Dynamic Adaptive Mesh Refinement for Topology Optimization* Shun Wang[†], Eric de Sturler[‡], Glaucio H. Paulino[§]

Abstract

We present an improved method for topology optimization with both adaptive mesh refinement and derefinement. Since the total volume fraction in topology optimization is usually modest, after a few initial iterations the domain of computation is largely void. Hence, it is inefficient to have many small elements, in such regions, that contribute significantly to the overall computational cost but contribute little to the accuracy of computation and design. At the same time, we want high spatial resolution for accurate three-dimensional designs to avoid postprocessing or interpretation as much as possible. Dynamic adaptive mesh refinement (AMR) offers the possibility to balance these two requirements. We discuss requirements on AMR for topology optimization and the algorithmic features to implement them. The numerical design problems demonstrate (1) that our AMR strategy for topology optimization leads to designs that are equivalent to optimal designs on uniform meshes, (2) how AMR strategies that do not satisfy the postulated requirements may lead to suboptimal designs, and (3) that our AMR strategy significantly reduces the time to compute optimal designs.

keywords: adaptive mesh refinement, topology optimization, iterative solvers.

1 Introduction

Topology optimization is a powerful structural optimization method that combines a numerical solution method, usually the finite element method, with an optimization algorithm to find the optimal material distribution inside a given domain [16, 20, 15, 14]. In designing the topology of a structure we determine which points in the domain should be material and which points should be void. However, it is known that, in the continuum setting, topology optimization leads to designs with intermediate densities. So continuous values between 0 and 1 replace discrete values (0 or 1) to represent the relative densities, and some form of penalization is used to obtain designs with almost discrete 0/1 material density distribution [3].

In topology optimization, problems are solved most commonly on fixed uniform meshes with a relatively large number of elements in order to achieve accurate designs [17, 12]. However, as void and solid regions appear in the design, it is more efficient to represent the holes with fewer large elements and the solid regions, especially the material surface, with more fine elements. Since the shape and position of holes and solid

^{*}This work was supported in part by the National Science Foundation under Grant DMR-03 25939 ITR through the Materials Computation Center at the University of Illinois at Urbana-Champaign.

[†]Department of Computer Science, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, U.S.A., wang-shun98@gmail.com,

[‡]Department of Mathematics, Virginia Tech, Blacksburg, Virginia 24061, U.S.A., sturler@vt.edu,

[§]Department of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, U.S.A., paulino@uiuc.edu.

regions are initially unknown, the most economical mesh representation for the design is unknown a priori. Therefore, adaptive mesh refinement (AMR) is very suitable for topology optimization. The purpose of AMR for topology optimization is to get the design that would be obtained on a uniformly fine mesh, but at a much lower computational cost by reducing the total number of elements and having fine elements only where and when necessary.

Highly accurate designs on uniform meshes may require so many elements that the solution of the optimization problem becomes intractable. However, AMR leads to high resolution in the mesh only when and where necessary. This makes it possible to obtain accurate designs with a modest number of elements and hence with a reasonable cost. Even when a design on a uniform mesh is computationally feasible, AMR tends to reduce the computational cost by reducing the required number of elements and by improving the conditioning of linear systems arising from the finite element discretization. Obviously, we do not want the use of AMR or the AMR procedure to alter the computed designs. However, there is a risk of this, since the mesh influences the computed deformations and sensitivities. It is imperative then that the solutions from the finite element analysis using AMR must be as accurate as those obtained on a uniform fine mesh. 1 Moreover, the final design must be governed by accurate sensitivities corresponding to those obtained on the finest mesh. If coarse mesh solutions drive or limit the design, suboptimal designs may result when designs optimal on a coarser mesh differ substantially from the optimal design on a (much) finer mesh. We will demonstrate that this occurs in quite simple cases. The early work in this area, though leading to acceptable designs in specific instances, does not satisfy these properties. We will propose relatively simple but essential changes to these methodologies that lead to AMR-based designs that are equivalent (up to some small tolerance) to designs on uniform fine meshes. In addition, our approach leads (in principle) to an overall more efficient method as we reduce the total number of elements further. The topology optimization may lead to a sequence of (intermediate) structures requiring high mesh resolution in different parts of the computational domain. Therefore, it is important to (1) allow the meshes at all levels to change continually (dynamic) and (2) to allow both mesh refinement and derefinement [23]. Derefinement is important for efficiency when the initial discretization needs to include relatively small elements in certain regions. This is important in a number of cases, which are elaborated upon below.

In the next section, we provide an assessment of previous AMR strategies, namely the implementations by Costa and Alves [8] and Stainko [22]. In Section 3, we provide a brief introduction to topology optimization. Next, in Section 4, we state the purpose of our AMR strategy for topology optimization and explain the requirements it poses. Based on these requirements, we propose a more robust and dynamic AMR strategy. We describe a number of implementation issues of our AMR strategy in Section 6. We briefly discuss the iterative solution of the large sparse linear systems arising in the finite element analysis in Section 5. In Section 7, we show numerical experiments that demonstrate the robustness and efficiency of our AMR strategy. The first experiment also explains why the refinement strategies by Costa and Alves [8] and Stainko [22] may lead to suboptimal designs. Finally, in Section 8, we present conclusions about our AMR strategy for topology optimization algorithms, and we mention some directions for future work.

2 Assessment of Previous AMR Strategies

Little research has been done in applying AMR to topology optimization. So, we start by briefly discussing two recent, important, papers in this area. The AMR method by Costa and Alves [8] goes through a predetermined, fixed sequence of optimizations and subsequent mesh refinements (they do not use derefinements),

 $^{^{1}}$ For comparison everywhere in this paper the element size for the uniform fine mesh is the same as the element size at the highest level of refinement in the AMR mesh.

always using (or assuming) a converged solution on a 'coarse mesh' to guide the refinement of that mesh and start the optimization on the next 'fine mesh'. Coarse meshes and the solutions on these coarse meshes are never revisited or updated after generating the next finer mesh. The method aims at refining the coarse mesh design. Hence the region with the fine(r) mesh that contains the material boundary is always confined to the coarse mesh region that has been determined before using only coarse mesh calculations. After a fixed number of optimization steps on a given mesh, they refine all material elements (density 0.5 or larger) and elements on the boundary between material elements and void elements (density less than 0.5). Furthermore, they refine elements that do not satisfy certain quality or solution error criteria. In addition, there are a few special cases that also lead to refinement. These refinements lead to accurate finite element solutions in material regions, a high mesh resolution on the material boundary and, therefore, accurate representation of this boundary, and larger elements in void regions reducing the amount of work. However, as reported by the authors, the 'optimal design' found by the method depends on the initial mesh and is not the same as the optimal design found using a uniform fine mesh [8]. Although the authors do not report this, we conjecture that the design found using the adaptively refined mesh is not an 'optimal design' on the uniform mesh, that is, it has higher compliance than the solution obtained on the uniform fine mesh. See also our numerical experiments below. Finally, only two-dimensional designs are treated, but conceptually we expect their algorithm to work similarly in three-dimensional designs.

Stainko follows a slightly different approach with respect to the refinements [22]. Mesh refinement is done only along the material boundary as indicated by the (regularization) filter. So, elements completely inside a material region or a void region are not refined. In principle this leads to a smaller number of elements and hence a reduced computation time. However, Stainko's procedure also progresses strictly from coarser meshes to finer meshes, and a coarse mesh is never updated after mesh refinement. So, just as in [8], the finest mesh, which contains the material boundary, is always confined to regions defined by (all) earlier refinements (all refinements are nested), each of which is based only on the corresponding coarse mesh computations. Stainko does not test whether the designs obtained are the same as those obtained on uniformly fine meshes; however, our experiments below show that, again, the designs will be depend on the initial mesh (resolution) and are not the same as optimal designs on the uniformly fine mesh at the maximum refinement level.

These approaches share two important choices that may lead to problems. First, both approaches solve the design problem on a fixed mesh until convergence before carrying out mesh refinement. After refinement on a given level, the mesh on that level remains fixed for the remainder of the optimization, and all further refinements are therefore constrained by the converged coarser level solutions. This works well in terms of refining the design, but for many design problems the optimal solution on a uniform fine(st) mesh is quite different from the converged solution on a coarser mesh. In that case, mesh refinement based only on the coarser level solution will erroneously confine the solution on the finer mesh to a smooth version of the coarser level solution. Therefore, the approaches proposed in [22, 8] may lead to suboptimal designs, as we will show in our numerical experiments.

Second, both approaches use only refinement but no derefinement, which may lead to inefficiencies. First, for designs with thin structures, the initial, coarsest, mesh must be fine enough to give a reasonable result. If fine elements that are no longer required cannot be removed as the design evolves, then more computational work than necessary will be performed. Second, in topology optimization approaches that use filtering for regularization, for an accurate design requiring a high resolution mesh, the (appropriate) filter will not work on the coarser meshes, because the filter radius, which should be a physical feature size independent of the mesh, will typically be too small. Hence, we must start with a relatively fine mesh. However, after a modest number of optimization steps, large regions will likely have become void and fine elements could be removed without problems. Again substantial computational overhead results from having to work with too many fine elements. Third, any AMR strategy that allows changes in the design beyond previously computed



Figure 1: Overview of the topology optimization algorithm with dynamic AMR.

coarse level designs and refines the mesh to accommodate such changes will be inefficient if fine elements in void regions cannot be removed.

Therefore, a more robust and efficient refinement strategy is needed. Hence, we propose a dynamic meshing strategy that includes both mesh refinement and derefinement everywhere in the computational domain. Our improved AMR strategy has two main components. First, we extend the refinement criteria from [8], refining all material elements and elements on the boundary, but with an additional layer of refinements around the material boundary (in the void-region). The thickness of the layer is a parameter. This way the fine level design can change shape arbitrarily in optimization steps between mesh refinements. Second, our AMR method updates coarse and fine meshes continually, so that small changes arising in the more accurate computations on finer meshes can change the shape of the design arbitrarily in the course of the optimization; the fine(r) meshes move with the material boundary. This means that our designs are really based on the accurate fine mesh computations and are not confined to regions fixed by earlier coarse mesh computations. Since we do continual mesh adaptation, we may have fine elements in regions that have become void at some point. Derefinement will remove those fine elements. Further details are given in the next subsection. This approach leads to designs on AMR meshes at greatly reduced cost that are the same as the designs that would have been obtained on a uniform fine mesh of the highest resolution (within a small tolerance). We will demonstrate this experimentally in section 7. Our approach also allows us to start with coarser meshes, since the coarse mesh solution does not need to be a good approximation to the final solution. Even when we start with a finer mesh for faster convergence or proper functioning of the regularization filter, derefinement allows us to remove fine elements that have become void (which tends to happen quite quickly).

3 A Brief Topology Optimization Review

In topology optimization we solve for the material distribution in a given computational design domain Ω . The topology optimization problem we consider here is to minimize the compliance of a structure under given loads as a function of the material distribution. To solve this problem numerically, we discretize the computational domain using finite elements, where we usually use a lower order interpolation for the density field (material distribution) than for the displacement field. The most common approach (also employed for this paper) is to use (bi-,tri-)linear interpolation for the displacement field and constant density in each element. The compliance minimization problem after finite element discretization is defined as

s.t.
$$\begin{split} \min_{\substack{\rho_e \in [\rho_e, 1], \forall e}} \boldsymbol{f}^T \boldsymbol{u} & (1) \\ \begin{cases} \boldsymbol{K}(\boldsymbol{\rho}) \boldsymbol{u} = \boldsymbol{f} & \text{for } \boldsymbol{x} \in \Omega \setminus \Omega_0, \\ \boldsymbol{u} = \boldsymbol{u}_0 & \text{for } \boldsymbol{x} \in \Omega_0, \\ \sum_e \rho_e V_e \leq V_0, \end{cases} \end{split}$$

where ρ_e is the density in element e, ρ is the vector of element densities, K is the stiffness matrix, a function of the discretized density field (ρ) , V_e is the volume of element e, V_0 is a maximum volume (fraction) allowed for the design, and Ω_0 is the part of the domain where the displacement is prescribed. To avoid singularity of the stiffness matrix, we enforce a small positive lower bound ρ_e on the element density, typically 10^{-3} .

As mentioned in the introduction, our discrete model must drive the continuous material distribution as much as possible to a 0/1 solution. We use the Solid Isotropic Material with Penalization (SIMP) method to make the undesirable intermediate densities between ρ (replacing 0) and 1 unfavorable [6]. In this case, the elasticity tensor is defined as a function of the element density,

$$\boldsymbol{E}_e = \rho_e^p \boldsymbol{E}_0,\tag{2}$$

where p is the penalization parameter. With p > 1, intermediate densities are unfavorable as they provide relatively little stiffness compared with their material cost. A common choice is p = 3, which results in intermediate material properties that satisfy the Hashin–Shtrikman bound for composite materials [10]. To avoid problems with local minima, we usually apply continuation on the parameter p, that is, we start with p = 1 and slowly increase p as the design converges.

The general scheme for topology optimization using AMR is illustrated in Figure 1. First, we set up the geometry, the finite element (FE) mesh, the loading and boundary conditions, and we initialize the density distribution ρ . Then, we start the optimization loop. In this loop, we assemble and solve the equilibrium equations $K(\rho)u = f$ in (1) using the FE discretization and a linear solver. Next, in the sensitivity analysis, we compute the derivatives of the objective function with respective to the design variables, $\partial c/\partial \rho_e$. After this, we can apply an optional low-pass filter to remedy the checkerboard problem [18, 19, 21], which can be also addressed by an alternative minimum length scale approach [9]. In the next step, we compute an update of the design variables. There are various optimization algorithms applicable to topology optimization. For this paper, we use Optimality Criteria (OC), a simple approach based on a set of intuitive criteria [6, 4]. After updating the design variables using a chosen optimization algorithm, we check the convergence of the design. Under certain conditions, to be discussed next, dynamic mesh adaptation is carried out before the (next) finite element analysis.

4 A Dynamic AMR Strategy

We base our algorithmic choices on a set of requirements on AMR codes for topology optimization. As stated above, the purpose of AMR for topology optimization is to get the design that would be obtained on a uniform fine mesh, but at a much lower computational cost by reducing the total number of elements and having fine elements only where (and when) necessary.

First, since the finite element analysis and the computation of sensitivities drive the changes in material distribution, they should be as accurate as on the uniform fine mesh. Therefore, we need a fine mesh that covers at least the material region and the boundary. Since the void regions have negligible stiffness they do not influence the (intermediate) linear finite element solutions and resulting sensitivity computations. Thus we do not need a fine mesh inside the void region, and we can use a refinement criterion similar to that of Costa and Alves [8]. At this point we focus on refinement and derefinement for shape only. Therefore, we are conservative with respect to accuracy, and we expect that, in future implementations, good error indicators will lead to further efficiency gains, in particular because of derefinement in solid material regions.

Second, the accurate computations on the finest level should drive the changes in the material distribution. This requires continual mesh adaptation so that computational results after refinements can drive updates to the material distribution, and designs are not confined by earlier coarse grid results. This also means that as the material region moves close to the boundary between fine and coarse(r) mesh, additional refinements allow for further evolution.

Third, we need to ensure that the design can change sufficiently in between mesh updates. Therefore, we maintain a layer of additional refinements around the material region (in the void region) and carry out continual mesh adaptation. Due to the additional layer of refinements and continual mesh updates, the design can change arbitrarily following the fine grid computations and resulting sensitivities, and it is not confined by earlier coarse grid results. To ensure that the design accurately reflects the fine mesh computations, we allow rapid refinements of the mesh early on when voids and material regions (and hence the boundary) develop, rather than delay refinements until later stages, when a suboptimal design might have developed.

Fourth, since the design can change substantially from its estimate on a coarse mesh, we may have fine elements in void regions. Those elements must be removed for efficiency, requiring derefinements of the mesh. To facilitate our strategy of continual mesh refinement and derefinement, we use a hierarchical representation of adaptive meshes.

We will now state our refinement and derefinement strategy in more detail. We adapt the mesh when CASE (i):

- 1. the relative change in the compliance is smaller than a given threshold, and
- 2. a given minimum number of optimization steps have been carried out since the last mesh update,

or when CASE (ii):

3. a given maximum number of optimization steps have been carried out without meeting conditions 1 and 2.

Condition 1 corresponds to a common convergence criterion for topology optimization that the maximum change in the design variables is smaller than a certain tolerance (which we usually set to 0.01). This condition is satisfied when the solution is near a local minimum, which might be caused by a no longer appropriate mesh. In that case, we must adapt the mesh to allow the design to change further. If the local minimum is not an artifact of the mesh, the design will remain the same after mesh adaptation. Condition 2



Figure 2: Refinement criteria for void element. Element a is marked for refinement, because it has solid elements within distance r_{AMR} ; element b is marked for derefinement.

prevents refinement and derefinement from happening too frequently. This is important as the solution needs to adapt to the changed mesh, so that the computed sensitivities reflect the design and not mesh artifacts. This also limits the cost of mesh adaptation. In our experiments this minimum number of optimization steps is set to five based on experience, and other values are possible. Regarding condition 3, in our experiments we adapt the mesh at least every ten optimization steps. This condition leads to faster convergence because it ensures that the mesh is appropriate for the material distribution. Using these conditions, we can start with a fairly coarse mesh, and we may carry out mesh (de)refinement before the design converges on any mesh if necessary.

We adapt our mesh according to the following procedure.

- 1. Mark all the elements for refinement or derefinement based on the following criteria:
 - If element e is solid, i.e., $\rho_e \in [\rho_s, 1]$, where ρ_s is a chosen density threshold, or element e is within a given distance r_{AMR} from a solid element we mark it for refinement.
 - If element e is void, i.e., $\rho_e \in [\rho, \rho_s]$, and there are no solid elements within distance r_{AMR} , we mark element e for derefinement. See Figure 2.
- 2. Check compatibility for the mesh that will be generated and make the following adjustments in two sweeps over all elements:
 - In the first sweep, we unmark elements marked for derefinement, if they have a sibling (an element generated by the same refinement) that is not marked for derefinement.
 - In the second sweep, we unmark elements marked for derefinement, if derefinement would lead to level two or higher edge incompatibility. We allow only level one incompatibility; see Figure 3 and the discussion in Section 6.

The above refinement criteria result in a layer of fine elements on the void side of the solid/void interface that allows the material to be redistributed locally. If a material boundary moves near the fine/coarse element interface, mesh refinement creates a new layer of fine elements around the current material surface to allow further local redistribution of the material. On the other hand, if some fine elements become void, these fine elements are removed by derefinement to keep the optimization efficient.

5 Iterative Solution Scheme

Although AMR significantly reduces the number of DOFs in the finite element simulation, we still have to solve a sequence of large linear systems, especially for three-dimensional designs. Moreover, because of the large difference in density between distinct parts of the computational domain and the elasticity tensor given by (2), with p = 3 toward the end of the optimization, the linear systems are very ill-conditioned. Hence, proper preconditioning is essential. In [24], we showed how to precondition the linear systems arising in topology optimization, and we also used *Krylov subspace recycling* [13] to reduce the number of iterations over multiple linear systems. We briefly mention the main ideas here.

To remedy the serious ill-conditioning in topology optimization problems, we explicitly rescale each stiffness matrix such that the diagonal coefficients are all equal, as is the case for a problem with homogeneous density. We rescale the stiffness matrix K by multiplying with a diagonal matrix on both sides,

$$\tilde{K} = D^{-1/2} K D^{-1/2}$$

where D is the diagonal of K. The importance of such scaling and why it helps has been explained for an idealized one-dimensional problem in [24]. We further reduce the condition number of the system matrix and the number of iterations for convergence by applying an incomplete Cholesky preconditioner with zero fill-in to the explicitly rescaled system,

$$ilde{K} pprox ilde{L} ilde{L}^T.$$

The finite element analysis in topology optimization requires the solution of a sequence of (usually) symmetric linear systems. In each optimization step, the algorithm updates the element densities, and after the first few optimization steps the changes in the design variables tend to be small from one optimization step to the next. Hence, the optimization leads to small changes from one linear system to the next, and the search space generated for one linear system provides important information for subsequent linear systems. First, the solution of one system can be used as an initial guess for the next system, reducing the initial residual. Second, an approximate invariant subspace derived from the Krylov space generated for one linear systems, improving the convergence rate of the iterative solver. This is the basic idea of Krylov subspace recycling; however, other subspaces may also be used for 'recycling' [13]. Since the linear systems discussed in this paper are symmetric, we use the Recycling MINRES algorithm (RMINRES) for Krylov subspace recycling [24]. Unfortunately, solving a sequence of problems on meshes that change periodically makes recycling more difficult. Although it is not hard to map relatively smooth eigenvectors from a mesh to an updated mesh, the combination of mesh adaptation and preconditioning seems to give accuracy problems. Recycling is still effective for AMR; however, it is not nearly as beneficial as on a static mesh, and its improvement is work in progress.

6 Implementation Issues

For the implementation of adaptive mesh refinement, we use the libMesh library [11] developed at the University of Texas at Austin and the Technische Universität Hamburg-Harburg. The libMesh library provides a C++ framework for numerical simulations of partial differential equations on serial and parallel platforms. It supports one-dimensional, two-dimensional, and three-dimensional finite element and finite volume simulations on adaptive meshes. The libMesh software uses PETSc [2, 1] for the solution of linear systems on both serial and parallel platforms. However, we use our own custom linear solvers with Krylov

subspace recycling and preconditioners as detailed in Section 5 and references [24, 13]. For compatibility with the libMesh package we have implemented the RMINRES method in the PETSc framework. For the incomplete Cholesky preconditioner we used routines provided by PETSc.

We have developed two-dimensional and three-dimensional topology optimization algorithms on top of **libMesh**. Currently, we use element-based design variables, the SIMP method for material interpolation [5], the OC method for optimization [6, 4], and Sigmund's filter technique [18, 19, 21] with some modifications for dealing with adaptive refinement. Following Stainko [22], we make a small modification in Sigmund's filter takes a distance and density weighted average of the sensitivities of all elements in a certain radius as

$$\widehat{\frac{\partial c}{\partial \rho_e}} = \frac{1}{\rho_e \sum_d H_{de}} \sum_d \rho_d H_{de} \frac{\partial c}{\partial \rho_d},\tag{3}$$

where $\partial c/\partial \rho_e$ is the sensitivity of the compliance with respect to the density of element e, and H_{de} is a distance weight defined as

$$H_{de} = \max\{r_{\min} - \operatorname{dist}(d, e), 0\}.$$
(4)

The parameter r_{\min} is a given radius for the filter (for the work reported here we use $r_{\min} = r_{AMR}$), and dist(d, e) is the distance between the centers of elements d and e. For a nonuniform mesh, we take the variation of element size into account by using the element volume to redefine the weight in the filter [22] as

$$\frac{\widehat{\partial c}}{\partial \rho_e} = \frac{1}{\rho_e \sum_d H_{de} V_d} \sum_d \rho_d H_{de} V_d \frac{\partial c}{\partial \rho_d}.$$
(5)

The filter radius r_{\min} is often a length scale independent of the mesh representation. Notice that the filter will be effectively deactivated if its size is smaller than that of the smallest element, i.e., no element has any neighbors within distance r_{\min} .

Because of the hierarchical data structure of libMesh, we must allow level-one mesh incompatibility. However, we avoid level-two and higher mesh incompatibility. For example, if the configuration in Figure 3(b) would result from mesh refinement, we refine the gray elements as well. If the configuration, in particular the gray elements, in Figure 3(b) would result from mesh derefinement, we avoid the derefinement. In this way, we limit mesh incompatibility to level-one mesh incompatibility. As indicated by the circled nodes in Figure 3(a), level-one mesh incompatibility results in hanging nodes. The libMesh package handles those hanging nodes by using the projection method to enforce constraints in the stiffness matrix. We divide the degrees of freedom (DOFs) into two groups. Group one consists of all the unconstrained DOFs, and group two consists of the constrained DOFs on the hanging nodes. The constrained DOFs can be computed by linear interpolation from unconstrained DOFs. If we define vector \tilde{u} on the unconstrained DOFs, then

$$\boldsymbol{u} = \begin{pmatrix} \tilde{\boldsymbol{u}} \\ \boldsymbol{P}\tilde{\boldsymbol{u}} \end{pmatrix} = \begin{bmatrix} \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{P} & \boldsymbol{0} \end{bmatrix} \begin{pmatrix} \tilde{\boldsymbol{u}} \\ \boldsymbol{0} \end{pmatrix}$$
(6)

is the mapping of \tilde{u} to all the DOFs, where P is the interpolation matrix. We compute \hat{u} by solving the projected system

$$\begin{bmatrix} I & P^T \\ 0 & 0 \end{bmatrix} K \begin{bmatrix} I & 0 \\ P & 0 \end{bmatrix} \hat{u} = \begin{bmatrix} I & P^T \\ 0 & 0 \end{bmatrix} f.$$
 (7)

Since libMesh does not drop the constrained DOFs in the linear system, the projected system in (7) is singular when there is any hanging node. Krylov subspace methods can handle such singularities as long as



Figure 3: Mesh incompatibility with examples of quad, triangle and hex elements: (a) level-one mesh incompatibility marked by circled nodes; (b) level-two mesh incompatibility marked by circled nodes. We allow level-one mesh incompatibility (see Section 6), but we avoid level-two and higher incompatibility by refining the gray coarse elements and by not derefining their children elements if these gray elements result from a potential derefinement.

the right hand side is consistent, but these singularities may cause problems for preconditioners. To avoid the singularities, we set the diagonal entries in the matrix corresponding to the constrained DOFs to 1 and solve

$$\left(\begin{bmatrix} I & P^T \\ 0 & 0 \end{bmatrix} K \begin{bmatrix} I & 0 \\ P & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & I \end{bmatrix} \right) \hat{u} = \begin{bmatrix} I & P^T \\ 0 & 0 \end{bmatrix} f.$$
(8)

In the end, we recover the constrained DOFs using the interpolation matrix:

$$\boldsymbol{u} = \begin{bmatrix} \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{P} & \boldsymbol{0} \end{bmatrix} \hat{\boldsymbol{u}}.$$
 (9)

7 Results and Discussion

We solve three problems to demonstrate the improvements of our new AMR scheme and verify that the computed designs using AMR meshes are equivalent to designs on uniform fine meshes.

For the first (2D) test problem, we compute the optimal design on a uniform fine mesh and on an adaptively refined mesh with both our AMR scheme and an approach following references [8, 22]. The highest level of refinement in the AMR meshes has the same element size as that in the uniform mesh. The results show that our scheme computes a solution equivalent to the optimal design on the uniform fine mesh (within a small tolerance), while the alternative AMR approach from [8, 22] does not. Moreover, the experiments elucidate how this suboptimal design arises from the strategy to only refine the results from a fixed coarse mesh.

For the second (3D) test problem, we compare the optimal design using an adaptive mesh and our AMR strategy with the optimal design on a uniform fine mesh for a relatively simple cantilever beam problem. Again the maximum refinement level for the AMR mesh has the same element size as the uniform, fine mesh.

We also use this test to show that our AMR strategy leads to faster convergence in both the linear iterations (finite element solution) and the nonlinear iterations (design optimization) as well as to a significant reduction in runtime (about a factor of three).

In the third test problem (also 3D), we compare the optimal design using an adaptive mesh and our AMR strategy with the optimal design on a uniform, fine mesh for a more complicated design problem. For all three test problems our AMR strategy leads to essentially the same design as is obtained on a uniform mesh, but at significantly reduced cost.

To evaluate the relative difference between two designs, we need a quantitative measure. We define the the relative difference between two designs as

$$D(\rho^{(1)}, \rho^{(2)}) = \frac{\int_{\Omega} |\rho^{(1)} - \rho^{(2)}| d\Omega}{\int_{\Omega} \rho^{(1)} d\Omega}.$$
(10)

We take $\rho(1)$ to indicate the design on the uniform fine mesh, and $\rho(2)$ to indicate the design on the AMR mesh. This difference can be computed in a number of ways. To simplify comparison, we take the uniform mesh to be the AMR mesh with maximum refinement at every point. So, we refine the AMR mesh to the same fine mesh level at every point (without changing the design), and then evaluate the 1-norm of the difference between the designs.

Test 1: 2D cantilever beam

We compute the optimal design for the 2D beam problem shown in Figure 4(a). We first compute the design on a uniform, fine mesh. Figure 4(b) shows an intermediate result, and Figure 4(c) the converged design. Note how the truss member at the lower-right corner has risen up noticeably from the intermediate result to the final design. An effective AMR procedure must be able to capture such an evolution in the design.

Next, we solve the same problem following the strategy mentioned in references [8, 22]. We start with a relatively coarse mesh (64×32) , and obtain the converged solution to the topology optimization problem shown in Figure 5(a). Then, we refine the mesh according to this coarse level result and we solve the optimization problem on this locally refined mesh until convergence, obtaining the solution shown in Figure 5(b). Next, we refine the mesh and solve again. Finally, we obtain the result on the finest mesh shown in Figure 5(c). The truss member at the lower-right corner has remained roughly at its original position on the coarsest mesh in spite of the high resolution of the design, causing the resulting design to differ significantly from the optimal design obtained on the uniform, fine mesh, even though the smallest element size in the meshes in Figure 5(c) is the same as the element size for the uniform mesh shown in Figure 4. This difference in material distribution is caused by the fine mesh discretization being confined to the region identified by the coarse mesh design. The mesh adaptation strategy only allows the fine mesh computation to refine the coarse mesh design. It does not allow the fine mesh computation to alter the design substantially, even if more accurate fine mesh computations indicate a better design. An additional problem is that the initial mesh needs to be relatively fine, such as the one in Figure 5(a), because a coarser initial mesh would lead to very poor solutions as the filter would be inactive at that mesh resolution. In this case, mesh adaptation with refinement only leaves fine elements that could be derefined for efficiency in the void regions.

Now, we solve the same problem, starting with the coarse mesh of Figure 5(a), but following our AMR strategy (Section 4). We allow multiple mesh adaptations on any level and we maintain a layer of fine elements on the void side of the solid/void interface. This leads to the results shown in Figure 6, with two intermediate results shown in Figures 6(a) and (b), and the final converged result in Figure 6(c). Note how the truss member at the lower-right corner moves up as the optimization progresses, just as for the



Figure 4: Topology optimization on a 256×128 uniform mesh: (a) problem configuration (the volume constraint V_0 is 50% of the domain volume); (b) an intermediate design; (c) final converged design.



Figure 5: Topology optimization on an adaptive mesh with only refinement on each level: (a) converged result on the coarsest mesh with 2048 elements; (b) converged result on the intermediate mesh with 5675 elements; (c) converged result on the final mesh with 20216 elements. Note the undesirable position of the truss member near the lower right corner, which remains nearly invariant during the evolution of the design.



(a)



(b)



Figure 6: Topology optimization on an adaptive mesh with continual dynamic refinement and derefinement on each level: (a)–(b) intermediate designs; (c) final converged design on a nonuniform mesh with 25229 elements, whose finest resolution is the same as the resolution of the uniform mesh in Figure 4. Notice that the truss member of the lower-right corner moves up as the AMR procedure progresses.

opt. step	$\ell_{\rm max}$	# elem	#unknowns	relative L_1 difference
80	1	2048	4290	21.16%
125	2	5675	11948	19.53%
200	3	20216	41824	19.42%
300	3	20216	41824	19.60%
400	3	20216	41824	19.66%
500	3	20216	41824	19.66%
600	3	20216	41824	19.65%
700	3	20216	41824	19.67%
800	3	20216	41824	19.66%
900	3	20216	41824	19.65%
1000	3	20216	41824	19.67%

Table 1: Mesh adaptation scheme following Costa and Alves [8].

Table 2: Dynamic AMR scheme

opt. step	$\ell_{\rm max}$	# elem	#unknowns	relative L_1 difference
27	1	2048	4290	21.13%
37	2	6113	12786	19.80%
100	3	24707	50560	17.77%
200	3	25040	51242	13.00%
300	3	25184	51550	5.00%
367	3	25229	51654	0.17%



Figure 7: 3D cantilever beam example with domain scale 2:1:1.

evolution of intermediate designs on the uniform mesh (reference). The figures also demonstrate how the mesh changes smoothly with the changes in material distribution. The smallest element size in the AMR meshes in Figure 6 is the same as the element size for the uniform mesh shown in Figure 4 (reference). Compared with the final solution shown in Figure 5, the solution obtained with our AMR strategy is closer to the solution obtained on the uniform mesh (reference). Indeed, based on the metric in (10), the relative difference between the designs in Figure 5(c) and Figure 4(c) is 19.6%, while the relative difference between the designs in Figure 5(c) and Figure 4(c). Furthermore, derefinement results in coarser elements in the void regions, cf. Figures 5(c) and 6(c). These results are summarized in Tables 1 and 2, where ℓ_{max} refers to the highest refinement level present in the mesh.

Test 2: 3D cantilever beam

We compute the optimal design for the three-dimensional cantilever beam, shown in Figure 7, with a volume constraint of 25%. Exploiting symmetry, we discretize only a quarter of the domain. We solve this problem on a (fixed) uniform mesh with $128 \times 32 \times 32$ B8 elements and also following our AMR strategy. The initial mesh for the AMR-based design has $64 \times 16 \times 16$ B8 elements. The final results are shown in Figure 8 with Figure 8(a) displaying the solution on a uniform, fine mesh, and Figure 8(8) displaying the AMR solution; note the large blocks in parts of the void region in Figure 8(b). The relative difference between these two designs is only 0.0909% (Eq. (10)). We use the preconditioned, recycling minimum residual solver (RMINRES) proposed in [24] to solve the linear systems arising from the finite element discretization for a given material distribution. The dimensions of the linear systems of equations for the adaptive mesh are less than half of those for the uniform, fine mesh. The difference is even larger early in the optimization iteration. Moreover, the number of RMINRES iterations for the linear systems. Therefore, using AMR reduces the solution time roughly by a factor of three; see the statistics in Figure 9.

Test 3: Cross-shaped domain

We compute the optimal design for the more complex three-dimensional test problem shown in Figure 10. For the cross-shaped domain, we compute the optimal design subject to the fixed boundary on the bottom front and back ends, and two loads on the left and right sides. The maximum volume allowed is 20% of the domain volume. We solve this problem both on a uniform mesh and on an adaptive mesh following our



Figure 8: Final solutions of the 3D cantilever beam problem (Figure 7) obtained using symmetry on a quarter of the domain as indicated by the mesh: (a) final solution on a fixed uniform mesh with $128 \times 32 \times 32$ elements; (b) AMR solution on a mesh with 57173 elements; the finest local resolution is the same as that of the uniform, fine mesh.



Figure 9: Comparison of linear solver statistics for the cantilever beam design problem on a uniform, fine mesh and on an adaptive mesh: (a) the number of unknowns in the linear systems arising from the finite element discretization; (b) the number of preconditioned MINRES and RMINRES(200,10) iterations (see below) for each optimization step; (c) solution times with MINRES and RMINRES(200,10) for the linear systems arising from finite element discretization at each optimization step. The parameters m and k in RMINRES(m,k) have the following meaning. The method recycles an approximate invariant subspace associated with the smallest k eigenvalues from one linear system to the next. In the solution of single linear system, the approximate invariant subspace is updated every m iterations.



Figure 10: A 3D compliance minimization problem in a cross-shaped domain with the bottom (shaded) front and back ends fixed and the bottom left and right ends pulled down. The volume constraint V_0 is 20% of the domain volume.

AMR strategy. The results are shown in Figures 11 and 12, respectively. The uniform mesh consists of 40960 B8 elements, while the final adaptive mesh consists of only 19736 B8 elements. Moreover, the optimization converges in over 200 steps on the uniform mesh, but in only 106 optimization steps on the adaptive mesh. The adaptive mesh refinement reduces the total solution time by more than a factor of three to about 30% of the solution time for the uniform mesh. Nonetheless, the relative difference between these two designs is only 2.58% (Eq. (10)).

8 Conclusions

In order to reduce the high computational cost of accurate three-dimensional designs by topology optimization we use adaptive mesh refinement. We propose several critical improvements to the approaches proposed by Costa and Alves [8] and Stainko [22] in order to attain better designs. In particular, we want to obtain the same optimal designs that would be obtained on a uniform, fine mesh with AMR discretization having significantly fewer elements but the same fine mesh resolution. The purpose of AMR is to reduce the cost for the (same) optimal design; we do not want to reduce the quality of designs. For large, complex, three-dimensional design problems we could not possibly use a uniform fine mesh at the desired resolution. Our approach requires a dynamic meshing strategy that involves continual refinements and derefinements following the strategy laid out in Section 4. Derefinements should also lead to further efficiency improvement by reducing the number of elements in void regions, especially for three-dimensional problems. Using three test problems, we demonstrate that our AMR algorithm achieves the desired designs that are within a small tolerance of those obtained on a uniform, fine mesh with the same finest level. Our AMR strategy significantly reduces the total runtime, nonlinear, and linear iterations with respect to using uniform meshes.

Important future work includes error estimation in the finite element analysis and mesh refinement and derefinement governed by both considerations of accurate design and error estimation. In addition, we plan to work on preconditioners that can be adapted with the mesh (rather than recomputed) and to improve the convergence rate of Krylov methods with subspace recycling [24, 13]. We also intend to extend the present AMR technique to multiphysics problems [7].



Figure 11: The optimal solution to the design problem shown in Figure 10 on a uniform finite element mesh with 40960 B8 elements. The quarter-mesh discretization is shown on the bottom figure.



Figure 12: The optimal solution to the design problem shown in Figure 10 on an adaptively refined mesh. The final mesh consists of 19736 B8 elements. The quarter-mesh discretization is shown on the bottom figure.

9 Acknowledgements

We are indebted to Hong Zhang and Mat Knepley from Argonne National Laboratory for their help with the PETSc library and to Roy Stogner, John Peterson, and Benjamin Kirk from the University of Texas at Austin for their help with the libMesh library. We also thank Cameron Talischi for insightful discussions which contributed to improve the present manuscript.

References

- S. Balay, K. Buschelman, V. Eijkhout, W. D. Gropp, D. Kaushik, M. G. Knepley, L. C. McInnes, B. F. Smith, and H. Zhang. PETSc users manual. Technical Report ANL-95/11 - Revision 2.1.5, Argonne National Laboratory, 2004.
- [2] S. Balay, K. Buschelman, W. D. Gropp, D. Kaushik, M. G. Knepley, L. C. McInnes, B. F. Smith, and H. Zhang. PETSc Web page, 2001. Http://www.mcs.anl.gov/petsc.
- [3] M. P. Bendsøe. Optimal shape design as a material distribution problem. Structural Optimization, 1(4):193-202, 1989.
- [4] M. P. Bendsøe and N. Kikuchi. Generating optimal topologies in structural design using a homogenization method. Computer Methods in Applied Mechanics and Engineering, 71(2):197–224, 1988.
- [5] M. P. Bendsøe and O. Sigmund. Material interpolation schemes in topology optimization. Archives of Applied Mechanics, 69(9–10):635–654, 1999.
- [6] M. P. Bendsøe and O. Sigmund. Topology Optimization: Theory, Methods and Applications. Springer-Verlag, Berlin, 2003. ISBN 3-540-42992-1.
- [7] R. C. Carbonari, E. C. N. Silva, and G. H. Paulino. Topology optimization design of functionally graded bimorph-type piezoelectric actuators. *Smart Materials and Structures*, 16:2605–2620, 2007. DOI 10.1088/0964-1726/16/6/065.
- [8] J. C. A. Costa Jr. and M. K. Alves. Layout optimization with h-adaptivity of structures. International Journal for Numerical Methods in Engineering, 58(1):83–102, 2003.
- [9] J. K. Guest, J. H. Prévost, and T. Belytschko. Achieving minimum length scale in topology optimization using nodal design variables and projection functions. *International Journal for Numerical Methods in Engineering*, 61(2):238–254, 2004.
- [10] Z. Hashin and S. Shtrikman. A variational approach to the theory of the elastic behaviour of multiphase materials. *Journal of the Mechanics and Physics of Solids*, 11:127–140, 1963.
- [11] B. S. Kirk, J. W. Peterson, R. H. Stogner, and G. F. Carey. libMesh: a C++ library for parallel adaptive mesh refinement/coarsening simulations. *Engineering with Computers*, 22(3):237–254, 2006.
- [12] J. Mackerle. Topology and shape optimization of structures using FEM and BEM: A bibliography (1999–2001). Finite Elements in Analysis and Design, 39(3):243–253, 2003.
- [13] M. L. Parks, E. de Sturler, G. Mackey, D. D. Johnson, and S. Maiti. Recycling Krylov subspaces for sequences of linear systems. SIAM Journal on Scientific Computing, 28(5):1651–1674, 2006.

- [14] G. H. Paulino and C. H. Le. A modified Q4/Q4 element for topology optimization. Structural and Multidisciplinary Optimization, 2008. In press.
- [15] G. H. Paulino, R. C. Page III, and E. C. N. Silva. A Java-based topology optimization program with web access: nodal design variable approach. In Proceedings of the 6th World Congress on Structural and Multidisciplinary Optimization (WCSMO6), Rio de Janeiro, Brazil, May 30 – June 3, 2005. International Society for Structural and Multidisciplinary Optimization, 2005.
- [16] S. F. Rahmatalla and C. C. Swan. A Q4/Q4 continuum structural topology optimization implementation. Structural and Multidisciplinary Optimization, 27:130–135, 2004. DOI 10.1007/s00158-003-0365-9.
- [17] G. I. N. Rozvany. Aims, scope, methods, history and unified terminology of computer-aided topology optimization in structural mechanics. *Journal for Structural and Multidisciplinary Optimization*, 21(2):90–108, 2001.
- [18] O. Sigmund. Design of Material Structures Using Topology Optimization. Ph.D. thesis, Department of Solid Mechanics, Technical University of Denmark, 1994.
- [19] O. Sigmund. On the design of compliant mechanisms using topology optimization. Mechanics of Structures and Machines, 25(4):495–526, 1997.
- [20] O. Sigmund. Topology optimization: a tool for the tailoring of structures and materials. A special issue of the Philosophical Transactions of the Royal Society: Science into the next Millennium (Issue III, Mathematics, Physics and Engineering), 358(1765):211-228, 2000.
- [21] O. Sigmund and J. Petersson. Numerical instabilities in topology optimization: a survey on procedures dealing with checkerboards, mesh-dependencies and local minima. *Journal for Structural and Multidisciplinary Optimization*, 16(1):68–75, 1998.
- [22] R. Stainko. An adaptive multilevel approach to the minimal compliance problem in topology optimization. Communications in Numerical Methods in Engineering, 22(2):109–118, 2006.
- [23] S. Wang. Krylov Subspace Methods for Topology Optimization and Adaptive Meshes. Ph.D. thesis, University of Illinois at Urbana-Champaign, Department of Computer Science, Urbana, Illinois 61801, September 2007.
- [24] S. Wang, E. de Sturler, and G. H. Paulino. Large-scale topology optimization using preconditioned Krylov subspace methods with recycling. *International Journal for Numerical Methods in Engineering*, 69(12):2441–2468, 2006.