Multiscale Modeling Using Goal-oriented Adaptivity and Numerical Homogenization. Part II: Numerical Results

by

Chetan Jhurani and L. Demkowicz
Part II: Numerical Results

Chetan Jhurani L. Demkowicz
Institute for Computational Engineering and Sciences
The University of Texas at Austin
Austin, Texas 78712

Abstract

This paper is the second in a series to develop a numerical homogenization method for heterogeneous media and integrate it with goal-oriented finite element mesh adaptivity. The first paper developed the mathematical formulation of local homogenization. This was done using an appropriate averaging of the Moore-Penrose pseudoinverse of the element stiffness matrix. Here we present numerical verification of this approach using a two dimensional conductivity problem with known analytical limit. The heterogeneity of the conductivity pattern resembles a chess-board. We also use this problem to analyze the choice of the norm in which homogenization error is minimized. Finally, we present two and three dimensional Step and Flash Imprint Lithography model problems which integrate homogenization with goal-oriented mesh adaptivity and Newton iterations for nonlinearity.

Contents

1 Introduction 2

2 Verification of Numerical Homogenization 2

3 Alternatives in Homogenization Error Functional 6

4 Convergence Rate with Uniform Mesh Refinements 7

5 Integration of Homogenization with Adaptivity and Newton Iterations 9
  5.1 Energy-oriented mesh adaptivity for a 2-D mesh . . . . . . . . . . . . . . . . . . . . 11
  5.2 Goal-oriented mesh adaptivity for a 2-D mesh . . . . . . . . . . . . . . . . . . . . 16
  5.3 Energy-oriented mesh adaptivity for a 3-D mesh . . . . . . . . . . . . . . . . . . . . 23
  5.4 Goal-oriented mesh adaptivity for a 3-D mesh . . . . . . . . . . . . . . . . . . . . 29
1 Introduction

In the first paper of this series, we presented mathematical formulation of a local numerical homogenization procedure to dimensionally reduce and approximately solve large nonlinear optimization problems posed on finite element meshes. In the current paper, we show numerical results verifying this method and its integration with goal-oriented mesh adaptivity and Newton iterations for nonlinearity.

The homogenization method is verified using a 2-D chessboard conductivity problem with a known homogenized limit [4]. The results provide evidence of the accuracy, robustness in presence of nonlinearities and mesh adaptivity. The adjoint solutions on coarse and fine meshes provide a basis of automatic goal-oriented adaptivity [3]. This gives rise to 1-irregular meshes with hanging nodes. These are handled using the constrained approximation techniques [2]. We present the details for 2-D and 3-D geometries in Section 5.

2 Verification of Numerical Homogenization

We verify the local numerical homogenization algorithm using a 2-D chessboard conductivity remove problem with a known homogenized limit [4]. If the conductivities of individual boxes of different colors are \( k_1 \) and \( k_2 \), then the effective conductivity is \( \sqrt{k_1 k_2} \) as box-width \( \epsilon \to 0 \), Figure 1. This conductivity pattern has been used for operator-dependent multigrid homogenization [5, 6]. However, in both the articles, the error due to homogenization was large when the two conductivities differed significantly.

Figure 1: A 2-D domain with chess-board pattern of conductivities \( k_1 \) and \( k_2 \) has a limiting conductivity \( \sqrt{k_1 k_2} \) as the width of the boxes \( \epsilon \to 0 \).

Using this analytical result, our goal is to form a pure Neumann problem with finite \( \epsilon \) that also has a computable definition of effective conductivity. We discretize this prob-
Conductivities

$k_1$

$k_2$

$\sqrt{k_1 k_2}$

$m$ small blocks on each side.

$m \gg 1$ and $m\epsilon < 1$, say 0.9.

Figure 2: A square box of width 1 and flux boundary conditions on all edges.

The pure Neumann problem is posed on a square domain of width 1 and a chess-board conductivity pattern with conductivities $k_1$ and $k_2$ in the interior, Figure 2. Uniform heat flows in from the left edge and flows out from the right edge. The magnitude of the flux is $f$. The top and bottom edges are insulated. To avoid boundary effects a thin layer of material near the boundary has conductivity equal to the homogenized limit $\sqrt{k_1 k_2}$. Since this is a pure Neumann problem, we have to fix a datum. We choose the minimum temperature in the domain to be exactly 0.

Figure 3(a) and Figure 3(b) show the conductivity pattern as a function of $x$ and $y$ and the temperature profile for 8 small boxes on each side ($\epsilon = 0.125$) and each small box discretized by 10 bilinear quads. Conductivity values are $k_1 = 1$ and $k_2 = 10$ and magnitude of imposed flux is 1.

The finite element solution shown in Figure 3(b) looks smooth. However, the analytical solution has singularities at all interior corners where the boxes of different conductivities meet. This is made clear by the finite element $x$ and $y$ derivatives of the temperature in Figures 4(a) and (b) respectively.

From the analytical homogenization result (as $\epsilon \to 0$) it is seen that the conductivity of the whole domain will be effectively $\sqrt{k_1 k_2}$. The limiting 2-D problem can be solved analytically as a 1-D problem. There will be no temperature variation in the vertical direction. The limiting solution will vary linearly in the horizontal direction.
Figure 3: (a) The conductivity pattern for $k_1 = 1$ and $k_2 = 10$ and $\epsilon = 0.125$ in a box of width 1. (b) The plot shows a finite element solution for the temperature when the magnitude of the imposed flux is 1 and the square is discretized by $80 \times 80$ bilinear quad elements.

Figure 4: (a) The finite element $x$ derivative of the function shown in Figure 3(b). (b) The finite element $y$ derivative of the same function.

The exact solution in the limit is

$$u(x, y) = (1 - x) \frac{f}{\sqrt{k_1 k_2}}, \quad (1)$$

where $u$ denotes the temperature, and $f$ is the magnitude of boundary flux. Using Equa-
tion (1), the maximum temperature in the box is at \( x = 0 \) and is equal to \( \frac{f}{\sqrt{k_1k_2}} \). Thus, a computable definition of effective conductivity is

\[
 k_{\text{eff}} := \frac{f}{\max_{x,y}(u(x,y)) - \min_{x,y}(u(x,y))} = \frac{f}{\max_{x,y}(u(x,y))}.
\]  

(2)

We compute \( k_{\text{eff}} \) for the finite element solution also. The local numerical homogenization method is used to upscale the whole domain into a single quad with bilinear shape functions. The output is a coarse-scale symmetric “stiffness” matrix of size 4 (the number of DOFs in the coarse-scale element). We can then extract the best conductivity from this stiffness matrix and compare it with the \( k_{\text{eff}} \) for the finite element solution using Equation (2). Denote the numerically homogenized conductivity \( k_{\epsilon} \) (because it will vary with \( \epsilon \)).

For a bilinear quad with conductivity \( k \) and vertex nodes ordered as \([ 1 = (0,0), 2 = (1,0), 3 = (0,1), 4 = (1,1) \])], the element stiffness matrix is

\[
 K = kK_0 \text{ where } K_0 = \frac{1}{6} \begin{bmatrix}
 4 & -1 & -1 & -2 \\
 -1 & 4 & -2 & -1 \\
 -1 & -2 & 4 & -1 \\
 -2 & -1 & -1 & 4
\end{bmatrix}
\]

The numerical homogenization algorithm will give the coarse-scale matrix \( \hat{K} \) of size \( 4 \times 4 \). In general it will not be proportional to \( K \) so we cannot extract a conductivity \( k_{\epsilon} \) for making a comparison. We use Frobenius matrix norm to get the best \( k_{\epsilon} \) such that \( \| K - \hat{K} \|_F^2 \) is minimum. This gives

\[
 k_{\epsilon} = \frac{K_0 : \hat{K}}{K_0 : K_0} = \frac{\text{trace}(K_0^T \hat{K})}{\text{trace}(K_0^T K_0)}
\]

where ‘:’ is the matrix inner product induced by the Frobenius norm and ‘trace’ is the matrix trace. Note that this extraction of a single number \( k_{\epsilon} \) is just for the comparison purposes of this section. For finite element assembly in a “real” problem we use the matrix \( \hat{K} \) obtained after homogenization.

For a fixed \( k_1 = 1 \) and variable \( k_2 > 1 \), Figure 5 shows the comparison between the limiting conductivity \( (\sqrt{k_2}) \) and \( k_{\epsilon} \) produced by the homogenization method. \( k_2 \) is varied from 1 to 100. The curves show that for this range and a fixed number of elements (1600) to resolve the solution, the two values are quite close. The difference increases for large contrast between \( k_1 \) and \( k_2 \) but it may be possible to rectify that by using smaller and more elements in the mesh to resolve the singularities in the solution derivatives. We do not attempt that here.
3 Alternatives in Homogenization Error Functional

In Section 3.3 of the first paper, we formulated the local numerical homogenization problem when a local self-equilibrated load is known. In Section 3.4 there we formulated the same problem by treating all loads equally. In both cases we had used a norm (given by a matrix $B$) to compare the local fine-scale and coarse-scale compliance matrices. Thus, we have to make two choices — whether a known load is used and which norm is used to compare coarse-scale and fine-scale solutions. Using the chess-board conductivity problem of Section 2, we present numerical evidence that the alternative in which the load is known, and we use a norm that compares errors only on the boundary of the domain is a better choice.

Consider the first choice, that the known local load be used. If we minimize the homogenization error for a particular load, we should get a better solution. This seems obvious. The choice in the case of norm needs a little explanation. As will be shown, if we compare errors only on the boundary (instead of the whole domain) we get a better solution. A finite element interacts with the rest of the domain through the boundary. For example, in the 1-D example of springs solved in Section 3.1 of the previous paper, the process of homogenization reduces the $N$ spring constants to just one. The rest of the domain (or the exterior) cannot know by interacting with an element what is there inside (at least in this 1-D example). In that sense, homogenization is exact. But even with the exact homogenization, the errors in the interior are not zero. Thus, they should not be expected to be small, and should not be compared.

Figure 6 shows the errors made by making these choices. The curves show the relative
errors between $k_\epsilon$ and expected exact $k = \sqrt{k_1 k_2}$ while $k_1 = 1$ fixed and $k_2$ is varied between 1 and 25.

Symbol $k_{F,SN}$ denotes the curve where the known self-equilibrated “force” (or “load”) is used in conjunction with a special norm. Here we use the boundary flux and the special weights the errors in the interior as 100 times less important than boundary errors. Symbol $k_{SN}$ denotes the curve where the load is not used, but the special norm is. Symbol $k_{F,N}$ denotes the curve where the load is used, but the norm is the $\ell_2$ norm. Symbol $k_N$ denotes the case where no load is used and the norm is the $\ell_2$ norm. As seen, using the known load is better than not using it. Similarly, using the weighted norm is better than not using the weighted norm.

Figure 6: The four curves show the relative errors between homogenized conductivity $k_\epsilon$ and analytic conductivity $\sqrt{k_1 k_2}$ for various choices made in defining the homogenization error. See text in Section 3 for details.

4 Convergence Rate with Uniform Mesh Refinements

We present the results of homogenization of a 2-D lattice with 21 particles on each side and “random” bonds. The bottom layer of particles is fixed with equal inter-particle distance 1.3 and the lattice relaxes under zero external forces. The objective is to compute the convergence rate of error in energy norm as the coarse mesh element size is reduced to the fine-scale elements. The steps of homogenization and nonlinear Newton iterations are integrated as shown in Figure 7. In this case, however, the mesh is always refined uniformly in $h$.

Figure 8 shows the lattice topology. The lattice consists of two kinds of harmonic bonds with different parameters (equilibrium length and stiffness). The bonds are randomly distributed. The darker color represents the first kind of bond with stiffness 0.4 and length 1.2.
Figure 7: Overall structure of integrating homogenization, mesh adaptivity, and Newton iterations for nonlinearity.

The lighter color signifies the second kind with stiffness 1 and length 1. Figure 9 shows an equilibrium solution starting from a square lattice as the initial guess.

We use various element sizes for the coarse mesh to homogenize the lattice. Figure 11 shows the results. The nonlinear problem is homogenized using load-independent homogenization (Section 3.4 in previous paper) with 1, 4, and 16 “square” elements with 400, 100, and 25 lattice “cells” in each element. As seen, the solutions obtained after homogenization match the fine-scale solution very well. Figure 10 shows the global relative error in $\ell^2$ norm when compared to the non-homogenized fine-scale solution.
Figure 8: A “random” 2-D lattice with 21 particles on each side.

Figure 9: An equilibrium solution for the lattice topology shown in Figure 8 and fixed bottom layer.

Figure 10: The global relative error in $\ell^2$ norm for various levels of homogenization shown in Figure 11. The exact solution is specified by 882 degrees of freedom.

5 Integration of Homogenization with Adaptivity and Newton Iterations

In this section, we show results that combine automatic goal-oriented $h$-adaptivity [3] with nonlinear iterations and local homogenization for Step and Flash Imprint Lithography [1]
Figure 11: An oblique view of the equilibrium solutions for the lattice shown in Figure 8 after homogenizing the lattice at various resolutions. The bottom-right lattice is the non-homogenized solution taken from Figure 9.

lattice problems. These three techniques are integrated by the logic shown in Figure 7. We present results for 2-D and 3-D lattices and compare meshes generated by energy-oriented and goal-oriented adaptivity.

Although the real SFIL lattice model is in 3-D, we show the progress of mesh refinements in 2-D first because of the clarity it provides. This 2-D lattice model has $128 \times 128$ cells. The base is fixed and the lattice is deformed to its minimum energy configuration for a sequence of coarse meshes. We run the algorithm two times but use a different strategy in both cases. First we refine solely to minimize error in energy. In the second case the refinements are to minimize an error estimate in a goal functional. As shown in Figure 12, the goal is the distance between top-right corner and the center of top edge. As shown in Figures 14(a) and 18(a), the initial mesh consists of 4 equal-sized elements. The analysis and results are presented in Sections 5.1 and 5.2.

The 3-D model, shown in Figure 13, depicts a SFIL lattice with rectangular features for imprinting. It consists of approximately 13000 unit cells and 38000 DOFs. The goal is the distance between the two vertical blocks measured. This distance is measured between coordinates $(12, 28, 4)$ and $(12, 24, 4)$. The initial mesh consists of equal-sized elements each of edge size 4, shown in Figures 24(a). See Sections 5.3 and 5.4 for analysis and results.
Figure 12: The figure shows a 2-D model with 16384 unit SFIL cells and fixed base. For goal-oriented adaptivity, the goal is the distance between top-right corner and the center of top edge. The numerical results for this model are shown in Figures 14 – 20.

Figure 13: The figure shows a 3-D model with approximately 13000 unit SFIL cells and fixed base. For goal-oriented adaptivity, the goal is the distance between coordinates (12, 28, 4), shown by the white circle, and (12, 24, 4). The numerical results for this model are shown in Figures 24 – 32.

5.1 Energy-oriented mesh adaptivity for a 2-D mesh

We show energy-oriented adaptivity results for the 2-D model shown in Figure 12. Figures 14 – 15 show the mesh as refinements proceed. Meshes are shown after the Newton iterations for that particular mesh have converged. As seen, the mesh refinements proceed to have smaller elements on the base, specifically near the two corners. This is expected because of a change of boundary condition — free “boundary” on vertical edges and fixed “boundary” on the base. By boundary we mean the molecules that form the topological
boundary of the lattice in analogy with a surface in continuum material.

Figure 14: Energy-oriented mesh adaptivity for a 2-D lattice of size 128 × 128 with fixed base boundary condition. Rest of the iterations are shown in Figure 15. Compare goal-oriented mesh adaptivity in Figures 18 – 19.
Figure 15: Energy-oriented mesh adaptivity for a 2-D lattice of size $128 \times 128$ with fixed base boundary condition. Previous iterations are shown in Figure 14. Compare goal-oriented mesh adaptivity in Figures 18 – 19.
Figure 16: The graphs show how the minimum energy and residual norm change as mesh is refined using energy-oriented adaptivity and Newton iterations proceed. (a) The kinks are present where mesh is refined and the instantaneous rate of decrease of energy is higher. (b) The residual decreases with Newton iterations and goes up again upon mesh refinements. This is because fine-scale becomes more important. Compare with Figure 21.
Figure 17: The graphs show the distribution of errors in various elements and the decrease of error in energy with the increasing number of DOFs for energy-oriented adaptivity. Compare with Figure 22.
Figure 16(a) shows convergence of error, measured as the difference of energy for current mesh and the minimum energy, as Newton iterations and mesh iterations proceed. The kinks are at iterations where the mesh is refined because the solution has numerically converged for the current mesh. Except while approaching the kinks (from the left) the reduction in error is smooth. In Figure 16(b), we plot the homogenized residual per DOF at each iteration. By homogenized residual we mean the vector that drives the Newton iterations. We divide by the number of DOFs because the number of DOFs increases as the mesh is refined. The residual goes up again upon mesh refinements because further details of the fine-scale are seen. The solution is the best in energy only for the coarser mesh.

Figure 17(a) shows \textit{a posteriori} error estimates in various elements for the last mesh. The variation in error in different elements is not too large, which is a good sign. Figure 17(b) is a plot of absolute error versus number of DOFs as the refinements proceed. The rate of decrease is almost constant throughout the iterations. Compare this with the plot in Figure 22 for goal-oriented adaptivity in which the corresponding curve is nearly flat.

5.2 Goal-oriented mesh adaptivity for a 2-D mesh

We show goal-oriented adaptivity results for the 2-D model shown in Figure 12. Figures 18–19 show the mesh as refinements proceed. As expected, the mesh refinements proceed to have smaller elements near the two points that are needed to compute the goal.
Figure 18: Goal-oriented mesh adaptivity for a 2-D lattice of size $128 \times 128$ with fixed base boundary condition. The goal is the distance between the top-right corner and center of top edge. Rest of the iterations are shown in Figure 19. Compare energy-oriented mesh adaptivity in Figures 14 – 15.
Figure 19: Goal-oriented mesh adaptivity for a 2-D lattice of size $128 \times 128$ with fixed base boundary condition. The goal is the distance between the top-right corner and center of top edge. Previous iterations are shown in Figure 18. Compare energy-oriented mesh adaptivity in Figures 14 – 15.

Figure 20 shows the meshes for the converged solution for energy-oriented and goal-oriented adaptivity. Figure 21(a) shows convergence of error, measured as the difference of energy for current mesh and the minimum energy, as Newton iterations and mesh iterations proceed. The kinks are at some of the iterations where the mesh is refined because the solution has numerically converged for the current mesh. The curve is much flatter than the curve shown in Figure 16(a) because the primary purpose of iterations is to reduce the error in goal. In Figure 21(b), we plot the homogenized residual per DOF at each iteration. By homogenized residual we mean the vector that drives the Newton iterations. We divide by the number of DOFs because as the mesh is refined the number of DOFs increases. The residual goes up again upon mesh refinements because further details of the fine-scale are seen. The solution is the best in energy only for the coarser mesh.

Figure 22(a) shows a posteriori error estimates in various elements for the last mesh. The variation in error in different elements is not too large, which is a good sign. Figure 22(b) is a plot of absolute error versus number of DOFs as the refinements proceed. The error is almost constant throughout the iterations. Compare this with the plot in Figure 17(b) for energy-oriented adaptivity in which the corresponding curve does not have flat regions.
Figure 20: Final meshes generated by energy-oriented adaptivity and goal-oriented adaptivity. The goal is the distance between top-right corner and the center of top edge.
Figure 21: The graphs show how the minimum energy and residual norm change as mesh is refined using goal-oriented adaptivity and Newton iterations proceed. (a) The kinks are present where mesh is refined and the instantaneous rate of decrease of energy is higher. (b) The residual decreases with Newton iterations and goes up again upon mesh refinements. This is because fine-scale becomes more important. Compare with Figure 16.
Figure 22: The graphs show the distribution of errors in various elements and the decrease of error in energy with the increasing number of DOFs for goal-oriented adaptivity. Compare with Figure 17.
Figure 23: The decrease in error estimate for goal-oriented mesh adaptivity and components of error estimate.
The error estimate in goal, however, decreases uniformly as seen in Figure 23(a). We also plot the error estimates for individual elements in Figure 23(b). The estimate is divided into two parts – the standard characterization and the term due to homogenization (Section 3.10 in the first paper). The error due to homogenization is larger by around 1 order of magnitude.

5.3 Energy-oriented mesh adaptivity for a 3-D mesh

We show energy-oriented adaptivity results for the 3-D model shown in Figure 13. Figures 24 – 25 show the mesh as refinements proceed. Meshes are shown after the Newton iterations for that particular mesh have converged. We start with a mesh that has equal elements of size 4. As seen, the mesh refinements proceed to have smaller elements where the lattice has abrupt changes, either in boundary conditions or the presence of topological features like corners or edges. The first refinements just take care of the four corners of the base (Figure 25(a)). Next come the four edges of the base and the 4 corners of the block placed on the base (Figure 25(b)). Similar to the 2-D model in Figures 14 – 15, the refinements happen near discontinuities in the boundary and boundary conditions. The final mesh is shown more clearly in Figure 26 with the view axis aligned to the coordinate axes.

Figure 27(a) shows convergence of error, measured as the difference of energy for current mesh and the minimum energy, as Newton iterations and mesh iterations proceed. The kinks are at iterations where the mesh is refined because the solution has numerically converged for the current mesh. Except while approaching the kinks (from the left) the reduction in error is smooth. In Figure 27(b), we plot the homogenized residual per DOF at each iteration. By homogenized residual we mean the vector that drives the Newton iterations. We divide by the number of DOFs because as the mesh is refined the number of DOFs increases. The residual goes up again upon mesh refinements because further details of the fine-scale are seen. The solution is the best in energy only for the coarser mesh. Figure 28(a) shows \textit{a posteriori} error estimates in various elements for the last mesh. The elements with lower number are the initial mesh elements. Some of them have not been refined yet and this explains larger error in the left of the graph. Figure 28(b) is a plot of absolute error versus number of DOFs as the refinements proceed. The rate of decrease is almost constant throughout the iterations. Compare this with the almost flat curve in Figure 34 for goal-oriented adaptivity.
Figure 24: Energy-oriented mesh adaptivity for a 3-D lattice shown in Figure 13 with fixed base boundary condition. Rest of the iterations are shown in Figure 25. Compare goal-oriented mesh adaptivity in Figures 29 – 30.
Figure 25: Energy-oriented mesh adaptivity for a 3-D lattice shown in Figure 13 with fixed base boundary condition. Previous iterations are shown in Figure 24. Compare goal-oriented mesh adaptivity in Figures 29 – 30.
Figure 26: Front, side, and top views of converged mesh generated by energy-oriented adaptivity iterations shown in Figures 24 and 25. Compare with Figure 31.
Figure 27: The graphs show how the minimum energy and residual norm change as mesh is refined using energy-oriented adaptivity and Newton iterations proceed. (a) The kinks are present where mesh is refined and the instantaneous rate of decrease of energy is higher. (b) The residual decreases with Newton iterations and goes up again upon mesh refinements. This is because fine-scale becomes more important. Compare with Figure 33.
Figure 28: The graphs show the distribution of errors in various elements and the decrease of error in energy with the increasing number of DOFs for energy-oriented adaptivity. Compare with Figure 34.


5.4 Goal-oriented mesh adaptivity for a 3-D mesh

We show energy-oriented adaptivity results for the 3-D model shown in Figure 13. Figures 29 – 30 show the mesh as refinements proceed. Meshes are shown after the Newton iterations for that particular mesh have converged. We start with a mesh that has equal elements of size 4. The goal is the distance between coordinates (12, 28, 4) and (12, 24, 4), see Figure 13. The initial guess is shown in Figure 24(a). As expected, the mesh refinements proceed to have smaller elements near these two points. Most of the larger elements away from these two points are not refined, even though they need to be refined for energy-oriented adaptivity (Figures 24 – 25). The final mesh is shown more clearly in Figure 31 with the view axis aligned to the coordinate axes.

Figure 29: Goal-oriented mesh adaptivity for a 3-D lattice shown in Figure 13 with fixed base boundary condition. The goal is the distance between the two blocks measured near the bottom. Rest of the iterations are shown in Figure 30. Compare energy-oriented mesh adaptivity in Figures 24 – 25.
Figure 30: Goal-oriented mesh adaptivity for a 3-D lattice shown in Figure 13 with fixed base boundary condition. The goal is the distance between the two blocks measured near the bottom. Previous iterations are shown in Figure 29. Compare energy-oriented mesh adaptivity in Figures 24 – 25.
Figure 31: Front, side, and top views of converged mesh generated by goal-oriented adaptivity iterations shown in Figures 29 and 30. The goal is the distance between the two blocks measured near the bottom. Compare with Figure 26.
Figure 32: Final meshes generated by energy-oriented adaptivity and goal-oriented adaptivity. The goal is the distance between the two blocks measured near the bottom.

Figure 32 shows the meshes for the converged solution for energy-oriented and goal-oriented adaptivity. Figure 33(a) shows convergence of error, measured as the difference of energy for current mesh and the minimum energy, as Newton iterations and mesh iterations proceed. The kinks are at some of the iterations where the mesh is refined because the solution has numerically converged for the current mesh. The curve is flat and has no kinks because the primary purpose of iterations is to reduce the error in goal and not reduce error in the energy. Compare the curve shown in Figure 27(a). In Figure 33(b), we plot the homogenized residual per DOF at each iteration. By homogenized residual we mean the vector that drives the Newton iterations. We divide by the number of DOFs because as the mesh is refined the number of DOFs increases. The residual goes up again upon mesh refinements because further details of the fine-scale are seen.
Figure 33: The graphs show how the minimum energy and residual norm change as mesh is refined using goal-oriented adaptivity and Newton iterations proceed. (a) The kinks are present where mesh is refined and the instantaneous rate of decrease of energy is higher. (b) The residual decreases with Newton iterations and goes up again upon mesh refinements. This is because fine-scale becomes more important. Compare with Figure 27.
Figure 34(a) shows \textit{a posteriori} error estimates in various elements for the last mesh. The initial part of the curve is for some of the original mesh elements that have not been refined. Since the adjoint solution is small in some of them, they stay coarse. Compare Figure 28(a) for the distribution of the error when we measure it in energy-norm. Figure 34(b) is a plot of absolute error versus number of DOFs as the refinements proceed. The error is almost constant throughout the iterations. Compare this with the plot in Figure 34(b) for energy-oriented adaptivity in which the corresponding curve does not have flat regions.

The error estimate in goal, however, decreases uniformly as seen in Figure 35(a). We also plot the error estimates for individual elements in Figure 35(b). The estimate is divided into two parts — the standard characterization and the term due to homogenization (Section 3.10 in the first paper). The error due to homogenization is larger by around 2 orders of magnitude.
Figure 34: The graphs show the distribution of errors in various elements and the decrease of error in energy with the increasing number of DOFs for goal-oriented adaptivity. Compare with Figure 28.
Figure 35: The decrease in error estimate for goal-oriented mesh adaptivity and components of error estimate (Section 3.10 in the first paper).

Acknowledgements

This work was supported by the Department of Energy under Grant No. DE-FG02-05ER25701. The authors would also like to thank Dr. J. Tinsley Oden, Dr. C. Grant Willson, Dr. Jon Bass, Dr. Serge Prudhomme, Dr. Paul T. Bauman, and Dr. Elizabeth Collister for many helpful discussions.
References


