Adaptive Modeling of Composite Structures:
Modeling Error Estimation
(1st edition)

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Abstract

The accurate simulation of the behavior of composite materials depends on many factors such as the character, size, topology, and mechanical properties of the microstructure, the definition of the domain of interest and the loads as well as the specification of accuracy desired and the goal of the simulation. There is, therefore, a need to develop a systematic technique to adaptively select the most appropriate scale that governs specific features of the response that are of interest. The concept of hierarchical modeling provides such a framework. In this approach, the accuracy of a given mathematical model, compared to a model of finer scale, is evaluated with the use of a posteriori estimates of the "modeling error" and these form the basis of an adaptive procedure.

This investigation focuses on the analysis of the equilibrium of linearly elastic heterogeneous bodies characterized by highly oscillatory elastic coefficients. The control of modeling error in such systems was studied in earlier works [37,32] using the HDPM : the Homogenized Dirichlet Projection Method. There, estimates of the error in the homogenized solutions in energy norms were used as a basis for an adaptive process of model selection. Following a brief review of the HDPM, we introduce an alternate method of model adaptation: the Hierarchical Adaptive Method for Model Enhancement and Refinement (HAMMER). In this method, we seek to generate a sequence of elasticity tensors such that the solutions they produce converge to the solution produced by the fine-scale microstructure.

We extend the theory of a posteriori estimation of modeling error to "quantities of interest", by which we mean local features of the response such as the average of stresses on material interfaces, boundary displacements, or mollified point-values of the displacement field, or any feature of the solution that can be characterized as a continuous linear functional on the space of functions to which the solution belongs. We establish computable upper and lower bounds on errors in such quantities of interest. This theory represents a significant departure from traditional error estimation techniques in that it enables the estimation of error in quantities such
as local displacements and displacement resultants such as interfacial strains and stresses. Preliminary results from 1-D numerical experiments demonstrating the effectiveness of the error estimates are given.

1 Introduction

Virtually all theories of heterogeneous media in mechanics and physics, including those pertaining to composite materials, involve (or support) mathematical models involving PDEs with rapidly oscillating coefficients. These spatial oscillations in coefficients may be non-periodic and may take place at scales small in comparison with characteristic lengths of the physical system under investigation. For many decades, it has been accepted as evident that the inclusion of such small-scale influences in the predictions of the global response of the system produces computational problems so large and complex that they cannot be resolved by available computing devices and procedures. Thus, averaging (homogenization) of these local properties has been viewed as a necessity. In the case of the elastostatics of composite materials, a considerable volume of work has been done on developing homogenization methods which accurately preserve certain global properties of the coefficients and large-scale features of the response.

There is a considerable volume of work on the computation of averaged properties of composites. Early works include those by Hill [20] and Hashin and Shtrikman [16–18]. A thorough survey of methods of analysis of composite materials, including a brief review of the history of this subject, can be found in [15]. Among texts on this subject, we mention those by Aboudi [1], Christensen [6], Herakovich [19] and Nemat-Nasser and Hori [29]. The concepts of Representative Volume Elements (RVEs) and Statistical Homogeneity (SH) have been the cornerstones of studies of overall properties of composites. These terms refer to representative samples of (e.g. unit cubes) of the material which exhibit properties “representative” of or “statistically equivalent” to the material as a whole. In [15], Hashin describes RVEs as being “large compared to typical phase region dimensions (e.g., fiber diameters and spacings).” Moreover, “in a SH composite, all global geometrical characteristics such as volume fractions, two-point correlations, etc. are the same in any RVE, irrespective of its position.” Additionally, “effective properties of a composite material define the relations between averages of field variables such as stress and strain” and “statistical homogeneity implies that body averages and RVE averages are the same.” However, it is well known that such RVEs do not exist for all composites and heterogeneous media. Moreover, even if an RVE were to be identified for a given composite material, no information about the local nature of field variables is provided by this approach (of computing overall properties).

Recently, some contemporary research has focused on developing fast and ef-
fective solution methods for direct micromechanical simulations. The tessellation-based Voronoi Cell Finite Element Method (VCFEM) has been proposed and studied in detail by Ghosh and coworkers [12,13]. In this method, heterogeneities are encapsulated in Voronoi Cells and these cells constitute the finite elements of the model. This method has been applied to both linear and nonlinear heterogeneous materials. Fu et al. [10] have studied the use of the Fast Multipole Method (FMM) for the boundary element solution of many particle problems. Meguid and Zhu [24] developed a special finite element for the analysis of heterogeneous materials with circular inclusions wherein element shape functions are supplemented by special Muskhelishvili functions. This approach of customizing the finite element basis functions has also been studied by Hou et al. [21,22] for elliptic problems with rough coefficients. In their multiscale finite element method (MFEM), basis functions are computed by solving the homogeneous version of the PDE at the element level with appropriate boundary conditions. The advantage that the MFEM has over the approach of Meguid and Zhu is that no restriction is placed on the shape of the inclusions. Cruz and Patera [7] have developed a parallel Monte-Carlo method to take into account possible randomness associated with the microstructure.

A related approach for treating heterogeneous media, developed in the late 1970s, is the method of homogenization of composites through asymptotic analysis; see Bensoussan et al. [5], Jikov et al. [23] and Sanchez-Palencia [34]. This approach assumes periodicity of microstructure. The computation of the homogenized properties of the composite are based upon the solution of periodic boundary value problems defined on a cell of the assumed period. A variety of mathematical results on the behavior of the homogenized solution as the size of the period becomes infinitesimally small can be found in the above works. The assumption of periodicity usually amounts to assuming an infinitely large composite body and ignores boundary layers in the case of finite domains. Asymptotic homogenization as an engineering tool has been explored by Kikuchi and coworkers [14,35]. As a first step toward accounting for microscale phenomena, these authors have used asymptotic corrections to enhance the homogenized solution. However, the proximity of the enhanced solution to the exact fine-scale solution is not explored. Such two-scale simulations have also been studied for elasto-plastic materials by Ghosh; Lee and Moorthy [11]. Fish and Belsky [8,9] have studied multigrid methods for the analysis of periodic heterogeneous media. Additional references to related work can be found in the references cited.

A rigorous approach for the analysis of periodic composite structures was presented by Morgan and Babuska [27,28,3] where equations of the type

\[-(a(x/\varepsilon)u'(x))' + b(x/\varepsilon)u(x) = f(x), \varepsilon\]

representing the size of a period, were analyzed using Fourier Transform ideas. The main features of their work are:

- A representation theorem for the solution \(u\) was developed in terms of \(\hat{f}\), the Fourier transform of the right hand side \(f\), and \(\phi(\varepsilon)\), the solution to a
local problem on a single cell. The function $\phi$ can be viewed as the Fourier transform of the Green's function of the operator $-\left(\frac{a(x/\varepsilon)}{(\cdot)^{1}} + b(x/\varepsilon)(\cdot)\right)$.

- Unlike classical asymptotic methods, $\varepsilon$ does not have to approach zero. However, results of asymptotic methods can be recovered as a special case of their results.
- One of the necessary conditions in their analysis is that the function $b(\cdot)$ be bounded below by a positive constant. This makes the approach unsuitable for elastostatics applications.

Existing literature on the analysis of heterogeneous materials is, generally speaking, divided into two general approaches. In one case, the scale of analysis (macro or micro) is selected \emph{a priori}. If the macro level is chosen, valuable microscale information is lost, whereas a direct microscale analysis of the macroscale problem is prohibitively expensive and, if at all possible, requires vast amounts of memory, storage and computational effort. For example, in the work of Babuska et al. [2], an accurate solution of a 2-D problem with roughly 1000 fibers requires $O(10^6)$ degrees of freedom. In the other case, two-scale analyses are performed by appealing to asymptotic homogenization and local corrections. The difficulty faced in this approach is that very restrictive assumptions are placed on the microstructure. These drawbacks suggest that the design of a successful methodology for the analysis of heterogeneous materials requires an adaptive selection of the scale of analysis in order to balance accuracy and computational cost.

Towards this end, the concept of hierarchical modeling was introduced by Oden and Zohdi in [37,32,36] as a methodology that provides a multilevel description of the physical phenomenon of interest based, when possible, on mathematical characterizations of the class of problems of interest. A hierarchy of descriptions of the physics of the problem is first set up, ranging from a coarse (long wave-length) description to the most detailed description contained in the class of models. Rather than heuristically choose a level of description from the hierarchy, \emph{a-posteriori} estimates of the modeling error associated with a particular description are derived and evaluated to enable the adaptive selection of a suitable characterization.

Based on this concept, a domain-decomposition method known as the Homogenized Dirichlet Projection Method (HDPM) has been developed [37,32]. In this method, the model at the coarsest level in the hierarchy is characterized by homogenized material properties and this is referred to as the homogenized problem. The adequacy of the solution to this homogenized problem, compared to the fine-scale solution, is then estimated using \emph{a-posteriori} modeling error estimates. In regions where the modeling error exceeds a preset tolerance, a finer-scale model is used and a correction to the homogenized solution is computed. Further studies on hierarchical modeling and HDPM have been carried out in [25,26,30,31]. We propose an alternate method of model adaptation that we refer to as the Hierarchical Adaptive Method for Model
Enhancement and Refinement (HAMMER). Our approach here is to generate a sequence of elasticity tensors such that the resultant sequence of solutions converges to the fine-scale solution. This method is described in detail later on in this work.

Interestingly, for a given preset tolerance, the final model resulting from the HDPM or any other adaptive modeling method depends on the definition of the error and the norm (or some other measure) used to quantify the error. Thus the choice of the error measure defines the goal of the simulation and different goals may well produce different models of the material and the associated boundary value problem. A principal contribution of the present paper is the establishment of a posteriori estimates of the error predicted by various coarse-scale models, particularly, the "homogenized" model, in "quantities of interest." The term "quantity of interest" signals the fact that we seek estimates of local quantities such as local strains, stresses, displacements, etc., rather than estimates in global energy norms as was done in [37,32,36]. Mathematically, we characterize such quantities as continuous linear functionals on the space of functions to which the fine-scale solution belongs. If the quantity of interest cannot be characterized by a continuous linear functional, we use regularization methods (e.g., mollification) to produce tractable approximations.

With estimates of errors of specific quantities of interest in hand, goal-oriented adaptive processes can be developed. In other words, the mathematical model of the material can be adaptively defined so as to deliver values of the quantities of interest, the accuracy of which meets certain preset error tolerances. An important feature of our theorems on estimation of modeling error is that we can derive upper and lower bounds on the modeling error in quantities of interest.

The outline of the presentation in this paper is as follows. We first present some preliminaries and notation and set up the model class of problems under consideration. In Section 3, we review, following [37] and [32], energy estimates of the error associated with the homogenized solution. We then present the theory for the estimation of the homogenization error in quantities of interest described by linear functionals on the space of admissible displacements. In Section 5, we describe the Homogenized Dirichlet Projection Method (HDPM) and the Hierarchical Adaptive Method for Model Enhancement and Refinement (HAMMER). Finally, we present results from one-dimensional numerical experiments on the performance of the various modeling error estimates. Numerical experiments illustrating model adaptivity in two dimensions will be presented in a forthcoming revised version of this paper.
2 Preliminaries

We begin with a mathematical characterization of a class of linear models of elastostatic deformation of heterogeneous elastic bodies. Let $\Omega \subset \mathbb{R}^N$, $N = 1, 2, 3$, denote an open bounded domain with a piecewise smooth boundary which is the region in space occupied by a material body. As usual, $H^1(\Omega)$ stands for the space of functions with distributional derivatives of order $\leq 1$ in $L^2(\Omega)$. Let $H^1(\Omega) \overset{\text{def}}{=} (H^1(\Omega))^N$ and $L^2(\Omega) \overset{\text{def}}{=} (L^2(\Omega))^N$ with the usual norms.

The body is assumed to be in static equilibrium under the action of body forces $f \in L^2(\Omega)$ and tractions $t \in L^2(\Gamma_t)$, where $\Gamma_t \subset \partial \Omega$. Zero displacements are prescribed on $\Gamma_u = \partial \Omega \setminus \Gamma_t$. Next, the body is assumed to be characterized by an elasticity tensor $E \in (L^\infty(\Omega))^{N^2 \times N^2}$ which satisfies the standard uniform ellipticity and symmetry conditions: $\exists \alpha_l, \alpha_u > 0$ such that $\forall A \in \mathbb{R}^{N \times N}$, $A = A^T$,

$$\alpha_l A : A \leq A : E(x)A \leq \alpha_u A : A, \quad \text{a.e. in } \Omega,$$

$$E_{ijkl} = E_{jikl} = E_{ijlk} = E_{klij} \quad 1 \leq i, j, k, l \leq N. \quad (1)$$

It is understood that $E$ is a highly oscillatory function of position $x$ over $\Omega$, not necessarily periodic. Then, according to the principle of virtual work, the elastostatics problem is characterized as follows:

\[
\begin{aligned}
\text{Find } u \in V(\Omega) \text{ such that } \\
B(u, v) = F(v) \quad \forall v \in V(\Omega), \\
\end{aligned}
\]

where the space of admissible functions $V(\Omega)$ is defined as

$$V(\Omega) \overset{\text{def}}{=} \{ v : v \in H^1(\Omega), v|_{\Gamma_u} = 0 \}. \quad (3)$$

The bilinear and linear forms in (2) are defined as

$$B(u, v) \overset{\text{def}}{=} \int_\Omega \nabla v : E \nabla u \, dx = \int_\Omega \text{tr} \left[ (\nabla v)^T E \nabla u \right] \, dx \quad (4)$$

and

$$F(v) = \int_\Gamma t \cdot v \, d\Gamma.$$
\[ \mathcal{F}(\nu) \overset{\text{def}}{=} \int_{\Omega} f \cdot \nu \, dx + \int_{\Gamma_t} t \cdot \nu \, ds. \]  

Under the stated assumptions, it is easily shown that (2) possesses a unique solution \( u \in V(\Omega) \). We shall refer to (2) as the fine-scale problem and to its solution \( u \) as the fine-scale solution.

The fine-scale problem can be made more amenable to computation through standard homogenization processes whereby \( E \) is replaced by a function \( E^0 \), often a constant, that is designed to characterize the macroscopic behavior of the structure. In the case of periodic media, asymptotic homogenization theory \([34,5]\) leads to local problems posed on a unit cell. The solutions to these local problems form the basis for computing the homogenized properties. In the case of non-periodic media, bounds on overall properties (the Hashin-Shtrikman bounds, for example) can be used to construct a homogenized material tensor. Assuming the homogenized material tensor also satisfies standard uniform ellipticity and symmetry conditions such as (1) (with different constants \( \alpha^0_t, \alpha^0_u \)), the homogenized problem reads

3 Analysis of the Modeling Error

The homogenized solution \( u^0 \) is obviously in error because material information is lost due to the process of homogenization. The homogenization or modeling error is defined as the difference between the fine-scale solution and the homogenized solution,
Here, we present upper and lower bounds in the energy norm of the homogenization error. The derivations of upper bounds in the energy norm follows [37].

### 3.1 Further Notation

We introduce additional notation for the definitions of the error estimates. The energy norm of a function \( v \in V(\Omega) \) is defined as

\[
\|v\|_{E(\Omega)} = B(v, v)^{1/2}
\]

where \( B : V(\Omega) \times V(\Omega) \to \mathbb{R} \) is defined in (4). Next, we define the inner product space

\[
L^2_{\text{sym}}(\Omega) \overset{\text{def}}{=} \{ A \in [L^2(\Omega)]^{N \times N} : A^T = A \},
\]

with the inner product

\[
((A, B)) = \int_{\Omega} A : B \, dx.
\]

The elasticity operator \( E \in [L^\infty(\Omega)]^{N^2 \times N^2} \) can be viewed as a \( L^2_{\text{sym}}(\Omega) \)-map and, with the stated assumptions of symmetry and uniform ellipticity on \( E \), we can define the following weighted inner product on \( L^2_{\text{sym}}(\Omega) \):

\[
((A, EB)) = ((E^T A, B)) = ((EA, B)).
\]

Also, under the stated assumptions, there exists \( E^{1/2} \in [L^\infty(\Omega)]^{N^2 \times N^2}, E^{1/2} : L^2_{\text{sym}}(\Omega) \to L^2_{\text{sym}}(\Omega) \) such that

\[
((A, EB)) = ((EA, B)) = ((E^{1/2} A, E^{1/2} B)).
\]
Finally, let

$$I_0 = (I - E^{-1} E^0).$$

(14)

Then, for $g \in V(\Omega)$, we define the associated linear residual functional $R_g : V(\Omega) \to \mathbb{R}$,

$$R_g(v) = -\int_\Omega \nabla v : E I_0 \nabla g \, dx, \quad v \in V(\Omega).$$

(15)

We repeatedly use the above functional throughout this work.

3.2 An energy estimate of the homogenization error

**Theorem 3.1** Let $u$ and $u^0$ be the solutions to problems (2) and (6) respectively. Then the following holds :

$$\zeta_{\text{low}} \leq \|e^0\|_E(\Omega) = \|u - u^0\|_E(\Omega) \leq \zeta_{\text{upp}},$$

(16)

where

$$\zeta_{\text{low}} \overset{\text{def}}{=} \frac{|R_{u^0}(u^0)|}{\|u^0\|_E(\Omega)}, \quad \zeta_{\text{upp}} \overset{\text{def}}{=} \left( (I_0 \nabla u^0, I_0 \nabla u^0) \right)_E^{1/2}. \quad (17)$$

**Proof.** The proof for the assertion $\|e^0\|_E(\Omega) \leq \zeta_{\text{upp}}$ can be found in [37] and is repeated here for completeness. First, it is seen that the modeling error $e^0$ satisfies

$$B(e^0, v) = R_{u^0}(v) = -\int_\Omega \nabla v : E I_0 \nabla u^0 \, dx, \quad \forall v \in V(\Omega).$$

(18)

We refer to the functional $R_{u^0}$ as the modeling residual. We see that
\[ \| e^0 \|_{E(\Omega)}^2 = B(e^0, e^0) = R_{u^0}(e^0) \]
\[ = - \int_{\Omega} \nabla e^0 : E I_o \nabla u^0 \, dx \]
\[ = - \int_{\Omega} E^2 \nabla e^0 : \frac{1}{2} I_o \nabla u^0 \, dx \]
\[ \leq \left\{ \int_{\Omega} E^2 \nabla e^0 : E^2 \nabla u^0 \, dx \right\}^{\frac{1}{2}} \]
\[ \leq \left\{ \int_{\Omega} \frac{1}{2} I_o \nabla u^0 : E^2 \nabla u^0 \, dx \right\}^{\frac{1}{2}} \]
\[ \leq \left\{ \int_{\Omega} \nabla e^0 : E \nabla u^0 \, dx \right\}^{\frac{1}{2}} \left\{ \int_{\Omega} I_o \nabla u^0 : E I_o \nabla u^0 \, dx \right\}^{\frac{1}{2}} \]
\[ \leq \| e^0 \|_{E(\Omega)} \sqrt{(I_o \nabla u^0, I_o \nabla u^0)}_E. \]

Next, it is straightforward to show that \( \| e^0 \|_{E(\Omega)} = \| R_{u^0} \|_{E'(\Omega)} \). But,

\[ \| R_{u^0} \|_{E'(\Omega)} \] \overset{\text{def}}{=} \sup_{v \in \mathcal{V}(\Omega) \setminus \{0\}} \frac{|R_{u^0}(v)|}{\| v \|_{E(\Omega)}} \geq \frac{|R_{u^0}(u^0)|}{\| u^0 \|_{E(\Omega)}}, \]

from which the assertion regarding the lower bound follows. \( \square \)

Thus, the homogenization error is bounded above and below by quantities that depend only on the homogenized solution \( u^0 \), the fine-scale microstructure \( E \), the homogenized elasticity tensor \( E^0 \) and the domain \( \Omega \).

**Remark 3.1** In the analysis presented here, it is nowhere assumed that \( E^0 \) is a constant. Thus the expression \( \zeta_{\text{low}} \leq \| e^0 \|_{E(\Omega)} \leq \zeta_{\text{upp}} \) is valid for any \( E^0 \) that is uniformly elliptic and symmetric.

### 4 Modeling Error in Quantities of Interest

Recent work in error estimation in the context of finite element analysis has focused on obtaining bounds on the numerical error in quantities of interest other than the energy norm [4,33]. In this section, we use a generalization of the approach of Prudhomme and Oden [33] to analyze the homogenization error in other quantities. We are interested in estimating \( L(e^0) = L(u) - L(u^0) \), where \( L \) is a continuous linear functional on \( \mathcal{V}(\Omega) \), \( L \in \mathcal{V}'(\Omega) \). For instance, \( L \) may represent something more localized than the global estimate (16), such as the average error in \( u \) or \( \nabla u \) over a small region in \( \Omega \). Some examples of linear functionals are
\[ L(v) = \int_\omega v \cdot n \, ds \] where \( \omega \subset \partial \Omega \) and \( n \) is the unit outward normal.

- \( L(v) = v(x_0), \, x_0 \in \Omega \) for one-dimensional problems.

Other examples can be found in the section on numerical examples later in this paper.

The first step in estimating \( L(e^0) \) is to relate the linear functional \( L \) to the source of the modeling error, i.e., the functional \( \mathcal{R}_{e^0} \). Toward this end, we assume the existence of an “influence function” \( w \) such that \( L(e^0) = \mathcal{R}_{e^0}(w) \) and using (18), we obtain \( L(e^0) = B(e^0, w) \). Noting that \( e^0 \in \mathcal{V}(\Omega) \), we pose the following global adjoint problem in order to obtain \( w \):

\[
\text{Find } w \in \mathcal{V}(\Omega) \text{ such that } \quad B(v, w) = L(v) \quad \forall v \in \mathcal{V}(\Omega) \tag{21}
\]

The adjoint problem (21) is of the same computational complexity as the original fine-scale problem (2) since both problems are governed by the same bilinear form. A natural way to simplify the adjoint problem is to pose the homogenized adjoint problem

\[
\text{Find } w^0 \in \mathcal{V}(\Omega) \text{ such that } \quad B^0(v, w^0) = L(v) \quad \forall v \in \mathcal{V}(\Omega) \tag{22}
\]

The solution to this homogenized adjoint problem will be referred to as the homogenized influence function. In what follows, we sometimes refer to the problems (2) and (6) as the primal fine-scale problem and primal homogenized problem, respectively. It is obvious that, under the stated assumptions on \( E \) and \( E^0 \), the functions \( w \) and \( w^0 \) exist and are uniquely defined.

It immediately follows that the modeling error in the influence function

\[
e^0 \overset{\text{def}}{=} w - w^0 \tag{23}
\]

satisfies

\[
B(v, e^0) = \mathcal{R}_{e^0}(v) \quad \forall v \in \mathcal{V}(\Omega) \tag{24}
\]
We also note that $\mathbf{e}^0$ satisfies the following relationship (analogous to (16)):

$$
\tilde{\zeta}_{\text{low}} \leq \| \mathbf{e}^0 \|_{E(\Omega)} = \| \mathbf{w}^0 - \mathbf{w}^0 \|_{E(\Omega)} \leq \tilde{\zeta}_{\text{upp}} 
$$

(25)

where

$$
\tilde{\zeta}_{\text{low}} \overset{\text{def}}{=} \frac{|\mathcal{R}_{\mathbf{w}^0}(\mathbf{w}^0)|}{\| \mathbf{w}^0 \|_{E(\Omega)}}, \quad \tilde{\zeta}_{\text{upp}} \overset{\text{def}}{=} \left( \langle \mathcal{I}_0 \nabla \mathbf{w}^0, \mathcal{I}_0 \nabla \mathbf{w}^0 \rangle \right)^{1/2} E.
$$

(26)

These preliminaries bring us to the following result:

**Theorem 4.1** Let $\mathbf{u}^0$ and $\mathbf{w}^0$ be the solutions to problems (6) and (22), respectively. Then,

$$
\eta_{\text{low}} \leq L(\mathbf{e}^0) \leq \eta_{\text{upp}}
$$

(27)

where

$$
\eta_{\text{low}} \overset{\text{def}}{=} \frac{1}{4} (\eta_{\text{low}}^+)^2 - \frac{1}{4} (\eta_{\text{upp}}^-)^2 + \mathcal{R}_{\mathbf{u}^0}(\mathbf{w}^0),
$$

(28)

$$
\eta_{\text{upp}} \overset{\text{def}}{=} \frac{1}{4} (\eta_{\text{upp}}^+)^2 - \frac{1}{4} (\eta_{\text{low}}^-)^2 + \mathcal{R}_{\mathbf{w}^0}(\mathbf{w}^0),
$$

(29)

with arbitrary $s \in \mathbb{R}^+$,

$$
\eta_{\text{upp}}^\pm \overset{\text{def}}{=} \sqrt{s^2 \tilde{\zeta}_{\text{upp}}^2 + 2 \langle \mathcal{I}_0 \nabla \mathbf{u}^0, \mathcal{I}_0 \nabla \mathbf{w}^0 \rangle} + s \tilde{\zeta}_{\text{upp}}^2,
$$

(30)

and

$$
\eta_{\text{low}}^\pm \overset{\text{def}}{=} \frac{|\mathcal{R}_{\mathbf{u}^0 \pm s \mathbf{w}^0}(\mathbf{u}^0 + \theta^\pm \mathbf{w}^0)|}{\| \mathbf{u}^0 + \theta^\pm \mathbf{w}^0 \|_{E(\Omega)}},
$$

(31)

where $\zeta_{\text{upp}}$ and $\tilde{\zeta}_{\text{upp}}$ are defined by (17) and (26), respectively, and $\theta^\pm$ is chosen so as to maximize $\eta_{\text{low}}^\pm$. 

12
PROOF. The error in the quantity of interest can be decomposed as

\[ L(e^0) = B(e^0, w) = B(e^0, e^0) + B(e^0, w^0) \]

\[ = B(se^0, s^{-1}e^0) + R_{u^0}(w^0), \quad (32) \]

where \( s \in \mathbb{R}^+ \) is an, as yet, unspecified positive scaling factor. Now, using a simple property of an inner product, we rewrite the expression (32) as

\[ L(e^0) = \frac{1}{4} \| se^0 + s^{-1}e^0 \|_{E(\Omega)}^2 - \frac{1}{4} \| se^0 - s^{-1}e^0 \|_{E(\Omega)}^2 + R_{u^0}(w^0). \quad (33) \]

The first two terms on the right hand side of (33) can be bounded above by noting that the quantity \( se^0 \pm s^{-1}e^0 \) satisfies

\[ B(se^0 \pm s^{-1}e^0, v) = R_{su^0 \pm s^{-1}w^0}(v), \quad \forall \ v \in V(\Omega), \quad (34) \]

and hence (in the spirit of Theorem 3.1),

\[ \| se^0 \pm s^{-1}e^0 \|_{E(\Omega)} \leq \eta^\pm_{\text{upp}}, \quad (35) \]

with,

\[ \eta^\pm_{\text{upp}} \overset{\text{def}}{=} \left\{ \int_{\Omega} \nabla (su^0 \pm s^{-1}w^0) : \nabla (su^0 \pm s^{-1}w^0) \right\}^{1/2} \]

\[ = \left\{ s^2_{\text{supp}} \pm 2((\mathcal{I}_0 \nabla u^0, \mathcal{I}_0 \nabla w^0))_E + s^{-2} \tilde{c}^2_{\text{supp}} \right\}^{1/2}. \quad (36) \]

To obtain a lower bound on the quantity \( se^0 \pm s^{-1}e^0 \), we note that

\[ \| se^0 \pm s^{-1}e^0 \|_{E(\Omega)} = \| R_{su^0 \pm s^{-1}w^0} \|_{E'(\Omega)} \geq \frac{|R_{su^0 \pm s^{-1}w^0}(v)|}{\|v\|_{E(\Omega)}}, \quad (37) \]

for any \( v \in V(\Omega) \setminus \{0\} \). In order to obtain the best possible lower bound, we use a linear combination of \( u^0 \) and \( w^0 \) of the form \( v = u^0 + \theta^\pm w^0 \), \( \theta^\pm \in \mathbb{R} \), in the above expression. By a simple extremization process, we find that the value
\[ \theta^\pm = \frac{B(u^0, w^0)R_{u^0}(su^0 \pm s^{-1}w^0) - B(u^0, u^0)R_{w^0}(su^0 \pm s^{-1}w^0)}{B(u^0, w^0)R_{w^0}(su^0 \pm s^{-1}w^0) - B(w^0, w^0)R_{u^0}(su^0 \pm s^{-1}w^0)} \]  

(38)

maximizes \( |R_{su^0 \pm s^{-1}w^0}(u^0 + \theta^\pm w^0)|/\|u^0 + \theta^\pm w^0\|_{E(\Omega)} \) and hence

\[ \|s\varepsilon^0 \pm s^{-1}\varepsilon^0\|_{E(\Omega)} \geq \eta_{\text{low}}^\pm \overset{\text{def}}{=} \frac{|R_{su^0 \pm s^{-1}w^0}(u^0 + \theta^\pm w^0)|}{\|u^0 + \theta^\pm w^0\|_{E(\Omega)}} \]  

(39)

with \( \theta^\pm \) given by (38). Note that this value of \( \theta^\pm \) is computable since it depends only on the homogenized solutions \( u^0 \) and \( w^0 \) and the material tensors \( E \) and \( E^0 \). The third term \( R_{w^0}(w^0) \) is seen to be exactly computable for the same reason.

**Remark 4.1** The scaling factor \( s \) is designed to balance the contributions of the primal (original) and adjoint problems to the modeling error in \( L \). It can be easily shown that the value

\[ s^* = \sqrt{\frac{\|\varepsilon^0\|_{E(\Omega)}}{\|\varepsilon^0\|_{E(\Omega)}}} \]  

(40)

is optimal in the sense that it minimizes the quantities \( \|s\varepsilon^0 + s^{-1}\varepsilon^0\|_{E(\Omega)} \) and \( \|s\varepsilon^0 - s^{-1}\varepsilon^0\|_{E(\Omega)} \). But, this optimal scaling factor \( s^* \) cannot be computed exactly since the modeling errors \( \varepsilon^0 \) and \( \varepsilon^0 \) are not known exactly. Hence, in our numerical experiments, we use

\[ s^* = \sqrt{\frac{\zeta_{\text{upp}}}{\zeta_{\text{upp}}}} \]  

(41)

as the upper bounds (16) and (25) have been observed to provide exceptionally accurate estimates of the modeling errors in the primal and adjoint solutions, respectively.

**Remark 4.2** From (33), we could propose the following estimates of the modeling error in the quantity of interest:

\[ L(e^0) \approx \eta_{\text{est,uppf}} \overset{\text{def}}{=} \frac{1}{4}(\eta_{\text{uppf}}^+)^2 - \frac{1}{4}(\eta_{\text{uppf}}^-)^2 + R_{w^0}(w^0), \]  

(42)
and

\[ L(e^0) \approx \eta_{\text{est,low}} \overset{\text{def}}{=} \frac{1}{4}(\eta_{\text{low}}^+)^2 - \frac{1}{4}(\eta_{\text{low}}^-)^2 + \mathcal{R}_{u^0}(w^0). \]  

(43)

Evidently, the accuracy of the bounds (27) and the estimates (42) and (43) of the modeling error in a given quantity of interest depends on the accuracy of the estimates \( \eta_{\text{low}}^+ \) and \( \eta_{\text{app}}^\pm \). This issue is addressed in more detail in Section 6.2.

5 Adaptive Modeling Methods

5.1 A Review of the Homogenized Dirichlet Projection Method (HDPM)

The Homogenized Dirichlet Projection Method is an adaptive non-overlapping domain decomposition scheme designed to improve the homogenized solution \( u^0 \) by posing local problems that take the fine-scale microstructure into account. This process is based on rigorous \textit{a posteriori} estimates of the energy error and is briefly described in this section.

We consider a non-overlapping partition \( \mathcal{P} \) of the domain \( \Omega \) into subdomains \( \Theta_k, k = 1 \ldots N(\mathcal{P}) \). The boundary \( \partial \Theta_k \) of each subdomain \( \Theta_k \) consists of a portion \( \Gamma_{kt} \) on which tractions are prescribed and a portion \( \Gamma_{ku} \) on which displacements are prescribed: \( \Gamma_{kt} = \Gamma_t \cap \partial \Theta_k, \Gamma_{ku} = \partial \Theta_k \setminus \Gamma_{kt} \).

Local function spaces are defined as

\[ V(\Theta_k) \overset{\text{def}}{=} \{ v : v \in V(\Omega), v|_{\Omega \setminus \Theta_k} = 0, v|_{\Gamma_{ku}} = 0 \}. \]  

(44)

The restriction of the homogenized solution to each subdomain is defined as \( u^0_k \overset{\text{def}}{=} u^0|_{\Theta_k} \). We denote by \( \hat{u}_k \) the solution to the following boundary value problem:

Find \( \hat{u}_k \in \{ u_k^0 \} + V(\Theta_k) \) such that

\[ B_k(\hat{u}_k, v_k) = F_k(v_k) \quad \forall v_k \in V(\Theta_k), \]  

(45)

for \( 1 \leq k \leq N(\mathcal{P}) \) with
We observe that the homogenized solution is used as Dirichlet data on the $\Gamma_{ku}$ portion of each subdomain's boundary. In particular, this data is used on the interior part of each subdomain's boundary given by $\partial \Theta \setminus \partial \Omega$. Finally, a global solution is constructed from the local solutions in the following manner:

\[
\text{\tilde{u}} \equiv u^0 + \sum_{k=1}^{N(P)} \mathcal{E}_k(\text{\tilde{u}}_k - u^0_k), \quad \tilde{u} \in V(\Omega),
\]

where $\mathcal{E}_k$ is an extension operator defined as $\mathcal{E}_k : V(\Theta_k) \ni v_k \rightarrow v \in V(\Omega)$, $v|_{\Theta_k} \equiv v_k$, $v|_{\partial \Theta \setminus \partial \Omega} = 0$. The function $\text{\tilde{u}}$ is referred to as the HDPM solution and the following result from [32] guarantees that the HDPM solution is indeed an improved solution.

**Theorem 5.1** Let $J(v) \equiv \frac{1}{2}B(v, v) - F(v)$ be the potential energy of $v \in V(\Omega)$. Then, $J(\text{\tilde{u}}) \leq J(u^0)$, and hence, $\|u - \text{\tilde{u}}\|_{E(\Omega)} \leq \|u - u^0\|_{E(\Omega)}$. □

The following result provides an upper bound on the difference between the fine-scale solution $u$ and the HDPM solution $\text{\tilde{u}}$.

**Corollary 5.1** Assume that $\nabla \cdot (E \nabla \text{\tilde{u}}_k), f \in H^{-1}(\Theta_k)$ and $(E \nabla \text{\tilde{u}}_k) \cdot n \in H^{-1/2}(\Gamma_{ku})$. Then, $\|u - \text{\tilde{u}}\|_{E(\Omega)} \leq \psi_{upp} \equiv \{2(J(\text{\tilde{u}}) - J(u^0)) + \epsilon_{upp}^2\}^{1/2}$. □

It can be seen that the term $(J(\text{\tilde{u}}) - J(u^0))$ is negative so that $\psi_{upp} \leq \epsilon_{upp}$ always. The next result is a sensitivity property that is very useful in selecting the subdomains on which the local problem (45) needs to be solved:

**Corollary 5.2** Let $I_0$ be as defined in (14). Then, for $1 \leq k \leq N(P)$, $\|\text{\tilde{u}}_k - u^0_k\|_{E(\Theta_k)} \leq \zeta_{k,upp} \equiv \{(\int_{\Theta_k} I_0 \nabla u^0 : E I_0 \nabla u^0\, dx)^{1/2}\}$. □

Proofs of the above statements and an adaptive algorithm designed to reduce the error in the energy norm between the fine-scale and HDPM solutions, by selectively solving the local problem (45), can be found in [32].

### 5.2 The Hierarchical Adaptive Method for Model Enhancement and Refinement (HAMMER)

In this section, we present a new method for adaptive model selection and refinement, and reduction of the modeling error. Our approach here is to
generate a sequence of elasticity tensors $E^{(i)}$ that are uniformly elliptic and symmetric so that the solutions $u^{(i)}$ they generate converge to the fine-scale solution $u$. First, without going into the details of how such a sequence is generated, we make the following observations.

- For a given $E^{(i)}$, let $u^{(i)} \in V(\Omega)$ be such that

\[
B^{(i)}(u^{(i)}, v) \overset{\text{def}}{=} \int_\Omega \nabla v : E^{(i)} \nabla u^{(i)} \, dx = F(v) \quad \forall v \in V.
\]

(48)

- Let the modeling error in $u^{(i)}$ be defined as $e^{(i)} \overset{\text{def}}{=} u - u^{(i)}$. It then follows from Sections 3 and 4 that the modeling error $e^{(i)}$ satisfies the equation

\[
B(e^{(i)}, v) = R_{u^{(i)}}(v) \quad \forall v \in V,
\]

(49)

and can be bounded above and below in the energy norm

\[
\zeta^{(i)}_{\text{low}} \leq \|e^{(i)}\|_{E(\Omega)} = \|u - u^{(i)}\|_{E(\Omega)} \leq \zeta^{(i)}_{\text{upp}},
\]

(50)

where,

\[
\zeta^{(i)}_{\text{low}} \overset{\text{def}}{=} \frac{|R_{u^{(i)}}(u^{(i)})|}{\|u^{(i)}\|_{E(\Omega)}}, \quad \zeta^{(i)}_{\text{upp}} \overset{\text{def}}{=} \left( (\mathcal{I}^{(i)} \nabla u^{(i)}, \mathcal{I}^{(i)} \nabla u^{(i)})_E \right)^{1/2},
\]

(51)

and $\mathcal{I}^{(i)} \overset{\text{def}}{=} I - E^{-1} E^{(i)}$.

- Given a quantity of interest expressed as a continuous linear functional $L \in V'(\Omega)$, let $w^{(i)} \in V(\Omega)$ be such that

\[
B^{(i)}(v, w^{(i)}) = L(v) \quad \forall v \in V,
\]

(52)

and define $\tilde{e}^{(i)} \overset{\text{def}}{=} w - w^{(i)}$. Then, $\tilde{e}^{(i)}$ satisfies the equation

\[
B(v, \tilde{e}^{(i)}) = R_{w^{(i)}}(v) \quad \forall v \in V,
\]

(53)

and can be bounded above and below in the energy norm

\[
\tilde{\zeta}^{(i)}_{\text{low}} \leq \|\tilde{e}^{(i)}\|_{E(\Omega)} = \|w - w^{(i)}\|_{E(\Omega)} \leq \tilde{\zeta}^{(i)}_{\text{upp}},
\]

(54)

where,
\[ \zeta_{\text{low}}^{(i)} \overset{\text{def}}{=} \frac{|\mathcal{R}_{\mathbf{w}^{(i)}}(\mathbf{w}^{(i)})|}{\|\mathbf{w}^{(i)}\|_{E(\Omega)}}, \quad \zeta_{\text{upp}}^{(i)} \overset{\text{def}}{=} \left( \left( \mathcal{I}^{(i)} \nabla \mathbf{w}^{(i)}, \mathcal{I}^{(i)} \nabla \mathbf{w}^{(i)} \right) \right)_{E}^{1/2}. \] (55)

- The modeling error in this quantity of interest \( L \) can be bounded above and below

\[ \eta_{\text{low}}^{(i)} \leq L(\mathbf{e}^{(i)}) \leq \eta_{\text{upp}}^{(i)} \] (56)

where

\[ \eta_{\text{low}}^{(i)} \overset{\text{def}}{=} \frac{1}{4} (\eta_{\text{low}}^{(i)})^2 - \frac{1}{4} (\eta_{\text{upp}}^{(i)})^2 + \mathcal{R}_{u^{(i)}}(\mathbf{w}^{(i)}), \]
\[ \eta_{\text{upp}}^{(i)} \overset{\text{def}}{=} \frac{1}{4} (\eta_{\text{upp}}^{(i)})^2 - \frac{1}{4} (\eta_{\text{low}}^{(i)})^2 + \mathcal{R}_{u^{(i)}}(\mathbf{w}^{(i)}), \] (57)

\[ \eta_{\text{upp}}^{\pm(i)} \overset{\text{def}}{=} \sqrt{s^2 (\zeta_{\text{upp}}^{(i)})^2 + 2 \left( \left( \mathcal{I}^{(i)} \nabla u^{(i)}, \mathcal{I}^{(i)} \nabla \mathbf{w}^{(i)} \right) \right)_{E} + s^{-2} (\zeta_{\text{upp}}^{(i)})^2}, \] (58)

and

\[ \eta_{\text{low}}^{\pm(i)} \overset{\text{def}}{=} \frac{\mathcal{R}_{su^{(i), \pm s^{-1}w}^{(i)}}(u^{(i)} \pm \theta_{\pm(i)}^{-1} w^{(i)})}{\|u^{(i)} \pm w^{(i)}\|_{E(\Omega)}}, \] (59)

with arbitrary \( s \in \mathbb{R}^+ \) and with \( \theta_{\pm(i)} \) obtained from (38) by replacing \( u^0 \) and \( w^0 \) with \( u^{(i)} \) and \( w^{(i)} \), respectively. The optimal value of the scaling factor \( s \) is given by

\[ s^* = \sqrt{\frac{\|\mathbf{e}^{(i)}\|_{E(\Omega)}}{\|\mathbf{e}^{(i)}\|_{E(\Omega)}}} \approx \sqrt{\frac{\zeta_{\text{low}}^{(i)}}{\zeta_{\text{upp}}^{(i)}}}. \] (60)

- Finally, the estimates of the modeling error in the quantity of interest proposed in Remark 4.2 are written as

\[ L(\mathbf{e}^{(i)}) \approx L_{\text{est,upp}}^{(i)} \overset{\text{def}}{=} \frac{1}{4} (\eta_{\text{upp}}^{(i)})^2 - \frac{1}{4} (\eta_{\text{low}}^{(i)})^2 + \mathcal{R}_{u^{(i)}}(\mathbf{w}^{(i)}), \]
\[ L(\mathbf{e}^{(i)}) \approx L_{\text{est,low}}^{(i)} \overset{\text{def}}{=} \frac{1}{4} (\eta_{\text{low}}^{(i)})^2 - \frac{1}{4} (\eta_{\text{upp}}^{(i)})^2 + \mathcal{R}_{u^{(i)}}(\mathbf{w}^{(i)}). \] (61)

Our approach towards generating a sequence \( \mathbf{E}^{(i)} \) of elasticity tensors is as follows: We begin with a sufficiently fine partition of the domain into non-overlapping subdomains and choose a homogenized elasticity tensor \( \mathbf{E}^0 \) as the first element of the sequence \( \mathbf{E}^{(i)} \), i.e., \( \mathbf{E}^{(0)} = \mathbf{E}^0 \). If the homogenized elasticity
tensor does not produce an acceptable solution, we change $E^0$ to $E$ locally on
the subdomains that contribute the most to the modeling error (according to
some error indicator). This results in a non-uniform material model, with the
exact microstructural representation in certain regions and the homogenized
model in the rest of the domain. This non-uniform characterization of the
material is denoted $E^{(1)}$ and used as the next element of the sequence of
elasticity tensors. We then solve (48) (this entails a global solve) to obtain
$u^{(1)}$, the next element of the sequence $u^{(i)}$. This process is repeated until the
global error tolerance is satisfied.

The advantage that the HAMMER has over the HDPM is that the homoge-
nized solution $u^0$ is used only to select the subdomains that need model refine-
ment and not to enforce boundary conditions. Thus, the final model generated
by this method is expected to show less dependence on the homogenized solu-
tion (the initial guess). Also, this method lends itself to easy iterative solution
since $u^{(i)}$ can be used as the initial guess to obtain $u^{(i+1)}$.

5.2.1 The HAMMER Algorithm

Step 1. Initialization. Given the initial data $\Omega$, $\Gamma_u$, $\Gamma_t$, $E$, $f$ and $t$, construct a
non-overlapping partition of the domain $P = \{ \Theta_k \}, k = 1, 2 \ldots N(P)$. Choose
a homogenized material tensor $E^0$. Specify error tolerance parameters $\alpha_{tol}$ and
$\beta_{tol}$.

Step 2. Begin Adaptive Loop. Set $E^{(0)} = E^0$ (the homogenized material prop-
erties), and for $i = 0, 1, \ldots$.

Step 3. Solution and Error Estimation. Compute $u^{(i)}$ by solving

$$B^{(i)}(u^{(i)}, v) = F(v) \quad \forall v \in V. \quad (62)$$

and compute

$$(\zeta_{k,upp}^{(i)})^2 = \sum_k (\zeta_{k,upp}^{(i)})^2 = \sum_k \int_{\Theta_k} T^{(i)} \nabla u^{(i)} : E T^{(i)} \nabla u^{(i)} \, dx \quad (63)$$

Step 4. Tolerance Test. If $\zeta_{k,upp}^{(i)} \leq \alpha_{tol} \|u^{(i)}\|_{E(\Omega)}$, STOP.

Step 5. Model Refinement. For $k = 1, 2 \ldots N(P)$, if

$$\zeta_{k,upp}^{(i)} > \beta_{tol} \left( \max_k (\zeta_{k,upp}^{(i)}) - \min_k (\zeta_{k,upp}^{(i)}) \right), \quad (64)$$

19
set \( E^{(i+1)}(x) = E(x), x \in \Theta_k \). Else, set \( E^{(i+1)}(x) = E^{(i)}(x), x \in \Theta_k \).

**Step 6. End Adaptive Loop.** Set \( i \leftarrow i + 1 \) and GOTO Step 3.

We now elaborate upon some of the steps in the above algorithm.

1. **Creation of a partition.** This is perhaps the most important step in the algorithm presented above and deserves further comment. The main goal of our approach is to use the microstructural representation of the material only when and where it is necessary. If the initial partition of the domain is too coarse, then the algorithm might lead to a material model that uses the fine-scale microstructure (almost) everywhere. On the other hand, if the initial partition is too fine (when the size of a subdomain approaches the microscale), then a large number of iterations may be needed to converge to the final material model.

Another important consideration in the creation of a partition of the domain is the numerical solution of the system of equations resulting from (48) due to, say, a finite element discretization. Typically, such problems cannot be solved on a workstation or a single-processor computer and require the use of parallel computers. The use of parallel machines usually requires a partition of the domain into subdomains (domain decomposition). Moreover, the complexity of the problem (48) changes at each iteration of the HAMMER, thus requiring the use of dynamic load balancing.

Of course, the numerical method that is used to solve (48) also plays a role in the partition of the domain. Different methods, e.g., \( h \), \( p \) or \( h-p \) finite element methods, POD methods, Fast Summation methods) introduce different constraints on the partitioning of the domain.

2. **Generation of \( E^0 \).** The homogenized elasticity tensor \( E^0 \) can be generated in several ways. For periodic media, the method of asymptotic analysis leads to a set of homogenized coefficients (see [34], Chap. 5). These coefficients are relatively inexpensive to compute since they only depend on the solution to an auxiliary problem posed on a unit-cell. For locally periodic media, this process can be carried out over each subdomain of the partition.

In the case of non-periodic media, one can, for instance, use the arithmetic average of the Hashin-Shtrikman bounds to generate \( E^0 \). For isotropic materials, the Hashin-Shtrikman bounds are functions of the Lamé parameters and volume fractions of the constituents. If the volume fractions of the constituents show considerable variation over the domain, a different \( E^0 \) can be generated for each subdomain.

3. **Selection of subdomains for model refinement.** In the algorithm presented above, we use an energy criterion (64) to select the subdomains that need model refinement. The criterion is designed such that whenever the global error tolerance is not met, at least one subdomain undergoes model refinement.
If the goal of the analysis is to reduce the error in a given quantity of interest \( L \in V'(\Omega) \), we note that

\[
|L(e^{(i)})| \leq |B(e^{(i)}, e^{(i)})| + |B(e^{(i)}, w^{(i)})| \\
\leq \|e^{(i)}\|_{E(\Omega)} \left( \|e^{(i)}\|_{E(\Omega)} + \|w^{(i)}\|_{E(\Omega)} \right) \\
\leq \zeta_{\text{up}}^{(i)} \left( \zeta_{\text{up}}^{(i)} + \|w^{(i)}\|_{E(\Omega)} \right),
\]

and hence the quantity \( \gamma_k = \zeta_{k,\text{up}}^{(i)} (\zeta_{\text{up}}^{(i)} + \|w^{(i)}\|_{E(\Omega)}) \) can be used as an error indicator in (64) in place of \( \zeta_{k,\text{up}}^{(i)} \).

(4) Solution schemes. The use of a non-uniform elasticity tensor, with the exact microstructure in some regions and the homogenized elasticity tensor in some regions, leads to a problem with disparate scales. The complexities associated with the numerical solution of such a problem, referred to sometimes as the problem of scale-bridging, are well known and a thorough study is in order.

6 Modeling Error Estimation: A One-dimensional Example

We study the performance of the various a posteriori estimators presented earlier for the following 1-D problem. Consider an elastic bar of unit length fixed at both ends and subjected to a constant body force. The primal fine-scale and homogenized problems are

\[-(E(x)u'(x))' = -1, u(0) = u(1) = 0 \quad \text{and} \quad -(E^o(x)u^o'(x))' = -1, u^o(0) = u^o(1) = 0.\]

The first linear functional we consider is

\[
L_1(v) = \int_a^b E' \, v' \, dx, \quad (a, b) = (0.75, 0.76),
\]

meaning that we are interested in the local (scaled) average value of the error in the stress in the given interval due to homogenization.

The second linear functional we consider is

\[
L_2(v) = v(x_0), \quad x_0 = 0.75.
\]

Here, we are interested in the pointwise value of the homogenization error.

The unit domain is partitioned into 10 equal subdomains and each subdomain is assumed to have 10 equal material intervals. For each interval, the material property is chosen at random to be either \( E = 1 \) or \( E = \tau \), where \( \tau \) is referred to as the mismatch ratio. Equal amounts of hard and soft material
are used. All of the following calculations are performed analytically. We use the harmonic average $\langle E^{-1} \rangle^{-1}$ as the homogenized modulus $E^0$ for both the primal and adjoint problems.

In the tables of values that follow, we use the exponential notation with four significant digits of the mantissa. The exponent is shown in parentheses.

6.1 Energy estimates of the modeling error

An effectivity index is a ratio of the estimated error to the actual error in various quantities. As a measure of the quality (effectivity) of a given a posteriori estimate, we introduce the following effectivity indices of the various energy estimates associated with the primal problem:

$$\lambda_{\text{low}} \overset{\text{def}}{=} \zeta_{\text{low}} / \|e^0\|_{E(\Omega)}, \quad \lambda_{\text{upp}} \overset{\text{def}}{=} \zeta_{\text{upp}} / \|e^0\|_{E(\Omega)},$$

$$\Lambda_{\text{upp}} \overset{\text{def}}{=} \psi_{\text{upp}} / \|u - \bar{u}\|_{E(\Omega)}, \quad \lambda_{k,\text{upp}} \overset{\text{def}}{=} \zeta_{k,\text{upp}} / \|\bar{u}_k - u^0_k\|_{E(\Theta_k)};$$

and the following associated with the adjoint problem:

$$\bar{\lambda}_{\text{low}} \overset{\text{def}}{=} \bar{\zeta}_{\text{low}} / \|e^0\|_{E(\Omega)}, \quad \bar{\lambda}_{\text{upp}} \overset{\text{def}}{=} \bar{\zeta}_{\text{upp}} / \|e^0\|_{E(\Omega)},$$

$$\bar{\lambda}^\pm_{\text{low}} \overset{\text{def}}{=} \bar{\eta}^\pm_{\text{low}} / \|s e^0 \pm s^{-1} e^0\|_{E(\Omega)}, \quad \bar{\lambda}^\pm_{\text{upp}} \overset{\text{def}}{=} \bar{\eta}^\pm_{\text{upp}} / \|s e^0 \pm s^{-1} e^0\|_{E(\Omega)}.$$  

Obviously, we hope that effectivity indices near unity can be obtained. Table 1 shows the effectivity indices for the energy estimates of the modeling error for the primal problem. We see that the upper estimates $\zeta_{\text{upp}}, \psi_{\text{upp}}$ and $\zeta_{k,\text{upp}}$ all perform remarkably well for all the mismatch ratios considered. Additionally, we note that the accuracy of the local sensitivity $\zeta_{k,\text{upp}}$ validates its use in Step 4 of the adaptive HDPM algorithm (see Section 5.3). The lower estimate $\zeta_{\text{low}}$, however, is seen to perform well only at higher mismatch ratios.

Next, we consider the performance of the energy estimates associated with the adjoint problems. Tables 2 and 3 show the effectivity indices for the adjoint problems defined by the functionals $L_1$ and $L_2$, respectively. For each linear functional, we show effectivity indices for the estimates $\bar{\zeta}_{\text{low}}$ and $\bar{\zeta}_{\text{upp}}$ as well as the estimates $\eta^\pm_{\text{low}}, \eta^\pm_{\text{upp}}, \eta_{\text{low}}$ and $\eta_{\text{upp}}$. Also, note that the last four estimates are evaluated for two cases. In one, no scaling is used or, equivalently, $s = s^{-1} = 1$ (recall Theorem 4.1). In the second case, we use the scaling factor $s = s^* \overset{\text{def}}{=} \sqrt{\bar{\zeta}_{\text{upp}} / \zeta_{\text{upp}}}$ (see Remark 4.1). The reason for considering the accuracy of the last four estimates will made be clear when we study the estimates of modeling error in the linear functionals $L_1$ and $L_2$. 

22
Table 1
Effectivity indices of upper and lower energy estimates of modeling error associated with the primal problem for the one-dimensional example.

<table>
<thead>
<tr>
<th>$\tau$</th>
<th>5</th>
<th>10</th>
<th>25</th>
<th>50</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda_{\text{low}}$</td>
<td>0.6866(0)</td>
<td>0.8306(0)</td>
<td>0.9288(0)</td>
<td>0.9638(0)</td>
<td>0.9817(0)</td>
</tr>
<tr>
<td>$\lambda_{\text{upp}}$</td>
<td>0.1008(1)</td>
<td>0.1004(1)</td>
<td>0.1002(1)</td>
<td>0.1001(1)</td>
<td>0.1000(1)</td>
</tr>
<tr>
<td>$\lambda_{k,\text{upp}}$ (min)</td>
<td>0.1000(1)</td>
<td>0.1000(1)</td>
<td>0.1000(1)</td>
<td>0.1000(1)</td>
<td>0.1000(1)</td>
</tr>
<tr>
<td>$\lambda_{k,\text{upp}}$ (max)</td>
<td>0.1137(1)</td>
<td>0.1085(1)</td>
<td>0.1039(1)</td>
<td>0.1021(1)</td>
<td>0.1010(1)</td>
</tr>
<tr>
<td>$\Lambda_{\text{upp}}$</td>
<td>0.1086(1)</td>
<td>0.1075(1)</td>
<td>0.1067(1)</td>
<td>0.1064(1)</td>
<td>0.1063(1)</td>
</tr>
</tbody>
</table>

Table 2
Effectivity indices of upper and lower energy estimates of modeling error associated with the adjoint problem $L_1$ for the one-dimensional example.

<table>
<thead>
<tr>
<th>$\tau$</th>
<th>5</th>
<th>10</th>
<th>25</th>
<th>50</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda_{\text{low}}$</td>
<td>0.9997(0)</td>
<td>0.9999(0)</td>
<td>0.1000(1)</td>
<td>0.1000(1)</td>
<td>0.1000(1)</td>
</tr>
<tr>
<td>$\lambda_{\text{upp}}$</td>
<td>0.1002(1)</td>
<td>0.1001(1)</td>
<td>0.1000(1)</td>
<td>0.1000(1)</td>
<td>0.1000(1)</td>
</tr>
</tbody>
</table>

$s = 1$

| $\lambda_{\text{low}}^+$ | 0.9497(0) | 0.9925(0) | 0.9995(0) | 0.9999(0) | 0.1000(1) |
| $\lambda_{\text{upp}}^+$ | 0.1005(1) | 0.1002(1) | 0.1001(1) | 0.1000(1) | 0.1000(1) |
| $\lambda_{\text{low}}^-$ | 0.9425(0) | 0.9920(0) | 0.9995(0) | 0.9999(0) | 0.1000(1) |
| $\lambda_{\text{upp}}^-$ | 0.1000(1) | 0.1000(1) | 0.1000(1) | 0.1000(1) | 0.1000(1) |

$s = s^*$

| $\lambda_{\text{low}}^+$ | 0.8574(0) | 0.9234(0) | 0.9679(0) | 0.9837(0) | 0.9918(0) |
| $\lambda_{\text{upp}}^+$ | 0.1008(1) | 0.1004(1) | 0.1002(1) | 0.1001(1) | 0.1000(1) |
| $\lambda_{\text{low}}^-$ | 0.8566(0) | 0.9055(0) | 0.9601(0) | 0.9797(0) | 0.9897(0) |
| $\lambda_{\text{upp}}^-$ | 0.1001(1) | 0.1001(1) | 0.1000(1) | 0.1000(1) | 0.1000(1) |

Again, it is seen that the upper estimates $\tilde{\zeta}_{\text{upp}}, \eta_{\text{upp}}^+$ and $\eta_{\text{upp}}^-$ display effectivity indices extremely close to unity. The performance of the lower bounds $\tilde{\zeta}_{\text{low}}$ shows a stronger dependence on the mismatch ratio and the linear functional under consideration. For instance, we see from Table 2 that for the linear functional $L_1$, $\tilde{\zeta}_{\text{low}}/\|\tilde{e}^0\|_{E(\Omega)} = 0.9997$, when $\tau = 5$. On the other hand, for the linear functional $L_2$, $\tilde{\zeta}_{\text{low}}/\|\tilde{e}^0\|_{E(\Omega)} = 0.7638$, when $\tau = 5$.

We expect that the effectivity index $\lambda_{\text{low}}^+ \overset{\text{def}}{=} \eta_{\text{low}}^+/\|se^0 \pm s^{-1}\tilde{e}^0\|_{E(\Omega)}$ will be closer to $\zeta_{\text{low}}/\|e^0\|_{E(\Omega)}$ or $\tilde{\zeta}_{\text{low}}/\|\tilde{e}^0\|_{E(\Omega)}$ depending on whether $se^0$ or $s^{-1}\tilde{e}^0$ is the dominant term. For the linear functional $L_1$, when $\tau = 5$, we find that $\|\tilde{e}^0\|_{E(\Omega)}/\|e^0\|_{E(\Omega)} = 2.214$ (with $s = 1$), whereas $\|s^{-1}\tilde{e}^0\|_{E(\Omega)}/\|se^0\|_{E(\Omega)} = \dots$
Table 3
Effectivity indices of upper and lower energy estimates of modeling error associated
with the adjoint problem $L_2$ for the one-dimensional example.

<table>
<thead>
<tr>
<th>$\tau$</th>
<th>5</th>
<th>10</th>
<th>25</th>
<th>50</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda_{\text{low}}$</td>
<td>0.7638(0)</td>
<td>0.8750(0)</td>
<td>0.9482(0)</td>
<td>0.9738(0)</td>
<td>0.9868(0)</td>
</tr>
<tr>
<td>$\lambda_{\text{upp}}$</td>
<td>0.1007(1)</td>
<td>0.1004(1)</td>
<td>0.1002(1)</td>
<td>0.1001(1)</td>
<td>0.1000(1)</td>
</tr>
</tbody>
</table>

$s = 1$

| $\lambda_{\text{low}}^+$ | 0.6779(0) | 0.8250(0) | 0.9262(0) | 0.9624(0) | 0.9810(0) |
| $\lambda_{\text{upp}}^+$ | 0.1002(1) | 0.1001(1) | 0.1000(1) | 0.1000(1) | 0.1000(1) |
| $\lambda_{\text{low}}^-$ | 0.7524(0) | 0.8686(0) | 0.9455(0) | 0.9724(0) | 0.9861(0) |
| $\lambda_{\text{upp}}^-$ | 0.1008(1) | 0.1004(1) | 0.1002(1) | 0.1001(1) | 0.1000(1) |

$s = s^*$

| $\lambda_{\text{low}}^+$ | 0.5683(0) | 0.7569(0) | 0.8947(0) | 0.9459(0) | 0.9726(0) |
| $\lambda_{\text{upp}}^+$ | 0.1000(1) | 0.1000(1) | 0.1000(1) | 0.1000(1) | 0.1000(1) |
| $\lambda_{\text{low}}^-$ | 0.7438(0) | 0.8636(0) | 0.9433(0) | 0.9713(0) | 0.9855(0) |
| $\lambda_{\text{upp}}^-$ | 0.1009(1) | 0.1005(1) | 0.1002(1) | 0.1001(1) | 0.1000(1) |

1.006, when scaling is used. As a consequence, the effectivity index $\lambda_{\text{low}}^+$ is
der lower (closer to the effectivity index $\zeta_{\text{low}}/\|e^0\|_{L^2(\Omega)}$) when scaling is used.

6.2 Modeling error in quantities of interest $L_1$ and $L_2$

Here, we examine the performance of the lower and upper bounds (27) and the
estimates (42) and (43) of the modeling error in quantities of interest $L_1$ and $L_2$
with $s = 1$ and $s = s^*$. For this purpose, we define $\eta_{\text{av}} = 1/2 (\eta_{\text{low}} + \eta_{\text{upp}})$, where
$\eta_{\text{low}}$ and $\eta_{\text{upp}}$ are defined in (28) and (29), respectively. Also, we introduce the
following effectivity indices:

\[
\gamma_{\text{low}} = \eta_{\text{low}}/L(e^0), \quad \gamma_{\text{upp}} = \eta_{\text{upp}}/L(e^0), \\
\gamma_{\text{av}} = \eta_{\text{av}}/L(e^0), \quad \gamma_{\text{est,upp}} = \eta_{\text{est,upp}}/L(e^0), \quad \gamma_{\text{est,low}} = \eta_{\text{est,low}}/L(e^0).
\]

In order to study the dependence of the above effectivity indices on the accu-
}racy of the various energy estimates presented earlier, we note that.
\[ \eta_{\text{low}} = \frac{1}{4}(\eta_{\text{low}}^+)^2 - \frac{1}{4}(\eta_{\text{low}}^-)^2 + \mathcal{R}_w(0), \]

\[ = \frac{1}{4}(\lambda_{\text{low}}^+ \|sE^0\|_{E(\Omega)})^2 - \frac{1}{4}(\lambda_{\text{upp}}^- \|sE^0 - s^{-1}E^0\|_{E(\Omega)})^2 + \mathcal{R}_w(0), \]

\[ L(e^0) \]

\[ = \frac{1}{4}\|sE^0 + s^{-1}E^0\|_{E(\Omega)}^2 - \frac{1}{4}\|sE^0 - s^{-1}E^0\|_{E(\Omega)}^2 + \mathcal{R}_w(0) \]

\[ - \frac{1}{4}(1 - (\lambda_{\text{low}}^+)^2)\|sE^0 - s^{-1}E^0\|_{E(\Omega)}^2 \]

\[ - \frac{1}{4}(\lambda_{\text{upp}}^-)^2 - 1\|sE^0 - s^{-1}E^0\|_{E(\Omega)}^2, \]

and hence,

\[ \gamma_{\text{low}} = 1 - \frac{1}{4}(1 - (\lambda_{\text{low}}^+)^2)\|sE^0 + s^{-1}E^0\|_{E(\Omega)}^2 / L(e^0) \]

\[ - \frac{1}{4}(\lambda_{\text{upp}}^-)^2 - 1\|sE^0 - s^{-1}E^0\|_{E(\Omega)}^2 / L(e^0). \]

(72)

Similarly,

\[ \gamma_{\text{upp}} = 1 + \frac{1}{4}(\lambda_{\text{upp}}^+)^2 - 1\|sE^0 + s^{-1}E^0\|_{E(\Omega)}^2 / L(e^0) \]

\[ + \frac{1}{4}(1 - (\lambda_{\text{low}}^+)^2)\|sE^0 - s^{-1}E^0\|_{E(\Omega)}^2 / L(e^0), \]

(73)

\[ \gamma_{\text{est, low}} = 1 - \frac{1}{4}(1 - (\lambda_{\text{low}}^+)^2)\|sE^0 + s^{-1}E^0\|_{E(\Omega)}^2 / L(e^0) \]

\[ + \frac{1}{4}(1 - (\lambda_{\text{low}}^-)^2)\|sE^0 - s^{-1}E^0\|_{E(\Omega)}^2 / L(e^0), \]

(74)

and

\[ \gamma_{\text{est, upp}} = 1 + \frac{1}{4}(\lambda_{\text{upp}}^+)^2 - 1\|sE^0 + s^{-1}E^0\|_{E(\Omega)}^2 / L(e^0) \]

\[ - \frac{1}{4}(\lambda_{\text{upp}}^-)^2 - 1\|sE^0 - s^{-1}E^0\|_{E(\Omega)}^2 / L(e^0). \]

(75)

From (72), we see that the \( \gamma_{\text{low}} \) can be expected to be close to unity only if the effectivity indices \( \lambda_{\text{low}}^+ \) and \( \lambda_{\text{upp}}^- \) are both very close to unity. For example,
if $\|se^0 + s^{-1}e^0\|^2_{E(\Omega)} / L(e^0)$ is $O(10^m)$ and $\|se^0 - s^{-1}e^0\|^2_{E(\Omega)} / L(e^0)$ is $O(10^n)$, then $(1 - (\lambda^+_{\text{low}})^2)$ and $((\lambda^-_{\text{upp}})^2 - 1)$ need to be $O(10^{-(n+2)})$ and $O(10^{-(m+2)})$, respectively, in order for $\eta_{\text{low}}$ to be reasonably close to unity. But, as already demonstrated, only the upper bound $\eta_{\text{upp}}$ has such accuracy. The effectivity index for the lower bound $\eta^+_{\text{low}}$ ranges between 0.8574 and 1.0000 for the functional $L_1$ and between 0.5653 and 0.9810 for $L_2$. Similar observations hold for the effectivity index $\gamma_{\text{upp}}$. Hence, the bounds $\eta_{\text{low}}$ and $\eta_{\text{upp}}$ can be expected to be accurate only if the ratio $\|se^0 \pm s^{-1}e^0\|^2_{E(\Omega)} / L(e^0)$ is very small.

Also, note that in the case of the effectivity index $\gamma_{\text{low}}$, the residual terms in (72) are of the same sign, since $\lambda^+_{\text{low}} < 1$ and $\lambda^-_{\text{upp}} > 1$. Hence, there is no possibility of a cancellation of errors. The same is true for the effectivity index $\gamma_{\text{upp}}$ of the upper bound. In the case of the estimates $\eta_{\text{est,low}}$ and $\eta_{\text{est,upp}}$, and the average of the bounds $\eta_{\text{av}}$, however, there is a cancellation of errors.

Table 4

<table>
<thead>
<tr>
<th>$\tau$</th>
<th>5</th>
<th>10</th>
<th>25</th>
<th>50</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>$|e^0 + e^0|^2_{E(\Omega)} / L(e^0)$</td>
<td>-0.5319(2)</td>
<td>-0.1964(3)</td>
<td>-0.1205(4)</td>
<td>-0.4819(4)</td>
<td>-0.1929(5)</td>
</tr>
<tr>
<td>$|e^0 - e^0|^2_{E(\Omega)} / L(e^0)$</td>
<td>-0.4583(2)</td>
<td>-0.1800(3)</td>
<td>-0.1162(4)</td>
<td>-0.4730(4)</td>
<td>-0.1911(5)</td>
</tr>
<tr>
<td>$\gamma_{\text{low}}$</td>
<td>0.2305(1)</td>
<td>0.1756(1)</td>
<td>0.1464(1)</td>
<td>0.1552(1)</td>
<td>0.1962(1)</td>
</tr>
<tr>
<td>$\gamma_{\text{upp}}$</td>
<td>-0.4145(0)</td>
<td>0.9914(-1)</td>
<td>0.3671(0)</td>
<td>0.2699(0)</td>
<td>-0.1448(0)</td>
</tr>
<tr>
<td>$\gamma_{\text{av}}$</td>
<td>0.9450(0)</td>
<td>0.9276(0)</td>
<td>0.9153(0)</td>
<td>0.9107(0)</td>
<td>0.9083(0)</td>
</tr>
<tr>
<td>$\gamma_{\text{est,low}}$</td>
<td>0.1024(1)</td>
<td>0.1015(1)</td>
<td>0.1007(1)</td>
<td>0.1004(1)</td>
<td>0.1002(1)</td>
</tr>
<tr>
<td>$\gamma_{\text{est,upp}}$</td>
<td>0.8661(0)</td>
<td>0.8405(0)</td>
<td>0.8237(0)</td>
<td>0.8178(0)</td>
<td>0.8148(0)</td>
</tr>
</tbody>
</table>

The results for the quantity of interest $L_1$ are given in Table 4, when the scaling factor $s = 1$, and in Table 5, when $s = s^*$. Since $L(e^0)$ is negative in this case, some of the effectivity indices are negative. From Tables 4 and 5, we observe that the terms $\|se^0 - s^{-1}e^0\|^2_{E(\Omega)} / L(e^0)$ and $\|se^0 - s^{-1}e^0\|^2_{E(\Omega)} / L(e^0)$ have magnitudes ranging approximately between 50 and 20000, when $s = 1$ and between 30 and 900, when $s = s^*$. Hence, the lower and upper bounds $\eta_{\text{low}}$ and $\eta_{\text{upp}}$ themselves do not always provide good estimates of the modeling error in the quantity of interest. Their average, $\eta_{\text{av}}$, behaves more consistently as a result of cancellation of errors. The estimates $\eta_{\text{est,upp}}$ and $\eta_{\text{est,low}}$ both show good effectivity indices owing to (a) the accuracy of the estimates $\eta_{\text{upp}}^\pm$ and $\eta_{\text{low}}^\pm$ (see Table 2), and (b) cancellation of errors.

The results for the quantity of interest $L_2$ are given in Table 6, when the scaling factor $s = 1$, and in Table 7, when $s = s^*$. While the behavior of the bounds $\eta_{\text{low}}$ and $\eta_{\text{upp}}$ is not unexpected, the effect of having inaccurate lower
Table 5
Effectivity indices of upper and lower bounds and estimates of modeling error in the quantity of interest $L_1$ with scaling $(s = s^*)$ for the one-dimensional problem.

<table>
<thead>
<tr>
<th>$\tau$</th>
<th>5</th>
<th>10</th>
<th>25</th>
<th>50</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{</td>
<td></td>
<td>e^0 + s^{-1}e^0</td>
<td></td>
<td>^2_{E(\Omega)}}{L(e^0)}$</td>
<td>-0.4083(2)</td>
</tr>
<tr>
<td>$\frac{</td>
<td></td>
<td>e^0 - s^{-1}e^0</td>
<td></td>
<td>^2_{E(\Omega)}}{L(e^0)}$</td>
<td>-0.3347(2)</td>
</tr>
<tr>
<td>$\gamma_{low}$</td>
<td>0.3722(1)</td>
<td>0.4205(1)</td>
<td>0.4519(1)</td>
<td>0.4629(1)</td>
<td>0.4684(1)</td>
</tr>
<tr>
<td>$\gamma_{upp}$</td>
<td>-0.1804(1)</td>
<td>-0.2331(1)</td>
<td>-0.2680(1)</td>
<td>-0.2803(1)</td>
<td>-0.2865(1)</td>
</tr>
<tr>
<td>$\gamma_{av}$</td>
<td>0.9591(0)</td>
<td>0.9369(0)</td>
<td>0.9195(0)</td>
<td>0.9129(0)</td>
<td>0.9095(0)</td>
</tr>
<tr>
<td>$\gamma_{est,low}$</td>
<td>0.1052(1)</td>
<td>0.1033(1)</td>
<td>0.1015(1)</td>
<td>0.1008(1)</td>
<td>0.1004(1)</td>
</tr>
<tr>
<td>$\gamma_{est,upp}$</td>
<td>0.8661(0)</td>
<td>0.8405(0)</td>
<td>0.8237(0)</td>
<td>0.8178(0)</td>
<td>0.8148(0)</td>
</tr>
</tbody>
</table>

Table 6
Effectivity indices of upper and lower bounds and estimates of modeling error in the quantity of interest $L_2$ without scaling $(s = 1)$ for the one-dimensional problem.

<table>
<thead>
<tr>
<th>$\tau$</th>
<th>5</th>
<th>10</th>
<th>25</th>
<th>50</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{</td>
<td></td>
<td>e^0 + e^0</td>
<td></td>
<td>^2_{E(\Omega)}}{L(e^0)}$</td>
<td>0.5023(1)</td>
</tr>
<tr>
<td>$\frac{</td>
<td></td>
<td>e^0 - e^0</td>
<td></td>
<td>^2_{E(\Omega)}}{L(e^0)}$</td>
<td>0.2982(2)</td>
</tr>
<tr>
<td>$\gamma_{low}$</td>
<td>0.2059(0)</td>
<td>0.5173(-1)</td>
<td>-0.5012(-1)</td>
<td>-0.8580(-1)</td>
<td>-0.1040(0)</td>
</tr>
<tr>
<td>$\gamma_{upp}$</td>
<td>0.4239(1)</td>
<td>0.4791(1)</td>
<td>0.5142(1)</td>
<td>0.5262(1)</td>
<td>0.5323(1)</td>
</tr>
<tr>
<td>$\gamma_{av}$</td>
<td>0.2222(1)</td>
<td>0.2422(1)</td>
<td>0.2546(1)</td>
<td>0.2588(1)</td>
<td>0.2610(1)</td>
</tr>
<tr>
<td>$\gamma_{est,low}$</td>
<td>0.3556(1)</td>
<td>0.3977(1)</td>
<td>0.4240(1)</td>
<td>0.4330(1)</td>
<td>0.4375(1)</td>
</tr>
<tr>
<td>$\gamma_{est,upp}$</td>
<td>0.8885(0)</td>
<td>0.8665(0)</td>
<td>0.8520(0)</td>
<td>0.8468(0)</td>
<td>0.8442(0)</td>
</tr>
</tbody>
</table>

bounds $\eta^\pm_{low}$ (see Table 3) results in the average $\eta_{av}$ and the estimate $\eta_{est,low}$ showing effectivity indices far from unity. The estimate $\eta_{est,upp}$ alone is seen to have reasonable effectivity indices.

7 Conclusions

The approach of hierarchical modeling generalizes many of the traditional methods of analysis of composite materials in that no periodicity of microscale constituents is assumed and the approach does not rely on the existence of RVEs. We have presented here a theory for estimation of modeling error in quantities of interest along with results from preliminary numerical experi-

27
Table 7
Effectivity indices of upper and lower bounds and estimates of modeling error in the quantity of interest $L_2$ with scaling ($s = s^*$) for the one-dimensional problem.

<table>
<thead>
<tr>
<th>$\tau$</th>
<th>5</th>
<th>10</th>
<th>25</th>
<th>50</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{|se^0 + s^{-1}e^0|^2_{L_2(\Omega)}}{L(e^0)}$</td>
<td>0.3355(1)</td>
<td>0.6565(1)</td>
<td>0.1596(2)</td>
<td>0.3153(2)</td>
<td>0.6265(2)</td>
</tr>
<tr>
<td>$\frac{|se^0 - s^{-1}e^0|^2_{L_2(\Omega)}}{L(e^0)}$</td>
<td>0.2815(2)</td>
<td>0.5811(2)</td>
<td>0.1467(3)</td>
<td>0.2939(3)</td>
<td>0.5881(3)</td>
</tr>
</tbody>
</table>

Elements on the performance of these estimates. A more detailed study of model adaptation based on the HAMMER and numerical experiments in two dimensions will be presented in a revised edition of this paper.

Acknowledgments We gratefully acknowledge the support of this work by the Office of Naval Research under grant N00014-95-1-0401 and by the NSF through NPACI, the National Partnership for Advanced Computational Infrastructure, grant 10152711.

References


28


