LINEAR ELASTIC MESH DEFORMATION VIA LOCALIZED ORTHOTROPIC MATERIAL PROPERTIES OPTIMIZED BY THE ADJOINT METHOD

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ABSTRACT

The finite element method has been shown to be a powerful tool in computational engineering with recent application to electromagnetics and fluid dynamics. However, achieving the high orders of accuracy easily available to the finite element method has proven difficult due to conforming higher-order meshes to curved geometries. If higher-order nodes are not placed on the surface of the geometry error is introduced into the simulated solution. This barrier is largely a non-issue for inviscid meshes where a mid-edge node can be projected onto the nearest geometry surface with minimal detrimental side effects. Viscous meshes however have to deform most of the boundary layers in order to avoid inverting the surface elements and to maintain an acceptable mesh quality. This research focuses on extending the application of the linear elastic analogy to this mesh movement problem by attributing orthotropic material properties individually to each node or element. This technique allows each node or element to behave differently under the stress of conforming to the boundary. These localized material properties are determined using the adjoint optimization method. To better determine mesh quality, a new mesh metric called Metric3 is introduced. This new metric resembles the included angle metric and is based on an element’s isoparametric transformation matrix.
DEDICATION

This dissertation is dedicated to my amazing wife Kristen Karman-Shoemake.
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CHAPTER 1

INTRODUCTION

The application of linear-elasticity to mesh movement is convenient considering the similarity of the problems being solved by the solid mechanics and meshing communities. The meshing community however is entirely concerned with solving for a displacement field subject to prescribed displacements on the boundary and with little regard to physical feasibility. For example the distribution of the Youngs Modulus in the field can continuously vary as a function of wall distance possibly taking values of no known materials. This approach has been successful when applied to finite volume (FV) mesh movement and is directly applicable to similar finite element (FE) problems.

The finite element method (FEM), while originally developed for structural mechanics, has been successfully applied to fluid dynamics and electromagnetics problems [1, 2]. But unlike traditional structural mechanics problems, E&M and especially CFD problems are primarily concerned with cases involving curved boundary definitions. In order to better approximate curved geometries, FEM has two options, H-refinement and P-refinement. H refinement simply inserts more elements into the mesh whereas P refinement elevates the order of interpolation across an element. The P-refined elements are referred to according to the order of the polynomial that interpolates them, e.g. linear (P1), quadratic (P2), cubic (P3), etc. Allowing each element to take responsibility
for its own order of interpolation within its domain is one of the greatest advantages of the finite element method [3].

The process of P refinement requires more consideration in order to see the full benefits of elevating the order. Consider a linear edge along a curved boundary and that this edge is increased in order from linear to quadratic. The simplest path to achieve this is to place the newly created node along the linear edge itself. The usual location is at the midpoint. Elevating every edge in the mesh in this way will result in a mesh of quadratic elements with straight edges. In general this will decrease the error in a solution, but this can be improved upon. An example of this can be seen in figure 1.1 from [4]. In this case an electromagnetic plane wave is incident on a perfect electric conductor (PEC) sphere. This scenario has an analytic solution against which the results are compared. In this short study, three very similar cases were run in which the mesh varied in the placement of the higher order nodes. Figure 1.1 shows the results. The P1 line represents the results obtained form a linear or finite volume style mesh. The P2 line represents the results obtained form a quadratic mesh in which the higher order nodes were placed at the midpoint of the linear edge. The P2_curved line represents the results obtained from a quadratic mesh originally elevated in the same fashion as the P2 mesh, but higher order nodes residing in the boundary edges were then placed onto the geometric definition of the sphere. Clearly, placing the higher order nodes on the geometry greatly improved the solution of the simulation.

However, this is an E&M case which does not have viscous effects requiring a boundary layer region of the mesh for boundaries representing physical walls. Suppose we are interested in the fluid dynamics of the same geometry. We limit this case to two dimensions so we will be considering a circle in a cross flow. The mesh describing this scenario would require a boundary
layer surrounding the circle in order to resolve the viscous effects. This mesh is depicted in figure 1.2. The circle depicted has a radius of one and initial wall spacing of 0.01.

Figure 1.1  Radar cross section of a perfect electric conducting sphere
Suppose we attempt the same process of elevating the mesh and placing the higher order nodes onto the geometry. The result of this is shown in figure 1.3. As we can see, the first layer of elements are inverted which invalidates the mesh. The mesh must be untangled in order to fix the inverted elements. Yano et. al in [5] demonstrated that the quality of the boundary layer impacts the accuracy of the flow solution. Thus the mesh must be untangled and in a way as to maximize the quality of the elements. The main techniques for handling this problem are to construct the mesh while incorporating the effects of boundary curvature or to construct the straight edge mesh and later incorporate the boundary curvature by untangling or deforming the straight edges. The former, a priori method, is very expensive and not currently robust whereas the latter, a posteriori method, makes use of existing meshing technology to begin elevating the mesh.
The main \textit{a posteriori} approaches are localized optimization, Winslow smoothing, and elastic smoothing. The optimization method used in \cite{6}, consists of identifying the region surrounding poor quality elements in the inviscid region of the mesh and moving the nodes in the region in such a way as to optimize the scaled Jacobian. Their objective function incorporated the log barrier method to enforce the Jacobians to stay within a desired range. If the poor quality element occurs in the boundary layer, a consistent deformation is applied to the entire stack containing the element. The method developed by Ruiz et. al in \cite{7} uses an objective function based on their distortion measure and an $L_2$ disparity measure between the nodes and the geometry. The surface nodes are allowed to move freely but the disparity measure drives the mesh to best fit the geometry. This allows for meshing on imperfect geometries. Lastly, Karman and Wyman \cite{8} extended weighted condition number smoothing to higher order meshes by computing the weight matrices based on
the unperturbed elevated mesh, subdividing the higher order elements into linear sub-elements, and smoothing by enforcing the sub-element shapes.

Fortunato and Persson [9] extended Winslow smoothing for unstructured higher order meshing. In place of the virtual control volumes traditionally used in Winslow smoothing, the undeformed elevated mesh is used as the computational mesh. The surfaces of the physical mesh are then projected and the Winslow equations are solved for the locations of the higher order physical mesh.

The solid mechanics approach views the mesh as an elastic solid on which boundary deformations are prescribed. Linear elasticity assumes small deformations making it unsuitable for large mesh movement problems. Persson and Peraire [10] successfully applied the nonlinear elastic approach using an adaptive Newton-Krylov solver which split the deformation into smaller steps. Moxey et. al [11] incorporate a thermal stress term used to control element quality and allow
for larger deformations. Poya et. al [12] present a unified approach to elasticity mesh movement encompassing classical linear elasticity, non-linear elasticity, incremental linear elasticity and propose the consistent incrementally linearized method. They then compared these approaches finding that the incremental linear approaches were the most robust, economical, and produced the best quality meshes. In [13], Turner compared linear elastic, hyperelastic, distortion, and the Winslow equation functionals and found that the elasticity functionals produced the highest quality meshes.

The goal of the work presented here is to explore orthotropic linear elasticity for the purpose of creating higher-order boundary conforming meshes. Similar to [11] with the thermal coefficient, the orthotropic material analogy provides more parameters with which to control the behavior of mesh movement than the isotropic material model alone. The following chapter discusses the governing equation of orthotropic linear elasticity, outlines multiple methods of specifying the orthotropic material parameters, defines three metrics used to evaluate mesh quality, and applies the adjoint optimization method to determine the optimal material properties.
CHAPTER 2

METHODOLOGY

2.1 Governing Equations

The governing equations describing linear-elastostatics can be expressed in tensor notation as

\[ \sigma_{ij} = -f_i \]
\[ \sigma_{ij} = C_{ijkl} \varepsilon_{kl} \]
\[ \varepsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}) \]

where \(\sigma_{ij}\) are the components of the stress tensor, \(f_i\) the applied body forces, \(C_{ijkl}\) the components of the stress-strain (constitutive) relation, \(\varepsilon_{ij}\) the components of the strain tensor, and \(u_i\) the components of the displacement.

These equations are covered in most solid mechanics texts. In this case, the derivations in [3,14] are used and go beyond the needs of the work presented. In the form above, the stress-strain relation is known as the elastic modulus tensor, or the stiffness tensor. The stiffness tensor can be inverted to form the compliance tensor \(S_{ijkl}\), which can be used in the equation \(\varepsilon_{ij} = S_{ijkl} \sigma_{kl}\). This is a 4th order tensor meaning that it consists of 16 entries in two dimensions and 81 entries in 3 dimensions. However, this is for the most general form. The stress and strain tensors are symmetric.
by definition and which means this must also be the case for the stiffness tensor. This symmetry requirement allows the stiffness tensor to be expressed in matrix form and cuts the number of unique entries down to 6 in two dimensions and 21 in three dimensions. For simplicity, the current work will only concern the two dimensional case. The stiffness form of the stress-strain relation may now be expressed in matrix form as

\[
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{12}
\end{pmatrix}
= 
\begin{pmatrix}
c_{11} & c_{12} & c_{13} \\
c_{21} & c_{22} & c_{23} \\
c_{31} & c_{32} & c_{33}
\end{pmatrix}
\begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\epsilon_{12}
\end{pmatrix}
\]

(2.4)

where \(\sigma_{11}\) is the normal stress applied to face 1 in the 1 direction, \(\sigma_{22}\) is the normal stress applied to face 2 in the 2 direction, and \(\sigma_{12}\) is the shear stress applied to face 1 in the 2 direction. The same convention applies to \(\epsilon\). The stiffness matrix in equation 2.4 pertains to fully anisotropic materials. This implies that a normal stress applied to the material can result in a shear strain and similarly an applied shear stress can result in a normal strain. Presently we will not allow these reactions to occur by forcing the responsible entries in the stiffness matrix to be zero. These are the off-diagonal entries in the 3rd column and the 3rd row. The compliance form, which follows, better serves to define the stress-strain relation in terms of qualitative material properties using the plane stress assumption.
The isotropic compliance matrix is obtained by setting

\[
\begin{bmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\epsilon_{12}
\end{bmatrix} = \begin{bmatrix}
\frac{1}{E_1} & -\frac{\nu_{12}}{E_2} & 0 \\
-\frac{\nu_{21}}{E_1} & \frac{1}{E_2} & 0 \\
0 & 0 & \frac{1}{2G_{12}}
\end{bmatrix}
\begin{bmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{12}
\end{bmatrix}
\]

(2.5)

The isotropic compliance matrix is obtained by setting

\[
E = E_1 = E_2
\]

\[
\nu = \nu_{12} = \nu_{21}
\]

\[
G = \frac{E}{2(1 + \nu)}
\]

(2.6)

Note that in two dimensions four material properties \((E_1, E_2, \nu_{21}, G_{12})\) are required in order to determine just as many unique entries in the compliance matrix. The variable \(\nu_{12}\) is not needed as the relation \(\nu_{12}/E_2 = \nu_{21}/E_1\) is required in order to maintain symmetry of the stress tensor [15]. Similarly in three dimensions, nine material properties are needed in order to determine nine unique entries in the compliance matrix. This is due to our current derivation taking place entirely with respect to an ideal reference frame. Thus the current form of the stress-strain relation only applies to situations in which the ideal reference frame of the material in consideration aligns with the global reference frame. A change of basis must be applied to the current compliance tensor in order to apply the current stress-strain relation to more interesting problems. This change of basis is covered in [14, 16]. In three dimensions it proceeds as follows. A transformation tensor \(\Omega_{ij}\) is defined as \(\Omega_{ij} = m_i \cdot e_j\) where \(m_i\) are the basis vectors in the ideal frame and \(e_i\) are the basis vectors...
of the global frame. We must evaluate

\[ C'_{ijkl} = \Omega_{ip}\Omega_{jq}\Omega_{kr}\Omega_{ls}C_{pqrs} \]  

(2.7)

in order to transform the stiffness tensor from the ideal frame into the global frame. Note that the entries in \( \Omega \) are directional cosines. As we will only be handling cases in two dimensions, the transformation from the ideal frame to the global frame is only a function of a rotation about the z axis, \( \theta \). Thus using the five values mentioned: \( E_1, E_2, \nu_{21}, G_{12}, \) and \( \theta \), any stiffness tensor describing an orthotropic material in an ideal frame can be transformed to join a global frame of reference.

Bower provides these transformations in matrix form for three dimensions along with the logic for developing the two dimensional transformation matrices [14]. Below is the rotation matrices used

\[
T = \begin{bmatrix}
c^2 & s^2 & 2cs \\
s^2 & c^2 & -2cs \\
-cs & cs & c^2 - s^2
\end{bmatrix},
\]

(2.8)

\[ C' = TCT^{-1} \]

(2.9)

where \( c = \cos(\theta) \) and \( s = \sin(\theta) \).
2.2 Discretization

The Galerkin formulation of the finite element method, using Lagrangian basis functions, is applied to the linear-elastic partial differential equation in order solve for the displacements of nodes in the mesh. This is a favorite problem of many introductory finite element texts, however most remain in the ideal frame or conflate the material directions with the global coordinate axes. This results in zeroes in the off diagonal entries of the third row and third column which is not the case after the change of basis shown in equation 2.9. As a thorough description of the system of equations being solved has not been shown yet, a derivation of the weak form follows, highlighting the transformed constitutive relations.

Beginning with the elastostatics equations in two dimensions,

\[
\frac{\partial \sigma_{11}}{\partial x_1} + \frac{\partial \sigma_{12}}{\partial x_2} + f_1 = 0 \tag{2.10}
\]

\[
\frac{\partial \sigma_{12}}{\partial x_1} + \frac{\partial \sigma_{22}}{\partial x_2} + f_2 = 0 \tag{2.11}
\]

we can define the differential operator \( D^T \) along with vectors \( \sigma \) and \( f \).

\[
D^T = \begin{bmatrix}
\frac{\partial}{\partial x} & 0 \\
0 & \frac{\partial}{\partial y}
\end{bmatrix}, \quad \sigma = \begin{bmatrix}
\sigma_{xx} \\
\sigma_{yy} \\
\sigma_{xy}
\end{bmatrix}, \quad f = \begin{bmatrix}
f_x \\
f_y
\end{bmatrix} \tag{2.13}
\]
This allows equation 2.10 to be expressed in matrix form as

\[ D^T \sigma + f = 0 \]  

(2.14)

In order to solve for the deformed locations of the mesh, the problem must be expressed in terms of displacements. A stress-strain relation along with a strain-displacement relation must be used to do this. The stress-strain relation was introduced earlier as \( \sigma = C \epsilon \). The strain-displacement relation can be written in tensor form as

\[ \epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \]  

(2.15)

This is the linearized form of the Lagrangian strain tensor. This relation assumes small displacements relative to the original configuration [17]. Again using Voigt notation, this can be written in matrix form as

\[ \epsilon = Du \]  

(2.16)

where the strain \( \epsilon \) and displacement \( u \) vectors are defined as

\[ \epsilon = \begin{pmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{xy} \end{pmatrix} \quad u = \begin{pmatrix} u_x \\ u_y \end{pmatrix} \]  

(2.17)
Thus equation 2.14 can be written as

\[ D^T C D u = -f \]  

(2.18)

Assuming \( C \) is a full matrix as in equation 2.9, equation 2.18 will expand to

\[
\frac{\partial}{\partial x} \left( c_{11} \frac{\partial u_x}{\partial x} + c_{12} \frac{\partial u_y}{\partial y} + c_{13} \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \right) + \frac{\partial}{\partial y} \left( c_{31} \frac{\partial u_x}{\partial x} + c_{32} \frac{\partial u_y}{\partial y} + c_{33} \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \right) = -f_x
\]

\[ (2.19) \]

\[
\frac{\partial}{\partial y} \left( c_{21} \frac{\partial u_x}{\partial x} + c_{22} \frac{\partial u_y}{\partial y} + c_{23} \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \right) + \frac{\partial}{\partial x} \left( c_{31} \frac{\partial u_x}{\partial x} + c_{32} \frac{\partial u_y}{\partial y} + c_{33} \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \right) = -f_y
\]

\[ (2.20) \]

The weak form is obtained by multiplying equation 2.18 by a weighting function \( w \) and integrating by parts to transfer differentiation from \( u \) onto \( w \) resulting in

\[
0 = \int_{\Omega_e} \left[ D^T(w)C' D u \right] d\Omega_e - \int_{\Omega_e} w f d\Omega_e - \int_{\Gamma_e} w t ds
\]

(2.21)

where

\[
D^T(w) = \begin{bmatrix}
\frac{\partial w}{\partial x} & 0 & \frac{\partial w}{\partial y} \\
0 & \frac{\partial w}{\partial y} & \frac{\partial w}{\partial x}
\end{bmatrix}
\]

(2.22)
The traction vector $t$ can be defined as

$$ t = nC'Du $$

(2.23)

where

$$ n = \begin{bmatrix} n_x & 0 & n_y \\ 0 & n_y & n_x \end{bmatrix} $$

(2.24)

Fortunately in the case of mesh movement, the boundary conditions are prescribed displacements which means the body forces and traction terms are dropped reducing the problem to

$$ 0 = \int_{\Omega_e} [D^T(w)C'Du] d\Omega_e $$

(2.25)

Integration is performed on each element using the Gauss-Legendre quadrature. The solution variables $u$ and physical coordinates $X$ are interpolated over an element as

$$ u_i(\xi, \eta) = \sum_{j} \hat{u}_{ij} \phi_j(\xi, \eta) $$

(2.26)

$$ X_i(\xi, \eta) = \sum_{j} \hat{X}_{ij} \phi_j(\xi, \eta) $$

(2.27)

where $N$ is the number of nodes in the element and the hatted variables $\hat{u}_{ij}, \hat{X}_{ij}$ are the $ith$ component of the values stored at the $jth$ node of the element. The transformation matrix from ideal space to
physical space is given by the Jacobian matrix

\[
J(\xi, \eta) = \frac{\partial X_i(\xi, \eta)}{\partial x_j} = \begin{bmatrix}
\frac{\partial x(\xi, \eta)}{\partial \xi} & \frac{\partial x(\xi, \eta)}{\partial \eta} \\
\frac{\partial y(\xi, \eta)}{\partial \xi} & \frac{\partial y(\xi, \eta)}{\partial \eta}
\end{bmatrix}
\]

which is easily inverted for use in changing the bounds of integration to the appropriate bounds of Gauss-Legendre quadrature.

After the elements have been integrated and the global system of equations has been assembled, the linear system is solved using the Conjugate Gradient method with ILU(0) preconditioning. Picard iterations are used to mitigate the error introduced from using of the infinitesimal strain tensor by taking many small steps to reach the full displacement prescribed to the boundary nodes.

2.3 Material Property Determination

As mentioned earlier, five parameters are required to describe a two dimensional orthotropic material in any orientation: \(E_1, E_2, \nu_{21}, G_{12}, \) and \(\theta\). In the following sections the most important parameter to be determined is \(\theta\). The other four may be left as user inputs or may be determined by the characteristics of the methods described below. The goal of the remainder of this section is to determine these orthotropic parameters locally within the interior of the mesh.

2.3.1 Discrete Material Property Determination

The goal is to devise a method with which to extract enough information from a general element in the mesh that at least \(\theta\) can be determined for use in evaluating the orientation of the stress-strain matrix for the element. An ellipse was chosen due to the fact that the semi-major and
semi-minor axes form an orthogonal basis. The magnitudes of the semi-major and semi-minor axes provide information with which $E_1$, $E_2$, $\nu_{21}$, and $G_{12}$ can be set, and the rotation of the ellipse can be used to determine $\theta$.

Multiple techniques are available for fitting an ellipse to data. Initially the singular value decomposition (SVD) was considered, however it does not produce desireable results for quadrilaterals that have been sheared, the resulting ellipse has undergone rotation in such a way as to orient the semi-major axis of the ellipse with the longest diagonal of the quadrilateral. The implications of this effect can be seen by considering an anisotropic quadrilateral element in the boundary layer. This element has been specifically created so that the long sides of the quad are approximately parallel to the closest boundary. This also provides a general direction of the semi-major axis of an ellipse as well as a value for $\theta$. Now suppose that the element has been sheared and resembles a parallelogram. Evaluating the SVD on this element would not result in the same value of $\theta$, an example of this is shown in figure 2.1.
Figure 2.1  Example of an SVD ellipse on a simple quadrilateral
The SVD also presents problems when considering triangular boundary layer regions. For consistency, an equivalence between a single anisotropic quad and two anisotropic triangles forming the same shape is desirable. Consider an anisotropic triangle in the boundary layer. In this case, evaluating the SVD on a triangle perfectly aligned with the boundary will not result in a semi-major axis that is parallel to the closest boundary. Attempts were made to remedy this by considering a virtual quad created by translating the point opposite the middle length edge, none of which resulted in satisfactory techniques that would handle general cases.

The ellipse fitting method used here, developed in [18] and stabilized in [19], is based on minimizing the algebraic distance from a set of points to an ellipse. Given the equation for the general form of a conic

\[ F = ax^2 + bxy + cy^2 + dx + ey + f = 0 \]  

(2.29)

the vector form of the equation can be written as

\[ F(x) = x^T a \]  

(2.30)
where

\[
\begin{pmatrix}
x^2 \\
x y \\
y^2 \\
x \\
y \\
1
\end{pmatrix}
\begin{pmatrix}
a \\
b \\
c \\
d \\
e \\
f
\end{pmatrix}
\]

\( (2.31) \)

The matrix \( D \) is formed as

\[
D =
\begin{bmatrix}
x_1^2 & x_1y_1 & y_1^2 & x_1 & y_1 & 1 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
x_i^2 & x_iy_i & y_i^2 & x_i & y_i & 1 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
x_N^2 & x_Ny_N & y_N^2 & x_N & y_N & 1
\end{bmatrix}
\]

\( (2.32) \)

The ellipse specific constraint

\[
4ac - b^2 = 1
\]

\( (2.33) \)

can be expressed in matrix form as

\[
a^T Ca = 1
\]

\( (2.34) \)
where

\[ C = \begin{bmatrix}
0 & 0 & 2 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 \\
2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix} \]  \hfill (2.35)

Letting \( S = D^T D \), then the eigensystem of

\[ Sa = \lambda Ca \] \hfill (2.36)

\[ a^T Ca = 1 \] \hfill (2.37)

can be solved using generalized eigenvectors. The eigenvector corresponding to the smallest positive eigenvalue contains the conic coefficients of the matrix of best fit [18]. The developments in [19] address the singularity of \( C \) and stiffness of \( S \) by separating the problem into quadratic and linear parts and thereby reducing the size of the eigensystem to be solved to a \( 3 \times 3 \). This was the method used to determine the ellipse coefficients from the elements.
Once the conic coefficients have been determined, the magnitude and direction of the major and minor axes are solved for using the matrix of the quadratic form below.

\[
M = \begin{bmatrix}
a & \frac{b}{2} \\
\frac{b}{2} & c
\end{bmatrix}
\]  

(2.38)

As provided in [20], the eigensystem is solved which produces eigenvectors for which the smallest eigenvalue corresponds to the semi-major axis. The semi-major axis \(a\) and semi-minor axis \(b\) are defined as

\[
a = \left( \frac{1}{\sqrt{\lambda_1}} \right)^2, \quad b = \left( \frac{1}{\sqrt{\lambda_2}} \right)^2, \quad \lambda_1 < \lambda_2
\]  

(2.39)

Experimentation has shown that providing the element vertices to this routine would not consistently produce the desired ellipse. For example, in figure 2.2 some of the ellipses would be rotated 90 degrees. A simple solution to this problem is to also provide the mid edge point locations. This guaranteed that the set of points to be fitted would not perfectly lie on an ellipse. In order to handle triangles, the virtual quad method described previously is used. Examples of the resulting ellipses for triangles and quadrilaterals are shown in figure 2.2. The ellipses have been scaled down 50% for visual clarity.
This approach assumes a well formed linear mesh boundary layer with respect to the curved geometry. This means that the direction of anisotropy in each boundary layer element will determine the state of the ellipse fit to that element. The ellipse is meant to be oriented such that the semi-minor axis is parallel to the average direction of displacement along the closest boundary edge.

### 2.3.2 Continuous Material Property Determination

In this section the determination of material parameters is not be determined by the pre-existing linear mesh but instead by the geometry itself. The material parameters are attributed to
each node in the mesh instead of to the element. This allows the material parameters within an element to vary with the same order polynomial as the element itself. In short, each node’s material parameters are determined by the wall distance to the closest boundary and the gradient of the wall distance. Computation of the wall distance will be described in detail in section 2.4.1.

In the previous section, all of the stiffness tensors for each element could be precomputed and stored for later use in the computation of the element stiffness matrix. In contrast to this, the stiffness tensor will not be computed until it is needed in the element stiffness matrix routine. This is due to the stiffness tensor varying over the element. Otherwise a stiffness tensor would have to be computed and stored for each quadrature point in each element. Regardless, at each quadrature point the stiffness tensor is computed by interpolating the wall distance at the quadrature point along with the gradient of the wall distance.

\[
d_{wi}(\xi, \eta) = \sum_j^N \hat{d}_{wij} \phi_j(\xi, \eta) \quad (2.40)
\]

\[
\frac{\partial d_{wi}(\xi, \eta)}{\partial x} = \sum_j^N \hat{d}_{wij} \frac{\partial \phi_j(\xi, \eta)}{\partial x} \quad (2.41)
\]

\[
\frac{\partial d_{wi}(\xi, \eta)}{\partial y} = \sum_j^N \hat{d}_{wij} \frac{\partial \phi_j(\xi, \eta)}{\partial y} \quad (2.42)
\]

Equation 2.40 shows how the wall distance is interpolated to the gauss-point. Similarly, equations 2.41 and 2.42 show how the gradient is computed.

The vector formed by the gradient of the wall distance can then be used to set \( \theta \) by solving for the angle between \( \nabla d_w \) and the x axis. The wall distance can be used to influence the values assigned to \( E_1, E_2, \nu_{21}, \) and \( G_{12} \). For example the Youngs Modulus values can be set as in equation
2.43 to inversely vary with the wall distance.

\[
E_1 = \frac{1}{d_w} \tag{2.43}
\]

2.4 Quality Metrics

Mesh quality metrics are a tool to quickly and inexpensively predict the accuracy of a solution on a given mesh. The quality metrics of straight edge meshes for finite difference and finite volume solvers do not provide any information about the curved higher order behavior of the elements. Bassi and Rebay in [21] demonstrated the necessity of curved boundary conforming elements, but the detrimental effects of introducing curved elements has also been shown in [22] and [2]. In order to quantify the effects of mesh curving the following metrics are proposed: the relative change in wall distance, the scaled Jacobian, and Metric3. The relative change in wall distance provides information concerning how well the deformed mesh has preserved the original wall spacing of the higher order nodes. The scaled Jacobian indicates the uniformity of space throughout an element and is widely used throughout the literature. Metric3 is introduced to supplement the scaled Jacobian by identifying poorly shaped elements that the scaled Jacobian does not identify.

2.4.1 Relative Change in Wall Distance

The deformation introduced by conforming high-order elements to curved boundaries is almost entirely contained to the boundary layer region of a mesh. The boundary layer was specifically built with prescribed wall spacings and element orientations as a priority. Even if the deformed
mesh is valid, if the wall spacing is largely affected or the boundary layer is no longer orthogonal then the mesh may not yield accurate simulation results. The state of the wall spacing is examined by computing the wall distance for each node in the mesh where wall distance $d_w$ is defined as

$$d_w = \| X(\xi) - p \|$$

(2.44)

where $p$ is the coordinate of a node in the mesh and $X(\xi)$ is the closest point on a boundary to $p$. The Gradient Descent Method was used to solve for the parametric coordinate $\xi$ that minimized the wall distance.

To avoid a brute force search of each edge for the closest point, an isotropic quad tree was used to narrow the search to a few candidates. Boundary nodes, $p_b$, were stored in the tree. After returning a boundary node $P$ when queried for the closest boundary nodes to $p_i$, the gradient descent search would then be performed on all boundary edges connected to $P$. The quadtree only covered the boundary as opposed to the entire mesh. This allows the search extent box for a point outside the quad tree to immediately be grown to a size such that part of the search extent box is adjacent to the quad tree’s extent box.

The original linear mesh and especially the boundary layer region of the mesh were created with specific desired qualities. The percent change in wall distance, $\Delta d_w$ defined below, was used to indicate how well these characteristics were maintained through the curving process.

$$\Delta d_w = \frac{d_{w\text{final}} - d_{w\text{initial}}}{d_{w\text{initial}}}$$

(2.45)
Figure 2.3 shows some results of using classical isotropic linear elasticity. Note that wall distance of the high-order nodes decreases while that of the element vertices increases. This results in a wave effect in the boundary layer near regions of surface curvature. This effect is present regardless of material properties.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{example.png}
\caption{Example of change in relative wall distance}
\end{figure}

### 2.4.2 Scaled Jacobian

The scaled Jacobian has become the standard metric for evaluating the quality of high-order elements. It was defined in [23] as

\[
J_s = \frac{J_{\min}}{J_{\max}}
\]  

(2.46)
where $J$ is the determinant of the transformation matrix. The diagonal components of the transformation, shown again in equation 2.47, are extensional components and the off diagonal components are shearing components. The Jacobian is a volume measure in three dimension and an area measure in two dimensions. Thus the scaled Jacobian is a subjective internal measure of the extremes of the area/volume transformation. For example figure 2.4 shows a mesh containing all straight edges. We would expect the worst elements in the mesh to be the rhomboid shaped elements. However the trapezoids in the last set of the boundary layer return the lowest scaled jacobian. This is due to the the trapezoid quads stretching space more along their long side compared to their short side. In fact, any well formed parallelogram regardless of the degree of shearing will return a perfect scaled Jacobian of one. This also applies to straight edge triangles as well. Among straight edge elements, the scaled Jacobian measure is very useful. The scaled Jacobian is specifically designed to report the relative variation of space within an element. While high scaled Jacobian values are important, they offer no insight into other aspects of an elements health which has encouraged the development of other quality metrics.

$$J(\xi, \eta) = \begin{vmatrix} \frac{\partial x(\xi, \eta)}{\partial \xi} & \frac{\partial x(\xi, \eta)}{\partial \eta} \\ \frac{\partial y(\xi, \eta)}{\partial \xi} & \frac{\partial y(\xi, \eta)}{\partial \eta} \end{vmatrix}$$ (2.47)
2.4.3 Metric3

In order to address the weakness of the scaled Jacobian measure, a new metric inspired by the interior angle or skewness from finite volume (FV) meshing has been developed. The evaluation of the FV interior angle involves visiting each corner of the element and computing the angle and storing the min and/or max as desired. Attempting to perform the same routine on a curved high-order element also requires an isoparametric transformation matrix. Suppose we wish to evaluate the interior angle of the corner at parametric coordinate \((\xi = 0, \eta = 0)\) of a highly curved element. Examining the contents of the transformation matrix will show that the first column vector points in the direction of taking a small step in \(\xi\). The second column vector points in the direction of taking a small step in \(\eta\). Normalizing these two vectors and taking the dot product yields the
interior angle

\[ M_3 = \max \left( \frac{c_1 \cdot c_2}{\|c_1\| \|c_2\|} \right) \]  \hspace{1cm} (2.48)

where \( c_1 \) and \( c_2 \) are the column vectors of the matrix in equation 2.47. Note that this procedure only relies on \( \xi \) and \( \eta \) which allows it to be performed at any location in an element. \( M_3 \) will return values of 0 where the local basis vectors are orthogonal and 1 where the local basis are identical. Thus \( M_3 \) can be used to examine the orthogonality of the local transformation of the isoparametric basis in physical space. This allows it to easily identify sheared elements as shown in figure 2.5.

Similar to the scaled Jacobian, \( M_3 \) is evaluated at the quadrature points of the element and the maximum value is attributed to the element. Note the \( M_3 \) values of the extruded region in figure 2.5 are identical. This is due to the quadrilaterals in the extruded region being geometrically similar in shape.
2.5 Adjoint Optimization

Discussed in section 2.1, 5 material parameters must be set for each element or node. This raises the question of how to assign them. Generalizations could be made based on initial cell shape or other mesh characteristics. To avoid resorting to trial and error, we can approach the problem of material determination as an optimization problem similar to [24]. In [24] the only design variables were the Youngs modulus for each element. The goal of that study was to achieve large boundary movement while maintaining cell quality in the smaller elements located in the boundary layer. In this case, the boundary movement is very small. For convenience, the following definitions are
made:

\[ ne = \text{number of elements} \quad (2.49) \]

\[ nn = \text{number of nodes} \quad (2.50) \]

\[ ndv = \text{number of design variables} \quad (2.51) \]

\[ ndvg = \text{number of design variable groups} \quad (2.52) \]

\[ \Upsilon = \text{physical dimension} = 2, 3 \quad (2.53) \]

The objective function to be minimized is defined in equation 2.54 and accumulates \( M_3 \) over the mesh.

\[ L = \sum_{i=1}^{ne} M_{3i} \quad (2.54) \]

Due to the large number of design variables and non-negligible solution time, a gradient based optimization method was used. Also due to the same factors and that only a single objective function is minimized, the adjoint method is preferred over the direct method as the direct method would require at least \( ndv \) solutions for a single optimization iteration. Following the process laid out in [24], the interior mesh displacements \( u \) are a function of prescribed boundary displacements \( u_b \), the initial coordinates \( x_0 \), and the five material properties \( E_1, E_2, \nu_{21}, G_{12}, \) and \( \theta \) assigned to
each element or node. Let \( l_{jk} \) denote the group of material properties such that

\[
l_j = \begin{pmatrix}
E_1 \\
E_2 \\
\nu_{21} \\
G_{12} \\
\theta
\end{pmatrix}
\]

for the \( j \)th element. The groups of material properties for the entire mesh will be coalesced into a single vector \( \beta \) such that

\[
\beta_i = l_{jk}
\]

where \( i = 1, \ldots, 5(ndv) \); \( j = 1, \ldots, ndv \); and \( k = 1, \ldots, 5 \). Thus the functional form of the mesh displacements can be written as

\[
u = u(x_0, u_b, \beta)
\]

The sensitivities of the objective function \( L(M_3) \) with respect to the the design variables \( \beta \) can be expressed as

\[
\frac{dL}{d\beta_i} = \frac{dL}{dM_3} \frac{dM_3}{dx_f} \frac{dx_f}{d\beta_i}
\]
where \( dL/dM_3 \) is a matrix of dimension of \( 1 \times ne \), \((dM_3/dxf)\) is a matrix of dimension \( ne \times (nn \times \Upsilon) \), and \((dx_f/\partial \beta_i)\) is a matrix of dimension \((nn \times \Upsilon) \times 1 \). The \( dL/dM_3 \) and \( dM_3/dxf \) factors are straightforward to evaluate. The \( dL/dM_3 \) is differentiated from equation 2.54. In this implementation \( dM_3/dxf \) was computed by visiting each element and central differencing \( M_3 \) for each node in the element. Although analytic expressions can be readily derived for this step, the finite differencing did not impose a noticeable time cost and was sufficiently accurate. The \( \partial x_f/\partial \beta_i \) is equivalent to

\[
\frac{\partial x_f}{\partial \beta_i} = \frac{\partial (x_0 + u)}{\partial \beta_i} = \frac{\partial x_0}{\beta_i} + \frac{\partial u}{\partial \beta_i} = \frac{\partial u}{\partial \beta_i} \tag{2.59}
\]

The term \( \frac{\partial x_0}{\partial \beta_i} \) is zero as the initial conditions \( x_0 \) have no dependence on \( \beta \). The second term \( \frac{\partial u}{\partial \beta_i} \) is the most difficult to obtain efficiently. Instead of finite differencing \( \frac{\partial u}{\partial \beta_i} \) which would be quite expensive to fill \( \frac{\partial u}{\partial \beta_i} \), we can differentiate the equation

\[ K(\beta)u = F(u_b) \tag{2.60} \]

with respect to \( \beta_i \) resulting in

\[
\frac{dK(\beta)}{d\beta_i}u + K(\beta)\frac{\partial u}{\partial \beta_i} = 0 \tag{2.61}
\]

Rearranging 2.61 we can isolate the solution sensitivity to the design variable \( \beta_i \) as

\[
\frac{\partial u}{\partial \beta_i} = -K(\beta)^{-1}\frac{dK(\beta)}{d\beta_i}u \tag{2.62}
\]
This has introduced an inverse of a large matrix. Nevertheless, substituting this back into equation 2.58 yields

\[
\frac{dL}{d\beta_i} = -\frac{dL}{dM_3} \frac{dM_3}{dx_f} K^{-1} \frac{dK(\beta)}{d\beta_i} u
\]  

(2.63)

Note that the product of the first two factors of the right hand side produce a vector of dimension \(1 \times (nn \times \Upsilon)\). Instead of evaluating the inverse of the stiffness matrix, we can form the adjoint equation

\[
\lambda^T = -\frac{dL}{dM_3} \frac{dM_3}{dx_f} K(\beta)^{-1}
\]  

(2.64)

Rearranging will produce

\[
K(\beta)^T \lambda = -\left( \frac{dL}{dx_f} \right)^T
\]  

(2.65)

which can easily be solved for \(\lambda\). This has reduced the amount of work from inverting the large sparse matrix \(K(\beta)\) to transposing \(K(\beta)\) and solving a linear system of equations. In this case, \(K(\beta)\) is already symmetric and square so the transpose in a non-issue. We can now substitute \(\lambda^T\) back into equation 2.63

\[
\frac{dL}{d\beta_i} = \lambda^T \frac{dK(\beta)}{d\beta_i} u
\]  

(2.66)
which must be evaluated for each design variable. Without using the adjoint method, the equation $K(\beta)u = 0$ would have to be computed $ndv + 1$ times just to perform a forward difference. The adjoint allows this to be reduced to a single solution evaluation for $u$, solving a linear system of equations for $\lambda$, and a matrix vector multiplication for each design variable. Once the objective sensitivities have been obtained, they are passed to the unconstrained quasi-Newton nonlinear equation solver from the Opt++ software package [25].

In section 2.3, element-wise and node-wise methods were developed for determining local material properties. Either may be used in the optimization method just described. The only difference being the number of design variables: element-wise has $ne \times 5$, node-wise has $nn \times 5$. The only part of the adjoint method this affects is $\frac{dK(\beta)}{d\beta_i}$. Considering the element-wise method, perturbing $\beta_i$ will only affect the element stiffness matrix of the element in which $\beta_i$ resides. Considering the node-wise method, the design variables attributed to an internal node of an element will similarly only affect the element stiffness matrix in which the node resides. Perturbing the design variables of a node residing on the boundary of an element will affect the element stiffness matrix of all of the elements in contact with that node. Results for each method will be presented.

### 2.5.1 Implementation

The implementation of the finite element solver used relied heavily on the object-oriented features of the C++ programming language. Being object-oriented allowed large portions of the code to be generalized in such a way as to be order-agnostic of the actual elements populating the mesh but to be routine-agnostic as well. Meaning that at run time the order of the elements could easily be changed as well as the material model and properties. Some sections of the code were expected
to be computationally expensive with no need for flexible run time behavior. These sections were
the linear system solve for the node displacements and the eigensystem decompositions for the
SVD, linear least squares, and matrix of the quadratic form of the ellipse. The ILU(0), compressed
matrix, and conjugate gradient features of simunova’s MTL4 [26] software were used to solve
the linear system of equations. A templated, statically sized, cache optimized, small dense matrix
library was implemented for general use in handling the small matrices involved in linear elasticity
and specifically for solving the aforementioned eigensystems. A detailed description is provided
in appendix A. Both the isotropic and orthotropic features of the finite element linear elastic solver
implemented were validated against sample problems provided in [3].
CHAPTER 3

RESULTS

The results presented here will be organized according to the rules for determining the local material properties. First a small study will be conducted to examine the general influence of each material property. Then results will be shown for globally prescribed material properties, discretely determined material properties, and continuously determined material properties. Finally results will be shown for discretely and continuously optimized material properties.

Within the globally defined material property section are subsections describing discrete and continuous material properties. This is due to the nature in which $\theta$ is determined. The other four material properties $E_1$, $E_2$, $\nu_{21}$, and $G_{12}$ are set according to the global values provided but $\theta$ is allowed to vary. The discrete method relies on the configuration of an element to determine $\theta$ which will be constant throughout that element. The continuous method relies on a point’s relation to the boundary to set $\theta$ which can vary from point. Thus the discrete material property method may be referred to as element-based and the continuous method as node-based.

As mentioned earlier, the quality metrics used to compare solutions will be the change in relative wall distance ($\Delta\%d_w$) for each node, the scaled Jacobian ($J_s$) of each element, and Metric3 ($M_3$) for each element. Due to the nature of this problem, mesh movement does not propagate very far into the interior of the mesh, thus there is very little difference in mesh quality far from the geometry regardless of the material properties used. In order to clearly see the effects of varying
the material properties, data from the quality metrics beyond a certain distance from the geometry is excluded from the histograms. All of the following cases have been scaled so that the extruded boundary layer is has a wall distance of 1.0. A distance of 0.25 from the surface was found to be appropriate to capture the information from the deformed elements and filter out the information from the undeformed elements.

### 3.1 Orthotropic Perturbation Study

The first method considered for determining the material properties is to supply a user input to globally set $E_1$, $E_2$, $\nu_{21}$, and $G_{12}$. The element-based method was used to set $\theta$ for each element. The first case is a viscous mesh of an eight point circle. The circular geometry was constructed with a radius of 1.0, initial wall spacing of 0.0001, and a farfield distance of 14.0. The domain was initialized using the T-Rex and Advancing Front Ortho features of Pointwise [27].

The P2 mesh curved using isotropic elasticity is shown in figure 3.1 and histograms and contour plots of the quality metrics are shown in figure 3.2. In this case the primary point of interest is the difference in the distance of the mid edge nodes to the geometry wall when compared to the vertex nodes. Figure 3.2a indicates that there are large populations of nodes near the geometry whose wall distance has increased or decrease by roughly 20%. Figure 3.2b shows the distribution in space of the offending nodes. This contour indicates that the vertices of the boundary layer elements are displaced away from the wall while the higher order nodes in the path of the boundary deformation are also displaced away from the wall, just not as far. For the first layer of elements there is a 40% difference in the wall distance of the off wall vertices and their shared edge midpoint.
Figure 3.1  8 point circle mesh
Figure 3.2  8 point circle: isotropic elasticity quality metrics data and contours
To better understand the effects of the orthotropic material properties, a small study was performed to investigate the impact each material property has on the quality of the curved mesh. The preceding result from the isotropic elasticity case, for which Young’s modulus and Poisson’s ratio were set to 1.0 and 0.45 respectively, was used as a baseline for comparison. This implies that the shear modulus $G$ has a value of 0.3448275 according to the definition of an isotropic material

$$G = \frac{E}{2(1 + \nu)}$$

The orthotropic material properties were then individually perturbed about the isotropic values. Shown below are the values used.

$$E_1 \in 0.5, 1.5$$

$$E_2 \in 0.5, 1.5$$  \hspace{1cm} (3.1)

$$\nu_{21} \in 0.4, 0.499$$  \hspace{1cm} (3.2)

$$G_{12} \in 0.2448275, 0.4448275$$  \hspace{1cm} (3.3)

The discrete material property method was used to set $\theta$.

For histogram plots pertaining to the perturbation study, the left column shows the results of the decreased value of the material property being discussed and the right column shows the results of the increased value. The effects of perturbing $E_1$ are shown in figure 3.3. In general varying $E_1$ only has a noticeable influence on the $\Delta \%d_w$. Compared to the isotropic results, the decreased value of $E_1$ only slightly contracts the range of the change in relative wall distance. However the
increased value of $E_1$ only slightly expands the range of $\Delta\%d_w$. Thus in this case, $E_1$ only has a minor influence. In figure 3.4, the effects of $E_2$ are indicated in all three metrics. The decreased value of $E_2$ expanded the range of $\Delta\%d_w$, shifted the peak of $J_s$ down, and shifted the population of $M_3$ up. The increased value of $E_2$ had the opposite effect of contracting the range of $\Delta\%d_w$, shifting the peak of $J_s$ up, and slightly decreasing the population of $M_3$. Therefore the increased value of $E_2$ has had a positive effect on the quality of the mesh. Close examination of figure 3.5 shows that the increased value of $\nu_{21}$ only marginally improves the state of the mesh. Figure 3.6 shows the decreased values of $G_{12}$ contract the range of $\Delta\%d_w$, shift the population of $J_s$ up, and shift the population of $M_3$ down. The increased value had the exact opposite effect. In summary, decreasing $G_{12}$ and increasing $E_2$ had the greatest effect on improving mesh quality while $nu_{21}$ had no impact and increasing $E_1$ had a negative impact.
Figure 3.3 Perturbation Study: effects of $E_1$ on quality metrics. Left column shows results for $E_1 = 0.5$ and right column shows results for $E_1 = 1.5$. First row shows $\Delta \%d_w$, second row shows $J_s$, third column shows $M_3$. 

(a) $\Delta \%d_w$

(b) $\Delta \%d_w$

(c) $J_s$

(d) $J_s$

(e) $M_3$

(f) $M_3$
Figure 3.4 Perturbation Study: effects of $E_2$ on quality metrics. Left column shows results for $E_2 = 0.5$ and right column shows results for $E_2 = 1.5$. First row shows $\Delta% d_w$, second row shows $J_s$, third row shows $M_3$. 
Figure 3.5 Perturbation Study: effects of $\nu_{21}$ on quality metrics. Left column shows results for $\nu_{21} = 0.45$ and right column shows results for $\nu_{21} = 0.499$. First row shows $\Delta \% d_w$, second row shows $J_s$, third row shows $M_3$. 
Figure 3.6  Perturbation Study: effects of $G_{12}$ on quality metrics. Left column shows results for $G_{12} = 0.2448275$ and right column shows results for $G_{12} = 0.4448275$. First row shows $\Delta \% d_w$, second row shows $J_s$, third row shows $M_3$. 
3.2 Globally Defined Material Properties

3.2.1 Viscous Circle

Using the above observations as guidelines, figure 3.7 shows the results of running the same viscous circle case with the following parameters $E_1 = 1$, $E_2 = 2.5$, $\nu_{21} = 0.4999$, and $G_{12} = 0.01$. For convenience let $I_{\text{ortho}} = < 1, 2.5, 0.4999, 0.01 >$ represent these material properties. The figures show that when compared to the isotropic elasticity: the difference between the minimum and maximum values of $\Delta \% d_w$ has been decreased from 40% to 15%, the majority of elements now have a scaled Jacobian value at or above 0.8 as opposed to 0.6, and $M_3$ shows a noticeable shift toward 0 as well as a decrease in the maximum value. Refining the mesh greatly improves the results.

To see the effects of h-refinement, the number of vertices on the geometry was increased from eight to sixteen and the isotropic results for this case are shown in figures 3.8. The improvements are that the range of the change in relative wall distance has been reduced to $(-7.5, 12)$, the entire population of $J_s$ is above 0.8, and the entire population of $M_3$ is below 0.2. However, 3.8d shows that the worst elements are closest to the surface. As shown in figure 3.9, the orthotropic element-based version of the sixteen point circle results in all of the quality metrics improving. The issue of the elements closest to the surface having the lowest scaled Jacobians has reversed as now the surface elements have the highest scaled Jacobian values. Results using the node-based method of determining $\theta$ are shown in figure 3.10. The node-based method shows an improvement in the range of $\Delta \% d_w$, decreased the distribution of $M_3$, and increased the distribution of $J_s$. Figure 3.11 shows the results for using a triangular discretization with the same orthotropic material properties. The triangular mesh was created by diagonalizing the sixteen point quadrilateral mesh. The change
in relative wall distance and scaled Jacobian metrics indicate that the mesh quality has improved yet the $M_3$ metric shows the opposite. The remaining cases presented will use P4 elements as they display more aspects of boundary conforming higher-order elements than P2 or P3 elements.
Figure 3.7 8 point circle using P2 quaerilaterals and element based orthotropic properties: $E_1 = 1.0, E_2 = 2.5, \nu_{21} = 0.4999, G_{12} = 0.01$
Scaled Jacobian

Number of Elements

(c)

(d)
Figure 3.8  16 point circle using P2 quadrilaterals and isotropic material properties
(a)

(b)
Figure 3.9 16 point circle using P2 quadrilaterals and element based orthotropic properties: $E_1 = 1.0, E_2 = 2.5, \nu_{21} = 0.4999, G_{12} = 0.01$
Figure 3.10 16 point circle using P2 quadrilaterals and node based properties: $E_1 = 1.0, E_2 = 2.5, \nu_{21} = 0.4999, G_{12} = 0.01$
Figure 3.11 16 point circle using P2 triangles and element based orthotropic properties: $E_1 = 1.0, E_2 = 2.5, \nu_{21} = 0.4999, G_{12} = 0.01$
3.2.2 Viscous Potato

The next case was created in order to examine the behavior of the orthotropic model on a less ideal geometry. The 'potato' mesh, shown in figure 3.12a, was specifically created to have both convex and concave regions along with a sharp point shown in figure 3.12d and some poorly created elements such as those shown in figure 3.12b located at the sharp curve along the top surface. For comparison the isotropic results are shown in figures 3.13 - 3.16. Applying the same globally defined material properties as the previous viscous circle case produces the results in figures 3.13, 3.17, and 3.21. These results mirror those of the viscous circle case in that the range of $\Delta d_w$ has decreased significantly from (-13,+22) for the isotropic case to (-3,+3) in the discrete case and (-3.5,+2) for the continuous case.

Both the discrete and continuous cases have outliers in $\Delta d_w$ caused by specific features of the mesh. Using the discrete method, the top curve caused the the lowest values of $\Delta d_w$ while the concave region caused the highest as can be seen in figures 3.18 and 3.19 respectively. For future reference, the sharp point on the bottom of the geometry has not caused any problems and is shown in figure 3.20. The continuous case handles the upper curve and concave quite well which can be seen in figure 3.22 and 3.23. The most extreme value of $\Delta d_w$ in these two regions was $-4\%$ along the upper curve. However, the sharp point caused the extremely low value $-16.5\%$ as seen in figure 3.24. Ostensibly this was due to allowing the stiffness tensor to rotate around the point in such a way as to 'weaken' the material properties of the nodes emanating from the point to stresses applied from either side of the point.

The scaled Jacobian and Metric3 both appear to have greatly benefited from the orthotropic models. The majority of scaled Jacobian values have increased from $\approx 0.75$ for the isotropic case to
above 0.8 for the element based and slightly further for the node based. Similarly, compared to the isotropic results both the element-based and node-based globally defined orthotropic models show a noticeable shift toward zero indicating that a significant amount of the population of elements in the boundary layer are closer to being right-angled.
Figure 3.12  Potato mesh
Figure 3.13  Potato using P4 quadrilaterals: isotropic elasticity results
Figure 3.14  Upper curve of the potato geometry using P4 quadrilaterals and isotropic elasticity

Figure 3.15  Upper concave region of the potato geometry using P4 quadrilaterals and isotropic elasticity
Figure 3.16  Bottom point region of the potato geometry using P4 quadrilaterals and isotropic elasticity
Figure 3.17  Potato using P4 quadrilaterals and element-based material properties
Figure 3.18  Upper curve of the potato geometry using P4 quadrilaterals and globally defined element-based material properties

Figure 3.19  Upper concave region of the potato geometry using P4 quadrilaterals and globally defined element-based material properties
Figure 3.20  Bottom point region of the potato geometry using P4 quadrilaterals and globally defined element-based material properties
Figure 3.21  Potato using P4 quadrilaterals and the node-based material properties
Figure 3.22  Upper curve of the potato geometry using P4 quadrilaterals and globally defined node-based material properties

Figure 3.23  Upper concave region of the potato geometry using P4 quadrilaterals and globally defined node-based material properties
Figure 3.24 Bottom point region of the potato geometry using P4 quadrilaterals and globally defined node-based material properties

3.2.3 30P30N Front Slat

The next geometry is the front slat of the 30P30N multi-element airfoil. The mesh contains 1980 elements, 1956 linear nodes, and 30,396 quartic nodes. The mesh has been constructed with a wall spacing of 0.0001 again using T-rex extrusion and the Advancing Front Ortho features of Pointwise. Figure 3.25 shows the level of refinement of the geometry, specifically the upper and lower sharp points. The isotropic elasticity results for this case are shown in figure 3.26. Along the leading edge the highest and lowest values of $\Delta \% d_w$ are approximately 26% and −9% respectively. The lowest value of $\Delta \% d_w = −13.7$ in the mesh occurs at the lower sharp point of the slat shown in figure 3.27. The level of refinement and large regions of low curvature serve as an obstacle to generalizing the state of the mesh into histogram form. The orthotropic material properties were set to $E_1 = 1.0$, $E_2 = 1.25$, $\nu_{21} = 0.499$, and $G_{12} = 0.05$ for the following cases.
The results of the element-based and node-based methods are shown in figures 3.28 and 3.30 respectively. Figure 3.32 shows the results of the node-based method on a triangular discretization. The histograms of the node-based cases in figures 3.30 and 3.32 show that there is an outlier with a relative wall distance around $-67$. The element-based case had a similar result but of only $-20\%$ change in wall distance. Again this is likely due to stresses being transmitted through the mesh and concentrated at the lower point. A closer view is shown in figure 3.31. Aside from the outlier, the change in relative wall distance has a very narrow range centered around zero. The high population at zero is due to the lack of curvature throughout large regions of the geometry. The $J_s$ and $M_3$ contour plots show that the effects of the mesh movement at the leading edge have not propagated into the regions of low curvature along the upper surfaces.

This triangular mesh was also created by diagonalizing the quadrilateral mesh meaning that all of the P1 nodes are in the exact same location. This provides an opportunity for comparison of the behavior of the $J_s$ and $M_3$ metrics in straight edged regions of the mesh. As noted earlier, for a straight edged triangle $J_s = 1$ where as a straight edge quadrilateral that is not a parallelogram will have $J_s < 1$. Thus the off body region of the quadrilateral mesh has $J_s$ values as low 0.4. This explains the existence of lower values of the quadrilateral scaled Jacobian histogram in figure 3.30d. A similar situation exists for the use of the $M_3$ metric. As a straight edge triangle will never have a $M_3$ value above 0.5, we can assume that in the triangular mesh the $M_3$ values above 0.5 are caused by poorly shaped elements. The straight edge quadrilaterals however can have any value between 0 and 1.
Figure 3.25  30P30N slat mesh
Figure 3.26  30P30N front slat using P4 quadrilaterals and isotropic material properties
Figure 3.27  Bottom point of the 30P30N front slat using P4 quadrilaterals and isotropic material properties
(a) 

(b)
Figure 3.28  30P30N front slat using P4 quadrilaterals and element-based material properties
Figure 3.29  Bottom point of the 30P30N front slat using P4 quadrilaterals and the element-based material properties
Scaled Jacobian

Number of Elements

(c)

(d)

99
Figure 3.30  30P30N front slat using P4 quadrilaterals and node-based material properties
Figure 3.31  30P30N front slat using P4 quadrilaterals and node-based material properties
(c)

(d)
Figure 3.32 30P30N front slat using P4 triangles and node-based material properties
3.3 Discretely Defined Material Properties

The results of allowing each element to determine the values of $E_1, E_2, \nu_{21}, G_{12}$ follow. The fifth material property, $\theta$ is determined in the same manner using the rotation of the ellipse formed from the P1 element described in section 2.3.1. The rules for determining the material properties follow. For a given element, let $a$ and $b$ represent the semi-major and semi-minor axes respectively of the ellipse constructed in section 2.3.1. Then define

$$a_s = \frac{1}{1 + \frac{b}{a+b}} \quad (3.4)$$
Also given master user input values of $E^*_1$, $E^*_2$, $\nu_{21}^*$, and $G^*_{12}$, the local values of $E^*_1$, $E^*_2$, $\nu_{21}^*$, and $G^*_{12}$ can be defined as

$$E_1 = a_s E^*_1 \quad (3.5)$$
$$E_2 = a_s E^*_2 \quad (3.6)$$
$$\nu_{21} = a_s \nu_{21}^* \sqrt{\frac{E_1}{E_2}} \quad (3.7)$$
$$G_{12} = a_s G^*_{12} \quad (3.8)$$

The factor $a_s$ was chosen such that $a_s$ would have approach one as the eccentricity of an ellipse increases. Defining the scaling factor in this way produces the effect that the elements closest to the surface will have material properties approaching the master values supplied. Moving away from the surface we can expect the resulting ellipses to decrease in eccentricity which will cause $b_s$ to decrease. The form of $\nu_{21}$ was developed by Lempriere [15] in order to ensure the system remained symmetric positive definite regardless of the values of $E_1$ and $E_2$. For the following results shown in figures 3.35 and 3.39 the master material properties supplied were

$$E^*_1 = 1.0 \quad (3.9)$$
$$E^*_2 = 2.5 \quad (3.10)$$
$$\nu^*_{21} = 0.499 \quad (3.11)$$
$$G^*_{12} = 0.02 \quad (3.12)$$
3.3.1 Viscous Potato

Applying the logic from equations 3.4 and 3.5 to the Potato case results in the distributions for $E_1$, $E_2$, $\nu_{21}$, and $G_{12}$ shown in figure 3.34. The results in figure 3.35 are an improvement over both the isotropic case and those from the globally defined element-based case in figure 3.17. The differences being that the range of $\Delta\%d_w$ has been reduced to $(-6, +2.5)$ with the majority of the population between $(-3, +1)$. The scaled Jacobian has improved with a population of over 200 with $J_s$ values above 0.9. Metric3 however has slightly declined.
Figure 3.34 Potato geometry using P4 quadrilaterals and element-based orthotropic material properties
Scaled Jacobian

Number of Elements

(c)

(d)
Figure 3.35 Potato geometry using P4 quadrilaterals and element-based orthotropic material properties
Figure 3.36  Upper curve of the potato geometry using P4 quadrilaterals and element-based material properties

Figure 3.37  Upper concave region of the potato geometry using P4 quadrilaterals and element-based material properties
3.3.2 30P30N Front Slat

Compared to the previous results in figure 3.28 there is very little difference except that the value of the outlier in 3.39a has been reduced from $-67\%$ to $-20\%$. The variation in $\Delta %d_w$ along the leading edge is in the range of $(-4, +1.15)$. The extremes of $\Delta %d_w$ again occur at the bottom point as shown in figure 3.40. The scaled Jacobian and Metric3 have both improved.
Figure 3.39  30P30N front slat using P4 quadrilaterals and discrete material properties
Figure 3.40 Bottom point of the 30P30N front slat using P4 quadrilaterals and discrete material properties

### 3.4 Continuously Defined Material Properties

Where the discrete material property determination used the existing mesh to supply information for setting the material parameters, the continuous method attempts to rely on the geometry. As described earlier this is accomplished by computing the wall distance $d_w$ as well as the gradient of the wall distance $\nabla d_w$. The wall distance will provide information with which to scale the values of $E_1, E_2, \nu_{21}, G_{12}$ and the vector formed from $\nabla d_w$ will serve to set $\theta$. Again, master values $E_1^*, E_2^*$,
\( \nu_{21}^* \) and \( G_{12}^* \) are defined by the user. The master values are then scaled using \( d_w \) and \( \nabla d_w \) as follows

\[
E_1 = \frac{1}{d_w} E_1^* \tag{3.13}
\]

\[
E_2 = \frac{1}{d_w} E_2^* \tag{3.14}
\]

\[
\nu_{21} = \frac{1}{d_w} \nu_{21}^* \sqrt{\frac{E_1}{E_2}} \tag{3.15}
\]

\[
G_{12} = \frac{1}{d_w} G_{12}^* \tag{3.16}
\]

Results for this approach are shown in figure 3.46 for which the following master values were used

\[
E_1^* = 1.0 \tag{3.17}
\]

\[
E_2^* = 2.5 \tag{3.18}
\]

\[
\nu_{12}^* = 0.499 \tag{3.19}
\]

\[
G_{12}^* = 0.02 \tag{3.20}
\]

### 3.4.1 Viscous Potato

The resulting distribution of continuously varying the orthotropic material properties with the inverse of the distance is shown in figure 3.41. Comparing the results in figure 3.42 to the globally defined case in figure 3.21 shows minor improvements. The outlier at the sharp point, originally at \(-16.4\), has moved closer to the surface with a value of \(-18.5\). Aside from this, the range of the majority of the population has slightly narrowed and the number of nodes with low
values of $\Delta^\%d_w$ has increased. The scaled Jacobian is unchanged but Metric3 shows that a number of elements have improved.
Figure 3.41 Inverse distance material property distribution on the potato geometry using P4 quadrilaterals and node-based orthotropic material properties
Figure 3.42   Potato geometry using P4 quadrilaterals and node-based orthotropic material properties
Figure 3.43  Upper curve of the potato geometry using P4 quadrilaterals and node-based material properties

Figure 3.44  Upper concave region of the potato geometry using P4 quadrilaterals and node-based material properties
3.4.2 30P30N Front Slat

Similar to the previous results for the 30P30N slat, the mesh has been compressed on to the lower point of the slat causing the outliers in the $\Delta \%d_w$ histogram shown in figure 3.46a. Aside from the outlier, the continuously varying material parameter method performed equivalently to the discretely determined material parameter method. The variation along the leading edge is again in the range ($-9\%$, $+4\%$) and, compared to the discretely determined method, the differences between the scaled Jacobian and Metric3 are negligible.
Figure 3.46  30P30N front slat using P4 quadrilaterals and continuous material properties
3.5 Adjoint Optimized Material Properties

The adjoint method described previously was applied to the mesh in figure 3.48. This mesh was constructed using normal extrusion specifically so that the grid lines are normal to the boundary. The wall spacing is 0.0001 with a growth rate 1.3. The domain is a $19 \times 11$ structured domain. The non-surface boundaries are frozen in order to emulate the existence of a larger encapsulating mesh without letting the problem size grow too large.

The baseline results using the isotropic material properties of $E = 1$, $\nu = 0.45$, and $G = 0.3448276$ are shown in figure 3.49. Here we can see that the range of $\Delta \% d_w$ is from $-10.6\%$ to $+11.6\%$ for a total variation of $21\%$ and that these extremes occur in the elements of regions with the greatest curvature. The scaled Jacobian ranges from roughly 0.75 to 0.95 center around
0.875 and with a peak population of 17. The $M_3$ metric has a range of roughly 0.5 to 2.5 with a peak population of 40 elements with a $M_3$ value of 1.5.

Figure 3.48  Small conic mesh
Figure 3.49 Small conic isotropic baseline
### 3.5.1 Discretely Defined Material Properties

The initial conditions of the discretely defined material properties case used the globally defined discrete method using values of $E_1 = 1$, $E_2 = 1.25$, $\nu_{21} = 0.402$, and $G_{12} = 0.1$. The resulting quality metrics of the optimized discrete material properties are shown in figure 3.50 and the resulting distribution of material properties is shown in figure 3.51. The quality metrics show that the range of $\Delta \% d_w$ has decreased to $(-6\%, +4.5\%)$ for a total variation of $10.5\%$, half that of the isotropic results. The range of $J_s$ has narrowed and the peak population of elements has increased and shifted toward $0.9$. The range of $M_3$ has not changed but the distribution has shifted toward $0$. Examining the contours show that the distribution of $\Delta \% d_w$ has not changed compared to the isotropic case. The scaled Jacobian and $M_3$ distributions appear to have changed only in the regions of high curvature.

The final state of the material properties shows that $E_1$ and $E_2$ had very little movement from their initial conditions. The transition of $E_2$ from $\approx 1$ is due to the eccentricity of the ellipse approaching $1$, indicating that the element is no longer anisotropic, and the isotropic values corresponding to the smallest Youngs’ modulus are used. Thus the initial conditions of $E_2$ were $1.25$ in the anisotropic region and $1$ in the inviscid region. The distribution of $G_{12}$ in space clearly indicates that the optimal solution requires lowering the shear modulus in the regions surrounding areas of high curvature. Furthermore, the optimization process determined that a thin layer of high $G_{12}$ values is beneficial. Lastly the distribution of $\nu_{21}$ shows that the solution benefits from slightly lowering the value of $\nu_{21}$ in the regions surrounding high curvature boundaries.
Figure 3.50  Adjoint optimized discrete material properties quality metrics
(a)

(b)
Figure 3.51 Adjoint optimized discrete material properties
Paying attention to the range of values in the figures 3.50 and 3.51 shows that there are extreme values of $E_2$, $G_{12}$ present in the data. Examining the surface elements reveals that these values are again concentrated along the regions of high boundary curvature. Figures 3.52 and 3.53 show the material properties and quality metrics of the second node up from the horizontal midline of the mesh. The reason for this configuration of material properties is due to the high values of $J_s$. This result is due to the scaled Jacobians indifference to sheared or parallelogram elements. The proposed quality metric $M_3$ was specifically created to indicate this situation as can be seen in figure 3.53c. The distribution of $\Delta\%d_w$ also show the detrimental effects of using the scaled Jacobian metric as the basis of the objective function. The shearing of this element has produced some of the lowest values of $\Delta\%d_w$ in the mesh.
Figure 3.52  Surface view of adjoint optimized discrete material properties
3.5.2 Continuously Defined Material Properties

The same values were used for the initial conditions of the continuously defined optimization case. The resulting quality metrics are shown in figures 3.54 and the optimized material properties in figure 3.55. The quality metrics tell roughly the same story as the discrete case. The range of $\Delta\%d_w$ has been reduced to $(-4.5, +4.5)$ and figure 3.54d shows that the entire population of scaled Jacobian values has shifted toward one as compared to the isotropic case. The histogram in figure 3.54f shows a small population of increased $M_3$ values indicating that the perpendicularity of elements is being sacrificed. This is confirmed by examining the region around the first surface point above the horizontal midline which is shown in figure 3.56.
Figure 3.54  Adjoint optimized continuous material properties quality metrics
Figure 3.55  Adjoint optimized continuous material properties
Figure 3.56 Near surface $M_3$ values of optimized continuous material property solution
CHAPTER 4
CONCLUSION

In this research the orthotropic material model was applied to linear elastic mesh movement for the purpose of conforming higher order meshes to curved boundaries. Multiple methods of determining orthotropic material properties were implemented. For each method the orientation of the stress-strain relation was set either by the configuration of the element or by the direction toward the nearest surface from a node. The four methods considered are referred to as global element-based, global node-based, discrete, and continuous. The elements-based methods relied on information in the existing linear mesh where as the node-based methods drew information from the boundary.

Three quality metrics were used to assess the quality of the resulting meshes. The scaled Jacobian \( J_s \), the change in relative wall distance \( \Delta \%d_{w} \), and Metric3 \( M_3 \). The scaled Jacobian indicated the relative ’smoothness’ of space within each element, the change in relative wall distance indicated the change in wall spacing from the original linear mesh to the final curved mesh, and Metric3 indicated the objective orthogonality of a curved element. Metric3 was introduced to specifically address the weakness of the scaled Jacobian to identify skewed elements.

The global element-based approach set the values of \( E_1, E_2, \nu_{21}, \) and \( G_{12} \) from user input and set \( \theta \) according to the ellipse fit to each element. The global node-based method set the same four material properties from user input and set \( \theta \) according to the angle between the vector
pointing from the node toward the closest point on the boundary. The discrete method set \( \theta \) along with the four material properties according to the eccentricity of the ellipse fit to the element. Similarly, the continuous method set \( \theta \) and the four material properties using the vector to the closest boundary point and the inverse of the distance to the closest boundary. Compared to the incremental linear elastic results using the isotropic material model, all four model showed that decreasing the magnitude of the shear modulus had the greatest impact on improving \( J_s, M_3 \), and \( \Delta \%d_w \) values. Among the four methods proposed the inverse-distance continuous method displayed the best results. Geometries containing sharp corners presented difficulties. Displacements along the curved boundaries induced stresses that were concentrated on the sharp corners of the mesh resulting in poor quality elements.

Optimizing the material properties for a simple curved geometry revealed a skin effect in which the material properties of the surface elements and nodes in the regions of high curvature had the most impact on the resulting mesh quality. The only material property modified by the optimization method outside of the surface elements was the shear modulus. However this was also contained to regions corresponding to high curvature at the surface.

4.1 Recommendations for Future Work

Having established the benefits of the orthotropic material model, additional improvements appear to be possible by incorporating boundary curvature information into the orthotropic material determination methods. This would allow sharp corners to be identified and handled accordingly. Similarly, the material properties in regions of curvature could be set according to the curvature. Further exploration of optimal orthotropic material properties around geometries with sharp corners
will improve the robustness of the orthotropic linear elastic mesh elevation technique. Application of the adjoint method to the anisotropic material model may indicate patterns with which further improvements may be made. The extension to three dimensions will allow the developed techniques to be applied to practical applications. Finally, the correlation between the proposed metric and the accuracy of flow solutions needs to be investigated.
REFERENCES


APPENDIX A

STATICALLY TYPED SMALL MATRIX LIBRARY
The small matrix class shown below was created as an introductory exercise in compile time metaprogramming. The goal of the class was to implement a small fast matrix library to solve for eigenvalues and eigenvectors that gave the compiler as many opportunities to optimize the routines as possible. The key points are that an instance of DenseMatrix is statically sized to the values of R, C, and T. These values must be provided at compile time which allows the compiler know exactly how big the loops within the subroutines will be along with the size values of the DenseMatrix being returned. For example, consider the matrix multiplication routine below and the product of a 3x2 matrix and a 2x1 matrix. The values of R, C, and N would be 3, 2, and 1 respectively. The compiler would be able to see this at compile time and would have the opportunity to optimize these loops. The other added benefit is the compile time error checking to ensure the proper size instances of DenseMatrix are being handled.

```cpp
template <size_t R, size_t C = 1, typename T = double>
class DenseMatrix
{
    protected:
        static const size_t rows_ = R;
        static const size_t cols_ = C;
        std::array<T> data_; 

};
```
template <size_t R, size_t C, class T>
T&
DenseMatrix<R, C, T>::operator()(size_t row, size_t col)
{
    // return get(row, col);
    return data_[row * cols_ + col];
}

template <size_t N, template <size_t, size_t, class> class mat>
const mat<R, N, T> operator*(const mat<C, N, T>& b) const
{
    mat<R, N, T> ret;
    for (size_t i = 0; i < R; ++i) {
        for (size_t k = 0; k < C; ++k) {
            for (size_t j = 0; j < N; ++j) {

161
ret(i, j) += (*this)(i, k) * b(k, j);

}

}

}

return ret;

}

}

}

}

}

}
X.setAll(0.0);
X.set(0) = 1.0;

mat<M,1,T> Y;
LUsolve<M>(B,Y,X);

c = transpose(Y)*X*invert(transpose(X)*X);

for (size_t i = 0; i < 100; ++i) {
    X = 1.0/Y.twoNorm()*Y;
    LUsolve<M>(B,Y,X);
    c = transpose(Y)*X*invert(transpose(X)*X);
}
T sigma = c.get(0,0);
ev = X;
lambda = 1.0/sigma + shift;
VITA

William Lawton Shoemake was born in August of 1987 in Nashville, Tennessee, to Jerry and Sandra Shoemake. He attended Centennial High School where he showed interest in physics and mathematics. He graduated in 2006 and attended the University of Tennessee at Chattanooga. Lawton earned a Bachelor of Science degree with a dual major in physics and mathematics in 2011. He also pursued his Master of Science degree in Computational Engineering at the University of Tennessee at Chattanooga. After graduation in 2013, he accepted a graduate research assistantship at the University of Tennessee at Chattanooga. Lawton graduated with a Ph.D. in Computational Engineering in December of 2017.