *SIAM J Appl Math*, 68(5):1268–1281, 2008.

[25] R. F. Sviercoski, C. L. Winter, and A. Warrick. An analytical effective tensor and its approximation properties for upscaling flows through generalized composites. *Adv Water Resour*, 33(7):728–739, 2010.

[26] A. Szymkiewicz. Calculating effective conductivity of heterogeneous soils by homogenization. *Arch Hydro-Eng Environ Mech*, 52(2):111–130, 2005.

[27] A. Szymkiewicz. *Modelling Water Flow in Unsaturated Porous Media*. Springer, 2013.

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