

ACHIEVING FINITE ELEMENT MESH QUALITY VIA
OPTIMIZATION OF THE JACOBIAN MATRIX NORM AND
ASSOCIATED QUANTITIES

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PART II - A FRAMEWORK FOR VOLUME MESH OPTIMIZATION
& THE CONDITION NUMBER OF THE JACOBIAN MATRIX

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Abstract. Three-dimensional unstructured tetrahedral and hexahedral finite element mesh optimization is studied from a theoretical perspective and by computer experiments to determine what objective functions are most effective in attaining valid, high quality meshes. The approach uses matrices and matrix norms to extend the work in Part I to build suitable 3D objective functions. Because certain matrix norm identities which hold for 2×2 matrices do not hold for 3×3 matrices, significant differences arise between surface and volume mesh optimization objective functions. It is shown, for example, that the equivalence in two-dimensions of the Smoothness and Condition Number of the Jacobian matrix objective functions does not extend to three dimensions and further, that the equivalence of the Oddy and Condition Number of the Metric Tensor objective functions in two-dimensions also fails to extend to three-dimensions. Matrix norm identities are used to systematically construct dimensionally homogeneous groups of objective functions. The concept of an ideal minimizing matrix is introduced for both hexahedral and tetrahedral elements. Non-dimensional objective functions having barriers are emphasized as the most logical choice for mesh optimization. The performance of a number of objective functions in improving mesh quality was assessed on a suite of realistic test problems, focusing particularly on all-hexahedral "whisker-weaved" meshes. Performance is investigated on both structured and unstructured meshes and on both hexahedral and tetrahedral meshes. Although several objective functions are competitive, the condition number objective function is particularly attractive. The objective functions are closely related to mesh quality measures. To illustrate, it is shown that the condition number metric can be viewed as a new tetrahedral element quality measure.

Key words. unstructured grid generation, finite element mesh, mesh optimization, smoothing, condition number

AMS subject classification. 65M50

1. Introduction

Optimization of three-dimensional unstructured meshes is studied from both a theoretical perspective and via computer experiments to determine what objective functions are most effective in achieving high quality finite element meshes. Unstructured mesh optimization is not a new subject, although much of the effort has been restricted to two-dimensions. In three dimensions [6], [9], [20], [3], [24] and others, have tackled the problem with varying degrees of depth. Some have concentrated upon using "smart" Laplacian smoothers in which a set of heuristics is developed to adjust the basic algorithm to move towards better meshes, often using tetrahedral

* THIS WORK WAS FUNDED BY THE DEPARTMENT OF ENERGY'S MATHEMATICS, INFORMATION AND COMPUTATIONAL SCIENCES PROGRAM (SC-31) AND WAS PERFORMED AT SANDIA NATIONAL LABORATORIES. SANDIA IS A MULTIPROGRAM LABORATORY OPERATED BY SANDIA CORPORATION, A LOCKHEED MARTIN COMPANY, FOR THE UNITED STATES DEPARTMENT OF ENERGY UNDER CONTRACT DE-ACO4-94AL85000.

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quality measures as a guide (a good summary of tetrahedral measures is given in [8]). A more systematic approach is attempted in the present work.

Currently, production meshing relies heavily on Laplace smoothing for unstructured meshes. Although frequently adequate for tetrahedral meshes, Laplace smoothing regularly fails to produce even a valid¹ mesh when applied to the all-hexahedral meshes arising from the "whisker weaver" [18]. Moreover, even when the mesh is valid, the quality, as measured by aspect ratio, skew, and scaled-jacobian quality metrics, is often very poor. This lack of quality serves as a major motivation for the present work. In structured meshing, considerable reliance is placed upon solving the partial differential equations that result from minimizing the harmonic map objective function. Although this is sometimes effective, it is much more so in two dimensions than in three, probably due to the lack of a theoretical guarantee of valid meshes in three-dimensions. Thus, even in structured meshing there is room for improvement in 3D smoothing techniques.

Optimization of unstructured hexahedral meshes is largely unexplored territory since such meshes have not been available until recently. The problem addressed is thus both novel and difficult because it requires automatic smoothing of three-dimensional structured or unstructured hexahedral, tetrahedral, and mixed element meshes.

This paper extends work reported in [15] which introduced the idea of using matrix norms to generate mesh quality objective functions and in Part I of this series of papers on mesh optimization [14]. In Part I the matrix norm idea was applied to unstructured surface triangular and quadrilateral finite element meshes. Surface objective functions were implemented and compared on various test problems. The Smoothness objective function was discovered to be equivalent to the condition number of the Jacobian matrix while the Oddy objective function was equivalent to the condition number of the metric tensor. The Oddy objective function gave the best over-all results.

Part I on *surface* mesh optimization is extended in this paper to *volume* mesh optimization. A separate paper on volume optimization is needed because many relationships which hold in 2D do not hold in 3D, and vice versa. This issue has not been critically examined before. The subject also deserves attention because in practice it is much harder to achieve good mesh quality in 3D than in 2D. This paper thus has two somewhat conflicting goals, namely, to systematically explore the space of possible 3D mesh objective functions derived from matrix norms, and to argue on theoretical grounds that there is one particular objective function, namely Condition Number (no longer equivalent to Smoothness), that is best suited for optimizing meshes. Although most readers will be interested primarily in the latter goal, the former goal is important because it shows how objective functions are related to one another.

Section 2 of this paper defines the 3D Jacobian and metric tensor matrices in terms of element edges. Section 3 shows that many well-known volume objective functions can be expressed in terms of matrix norms. Section 4 uses 3D matrix norm identities to form dimensionally homogeneous groups of objective functions and defines several new objective functions. Section 5 describes the ideal element types in terms of matrices and introduces the idea of differentiation of a scalar function with respect to a matrix in order to create objective functions which have the ideal elements as stationary points. Because non-dimensional objective functions appear to be the

¹ By valid it is meant that the elements are properly oriented with locally positive jacobian determinant.

most effective in improving mesh quality, Section 6 focuses on identifying as many non-dimensional objective functions as possible and discusses relationships between them and gives reasons why, among all the non-dimensional objective functions, the Jacobian condition number is one of the most attractive. Section 7 considers optimization of tetrahedral meshes and studies the Jacobian condition number as a tetrahedral quality measure. Section 8 presents the results of numerical optimization experiments performed with the CUBIT code. Section 9 is the summary and conclusion.

2. Building Blocks for Nodally-Based Volume Objective Functions

For reasons discussed in Part I, attention is focused not on the mesh elements but rather on the nodes of the mesh and the edges emanating from a given node. The mesh optimization is a series of local optimization problems, one for each free node of the mesh.

Let M be the number of elements attached to a given interior node of the mesh whose spatial position is to be "optimized" and let \mathcal{M} be the set of integers $m = 0, 1, 2, \dots, M - 1$.² Assume for the rest of this paper that $m \in \mathcal{M}$. Let the given node be associated with the vector $x \in R^3$. It is assumed that each of the M elements is attached to the interior node by 3 neighboring vertices³. Let the three neighbor nodes associated with the m^{th} element be $x_{m,k} \in R^3$ with $k = 1, 2, 3$. To achieve control over mesh quality, the local objective function $f(x)$ needs to be based, not directly on x , but rather on the important geometric entities associated with the node. The critical quantities for the m^{th} element are:

1. The 3 edge vectors, $e_{m,k}$, in the plane:

$$e_{m,k} = x_{m,k} - x$$

2. The Jacobian matrix:

$$J_m = [e_{m,1}, e_{m,2}, e_{m,3}] = \begin{pmatrix} x_{m,1} - x & x_{m,2} - x & x_{m,3} - x \\ y_{m,1} - y & y_{m,2} - y & y_{m,3} - y \\ z_{m,1} - z & z_{m,2} - z & z_{m,3} - z \end{pmatrix},$$

and the metric tensor:

$$G_m = J_m^T J_m.$$

3. Finally, define for each of the m-elements:

$$g_m = \det G_m,$$

and the Jacobian determinant

$$j_m = \det J_m = e_{m,1} \cdot (e_{m,2} \times e_{m,3}).$$

Then $j_m^2 = g_m$ and j_m is six times the local volume of the m-th tetrahedron enclosed by the corresponding triad of edges. For shorthand, let $|j_m| = \sqrt{g_m}$. It is important to distinguish between j_m and $\sqrt{g_m}$ because the former can be negative or positive,

² According to [4], the total number of edges or vertices attached to the interior node is $\frac{1}{2}(M+4)$. M can be as large as 40 in the all-hexahedral whisker-weaved meshes.

³ This assumption eliminates unusual element types such as pyramids and knives for the present.

with negative j_m signifying inverted (also called tangled, folded, or invalid) elements. A mesh with all-positive j_m is generally the minimum quality criterion for a mesh. If $j_m \leq 0$ for some element then the mesh is considered *invalid*.

Recent work in continuum variational methods of mesh generation has shown that a powerful approach to the construction of objective functions involves the use of matrices and matrix norms [15]. The Jacobian matrix is the fundamental quantity that describes all the first-order mesh qualities (length, areas, and angles) of interest, therefore, it is appropriate to focus the building of objective functions on the Jacobian matrix or the associated metric tensor. Many of the well-known objective functions in structured mesh optimization can be cast in the form of norms of matrices. One advantage of expressing objective functions in terms of matrix norms is that it is relatively straightforward to generalize a surface mesh objective function to a volume mesh objective function. New non-geometric interpretations of previously known objective functions become available using matrix norms. Another advantage is that matrices permit easy introduction of weighted forms of objective functions for anisotropic mesh quality measures. For these reasons, objective functions constructed from matrices are emphasized.

The matrices of interest must be converted to scalars to create objective functions. This can be done using the trace, determinant, or matrix norms. There are several matrix norms but, for mesh generation, the Frobenius norm has proven the most useful and most easily implemented. Let A be a 3×3 matrix, then the Frobenius norm of A is $\|A\|_F = (\text{tr}(A^T A))^{\frac{1}{2}}$. The norm-squared is the sum of the square of the elements in the matrix, which is why the Frobenius norm lends itself so readily to the construction of objective functions for meshing. For the rest of this paper the F subscript is omitted since all the norms will be Frobenius norms. The following matrix properties prove useful in analyzing the objective functions used in the present approach. Let $A_{3 \times 3}$ be a real matrix with determinant α non-zero and let $\text{adj}A = \alpha A^{-1}$ be the adjoint matrix of A . Then

$$\|A^{-1}\| = \|\text{adj}A\| / |\alpha|.$$

Note that, in contrast to the case for $A_{2 \times 2}$, $\|A\| \neq \|\text{adj}A\|$ for $A_{3 \times 3}$. The *condition number* of A is the dimensionless quantity

$$\kappa(A) = \|A\| \|A^{-1}\| = \kappa(A^{-1}).$$

The following matrices are useful:

$$\text{Diag}A = \begin{cases} A_{ij} & \text{if } i = j \\ 0 & \text{else} \end{cases}$$

which is the matrix formed from the diagonal elements of A , and

$$\text{Offdiag}A = A - \text{Diag}A$$

which is the matrix consisting of the off-diagonal elements of A .

Let f_m be a scalar quality metric for the m^{th} triad attached to the center node, derived from the building blocks in this section. For example

$$f_m(x, y, z) = f(A_m(x, y, z))$$

where the A_m are the Jacobian matrices constructed from the adjacent edges. Consider the vector $\mathbf{f} = (f_0, f_1, \dots, f_{M-1}) \in R^M$. The p -norm of \mathbf{f} is

$$\|\mathbf{f}\|_p = \left(\sum_m |f_m|^p \right)^{1/p}$$

with $p \geq 1$. Usually $p = 1, 2$ will be used, but the ℓ_∞ norm:

$$\|\mathbf{f}\|_\infty = \max_m \{|f_m|\}$$

is also a useful norm because it enables optimization of worst-case mesh quality measures instead of average measures. The ℓ_∞ norm will be considered further in the next paper in connection with mesh untangling.

The general form of the local mesh objective functions in this work is $\|\mathbf{f}\|_p$. For $p = 2$, the minimizations are unconstrained, three-variable, and have smooth objective functions on some domain. The necessary condition for a minimum to exist are (i) the gradient of the objective function is zero at the minimum, and (ii) the Hessian is positive semi-definite at the minimum [11]. Sufficient conditions require that the Hessian be positive definite.

With this form of the objective function chosen, it remains only to determine the choice of the function f which takes $A_{3 \times 3}$ to a scalar. Objective functions will thus be posed in the form $f = f(A)$, where A is tacitly recognized as the Jacobian matrix.

3. Known Volume Objective Functions Expressed as Matrix Norms

A number of previously proposed 3D objective functions can be expressed in terms of matrices and matrix norms. Some of these are summarized in this section.

p-Length, $(length)^{2p}$.

Let p be a positive integer.

$$f_{p\text{-Length}}(A) = \|A\|^{2p}.$$

For $p = 1$, Length is the sum of the squares of the three edge lengths. Length is important because it is the objective function for Laplacian smoothing. This objective function is widely used due to its simplicity but it is recognized that it does not consistently produce valid meshes. Length is also the sum of the eigenvalues (trace) of the metric tensor.

For $p = 2$, this objective function is closely related to, but not identical with, the "Length-weighted Laplacian" smoother [7].

Norm of the Metric Tensor, $(length)^4$.

$$f_{NMT}(A) = \|A^T A\|^2.$$

NMT has no simple geometric interpretation (it is the sum of the three edge lengths to the fourth power plus the sum of the squares of the pairwise projected edge lengths). However, as shown in [15], because $A^T A$ is symmetric, the square of the norm of the metric tensor is the sum of the squares of its eigenvalues. Minimization of this functional should make the eigenvalues of the metric tensor equal (in a least-squares sense). This, in turn, means that the metric tensor will be made proportional to a

rotation matrix, giving near-equal aspect ratios and orthogonality. To our knowledge, this objective function has never been tried in 3D, but it is an obvious extension of the work in [16].

Off-Diagonal, $(length)^4$.

The Off-Diagonal objective function:

$$f_{OffDiag}(A) = |Offdiag A^T A|^2$$

attempts to equidistribute the face angles about a node. Although geometrically appealing, Off-Diagonal suffers the great drawback that it is non-convex in general, i.e., the minimal mesh does not always exist. To make practical use of Off-diagonal requires combining it with other objective functions to get convexity. For this paper Off-diagonal is combined with 2-Length since they both have dimensions of $(length)^4$. This objective function has been proposed by some for structured 3D mesh generation but has not been used extensively.

Volume, $(length)^6$.

The Volume objective function makes locally equal element volumes:

$$f_V(A) = \alpha^2.$$

In the continuum the volume objective function is non-elliptic, so non-smooth grids result. This property carries over to the discrete optimization function for volume. Volume has been proposed in [5], [6], and others.

Adjoint of the Jacobian Matrix $(length)^4$.

$$f_{adjoint}(A) = |adj A|^2 = \alpha^2 |A^{-1}|^2.$$

The geometric interpretation of this objective function can be found by noting that

$$|adj J_m|^2 = |e_{m,1} \times e_{m,2}|^2 + |e_{m,2} \times e_{m,3}|^2 + |e_{m,3} \times e_{m,1}|^2,$$

i.e., $|adj J_m|^2$ is twice the sum of the squares of the areas of the three triangular faces lying between the three edges. The adjoint is also the second-invariant of the characteristic polynomial of G_m . This objective function was used in a group of objective functions in [13].

Smoothness, $(length)^1$.

The Smoothness objective function derives by analogy to variational structured mesh generation [2]:

$$f_S(A) = \alpha |A^{-1}|^2.$$

When writing the Smoothness objective function for surface meshes in Part I in terms of matrix norms, it was found that $f_S(A) = f_{IS}(A) = \kappa(A)$ because the norm of the adjoint was equal to the norm of the matrix. This does not hold in three dimensions, and therefore, there are three objective functions to consider while in 2D there was only one.

Inverse Smoothness, $(length)^{-1}$.

This objective function is an ad-hoc generalization that appears in [1] and others:

$$f_{IS} = |A|^2 / \alpha.$$

Note that $f_{IS}(A) = f_{IS}(A^{-1})$.

The Oddy Metric, $(length)^0$.

In Part I on surface meshes, the condition number of the metric tensor was shown to be equivalent to an objective function based on the Oddy metric [19]. This equivalence does not hold in three-dimensions, thus there is another objective function to consider:

$$f_{Oddy}(A) = \alpha^{-4/3} \{ |A^T A|^2 - (1/3) |A|^4 \}.$$

This objective function is infinite for invalid meshes and is zero for the identity or rotation matrices.

These previously known objective functions are included in the numerical tests given later in this paper, but first several new objective functions suggested by the matrix norm approach are introduced.

4. Volume Objective Functions from Dimensionally Homogeneous Groups

The objective functions of the previous section do not exhaust the myriad possibilities that arise by approaching mesh optimization via matrix norms. This section seeks to answer two questions (1) are there some other potentially useful objective functions that have so far been over-looked, and (2) is there a way to group objective functions in some rational way? Brackbill suggested combining continuum objective functions into a group to control smoothness, area, or orthogonality [2] but found that it was difficult to select the constants in these combinations due to dimensional inhomogeneity of the objective functions. As shown in Part I, this limitation can be partly overcome by combining objective functions having the same dimension⁴. This idea is extended further here by giving a systematic way to construct dimensionally homogeneous groups via certain identities which hold for arbitrary 3×3 matrices (these identities do not hold for 2×2 matrices). There are two identities that appear rather fundamental, and from which many others can be constructed. The first has dimensions $(length)^2$:

$$|A|^2 + 2 \operatorname{tr}(\operatorname{adj} A) \equiv (\operatorname{tr} A)^2 + (1/2) |A - A^T|^2$$

and can be derived from a trivial matrix identity. The second has dimensions $(length)^3$:

$$(\operatorname{tr} A)^3 + 3 \alpha \equiv \operatorname{tr}(A^3) + 3 (\operatorname{tr} A) \operatorname{tr}(\operatorname{adj} A)$$

and can be derived from the fact that every matrix satisfies its own characteristic polynomial. These identities are not particularly useful in themselves because the objective functions they suggest (e.g. $\operatorname{tr} A$) have geometrical interpretations that do not correspond to a useful element quality measure. Replacing A with $A^T A$ in these

⁴ By *dimension* reference is made to the idea that if the matrix A has a particular set of units (say length), then the units of other related matrices and norms are determined.

identities, one can obtain two other identities having dimensions of $(length)^4$ and $(length)^6$ which contain norms upon which useful objective functions can be based:

$$\begin{aligned} |A^T A|^2 + 2\alpha^2 |A^{-1}|^2 &\equiv |A|^4, \\ 3|A|^2 |A^T A|^2 - |A|^6 + 6\alpha^2 &\equiv 2|AA^T A|^2. \end{aligned}$$

The identities given in this section suggest dimensionally homogeneous groups of objective functions. Let $c_1, c_2, c_3,$ and c_4 be arbitrary real constants.

Group Six, $(length)^6$.

$$f_6(A) = 3c_1 |A|^2 |A^T A|^2 - c_2 |A|^6 + 6c_3 \alpha^2.$$

Note that if $c_1 = c_2 = c_3 = 1/2$ then one obtains the other objective function, $|AA^T A|^2$, in the $(length)^6$ identity, which is why it is left out of this group.

Group Four, $(length)^4$.

$$f_4(A) = c_1 |A^T A|^2 - c_2 |A|^4 + c_3 \alpha^{4/3}.$$

Group Two, $(length)^2$.

$$f_2(A) = c_1 |A|^2 + 2c_2 \text{tr}(\text{adj}A) - c_3 (\text{tr}A)^2 + c_4 \alpha^{2/3}.$$

A method for choosing the constants in these groups is given in the next section.

5. The Ideal Element - A Geometric View

Every matrix A with column vectors $a_i, i = 1, 2, 3$ has the following factorization:

$$A = D Q^T$$

where

$$\begin{aligned} A &= [a_1, a_2, a_3], \\ D &= \text{diag}(d_1, d_2, d_3), \\ Q &= [a_1/d_1, a_2/d_2, a_3/d_3], \end{aligned}$$

and $d_i = |a_i|$. The normalized column vectors of A are contained in Q and the lengths in D . Thus $|Q|^2 = 3$ because the column vectors comprising Q are of unit length. The quantity $\det(Q)$ is referred to in the CUBIT code as the *scaled jacobian* quality measure. It varies from minus one to plus one. Positive scaled jacobian is considered the minimal quality permitted for a mesh, while negative values of the scaled jacobian signify that invalid elements exist.

The matrix A determines the geometric quality of the corresponding element. In the absence of anisotropy, each edge of the element should have equal length. This requirement corresponds to making the diagonal matrix D have equal positive entries, i.e., $D = \Delta I$ for some $\Delta > 0$ and I the 3×3 identity matrix. The proper choice for Q depends on the element type. For a hexahedral element, the edges of the element

should be orthonormal, hence we require $Q^T = R$ for some rotation matrix R where $R^T R = I$ and $\det(R) = +1$ to maintain proper orientation.

Thus, for an isotropic hexahedral element the ideal matrix has the form

$$A = \Delta R$$

where R is an orthogonal matrix with $\det(R) = 1$ and $\Delta > 0$. If A has this form then

- the column vectors of A are orthogonal,
- the lengths of the columns vectors are equal, and
- the volume of the region spanned by the 3 vectors is positive, and
- the corner of the element defined by A matches the corner of a cube.

Although the form of the ideal A has been determined, the scalar Δ and the matrix R have not been specified. These control the element size and orientation, respectively. With isotropic meshes, it is not desirable to specify the size and orientation of each element of the mesh, rather, the optimization procedure should do this. To eliminate these two quantities, note that the following relationship holds for the ideal element:

$$A^T A = \Delta^2 I.$$

The determinant of the left-hand-side of this expression is α^2 and therefore,

$$\Delta^2 = \alpha^{2/3}.$$

The ideal matrix is then

$$A = \alpha^{1/3} R.$$

Because the Frobenius matrix norm is invariant to rotations, i.e.,

$$|MR| = |RM| = |M|$$

for any matrix M , the rotation matrix in the ideal will not need to be specified.

The ideal matrix for tetrahedral elements will be discussed in section 7.

Not all of the objective functions described so far are minimized by the ideal A . Although it is neither necessary nor sufficient to require that an objective function be minimized by the ideal, doing so is a rational approach to designing objective functions. Consider the function $f(A)$ taking 3×3 matrices to a scalar. Differentiation of f with respect to A can be defined to be the following 3×3 matrix:⁵

$$[\partial f / \partial A]_{ij} = \partial f / \partial A_{ij}.$$

Derivatives for relevant functions $f(A)$ are given in Appendix I. The matrix function has a stationary point when $\partial f / \partial A = 0$, with 0 the 3×3 zero matrix.

Applying the differentiation formula to the Length objective function we find that $A = 0$ is the minimizer. Of course, $A = 0$ is not attained in practice because the admissible set of A 's are required to satisfy the boundary data. It is reasonable to ask if the Length objective function can be modified in some way to give the ideal as the minimizer. Length is part of the Group Two objective function of the previous

⁵ Of course, Sufficient smoothness must be assumed.

section, so let us ask if one can choose the constants c_i to give the desired minimizer. This is indeed possible, and can also be done for the other Group objective functions:

$$\begin{aligned} f_L(A) &= |A|^2 - 3\alpha^{2/3}, \\ f_{2L}(A) &= |A^T A|^2 - 3\alpha^{4/3}, \\ f_{3L}(A) &= |AA^T A|^2 - 3\alpha^2, \end{aligned}$$

The Smoothness and Inverse Smoothness objective functions must also be modified slightly to have the ideal as the minimizer:

$$\begin{aligned} f_S(A) &= \alpha^{2/3} |A^{-1}|^2, \\ f_{IS}(A) &= \alpha^{-2/3} |A|^2. \end{aligned}$$

Empirical results confirm that, in general, mesh quality is improved with these modified objective functions, when compared to their original forms.

6. Non-Dimensional Objective Functions

The non-dimensional objective functions are interesting because they are scale-independent and are the lowest-order objective functions having barriers⁶. Furthermore, they can be symmetrized so that $f(A) = f(A^{-1})$. This means that both the local map from the logical to the physical region and the local inverse map from the physical to the logical region are well-conditioned. Begin by defining the following three non-dimensional objective functions:

$$\begin{aligned} f_1(A) &= \alpha^{-2/3} |A|^2, \\ f_2(A) &= \alpha^{-4/3} |A^T A|^2, \\ f_3(A) &= \alpha^{-2} |AA^T A|^2, \end{aligned}$$

and their three counterparts:

$$\begin{aligned} \hat{f}_1(A) &= f_1(A^{-1}) = \alpha^{2/3} |A^{-1}|^2, \\ \hat{f}_2(A) &= f_2(A^{-1}) = \alpha^{4/3} |(A^T A)^{-1}|^2, \\ \hat{f}_3(A) &= f_3(A^{-1}) = \alpha^2 |(AA^T A)^{-1}|^2. \end{aligned}$$

The functions f_1 and \hat{f}_1 are recognized as the dimensionless versions of inverse Smoothness and Smoothness, respectively.

These objective functions serve as building blocks for some of the other known non-dimensional objective functions, suggest new non-dimensional functions, and help create some interesting non-dimensional identities involving mesh objective functions. For example, one can build *symmetric* objective functions by combining f_i with \hat{f}_i . Three condition numbers are immediate:

$$\begin{aligned} \kappa^2(A) &= f_1 \hat{f}_1, \\ \kappa^2(A^T A) &= f_2 \hat{f}_2, \\ \kappa^2(AA^T A) &= f_3 \hat{f}_3. \end{aligned}$$

⁶ By a barrier it is meant a set of matrices in the domain for which the objective function becomes infinite.

The building blocks are related to one another through the following identities:

$$\begin{aligned} f_2 &= f_1^2 - 2 \hat{f}_1, \\ \hat{f}_2 &= \hat{f}_1^2 - 2 f_1, \\ f_3 &= f_1^3 - 3 \kappa^2(A) + 3, \\ \hat{f}_3 &= \hat{f}_1^3 - 3 \kappa^2(A) + 3. \end{aligned}$$

The condition number objective functions are related through the following identities:

$$\begin{aligned} \kappa^2(A) &= 3 + f_1 f_2 - f_3 = 3 + \hat{f}_1 \hat{f}_2 - \hat{f}_3, \\ \kappa^2(A^T A) &= \kappa^4(A) + 4 \kappa^2(A) - 2 f_1^3 - 2 \hat{f}_1^3. \end{aligned}$$

$\kappa^2(AA^T A)$ can be similarly expressed in terms of lower-order objective functions.

Let f_O be the Oddy objective function, then

$$\begin{aligned} f_O(A) &= (2/3) f_1^2 - 2 \hat{f}_1, \\ \hat{f}_O(A) &= f_O(A^{-1}) = (2/3) \hat{f}_1^2 - 2 f_1, \\ (1/4) f_O \hat{f}_O &= (1/9) \kappa^4(A) + \kappa^2(A) - (1/3) (f_1^3 + \hat{f}_1^3), \end{aligned}$$

The last objective function will be referred to as the *symmetric* Oddy objective function. Let $w_n = (n - 3)/3$ with n an integer and define the following symmetric objective functions:

$$S_n = (w_n f_1^2 - 2 \hat{f}_1) (w_n \hat{f}_1^2 - 2 f_1).$$

Then for $n = 0, 1, 2, 3$ one obtains the $\kappa^2(A^T A)$, Symmetric Oddy, S_2 - a new symmetric objective function, and $\kappa^2(A)$, respectively, showing that these objective functions are all part of the same family. Another interesting family can be obtained from the three objective functions f_L, f_{2L}, f_{3L} , and their respective counterparts to give three more symmetric dimensionless objective functions:

$$\begin{aligned} f_L \hat{f}_L &= (f_1 - 3) (\hat{f}_1 - 3) = \kappa^2(A) - 3 (f_1 + \hat{f}_1) + 9, \\ f_{2L} \hat{f}_{2L} &= (f_2 - 3) (\hat{f}_2 - 3), \\ f_{3L} \hat{f}_{3L} &= (f_3 - 3) (\hat{f}_3 - 3). \end{aligned}$$

Proposition

The ideal matrix is a stationary point of $\kappa(A)$, $\kappa(A^T A)$, and the other non-dimensional objective functions given in this section.

Proof

All of the dimensionless objective functions can be expressed as combinations of f_1 and \hat{f}_1 and the ideal is a stationary point of the latter two functions. §

Observation

Let $A_{3 \times 3}$ with $\alpha > 0$. Let $f(A) > 0$ be a non-dimensional objective function such that $\lim_{\alpha \rightarrow 0} f(A)$ is unbounded but $f(A)$ is bounded for A in some set of matrices having positive determinant. Then the volume α associated with A is bounded below by a positive constant. §

The non-dimensional objective functions described in this section appear quite attractive, having a number of favorable theoretical properties. The objective function

$\kappa(A)$ in particular enjoys all of these nice properties, including symmetry. A geometric interpretation of this objective function can be found by noting that

$$\kappa(A) = |A| |adj A| / |\alpha|,$$

i.e., the condition number is the square root of the product of the sum of the squares of the edge-lengths and the sum of the squares of the adjacent face areas, divided by six times the volume of the tetrahedron defined by the edges. This is similar to, but not identical with, the objective function given in [10], page 11, for a tetrahedral quality measure.

Minimizing the condition number of A would seem to be a good idea because this maximizes the distance to the set of singular matrices ([12], page 26). In view of this, $\kappa(A)$ is the first objective function we know of that directly states that invalid meshes are to be avoided⁷.

Because condition number is the simplest symmetric non-dimensional objective function, close attention was paid to its performance in the empirical tests given in section 8.

7. Optimization of Tetrahedral Meshes.

The ideal isotropic tetrahedral element is the the unit equilateral tetrahedron. For isotropic tetrahedral elements the ideal matrix A again has $D = \Delta I$. However, the columns of Q should not be orthonormal. Instead let us require $Q^T = RW$ where R is a rotation matrix and

$$(1) \quad W = \begin{pmatrix} 1 & 1/2 & 1/2 \\ 0 & \sqrt{3}/2 & \sqrt{3}/6 \\ 0 & 0 & \sqrt{2}/\sqrt{3} \end{pmatrix}$$

This matrix is derived from examining the edge vectors of the ideal tetrahedron. Since $\det(W) = \sqrt{2}/2$, the ideal must have the form

$$\begin{aligned} A &= (\sqrt{2}\alpha)^{1/3} RW, \\ A^T A &= (\sqrt{2}\alpha)^{2/3} W^T W. \end{aligned}$$

The objective functions given in the previous sections should be weighted for the tetrahedral case in order that the tetrahedral ideal is a stationary point. If $f(A)$ is minimized by $A = A_{ideal}$ then $f(AW^{-1})$ is minimized by $A = A_{ideal}W$. Thus, for example, the modified length objective function for tetrahedra reads

$$f_L(A) = |AW^{-1}|^2 - 3(\sqrt{2}\alpha)^{2/3}.$$

The matrix AW^{-1} forms the linear transformation between the ideal tetrahedral element and the element defined by the matrix A .

In this section, however, attention is mainly focused on the Jacobian condition number objective function as it applies to tetrahedral elements. The weighted condition number objective function for tetrahedra is

$$\kappa(AW^{-1}) = |AW^{-1}| |WA^{-1}|.$$

⁷ We speculate that all of the non-dimensional objective functions having barriers measure distance from the set of singular matrices.

Proposition.

Let A_i , $i = 0, 1, 2, 3$ be the matrix associated with node i of a tetrahedral element. Then $f(A_i W^{-1}) = C$, where C is a constant independent of i and f is any of the objective functions discussed in this paper.

Proof.

A sketch of a proof goes like this: one can first show that there exist matrices M_i such that $A_i = A_0 M_i$. One can also show that there exist rotation matrices such that $M_i W^{-1} = W^{-1} R_i$. Then

$$|A_i W^{-1}| = |A_0 M_i W^{-1}| = |A_0 W^{-1} R_i| = |A_0 W^{-1}|.$$

A similar result holds for $|(A_i W^{-1})^{-1}|$ and for $\det(A_i W^{-1})$. §

Thus, for each objective function a single number can be associated with any given tetrahedron. Adopting the definition of a tetrahedral shape measure given in [8], any of the dimensionless objective functions are valid shape measures provided (i) $1/f$ is used, and (ii) there is a unique, global maximum. The latter requirement is not proven here but is likely to hold for most of the dimensionless objective functions. If the weight W were not included in the argument of the objective function, the function would no longer be invariant under a change of node.

$\kappa(A)$ is somewhat similar to the Q_K tetrahedral measure reported in [10], page 11. But $\kappa(AW^{-1})$ is neither identical to Q_K nor can it be expressed in terms of any combination of the quality metrics given in [21]. Thus $\kappa(AW^{-1})$ is a new tetrahedral element quality measure. To emphasize this point, tests A-D from [21] were performed, to show how the condition number quality measure varies with distortions of a tetrahedron⁸ (see Table 1).

The key feature to note in the table is that the condition number quality measure behaves similarly to other tetrahedral quality measures.⁹ We suspect, but have not proved, that $\kappa(AW^{-1})$ can be shown to be an *equivalent* tetrahedral quality measure to Q_K in the sense defined in [17]. At the very least, then, the situation for using condition number as a tetrahedral quality measure is paraphrased from [8]: "since it is impossible to fill an arbitrary volume with equilateral tetrahedra, equivalent quality measures will perform similarly, but with somewhat different results". The "somewhat different" results will be seen in section 10 where numerical experiments are performed to determine which objective function gives the best overall mesh quality.

As a final observation, note that most of the tetrahedral quality measures given in [21] and [8] cannot be expressed in terms of matrix norms. Three exceptions are the Mean Ratio η , which is roughly $(\alpha^{-2/3} |A|^2)^{-1}$, γ , approximately $|A|^{3/2} / \alpha$, and the κ measure, which is roughly $(\alpha^{2/3} |A^{-1}|^2)^{-3}$.

8. Empirical Tests.

The theory presented has identified a number of promising objective functions, but is unable to determine, for example, whether $\kappa(A)$ or $\kappa(A^T A)$ will produce superior mesh quality. To explore this question, computer experiments on realistic problems are needed. Many of the objective functions considered in this paper were implemented within the CUBIT code. All of the objective functions can be evaluated in terms of just three matrix functions, the determinant, the norm, and the norm of the adjoint. Evaluating the gradient of an objective function entails an indirect approach because if one attempts to write out the complete expression an unwieldy number of terms

⁸ A normalization factor of $1/3$ was included in the definition so that the ideal element gave $\kappa = 1$.

⁹ Note that $\kappa(AW^{-1})$ is symmetric about the apex distance and has values close to γ .

TABLE 1
Sensitivity of Condition Number Quality Measures to Tests A, B, C, and D

Apex Dist (A)	κ	Angle (B)	κ	LM (C)	κ	Angle (D)	κ
0.25	2.03	0	1.00	1.00	1.00	90	1.00
0.50	1.22	15	1.02	0.75	1.04	75	1.02
1.00	1.00	30	1.11	0.50	1.22	60	1.11
2.00	1.22	45	1.29	0.30	1.74	45	1.29
3.00	1.61	60	1.73	0.20	2.47	30	1.73
4.00	2.03	75	3.21	0.10	4.77	15	3.21

results. For example, $|A|^2$ contains 9 terms which must be differentiated, $|adj A|^2$ has 27, while α has 6. When differentiated, these objects contain 9, 54, and 18 terms, respectively. $\kappa^2(A)$ contains upwards of 324 non-differentiated terms in the numerator alone, if everything is expanded fully. The difficulty may be avoided by making use of the idea of differentiating a scalar function of a matrix introduced in the previous section. Let

$$F(x, y, z) = \sum_m f(J_m(x, y, z))$$

be a mesh objective function. Then the chain rule shows that

$$\partial F / \partial x = \sum_m \text{tr} \{ (\partial f / \partial J_m)^T (\partial J_m / \partial x) \}$$

and, because $\partial J_m / \partial x$ is readily computed,

$$\nabla F = - \sum_m (\partial f / \partial J_m) u,$$

where $u^T = [1, 1, 1]$. A sufficient condition for a stationary point is thus $\partial f / \partial J_m = 0$ for all m . This is one reason why objective functions should be zero at the ideal element. Of course, the gradient method is only applicable for $1 < p < \infty$. For the non-differentiable cases, a non-gradient method is employed.

Several sets of optimization tests were performed focusing on different geometries, element types, and mesh connectivities. These tests included (1) all-hexahedral unstructured, whisker-weaved meshes (three geometries, including those shown in figures 1 and 2), (2) all-hexahedral semi-structured swept meshes (three geometries, including that in figure 3), (3) all-tetrahedral meshes (three geometries, including those in figures 1 and 2), and (4) a tetrahedral mesh using an l-infinity norm (the same geometry as in figure 1). The investigation began with about twenty objective functions which were tested on the "knee" geometry. The results are shown in Table 2. The list was then reduced to include only those objective functions having barriers since this is a critical requirement of any robust optimizer (see Table 3). Among those having barriers there were several which performed particularly well, so the list was further reduced. To compare results between objective functions several quality measures were used. For hexahedral elements these were: aspect ratio [22], skew [22], Oddy's metric [19], condition number, and minimum scaled Jacobian. For tetrahedral elements, these were: gamma [21], condition number, and minimum scaled Jacobian. Except for the minimum scaled the Jacobian, smaller numbers in the tables indicate superior mesh quality. Results were also compared against two volume smoothers

already in CUBIT namely, Laplacian smoothing and Equipotential [23].

Although only a very limited set of tests could be performed, the following observations are made:

- As expected, objective functions having barriers maintain valid meshes whereas those without barriers did not consistently do so,
- All of the objective functions having barriers gave meshes notably superior to those smoothed with CUBIT's original Laplacian and Equipotential algorithms. This was especially true on the whisker-weaved meshes,
- The objective functions that were modified to make the ideal a stationary point (like f_S and f_{IS}) generally performed better than the original objective functions, but not always,
- The weighted objective functions, $f(AW^{-1})$, consistently improved tetrahedral mesh quality over the unweighted objective functions, $f(A)$, though not dramatically,
- It is currently rare to achieve excellent quality by optimizing the whisker-weaved meshes, although the quality is much improved with the non-dimensional objective functions compared to the unoptimized mesh. For example, the minimum scaled Jacobian was typically +0.003 in the unoptimized mesh and +0.300 in the optimized mesh. Hexahedral element swapping techniques to change mesh connectivity may be considered in the future to further improve quality,
- In terms of relative efficiency, it was found that objective functions which use the metric tensor were noticeably slower than those which use the Jacobian matrix (see Table 3). The fastest objective function based on the metric tensor was Oddy(A),
- On Swept meshes, Oddy performed very well, whereas on whisker-weaved meshes it lagged quite a few others (see table 4),
- Somewhat surprisingly, quality achieved with the Smoothness objective function was noticeably less than a half dozen other objective functions also having barriers. Smoothness was also the slowest of the objective functions based on the Jacobian matrix,
- Condition number of the Jacobian matrix, condition number of the metric tensor, inverse smoothness, and Oddy (all in their weighted forms) appeared to give the best quality of all the objective functions tried on tetrahedral meshes. An ℓ_∞ norm was used in this test. These objective functions also performed well on hexahedral meshes.

9. Summary and Conclusions.

This paper applied the matrix norm idea to design objective functions for finite element *volume* mesh optimization. Traditional volume objective functions such as length, volume, and smoothness can be expressed in terms of matrix norms. In two dimensions, smoothness, inverse smoothness, and condition number of the jacobian matrix are identical objective functions, while in three dimensions they become three distinct objective functions because the norm of the adjoint matrix is no longer equal to the norm of the matrix. Similarly, in two dimensions oddy and the condition number of the metric tensor give the same objective function while in three dimensions they are distinct.

Two fundamental matrix norm identities were presented having dimensions of length⁴ and length⁶. These show the relationship between a number of objective

functions and how dimensionally homogeneous groups of objective functions can be formed. The arbitrary constants in these groups can be determined by introducing the matrix corresponding to the ideal mesh element. The constants were chosen so that the ideal matrix is a stationary point of any given objective function. For example, the power of α in the smoothness and inverse smoothness objective functions was adjusted to make the ideal a stationary point.

Non-dimensional objective functions with barriers seem to be the most logical choice for mesh objective functions because they are scale invariant and avoid inverted elements. Several non-dimensional matrix norm identities were derived in terms of smoothness and inverse smoothness to show how other non-dimensional objective functions were related to one another. For example, the condition number of the metric tensor can be expressed in terms of the condition number of the jacobian matrix, smoothness, and inverse smoothness. Given the wealth of potential non-dimensional objective functions the condition number of the jacobian matrix was preferred because it is the simplest of the symmetric non-dimensional objective functions and because it is a measure of the distance of a given matrix to the set of singular matrices.

The ideal matrix corresponding to tetrahedral elements was related to a matrix W derived from considering the equilateral tetrahedral element. Objective functions for tetrahedral elements expressed in terms of the matrix AW^{-1} have the ideal matrix as a stationary point. For each such objective function it was shown that a single number, independent of the node at which it is computed, could be assigned to a given tetrahedral element. To illustrate, the condition number of the jacobian for tetrahedral elements was subjected to the distortions given in [21], the numerical results being very similar to the other tetrahedral quality measures given in that reference.

Finally, many of the objective functions were implemented in the CUBIT code and empirically tested using unstructured all-hexahedral whisker-weaved meshes, semi-structured swept meshes, and an all-tetrahedral mesh. Ultimately, the list of objective functions could not be reduced to just one objective function as several were competitive. In terms of dimension, the non-dimensional objective functions performed best. Of these, Oddy, condition number of the metric tensor, and others based on the metric tensor gave good mesh quality but, due to their relative slowness, are less attractive. Probably the two best overall objective functions were Condition Number of the Jacobian Matrix and Inverse Smoothness (with $\alpha^{2/3}$).

Although this study has clarified a number of issues, there remain several others that must be addressed before the matrix norm approach can realize its full potential. Efficiency issues related to the optimization algorithm need further consideration. In addition, barrier-based objective functions require that one optimize beginning with a valid mesh. If this is not done, the resulting mesh will likely contain inverted elements. Part III will consider ways to create valid meshes from invalid meshes so that barrier-based objective functions can further improve mesh quality. Because the objective functions in this paper are based only on interior nodes, the current approach does not guarantee good mesh quality on the boundary of the domain. This also will be addressed in Part III.

Acknowledgements

This work was made possible through the MICS program office directed by Fred Howes and managed at Sandia Laboratories by David Womble. We would also like to thank

department manager Rob Leland for his support and CUBIT team members Scott Mitchell and Nate Folwell for providing many whisker-weaved mesh examples.

REFERENCES

- [1] J.G. Tinoco, P. Barrera, *Smooth and Convex Grid Generation over General Plane Regions*, to appear in *Mathematics and Computers in Simulation*, Elsevier, 1998.
- [2] J. Brackbill, J. Saltzman, *Adaptive zoning for singular problems in two dimensions*, *J. Comp. Phys.*, 46, pp342-368, 1982.
- [3] S. Canann, J. Tristano, M. Staten, *An Approach to Combined Laplacian and Optimization-Based Smoothing for Triangular, Quadrilateral, and Quad-Dominant Meshes*, Proceedings of the 7th International Meshing RoundTable, pp479-494, Detroit, 1998.
- [4] G. Carey, *Computational Grids*, Taylor & Francis, 1997.
- [5] J. Castillo, *A discrete variational method*, *SIAM J. Sci. Stat. Comput.*, Vol. 12, No. 2, pp454-468, 1991.
- [6] C.L. Chen, K.Y. Szema, and S.R. Chakravarthy, *Optimization of Unstructured Grid*, AIAA 95-0217, 33rd Aerospace Sciences Meeting, January 1995, Reno NV.
- [7] *CUBIT Mesh Generation Environment*, SAND94-1100, Sandia National Laboratories, Albuquerque, NM 87185.
- [8] J. Dompierre, P. Labbe, F. Guibault, and R. Camerero, *Proposal of Benchmarks for 3D Unstructured Tetrahedral Mesh Optimization*, pp459-478, Proceedings of the 7th International Meshing RoundTable '98, Dearborn MI, October 26-28, 1998.
- [9] L. Freitag, M. Jones, and P. Plassman, *An efficient parallel algorithm for mesh smoothing*, In Proceedings of the Fourth International Meshing RoundTable, Sandia National Laboratories, pp47-58, 1995.
- [10] P.L. George and H. Borouchaki, *Delaunay Triangulation and Meshing*, Hermes, Paris, 1998.
- [11] P. Gill, W. Murray, M. Wright, *Practical Optimization*, Academic Press, 1981.
- [12] G. Golub and C. Van Loan, *Matrix Computations*, Johns Hopkins University Press, 1983.
- [13] O.P. Jacquotte, J. Cabello, *A variational method for the optimization and adaption of grids in computational fluid dynamics*, in *Numerical Grid Generation in Computational Fluid Mechanics '88*, S. Sengupta, et. al., eds., pp405-413, PineRidge Press, Swansea UK, 1988.
- [14] P. Knupp *Achieving Finite Element Mesh Quality via Optimization of the Jacobian Matrix Norm and Associated Quantities, Part I - A Framework for Surface Mesh Optimization*, submitted for publication.
- [15] P. Knupp, N. Robidoux, *A Framework for Variational Grid Generation: Conditioning the Jacobian Matrix with Matrix Norms*, submitted for publication.
- [16] G. Liao, *Variational Approach to Grid Generation*, *Num. PDE's*, 8, pp143-147, 1992.
- [17] A. Liu and B. Joe, *Relationship between tetrahedron quality measures*, *Bit*, 34:268-287, 1994.
- [18] N.T. Folwell and S.A. Mitchell, *Reliable Whisker Weaving via Curve Contraction*, pp365-378, Proceedings of the 7th International Meshing RoundTable, Dearborn MI, 1998.
- [19] A. Oddy, J. Goldak, M. McDill, M. Bibby, *A distortion metric for isoparametric finite elements*, *Trans. CSME*, No. 38-CSME-32, Accession No. 2161, 1988.
- [20] V.N. Parthasarathy and S. Kodiyalam, *A constrained optimization approach to finite element mesh smoothing*, *Finite Elements in Analysis and Design*, 9, p309-330, 1991.
- [21] V.N. Parthasarathy, C.M. Graichen, and A.F. Hathaway, *A comparison of tetrahedron quality measures*, *Finite Elements in Analysis and Design*, Vol. 15, pp255-261, 1993.
- [22] J. Robinson, *CRE method of element testing and the Jacobian shape parameters*, *Eng. Comput.*, Vol 4, pp113-118, June 1987.
- [23] R.E. Tipton, *Grid Optimization by Equipotential Relaxation*, unpublished, Lawrence Livermore National Laboratory, 1990.
- [24] P. Zavattieri, *Optimization Strategies in Unstructured Mesh Generation*, *Intl. J. Num. Meth. Engr.*, Vol. 39, p2055-2071, 1996.

Appendix I: Derivatives of Objective Functions

$$\begin{aligned} \frac{\partial}{\partial A} |A|^2 &= 2A, \\ \frac{\partial}{\partial A} \text{trace}(A) &= I, \\ \frac{\partial}{\partial A} \text{trace}(A^n) &= n(A^{n-1})^T, \\ \frac{\partial \alpha^n}{\partial A} &= n\alpha^n A^{-T}, \\ \frac{\partial}{\partial A} |A|^4 &= 4|A|^2 A, \\ \frac{\partial}{\partial A} |A^T A|^2 &= 4A A^T A, \\ \frac{\partial}{\partial A} |\text{OffDiag} A^T A|^2 &= 4A \text{OffDiag}(A^T A), \\ \frac{\partial}{\partial A} |\text{adj} A|^2 &= 2A \{|A|^2 I - A^T A\}, \\ \frac{\partial}{\partial A} |A^{-1}|^2 &= 2\alpha^{-2} A \{|A|^2 I - A^T A - \alpha^2 |A^{-1}|^2 (A^T A)^{-1}\}, \\ \frac{\partial}{\partial A} \text{trace}(\text{adj} A) &= (\text{trace} A) I - A^T, \\ \frac{\partial}{\partial A} |A A^T A|^2 &= 6A A^T A A^T A, \\ \frac{\partial}{\partial A} |A W^T|^2 &= 2A W^T W, \\ \frac{\partial}{\partial A} |W A|^2 &= 2W^T W A. \end{aligned}$$

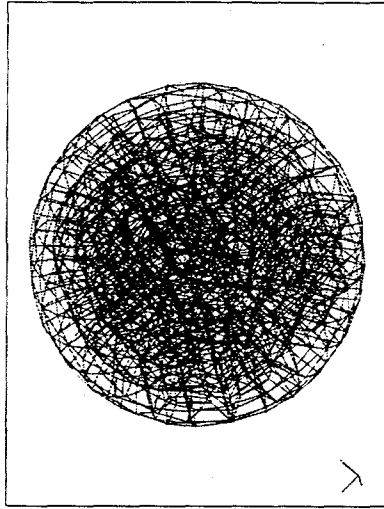


FIG. 1. Initial WW Hexahedral Mesh on Sphere Geometry

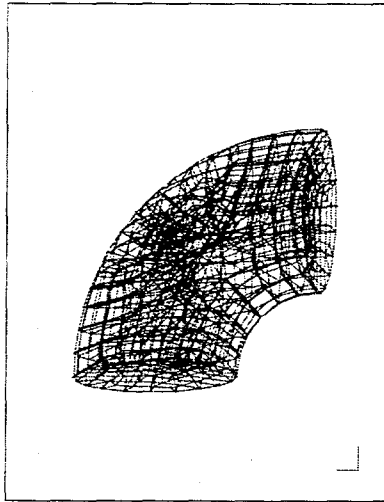


FIG. 2. Initial WW Hexahedral Mesh on Knee Geometry

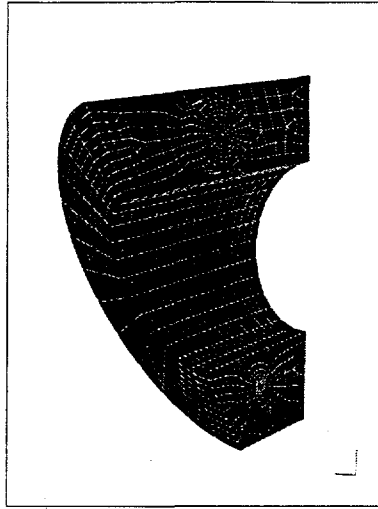


FIG. 3. Initial Swept Hexahedral Mesh on Curved Geometry

TABLE 2
Average Quality Metrics for Hexahedral Mesh (Knee Geometry)

Method	Aspect	Skew	Oddy	Scaled J	Valid?
Whisker Weave	1.496	0.4594	7119	0.6225	No
Laplacian	1.493	0.4597	7116	0.6229	No
Equipotential	1.976	0.5386	12900	0.5394	No
Length, $ A ^2$	1.520	0.4106	4270	0.6680	No
$ A ^2 - 3\alpha^{2/3}$	1.486	0.4082	4267	0.6757	No
2-Length, $ A ^4$	1.482	0.4357	5690	0.6530	No
NMT $ A^T A ^2$	1.513	0.4468	8532	0.6334	No
Volume, α^2	1.608	0.5019	4271	0.5983	No
$ OffDiagA^T A ^2$	1.480	0.4648	4273	0.6278	No
$ adjA ^2$	1.453	0.4172	1430	0.6729	No
$ AA^T A ^2 - 3\alpha^2$	1.834	0.4860	3708	0.5479	No
$ A^T A ^2 - 3\alpha^{4/3}$	1.688	0.4722	55460	0.5427	No
Smoothness, $\alpha A^{-1} ^2$	1.556	0.4127	25.7	0.6669	Yes
$\alpha^{2/3} A^{-1} ^2$	1.472	0.3872	9.396	0.6861	Yes
$ A^{-1} ^2$	1.446	0.3994	6.755	0.6911	Yes
$ A ^2 / \alpha$	1.419	0.3905	5.836	0.6962	Yes
$\alpha^{-2/3} A ^2$	1.441	0.3888	2847	0.6911	Yes
$\alpha^{-4/3} A^T A ^2$	1.551	0.4153	13.41	0.6592	Yes
Oddy(A)	1.448	0.4109	1426	0.6761	Yes
Oddy(A^{-1})	1.669	0.4371	23.2	0.6328	Yes
$\kappa(A)$	1.453	0.3929	8.760	0.6889	Yes
$\kappa(A^T A)$	1.465	0.4096	8.115	0.6778	Yes

TABLE 3
Average Quality Metrics for WW Hexahedral Mesh (Sphere Geometry) - Barriers Only

Method	Aspect	Skew	Oddy	$\kappa(A)$	Scaled J	Valid?	Rel CPU
Whisker Weave	1.533	0.3452	1867	622	0.6877	No	-
Laplacian	1.528	0.3438	1867	622	0.6888	No	-
Equipotential	2.113	0.5007	5600	1865	0.5482	No	-
$ A ^2/\alpha$	1.434	0.2955	3.559	1.424	0.7441	Yes	0.86
$\kappa(A)$	1.467	0.2782	4.133	1.447	0.7529	Yes	1.00
$\alpha^{2/3} A^{-1} ^2$	1.480	0.2744	4.733	1.469	0.7549	Yes	1.51
$\kappa(A^T A)$	1.470	0.2829	4.178	1.451	0.7522	Yes	3.18
$\alpha^{-4/3} A^T A ^2$	1.514	0.2822	5.374	1.501	0.7513	Yes	7.47
Smoothness, $\alpha A^{-1} ^2$	1.523	0.2735	5.003	1.492	0.7533	Yes	2.26
Oddy(A^{-1})	1.548	0.2877	6.084	1.532	0.7476	Yes	12.8
Oddy(A)	1.466	0.3072	3.579	1.457	0.7319	Yes	3.02
$\alpha^{-2/3} A ^2$	1.467	0.2854	3.770	1.441	0.7471	Yes	0.60
$ A^{-1} ^2$	1.438	0.3068	3.801	1.429	0.7418	Yes	2.27

TABLE 4
Average Quality Metrics for Swept Hexahedral Mesh (Curved Geometry)

Method	Aspect	Skew	Oddy	$\kappa(A)$	Scaled J	Valid?
Sweep	7.68	0.130	524	4.25	0.930	Yes
Laplacian	3.89	0.600	3e+05	9e+04	0.228	No
Equipotential	6.21	0.314	1023	288	0.823	No
$ A ^2/\alpha$	6.00	0.246	168	3.22	0.880	Yes
$\kappa(A)$	6.38	0.167	230	3.42	0.919	Yes
$\alpha^{2/3} A^{-1} ^2$	6.75	0.148	791	3.88	0.896	Yes
$\kappa(A^T A)$	6.31	0.224	240	3.50	0.891	Yes
$\alpha^{-4/3} A^T A ^2$	7.51	0.167	468	4.14	0.918	Yes
Smoothness, $\alpha A^{-1} ^2$	7.68	0.140	508	4.21	0.931	Yes
Oddy(A^{-1})	7.56	0.168	491	4.19	0.916	Yes
Oddy(A)	5.71	0.363	148	3.26	0.804	Yes
$\alpha^{-2/3} A ^2$	5.93	0.264	162	3.21	0.870	Yes
$ A^{-1} ^2$	6.36	0.177	231	3.43	0.913	Yes

TABLE 5
Worst-Case Quality Metrics for Tetrahedral Mesh (Sphere Geometry) - ℓ_∞ norm

Method	β	γ	$\kappa(A)$	Scaled J
Tetrahedral Mesh	4.232	4.764	3.579	0.1377
Laplacian	5.750	376.	297.	0.0024
$ A ^2/\alpha$	3.965	4.345	3.790	0.1613
$\kappa(A)$	4.263	5.155	2.989	0.1004
$\alpha^{2/3} A^{-1} ^2$	4.757	5.855	3.033	0.0883
$\kappa(A^T A)$	4.262	5.146	2.989	0.1013
Smoothness, $\alpha A^{-1} ^2$	4.405	4.777	3.044	0.1136
Oddy(A^{-1})	6.124	6.406	3.156	0.0779
Oddy(A)	3.864	4.153	3.607	0.1740
$\alpha^{-2/3} A ^2$	3.866	3.986	3.300	0.1574