NUMERICAL AVERAGING OF NON-DIVERGENCE STRUCTURE ELLIPTIC OPERATORS*

BRITTANY D. FROESE† AND ADAM M. OBERMAN‡

Abstract. Many important equations in science and engineering contain rapidly varying operators that cannot be practically sufficiently resolved for accurate solutions. In some cases it is possible to obtain approximate solutions by replacing the rapidly varying operator with an appropriately averaged operator. In this paper we use formal asymptotic techniques to recover a formula for the averaged form of a second order, non-divergence structure, linear elliptic operator. For several special cases the averaged operator is obtained analytically. For genuinely multi-dimensional cases, the averaged operator is also obtained numerically using a finite difference method, which also has a probabilistic interpretation.

Key words. Homogenization, partial differential equations, elliptic partial differential equations, diffusions, finite difference methods.

AMS subject classifications. 35J15, 35B27, 65L12.

1. Introduction

Second order elliptic equations — in both divergence and non-divergence form — frequently arise in science and engineering [6]. When the operators involved vary rapidly on a small spatial scale these problems carry an additional challenge since it is generally not practical to resolve the computational domain finely enough to capture the behaviour of the operator. A resolution to this challenge is to replace (homogenize) the original operator with a different, slowly varying operator with solutions that are close to the solutions of the original problem.

In the divergence structure case, the homogenized operator is obtained by solving a cell problem. In the non-divergence stucture case studied herein, the homogenized operator is obtained by averaging the coefficients against the invariant measure, which is the solution of an adjoint problem. As a result, in this case, the procedure is called averaging. (There is some inconsistency in the literature concerning terminology; we follow [8].)

1.1. Contents. The first section of this paper is introductory. Section two gives the theoretical basis for the averaging formula. Section three provides explicit analytical solutions. Section four gives a comparison with known analytical results in the divergence structure case, when these are available. Section five is numerical; it begins with a discussion of the discretization and follows with numerical computations. The final section gives the conclusions.

1.2. Goals of this paper. Let L^ϵ denote the following non-degenerate elliptic differential operator

$$L^\epsilon = -\sum_{i,j=1}^n a_{ij}(x/\epsilon)\frac{\partial^2}{\partial x_i x_j} + \sum_{i=1}^n b_i(x/\epsilon)\frac{\partial}{\partial x_i} + c(x/\epsilon) \tag{1.1}$$

Here we assume that the coefficients $A = (a)_{ij}$, $b = (b)_i$, and c are periodic of period one in all their arguments and belong to $C^1(\mathbb{R}^n)$. We study the problem

$$\begin{cases} L^\epsilon u^\epsilon = f(x), & \text{for } x \in U \\ u^\epsilon = g(x), & \text{for } x \in \partial U \end{cases} \tag{PDE}^\epsilon$$

in a bounded domain $U \subset \mathbb{R}^n$ with smooth boundary ∂U. Here for simplicity, $f(x)$, $g(x)$ are continuous functions on U, ∂U, respectively.

Our goal is approximation of $(\text{PDE})^\epsilon$ for small ϵ using a homogeneous operator on a coarsely resolved finite difference grid. This goal is accomplished by recovering, using both analytical and numerical techniques, the averaged operator which is the limit of the operators L^ϵ as $\epsilon \to 0$.

In the first part of this paper we use formal asymptotic calculations to recover an analytic formula for the averaged operator (first obtained by Freidlin [3] using probabilistic methods). The averaged operator is given in terms of the invariant distribution for the dynamics, which is the solution of a PDE involving the adjoint operator. In several special cases we obtain explicit representations of the invariant distribution so that the averaged operator can be expressed in closed form. These special cases require additional structure on the coefficients.

In the general, genuinely multidimensional case, there is no analytical formula for the invariant distribution available. However, the PDE for the invariant distribution can be solved numerically on a relatively coarse grid. Numerical examples are computed, the method is validated by recovering the known solutions, and new examples are computed.

1.3. Related work.   Homogenization (and averaging to a lesser extent) have received much attention in recent years; see the books [4, 8, 1] and the survey [2]. We are grateful to the authors of [8], which influenced our approach.

Early work by Freidlin [3] used probabilistic methods to average the inhomogeneous, non divergence-structure equation $(\text{PDE})^\epsilon$. The non-divergence equation has a probabilistic interpretation. Freidlin averaged the operator by considering the limiting distribution of the underlying stochastic differential equation. The operator is the generator for the diffusion and arises as the backward Kolmogorov equation. The evolution of densities satisfies the Fokker-Planck equation, which involves the adjoint operator; see also [8, Chapter 6].

There is considerably more work on divergence structure equations, either in the variational form

$$-\nabla \cdot (A(x/\epsilon)\nabla u) = f \tag{1.2}$$

or expanded into the singular form (see notation in the next section)

$$-A(x/\epsilon) : D^2 u + \frac{1}{\epsilon} b(x/\epsilon) \cdot \nabla u = f. \tag{1.3}$$

While the problems $(\text{PDE})^\epsilon$ and (1.3) are equivalent for fixed ϵ, provided the coefficients are smooth enough, we note that the non-divergence structure equation $(\text{PDE})^\epsilon$ and the expanded divergence structure equation (1.3) are different in the limit $\epsilon \to 0$. This difference is due to the coefficient ϵ^{-1} of the drift term b in the divergence structure problem. References to works in the divergence structure setting can be found in the textbooks mentioned above. We draw the attention of the reader to the recent work [7].

In very simple cases, both the divergence structure and non-divergence structure operators average (homogenize) to the harmonic mean. However, in general the results are different. For example, in the simple case of separable operators, where analytical results are available, the results are different; see section 3.3.

2. The averaging formula

In this section we use formal asymptotic calculations and PDE methods to average the operator (1.1). This section uses an argument similar to Part II of [8] and [2], which gave the homogenization formula for divergence structure elliptic equations. The formal calculations can be made rigorous, following the method of Part III of [8].

We use the notation

$$(D^2)_{ij} = \frac{\partial^2}{\partial x_i x_j}, \qquad \nabla = (\partial x_1, \ldots, \partial x_n)$$

for the Hessian operator and the gradient operator, respectively. We use

$$M : N = tr(M^T N) = \sum_{i,j=1}^{n} M_{ij} N_{ij}$$

for the inner product between matrices and $b \cdot d = \sum_{i=1}^{n} b_i d_i$ for the dot product of vectors. We rewrite L^ϵ defined in (1.1) as

$$L^\epsilon = -A(x/\epsilon) : D^2 + b(x/\epsilon) \cdot \nabla + c(x/\epsilon),$$

and we use angle brackets to denote the average over one periodic domain $\Omega = [0,1]^n$,

$$\langle v \rangle = \frac{\int_\Omega v}{|\Omega|}.$$

2.1. The Fredholm Alternative and the invariant distribution. For completeness, we recall the Fredholm Alternative. Consider the operator

$$L_0(x) = -A(x) : D^2$$

where the coefficient matrix, $A(x)$, is periodic, C^1, and uniformly positive definite. The adjoint operator, which is also periodic, acts on a function $v(x) \in C^2(\Omega)$ by

$$L_0^*(x)v(x) = -D^2 : (A(x)v(x)).$$

THEOREM 2.1 (The Fredholm Alternative [8]). *Consider the operator $L_0(x) = -A(x) : D^2$, where the coefficient matrix is periodic, C^1, and uniformly positive definite. Exactly one of the following conditions holds.*

1. *The equation $L_0 u = f$ has a unique periodic solution for every $f \in L_{per}^2(\Omega)$.*

2. *The homogeneous equation $L_0 u = 0$ has a non-trivial periodic solution, the nullspaces of L_0 and its adjoint L_0^* have the same dimension, and the inhomogeneous equation $L_0 u = f$ is solvable if and only if*

$$\langle f v \rangle = 0 \text{ for all } v \text{ in the kernel of } L_0^*.$$

Since the kernel of the operator L_0 is one-dimensional (consisting only of constants), the kernel of the adjoint L_0^* is also one-dimensional by the Fredholm Alternative. Thus the *invariant distribution*, ρ^∞, is uniquely prescribed as the unique element of the kernel of the adjoint operator L_0^* [8, Theorem 6.16]

$$L_0^* \rho^\infty = -D^2 : (A\rho^\infty) = 0, \qquad \text{in } \Omega \tag{2.1}$$

which satisfies the normalisation condition

$$\langle \rho^\infty \rangle = 1, \qquad \rho^\infty \text{ is periodic in } y. \tag{2.2}$$

This leads to the following solvability condition.

THEOREM 2.2 (Solvability Condition). *Consider the operator* $L_0(x) = -A(x):$ D^2, *where the coefficient matrix is periodic,* C^1, *and uniformly positive definite. The equation*

$$L_0 u = f, \qquad u \text{ is periodic}$$

has a solution if and only if f is orthogonal to the nullspace of the adjoint operator, which can be verified by

$$\langle \rho^\infty f \rangle = 0,$$

where ρ^∞ is the invariant distribution.

2.2. The averaged coefficients.
THEOREM 2.3. *Let the operator L^ϵ be as in (1.1). Let ρ^∞ be the invariant distribution, given by the unique solution of (2.1), (2.2). Formally, in the limit $\epsilon \to 0$, solutions of equation (PDE)$^\epsilon$ converge to solutions of the averaged equation*

$$\begin{cases} \bar{L}u = f(x), & \text{for } x \in U \\ u = g(x), & \text{for } x \in \partial U, \end{cases} \tag{PDE}$$

where

$$\bar{L} = -\bar{A} : D^2 + \bar{b} \cdot \nabla + \bar{c}$$

has coefficients given by averaging the original coefficients against the invariant distribution

$$\bar{A} = \langle \rho^\infty A \rangle, \qquad \bar{b} = \langle \rho^\infty b \rangle, \qquad \bar{c} = \langle \rho^\infty c \rangle. \tag{2.3}$$

In addition, formally,

$$u^\epsilon(x) = u_0(x) + O(\epsilon^2). \tag{2.4}$$

Proof. We begin the analysis by introducing a new variable

$$y = x/\epsilon,$$

where ϵ is the size of the small cells on which the coefficients vary. We assume the two scales x and y are independent and write the coefficients as

$$A(x/\epsilon) = A(y), \qquad b(x/\epsilon) = b(y), \qquad c(x/\epsilon) = c(y).$$

Since we are treating the two spatial scales as independent, rewrite the partial derivative ∂_{x_i} as

$$\partial_{x_i} + \frac{1}{\epsilon}\partial_{y_i}.$$

Equation $(\mathrm{PDE})^\epsilon$ then becomes

$$
\begin{aligned}
&-\frac{1}{\epsilon^2}A:D_y^2 u^\epsilon \\
&+\frac{1}{\epsilon}\left(-2A:\nabla_x\nabla_y^T u^\epsilon + b\cdot\nabla_y u^\epsilon\right) \\
&+\left(-A:D_x^2 u^\epsilon + b\cdot\nabla_x u^\epsilon + cu^\epsilon\right)=f.
\end{aligned}
\tag{2.5}
$$

Now we look for a solution of the form

$$
\begin{aligned}
u^\epsilon(x)&=u_0(x,x/\epsilon)+\epsilon^2 u_2(x,x/\epsilon)+\ldots \\
&=u_0(x,y)+\epsilon^2 u_2(x,y)+\ldots
\end{aligned}
\tag{2.6}
$$

A term of $O(\epsilon)$ is not needed, as the asymptotics verify. Substituting this solution form into the PDE (2.5) we obtain

$$\frac{1}{\epsilon^2}L_0 u_0 + \frac{1}{\epsilon}L_1 u_0 + (L_0 u_2 + L_2 u_0) + O(\epsilon) = f. \tag{2.7}$$

Here we have defined the operators

$$
\begin{aligned}
L_0 &= -A:D_y^2 \\
L_1 &= -2A:\nabla_x\nabla_y^T + b\cdot\nabla_y \\
L_2 &= -A:D_x^2 + b\cdot\nabla_x + c.
\end{aligned}
$$

To ensure that u^ϵ satisfies the required boundary conditions we also enforce the appropriate boundary conditions on the terms in the asymptotic expansion (2.6). For the leading order term we require

$$
\begin{cases}
u_0 = g(x) & \text{on } \partial U \\
u_0 & \text{periodic in } y.
\end{cases}
$$

For $k>0$ we enforce

$$
\begin{cases}
u_k = 0 & \text{on } \partial U \\
u_k & \text{periodic in } y.
\end{cases}
$$

We first look at the leading order, $O(\frac{1}{\epsilon^2})$, terms in (2.7) to obtain the equation

$$
\begin{cases}
-A:D_y^2 u_0 = 0 \\
u_0 \text{ is periodic in the } y \text{ variable.}
\end{cases}
$$

Because of the periodic boundary conditions (in y), the solution of this equation will be independent of the y variable:

$$u_0 = u_0(x)$$

Next we consider the $O(\frac{1}{\epsilon})$ terms in (2.7) to obtain

$$-2A:\nabla_x\nabla_y^T u_0 + b\cdot\nabla_y u_0 = 0.$$

This is automatically satisfied since u_0 is independent of y.

Finally, we consider the $O(1)$ terms in (2.7) to obtain the equation

$$-A:D_y^2 u_2 = A:D_x^2 u_0 - b\cdot\nabla_x u_0 - cu_0 + f. \qquad (2.8)$$

We can now use Theorem 2.2 to obtain a solvability condition for (2.8):

$$\int_\Omega \rho^\infty \left(A:D_x^2 u_0 - b\cdot\nabla_x u_0 - cu_0 + f\right) dy = 0.$$

Because u_0 and f are independent of the y variable and the solution of the adjoint problem is normalized we can integrate the last equation to obtain

$$-\bar{A}:D_x^2 u_0 + \bar{b}\cdot\nabla_x u_0 + \bar{c}u_0 = f, \qquad (2.9)$$

where the averaged coefficients are given by (2.3)

$$\bar{A} = \langle\rho^\infty A\rangle, \qquad \bar{b} = \langle\rho^\infty b\rangle, \qquad \bar{c} = \langle\rho^\infty c\rangle.$$

Returning now to the asymptotic expansion for u^ϵ (2.6), we see that (2.4) holds, where u_0 satisfies the averaged Equ. (2.9). □

3. Explicit solutions

In this section we consider a number of special cases for which we can solve the adjoint problem (2.1) exactly. In these cases we can generate explicit formulas for the averaged operators.

We provide a visual representation of several of these operators by plotting the ellipses given by the equation $y^T A y = 1$. The shading of these pictures is such that lighter colouring corresponds to larger entries in the coefficient matrix.

REMARK 3.1. Since the lower order terms average in the same way as the coefficient matrix, but do not affect the formula for the invariant distribution, we omit them to shorten the exposition.

3.1. Multiples of a constant coefficient matrix. One of the simplest cases involves a coefficient matrix that is a (variable) scalar multiple of a constant matrix

$$A(x/\epsilon) = a(x/\epsilon)B,$$

which yields the harmonic mean

$$\bar{A} = \langle a(y)^{-1}\rangle^{-1} B. \qquad (3.1)$$

A typical example is illustrated in figure 3.1, which is the piecewise constant periodic checkerboard.

As a special case we recover the well-known one-dimensional result which follows. The operator

$$-a(x/\epsilon)u_{xx}^\epsilon = f$$

homogenizes to the harmonic mean

$$\bar{a} = \left\langle a(y)^{-1} \right\rangle^{-1}. \tag{3.2}$$

Proof. [Calculation] The adjoint problem (2.1) becomes

$$-B : D_y^2(a(y)\rho^\infty(y)) = 0$$

with solution $\rho^\infty(y) = a(y)^{-1} \left\langle a(y)^{-1} \right\rangle^{-1}$ yielding (3.1). In particular (since B is constant) we see that each element in the coefficient matrix homogenizes to its harmonic mean:

$$\bar{a}_{i,j} = \left\langle a(y)^{-1} b_{ij}^{-1} \right\rangle^{-1} = \left\langle a_{ij}(y)^{-1} \right\rangle^{-1}. \tag{3.3}$$

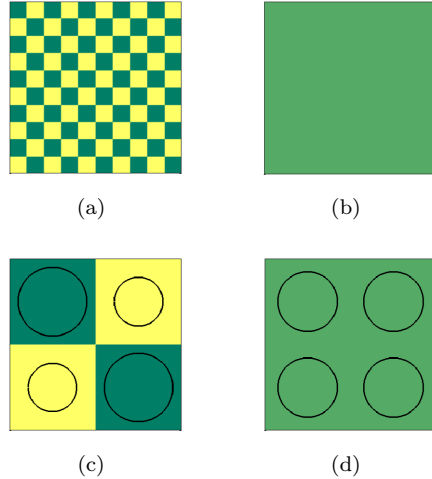<p style="text-align:right">□</p>

FIG. 3.1. *A visual representation of a piecewise constant multiple of the laplacian on a periodic checkerboard. (a) The original grid. (b) The homogenized grid. (c) The original operator on one small cell. (d) The homogenized operator on one small cell.*

3.2. A special case: layered material. Next we consider the special case of a layered material, where the coefficient matrix is a function of only one variable:

$$A(y) = A(y_1).$$

See figure 3.2 for a visualization of the operator.

The adjoint equation is now

$$-D_y^2(A(y_1)\rho^\infty(y)) = 0,$$

which has the solution

$$\rho^\infty(y) = a_{11}(y_1)^{-1} \left\langle a_{11}(y_1)^{-1} \right\rangle^{-1}.$$

Thus the averaged coefficient matrix from (2.3) is

$$\bar{A} = \left\langle a_{11}^{-1} \right\rangle^{-1} \left\langle a_{11}^{-1} A \right\rangle. \tag{3.4}$$
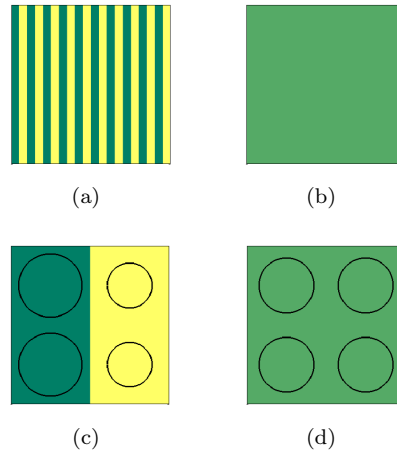
FIG. 3.2. *A visual representation of a piecewise constant multiple of the laplacian on a layered material. (a) The original grid. (b) The homogenized grid. (c) The original operator on one small cell. (d) The homogenized operator on one small cell.*

3.3. A special case: separable, diagonal coefficient matrix. We also consider the case where the coefficient matrix is diagonal and has separable entries. That is, the matrix can be expressed as a product of diagonal matrices of the form

$$A(y) = \prod_{j=1}^{n} A^j(y_j)$$

and each entry on the diagonal of the resulting matrix can be written as

$$A_{ii}(y) = \prod_{j=1}^{n} A_{ii}^j(y_j).$$

See figure 3.3 for a visualisation of such an operator. The averaged coefficients are

$$\bar{A} = \left\langle \frac{1}{\prod\limits_{j=1}^{n} A_{jj}^j(y_j)} A \right\rangle \left\langle \frac{1}{\prod\limits_{j=1}^{n} A_{jj}^j(y_j)} \right\rangle^{-1} \tag{3.5}$$

as can be verified by the calculation which follows.

Proof. [Calculation] In this case, the adjoint equation (2.1) takes the form

$$-\sum_{i=1}^{n} \left(\prod_{j=1}^{n} A_{ii}^j(y_j) \rho^\infty(y) \right)_{y_i y_i} = 0.$$

Since the coefficients are separable, the invariant distribution will also be separable:

$$\rho^\infty = \frac{1}{\prod\limits_{j=1}^{n} A_{jj}^j(y_j)} \left\langle \frac{1}{\prod\limits_{j=1}^{n} A_{jj}^j(y_j)} \right\rangle^{-1}$$
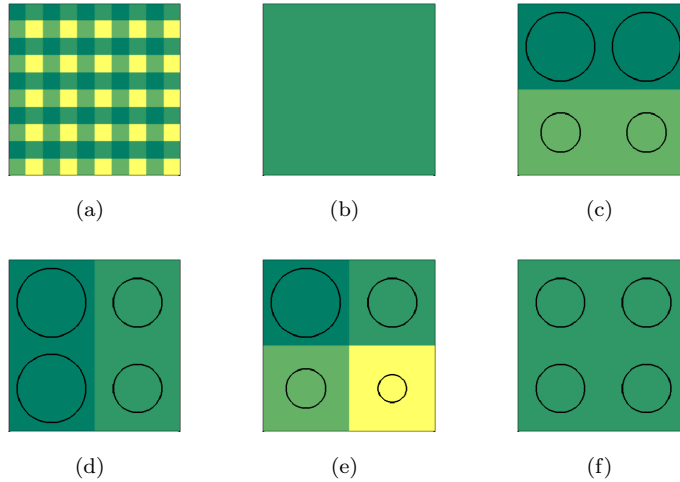
FIG. 3.3. *A visual representation of a separable operator. (a) The original grid. (b) The homogenized grid. (c) The vertical structure of the operator on one small cell. (d) The horisontal structure of the operator on one small cell. (e) The original operator on one small cell. (f) The averaged operator on one small cell.*

and the result follows by averaging using (2.3).   □

4. Comparison with divergence structure results

A given coefficient matrix, A, can be used to generate either the non-divergence structure operator (1.1)

$$L^\epsilon u = -A(x/\epsilon) : D^2 u,$$

or the divergence structure operator (1.2)

$$L^\epsilon_{div} u = -\nabla \cdot (A(x/\epsilon)\nabla u).$$

Only in very simple cases will the coefficient matrix A homogenize to the same operator for both the divergence and non-divergence case. The main example where the results are the same is the one-dimensional case, where the coefficient matrix homogenizes to the harmonic mean for both problems [8], (3.2). However, in general the two operators will result in different homogenized coefficients.

For the convenience of the reader we compare the explicit solutions of 3 to known results for the divergence structure problem.

4.1. A layered material. First we consider a two-dimensional layered material. The divergence structure result is given in [8]. Although most elements of the coefficient matrix average in the same way for both problems, one element is different. In the non-divergence structure case we obtain from (3.4)

$$\bar{a}_{22} = \left\langle a_{11}^{-1} \right\rangle^{-1} \left\langle \frac{a_{22}}{a_{11}} \right\rangle.$$

The divergence case, on the other hand, yields

$$\bar{a}_{22}^{div} = \left\langle \frac{a_{21}}{a_{11}} \right\rangle \left\langle \frac{a_{12}}{a_{11}} \right\rangle \left\langle a_{11}^{-1} \right\rangle^{-1} + \left\langle a_{22} - \frac{a_{12}a_{21}}{a_{11}} \right\rangle.$$

4.2. A separable material.   We can also consider a two-dimensional separable operator that is a scalar multiple of the identity.

$$A(x/\epsilon) = a_1(x_1/\epsilon)a_2(x_2/\epsilon)I$$

This is a special case of both the constant operator of 3.1 and the separable case of 3.3. In either case, the coefficients for the non-divergence structure problem homogenizes to the constant multiple of the identity, given by a generalized harmonic mean,

$$\bar{A} = \langle a_1^{-1}a_2^{-1}\rangle^{-1}I,$$

where I denotes the identity matrix. In the divergence problem, which is considered in [4], the homogenized coefficients are not all equal and are obtained from a combination of the harmonic and arithmetic means of the coefficients.

$$\bar{A}_{11}^{div} = \langle a_2\rangle\langle a_1^{-1}\rangle^{-1}$$
$$\bar{A}_{22}^{div} = \langle a_1\rangle\langle a_2^{-1}\rangle^{-1}.$$

5. Numerical results

Although there are a number of situations in which we can write down an explicit representation of the averaged coefficients, this is not always possible. However, the homogenization result can be implemented numerically. To accomplish this we need only solve one linear equation (2.1), along with the normalization constraint (2.2). The computational effort is comparable (arguably less) to the effort for the divergence structure problem, where n equations must be solved for the cell problem.

The finite difference schemes we use have a natural interpretation as a discrete space Markov chain approximation of the underlying diffusion process. Consequently, one approach to interpreting the numerical method would be to use Markov chain approximations along the lines of [5, 10, 9]. Here we will focus on the PDE aspects in order to discretize the problem. To present the ideas in the simplest setting, we perform the discretization in two dimensions; the generalisation to higher dimensions is accomplished by standard techniques.

In this section we numerically average several test problems and solve the averaged equations. We demonstrate that the approach presented in this paper does correctly average the non-divergence structure elliptic operator and compute the operators in some cases where the exact formula is not known. We begin by validating the approach: we demonstrate numerically that the solutions of the original equation

$$A(x/\epsilon) : D^2 u^\epsilon = f$$

converge pointwise to the solutions of the averaged equation

$$\bar{A} : D^2 u = f$$

in the limit as $\epsilon \to 0$.

A further goal of this section is to investigate the relationship between cell resolution and accuracy of both the computed averaged operators and the solutions of the averaged equations.

Notation for this section. Below, the diagonal matrix whose j^{th} diagonal element is given by the jth element of the vector a is denoted by $\operatorname{diag}(a)$. We use $\mathbf{0}, \mathbf{1}$ for vectors whose elements are identically zero or one respectively. The identity matrix is represented by I.

5.1. Discretization and numerical solution. We will be solving the non-divergence form equation $(\text{PDE})^\epsilon$. This is discretized using centred differences and the linear system was solved directly (in this case using the default Matlab backslash solver). In all cases, the computational domain is the unit square $[0,1] \times [0,1]$.

We also want to solve equation (2.1) for the invariant distribution. Let $\rho = (\rho_{ij})$ be a grid vector indexed by the grid coefficients. The fact that the grid vector ρ approximates the solution ρ^∞ at the corresponding grid points,

$$\rho_{ij} = \rho^\infty(hi, hj) + O(h^2)$$

will follow from the standard linear finite difference analysis. After discretizing the two-dimensional adjoint equation (2.1) by standard centered finite differences, with spatial resolution, h, we obtain a finite dimensional linear equation:

$$M\rho = 0, \tag{5.1}$$

where M is a linear operator defined below, along with the discretization of the constraint (2.2)

$$\sum_{i,j} \rho_{ij} h^2 = 1. \tag{5.2}$$

The matrix M is obtained by combining the finite difference operators, for each term as follows. To shorten the formulas, write the grid matrix $A = A_{ij}$ as a collection of scalar functions for each component

$$A = A_{ij} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}_{ij} = \begin{pmatrix} q_{ij} & s_{ij} \\ s_{ij} & r_{ij} \end{pmatrix}.$$

Then define the linear operators

$$Q = \text{diag}(q_{ij}), \qquad R = \text{diag}(r_{ij}), \qquad S = \text{diag}(s_{ij}),$$

which correspond to scalar multiplication. Next define $D_{y_1 y_1}, D_{y_1 y_2}, D_{y_2 y_2}$ to be the linear operators corresponding to the finite difference operators for the second derivatives. Equation (5.1) then takes the form

$$(D_{y_1 y_1} Q + D_{y_2 y_2} R + 2 D_{y_1 y_2} S) \rho = 0. \tag{5.3}$$

Writing out the operator more explicitly, term by term, results in

$$(D_{y_1 y_1} Q\rho)_{ij} = \frac{1}{h^2} \left(q_{i+1,j}\rho_{i+1,j} + q_{i-1,j}\rho_{i-1,j} - 2q_{i,j}\rho_{i,j} \right)$$

$$(D_{y_2 y_2} R\rho)_{ij} = \frac{1}{h^2} \left(r_{i,j+1}\rho_{i,j+1} + r_{i,j-1}\rho_{i,j-1} - 2r_{i,j}\rho_{i,j} \right) \tag{5.4}$$

$$2(D_{y_1 y_2} S\rho)_{ij} = \frac{2}{h^2} \left(s_{i+1,j+1}\rho_{i+1,j+1} + s_{i-1,j-1}\rho_{i-1,j-1} \right.$$

$$\left. - s_{i+1,j-1}\rho_{i+1,j-1} - s_{i-1,j+1}\rho_{i-1,j+1} \right).$$

Equation (5.3) can be solved by a direct method, enforcing the single constraint (5.2). For simplicity, we solved the equation iteratively by a Gauss-Seidel method. Since the operator preserves mass, even at the discrete level, the constraint (5.2) was satisfied by choosing initial data which satisfied the constraint.

5.2. Multiples of a constant coefficient matrix.   We begin with a simple example, where the coefficient matrix is a (variable) scalar multiple of a constant matrix. That is,

$$A = p(y)K,$$

where K is a constant matrix.

We have already showed that the solution (3.1) of the adjoint equation is simply

$$\rho^\infty(y) = p(y)^{-1} \langle p(y)^{-1} \rangle^{-1}.$$

It is easy to see that this will also be a steady state solution of the discretized equation no matter what cell resolution we use. To demonstrate this, we make the following replacements in the discretized Equ. (5.4):

$$Q = k_{11}P, \qquad R = k_{22}P, \qquad S = k_{12}P.$$

Here $P = \text{diag}(p)$ is a diagonal matrix and k_{11}, k_{22}, k_{12} are constant. The proposed steady state solution in discrete form is

$$\rho^\infty = P^{-1}\mathbf{1}\langle P^{-1}\mathbf{1}\rangle^{-1}.$$

Substituting these expressions into the discrete Equ. (5.4) we find that

$$\begin{aligned}
D_{y_1 y_1} Q \rho^\infty &= D_{y_1 y_1} k_{11} P P^{-1} \mathbf{1} \langle P^{-1}\mathbf{1}\rangle^{-1} \\
&= k_{11} \langle P^{-1}\mathbf{1}\rangle^{-1} D_{y_1 y_1} \mathbf{1} \\
&= \mathbf{0},
\end{aligned}$$

where the last step holds since the rows of $D_{y_1 y_1}$ sum to one. The other terms vanish similarily, showing that (3.1) is in fact the steady state solution of the discrete iterative scheme (5.4) regardless of how well or poorly the cell is resolved.

We now choose a specific example where the coefficient matrix is piecewise constant in a checkerboard pattern. The coefficient matrix will vary between

$$A_1 = \begin{pmatrix} 2 & 1 \\ 1 & 4 \end{pmatrix} \qquad A_2 = \begin{pmatrix} 4 & 2 \\ 2 & 8 \end{pmatrix} = 2A_1.$$

See figure 5.1(a) for a surface plot of the resulting solution. Using the formula (3.3), we expect that the coefficient matrix should average to

$$\bar{A} = \begin{pmatrix} 8/3 & 4/3 \\ 4/3 & 16/3 \end{pmatrix}.$$

We set a forcing $f = 50$, enforce zero Dirichlet boundary conditions, and run through different values of ϵ to investigate the convergence of solutions of the original equation to solutions of the averaged equation as $\epsilon \to 0$.

Convergence results are presented in Table 5.1 and figure 5.1(b). These computations are consistent with the assertion that the solutions of the original equation $(\text{PDE})^\epsilon$ do, in fact, converge to the solutions of the averaged equation (2.3) as $\epsilon \to 0$. Furthermore, the convergence appears to be second order in ϵ. That is, the exact solution of $(\text{PDE})^\epsilon$ is given by

$$u^\epsilon = \bar{u} + O(\epsilon^2),$$

consistent with (2.4).

ϵ	$\|u - \bar{u}\|_2$
1/3	5.474×10^{-3}
1/5	2.003×10^{-3}
1/7	1.029×10^{-3}
1/9	6.250×10^{-4}
1/11	4.194×10^{-4}
1/13	3.008×10^{-4}
1/15	2.262×10^{-4}
1/17	1.763×10^{-4}
1/19	1.412×10^{-4}
1/21	1.157×10^{-4}
1/23	9.648×10^{-5}
1/25	8.169×10^{-5}

TABLE 5.1. *Results for a coefficient that is a multiple of a constant matrix. The error gives the L^2 difference between the solution of the averaged equation and the solution of the original equation for a given value of ϵ.*
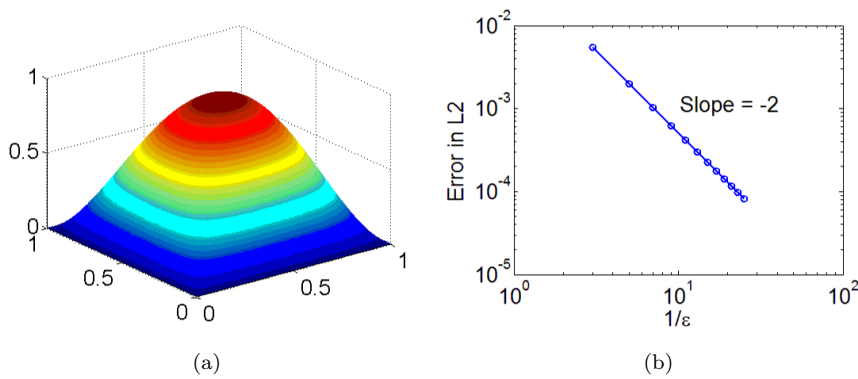

(a)   (b)

FIG. 5.1. *Results for a coefficient that is a multiple of a constant matrix. (a) A surface plot of the solution on the fully resolved grid (25×25 cells of 24×24 grid points). (b) Log-log plot of L^2 difference between solutions of averaged equation and original equation.*

5.3. A layered material. Next we consider a layered material, where the coefficient matrix varies in vertical stripes. That is, $A(y_1, y_2) = A(y_1)$. For this example we allow the coefficients to vary between the following two matrices:

$$A_1 = \begin{pmatrix} 2 & 1 \\ 1 & 4 \end{pmatrix} \qquad A_2 = \begin{pmatrix} 20 & 0 \\ 0 & 1 \end{pmatrix}.$$

Again we set the forcing to $f = 50$ and enforce zero Dirichlet boundary conditions. The resulting solution is plotted in figure 5.2.

According to (3.4) the homogenized coefficient matrix should be

$$\bar{A} = \begin{pmatrix} 40/11 & 10/11 \\ 10/11 & 41/11 \end{pmatrix}.$$

The difference between the solutions of the original Equ. $(\text{PDE})^\epsilon$ and the homogenized

Equ. (2.3) (measured in L^2) are presented in Table 5.2 and figure 5.2. As in the first example, we observe quadratic convergence as $\epsilon \to 0$.

ϵ	$\|u - \bar{u}\|_2$
1/3	1.565×10^{-2}
1/5	5.609×10^{-3}
1/7	2.867×10^{-3}
1/9	1.740×10^{-3}
1/11	1.168×10^{-3}
1/13	8.384×10^{-4}
1/15	6.312×10^{-4}
1/17	4.924×10^{-4}
1/19	3.948×10^{-4}
1/21	3.237×10^{-4}
1/23	2.702×10^{-4}
1/25	2.289×10^{-4}

TABLE 5.2. *Results for a layered material. The error gives the L^2 difference between the solution of the averaged equation and the solution of the original equation for a given value of ϵ.*
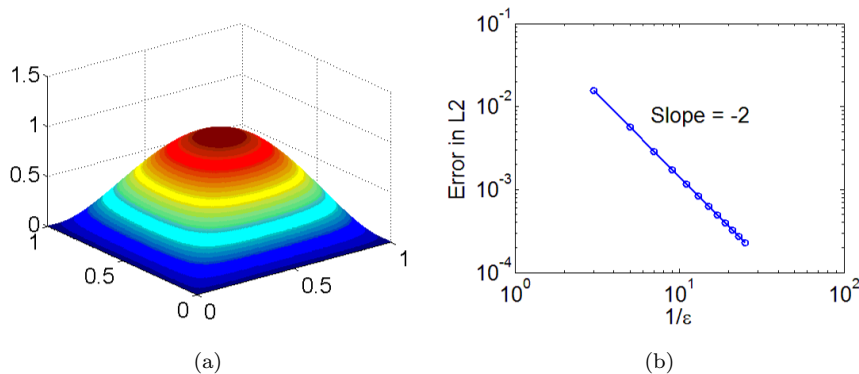

(a)   (b)

FIG. 5.2. *Results for a layered material. (a) A surface plot of the solution on the fully resolved grid (25×25 cells of 24×24 grid points). (b) Log-log plot of L^2 difference between solutions of the averaged equation and original equation.*

5.4. A separable, diagonal coefficient matrix. Next we consider a separable, diagonal coefficient. We again choose a piecewise constant coefficient matrix. In this case, each cell is divided into quarters with the following coefficients:

$$A_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad A_2 = \begin{pmatrix} 2 & 0 \\ 0 & 4 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$A_3 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 20 & 0 \\ 0 & 1 \end{pmatrix} \qquad A_4 = \begin{pmatrix} 2 & 0 \\ 0 & 4 \end{pmatrix} \begin{pmatrix} 20 & 0 \\ 0 & 1 \end{pmatrix}.$$

As before we set $f = 50$ with $u = 0$ on the boundary. See figure 5.3(a) for a surface plot of the solution.

According to (3.5), the homogenized coefficients should be

$$\bar{A} = \begin{pmatrix} 14 & 0 \\ 0 & 2 \end{pmatrix}.$$

As in the previous examples, we observe $O(\epsilon^2)$ convergence to the solution of the averaged equation; see Table 5.3 and figure 5.3(b).

ϵ	$\|u - \bar{u}\|_2$
1/3	6.105×10^{-2}
1/5	2.337×10^{-2}
1/7	1.214×10^{-2}
1/9	7.405×10^{-3}
1/11	4.984×10^{-3}
1/13	3.582×10^{-3}
1/15	2.698×10^{-3}
1/17	2.106×10^{-3}
1/19	1.689×10^{-3}
1/21	1.385×10^{-3}
1/23	1.156×10^{-3}
1/25	9.794×10^{-4}

TABLE 5.3. *Results for a coefficient matrix with separable entries. The error gives the L^2 difference between the solution of the averaged equation and the solution of the original equation for a given value of ϵ.*
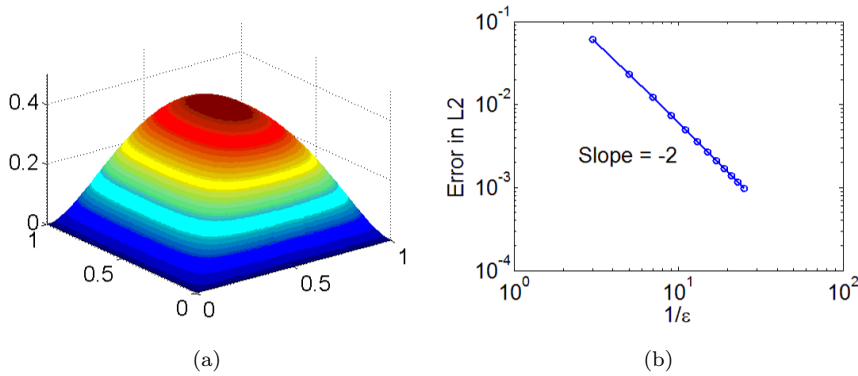

(a)   (b)

FIG. 5.3. *Results for a coefficient matrix with separable entries. (a) A surface plot of the solution on the fully resolved grid (25×25 cells of 24×24 grid points). (b) Log-log plot of L^2 difference between solutions of the averaged equation and original equation.*

5.5. A more general linear operator. In all the examples we have considered so far we have assumed that the coefficients of the drift and source terms (b, c in

(1.1)) are equal to zero. Here we consider a more general operator where these terms are present in the equation. We choose the same coefficient matrix used in section 5.2, which is a scalar multiple of a constant matrix. The remaining coefficients do not need to have this property (i.e., b need not be a multiple of a constant vector) in order for the analysis in section 3.1 to apply. In particular we consider the coefficients:

$$A_1 = \begin{pmatrix} 2 & 1 \\ 1 & 4 \end{pmatrix} \qquad b_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad c_1 = 1$$

$$A_2 = \begin{pmatrix} 4 & 2 \\ 2 & 8 \end{pmatrix} \qquad b_2 = \begin{pmatrix} 2 \\ 4 \end{pmatrix} \qquad c_1 = 2.$$

As before we let $f = 50$ and enforce zero Dirichlet boundary conditions. The solution is plotted in figure 5.4(a).

The analysis in section 3.1 is easily extended to this situation, and predicts the following averaged coefficients:

$$\bar{A}_1 = \begin{pmatrix} 8/3 & 4/3 \\ 4/3 & 16/3 \end{pmatrix} \qquad \bar{b}_1 = \begin{pmatrix} 4/3 \\ 8/5 \end{pmatrix} \qquad \bar{c}_1 = 4/3.$$

Convergence results are contained in Table 5.4 and figure 5.4. As before, we observe quadratic convergence as $\epsilon \to 0$.

ϵ	$\|u - \bar{u}\|_2$
1/3	5.486×10^{-3}
1/5	2.008×10^{-3}
1/7	1.031×10^{-3}
1/9	6.263×10^{-4}
1/11	4.203×10^{-4}
1/13	3.014×10^{-4}
1/15	2.267×10^{-4}
1/17	1.767×10^{-4}
1/19	1.415×10^{-4}
1/21	1.159×10^{-4}
1/23	9.669×10^{-5}
1/25	8.187×10^{-5}

TABLE 5.4. *Results for a general elliptic operator. The error gives the L^2 difference between the solution of the averaged equation and the solution of the original equation for a given value of ϵ.*

5.6. Non-zero boundary conditions.   In all the examples we have studied so far we have enforced zero Dirichlet boundary conditions. Now we demonstrate numerically that the approach presented in this paper also works for non-constant Dirichlet boundary conditions.

In this example we use the y-periodic coefficient matrix with entries

$$a_{11}^\epsilon = \frac{1}{\cos\left(\frac{2\pi x_1}{\epsilon} - \frac{\pi}{\epsilon}\right)\left[\cos\left(\frac{\pi}{\epsilon}\right) - \cos\left(\frac{2\pi x_2}{\epsilon} - \frac{\pi}{\epsilon}\right)\right] + 4}$$

$$a_{22}^\epsilon = \frac{1}{\cos\left(\frac{2\pi x_2}{\epsilon} - \frac{\pi}{\epsilon}\right)\left[\cos\left(\frac{\pi}{\epsilon}\right) - \cos\left(\frac{2\pi x_1}{\epsilon} - \frac{\pi}{\epsilon}\right)\right] + 4}$$

$$a_{12} = 0.$$
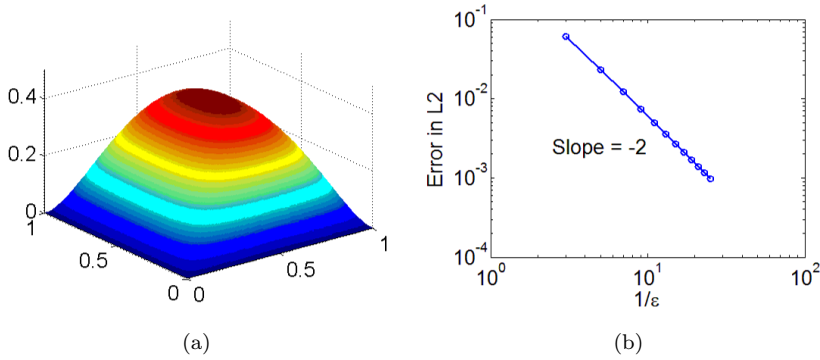
(a)   (b)

FIG. 5.4. *Results for a general elliptic operator. (a) A surface plot of the solution on the fully resolved grid (25 × 25 cells of 24 × 24 grid points). (b) Log-log plot of L^2 difference between solutions of the averaged equation and original equation.*

We set forcing

$$f = -2$$

and enforce the boundary conditions

$$u = 2x_1^2 + 2x_2^2 \qquad x_1 = 0, x_1 = 1, x_2 = 0, x_2 = 1.$$

This problem has the exact solution

$$u^\epsilon = \frac{\epsilon^2}{4\pi^2}\left[\cos\left(\frac{\pi}{\epsilon}\right) - \cos\left(\frac{2\pi x_1}{\epsilon} - \frac{\pi}{\epsilon}\right)\right]\left[\cos\left(\frac{\pi}{\epsilon}\right) - \cos\left(\frac{2\pi x_2}{\epsilon} - \frac{\pi}{\epsilon}\right)\right] + 2x_1^2 + 2x_2^2.$$

We fix $\epsilon = 1/499$ and look at the relationship between cell resolution and solution accuracy. This solution is plotted in figure 5.5(a).

The convergence results are presented in Table 5.5 and figure 5.5(b). It is evident from the log-log plot of error that for fixed (small) ϵ, the error is linearly dependent on the spatial step size used to solve the cell problem (2.1).

5.7. Random coefficients.   So far we have considered operators that vary periodically. However, the averaging method discussed in this article can also be applied to average random operators. While we avoid the analysis, we can compute the invariant distribution in this case.

Next we consider the case where the coefficient matrix at each point is randomly chosen (with equal probability) to be one of two constant operators. Since the operator no longer varies periodically, it is now neccessary to solve for the invariant distribution in the entire domain. As before, we enforce periodic boundary conditions. In order to compute the averaged coefficients, we solve for the invariant distribution with K different randomly chosen coefficients A^i and compute the averaged coefficients

$$\bar{A}^i = \left\langle \rho^\infty A^i \right\rangle.$$

$1/h$	$\bar{a}_{11}$	$\bar{a}_{22}$	$\|u - \bar{u}\|_2$
10	0.24514	0.24514	6.527×10^{-3}
50	0.24891	0.24891	1.437×10^{-3}
90	0.24939	0.24939	8.103×10^{-4}
130	0.24958	0.24958	5.607×10^{-4}
170	0.24967	0.24967	4.290×10^{-4}
210	0.24973	0.24973	3.499×10^{-4}
250	0.24978	0.24978	2.907×10^{-4}
290	0.24981	0.24981	2.531×10^{-4}
330	0.24983	0.24983	2.239×10^{-4}
370	0.24985	0.24985	1.989×10^{-4}
410	0.24986	0.24986	1.792×10^{-4}
450	0.24988	0.24988	1.630×10^{-4}
490	0.24989	0.24989	1.494×10^{-4}

TABLE 5.5. *Results for a problem with non-constant boundary conditions homogenized on a cell with spatial resolution h. The averaged coefficients are $\bar{a}_{11}, \bar{a}_{22}, \bar{a}_{12}$. The error gives the L^2 difference between the solution of the homogenized equation and the solution of the original equation.*
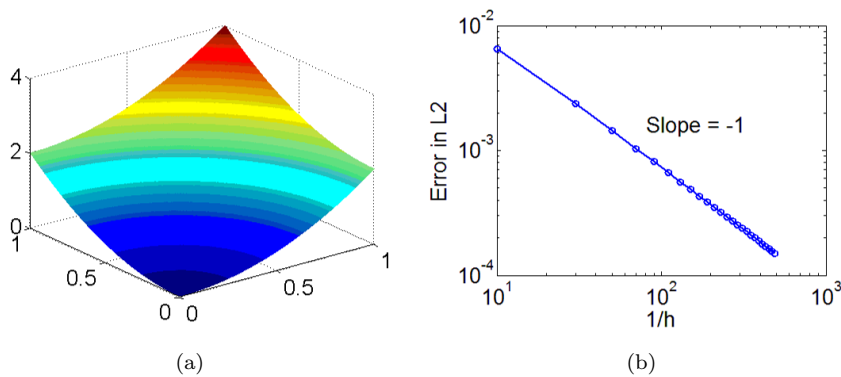

(a)   (b)

FIG. 5.5. *Results for a problem with non-constant boundary data averaged on a cell with spatial resolution h. (a) A surface plot of the exact solution (with $\epsilon = 1/499$). (b) Log-log plot of L^2 difference between solutions of the averaged equation and original equation.*

The results of these trials are averaged to compute the averaged coefficient matrix for the general random problem.

$$\bar{A} = \frac{1}{K} \sum_{i=1}^{K} \bar{A}^i.$$

In the following computations, we average the coefficients over $K = 10$ trials. To demonstrate that this approach correctly averages the random operator we will solve for twenty different random coefficient matrices and compute the mean difference between the solutions of the random and averaged problems.

In particular, we randomly vary between the following two coefficient matrices:

$$A_1 = \begin{pmatrix} 2 & 1 \\ 1 & 4 \end{pmatrix} \quad A_2 = \begin{pmatrix} 20 & 0 \\ 0 & 1 \end{pmatrix}.$$

We enforce zero Dirichlet boundary conditions and set forcing $f = 30$.

Results are shown in Table 5.6 and figure 5.6. We see that as the number of grid points is increased, the solution of the random equation approaches (on average) the solution of the averaged equation. Moreover, the average difference between the two solutions is $O(h)$.

N	$\bar{a}_{11}$	$\bar{a}_{22}$	$\bar{a}_{12}$	$\|u - \bar{u}\|_2$	$\langle \|u - \bar{u}\|_2 \rangle$
8	6.834	3.194	0.731	2.747×10^{-2}	3.635×10^{-2}
16	6.745	3.209	0.736	2.622×10^{-2}	2.146×10^{-2}
24	6.657	3.224	0.741	9.839×10^{-3}	1.699×10^{-2}
32	6.628	3.229	0.743	9.934×10^{-3}	9.940×10^{-3}
40	6.672	3.221	0.740	1.923×10^{-2}	8.358×10^{-3}
48	6.683	3.220	0.740	5.064×10^{-3}	6.583×10^{-3}
56	6.538	3.244	0.748	4.283×10^{-3}	6.029×10^{-3}
64	6.496	3.251	0.750	5.144×10^{-3}	6.624×10^{-3}
72	6.624	3.229	0.743	5.976×10^{-3}	5.100×10^{-3}
80	6.636	3.227	0.742	3.008×10^{-3}	4.009×10^{-3}
88	6.594	3.234	0.745	3.239×10^{-3}	3.454×10^{-3}
96	6.592	3.235	0.745	3.821×10^{-3}	3.902×10^{-3}
104	6.564	3.239	0.746	2.369×10^{-3}	3.145×10^{-3}
112	6.574	3.238	0.746	2.870×10^{-3}	2.979×10^{-3}
120	6.572	3.238	0.746	3.141×10^{-3}	2.986×10^{-3}

TABLE 5.6. *Results for a problem with random coefficients on an $N \times N$ grid. The averaged coefficients are $\bar{a}_{11}, \bar{a}_{22}, \bar{a}_{12}$. The errors include the L^2 difference between the solution of the homogenized equation and the solution of a random equation as well as the average difference over 20 trials.*
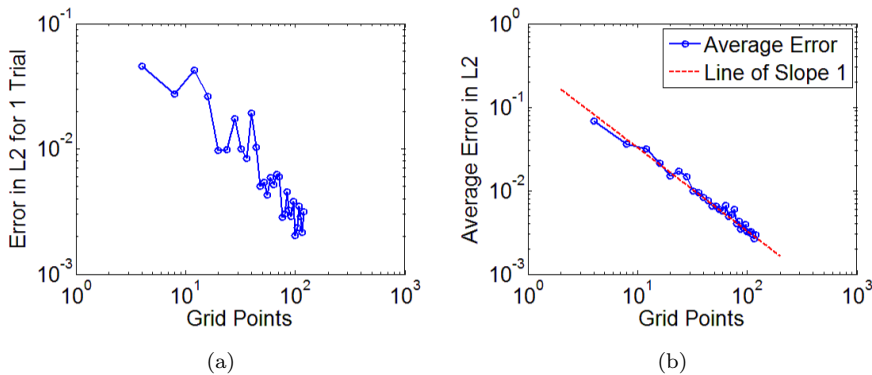

(a)   (b)

FIG. 5.6. *Results for a problem with random coefficients. (a) Log-log plot of the L^2 difference between the homogenized solution and a random solution. (b) Log-log plot of the average L^2 difference between the homogenized solution and a random solution over 20 trials.*

6. Conclusions

We recovered a simple formula for the averaged operator of the non-divergence structure elliptic operator with rapidly varying, periodic coefficients. This formula was

available in the literature using probabilistic techniques; we gave a formal derivation using partial differential equation techniques. The derivation can be made rigorous. We also presented several special cases where the adjoint problem could be solved in closed form, leading to a closed form result for the averaged operator. This could be accomplished for a wider set of examples than in the divergence structure case. We also showed that the homogenized operators are generally different between the two cases.

The second part was numerical computations. The adjoint equation was discretized using finite differences, and solved using a Gauss-Seidel method. The effort involved in solving this problem is comparable (or less) to the corresponding problem in the divergence structure case. The numerics were validated for finite ϵ against resolved numerical solutions. The formal asymptotic convergence rate $O(\epsilon^2)$ was also validated.

REFERENCES

[1] D. Cioranescu and P. Donato, *An Introduction to Homogenization*, Oxford Lecture Series in Mathematics and its Applications, The Clarendon Press Oxford University Press, New York, 17, 1999.

[2] B. Engquist and P.E. Souganidis, *Asymptotic and numerical homogenization*, Acta Numer., 17, 147-190, 2008.

[3] M.I. Freidlin, *Dirichlet's problem for an equation with periodic coefficients depending on a small parameter*, Theory Prob. Appl., 9, 121-125, 1964.

[4] M.H. Holmes, *Introduction to Perturbation Methods*, Texts in Applied Mathematics, Springer-Verlag, New York, 20, 1995.

[5] H.J. Kushner and P. Dupuis, *Numerical Methods for Stochastic Control Problems in Continuous Time*, Applications of Mathematics (New York), Stochastic Modelling and Applied Probability, Springer-Verlag, New York, second edition, 24, 2001.

[6] G.W. Milton, *The Theory of Composites*, Cambridge Monographs on Applied and Computational Mathematics, Cambridge University Press, Cambridge, 6, 2002.

[7] H. Owhadi and L. Zhang, *Homogenization of parabolic equations with a continuum of space and time scales*, SIAM J. Numer. Anal., 46(1), 1-36, 2007/08.

[8] G.A. Pavliotis and A.M. Stuart, *Multiscale Methods*, Texts in Applied Mathematics, Averaging and homogenization, Springer, New York, 53, 2008.

[9] H. Wang, *Convergence of a numerical method for solving discontinuous Fokker-Planck equations*, SIAM J. Numer. Anal., 45(4), 1425-1452 (electronic), 2007.

[10] H. Wang, C.S. Peskin and T.C. Elston, *A robust numerical algorithm for studying biomolecular transport processes*, J. Theoret. Biol., 221(4), 491-511, 2003.