Applied Mathematical Modelling 47 (2017) 600–618

Contents lists available at ScienceDirect

Applied Mathematical Modelling

journal homepage: www.elsevier.com/locate/apm

Macroscale modelling of multilayer diffusion: Using volume averaging to correct the boundary conditions

E.J. Carr[a,*], I.W. Turner[a,b], P. Perré[c]

[a] School of Mathematical Sciences, Queensland University of Technology (QUT), Brisbane, Australia
[b] Australian Research Council Centre of Excellence for Mathematical and Statistical Frontiers (ACEMS), Queensland University of Technology (QUT), Brisbane, Australia
[c] LGPM, CentraleSupélec, Université Paris-Saclay, Châtenay-Malabry, France

ARTICLE INFO

Article history:
Received 14 July 2016
Revised 13 January 2017
Accepted 21 March 2017
Available online 31 March 2017

Keywords:
Multilayer diffusion
Composite medium
Macroscale
Volume averaging
Homogenization
Boundary conditions

ABSTRACT

This paper investigates the form of the boundary conditions (BCs) used in macroscale models of PDEs with coefficients that vary over a small length-scale (microscale). Specifically, we focus on the one-dimensional multilayer diffusion problem, a simple prototype problem where an analytical solution is available. For a given microscale BC (e.g., Dirichlet, Neumann, Robin, etc.) we derive a corrected macroscale BC using the method of volume averaging. For example, our analysis confirms that a Robin BC should be applied on the macroscale if a Dirichlet BC is specified on the microscale. The macroscale field computed using the corrected BCs more accurately captures the averaged microscale field and leads to a reconstructed microscale field that is in excellent agreement with the true microscale field. While the analysis and results are presented for one-dimensional multilayer diffusion only, the methodology can be extended to and has implications on a broader class of problems.

1. Introduction

Mathematical models taking the form of partial differential equations (PDEs) involving small-scale variation in coefficients are ubiquitous in engineering and scientific disciplines. Popular applications include heat conduction in composite materials [1], groundwater flow and contaminant transport in heterogeneous aquifers [2,3] and oil recovery in subsurface reservoirs [4], where the spatial heterogeneity of the conductivity/permeability dictates the flow behaviour. For such problems, direct numerical solution of the governing equations via a discretisation of the domain yields a prohibitively large number of mesh elements and hence a discrete system which is exorbitantly expensive to solve [5]. Such numerical issues motivate the need for a macroscale approach.

In this work, the microscale refers to the usual scale at which transport phenomena is described, namely the classical macroscopic or continuum scale, where for example the laws of Fourier and Darcy hold. On the other hand, the macroscale refers to a larger scale where the heterogeneous medium can be replaced by an equivalent or effective homogeneous medium [6]. We assume that the boundary conditions (BCs) at the microscale are known or can be controlled (i.e., the parameters appearing in the BCs are measurable) with our goal being to develop a macroscale model, whose solution $U(x, t)$ provides a good approximation to the smoothed/averaged behaviour of the microscale field $u(x, t)$ (in some sense).

* Corresponding author.
E-mail addresses: elliot.carr@qut.edu.au, ecarr.maths@gmail.com (E.J. Carr), i.turner@qut.edu.au (I.W. Turner), patrick.perre@centralesupelec.fr (P. Perré).

http://dx.doi.org/10.1016/j.apm.2017.03.044

Consider, for example, the diffusion equation in a heterogeneous medium:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\kappa(x)\frac{\partial u}{\partial x}\right), \quad l_0 < x < l_m, \tag{1}$$

where the diffusivity $\kappa(x)$ varies over a microscale which is small relative to the length of the domain $l_m - l_0$. Formulating a macroscale model of (1) can be achieved in several ways. The simplest approach is to assume that the diffusivity $\kappa(x)$ can be replaced by an averaged or effective value κ_{eff}, which is constant (or varies slowly with the spatial coordinate x):

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial x}\left(\kappa_{\text{eff}}\frac{\partial U}{\partial x}\right), \quad l_0 < x < l_m. \tag{2}$$

Note that solving macroscale equations such as (2) require significantly less computational effort compared with solving microscale equations such as (1) over the entire domain as the grid resolution is not constrained by the small-scale heterogeneous geometry.

A more rigorous approach is to use upscaling methods such as homogenization [7] and volume averaging [8] to derive the macroscale equation. A recent and comprehensive comparison between both approaches is given by Davit et al. [9]. For volume averaging in one spatial dimension, we define the averaging operator:

$$\langle u\rangle(x,t) = \frac{1}{2\delta}\int_{x-\delta}^{x+\delta} u(\zeta,t)\; d\zeta, \tag{3}$$

which replaces $u(x, t)$ by its local average in a small interval of length 2δ around each point x. The central idea of volume averaging is to obtain an approximation to the averaged field $\langle u\rangle(x, t)$ (without computing the microscale field $u(x, t)$) by deriving a macroscale equation through direct spatial averaging of the microscale equation via application of the operator (3). Various theorems for interchanging averaging and differential operators then permit a macroscale equation to be determined, the solution of which approximates $\langle u\rangle(x, t)$.

The idea behind homogenization is less intuitive. Given that there are two inherent length scales in the problem, the idea is to introduce a second spatial variable $y = x/\varepsilon$ (scale of the heterogeneities) and consider the family of problems parameterised by ε. Assuming the solution $u_\varepsilon(x, y, t)$ has an expansion of the form:

$$u_\varepsilon(x,y,t) = u_0(x,y,t) + \varepsilon u_1(x,y,t) + \varepsilon^2 u_2(x,y,t) + \cdots, \tag{4}$$

homogenization seeks the asymptotic solution as $\varepsilon \to 0$ (i.e., letting the heterogeneities tend to zero). Ultimately, for the diffusion equation (1), both approaches lead to the same macroscale Eq. (2), where the the effective diffusion coefficient κ_{eff} is given by the harmonic average of the microscale diffusivity [10]. In the method of volume averaging, the macroscale field $U(x, t)$ is an approximation to the averaged field $\langle u\rangle(x, t)$ while in the homogenization method $U(x, t)$ is equal to the leading order approximation $u_0(x, t)$ in the expansion (4) (which can be shown to be independent of the small length scale y).

In this paper, we aim to answer the following important question: given a set of BCs on the microscale, what form should the BCs on the macroscale take? In other words, what choices for the macroscale BCs give the best match between the macroscale and microscale fields? Traditionally, the microscale BCs do not play any role in the derivation of the macroscale equation in neither volume averaging nor homogenization. As pointed out by Pavliotis and Stuart [10], the microscale BCs are "irrevelant" in the homogenization procedure as they do not enter into the analysis: exactly the same macroscale equation is generated regardless of the form of the microscale BCs. For both approaches (volume averaging and homogenization), usually the macroscale BCs imposed are of the same type as the microscale BC. For example, if a Dirichlet BC is applied on the microscale field then the same Dirichlet condition is imposed on the macroscale field [5,9–14]. If the microscale flux at the boundary is specified and assigned a constant value then the macroscale flux at the same boundary is assumed equal to that constant [5,11,12,15][1].

In the context of homogenization by asymptotic expansion, for certain differential operators and sets of BCs it is possible to rigorously prove convergence of the sequence of microscale solutions $u_\varepsilon(x, y, t)$ towards $u_0(x, t)$ in the limit $\varepsilon \to 0$ [7,10]. This, of course, assumes that the ratio of the microscale to macroscale length scales is infinitesimally small, which is often a flawed assumption in many real-world problems.

As a means of validating the macroscale model and corresponding BCs, in this work we use the solution of the microscale model as the reference solution (referred to by Davit et al. [9] as validation by direct numerical simulation)[2]. Two examples that raise concerns about the common choices for the macroscale BCs are given in Fig. 1. In Example 1, three snapshots of the microscale field $u(x, t)$ are given with a Dirichlet BC imposed at the left boundary. Overlayed is an averaged (macroscale) field computed by averaging $u(x, t)$ via the operator (3). Observe that $\langle u\rangle(x, t)$ satisfies a similar evolution law to the microscale field, however, it clearly does not satisfy the Dirichlet BC specified on the microscale at the left boundary[3]. In Example 2, the Dirichlet condition at the right boundary is modified to a Robin condition. Applying the same Robin

[1] For example, for the diffusion equations (1) and (2) the microscale BCs $u(x,t) = a$ and $\kappa_1 \frac{\partial u}{\partial x} = q$ at $x = 0$ traditionally lead to macroscale BCs of $U(x,t) = a$ and $\kappa_{\text{eff}} \frac{\partial U}{\partial x} = q$ being proposed at $x = 0$, respectively.

[2] For example, for the diffusion problem, to validate the macroscale model, the macroscale field $U(x, t)$ is compared to the microscale field $u(x, t)$.

[3] Unless $\delta = 0$, the average of the microscale field over the interval $[0, \delta]$ is less than 1. Also, for the macroscale field to pass through the centre of the oscillations, $\langle u\rangle(0, t)$ cannot be equal to 1 for all $t > 0$.