Novel Mesh Quality Improvement Systems for Enhanced Accuracy and Efficiency of Adaptive Finite Element Electromagnetics with Tetrahedra

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Abstract

Finite element accuracy and efficiency can be directly affected by mesh quality. When employing $h$-adaptive solution strategies, a mesh improvement stage is required in order to ensure high quality tetrahedra. However, mesh improvement techniques and quality indicators are often based on purely geometrical considerations. Recent work has focused on theoretically linking mesh quality criteria to interpolation and discretization errors. The potential benefits and related costs of a family of new mesh quality improvement systems are investigated using a set of electromagnetic benchmarks and mesh quality measures directly associated with finite element accuracy and efficiency. The new techniques are shown to outperform the existing mesh smoothing techniques in both mesh quality improvement and computational cost. The significant gains in finite element accuracy and efficiency are highlighted through theoretical and experimental results.
Résumé

La précision et l'efficience de la méthode des éléments finis sont directement liées à la qualité du maillage. Donc, les stratégies d'amélioration du maillage jouent un rôle considérable dans le cadre de la $h$-adaptation. Cependant, les méthodes d'amélioration du maillage de même que les indicateurs de qualité sont souvent basés sur des critères purement géométriques. Des liens théoriques entre la qualité du maillage et les erreurs d'interpolation et de discrétisation ont été établis récemment. Or, de nouvelles méthodes pour l'amélioration du maillage éléments finis sont présentées. Des tests d'évaluation de performance électromagnétiques, ainsi que des mesures de qualité liées à la précision et l'efficience de l'analyse par éléments finis sont employés pour démontrer l'efficacité des nouvelles méthodes. Les nouvelles méthodes ont la capacité de surpasser les méthodes existantes dans l'amélioration du maillage et la réduction des coûts. Des résultats théoriques et expérimentaux servent à souligner les gains considérables dans la précision et l'efficience de la méthode des éléments finis.
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Chapter 1

Introduction

The analysis and design of electric and magnetic devices is often governed by the tradeoff between accuracy and cost. In theory, powerful and sophisticated numerical methods are capable of resolving a wide range of complex problems in science and engineering. However, practical implementations are frequently intractable due to the associated computational costs.

Finite element methods are a well-established class of numerical methods that are particularly well-suited for problems in computational electromagnetics. However, the computational bottlenecks associated with large-scale problems and potential real-time applications are daunting. The applicability of finite element methods to next-generation problems, such as nanotechnology, relies on a mastery of strategies for mitigating computational costs. Unlocking the full potential of finite element methods also relies on a clear understanding of what influences accuracy. While an increase in accuracy is expected for a corresponding increase in cost, certain subtle effects may play a larger role than previously thought. A thorough understanding of finite element accuracy may reveal hidden inefficiencies and lead to significant advances. Thus, a two-pronged approach that simultaneously targets increases in accuracy and decreases in cost is a promising alternative.
1.1 The Finite Element Method

The finite element method is an indispensable tool in the study and evaluation of problems involving differential and integral equations. Specifically, the finite element method can be used to successfully solve complex differential and integral equations that arise in describing an electromagnetic system [1]. It has applications in a wide range of fields in science and engineering and is typically used to simulate the performance of devices before building prototypes. The finite element method is very versatile and is able to handle static, quasi-static, transient and wave problems, in problem spaces of complex geometry and in virtually all material regions [1]. Given its strong theoretical foundations and favorable characteristics, it is sometimes regarded as one of the most powerful numerical analysis techniques available today.

The starting point of any finite element analysis is an initial mesh of the problem region. Although numerous types of elements may be used for discretization, tetrahedral meshes are often preferred in computational electromagnetics. The essence of the finite element method lies in the local nature of the approximating functions. Differential or integral equations that describe the physical system are solved using a piecewise polynomial solution that models the problem [1]. The steps associated with a typical analysis may be summarized as follows: (i) the problem region is discretized using tetrahedra; (ii) a model of the solution is constructed over each element by an approximating function (uniquely defined by a set of parameters); and (iii) the parameters are computed based on global constraints (boundary conditions).
Thus, finite element analysis relies on the discretization of a continuous problem and leads to a solution consisting of a finite set of numerical values. Finite element solutions are inherently approximate. The accuracy of the solution generally depends on the order of the approximating functions, on the number and distribution of unconstrained parameters (e.g., tetrahedra) in the problem region, and on the mesh quality. From engineering experience, it is generally understood that poor quality elements are those that diverge significantly from the ideal equilateral tetrahedron. However, four decades after the invention of finite element methods, the precise relationships between mesh quality and solution accuracy and efficiency are yet to be thoroughly understood.

The computational effort required for the electromagnetic analysis of complex systems can be prohibitive. For instance, it is not uncommon to encounter computational costs of $O(n^3)$ in some finite element implementations, where $n$ is proportional to the number of degrees of freedom (DOF) in the problem domain (e.g., number of tetrahedral elements in the mesh) [1]. The use of adaptive finite element methods is particularly valuable in this regard.

1.2 Adaptive Finite Element Methods

While finite element methods are presently employed extensively for electromagnetic analysis and design, the use of adaptive finite element methods (AFEMs) has increased considerably in recent years. Today, the focus is on the research and development of efficient and reliable three-dimensional methods for the analysis of realistic systems [1]. The primary advantage of AFEMs is the accurate computational analysis of large continuum problems for only a relatively small fraction of the cost of non-adaptive finite
element methods [1]. AFEMs have been shown to significantly alleviate computational bottlenecks by intelligently evolving the distribution of elements in the problem region and ensuring high accuracy (Fig. 1.1). AFEMs strive to achieve the maximum increase in accuracy for each additional DOF. A uniform increase in DOF throughout the problem region could yield accuracy comparable to AFEMs. Often, this is a wasteful proposition. Consider a case where the finite element solution error is non-uniform in the problem region; a uniform refinement would produce additional free parameters in regions which are sufficiently well resolved. Regions of high error would not be treated in an efficient way. Furthermore, the structure of an initial discretization is sometimes insufficient for resolving physical behavior in practical systems. Uniform refinements do not allow for this initial discretization to be modified and can incur exorbitant costs. AFEMs strive to achieve a specific level of accuracy for the minimum computational cost by intelligently evolving the mesh.

![Tetrahedral mesh of microstrip filter structure, before and after adaptation](image)

**Figure 1.1:** Tetrahedral mesh of microstrip filter structure, before adaption (a) and after adaption (b) [1].
AFEMs may be described as an adaptive feedback loop that consists of five basic steps:

1. Construction of an inexpensive initial mesh;
2. Finite element processing, resulting in a finite element solution;
3. If the termination criteria have not been satisfied (e.g., accuracy, memory limits), an error estimator determines which regions represent the highest error in the solution;
4. Identification of regions of inadequate discretization by examining error distribution;
5. Update of finite element discretization by adding (or removing) DOF. (Go to step 2.)

Each of these five steps is a research area in its own right. The method for updating a discretization (step 5) has been the focus of extensive research [1]. Currently, there are four main paradigms commonly employed within the adaptive feedback loop: (i) $h$-type; (ii) $p$-type; (iii) $hp$-type; and (iv) $r$-type. The $h$-type adaption model is conceptually simple and consists of adding elements to improve the discretization. Alternatively, $p$-type adaption increases the degree of approximation over elements within the mesh. The $hp$-type adaption approach combines the two previous models. Finally, $r$-type adaption repositions nodes within the mesh to achieve an increase in solution accuracy.

When employing first-order tetrahedral elements within the $h$-type adaption context, a more specific flowchart applies (Fig. 1.2). The update of the discretization is accomplished through mesh refinement whereby elements are added to the discretization in order to increase resolution. Mesh improvement is performed immediately after refinement to mitigate the difficulties associated with poor quality tetrahedral elements. Finite element processing is then performed on the adapted mesh and is repeated until termination criteria are satisfied.
1.3 Mesh Improvement within $h$-adaptive Finite Element Methods

AFEMs incorporating $h$-type adaption have been used successfully for various types of engineering applications. For problems where singularities in the mathematical field solutions exist (such as those at sharp material edges and corners), $h$-type adaption models have been particularly useful [1]. The $h$-type adaption model is concerned with adapting the size of the elements, while keeping constant the order of the approximating functions over the elements. The increase in free parameters is thus accomplished by increasing the number of elements in the mesh (i.e., refining the mesh). Thus, $h$-type adaptive refinement is conceptually straightforward. However, an effective implementation can be subject to practical limitations. The manner in which new elements are defined can affect the quality of the resulting mesh. For instance, the formation of poorly shaped elements (e.g., long, thin elements or flat elements) can
severely compromise the accuracy of the solution and the efficiency with which it is computed [40-45]. A mesh improvement stage is a required component for mitigating the problems associated with poor quality elements. Considerable attention has been given to mesh improvement in recent years. Accordingly, various mesh quality improvement strategies have been proposed in order to eliminate poor quality elements that are formed as a result of mesh generation and \( h \)-adaptive mesh refinement [22, 25-28, 30]. Among the most promising mesh quality improvement methods for three-dimensional meshes are smoothing-based techniques [22, 26-27]. These techniques reposition individual vertices within the mesh to improve local mesh quality, without changing the mesh topology.

1.4 Motivation for the Research

Mesh quality can affect both finite element solution accuracy and efficiency [22-28, 32-46]. In the \( h \)-type adaption context (first-order tetrahedral elements), mesh quality improvement is often a pre-requisite for successful finite element analysis [32-46]. Understanding the relationship between mesh quality and finite element accuracy and efficiency is crucial. However, this relationship is rarely treated adequately [42-44]. Deciphering the correlation between mesh quality and interpolation error, discretization error, and matrix conditioning is an important step toward improving finite element accuracy at reduced computational cost [40-44].

Discretization error is the measure of finite element accuracy that is the most closely linked with practical applications: it measures the difference between a finite element solution and the true solution [37]. Generally, it is not possible to achieve pointwise
bounds on discretization error as a function of mesh quality [40]. Even global bounds on
discretization error usually cannot be achieved without bounds on interpolation error.
Two types of interpolation error are most important for practical applications: (i) errors in
the interpolated function; and (ii) errors in the interpolated gradient [37]. Pointwise and
global bounds on both interpolation errors are dependent on element quality [40]. The
impact of a single poor quality element on interpolation error is entirely local. However,
the corresponding finite element solution may be in error throughout the entire mesh
(high discretization error) [40]. Hence, mesh quality improvement is a critical stage of a
finite element analysis.

A further aspect to consider is finite element matrix conditioning. Good conditioning is a
key factor in ensuring an efficient solution of the resulting linear systems of equations.
Indeed, round-off errors in many classes of solvers are sensitive to matrix conditioning. A
single elemental stiffness matrix with large maximum eigenvalue raises the maximum
eigenvalue of the global matrix equally high [40]. Thus, a handful of bad quality elements
can be deleterious to finite element matrix conditioning. The efficiency of certain solvers,
such as Jacobi or steepest descent, suffers whenever the condition number is large (even
when a single eigenvalue is to blame). Krylov subspace methods, such as the conjugate
gradient (CG) method applicable to symmetric positive definite (SPD) systems, are often
superior in this regard. The CG method can circumvent each bad eigenvalue with one
extra iteration, after which it performs as well as if the bad eigenvalue were not present at
all [40]. Nevertheless, the effects of a small number of bad elements on both finite
element accuracy and efficiency cannot be disregarded.
1.5 Thesis Objectives

The focus of this thesis centers around mesh improvement systems within the $h$-adaptive finite element context. The main thrusts are twofold: (i) to develop a new family of mesh smoothing systems that outperform existing techniques in terms of finite element mesh quality improvement, and (ii) to thoroughly investigate the impact of these systems on the resulting finite element accuracy and efficiency.

1.6 Thesis Outline

In Chapter 2, the state-of-the-art in mesh generation and mesh refinement will be addressed. Chapter 3 will focus on the various mesh improvement strategies that are currently employed in the context of $h$-adaption. In Chapter 4, a new family of four smoothing-based mesh quality improvement systems for tetrahedral meshes will be presented and evaluated using conventional mesh quality measures. A thorough discussion of the impact of mesh quality on solution accuracy and efficiency will be presented in Chapter 5. This theory will then be applied toward evaluating the new mesh smoothing techniques. In particular, the focus will be on their potential advantages and related costs for $h$-type adaptive finite element electromagnetic analysis. Finally, conclusions and a summary of original contributions will be presented in Chapter 6.
Chapter 2

Tetrahedral Mesh Generation and Refinement

Mesh generation involves the creation of an initial discretization of the problem domain. This is often regarded as one of the most difficult aspects of the finite element method. In two dimensions, triangular mesh generation is considered a closed problem [12]. In three dimensions, the general principles of tetrahedral mesh generation are known. However, rigorous theoretical guarantees and proofs are not available in many cases [11]. Mesh generation applications are abundant and diverse. In addition to computational applications in engineering, mesh generation is also used in disciplines such as solid modeling, computer graphics, biomechanics, and cartography [12]. While mesh generation is responsible for the creation of an initial discretization, the mesh refinement stage updates this discretization by adding or removing elements. Both mesh generation and mesh refinement are intrinsic components of a finite element analysis system and will be explored in this chapter.

2.1 Tetrahedral Mesh Generation Techniques

A tetrahedron is a simplex and has many favorable properties. Complete polynomial expansion functions can be defined over tetrahedra with relative ease [11, 12]. The tetrahedron is the most flexible element for covering complex topologies in three dimensions. Ease of refinement is also an important attribute [15]. This section will examine different approaches to the tetrahedral mesh generation problem.
2.1.1 The Octree Method

There exist various approaches for meshing a region using tetrahedra. Early attempts focused on the octree method [2, 3]. This technique involves the use of cubes to discretize the problem domain. Subsequently, the cubes are subdivided into tetrahedra until the desired resolution is achieved. It is obvious that some form of boundary recovery technique must be employed. This usually involves a large number of surface intersection calculations, with no direct control over the triangulation of the boundary surface. Thus, the recovery of the boundary surface is often problematic [2, 3].

2.1.2 The Advancing Front Method

The advancing front method uses the triangular surface mesh of the problem domain as a starting point [4, 5]. The main virtue is that the surface triangulation remains intact throughout the entire procedure and the resulting mesh is boundary conforming. However, considerable effort is devoted to creating an optimal surface mesh. Once the surface mesh is established, a tetrahedron is constructed by placing a vertex in the domain and connecting it to a surface triangle. An optimal location is chosen for each inserted vertex. Alternatively, an existing vertex may be chosen for connection with an existing triangular face of the front. After each new tetrahedron is created, intersection checks are required to verify that it is not in conflict with an existing element [4, 5]. Every subsequent step builds on the previous one, gradually extending the mesh until it covers the entire domain. The difficulty lies in the final stages of the algorithm, where the last pieces of empty space must be discretized [4, 5]. These last tetrahedra often exhibit very poor quality and user intervention is sometimes required [4].
2.1.3 The Delaunay Method

The Delaunay tetrahedralization is a fundamental structure of computational geometry [6-12]. Intense research on Delaunay-based mesh generation has led to the development of many successful Delaunay mesh generation software packages [8-12]. Delaunay-based methods for generating a tetrahedral mesh are the most widely accepted.

The tetrahedralization of a set \( D \) of \( N \) vertices is the decomposition of the convex hull of \( D \) into tetrahedra such that, the vertices of the tetrahedra are in \( D \) and the intersection of two tetrahedra is either empty, a vertex, an edge, or a face. Of all the possible tetrahedralizations of the set \( D \), the Delaunay tetrahedralization is the one that conforms to the Delaunay criterion. By definition, the circumsphere of a tetrahedron is the sphere that intersects all four vertices of the tetrahedron. The Delaunay criterion requires that no tetrahedron circumsphere contain mesh vertices in its interior ("empty-sphere criterion"). If five or more vertices lie on a circumsphere, then more than one tetrahedralization of the set of vertices satisfies the Delaunay criterion. A large percentage of slivers (four nearly coplanar vertices) can be created in three dimensions due to this arbitrariness [30].

Despite the simplicity of the Delaunay criterion, there is no guarantee that a Delaunay tetrahedralization will conform to specific boundary triangles and edges [8]. Extra vertices and local transformations may be required [7, 24]. The Delaunay criterion simply prescribes a method for connecting a set of vertices. Various ways of inserting vertices into the domain have been studied [8]. For instance, insertion at a tetrahedron's centroid and circumsphere have both been proposed as viable schemes [20].
One popular method for creating a Delaunay tetrahedral mesh is incremental vertex insertion combined with the Bowyer/Watson algorithm [11, 12]. The Bowyer/Watson algorithm relies on Delaunay's empty-sphere criterion whereby no tetrahedron circumsphere may contain a vertex of the mesh [11]. In this scheme, the initial Delaunay tetrahedralization may consist of a rectangular cylinder constructed from five tetrahedra. The rectangular cylinder encloses the entire region to be meshed. The eight vertices that define this bounding box and all tetrahedra incident on these eight vertices are removed only after all problem region vertices have been inserted and boundary recovery has been performed. When a vertex is inserted into an existing Delaunay tetrahedralization, the tetrahedra that contain this new vertex in their circumsphere are deleted (special treatment of degeneracies is required). The resulting cavity is remeshed by connecting this vertex to the faces lining the cavity.

All decisions are based on floating-point arithmetic. The numerical computations associated with cavity construction are very sensitive to round-off errors [8]. Even if all floating-point operations are performed in 64-bit arithmetic, incorrect decisions may still occur [7]. These errors may lead to the formation of disjoint, non-convex, or intersecting tetrahedra. Consistency checks have been developed for evaluating the validity of the mesh after vertex insertion [6, 8].

In general, the desired surface triangulation will not exist within the bounding box. It follows that a boundary recovery phase must attempt to reconstruct the desired boundary faces [11]. Due to the recovery process, the tetrahedralization will no longer be Delaunay.
These boundary recovery techniques usually involve strategic vertex insertions and local transformations based on edge and face swapping [7, 24]. If a mesh does not entirely conform to the Delaunay criterion, extra attention must be given to the cavity construction algorithm [6]. The Bowyer/Watson algorithm applied to such a mesh has the potential of creating a non-convex insertion cavity. One approach that overcomes these difficulties is to expand the insertion cavity outward, starting with the element containing the inserted vertex [6]. Checks are performed in order to ensure that the final insertion cavity is convex. However, this approach runs into difficulties in three dimensions when the problem domain is non-convex [6]. In practice, the Bowyer/Watson algorithm results in the formation of a large percentage of slivers [9, 10]. The creation of slivers can be reduced, but rarely eliminated altogether [9, 10, 25, 30].

A second method for creating a Delaunay tetrahedral mesh is incremental vertex insertion and local transformations [24]. A vertex that is inserted into an existing discretization either falls on a face, an edge, or inside a tetrahedron. Depending on its location, the inserted vertex is connected to the existing discretization in a way that will produce a conforming mesh. The new local configuration is evaluated for the Delaunay criterion. If the Delaunay criterion is violated, local transformations are performed on the local configuration of tetrahedra. Based on Delaunay’s lemma, these local transformations can be used to establish local Delaunay conformity [24].
**Delaunay's Lemma.** Consider a set of simplexes that divide uniformly the space $R^n$ and have in common a subsimplex or the empty set. A necessary and sufficient condition that no circumscribed sphere of a simplex contains in its interior a node of a simplex is that this holds for every pair of simplexes that have in common a face in $(n-1)$ dimensions. In other words, for every such pair of simplexes, the node of each simplex is not contained in the interior of the circumscribed sphere of the other simplex.

Several five-vertex configurations may exist in the modified region (Fig. 2.1). Only two pairs of these configurations are transformable, namely $1A/1B$ and $3A/3B$. In other words, the local transformations $1A$-to-$1B$, $1B$-to-$1A$, $3A$-to-$3B$, and $3B$-to-$3A$ can be performed [24, 25]. If a transformable configuration does not satisfy Delaunay’s criterion, local transformations are used to establish Delaunay conformity. Local transformations are also employed within the mesh improvement context to achieve local optimality (discussed in Chapter 3).

Three-dimensional Delaunay meshes are common in computational electromagnetics. Their advantages include, (i) the smallest possible min-containment radius (radius of the smallest sphere that encloses the tetrahedral element), (ii) the circumspheres of the tetrahedra incident on an interior vertex are the closest to that vertex, and (iii) the weighted average of the square of edge lengths is minimized [6-12]. In this sense, Delaunay meshes correspond to an “optimal” discretization of a set of points [1]. The Delaunay algorithm also benefits from fast processing of large problem sizes due to the simplicity of the empty-sphere property.
2.2 Mesh Refinement

The $h$-type adaption model requires an efficient mesh refinement technique for reducing the local element size. The finer the mesh, the better the resolution of the physical phenomenon. Three of the most popular refinement techniques are templates [21], bisection of edges [13-19], and Delaunay refinement [20].

2.2.1 Templates

Tetrahedra can be refined based on a fixed template approach. For example, octasection would produce eight tetrahedra for each divided one. This approach reduces versatility, as elements are always divided in the same way and the degree of division is fixed [21]. To produce a conforming mesh, additional operations must be performed which increase the complexity of the algorithm [21].
2.2.2 Edge Bisection

Edge bisection refines the mesh on an elemental basis and no searching is required if appropriate data structures are used [14, 16, 17]. Bisection does not require the initial mesh to be Delaunay and is conceptually straightforward. In this approach, one or more edges of a tetrahedron are split in half. In the case of single-edge bisection, the target tetrahedron is split into two tetrahedra (Fig. 2.2). Once the target tetrahedron has been bisected, a recursive procedure further refines the mesh to re-establish conformity.

Bisection algorithms range from the very simple, to the more involved [13-19]. The merits of longest-edge bisection have been known for quite some time [14, 16, 17]. For example, experimental results show that the poorest aspect ratios resulting from longest-edge bisection are very close to the poorest aspect ratios of the initial mesh [14].

![Figure 2.2: Bisection of a tetrahedron [18].](image)

Certain bisection algorithms attempt to increase efficiency by reducing the expansion of the embedded region [15]. In other cases, emphasis is placed on producing element size transitions that are smooth throughout the entire mesh [13]. Arnold et al. propose a method in which the refinement edge is not restricted to the longest edge within the tetrahedron [18]. In this approach, all the solid angles of all descendant tetrahedra remain bounded below by a positive constant depending on the tetrahedra in the initial mesh [18]. In this sense, the quality of tetrahedra does not degenerate as a result of refinement.
Rivara proposes a sophisticated method for implementing the traditional longest-edge bisection algorithm [17]. This new refinement approach is applicable in both two and three dimensions. In both cases, it is based on the definition of the “longest edge propagation path” (LEPP) of a triangle or tetrahedron. The LEPP-based approach leads to an efficient, non-recursive and robust implementation [17]. Its non-recursive nature allows for the possibility of a parallel implementation given appropriate data structures. Rivara defines the LEPP of any tetrahedron $t_i$ as “the set of all neighbor tetrahedra (by the longest edge) having respective longest edge greater than or equal to the longest edge of the preceding tetrahedron in the path” [17]. In three dimensions, this path propagates in many directions (Fig. 2.3). A terminal tetrahedra set is defined by Rivara as “the set of all the tetrahedra of the mesh that share their common longest edge” [17]. The LEPP of a tetrahedron will have a finite number of terminal tetrahedra sets.

Essentially, the LEPP-based refinement of a target tetrahedron is carried out by the repetitive longest-edge bisection of the terminal tetrahedra sets until the target tetrahedron is divided [17]. This produces the traditional longest-edge bisection without the creation of temporary non-conforming vertices. Computational cost is reduced by the use of efficient data structures for managing neighbor tetrahedra [17]. A two-dimensional example of the bisection algorithm (with target triangle $t_0$) is shown in Fig. 2.3. A simpler scheme would divide $t_0$ along its longest edge, and subsequently bisect $t_i$ to maintain conformity. Notice however that the LEPP-based approach produces a smooth gradation in element size and better quality elements [14, 17]. In three dimensions the results are analogous [17].
2.2.3 Delaunay Refinement

Delaunay vertex insertion strategies may also be used to reduce local element size. Shewchuk presents a Delaunay refinement algorithm (Bowyer/Watson-based) that creates a conforming mesh with a bound on circumradius-to-shortest edge ratio of two [20]. Vertex insertion is performed at the circumcenter of a poor quality tetrahedron. However, sliver tetrahedra can have a circumradius-to-shortest edge ratio below two [9, 10, 20]. The volume of a sliver can be arbitrarily close to zero, as all four of its vertices lie virtually in the same plane. In practice, a large percentage of slivers are created, and mesh improvement techniques do not always succeed in removing them [20]. In addition, Shewchuk's algorithm must handle the complexities of cavity creation [6]. Although the use of Delaunay refinement within an h-type adaption model is promising [8-12], the computational cost of the Delaunay operation at every adaptive step can be prohibitive.

Figure 2.3: Two-dimensional LEPP-based bisection: (a) initial triangulation; (b) first step; (c) second step; (d) final triangulation [17].
While the Delaunay algorithm generates the "optimal" discretization for a given set of vertices, the mesh quality may still not be sufficient to obtain the desired level of accuracy, nor a practicable solution efficiency. This highlights the importance of the mesh improvement stage.
Chapter 3

Mesh Quality Improvement Systems

Mesh generation and mesh refinement both have a significant impact on the quality of tetrahedral elements in the discretization. While much work has been done to perfect these stages of $h$-adaptive finite element analysis, subsequent mesh quality improvement is often required. Indeed, the accuracy and efficiency of the finite element solution is directly affected by mesh quality. The problem in three dimensions is more severe than in two, since tetrahedra can exhibit poor quality in more ways than triangles. Some examples of poorly shaped tetrahedra are shown in Fig. 3.1.

![Examples of poorly shaped tetrahedra](image)

Figure 3.1: Examples of poorly shaped tetrahedra [33].

A mesh improvement system typically consists of a combination of the two main categories of mesh improvement techniques, namely local transformations [22-25] and smoothing [26-28]. Local transformations change element connectivities. In contrast, mesh smoothing repositions mesh vertices in order to achieve an increase in mesh...
quality. The particular transformations and smoothing approaches that are selected, as well as how they are combined are critical to the resulting mesh quality. An example of a combined mesh improvement system is shown in Fig. 3.2.

![Combined mesh improvement system diagram](image)

**Figure 3.2: Combined mesh improvement system.**

### 3.1 Local Transformations

Mesh improvement by local transformations modifies the mesh topology. The local transformations $1A$-$to$-$1B$, $1B$-$to$-$1A$, $3A$-$to$-$3B$, and $3B$-$to$-$3A$ were first discussed in Section 2.1.3. In addition to the mesh generation application previously described, local transformations can also be used to optimize a particular tetrahedron quality measure. The transformations are closely associated with the possible configurations of five distinct, noncoplanar three-dimensional vertices, $a$, $b$, $c$, $d$, and $e$. The related configurations first appeared in Fig. 2.1 and are repeated in Fig. 3.3 for convenience. In the top three configurations (1A, 1B, and 2), no four vertices are coplanar. The remaining bottom four configurations represent all possible cases where four vertices ($a$, $b$, $d$, $e$) are coplanar. As discussed in Section 2.1.3, only the pairs $1A/1B$ and $3A/3B$ are transformable.
Mesh improvement using local transformations is based on examining interior faces and their associated five-vertex configurations. Given an interior face, one could proceed by determining the two tetrahedra incident on it. From this, the location of each of the five relevant vertices would be available. The type of configuration can be determined using barycentric coordinates [25]. If the configuration corresponds to either 1A, 1B, 3A, or 3B, a check can be performed to determine whether a transformation is beneficial. The operation is carried out only if it will benefit mesh quality. Subsequently, all faces in the five-vertex configuration other than the faces involved in the swap, will also need to be evaluated for optimality. This corresponds to the faces forming the convex hull of the five-vertex configuration. If the associated five-vertex configuration of the face corresponds to either 1A, 1B, 3A, or 3B, then it is considered transformable.
A description of the mechanics of these local transformations is now in order. The $1A/1B$ transformation involves swapping face $abc$ (in $1A$) for faces $ade$, $bde$, and $cde$ (in $1B$), or vice versa. The $3A/3B$ transformation involves swapping face $abc$ (in $3A$) for face $cde$ (in $3B$), or vice versa. For the $3A/3B$ case, the two coplanar faces must be on a boundary or incident on another pair of tetrahedra that can be transformed to preserve conformity.

One special case that should be mentioned arises in configuration $1B$. When face $dea$ is examined, the two tetrahedra incident on it are $deab$ and $deac$. It may occur that $debc$ is not present in the tetrahedralization. In other words, one or more faces may be incident on edge $de$ between faces $deb$ and $dec$. In order for a $1B$-to-$1A$ transformation to be possible, the extra faces must be removed. Moreover, the $1A$-to-$1B$ transformation is only valid if the eventual edge $de$ is interior to the two tetrahedra.

In the mesh improvement context, the goal of performing a local transformation is to locally optimize a quality measure of the local five-vertex configuration. For instance, one could allow a transformation to proceed only if it increases the worst quality measure of all tetrahedra involved in the transformation. Maximizing the minimum sine of dihedral angles (angles inside the tetrahedron, formed by pairs of adjacent triangular faces) is a common objective function. Alternatively, Delaunay’s empty-sphere criterion could be used to select the configuration in which no tetrahedron in the local five-vertex tetrahedralization contains the other vertex in its circumsphere. Once all transformable faces have been optimized, the overall tetrahedralization is considered “locally optimal” [25]. This does not necessarily correspond to a globally optimal tetrahedralization. There is no straightforward way of determining the level of global optimality.
3.2 Smoothing

Mesh smoothing techniques have been shown to be effective in improving tetrahedral meshes [22, 26-28]. These techniques reposition individual vertices to improve local mesh quality without changing the mesh topology. Typically, several iterations of smoothing are performed to improve the overall quality of the mesh. Smart-Laplacian smoothing and optimization-based smoothing are two variants that have received much attention [22, 26-28]. While optimization-based approaches yield an optimal local submesh, the associated computational costs can be daunting [27].

3.2.1 Smart-Laplacian Smoothing

Laplacian smoothing is a conceptually simple and computationally inexpensive smoothing algorithm. In its simplest form, Laplacian smoothing involves the repositioning of an internal vertex to the average location of any vertex connected to it by an edge. This approach is based on the assumption that all tetrahedra connected to the free vertex are nearly equilateral and of roughly the same volume. In this case, the movement of the vertex to the centroid would maximize local aspect ratios [27]. Based on this idea, one expects that repositioning the vertex to the centroid is always the correct choice for increasing local quality. However, if poorly shaped tetrahedra exist in the mesh, Laplacian smoothing will often lead to invalid meshes [22]. Smart-Laplacian smoothing repositions a vertex to the average location of the vertices connected to it by edges only if the quality of the local submesh is improved according to a specific quality measure [27]. This enhanced version remains easy to implement and computationally inexpensive, yet still yields non-optimal results.
3.2.2 Optimization-based Smoothing

Optimization-based approaches formulate the smoothing operation as a non-smooth optimization problem, and use an analog of the steepest descent method for smooth functions to maximize or minimize a given mesh quality measure [26-28]. These approaches are much more computationally expensive (approximately 10 times more expensive than smart-Laplacian [27]), but yield optimal results. The quality of the mesh is guaranteed to improve as a result of the operation and invalid meshes are not created.

Optimization-based smoothing is based on functions that represent the element quality measure to be optimized. These functions are usually written $f_j(x)$, where $x$ is the position of the free vertex. For a given optimization problem, $f_j(x)$, $j=1,...,n$, is the set of element quality functions that vary with $x$. The active value is defined as the minimum of all function values at $x$. The active set is the set of functions that obtain the active value. For example, when maximizing the minimum dihedral angles, $n$ is equal to the number of tetrahedra containing the vertex multiplied by 6. The goal of optimization-based smoothing is to find the position $x^*$ that maximizes the composite function $g(x) = \min [f_j(x)]$, for $1 \leq j \leq n$ (a one-dimensional slice through $g(x)$, denoted by $h$, is shown in Fig. 3.4). This is equivalent to searching for a location where the minimum quality measure is greater than anywhere else, while maintaining a valid mesh. In general, $g(x)$ is discontinuous when the function attaining a minimum changes. To solve this non-smooth optimization problem, one can employ a method that is analogous to the steepest descent method for smooth functions [26, 27]. Various approaches to optimization-based smoothing that target different quality measures have been proposed [26-28].
3.2.3 The Advantages of Combined Techniques

The best quality meshes are created using combinations of local transformations and smoothing [22, 25]. When used individually, local transformations fail to eliminate all very large and very small angles [22]. Conversely, smoothing strategies sometimes encounter difficulties because they do not alter the underlying poor mesh connectivity [22]. An initial sweep of local transformations is helpful for improving the connectivity of the mesh and usually allows for greater gains in tetrahedron quality during subsequent smoothing operations [22]. In the chapters that follow, the focus will be on developing novel smoothing-based mesh improvement systems for enhanced accuracy and efficiency of \( h \)-adaptive finite element electromagnetics.
Chapter 4

A New Family of Combined Mesh Improvement Systems

The smoothing component of a mesh improvement system may be implemented as either a single technique or a combination of various smoothing approaches. Combinations of smart-Laplacian smoothing and optimization-based smoothing have performed favorably for many types of meshes [22, 27]. The resulting improvement in mesh quality is often comparable to optimization-based smoothing performed alone, but at only a fraction of the cost [22, 27]. In fact, it has been suggested that combined approaches can produce higher quality meshes than pure optimization-based smoothing [27].

4.1 Existing Combined Smoothing Techniques

Several combined mesh smoothing approaches have been presented in the literature [22, 26, 27]. Most notably, the combined approaches C1, C2, C3, and C4 have been shown to be effective and efficient for improving mesh quality [22, 27]. Before describing the algorithmic details of these four existing approaches, a few preliminary issues must be addressed. Prior to any operations on mesh vertices, a threshold value is established for the entire mesh. For instance, if the objective is to maximize the minimum dihedral angles in the mesh (angles inside the tetrahedron, formed by pairs of adjacent triangular faces), the threshold would take on a value in degrees (e.g., 10°). Once this threshold has been established, smoothing takes place over several passes. During each pass, the same algorithm is applied to each vertex of the mesh in turn. Each vertex has a local submesh and an active value associated with it. The local submesh consists of the union of all
tetrahedra that are incident upon it. The active value is the poorest quality measure value within the local submesh under consideration (e.g., smallest dihedral angle). A description of the existing techniques is now in order.

C1: If the active value exceeds the threshold, smart-Laplacian smoothing is used; otherwise optimization-based smoothing is used.

C2: Smart-Laplacian smoothing is used as the initial step. If the active value exceeds the threshold, go to next vertex; otherwise, optimization-based smoothing is used.

C3: If the active value exceeds the threshold no smoothing is performed (go to next vertex); otherwise smart-Laplacian smoothing is employed. If the threshold is still not exceeded following smart-Laplacian, optimization-based smoothing is used.

C4: Same as C2, but with a floating threshold.

We notice that C4 is equivalent to C2, except that C4 employs a floating threshold. In other words, the threshold value is updated after each smoothing pass. For instance, in the case of a strategy that maximizes the minimum dihedral angles, the threshold may be updated to the global minimum dihedral angle in the mesh plus a constant. A major advantage of the floating threshold strategy is that the threshold value is automatically adjusted for targeting the extremal angles in the mesh.
Upon closer examination of C1-C4, it is apparent that they are formulated using five fundamental operations:

1. Smart-Laplacian smoothing (unconditional);
2. Optimization-based smoothing (unconditional);
3. Smart-Laplacian smoothing if the active value does not satisfy the threshold;
4. Optimization-based smoothing if the active value does not satisfy the threshold;
5. Optimization-based smoothing if the active value does not satisfy the threshold, otherwise smart-Laplacian smoothing.

For example, C2 is equivalent to (1,4). For the case of six smoothing passes, the existing techniques can be rewritten as follows,

C1: (5)-(5)-(5)-(5)-(5)-(5);
C2: (1,4)-(1,4)-(1,4)-(1,4)-(1,4)-(1,4);
C3: (3,4)-(3,4)-(3,4)-(3,4)-(3,4)-(3,4);
C4: (1,4)-(1,4)-(1,4)-(1,4)-(1,4)-(1,4).

4.2 Proposed Smoothing Techniques

A few observations can now be made which will lead to the formulation of the new mesh smoothing techniques D1, D2, D3, and D4. The technique C4 uses a floating threshold and is the recommended smoothing technique [22, 27], whereas the others have a fixed threshold value. Furthermore, within a given smoothing pass, a sequence of two fundamental operations is performed on each vertex (with the exception of C1). When a floating threshold is being used, the threshold value is not updated until these two operations have been applied to each vertex in turn. Thus, the threshold is not updated
after the first operation and information about the current mesh quality is not available to the second operation. As well, C1-C4 always attack the smoothing problem using at most two types of fundamental operations. For instance, over six passes, the C4 technique depends on the combined effort of only two fundamental operations, (1) and (4), to solve the smoothing problem.

The new smoothing techniques D1-D4 are formulated to explore promising variations on the characteristics described above. They can be expressed in terms of fundamental operations as follows,

\[ \text{D1: (3)-(5)-(4)-(3)-(5)-(4);} \]
\[ \text{D2: (3)-(4)-(3)-(4)-(3)-(4);} \]
\[ \text{D3: (3)-(4)-(5)-(5)-(1)-(1);} \]
\[ \text{D4: (1)-(1)-(5)-(5)-(3)-(4).} \]

As can be readily observed, a single fundamental operation is applied over each smoothing pass (for a total of six passes). Moreover, a floating threshold is used for each new technique and is updated after each fundamental operation. In addition, the type of fundamental operation from one pass to the next is variable (as is the ordering). In D1, the threshold is used in the decision process during each smoothing pass. The tendency is to move from the less effective smart-Laplacian smoothing to the more effective optimization-based smoothing over three passes. The following three passes repeat this sequence of steps. In the D2 technique, the fundamental operations alternate between the least computationally expensive and most expensive, while decision-making continues to be based on a floating threshold. D3 employs four different operations in an order which
strives to maximize their combined effectiveness. In this case, the operations that target the largest number of elements are placed towards the end, and early smoothing passes are less computationally expensive. D4 uses a strategy opposite to D3. It should be noted that the second fundamental operation (optimization-based smoothing without condition) was never employed in D1-D4. The extremely high computational cost of this operation precluded it from being used alone within a smoothing pass. The effectiveness of these new approaches is examined in the following sections.

4.3 Unit Cube Benchmark System

A basic benchmark example is considered, in order to evaluate the potential benefits of the new smoothing approaches D1, D2, D3, and D4. The problem consists of a unit cube with an initial mesh of 25,688 tetrahedra; a standard problem for mesh quality analysis [22, 26, 27]. In practice, maximizing the minimum sine of dihedral angles of the incident tetrahedra has been shown to effectively eliminate extremal angles [22, 27], and is used as an objective function in this work. The initial threshold value is set to 10°. For those techniques that use a floating threshold, the threshold value is updated to the global minimum dihedral angle in the mesh plus 5° after each smoothing pass. Smoothing is performed over six passes. The results for the benchmark problem are summarized in Table 4.1. Global minimum and maximum dihedral angles, a dihedral angle distribution and total time required to perform smoothing over six passes are presented. The C1 and C3 techniques can be modified to employ a floating threshold. The notation C1f and C3f is used for referring to these modified versions. They are included for additional insight.
Table 4.1: Numerical results for unit cube benchmark system.

<table>
<thead>
<tr>
<th>Case</th>
<th>Min. dihedral</th>
<th>Max. dihedral</th>
<th>% Dihedral angles &lt; 6°</th>
<th>12°</th>
<th>18°</th>
<th>162°</th>
<th>168°</th>
<th>174°</th>
<th>Time (ms)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Init.</td>
<td>0.369°</td>
<td>179°</td>
<td>0.0912</td>
<td>0.514</td>
<td>1.35</td>
<td>0.284</td>
<td>0.111</td>
<td>0.0193</td>
<td>N/A</td>
</tr>
<tr>
<td>D1</td>
<td>16.2°</td>
<td>158°</td>
<td>0</td>
<td>0</td>
<td>0.132</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>8.88</td>
</tr>
<tr>
<td>D2</td>
<td>13.5°</td>
<td>161°</td>
<td>0</td>
<td>0</td>
<td>0.332</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>7.92</td>
</tr>
<tr>
<td>D3</td>
<td>13.3°</td>
<td>161°</td>
<td>0</td>
<td>0</td>
<td>0.414</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>7.95</td>
</tr>
<tr>
<td>D4</td>
<td>14.8°</td>
<td>159°</td>
<td>0</td>
<td>0</td>
<td>0.0944</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>10.1</td>
</tr>
<tr>
<td>C1</td>
<td>10.1°</td>
<td>164°</td>
<td>0.0243</td>
<td>0.553</td>
<td>0.0143</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>8.56</td>
</tr>
<tr>
<td>C2</td>
<td>10.0°</td>
<td>164°</td>
<td>0.0344</td>
<td>0.612</td>
<td>0.0182</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>8.35</td>
</tr>
<tr>
<td>C3</td>
<td>10.0°</td>
<td>165°</td>
<td>0.132</td>
<td>1.07</td>
<td>0.0712</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>4.73</td>
</tr>
<tr>
<td>C4</td>
<td>16.7°</td>
<td>158°</td>
<td>0</td>
<td>0</td>
<td>0.00711</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>18.7</td>
</tr>
<tr>
<td>C1f</td>
<td>17.0°</td>
<td>158°</td>
<td>0</td>
<td>0</td>
<td>0.00843</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>18.7</td>
</tr>
<tr>
<td>C3f</td>
<td>16.9°</td>
<td>159°</td>
<td>0</td>
<td>0</td>
<td>0.00584</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>18.1</td>
</tr>
</tbody>
</table>

The success of a mesh smoothing technique relies upon the creation of high quality meshes at low computational cost. In order to evaluate the performance of the new techniques vis-à-vis the existing C1-C4, Clf, and C3f, both quality performance and computational time performance will be examined simultaneously. From Table 4.1, it is evident that D1-D4 yield a significantly improved quality mesh compared to the initial mesh. All extremal angles are essentially eliminated by these new techniques. It is also apparent that D1-D4 are more effective at removing the extremal angles than C1-C3 for this benchmark system. C3 is the poorest performer of all. However, C4, C1f, and C3f produce a comparable quality mesh to the new techniques. It is also apparent that C1-C3 require computational time similar to D1-D4. Furthermore, C4, C1f, and C3f are approximately twice as costly as any of the other tested techniques. Overall, it seems that D1-D4 are either superior or equivalent to the existing techniques in both mesh quality improvement and computational cost. Figs. 4.1-4.6 show the percentage of angles in each six degree bin (30 bins total) for varying techniques and levels of magnification.
Figure 4.1: Distribution of dihedral angles for C1-C4.

Figure 4.2: Distribution of dihedral angles for D1-D4.
Figure 4.3: Distribution of dihedral angles comparison of D1-D4 and C4.

Figure 4.4: Distribution of dihedral angles comparison of D1-D4 and C4 (small angles).
Figure 4.5: Distribution of dihedral angles comparison of D1-D4 and C4 (mid-angles).

Figure 4.6: Distribution of dihedral angles comparison of D1-D4 and C4 (large angles).
Fig. 4.1 shows that C4 is the most successful technique out of C1-C4 for eliminating extremal angles. Fig. 4.2 confirms that D1-D4 effectively remove all extremal angles from the initial mesh. Hence, Figs. 4.3-4.6 compare the quality performance of D1-D4 and C4. The general profile of the compared techniques can be seen in Fig. 4.3. Fig. 4.4 specifically focuses on small dihedral angles. Both new and existing techniques are successful at eliminating angles below 10°. There is a minor divergence in the performance between 10° and 15°. Fig. 4.6 provides a comparison of performance for large angles. All angles above 160° are eliminated equally well by D1-D4 and C4. Below this value, a minor divergence occurs.

The minor divergences that were observed between D1-D4 and C4, generally occur at the outer limits of what is considered “extremal”. It could be argued that the removal of these angles is crucial and that C4 should be accorded extra merit for its slightly better performance in this regard. However, if one considers that C4 is twice as computationally expensive as D1-D4, it is expected that D1-D4 would surpass C4 for these outer extremal angles given a few additional iterations.

It is also worthwhile to note that the initial unit cube mesh had a relatively high quality to begin with. However, even a very small number of very poor quality tetrahedral elements can significantly degrade solution accuracy and efficiency [40-44].
4.4 Cuboidal Capacitor Benchmark System

The second benchmark system consists of a series of three test cases based on an electrostatic benchmark problem: one-eighth of an air-filled, concentric, cuboidal capacitor – the 3-D analog to the standard 2-D “L” benchmark problem used for adaptive mesh quality analysis [31]. The corresponding geometry is shown in Fig. 4.7 (along with a vertex distribution for test case #3). The conductor boundary conditions are 1V on the small, inner cube and 0V on the outer cube. The symmetry planes are defined by $x=0$, $y=0$, and $z=0$ between the two conductors.

![Cuboidal capacitor 3-D test problem](image)

Figure 4.7: Cuboidal capacitor 3-D test problem (one-eighth geometry) and vertex distribution for adaptively refined mesh (test case #3).

Test case #1 deals with an initial mesh of the problem region (25,154 tetrahedra). Test case #2 (25,644 tetrahedra) focuses on the more demanding scenario of poor quality tetrahedra resulting from uniform refinement of an initial mesh. Test case #3 extends the previous case by an adaptive refinement, focusing elements near the inner conducting cube (26,316 tetrahedra). Just as for the unit cube benchmark, the objective is to
maximize the minimum sine of dihedral angles of the tetrahedra incident on the vertex under consideration [22, 27]. The initial threshold value is set to 10°. For those techniques that use a floating threshold, the threshold value is updated to the global minimum dihedral angle in the mesh plus 5° after each smoothing pass. Smoothing is performed over six passes.

The results for the three test cases are summarized in Tables 4.2-4.4. Global minimum and maximum dihedral angles, a dihedral angle distribution and total time required to perform smoothing over six passes are presented. For reference, Figs. 4.8-4.9 show the percentage of angles in each six degree bin (30 bins total) for test case #1 and test case #3, respectively.

The test case #1 results in Table 4.2 are somewhat similar to the unit cube benchmark results in Table 4.1. The respective meshes have comparable quality and number of tetrahedra. In fact, Table 4.2 directly corroborates the earlier observation that D1-D4 are either superior or equivalent to the existing techniques in both mesh quality improvement and computational cost. Although the initial mesh associated with test case #1 has a relatively high quality, even very few poor tetrahedral elements can be detrimental to solution accuracy and efficiency [40-44].
Table 4.2: Numerical results for cuboidal capacitor test case #1.

<table>
<thead>
<tr>
<th>Case</th>
<th>Min. dihedral</th>
<th>Max. dihedral</th>
<th>% Dihedral angles &lt; 6°</th>
<th>% Dihedral angles &gt; 12°</th>
<th>% Dihedral angles &gt; 18°</th>
<th>% Dihedral angles &gt; 162°</th>
<th>% Dihedral angles &gt; 168°</th>
<th>% Dihedral angles &gt; 174°</th>
<th>Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Init</td>
<td>0.854</td>
<td>179</td>
<td>0.114</td>
<td>0.510</td>
<td>1.25</td>
<td>0.280</td>
<td>0.111</td>
<td>0.0232</td>
<td>N/A</td>
</tr>
<tr>
<td>D1</td>
<td>14.3</td>
<td>159</td>
<td>0</td>
<td>0</td>
<td>0.0321</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>8.48</td>
</tr>
<tr>
<td>D2</td>
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<td>160</td>
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<td>0</td>
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<td>6.69</td>
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<tr>
<td>D3</td>
<td>15.1</td>
<td>161</td>
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<td>0.188</td>
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<td>0</td>
<td>0</td>
<td>8.33</td>
</tr>
<tr>
<td>D4</td>
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<td>158</td>
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<td>0</td>
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</tr>
<tr>
<td>C1</td>
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<td>0.0175</td>
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<tr>
<td>C2</td>
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<td>0.0358</td>
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<td>0.0199</td>
<td>0</td>
<td>0</td>
<td>7.67</td>
</tr>
<tr>
<td>C3</td>
<td>10.1</td>
<td>165</td>
<td>0</td>
<td>0.113</td>
<td>0.983</td>
<td>0.0662</td>
<td>0</td>
<td>0</td>
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<tr>
<td>C4</td>
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<td>0</td>
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</tr>
<tr>
<td>C1f</td>
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<td>158</td>
<td>0</td>
<td>0.00693</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
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<tr>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>13.7</td>
</tr>
</tbody>
</table>

Table 4.3 is associated with test case #2. The initial mesh quality is significantly worse than in test case #1. All techniques produce similar quality angle distributions, with D1, D3, D4, and C4 producing slightly better percentages of angles less than 18°. C4 required 25.1 s to complete its task. Notice, however, that D1, D3, and D4 required less than half that time to achieve comparable results. This highlights the computational cost advantages of the new techniques.

Table 4.4 shows that the test case #3 initial mesh quality is very poor. It is clear that global minimum and maximum dihedral angles benefit most from D1-D4. Also, D1 and D4 are the most successful at reducing the percentage of dihedral angles smaller than 6°. Remarkably, D1-D4 are the only techniques capable of eliminating dihedral angles greater than 174°. All the while, they maintain a computational cost that is greatly reduced compared to the existing techniques. This third test case clearly indicates the mesh quality improvement benefits of the new techniques versus the existing techniques.
Table 4.3: Numerical results for cuboidal capacitor test case # 2.

<table>
<thead>
<tr>
<th>Case</th>
<th>Min. dihedral</th>
<th>Max. dihedral</th>
<th>% Dihedral angles &lt; 6°</th>
<th>% Dihedral angles &gt; 162°</th>
<th>% Dihedral angles &gt; 168°</th>
<th>% Dihedral angles &gt; 174°</th>
<th>Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Init.</td>
<td>0.0112</td>
<td>179</td>
<td>10.0</td>
<td>9.62</td>
<td>6.97</td>
<td>3.96</td>
<td>N/A</td>
</tr>
<tr>
<td>D1</td>
<td>2.63</td>
<td>176</td>
<td>0.0431</td>
<td>0.532</td>
<td>0.0711</td>
<td>0.0155</td>
<td>11.0</td>
</tr>
<tr>
<td>D2</td>
<td>2.63</td>
<td>176</td>
<td>0.0422</td>
<td>0.805</td>
<td>0.115</td>
<td>0.0155</td>
<td>13.0</td>
</tr>
<tr>
<td>D3</td>
<td>2.67</td>
<td>176</td>
<td>0.0423</td>
<td>0.528</td>
<td>0.0764</td>
<td>0.0154</td>
<td>11.6</td>
</tr>
<tr>
<td>D4</td>
<td>3.05</td>
<td>175</td>
<td>0.0365</td>
<td>0.578</td>
<td>0.0727</td>
<td>0.0123</td>
<td>11.0</td>
</tr>
<tr>
<td>C1</td>
<td>3.43</td>
<td>169</td>
<td>0.0238</td>
<td>0.438</td>
<td>0.0409</td>
<td>0.00867</td>
<td>48.5</td>
</tr>
<tr>
<td>C2</td>
<td>3.56</td>
<td>175</td>
<td>0.0241</td>
<td>0.476</td>
<td>0.0398</td>
<td>0.00923</td>
<td>37.7</td>
</tr>
<tr>
<td>C3</td>
<td>3.56</td>
<td>175</td>
<td>0.0207</td>
<td>0.628</td>
<td>0.0334</td>
<td>0.00934</td>
<td>40.3</td>
</tr>
<tr>
<td>C4</td>
<td>3.56</td>
<td>175</td>
<td>0.0165</td>
<td>0.525</td>
<td>0.0425</td>
<td>0.00890</td>
<td>25.1</td>
</tr>
<tr>
<td>C1f</td>
<td>3.43</td>
<td>175</td>
<td>0.0199</td>
<td>0.524</td>
<td>0.0404</td>
<td>0.00865</td>
<td>34.4</td>
</tr>
<tr>
<td>C3f</td>
<td>3.56</td>
<td>175</td>
<td>0.0223</td>
<td>0.775</td>
<td>0.0507</td>
<td>0.00891</td>
<td>28.0</td>
</tr>
</tbody>
</table>

Table 4.4: Numerical results for cuboidal capacitor test case # 3.

<table>
<thead>
<tr>
<th>Case</th>
<th>Min. dihedral</th>
<th>Max. dihedral</th>
<th>% Dihedral angles &lt; 6°</th>
<th>% Dihedral angles &gt; 162°</th>
<th>% Dihedral angles &gt; 168°</th>
<th>% Dihedral angles &gt; 174°</th>
<th>Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Init.</td>
<td>0.0127</td>
<td>179</td>
<td>10.3</td>
<td>9.54</td>
<td>6.83</td>
<td>3.86</td>
<td>N/A</td>
</tr>
<tr>
<td>D1</td>
<td>5.25</td>
<td>173</td>
<td>0.00654</td>
<td>0.507</td>
<td>0.0421</td>
<td>0</td>
<td>23.0</td>
</tr>
<tr>
<td>D2</td>
<td>4.73</td>
<td>174</td>
<td>0.0184</td>
<td>0.759</td>
<td>0.0654</td>
<td>0</td>
<td>24.2</td>
</tr>
<tr>
<td>D3</td>
<td>5.25</td>
<td>173</td>
<td>0.0113</td>
<td>0.550</td>
<td>0.0722</td>
<td>0</td>
<td>18.1</td>
</tr>
<tr>
<td>D4</td>
<td>5.89</td>
<td>172</td>
<td>0.00352</td>
<td>0.566</td>
<td>0.0387</td>
<td>0</td>
<td>18.9</td>
</tr>
<tr>
<td>C1</td>
<td>0.0147</td>
<td>179</td>
<td>0.0118</td>
<td>0.544</td>
<td>0.0471</td>
<td>0.00336</td>
<td>59.8</td>
</tr>
<tr>
<td>C2</td>
<td>3.12</td>
<td>176</td>
<td>0.00804</td>
<td>0.460</td>
<td>0.0279</td>
<td>0.00293</td>
<td>45.6</td>
</tr>
<tr>
<td>C3</td>
<td>3.12</td>
<td>176</td>
<td>0.0107</td>
<td>0.637</td>
<td>0.0374</td>
<td>0.00283</td>
<td>46.7</td>
</tr>
<tr>
<td>C4</td>
<td>3.12</td>
<td>176</td>
<td>0.00876</td>
<td>0.533</td>
<td>0.0508</td>
<td>0.00285</td>
<td>27.8</td>
</tr>
<tr>
<td>C1f</td>
<td>0.0133</td>
<td>179</td>
<td>0.0844</td>
<td>0.693</td>
<td>0.171</td>
<td>0.00477</td>
<td>30.8</td>
</tr>
<tr>
<td>C3f</td>
<td>3.12</td>
<td>176</td>
<td>0.0109</td>
<td>0.820</td>
<td>0.0575</td>
<td>0.00290</td>
<td>30.5</td>
</tr>
</tbody>
</table>
Figure 4.8: Distribution of dihedral angles for test case # 1.

Figure 4.9: Distribution of dihedral angles for test case # 3.
Chapter 5

Theoretical Evaluation of New Mesh Improvement Systems

It is well known that the accuracy and efficiency of the finite element method can be directly affected by very few poor quality tetrahedral elements [32, 40-44]. For instance, a single poor quality element can cause the solution to be strongly in error throughout the entire mesh and lead to ill-conditioned finite element matrices. The effects of ill-conditioning are often related to a slowdown of iterative solvers and large round-off errors in the finite element solution [40]. Moreover, the definition of “high quality” is usually subjective and has not been thoroughly characterized. In the computational geometry and computer science spheres, poor quality is often synonymous with a large deviation from the equilateral shape. A purely geometric indicator based on this concept does not fully characterize the impact of mesh quality on finite element accuracy and efficiency. In particular, geometric quality measures do not address the full mathematical connections between mesh geometry, interpolation errors, discretization errors, and matrix conditioning. Several decades after the invention of the finite element method, these connections are yet to be solidified.

Recent efforts have led to error bounds and first-order tetrahedral element quality measures based on the theory of interpolation error, discretization error, and matrix conditioning. Using these new indicators, one may directly evaluate the performance of mesh improvement systems in terms of finite element accuracy and efficiency. One may also employ the indicators as mesh improvement objective functions.
To achieve the highest levels of efficacy, carefully selected quality measures may be used for “guiding” a stage of the finite element process and making locally optimal changes at the outset. This is in contrast to blindly applying the same algorithm, regardless of the local situation. For example, an unguided mesh refinement would apply the same technique (e.g., edge bisection) to each element in the tetrahedral mesh without considering the prevailing quality of the local tetrahedra at each step. Inherent in this unguided operation is the assumption that the mesh will be repaired afterward. The extra cost and difficulty associated with repairing a poor mesh may well be avoided by using guided operations.

No matter the context, it is clear that mesh quality evaluations are essential for achieving optimal accuracy and efficiency in multiple stages of finite element analysis. The following examines various mesh quality indicators for the elements most often used in \( h \)-type adaption: first-order tetrahedral elements.

### 5.1 Geometric Mesh Quality Measures

Geometric mesh quality measures evaluate the shape of tetrahedra based on purely geometric characteristics. Although their use is widespread in the computational geometry and computer science domains, geometric measures are not sufficient to fully characterize tetrahedra in the context of finite element accuracy and efficiency. Commonly used benchmark tests for geometric quality measures are based on a specific distortion of an equilateral tetrahedron [33, 34]. For instance, a common basis for comparison is a tetrahedral element with three fixed vertices and a fourth mobile vertex \( v \). The quality \( Q \) of such a tetrahedral element is dependent on \( v \) (i.e., \( Q(v) \)). In order to
further facilitate comparisons between measures, certain baseline characteristics have been established. A quality measure that satisfies the following three conditions is considered “fair” [34]:

(i) All degenerate elements (i.e., having all vertices in the same plane) have a $Q = 0$;
(ii) Scale-invariance: elements with different sizes and same shape have identical $Q$;
(iii) Normalization: $Q$ has a maximum value of one (equilateral tetrahedron).

Geometric measures often employ a ratio of quantities such as volume, edge lengths and radii of spheres associated with the tetrahedral shape. The circumsphere radius $R_c$ is the radius of the sphere passing through all four vertices of a tetrahedron. The insphere radius $R_i$ is the radius of the sphere inscribed in a tetrahedron such that each face of the tetrahedron is tangent to the sphere. Both are common quantities associated with tetrahedral shape. A normalized version of the ratio of these two quantities,

$$\alpha = \frac{3R_i}{R_c},$$  \hspace{1cm} (5.1)

achieves a value of one for equilateral tetrahedra [33]. Elements having a lower value are considered poorer quality. The $\alpha$ measure correctly identifies tetrahedra that diverge from the equilateral shape for four common cases [33]. Similar performance can be achieved using a ratio of tetrahedral volume $V$ to cubed average edge length $l_{\text{avg}}^3$ [35],

$$\beta = 6\sqrt{2} \frac{V}{l_{\text{avg}}^3}. \hspace{1cm} (5.2)$$

In general, a quality measure should be as computationally inexpensive as possible due to repeated evaluations during the adaptive finite element process. A variant of the $\beta$
measure uses the \textit{rms} edge length $l_{rms}$ to improve computational efficiency [33]. The $\alpha$ measure and both versions of the $\beta$ measure are fair and succeed in identifying distorted tetrahedra with similar fidelity. A notable (non-fair) measure,

$$\omega = \frac{l_{\text{min}}}{l_{\text{max}}}$$  \hspace{1cm} (5.3)

is only sensitive to major distortions of an edge length from the equilateral baseline case and does not penalize slivers significantly enough [33]. Similarly, the ratio

$$\tau = \frac{l_{\text{max}}}{2R}$$  \hspace{1cm} (5.4)

is only successful in one of four standard benchmark test cases [33]. In fact, it often prefers slivers over equilateral tetrahedra.

The preceding discussion is concerned solely with distortions from the equilateral shape. Although non-equilateral tetrahedra are known to negatively impact finite element accuracy and efficiency, neither the successful measures $\alpha$ and $\beta$, nor the unsuccessful ones are sufficient for evaluating tetrahedra in the finite element context. This is attributable to the fact that none of the geometric measures is theoretically linked to interpolation errors, discretization errors, or matrix conditioning. Although extensive reviews of geometric mesh quality indicators may be found in the literature, they are generally of limited use for the finite element practitioner [37]. The following section will discuss indicators and error bounds that are theoretically linked to a tetrahedral element's fitness for interpolation, discretization, and matrix conditioning. These theoretical indicators will be used to corroborate the mesh quality improvement capabilities of the new mesh smoothing techniques D1, D2, D3, and D4.
5.2 Interpolation Error

Interpolation fitness is of utmost importance to finite element accuracy. In fact, discretization error often cannot be bounded without bounds on interpolation error. Much of the work on error estimators is based on functional analysis and embedding theorems [38, 39]. Rules of thumb can occasionally be drawn from these mathematical results. For instance, when dealing with triangular finite element meshes, small angles are not harmful to interpolation and discretization errors, whereas large angles should be avoided altogether [38]. Furthermore, it is also known that small angles can negatively impact stiffness matrix conditioning and solution efficiency. Based on these observations, one may conclude that the sine of dihedral angles in a triangular mesh should be bounded away from 0. However, functional analysis often leads to error estimators that are asymptotic in nature and that ignore the constants associated with error bounds. It is not clear how these results could be used in the mesh improvement context for making very fine distinctions between finite elements. Beyond the theoretical realm, these estimators have limited usefulness. Conversely, constructing mesh quality measures based on precise (nearly tight) error bounds is a plausible alternative [40].

To focus ideas, consider a problem domain \( \Omega \) along with an associated tetrahedral mesh \( T \). The true solution \( u_*(r) \) is a continuous scalar function defined over \( T \). Let \( \widetilde{u}_i(r) \) correspond to a piecewise linear approximation of \( u_*(r) \), where \( \widetilde{u}_i(v) = u_*(v) \) at each vertex \( v \) in \( T \). The approximation \( \widetilde{u}_i(r) \) is linear over each tetrahedron in \( T \).
When investigating the interpolation fitness of first-order tetrahedral finite elements, interpolation error is discussed in two veins: (i) the difference between the interpolated function and exact solution; and (ii) the difference between the gradient of the interpolated function and the gradient of the exact solution [40]. In particular, errors in the gradient are very sensitive to element size and shape, and are known to directly influence discretization errors [40]. Evaluated within an infinity norm, the two types of interpolation errors may be written as $\| \tilde{u}_j - u_* \|_\infty$ and $\| \nabla \tilde{u}_j - \nabla u_* \|_\infty$. These two expressions correspond to the maximum pointwise interpolation error over an element and the maximum pointwise error in the interpolated gradient over an element, respectively.

The general mathematical framework surrounding interpolation error bounds will now be described. One or more assumptions must first be made about the scalar function $u_*(r)$ being approximated over the mesh $T$. This assumption may be based on a property that $u_*(r)$ is known to satisfy throughout the problem domain or a quantity that is readily available during error estimation [40]. One possibility is to combine a smoothness constraint with a constraint on curvature within each first-order tetrahedral element. The curvature constraint would restrict the magnitude of the directional second derivative of $u_*(r)$ to not exceed $k_{loc}$ (per-element curvature bound) anywhere in a given first-order tetrahedral element. Of course $k_{loc}$ may vary from one element to the next. The curvature constraint may be expressed in the form,

$$|\tilde{u}_d'(r)| \leq k_{loc}$$

(5.5)
where \( d \) is the unit direction vector. It can be shown that

\[
u^*_d(r) = d^\top H(r)d
\]  
(5.6)

where \( H(r) \) is the Hessian matrix of \( u_*(r) \) [40]. This constraint on \( u_*(r) \) allows for the derivation of bounds on interpolation errors over a first-order tetrahedral finite element (Table 5.1). The min-containment radius \( R_{mc} \) refers to the radius of the smallest sphere that encloses the tetrahedral element. \( R_c \) is the radius of the circumsphere of the element. \( A_f \), \( V_t \), and \( l_{ij} \) are the area of a triangular face of the tetrahedron, volume of the tetrahedron and length of an edge connecting vertices \( v_i \) and \( v_j \), respectively. When \( k_{loc} \) is not available for the element of interest, a comparison of elements can be made by dropping this factor.

<table>
<thead>
<tr>
<th>Interpolation error</th>
<th>Upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>( |\vec{u}<em>i - u</em>*|_w )</td>
<td>( k_{loc} \frac{R_{mc}^2}{2} )</td>
</tr>
<tr>
<td>( |\nabla \vec{u}<em>i - \nabla u</em>*|_w )</td>
<td>( k_{loc} \frac{1}{6V} \sum_{1 \leq j \leq 4} A_i A_j l_{ij}^2 + \max_j \sum_{j \neq i} A_j l_{ij} ) ( \frac{\sum_{m=1}^4 A_m}{2} )</td>
</tr>
</tbody>
</table>

The upper bound on \( \|\vec{u}_i - u_*\|_w \) was shown to be tight; for any tetrahedron with min-containment radius \( R_{mc} \), there exists a function \( u_*(r) \) such that [39],

\[
\|\vec{u}_i - u_*\|_w = k_{loc} \frac{R_{mc}^2}{2}.
\]  
(5.7)

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It is worthwhile to note that the Delaunay algorithm in three dimensions minimizes the maximum $R_{mc}$, as compared with all other tetrahedralizations of the arbitrary set of vertices [7]. For a tetrahedral mesh having $k_{loc}$ identical for each element, the Delaunay algorithm minimizes the maximum bound on interpolation error over the mesh [40].

Refinement by longest-edge bisection can be justified by observing that for a tetrahedron $R_{mc} \leq \sqrt{3/8}l_{max}$ [40]. A looser upper bound on interpolation error can then be expressed,

$$\|\tilde{u}_i - u_*\|_\infty \leq \frac{3k_{loc}l_{max}^2}{16}.$$ 

(5.8)

Based on this result, a case can be made for targeting the maximum edge length during refinement until all edges are shorter than an a priori tolerance. The alternative upper bound in Eq. (5.8) is also easier to compute than $R_{mc}$.

Table 5.1 also lists bounds for the maximum pointwise error in the interpolated gradient over an element, $\|\nabla \tilde{u}_i - \nabla u_*\|_\infty$. Typically, bounds on finite element discretization error can only be obtained if both interpolation errors are bounded. The finite element approximation and $\tilde{u}_i(r)$ are both piecewise linear functions. In general, the two functions differ because the finite element approximation does not equal the true solution at the mesh vertices. Notice from Table 5.1 that the bounds on $\|\nabla \tilde{u}_i - \nabla u_*\|_\infty$ are quite sensitive to poorly shaped elements. This error can grow without bound for elements approaching zero volume. Further insight can be gained by examining a weaker upper bound,
where $\theta_{kl}$ is the dihedral angle at the edge connecting $v_k$ and $v_l$, and $i, j, k, l$ are distinct in each term of the summation [40]. The appearance of $\sin \theta_{kl}$ in the denominator suggests that an infinite error may result from dihedral angles approaching 0° or 180°. However, the behavior of the opposite edge $l_{i,j}$ must also be taken into account. If the length of $l_{i,j}$ approaches zero at the same rate as $\sin \theta_{kl}$, the bound does not approach infinity. For the specific case of a dihedral angle approaching 0° and an opposite edge that is not, a large dihedral angle must also exist within the tetrahedron. For a dihedral angle approaching 180°, the opposite edge is becoming longer. Thus, tetrahedra having a dihedral angle approaching 180° have upper bounds on $\| \nabla u_i - \nabla u_* \|$ that are arbitrarily large. To summarize these two problematic cases, dihedral angles near 180° should be avoided altogether, whereas angles near 0° are only harmful when a large angle is present as well. Nevertheless, small dihedral angles degrade finite element matrix conditioning and finite element efficiency [40].

Quality measures may directly be formulated from the bounds on interpolation error in Table 5.1. Taking the reciprocal of the bounds leads to measures that are sensitive to both size and shape (Table 5.2). Maximizing an element’s measure is equivalent to minimizing its error bound. The $k_{loc}$ factor could be dropped, but is included to emphasize the direct link to the error bounds.
Table 5.2: Quality measures based on interpolation error bounds for first-order tetrahedra.

<table>
<thead>
<tr>
<th>Interpolation error</th>
<th>Upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>$|\tilde{u}<em>j - u</em>*|_{\infty}$</td>
<td>$\left[ k_{loc} \frac{R_{mc}^2}{2} \right]^{-1}$</td>
</tr>
<tr>
<td>$|\nabla \tilde{u}<em>j - \nabla u</em>*|_{\infty}$</td>
<td>$\left[ k_{loc} \frac{1}{6V} \sum_{1 \leq i \leq 4} A_i f_i^2 + \max_j \sum_{j \neq i} A_j f_j \sum_{m=1}^{4} A_m \right]^{-1}$</td>
</tr>
</tbody>
</table>

Two useful properties of quality measures that facilitate inclusion into a mesh smoothing system and prevent difficulties with optimization-based smoothing are, (i) the gradient of the quality measure is non-zero and finite for degenerate elements; and (ii) the quality measure is a smooth function of the free vertex $v$ [40]. Optimization-based mesh smoothing algorithms rely on gradient evaluations of the quality measure to choose search directions. The gradient property is critical when optimization-based smoothing attempts to optimize zero gradient degenerate elements. Infinite gradients would lead to numerical difficulties. The non-zero (finite) gradient condition for degenerate elements is satisfied by all measures in Table 5.2. The smoothness condition constrains the type of optimizer (smooth or non-smooth) that can be used to solve the smoothing problem. Although non-smooth optimization algorithms are available, they are typically more computationally expensive than algorithms for optimization of smooth functions. A trivial example of a non-smooth quality measure is the minimum dihedral angle. It has a gradient that changes abruptly as the identity of the minimum angle changes. It follows that this measure cannot be optimized using conventional smooth optimizers.
Scale-invariance should also be considered when evaluating quality measures. Although interpolation errors are intrinsically tied to both size and shape, it is often desirable to evaluate the impact of poor quality alone. Scale-invariant measures are most appropriate when comparing meshes based solely on element quality. Typically, the mesh improvement module receives a mesh from the refinement module. Presumably, the mesh refinement module possesses information about the ideal sizes of elements (e.g., from an error estimator) and the refinement is part of an overall adaptive scheme that has established a certain grading of element sizes throughout the mesh. In such a case, the function of the mesh improvement stage is to remove poorly shaped tetrahedral elements without regard for element size. Scale-invariant measures are useful in this situation. In essence, scale-invariance isolates the performance of the mesh improvement module from both the mesh generation and mesh refinement stages. Scale-invariant measures may be formulated based on the size-and-shape measures in Table 5.2. This can be accomplished by a procedure that scales the element uniformly until reaching unit volume, and then evaluates its quality using the size-and-shape measure [40]. This way, an element's error bound is compared with the bound of other elements that are the same size. Incorporating the smoothness, scale-invariance and gradient properties into the $\| \nabla \bar{u}_T - \nabla u_* \|_m$ measure in Table 5.2, and dropping the constants yields,

$$Q_s = V \left[ \sum_{m=1}^{4} A_m \left( \sum_{I \in \mathbb{S}_{1,4}} A_{I,E}^2 \right)^{3/4} \right]^{1/4}$$

(5.10)
Error bounds and quality measures can be valuable for guiding many stages of the finite element process, including mesh generation, mesh refinement, and mesh improvement (smoothing and local transformations). A single bound or measure can be used, or an element may be required to pass separate tests for different criteria. Extreme cases arise where the ideal elements for interpolation, discretization, and matrix conditioning are diametrically opposed. Although optimization-based smoothing only allows for a single objective function, several measures can be “combined”. The weighted harmonic mean,

\[ \frac{1}{Q_c} = \frac{\omega}{Q_1} + \frac{1-\omega}{Q_2} \]  

(5.11)

where \( Q_c \) is the combined quality measure and \( \omega \) is chosen to regulate the relative importance of \( Q_1 \) and \( Q_2 \) is a straightforward way of performing this combination [40]. If an element obtains a low value for either of the two measures, this low value will dominate the combined measure.

5.3 Discretization Error

Finite element accuracy is governed by the difference between the finite element approximation \( \tilde{u} \), and the true solution \( u \). This discretization error arises due to the approximation of a continuous partial differential equation by a discrete system of linear equations resulting from the finite element method. The impact of mesh quality on accuracy is clear for the case of triangular finite elements. Many celebrated papers have been published (e.g., [38]), recommending constraints on a triangular mesh that will help mitigate problems with accuracy. Among the many recommendations, one may mention the avoidance of flat elements and extremal angles, as well as bounds on the ratio of maximum element edge length to the diameter of the inscribed circle [41].
The relationship between discretization error and tetrahedral mesh quality cannot be fully characterized without knowledge of the partial differential equation being solved [40]. There exists a close link between discretization and interpolation errors. Strategies for reducing interpolation error often have a similar effect on discretization error. The bounds on $\|\tilde{u}_i - u_*\|_{\infty}$ can be reduced by using smaller elements (i.e., $l_{\text{max}}$ dependency in Eq. (5.8)). However, the error $\|\nabla \tilde{u}_i - \nabla u_*\|_{\infty}$ is much more sensitive to poor tetrahedral shape and grows without bound for angles approaching 180° [40]. Typically, the discretization error cannot be bounded unless both interpolation errors are bounded.

The finite element solution $\tilde{u}(r)$ for first-order tetrahedral elements is a piecewise linear approximation over the problem domain $\Omega$. However, unlike the interpolating function $\tilde{u}_i(r)$, the finite element approximation is not constrained to be equal to the true solution at the vertices of each tetrahedral element. Consequently, the finite element solution has the potential to approximate the exact solution more accurately than the interpolating function. Clearly, the bounds on interpolation error are not directly applicable to the discretization error.

Discretization errors are sometimes measured within a specific norm. For electrostatic and magnetostatic problems, this norm is usually the field energy (over an element $\Gamma$),

$$
\left\| \tilde{u}_i \right\|_{\epsilon_{\Gamma}} = \left( \int_{\Gamma_i} |\nabla \tilde{u}_i|^2 \, dV \right)^{1/2}.
$$

(5.12)

The finite element method finds the approximation that minimizes the discretization error over the entire problem domain $\Omega$ (within the energy norm).
Since the finite element solution \( \tilde{u} \) is optimal, a global bound on discretization error can be obtained via bounds on interpolation error as follows,

\[
\| \tilde{u} - u_* \|_E \leq \left( \int_{\Omega} \| \nabla \tilde{u} - \nabla u_* \|^2 dV \right)^{1/2} \leq \sum_{i \in \text{cells}} V_i \left\| \nabla \tilde{u}_i - \nabla u_* \right\|^2_{\text{ext}}^{1/2}.
\]  

(5.14)

It is normally expected that the finite element solution converges to the true solution as the size of the elements in the mesh tends to zero. However, this outcome only holds if both interpolation errors go to zero as well. In general, dihedral angles approaching 180° and large tetrahedral elements (large \( l_{\text{max}} \)) can significantly worsen the discretization error. The inequality in Eq. (5.14) applies to electrostatic and magnetostatic problems that employ the energy norm. In other formulations, the relative influence of the two interpolation errors will depend on the coefficients of the partial differential equation.

Discretization error can also be investigated by examining finite element stiffness matrices [37, 42-44]. Tsukerman compares the interpolating function \( \tilde{u}_i(r) \) to the first-order Taylor approximation \( \tilde{u}_r \) of the exact potential around a point \((x_0, y_0, z_0)\) in a given tetrahedral element [37],

\[
\tilde{u}_r(r) = u_*(r_0) + \nabla u_*(r_0) \cdot (r - r_0).
\]  

(5.15)

Notice that the approximations of node values by both \( \tilde{u}_i \) and \( \tilde{u}_r \) are shape independent. However, it can be shown that the energy norm approximation of \( u_* \) by Taylor approximation is uniform and shape independent, whereas the approximation by the
interpolating function may depend on shape [37]. These two key observations lead to the formulation of a quality measure for tetrahedral node elements [37, 42-44].

Hence, \( \tilde{u}_f \) may be worse than \( \tilde{u}_r \), in the energy norm approximation of \( u_r \),

\[
\| \tilde{u}_f - u_r \|_E \geq \| \tilde{u}_r - u_r \|_E .
\]  

(5.16)

Tsukerman attributes this apparent discrepancy to the eigenvalues of the finite element stiffness matrix. If the stiffness matrix has a large eigenvalue, the energy norm difference between \( \tilde{u}_f \) and \( \tilde{u}_r \) may become correspondingly large [37]. Although it is known that poorly conditioned finite element matrices lead to problems with the efficiency of iterative solvers, this new theory indicates that ill-conditioning is also a source of reduced accuracy. Tsukerman proposes a new “general accuracy condition” based on the maximum eigenvalue of the element stiffness matrix. Hence, the following global bound on discretization error can be used as an a priori measure of finite element mesh quality,

\[
\| \tilde{u} - u \|_E \leq \| \tilde{u}_f - u_r \|_E \leq c \left( \sum_{t=\text{mesh}} V_t \left( \lambda_{\text{max}}(A_t) l_{\text{max}}^{2\kappa} + l_{\text{max}}^{2(m+1-p)} \right) \right)^{\frac{1}{2}}.
\]  

(5.17)

In Eq. (5.17), \( c \) is a generic constant (independent of element shape) which is not necessarily the same in all occurrences, \( \hat{A}_t \) is the usual element stiffness matrix divided by the element volume \( V_t \), \( l_{\text{max}} \) is the maximum edge length of the element and \( \lambda_{\text{max}}(\cdot) \) is the maximum eigenvalue operator [43]. The term \( m \) denotes the order of the local Taylor approximation, \( \kappa \) is the order of the Taylor approximation of the DOF of the exact solution. For first-order tetrahedral node elements, \( m=1 \) and \( \kappa=2 \). The \( p \) term is the order of the highest derivative included in the energy norm (\( p=1 \) for field energy).

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Furthermore, Eq. (5.17) leads to a “minimum-maximum” angle condition between edges and faces, which states that these angles should be bounded away from $0^\circ$ and $180^\circ$. Additional results confirm that the maximum eigenvalue of the stiffness matrix and matrix conditioning play a significant role in finite element interpolation fitness [43].

Tsukerman identifies a quality measure that links geometric and algebraic accuracy criteria: the minimum singular value $\sigma_{\text{min}}$ of the element “edge shape matrix” $E$ [42]. This indicator provides a measure of the flatness of a tetrahedral element, while also being directly related to the maximum eigenvalue of the scaled stiffness matrix $\hat{A}_i$ on which the original error estimate in Eq. (5.17) is based. In fact, $\sigma_{\text{min}}^2$ is reciprocal to the maximum eigenvalue of $\hat{A}_i$ (which governs the interpolation error).

The $E$ matrix is three-by-six and has unit vector columns directed along the element edges (in either of the two possible directions),

$$
E = \begin{bmatrix}
e_{1x} & e_{2x} & e_{3x} & e_{4x} & e_{5x} & e_{6x} \\
e_{1y} & e_{2y} & e_{3y} & e_{4y} & e_{5y} & e_{by} \\
e_{1z} & e_{2z} & e_{3z} & e_{4z} & e_{5z} & e_{6z}
\end{bmatrix}.
$$

It can be shown that the minimum singular value $\sigma_{\text{min}}$ of $E$ is sufficient to characterize the first-order finite element approximation of the potential over tetrahedral node elements (with a minimum value of zero for invalid tetrahedra that have six coplanar edges) [42]. More specifically, the finite element interpolation error over a single element $t$ is governed by,

$$
\|\hat{\mathbf{u}}_i - \mathbf{u}_i\|_{L_2} \leq c_l \max_{i} \sigma_{\text{min}}^{-1} (E_i) \sqrt{V_i},
$$

(5.19)
or for the whole domain,

\[ \| \bar{u} - u_i \| \leq \| \bar{u}_f - u_i \| \leq c \sqrt{V} \Omega_{\max} \sigma_{\min}^{-1}(E_i)^{1}_{\max}, \]  

(5.20)

where \( \sigma_{\min}(\cdot) \) is the minimum singular value operator [42]. Note that Krizek gives an equivalent criterion (asymptotically) from the geometric perspective: the maximum dihedral angle and the maximum planar angle in all four triangular faces should be bounded away from 180° [45].

In section 5.2, pointwise bounds on interpolation error were localized to individual elements. The bounds on discretization error are all global in nature, as pointwise bounds are not easy to derive. Typically, a poor quality element can cause substantial discretization errors in nearby elements [40].

### 5.4 Finite Element Efficiency and Stiffness Matrix Conditioning

The performance of a finite element analysis system is usually governed by the tradeoff between accuracy and efficiency. A high computational efficiency is crucial for a successful analysis and is directly influenced by mesh quality. The condition number of finite element matrices plays a central role in determining how much computational effort will be required to solve a system of linear equations and how large the associated round-off errors will ultimately be [40]. It follows that the link between mesh quality and stiffness matrix conditioning is an important one to address. Understanding this relationship leads to the formulation of mesh quality criteria for evaluating the fitness of tetrahedral elements in terms of finite element efficiency.
The solution of systems of linear equations arising from finite element analysis is a research area in its own right. Both iterative and direct methods are used in the finite element context to solve systems of the form \( Ax = b \). Indeed, solving large and sparse systems of linear equations is perhaps the most computationally expensive aspect of finite element analysis. While direct methods can arrive at a solution after a predetermined number of steps, iterative methods construct successive approximations to the true solution. Iterative methods are usually best suited for large and sparse systems because neither the factorization, nor the storage of \( A \) is required. The family of Krylov subspace methods is a class of iterative methods that is widely used (e.g., conjugate gradient method). The main computational kernels associated with Krylov subspace methods are inner products and matrix-vector products. The speed of convergence of iterative methods depends on the conditioning of the global stiffness matrix, with large condition number leading to slower performance [40]. Direct methods are more susceptible to round-off error in floating-point computations than to a slowdown. The size of the round-off error is linked to the global stiffness matrix condition number. Typically, Gaussian elimination loses accuracy at the rate of one decimal digit for every digit in the integer part of the condition number [40].

The relationship between element shape and matrix conditioning depends on the partial differential equation being considered. Poisson’s equation will be used here to clarify this link. Poisson’s equation may be written in the form

\[-\nabla^2 f(r) = g(r), \]

(5.21)
where \( g(r) \) is a known function of \( r \) and the goal is to find an approximation \( h(r) \) of \( f(r) \) subject to specific boundary conditions [40]. A four-by-four stiffness matrix \( S_{loc} \) is constructed for each linear tetrahedral element. A global \( n \)-by-\( n \) stiffness matrix \( S \) for the entire mesh is constructed via the matrix assembly process (where \( n \) is the number of mesh vertices). The computational effort required to solve the resulting system of linear equations is proportional to the condition number \( \kappa_S \) of \( S \), where

\[
\kappa_S = \frac{\lambda^{S}_{\text{max}}}{\lambda^{S}_{\text{min}}}. 
\]  

(5.22)

Thus, it is useful to characterize how the maximum and minimum eigenvalues of \( S \) are affected by tetrahedral mesh quality. Typically, \( \lambda^{S}_{\text{min}} \) is tied to the properties of the physical system. However, it can be shown that a lower bound for \( \lambda^{S}_{\text{min}} \) is proportional to the smallest element volume in the mesh and an upper bound is proportional to the greatest element volume [46]. In practice, the eigenvalue \( \lambda^{S}_{\text{max}} \) tends to have a much more pronounced effect on condition number than \( \lambda^{S}_{\text{min}} \). In fact, it can be shown that,

\[
\max_i \lambda^{S_{loc}}_{\text{max}} \leq \lambda^{S}_{\text{max}} \leq m \max_i \lambda^{S_{loc}}_{\text{max}},
\]  

(5.23)

where \( m \) is the maximum number of elements meeting at a single vertex in the mesh [40]. Thus, \( \lambda^{S}_{\text{max}} \) strongly depends on the maximum \( S_{loc} \) eigenvalues from among all element stiffness matrices [40]. Further analysis would yield a relationship describing the dependence of \( \lambda^{S_{loc}}_{\text{max}} \) on tetrahedral shape [40],

\[
\sum_{i=1}^{4} \frac{A_i^2}{27V} \leq \lambda^{S_{loc}}_{\text{max}} \leq \sum_{i=1}^{4} \frac{A_i^2}{9V}.
\]  

(5.24)
From Eqs. (5.23) and (5.24), it is evident that a single badly shaped element (approaching zero volume) can make $\lambda_{\max}^{\delta}$ arbitrarily large and severely compromise finite element solution efficiency. Furthermore, the impact of scale-variance should also be well understood. A uniform scaling of a tetrahedron will cause $\lambda_{\max}^{\delta}$ to grow linearly with the longest edge $l_{\max}$. In the context of Poisson’s equation, the shapes of the largest tetrahedra in the mesh may be more important than the shapes of the smaller ones.

To summarize, tetrahedral elements should be “small” and non-flat in order to keep a reasonable upper bound on $\lambda_{\max}^{\delta}$. Meanwhile, “very small” tetrahedral elements should be avoided so that a reasonable lower bound on $\lambda_{\min}^{\delta}$ remains intact. In general, poor quality meshes and highly non-uniform meshes are not conducive to a well-conditioned global stiffness matrix, nor to high efficiency of the finite element method.

5.5 Evaluation of New Mesh Improvement Systems

The proposed mesh improvement systems D1, D2, D3, and D4 were shown to outperform previous combined mesh smoothing techniques in both geometric mesh quality and computational cost [32]. This section focuses on evaluating the performance of the new family of mesh smoothing systems using a suite of mesh quality indicators. A description of the selected elemental mesh quality indicators $M_1 - M_5$ is now in order.

Parthasarathy proposed a variation on the $\beta$ measure in Eq. (5.2), in which average edge length is replaced by the $rms$ edge length to reduce cost [33].
As discussed in Section 5.1, $M_i$ is a fair, purely geometric measure that has fidelity comparable to the $\beta$ measure. The $M_i$ measure attains a value of one for equilateral tetrahedra and a value of zero for degenerate elements.

The shape of elements is usually controlled by the need to bound $\|\nabla \tilde{u}_i - \nabla u_\ast\|_\infty$. While the bounds on $\|\tilde{u}_i - u_\ast\|_\infty$ can be reduced by using smaller elements (i.e., $l_{\text{max}}$ dependency in Eq. (5.8)), the error $\|\nabla \tilde{u}_i - \nabla u_\ast\|_\infty$ is much more sensitive to poor tetrahedral shapes. In fact, $\|\nabla \tilde{u}_i - \nabla u_\ast\|_\infty$ grows without bound for angles approaching $180^\circ$ [40]. Shewchuk's scale-invariant measure (given in Eq. (5.10)) is used here to evaluate interpolation fitness. For convenience, it is renamed $M_2$,

$$M_2 = V_i \left[ \frac{\sum_{m=1}^{4} A_m}{\sum_{1 \leq i < j \leq 4} A_i A_j l_{ij}^2} \right]^{\frac{3}{2}}. \quad (5.26)$$

The normalized Baker quality criterion has a solid theoretical basis linking it to approximation accuracy for first-order tetrahedral finite elements [47]. In particular, the measure is fair and associated with interpolation error bounds suggested by approximation theory,

$$M_3 = 2\sqrt{6} \left( \frac{R_i}{l_{\text{max}}} \right). \quad (5.27)$$
As described in Section 5.3, Tsukerman’s minimum singular value of the edge shape matrix $E$ is theoretically linked to finite element accuracy. It is restated here as $M_4$,

$$M_4 = \sigma_{\text{min}}(E_i).$$

(5.28)

The final measure is related to the fitness of tetrahedral elements for stiffness matrix conditioning. In fact, $M_5$ is closely tied to Eq. (5.24) and follows from the discussion in Section 5.4 [40],

$$M_5 = \frac{V}{A_{\text{rms}}}^{\frac{1}{3}},$$

(5.29)

A benchmark system for Laplace’s equation (analogous to test case #2 in Section 4.4) is used to draw comparisons between the mesh smoothing techniques. This cuboidal capacitor electrostatic benchmark system (25,483 tetrahedra) focuses on the more demanding scenario of poor quality tetrahedra resulting from uniform refinement of an initial mesh. The corresponding geometry is shown in Fig. 4.7 (p. 38). The conductor boundary conditions are 1V on the small, inner cube and 0V on the outer cube.

In Table 5.3, mesh quality before and after smoothing is compared using the $M_1-M_5$ suite of mesh quality indicators. Computational cost and $\text{rms} \%$ error are also presented, with three significant figures used throughout. The $\text{rms} \%$ error was calculated using approximately 15,000 equally spaced sampling points throughout the cuboidal region. The accompanying Figs. 5.1-5.12 provide a graphical perspective on the numerical results of Table 5.3, as well as distributions of the $M_1-M_5$ indicators for selected mesh improvement techniques.
Time costs presented in Table 5.3 and Fig. 5.1 re-confirm the computational benefits of D1-D4 over the existing techniques. The results in Table 5.3 also show that D1-D4 outperform C1-C3f for the entire suite of indicators. Recall that $M_1-M_3$ cover the spectrum of theoretical solution accuracy, geometric mesh quality, and theoretical solution efficiency. At the same time, the new techniques provide an improved $rms$ % error throughout the entire cuboidal region compared to both the initial $rms$ error of 3.70%, and relative to the existing techniques. This practical finding corroborates the results associated with the theoretical mesh quality indicators. From Figs. 5.3-5.12, it is also apparent that the $M_1-M_3$ indicators all classify the new techniques in the same order of effectiveness: D4, D1, D3, and D2. While the $rms$ % error also identifies D1-D4 as the superior techniques, the same ordering is not apparent. It should be recalled that this $rms$ % error measure was evaluated over discrete sampling points, with only 0.03% separating first (D3) from fourth (D4). In general, D1-D4 are seen to outperform all other mesh smoothing techniques for the standard cuboidal capacitor benchmark system. Thus, D1-D4 are recommended for improved finite element solution accuracy and efficiency.
Table 5.3: Numerical results for cuboidal capacitor benchmark system.

<table>
<thead>
<tr>
<th>Case</th>
<th>Initial</th>
<th>Final</th>
<th>Mean</th>
<th>Min.</th>
<th>Max.</th>
<th>Mean</th>
<th>Final</th>
<th>Mean</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Time (s)</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>6.05</td>
<td>5.01</td>
<td>7.12</td>
<td>6.90</td>
</tr>
<tr>
<td>% Error</td>
<td>N/A</td>
<td>3.70</td>
<td>N/A</td>
<td>N/A</td>
<td>3.09</td>
<td>3.11</td>
<td>3.08</td>
<td>3.11</td>
</tr>
<tr>
<td>M1</td>
<td>0.334e-3</td>
<td>1.00</td>
<td>0.736</td>
<td>1.02e-2</td>
<td>1.00</td>
<td>0.769</td>
<td>0.760</td>
<td>0.769</td>
</tr>
<tr>
<td>M2</td>
<td>6.52e-05</td>
<td>0.165</td>
<td>0.129</td>
<td>1.71e-3</td>
<td>0.165</td>
<td>0.134</td>
<td>0.133</td>
<td>0.134</td>
</tr>
<tr>
<td>M3</td>
<td>2.85e-4</td>
<td>0.999</td>
<td>0.639</td>
<td>8.46e-3</td>
<td>0.999</td>
<td>0.672</td>
<td>0.661</td>
<td>0.671</td>
</tr>
<tr>
<td>M4</td>
<td>3.89e-4</td>
<td>1.41</td>
<td>0.952</td>
<td>1.23e-2</td>
<td>1.41</td>
<td>0.989</td>
<td>0.980</td>
<td>0.989</td>
</tr>
<tr>
<td>M5</td>
<td>1.71e-4</td>
<td>0.414</td>
<td>0.331</td>
<td>4.99e-3</td>
<td>0.414</td>
<td>0.343</td>
<td>0.340</td>
<td>0.343</td>
</tr>
</tbody>
</table>

*The "% Error" row contains rms values rather than mean values.*
Figure 5.1: Cost of mesh improvement systems for cuboidal capacitor benchmark.

Figure 5.2: The rms % error for cuboidal capacitor benchmark.
Figure 5.3: Mean $M_1$ geometric mesh quality indicator for cuboidal capacitor benchmark.

Figure 5.4: Distribution of $M_1$ geometric quality indicator for cuboidal capacitor benchmark.
Figure 5.5: Mean $M_2$ solution accuracy indicator for cuboidal capacitor benchmark.

Figure 5.6: Distribution of $M_2$ solution accuracy indicator for cuboidal capacitor benchmark.
Figure 5.7: Mean $M_3$ solution accuracy indicator for cuboidal capacitor benchmark.

Figure 5.8: Distribution of $M_3$ solution accuracy indicator for cuboidal capacitor benchmark.
Figure 5.9: Mean $M_s$ solution accuracy indicator for cuboidal capacitor benchmark.

Figure 5.10: Distribution of $M_s$ solution accuracy indicator for cuboidal capacitor benchmark.
Figure 5.11: Mean $M_3$ solution efficiency indicator for cuboidal capacitor benchmark.

Figure 5.12: Distribution of $M_3$ solution efficiency indicator for cuboidal capacitor benchmark.
Chapter 6

Conclusion

Mesh quality improvement is particularly important in $h$-adaptive finite element electromagnetics. The mesh generation and mesh refinement stages are prone to the creation of poor quality tetrahedra, which can significantly degrade solution accuracy and efficiency. For this reason, powerful and efficient mesh improvement systems are often a pre-requisite for successful $h$-adaptive finite element analysis.

Novel smoothing-based mesh improvement techniques D1, D2, D3, and D4 for $h$-adaptive finite element analysis with tetrahedra were described in Chapter 4. Through a series of standard electromagnetic benchmark tests, the new techniques were shown to significantly improve mesh quality while greatly reducing computational cost. In fact, D1-D4 were able to outperform or match the existing techniques in both computational cost and mesh quality improvement.

The links between mesh quality, and finite element accuracy and efficiency were explored in Chapter 5. A suite of finite element mesh quality indicators based on the theory underlying interpolation error, discretization error, and matrix conditioning were presented. Based on the suite of theoretical mesh quality indicators, techniques D1-D4 outperformed the existing mesh smoothing techniques in both finite element accuracy and efficiency, while achieving a significant reduction in cost. Experimental data corroborated the theoretical results.
6.1 Original Contributions Appearing in Publications

The new mesh smoothing techniques and related research described in Chapter 4 will appear in an upcoming issue of IEEE Transactions on Magnetics [32]. The research and findings were also the basis for a conference paper [48] and poster presentation at COMPUMAG 2003 (the 14th Conference on the Computation of Electromagnetic Fields). COMPUMAG 2003 was held in Saratoga Springs (USA), July 13-17, 2003.

The research and experimental results related to the impact of mesh quality improvement systems on finite element accuracy and efficiency (as discussed in Chapter 5) have been accepted for publication in conference proceedings and oral presentation at CEFC 2004 (11th Biennial IEEE Conference on Electromagnetic Field Computation). CEFC 2004 will be held in Seoul (Korea), June 6-9, 2004.

Parallel and distributed processing for \( h-p \) adaptive finite element analysis was investigated in an invited conference paper and oral presentation at COMPUMAG 2003 [49]. This contribution will also appear in IEEE Transactions on Magnetics [50].
6.2 Future Work

There are many opportunities for future research. The mesh smoothing systems could be modified such that a successful theoretical measure is used for guiding the mesh improvement stage, rather than for evaluating the results a posteriori. This strategy could be expanded for guiding not only improvement, but mesh generation and refinement as well. Methods for reducing the cost of computing the theoretical indicators would be useful in this context. The potential benefits of incorporating local transformations into the mesh improvement framework should be assessed.

More general avenues of research include, evaluating linear element effectiveness for time dependent problems, the effect of element gradation on the finite element approximation, and combined techniques for targeting several objective functions. Error bounds and mesh quality indicators for higher-order tetrahedral elements should also be investigated. The ultimate test of any algorithm or software is its acceptance and use by the research and industrial communities. The application of the new techniques to sophisticated electromagnetic devices and problems of industrial interest could be a next step in this direction.
References


