NUMERICAL METHODS FOR MULTISCALE INVERSE PROBLEMS

CHRISTINA FREDERICK¹ AND BJÖRN ENGQUIST²

Abstract. We will consider inverse problems for multiscale partial differential equations of the form $-\nabla \cdot (a^\epsilon \nabla u^\epsilon) + b^\epsilon u^\epsilon = f$ in which solution data is used to determine coefficients in the equation. Such problems contain both the general difficulty of finding an inverse and the challenge of multiscale modeling, which is hard even for forward computations. The problem in its full generality is typically ill-posed and one approach is to reduce the dimensionality of the original problem by just considering the inverse of an effective equation without microscale $\epsilon$. We will here include microscale features directly in the inverse problem. In order to reduce the dimension of the unknowns and avoid ill-posedness, we will assume that the microscale can be accurately parametrized by piecewise smooth coefficients. We indicate in numerical examples how the technique can be applied to medical imaging and exploration seismology.

1. Introduction

Inverse problems for partial differential equations pose a huge computational challenge, in particular when the coefficients are of multiscale form. An application is medical imaging, where high resolution reconstructions are obtained using photo-acoustic effects of optical and ultrasonic waves [5, 6]. We also consider examples in reflection seismology [16], where accurate models of seismic wave propagation in the Earth’s sedimentary crust must account for a wide spectrum of time and spatial scales. The mathematical formulation is as follows.

For a bounded, connected domain, $\Omega \subset \mathbb{R}^n$ with Lipschitz boundary, we will consider the Dirichlet problem

$$-\nabla \cdot (a^\epsilon \nabla u^\epsilon) + b^\epsilon u^\epsilon = f \quad \text{in } \Omega \quad u^\epsilon = g \quad \text{on } \partial \Omega.$$  \hspace{1cm} (1.1)

Here $a^\epsilon(x) = a(x, x/\epsilon)$ and $b^\epsilon(x) = b(x, x/\epsilon)$ are matrices with bounded, measurable elements, and the functions $a(x, y)$ and $b(x, y)$ are assumed to be periodic in the second variable. The constant $0 < \epsilon << 1$ represents the ratio of scales in the problem. Furthermore, we assume $f$ and $g$ are smooth, bounded functions.

When faced with balancing computational cost with accuracy, most approaches only deal with scientific models of large scale behavior and, for example, account

¹Department of Mathematics, The University of Texas at Austin, 1 University Station C1200, Austin, Texas 78712 USA (c frederick@math.utexas.edu).
²The Institute for Computational Engineering and Sciences, 201 East 24th St, Stop C0200, Austin, Texas 78712 USA (engquist@math.utexas.edu).
for microscopic processes by using effective or homogenized equations to simplify computations. Homogenization theory [7, 11] provides the form of the effective problem corresponding to (1.1); as \( \epsilon \to 0 \) \( u^\epsilon \rightharpoonup U \) in \( H_0^1(\Omega) \), where \( U \) is the solution to an equation of the form

\[
- \nabla \cdot (A \nabla U) + b^0 U = f \text{ in } \Omega \quad U = g \text{ on } \partial \Omega.
\] (1.2)

The full inverse problem is to determine the function \( a^\epsilon \) from measurements of the solution to the forward problem on the full domain or part of the domain, for example, on the boundary. The observed data is assumed to be of the form \( d = F(u, \nabla u, x) \), where \( F \) is the observation operator. A common approach is to formulate this problem as a PDE-constrained optimization problem of the form

\[
\begin{align*}
\min_{a^\epsilon, u^\epsilon} \quad & J(a^\epsilon, u^\epsilon) := \frac{1}{2} \| F(u^\epsilon, \nabla u^\epsilon, x) - d \|^2 + \alpha R(a^\epsilon) \\
\text{subject to} \quad & c(a^\epsilon, u^\epsilon) = 0.
\end{align*}
\] (1.3)

The constraint \( c(a^\epsilon, u^\epsilon) = 0 \) is satisfied when \( u^\epsilon \) solves the state equation (1.1). The choice of a regularization functional \( R \) and the constant \( \alpha \geq 0 \) is a research topic on its own, and in this work we concentrate on issues concerning the data fidelity term by setting \( \alpha = 0 \).

Full inversion has a high computational cost and is typically ill-posed; a number of different sequences \( a^\epsilon \) give the same homogenized solution \( U \), \( \lim_{\epsilon \to 0} u^\epsilon = U \). In [14], the full inverse problem (1.3) is replaced with an effective inverse problem, formulated as

\[
\begin{align*}
\min_{A, U} \quad & J^0(A, U) := \frac{1}{2} \| F(U, \nabla U, x) - d \|^2 + \alpha R(A) \\
\text{subject to} \quad & c^0(A, U) = 0,
\end{align*}
\] (1.4)

where the constraint \( c^0(A, U) = 0 \) is satisfied when \( U \) solves the state equation (1.2).

This paper explores the possibility of explicitly including the microscale components of the forward model in the inversion process by assuming a priori knowledge of the microstructure in the form of a low dimensional parametrization. This is achieved by imposing the additional constraint \( a^\epsilon(x) = a(m(x), x/\epsilon) \), where \( a \) is known and \( m \) is to be determined. The problem (1.3) is then replaced by

\[
\begin{align*}
\min_{m, u^\epsilon} \quad & J(a^\epsilon, u^\epsilon) \\
\text{subject to} \quad & c(a^\epsilon, u^\epsilon) = 0, \\
& a^\epsilon(x) = a(m(x), x/\epsilon).
\end{align*}
\] (1.5)

The following is a summary of the different numerical approaches for microscale inversion.

I. **Full inverse problem.** The full inverse problem (1.3) is ill-posed and computationally expensive. Therefore, we omit this case from our computations.

II. **Directly inverting the effective model** (1.4) for a microscale parameter can be done in two ways.
a. **Analytic solver.** If the closed form of the effective coefficient $A(m(x))$ corresponding to $a(m(x), x/\epsilon)$ is known, the effective inverse problem can also be formulated in terms of microstructure. Here, forward solvers use the analytic form of the effective equation to compute solutions on a coarse grid to find the solution to the optimization problem

$$\min_{m,U} J^0(A,U) \quad \text{subject to} \quad c^0(A,U) = 0, \quad A = A(m).$$

(1.6)

b. **HMM.** Often, the explicit form of the homogenized coefficient corresponding to $a^\epsilon$ is not known, and therefore the term $A_{m(x)}$ in (1.6) cannot be directly computed. This issue can be overcome numerically with the heterogeneous multiscale method, or HMM, introduced by E and Engquist [9]. HMM provides a framework for the design of methods that capture macroscale properties of a system using microscale information.

$$\min_{m,U} J^0(A_{HMM},U_{HMM}) \quad \text{subject to} \quad c^H(a^\epsilon,U_{HMM}) = 0, \quad a^\epsilon(x) = a(m(x), x/\epsilon).$$

(1.7)

Here, the constraint $c^H(a^\epsilon,U_{HMM}) = 0$ is satisfied when $U_{HMM}$ is the HMM solution corresponding to (1.1). The advantage of HMM is the ability to evaluate the functional $J^0(A_{HMM},U_{HMM})$ without explicit knowledge of $A_{HMM}$.

### III. Two-stage solver.

Another option is to first solve the minimization problem (1.4) and then determine the microscale parameter from the recovered effective coefficient. This idea is formulated as a two-stage procedure,

$$\left\{ \begin{array}{l}
\hat{A},\hat{U} = \arg\min_{A,U} J^0(A,U) \quad \text{subject to} \quad c^0(A,U) = 0 \\
\min_{m} \|A(m) - \hat{A}\|^2.
\end{array} \right.$$  

(1.8)

The paper is organized as follows. In section §2 we provide theory for inverse problems for elliptic equations and prove uniqueness of microscale inversion of the effective equation corresponding to certain models. In §2.1 we present results for anisotropic inverse conductivity problems from [4] corresponding to a parametrized conductivity. In §3 we describe the finite element heterogeneous multiscale method. Numerical results are provided in §4. In section §5 we consider problems from medical imaging, quantitative photoacoustic tomography. In section §6 we provide numerical results for inverse scattering problems. Then we conclude in §7.

#### 2. Analysis ($b^\epsilon = 0$)

Let $\Omega$ be a bounded region in $\mathbb{R}^n$, $n \geq 2$. We consider the solution to the equation

$$-\nabla \cdot (\gamma \nabla u) = 0 \quad \text{in} \quad \Omega.$$  

(2.1)

The coefficient $\gamma$, referred to as the conductivity, is in general a real, positive definite symmetric, $n \times n$ matrix; if $\gamma$ is scalar we say that the conductivity is isotropic, in all other cases it is called anisotropic. In the next sections we will
model multiscale and effective conductivities by \( \gamma(x) = a'(x) \) and \( \gamma(x) = A(x) \) respectively. Our aim is to determine \( \gamma \) using multiple boundary measurements.

**Definition 2.1.** For \( f, g \in H^{1/2}(\partial \Omega) \) let \( u \in H^1(\Omega) \) be the weak solution to (2.1) subject to \( u|_{\partial \Omega} = f \), and let \( v \) be an arbitrary function in \( H^1(\Omega) \) that satisfies \( v|_{\partial \Omega} = g \). The Dirichlet-to-Neumann map \( \Lambda_\gamma : H^{1/2}(\partial \Omega) \to H^{-1/2}(\partial \Omega) \) is defined by

\[
\langle \Lambda_\gamma f, g \rangle = \int_\Omega \gamma \nabla u \cdot \nabla v.
\]

In the anisotropic case, the inverse problem is to recover conductivities \( \gamma \) up to the action of a class of diffeomorphisms. In order to obtain logarithmic stability estimates, regularity assumptions are made. A summary of these results is found in [2]. One idea is to replace these a-priori regularity assumptions with assumptions of a different character that are more suited for applications and give rise to better stability estimates. Similarly, one could search for functionals associated with the unknown conductivity that carry relevant physical information. This approach was investigated in [3], where it was shown that the average conductivity \( \frac{1}{|\Omega|} \int_\Omega \gamma \) is not continuously dependent on the map \( \Lambda_\gamma \).

In this work we search for other descriptions of the conductivity that result in stable dependence on boundary measurements.

### 2.1. Conductivities with special anisotropy.

In the case where the conductivity matrix \( \gamma \) has more structure, results in [4] show that we can infer more about the uniqueness of the solution to the inverse problem. We impose the form \( \gamma(x) = A(m(x)) \) for a scalar function \( m(x) \). Then, \( m \to A(m) \) is a matrix-valued function with derivative \( D_mA \).

**Definition 2.2.** Given \( E > 0 \), and denoting the class of \( n \times n \) real valued symmetric matrices by \( \text{Sym}_n \), we say that \( A \in \mathcal{H}^\infty \) if \( A, D_mA \in W^{1,\infty}(\lambda^{-1}, \lambda], \text{Sym}_n \) and the following conditions hold for all \( m \in (\lambda^{-1}, \lambda] \):

\[
\begin{align*}
\lambda^{-1}|\xi|^2 &\leq A(m)\xi \cdot \xi \leq \lambda|\xi|^2 \quad \text{for all } \xi \in \mathbb{R}^n, \\
D_mA(m)\xi \cdot \xi &\geq E^{-1}|\xi|^2 \quad \text{for all } \xi \in \mathbb{R}^n.
\end{align*}
\tag{2.2}
\]

The condition (2.2) describes the monotonicity of the coefficient with respect to the parameter. The following theorem, adapted to our context, is from [4]. It gives a global uniqueness result of \( A(m) \) among piecewise analytic perturbations.

**Theorem 2.1 (Alessandrini, Gaburro 2001).** Suppose \( A \in \mathcal{H}^\infty \) and suppose \( \lambda^{-1} \leq m_1(x), m_2(x) \leq \lambda \) for all \( x \in \Omega \), and \( \|m_1\|_{W^{1,\infty}(\Omega)}, \|m_2\|_{W^{1,\infty}(\Omega)} \leq E \). Suppose also that \( \Omega \) can be partitioned into a finite number of domains \( \{\Omega_j\}_{j \leq N} \) with \( m_1 - m_2 \) analytic on each \( \overline{\Omega}_j \). Then, \( \Lambda_{A(m_1)} = \Lambda_{A(m_2)} \) implies that \( A(m_1) = A(m_2) \) in \( \Omega \).

In the proof of Theorem 2.1, it is shown that \( m_1 = m_2 \) on each \( \overline{\Omega}_j \). We will use this result to describe microscale parameter recovery from the Dirichlet-to-Neumann map corresponding to an effective equation.
2.2. Inverse homogenization. The first example we will consider is the Dirichlet problem

\[-\nabla \cdot (a^\varepsilon \nabla u^\varepsilon) = f \text{ in } \Omega, \quad u^\varepsilon = 0 \text{ on } \partial \Omega. \quad (2.3)\]

The goal of inverse homogenization is to recover the coefficient \(a^\varepsilon\) from coarse scale data \(d\) of the form \(d = H(U, \nabla U, x)\), where \(U\) is the solution to the homogenized problem

\[-\nabla \cdot (A \nabla U) = f \text{ in } \Omega, \quad U = 0 \text{ on } \partial \Omega. \quad (2.4)\]

In [8], the problem is re-cast using the geometric framework underlying homogenization. Here, we will parametrize the conductivity itself in order to reformulate the problem as an optimization problem with a low dimensional search space.

2.2.1. Microscale Parametrization. Explicit solutions of the homogenized equation (1.2) can be found for problems in the case \(n = 1\), and also in certain higher dimensional models that have a one-dimensional character, such as those describing layered media [11]. We will use the following examples of models that include a microscale parametrization, depicted in Figure 1. In order to comply with the assumptions in the previous section, we let \(m\) be a bounded scalar function \(-1 \leq m(x) < 1 < \lambda\) for all \(x \in \Omega\).

In the first two cases, \(a(x, y) \in L^\infty((\lambda^{-1}, 1) \times \mathbb{R}^2)\) is a positive function that is \(Y\)-periodic in \(y\), \(Y = [0, 1) \times [0, 1)\). Then, the conductivity \(a^\varepsilon\) is characterized by \(a^\varepsilon(x) = a(m(x), x/\varepsilon)\).

A. Volume fraction. An example of a function that characterizes a two-phase medium that takes values determined by the functions \(a_1\) and \(a_2\), with the respective volume fractions \(\xi\) and \(1 - \xi\) respectively, and \(a_i(y) = a_i(y_2)\) \(1\)-periodic for \(i = 1, 2\). Then,

\[a(\xi, y) = \begin{cases} a_1(y_2) & 0 \leq y < \xi \\ a_2(y_2) & \xi \leq y < 1 \end{cases}. \quad (2.6)\]

B. Amplitude. Here we include a damping term \(\xi\) that restricts the oscillations of a multiscale function. For \(a_0 > 0\) and a \(1\)-periodic function \(a_1 \in L^\infty(\mathbb{R})\),

\[a(\xi, y) = a_0 + \xi a_1(y). \quad (2.7)\]

C. Angle. The assumption (2.5) is modified in the third case. Here, the conductivity \(a^\varepsilon\) is characterized by a \(Y\)-periodic function \(\hat{a} \in L^\infty(\mathbb{R}^2)\), and a spatially varying rotation matrix \(\sigma_{m(x)}\),

\[a^\varepsilon(x) = \hat{a}(\sigma_{m(x)}x/\varepsilon), \quad \sigma_{\xi} = \begin{pmatrix} \cos \xi & \sin \xi \\ -\sin \xi & \cos \xi \end{pmatrix}. \quad (2.8)\]
2.2.2. Effective coefficients. In this section we will derive the closed form of the homogenized coefficient matrix $A = A(m(x))$ corresponding to $a'$. The following lemma describes the effective coefficient corresponding almost periodic functions. The averaging operator is denoted $\langle f \rangle_Y = \frac{1}{|Y|} \int_Y f(y)dy$, where $|Y|$ is the volume of the set $Y \subset \mathbb{R}^2$.

**Lemma 2.1.** Suppose $a'(x) = \tilde{a}(x, x/\varepsilon)$, where $\tilde{a}(x, y)$ is smooth in $x$ and is only a function of $x$ and $y_2$, $\tilde{a}(x, y) = \tilde{a}(x, y_2)$. Also, suppose that $\tilde{a}(x, \cdot)$ is $Y-$periodic, $Y = [0, 1)$. Then, the homogenized coefficient corresponding to $a'$ is $A(x)$ defined by

$$A(x) = \text{diag}(\langle \tilde{a}(x, \cdot) \rangle_Y, (\langle \tilde{a}(x, \cdot) \rangle_Y)^{-1}).$$

**Proof.** Homogenization theory for locally periodic functions [11, 13] provides the explicit form of $A(x)$, the homogenized coefficient corresponding to $a'(x)$

$$A(x) = \int_Y (\tilde{a}(x, y) + \tilde{a}(x, y)\nabla_y \chi)dy,$n$$

where $\chi = (\chi_1, \chi_2)$ solves the cell problems:

$$-\nabla_y \cdot (\tilde{a}(x, y)\nabla_y \chi) = \nabla_y \cdot \tilde{a}(x, y)Id$$

with the constraint $\chi(x, y)$ is $Y-$periodic in the second variable and $\int_Y \chi(x, y)dy = 0$. Since we further assumed that $\tilde{a}$ is a function of only $x$ and $y_2$, $\tilde{a} = \tilde{a}(x, y_2)$, the solutions to the cell problem (2.11) are of the form $\chi = (\chi_1(x, y_2), \chi_2(x, y_2))$. Therefore, (2.11) is equivalent to

$$-\frac{\partial}{\partial y_2}(\tilde{a}(x, y_2)\frac{\partial}{\partial y_2} \chi_1) = 0,$$

$$-\frac{\partial}{\partial y_2}(\tilde{a}(x, y_2)\frac{\partial}{\partial y_2} \chi_2) = \frac{\partial}{\partial y_2} \tilde{a}(x, y_2).$$

Integration from 0 to $y_2$ gives

$$\tilde{a}(x, y_2) \frac{\partial \chi_1}{\partial y_2} = c_1$$

$$\tilde{a}(x, y_2) \frac{\partial \chi_2}{\partial y_2} = -\tilde{a}(x, y_2) + d_1$$

**Figure 1.** (left to right) Oscillatory conductivities with spatially varying volume fraction, amplitude, and angle.
for some constant functions \(c_1(x), d_1(x)\). Since \(\tilde{a}\) is strictly positive, we can divide (2.12) and (2.13) by \(\tilde{a}(x, y_2)\) and integrate from 0 to \(y_2\) again

\[
\chi_1 = c_1 \int_0^{y_2} \frac{1}{\tilde{a}(x, \xi)} d\xi + c_2 \\
\chi_2 = -y_2 + d_1 \int_0^{y_2} \frac{1}{\tilde{a}(x, \xi)} d\xi + d_2.
\]

Now, using periodicity, \(\chi_l(x, 0) = \chi_l(x, 1)\) it follows that \(c_1 = 0\), and \(d_1 = \langle \tilde{a}(x, \cdot)^{-1} \rangle_Y^{-1}\). Therefore (2.12) and (2.13) become

\[
\tilde{a}(x, y_2) \frac{\partial \chi_1}{\partial y_2} = 0 \\
\tilde{a}(x, y_2) \frac{\partial \chi_2}{\partial y_2} = -\tilde{a}(x, y_2) + \langle \tilde{a}(x, \cdot)^{-1} \rangle_Y^{-1}
\]

Substituting these expressions into (2.10) results in the closed form for the effective coefficient (2.9).

Now we can describe the homogenized coefficients corresponding to \(a^\prime\) of the form (2.6) and (2.7).

**Effective volume fraction.** Applying Lemma 2.1 for \(\tilde{a}(x, \cdot) = a_1\chi_{[0,m(x)]} + a_2\chi_{[m(x),1)}\) results in the expression

\[
A(m(x)) = \text{diag}(\langle a_1\chi_{[0,m(x)]} + a_2\chi_{[m(x),1)} \rangle_Y, \langle a_1^{-1}\chi_{[0,m]} + a_2^{-1}\chi_{[m,1)} \rangle_Y^{-1}). \tag{2.14}
\]

**Effective amplitude.** Applying Lemma 2.1 for \(\tilde{a}(x, \cdot) = a_0 + m(x)a_1\) results in the expression

\[
A(m(x)) = a_0 I_d + m(x)\text{diag}(\langle a_1 \rangle_Y, \langle a_1^{-1} \rangle_Y^{-1}). \tag{2.15}
\]

Now that we can describe the dependence of the effective coefficient on the microscale parameter, we prove uniqueness of the solution to the inverse homogenization problem using Theorem 2.1.

**Theorem 2.3.** For \(a^\prime\) of the form (2.6) and (2.7), the microscale parameter \(m(x)\) is completely determined by the Dirichlet-to-Neumann map corresponding to the homogenized equation.

**Proof.** We check the monotonicity assumption (2.2), for the effective volume fraction (2.14),

\[
D_m A(m) = \text{diag} \left( (a_1 - a_2)(m), \frac{(a_2^{-1} - a_1^{-1})(m)}{\langle a_1^{-1}\chi_{[0,m]} + a_2^{-1}\chi_{[m,1]} \rangle^2} \right)
\]

and also for the effective amplitude (2.15),

\[
D_m A(m) = \text{diag} \left( \langle a_1 \rangle_Y, \langle a_1^{-1} \rangle_Y^{-1} \right).
\]

In both cases, \(D_m A(x, m)\) is a diagonal matrix with positive entries, and the assumptions of Theorem 2.1 are satisfied.

We also will describe the effective coefficient corresponding to a parametrization of the angle (2.8).
Figure 2. Piecewise polynomials are used to model cell structures that result in a spatially varying membrane thickness (left) and composition (right).

**Lemma 2.2.** If we assume that \( \hat{a} > 0 \) is function of only one variable, \( \hat{a} = \hat{a}(y_2) \), and \( m \) is a constant function, again denoted \( m \), the homogenized coefficient corresponding to (2.8) has the following form:

\[
A(m) = \langle \hat{a} \rangle \text{Id} + \left( \langle \hat{a}^{-1} \rangle^{-1} - \langle \hat{a} \rangle \right) \begin{pmatrix} \cos^2 m & \cos m \sin m \\ \cos m \sin m & \sin^2 m \end{pmatrix}.
\]  

**(2.16)**

**Proof.** Let \( \sigma = \sigma_m \). The homogenized coefficient corresponding to \( \hat{a} \) is a known matrix \( \hat{A} = \text{diag} \langle \hat{a} \rangle_{[0,1]}, \langle \hat{a}^{-1} \rangle_{[0,1]} \). Consider the scalar problems

\[
\int_X \nabla \psi \cdot \hat{a}(x/\epsilon) \nabla u^\epsilon dx = 0, \quad \forall \psi \in H_0^1(X); \quad u^\epsilon \in H_0^1(X)
\]

\[
\int_X \nabla \psi \cdot \hat{A} \nabla U dx = 0, \quad \forall \psi \in H_0^1(X); \quad U \in H_0^1(X)
\]

Now consider the change of variables \( x = \sigma y \) where \( \sigma \) is an orthogonal transformation from \( \mathbb{R}^2 \) to \( \mathbb{R}^2 \). We obtain the Dirichlet problems for \( Y = \sigma^{-1} X \)

\[
\int_Y \nabla_y \psi \cdot \hat{a}(\sigma y/\epsilon) \nabla_y u^\epsilon(\sigma y) dy = 0
\]

\[
\int_Y \nabla_y \psi \cdot \sigma \hat{A} \sigma^{-1} \nabla_y U(\sigma y) dy = 0
\]

Since \( u^\epsilon(\sigma y) \rightharpoonup U(\sigma y) \) in \( H_0^1(Y) \), it follows that the homogenized coefficient for \( a^\epsilon(x) \) is \( \sigma \hat{A} \sigma^{-1} \).

**Remark 2.4.** In this case, \( D_m A = (\langle \hat{a}^{-1} \rangle^{-1} - \langle \hat{a} \rangle) \begin{pmatrix} -\sin 2m & \cos 2m \\ \cos 2m & \sin 2m \end{pmatrix} \), has eigenvalues \( \pm 1 \). Therefore, the monotonicity assumption of Theorem 2.1 cannot be directly applied. We will describe the numerical results that indicate the possibility of microstructure inversion.
2.3. **Unknown homogenized coefficient.** In two dimensions, the homogenized form of $a^\epsilon$ is generally not known explicitly. We will consider two examples that can be used to model periodic cell structures. A typical cell is modeled by the set $Y = [0, 1] \times [0, 1]$. The interior of a cell is the set $Y' \subset Y$, and $a_1, a_2 \in L^\infty(\mathbb{R}^2)$ are $Y-$periodic functions.

**D. Cell wall thickness.** In the first example we again consider a spatially varying parameter that determines the thickness of the cell walls,

$$a^\epsilon(x) = a(m(x), x/\epsilon), \quad a(\xi, y) = \begin{cases} a_1(y) & y \in \xi Y' \\ a_2(y) & \text{otherwise} \end{cases}. \quad (2.17)$$

**E. Cell composition.** In the second consider a configuration of cells with a fixed geometry that possess spatially varying compositions,

$$a^\epsilon(x) = a(m(x), x/\epsilon), \quad a(\xi, y) = \begin{cases} \xi a_1(y) & y \in Y' \\ a_2(y) & \text{otherwise} \end{cases}. \quad (2.18)$$

For a fixed $m \in (0, 1)$, $a(m, \cdot)$ satisfies the condition of cubic symmetry, and therefore the homogenized matrix $A(m)$ is isotropic, that is, $A(m) = \bar{a}(m, x)Id$ (see [11]). A rough estimate of $\bar{a}(x)$ is given by the Voigt-Reiss inequality,

$$\langle a(m, \cdot)^{-1} \rangle^{-1} \leq \bar{a}(m, x) \leq \langle a(m, \cdot) \rangle.$$ 

Although the explicit form of the effective coefficient is not known, a numerical approximation of the effective problem can be estimated with multiscale methods such as HMM, described in the next section. Our numerical results indicate that microscale details can be gleaned from coarse boundary measurements.

3. **Finite element heterogeneous multiscale method**

The problem (1.1) is well studied in homogenization theory [7, 11], and demonstrates the application of these homogenization techniques in multiscale computation. Numerical methods such as the finite element heterogeneous multiscale method (FE-HMM) [1, 9] approximate the solution to an effective problem (1.2) using grids with typical macroscale spacing $H > \epsilon$ without explicit knowledge of the homogenized coefficient.

We will introduce FE-HMM in a basic setting. First, the effective model (1.2) is discretized using a $P_1$ finite element method with triangulation $\mathcal{T}_H$ of element size $H$. The resulting macroscale bilinear form is defined for functions $V$ and $W$ lying in the finite element space $X_H$,

$$\mathcal{B}(V, W) := \int_{\Omega} \nabla V(x) \cdot A_{HMM}(x) \nabla W(x) dx + \int_{\Omega} b^0 W V dx,$$

where $A_{HMM}, b^0$ are effective coefficients, but $A_{HMM}$ is not known explicitly. This term is approximated using numerical quadrature for a set of quadrature points,
\begin{align}
&\{x_l\}, \text{ and weights, } \{\omega_l\}, \\
&B(V, W) \simeq \sum_{K \in T_h} |K| \sum_{x_l \in K} \omega_l \left( (\nabla V \cdot A_{HMM} \nabla W)(x_l) + (b^0 W)(x_l) \right), \quad (3.1)
\end{align}

where $|K|$ is the measure of $K$.

A microscale solver is then used to estimate the stiffness matrix when the effective coefficient $A_{HMM}$ is not known. The effective behavior of $a^\epsilon$ is captured locally by solving the cell problems

\begin{equation}
-\nabla \cdot (a^\epsilon \nabla v_l^\epsilon) = 0 \text{ in } I_\delta(x_l) := x_l \pm \frac{\delta}{2},
\end{equation}

with the boundary condition $v_l^\epsilon = V_l$ on $\partial I_\delta(x_l)$, where $V_l$ is the linear approximation of $V$ at $x_l$. In this work, we choose a $P_1$ finite element method with triangulations $T_h$ of the subdomains $I_\delta(x_l)$. The spacing $h < \epsilon$ is chosen sufficiently small in order to resolve the microscale.

Then, the term $(\nabla V \cdot A_{HMM} \nabla W)(x_l)$ in (3.1) can be estimated by

\begin{equation}
(\nabla V \cdot A_{HMM} \nabla W)(x_l) \simeq \frac{1}{\delta^n} \int_{I_\delta(x_l)} \nabla v_l^\epsilon \cdot (a^\epsilon \nabla w_l^\epsilon) dx.
\end{equation}

The HMM bilinear form is then defined by

\begin{equation}
B_{HMM}(V, W) := \sum_{K \in T_h} \frac{|K|}{\delta^n} \sum_{x_l \in K} \omega_l \left( \int_{I_\delta(x_l)} \nabla v_l^\epsilon \cdot (a^\epsilon \nabla w_l^\epsilon) dx + (b^0 W)(x_l) \right).
\end{equation}

Finally, we have that the HMM solution, $U_{HMM}$, solves the problem

\begin{align*}
&\min_{V \in X_h} B_{HMM}(V, V) - (f, V).
\end{align*}

In [12], analysis errors for HMM are given for model problems with no lower order terms, $b^\epsilon = 0$. The results for the deterministic setting are summarized below.

\textbf{Theorem 3.1 (Ming, Zhang 2005).} Denote by $U, U_{HMM}$ the solutions to (2.4) and the HMM solution, respectively. Let

\begin{align*}
e(\text{HMM}) &= \max_{x_l \in K, K \in T_h} \| A(x_l) - A_{HMM}(x_l) \|, \\
&\text{where } \| \cdot \| \text{ is the Euclidean norm. If } U \text{ is sufficiently smooth, and } \lambda I \leq a^\epsilon \leq \Lambda I \text{ for } \lambda, \Lambda > 0, \text{ then there exists a constant } C \text{ independent of } \epsilon, \delta \text{ and } H \text{ such that}
\end{align*}

\begin{align*}
&\| U - U_{HMM} \|_1 \leq C \left( H^k + e(\text{HMM}) \right), \\
&\| U - U_{HMM} \|_0 \leq C \left( H^{k+1} + e(\text{HMM}) \right).
\end{align*}

Then $U_{HMM} \to U$ as $e(\text{HMM}) \to 0$. For the periodic homogenization problem it is also shown that

\begin{align*}
e(\text{HMM}) &\leq \begin{cases} 
C_\epsilon & I_\delta(x_l) = x_l + \epsilon I \\
C(\frac{\epsilon}{\delta} + \delta) & \text{otherwise}
\end{cases}
\end{align*}
These results show that the HMM solution is a good approximation to the homogenized solution. In the next section we show numerical results for microscale parameter recovery using HMM as a forward solver.

4. Numerical Inversion

Here we compute solutions to the effective equation (1.6) using an analytic forward solver (II a.), HMM (II b.). The inversion results also include a two-stage solver (III) for the minimization problem (1.8). The model problems (1.1), (1.2) are solved for \( f = 0 \), and imposed Dirichlet boundary conditions, \( \{g_1, \ldots, g_K\} \).

4.1. Forward solvers. Let \( \mathcal{T}_h \) be a regular triangulation of \( \Omega \) with resolution \( h \), and let \( X_h \) be the standard piecewise linear finite element space. The finite element solution \( u_h^{(k)} \in g^{(k)} + X_h \) to the full problem (2.3) has the variational formulation

\[
\int_{\Omega} \nabla v(x) \cdot a^{e}(x) \nabla u_h^{(k)}(x) dx + \int_{\Omega} b^{e}(x) u_h^{(k)}(x) dx = 0 \quad \text{for all } v \in X_h.
\]

The finite element solution \( U^{(k)} \in g^{(k)} + X_H \) to the effective problem (2.4) satisfies

\[
\int_{\Omega} \nabla V(x) \cdot A^{e}(x) \nabla U^{(k)}(x) dx + \int_{\Omega} b^0(x) U^{(k)}(x) dx = 0 \quad \text{for all } V \in X_H. \tag{4.1}
\]

From the previous section, we have that the FE-HMM solution \( U_{\text{HMM}}^{(k)} \in g^{(k)} + X_H \) satisfies

\[
\int_{\Omega} \nabla V(x) \cdot A_{\text{HMM}}^{e}(x) \nabla U_{\text{HMM}}^{(k)}(x) dx + \int_{\Omega} b^0(x) U_{\text{HMM}}^{(k)}(x) dx = 0 \quad \text{for all } V \in X_H, \tag{4.2}
\]

where \( A_{\text{HMM}}^{e} \) is estimated by microscale solvers on local subdomains.

4.2. Discrete inverse problem. Denote the boundary nodes of the coarse mesh by \( \mathcal{V}_B \). For each \( 1 \leq k \leq K \), coarse predictions are of the form

\[
F^{(k)} = A \nabla U^{(k)} \cdot n|_{\mathcal{V}_B}, \quad F_H^{(k)} = A_{\text{HMM}}^{e} \nabla U_{\text{HMM}}^{(k)} \cdot n|_{\mathcal{V}_B}, \tag{4.3}
\]

where \( n \) is the unit normal vector to \( \partial \Omega \).

I. We set the observed Neumann data to be of the form

\[
d^{(k)} = \Pi^H a^{e} \nabla u^{(k)} \cdot n|_{\mathcal{V}_B}, \tag{4.4}
\]

where \( \Pi^H \) is a projection operator from \( X_h \) onto \( X_H \).

II. The discrete Dirichlet-to-Neumann maps \( \Lambda_A^{V_B} \) and \( \Lambda_{A_{\text{HMM}}}^{V_B} \) are determined by the Dirichlet conditions \( g^{(k)} \) and predictions from coarse scale solvers, \( F^{(k)} \) and \( F_H^{(k)} \) in (4.3).

a. The discrete problem corresponding to the effective inverse problem (1.6) is

\[
\begin{align*}
\text{minimize} & \quad \| \Lambda_A^{V_B} - d \| \\
\text{subject to} & \quad C^0(A, U) = 0, \\
A & = A(m),
\end{align*} \tag{4.5}
\]
where \( C^0 \) is satisfied when \( U \) solves (4.1).

b. The HMM-reduced model (1.7) becomes

\[
\begin{align*}
\minimize_{m,U_{HMM}} & \quad \|A_{HMM}^V - d\| \\
\text{subject to} & \quad C^H(A_{HMM},U_{HMM}) = 0, \\
& \quad a^e(x) = a(m(x), x/\varepsilon),
\end{align*}
\]

(4.6)

where \( C^H \) is satisfied when \( U_{HMM} \) solves (4.2).

III. Finally, the two-stage procedure (1.8) is discretized as

\[
\begin{align*}
(\hat{A}, \hat{U}) = \arg \minimize_m & \quad \|A^V_{HMM} - d\| \text{ subject to } C^0(A,U) = 0 \\
& \quad \|A(m) - \hat{A}\|
\end{align*}
\]

(4.7)

4.3. Numerical Results (\( b^e = 0 \)). In §2, the parameter \( m \) is chosen to be an arbitrary scalar function that satisfies the requirements of Theorem 2.1. In the numerical examples, the function \( m \in L^\infty(\mathbb{R}^2) \) is defined for a vector \( \hat{m} \in \mathbb{R}^N \) and piecewise linear basis functions \( \{l_k\} \) defined for a partition \( \{\Omega_k\} \subset \Omega, 1 \leq k \leq N, \cup \Omega_k = \Omega \),

\[
m(x) = \sum_{k=1}^N \hat{m}_k l_k(x).
\]

(4.8)

The problems (1.1), (1.2) are discretized on the domain \( \Omega = [0,2] \times [0,2] \). We set \( f = 0 \) and prescribe Dirichlet boundary conditions, \( G = \{g_1, \ldots, g_K\} \). The coefficient \( a^e \) is defined for a given vector \( m^* \in \mathbb{R}^N \) by (4.8) using the partition \( \Omega_k = \left[ \frac{2(k-1)}{N}, \frac{2k}{N} \right] \times [0,2], 1 \leq k \leq N \).

In the following numerical experiments we use the \( K = 4 \) boundary conditions \( \{x^2, y^2, xy, (xy)^2\} \), and set the constants \( \epsilon = 1/60, H = 1/12, h = 1/256 \). The microscale problems (3.2) in HMM are solved on the subdomains \( I_\delta(x_l) = x_l + 3\epsilon I_d \). The projection operator \( \Pi^H \) is set to be convolution with a smoothing kernel. The optimization problems (4.5) – (4.7) are performed using the MATLAB \texttt{lsqnonlin} function. The error is computed using the formula \( \|m^* - \hat{m}\| \).

Error in recovered microscale inversion of (2.3):

| # unknowns | Analytic | HMM | Two-stage |
|------------|----------|-----|-----------|
| 1          | 0.01654417 | 0.02539143 | 0.10816459 |
| 2          | 0.09828509 | 0.08513511 | 0.16240264 |
| 3          | 0.10929754 | 0.10148560 | 0.27615110 |
| 4          | 0.11633237 | 0.10527977 | 0.32224688 |
| 5          | 0.17736705 | 0.15733702 | 0.42772383 |
| 6          | 0.42557205 | 0.18798622 | 0.38027366 |
B. Amplitude

| # unknowns | Analytic | HMM | Two-stage |
|------------|----------|-----|-----------|
| 1          | 0.01233656 | 0.01577666 | 0.01213464 |
| 2          | 0.01986943 | 0.02625374 | 0.12929148 |
| 3          | 0.04743092 | 0.05540454 | 0.32575215 |
| 4          | 0.07635345 | 0.06861825 | 0.48210484 |
| 5          | 0.36012401 | 0.36383803 | 0.55689244 |
| 6          | 0.52969666 | 0.54096046 | 0.73761752 |

C. Angle

| # unknowns | Analytic | HMM | Two-stage |
|------------|----------|-----|-----------|
| 1          | 0.03621115 | 0.04599242 | 0.04225760 |
| 2          | 0.05374923 | 0.06188072 | 0.14315285 |
| 3          | 0.07829441 | 0.09554321 | 0.26518266 |
| 4          | 0.06354117 | 0.06750427 | 0.24979234 |
| 5          | 0.26919343 | 0.28371626 | 1.39133602 |
| 6          | 0.48579157 | 0.49334067 | 0.70127957 |

These results for the inverse conductivity problem are important to other applications where surface measurements of a medium are used to describe characteristics of the interior. Similar model work in a variety of other areas, including exploration geophysics, mine and rock detection, and reservoir modeling. In the next sections we will explore numerical results corresponding to medical imaging and geophysics.

5. Medical imaging \((b^\varepsilon > 0)\)

Multiscale features play an important role in problems in most areas of science and engineering. An example we will consider is from [10]:

\[
\begin{align*}
- \nabla \cdot (a^\varepsilon(x, \lambda) \nabla u^\varepsilon) + \sigma(x, \lambda) u^\varepsilon &= 0 & x \in \Omega \\
u^\varepsilon &= g & x \in \partial\Omega.
\end{align*}
\]  

(5.1)

Here, \(\Omega \subset \mathbb{R}^d\) is a bounded, open domain with smooth boundary, \(a^\varepsilon\) and \(\sigma\) are diffusion and absorption coefficients that are dependent on the wavelength \(\lambda\). Denoting the Grüneisen coefficient (see [5, 6]) by \(\Gamma(x)\), the objective of qPAT is to recover \((a^\varepsilon, \sigma, \Gamma)\) from the observed data for a given number of illuminations \(g\). We will modify the numerical examples from [5, 6] by including microscale components.

Then, the wavelength dependent Grüneisen and absorption coefficients are (see Figure 3) are \(\sigma(x, \lambda) = \sum_{i=1}^{2} \beta_i(\lambda) \sigma_i\), \(\beta_1(\lambda) = \frac{\lambda}{\lambda_0}, \beta_2(\lambda) = \frac{\lambda}{\lambda_0^2}\). The wavelength diffusion coefficient is based on \(a^\varepsilon\) in (2.17) and (2.18), and is denoted \(a^\varepsilon(x, \lambda) = (\lambda/\lambda_0)^{3/2} a^\varepsilon(x)\). Observed data is of the form \(F(u, \nabla u, x) = \Gamma(x) \sigma(x) u(x)\), \(x \in \Omega\).

Because the explicit form of the effective coefficient is unknown, HMM is used as a forward solver. The Dirichlet data is of the form \(g_K\), for \(K = 1\) and three
wavelengths are used, \( \lambda_0 = .3, \lambda \in \Lambda := \{.2, .3, .4\} \). \( \epsilon = 1/60 \), \( H = 1/12 \), \( h = 1/256 \). Four illuminations are used for each wavelength.

**Table 1.** Error in recovered microscale inversion of (5.1) using FE-HMM.

| # unknowns | D. Cell wall thickness | E. Composition |
|------------|------------------------|----------------|
| 1          | 0.05368672             | 0.03365713     |
| 2          | 0.09809018             | 0.03679930     |
| 3          | 0.16055524             | 0.06666732     |
| 4          | 0.19781079             | 0.05148374     |
| 5          | 0.35063360             | 0.09036330     |
| 6          | 0.35667525             | 0.14959667     |

6. **Seismic waveform inversion \( (b^r < 0) \)**

Let \( \Omega = [0,2]^2 \). We consider the 2D variable coefficient Helmholtz equation

\[
\nabla \cdot (a(x)\nabla u) + \omega^2 u(x) = f(x) \quad x \in \Omega, \tag{6.1}
\]

where \( f(x) = \delta(x - x_s) \) represents a point source located at \( x_s \in \Omega \). We impose the boundary conditions

\[
a\nabla u \cdot n - iku = 0 \quad \text{on } \partial\Omega, \quad k = \omega a^{-1/2}.\]

In the numerical simulation, the parameters used are \( \epsilon = 1/100, H = 1/30, h = 1/512 \), and two wavelengths \( \omega \in \{.02\pi, 2\pi\} \). The following is a summary of the errors in microscale inversion of the effective model corresponding to (6.1).
Figure 4. Solutions to (6.1) for $\omega = .02\pi$ (left), $\omega = 2\pi$ (right) and $a = a^\epsilon$ in (2.7).

| N | A. Vol. frac. | B. Amp. | C. Angle |
|---|---------------|---------|----------|
|   | Analytic  | HMM     | Analytic | HMM     | Analytic | HMM     |
| 1 | 0.01600791 | 0.00479021 | 0.00383418 | 0.00565930 | 0.17015129 | 0.04220992 |
| 2 | 0.01818027 | 0.01594484 | 0.01319153 | 0.01619181 | 0.04816221 | 0.03141378 |
| 3 | 0.1408450 | 0.04590868 | 0.07428310 | 0.02316657 | 0.08764245 | 0.05826443 |
| 4 | 0.20210267 | 0.10937484 | 0.19077256 | 0.14657290 | 0.38442773 | 0.23623349 |
| 5 | 0.39181729 | 0.20548307 | 0.39831642 | 0.39190638 | 0.41889290 | 0.25488886 |
| 6 | 0.58806074 | 0.18695132 | 0.34706439 | 0.40082310 | 0.29390696 | 0.68871342 |

Remark 6.1. These techniques can be used to describe problems in reflection seismology. Here the representation of $m$ is of the form

$$m(x) = \sum_{k=1}^{N} \hat{m}_k \varphi_k(x).$$

(6.2)

where $\{\varphi_k\}$ is a spline basis.

Figure 5. Layered media example. Splines are used to model the angle, amplitude, and thickness of the layers. The discontinuities can be used to model faults in earths subsurface.
7. Conclusion

We presented in this paper theoretical and numerical techniques for solving inverse problems corresponding to multiscale partial differential equations. Such inverse problems are often reduced to well-posed problems through the use of effective forward models. Obtaining these models can result in the loss of microscale information due to averaging or homogenization. In our approach, we use effective forward models and constrain the search space to a low dimensional parameter space $m \in \mathbb{R}^N$. For higher dimensional $m$, other minimization techniques must be used, as for example, adjoint-state based methods in geophysical applications ([15]).

Using recovery results for inverse conductivity problems with special anisotropy [4], we prove for certain microstructure models, the Dirichlet-to-Neumann map corresponding to the effective equation uniquely determines a microscale parameter. We provided numerical justification that indicates that multiscale methods, such as the heterogeneous multiscale method (HMM) can be used to make forward predictions that prove useful in these microscale recovery problems, even when the explicit form of the effective equation is not known. We also provide results that demonstrate the performance of these techniques applied to models arising in medical imaging and exploration seismology.

Acknowledgements

This work has greatly benefited from discussions with Kui Ren and the expertise of Pingbing Ming and Fen Yang Tang. This research was supported in part by NSF grant DMS-1217203 and the Texas Consortium for Computational Seismology. CF was also supported in part by NSF grant DMS-1317015.

References

[1] A. Abdulle, W. E, B. Engquist, and E. Vanden-Eijnden, The heterogeneous multiscale method, Acta Numerica, 21 (2012), pp. 1–87.
[2] G. Alessandrini, Open issues of stability for the Inverse Conductivity Problem, Journal Inverse Ill-Posed Problems, 15 (2007), pp. 1–10.
[3] G. Alessandrini and E. Cabib, EIT and the average conductivity, J. Inverse Ill-Posed Probl, 15 (2008), pp. 1–10.
[4] G. Alessandrini and R. Gaburro, Determining conductivity with special anisotropy by boundary measurements, SIAM Journal on Mathematical Analysis, 33 (2001), pp. 153–171.
[5] G. Bal and K. Ren, Multi-source quantitative PAT in diffusive regime, Inverse Problems, 27 (2011), pp. 1–24.
[6] ———, On multi-spectral quantitative photoacoustic tomography in diffusive regime, Inverse Problems, 28 (2012), p. 025010.
[7] G. Bensoussan, Alain and Lions, Jacques Louis and Papanicolaou, Asymptotic Analysis for Periodic Structures, vol. 5 of Studies in Mathematics and its Applications, North-Holland Pub. Co.(Amsterdam and New York and New York), 1978.
[8] M. Desbrun, R. Donaldson, and H. Owhadi, Discrete geometric structures in homogenization and inverse homogenization with application to eit, arXiv preprint arXiv:0904.2601, (2009).
[9] W. E and B. Engquist, The heterogeneous multiscale methods, Communications in Mathematical Sciences, 1 (2003), pp. 87–132.
[10] J. Fish, V. Filonova, and S. Kuznetsov, *Micro-inertia effects in nonlinear heterogeneous media*, International Journal for Numerical Methods in Engineering, 91 (2012), pp. 1406–1426.

[11] V. V. Jikov, S. M. Kozlov, and O. A. Oleinik, *Homogenization of Differential Operators and Integral Functionals*, Springer, 2011.

[12] P. Ming and P. Zhang, *Analysis of the Heterogeneous Multiscale Method for Elliptic Homogenization Problems*, Journal of the American Mathematical Society, 18 (2005), pp. 121–156.

[13] G. Pavliotis and A. Stuart, *Multiscale Methods: Averaging and Homogenization*, vol. 53, Springer, 2008.

[14] G. Pavliotis, A. Stuart, and J. Nolen, *Multiscale modelling and inverse problems*, in Numerical Analysis of Multiscale Problems, R. Graham, Ivan G. and Hou, Thomas Y. and Lakkis, Omar and Scheichl, ed., Springer Berlin Heidelberg, 2012, pp. 1–34.

[15] R.-E. Plessix, *A review of the adjoint-state method for computing the gradient of a functional with geophysical applications*, Geophysical Journal International, 167 (2006), pp. 495–503.

[16] W. W. Symes, *The seismic reflection inverse problem*, Inverse Problems, 25 (2009).