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DEFORMATION AND QUALITY MEASURES FOR TETRAHEDRAL MESHES

Timothy J. Baker[*]

[*]Department of MAE
Princeton University
Princeton, NJ 08544, U.S.A.
e-mail: baker@tornado.princeton.edu

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Abstract. *A deformation measure is derived that can be used to assess the degree of stretching or compression in a time evolving unstructured mesh. Mesh quality measures for static meshes can then be obtained by considering any fixed element as resulting from the deformation of a reference equilateral element. These results are generalized to create a family of element shape measures based on unitarily invariant matrix norms.*

1 INTRODUCTION

It is generally accepted that a bad quality mesh is a considerable handicap when computing a finite element solution. Difficulties often arise in the robustness of the computation and spurious solution errors can occur in the numerical computation. Although everyone has a subjective feel for what constitutes a good quality mesh, it is not at all obvious how this property (or properties) should be captured by an objective measure. One can separate the question into two distinct issues. First, each element should be well shaped. For isotropic meshes this means that the elements should have a low aspect ratio. Second, a smooth gradation in mesh size is desirable. In other words, the change in element size between neighboring elements should be small relative to the size of an individual element.

In this paper we examine the first criterion, namely the quality of an individual element, and restrict ourselves to unstructured meshes made up of triangles or tetrahedra. Several measures of element quality have been proposed [1] and combinations of different quality measures have been used to distinguish the various ways in which a triangular or tetrahedral element can become degenerate (*i.e.* have zero volume) [2]. Most of the element quality measures that have been proposed are formed from non-dimensional ratios of particular geometric characteristics (*e.g.* ratio of circum-radius to in-radius, ratio of maximum to minimum edge length). More recently, element quality measures have been constructed from matrix norms [3].

Consider a tetrahedron whose vertices are given by the points with position vectors $\mathbf{x}_n$ where $n = 0, 1, 2, 3$. The position vector $\mathbf{x}_n$ is a column vector of the three coordinates ($\mathbf{x}_n^T = (x_n, y_n, z_n)$). The edge matrix T_n is defined as

$$T_n = (-1)^n(\mathbf{x}_{n+1} - \mathbf{x}_n,\ \mathbf{x}_{n+2} - \mathbf{x}_n,\ \mathbf{x}_{n+3} - \mathbf{x}_n) \tag{1}$$

where addition in the indices is to be interpreted as modulo four (*i.e.* $\mathbf{x}_{n+4} \equiv \mathbf{x}_n$). Thus, T_n is formed by the three edge vectors joining the vertex at $\mathbf{x}_n$ to each of the three remaining vertices. The determinant $|T_n|$ of the matrix is equal to six times the volume of the tetrahedron (twice the area of the triangle in the 2D case). If a right handed rule is assumed for the edge ordering then $|T_n| > 0$ for elements with positive volume.

In reference [4] the matrix T_n is used as the starting point to define a deformation matrix whose singular values provide information about the compression and stretching of the triangular or tetrahedral elements in a time evolving mesh. A typical time dependent problem is presented in figure 1 which shows a mesh of triangles surrounding a disk placed at the left hand end of a duct.

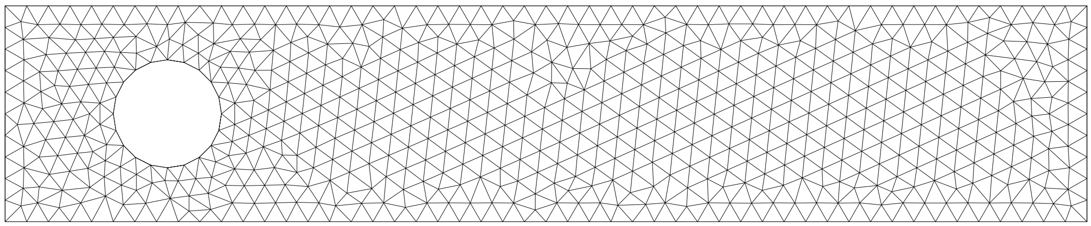

Figure 1: Original mesh for disk inside duct.

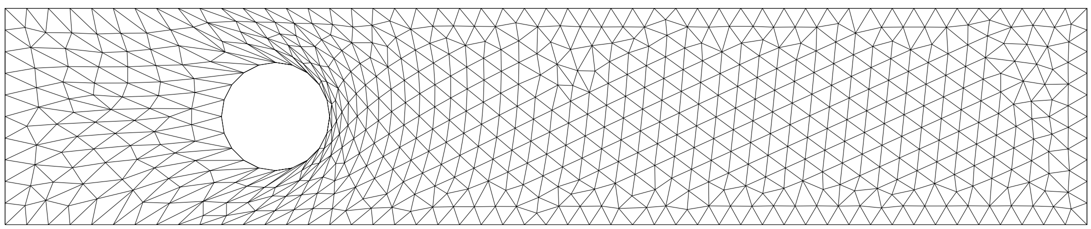

Figure 2: Mesh after translating disk 1 diameter to the right.

A mesh movement (r-refinement) procedure, based on solving the equilibrium equations for a stress field, translates the disk to the right. Figure 2 shows the resulting mesh after moving the disk a distance of one diameter. Further movement would create elements with negative volumes. Using the the mesh deformation measure defined in reference [4] it is possible to identify the elements that are severely distorted and remove these by an edge collapse procedure. The resulting mesh is shown in figure 3. Finally, a new high quality mesh is created by inserting new points by means of a Delaunay refinement procedure (see figure 4). This cycle of mesh movement, element removal and mesh refinement can be repeated as often as necessary until the disk has reached the right hand end of the duct (see figure 5) [4].

In order to define a shape measure for an element T in a fixed mesh of triangles or tetrahedra one can construct the deformation matrix corresponding to the transformation of a reference equilateral element (regular tetrahedron in 3D, equilateral triangle in 2D) to the given element T. This is the approach adopted by Freitag and Knupp [3] who derived an element shape measure based on the Frobenius norm. In the following we show how the deformation measure described in reference [4] and the shape measure of reference [3] fit within the same general framework and demonstrate that the approach presented in reference [4] leads to an alternative shape measure based on the condition number associated with the spectral norm. We then generalize these results to define a family of shape measures based on unitarily invariant matrix norms.

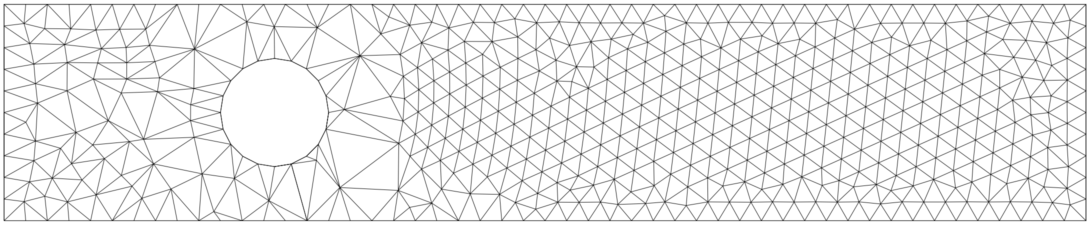

Figure 3: Mesh after disk translation of 1 diameter and mesh coarsening.

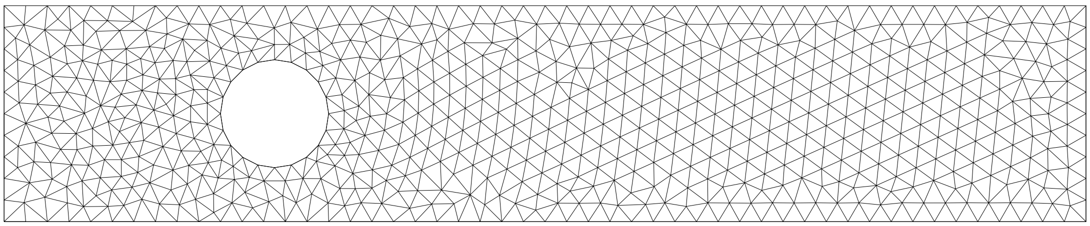

Figure 4: Mesh after 1 complete cycle of movement and modification.

2 ELEMENT DEFORMATION MEASURE

In the definition of the edge matrix T_n, given by equation (1), the vertex n plays a special role. We shall call this the corner vertex for the edge matrix T_n. Let F be the elementary column exchange matrix

$$F = \begin{pmatrix} 1 & 1 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \tag{2}$$

It follows that

$$T_{n+1} = T_n F = T_0 F^n \tag{3}$$

For any given element we have a sequence of $d+1$ edge matrices $T_n, n = 0, \ldots, d$ where $d = 2$ for a triangle and $d = 3$ for a tetrahedron. It is clear that any intrinsic property of the element, such as a deformation measure or shape measure, should not depend on the choice of the corner vertex.

Suppose that the element defined by the edge matrix T_n is mapped, under the action of an r-refinement procedure, to an element whose corresponding edge matrix is $\tilde{T}_n$. We define the deformation matrix associated with this mapping by

$$\tilde{T}_n = A_n T_n \text{ so that } A_n = \tilde{T}_n T_n^{-1} \tag{4}$$

Then,

$$A_{n+1} = \tilde{T}_{n+1} T_{n+1}^{-1} = \tilde{T}_n F F^{-1} T_n^{-1} = A_n \tag{5}$$

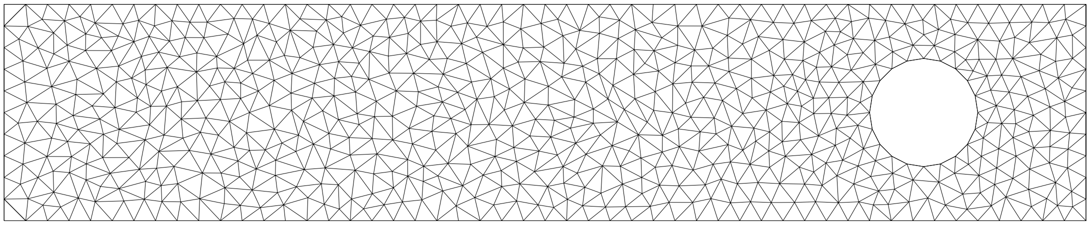

Figure 5: Mesh after 7 complete cycles of movement and modification.

The matrix A_n is therefore independent of the choice of the corner vertex n and we may write A for the deformation matrix. In the notation of reference [4], $T_n \equiv M_1^T$ and $\tilde{T}_n \equiv M_2^T$. The deformation matrix defined in reference [4] is not invariant under a change of corner vertex, a situation that is remedied here by defining the edge matrix T_n to be the transpose of the edge matrix in reference [4].

We can now use the polar decomposition theorem to write A as $A = PU$ where U is a unitary matrix representing pure rotation and P is a positive definite matrix whose eigenvalues correspond to the modes of element distortion. An eigenvalue larger than 1 represents a stretching while a compression is indicated by an eigenvalue less than 1. The eigenvalues of the dilatation matrix P, also known as the singular values of A, are found by taking the square root of the eigenvalues of AA^T. Note that A^TA and AA^T have the same eigenvalues even though their eigenvectors will generally be different.

Let σ_{max} and σ_{min} be the maximum and minimum singular values of A (*i.e.* the maximum and minimum eigenvalues of the dilatation matrix P). If A corresponds to a pure rotation then $\sigma_{max} = \sigma_{min} = 1$ and a uniform scaling by a factor μ would result in $\sigma_{max} = \sigma_{min} = \mu$.

When distortion is so severe that an eigenvalue of the dilatation matrix P becomes zero, the determinant of A and hence also the determinant of the new edge matrix $\tilde{T}_n$ is zero. It follows that the volume of the element has shrunk to zero and any further deformation will create elements with negative signed volumes. In practice, it seems prudent to repeat the mesh movement with a smaller boundary deformation if any singular values fall below 0.1 in size.

It is sometimes useful to know which elements are deforming in a manner that is predominantly compression or, on the other hand, predominantly stretching. We can make such an assessment based on the dilatation matrix. If none of the singular values is much larger than 1 but at least one singular value is much less than 1, the element can be regarded as undergoing a compression. Conversely, if none of the singular values is much less than 1 but at least one singular value is much larger than 1, the element is being stretched.

3 ELEMENT SHAPE MEASURES

In order to derive a shape measure based on the edge matrix, we start by considering the deformation matrix relative to a reference equilateral element (*i.e.* regular tetrahedron in 3D, equilateral triangle in 2D). Let T_n be an edge matrix for the element T and let W be the reference equilateral element. The associated deformation matrix is

$$A_n = T_n W^{-1} \tag{6}$$

In this case, since W is a fixed edge matrix, A_n will depend on the corner vertex n. However,

$$A_{n+1} = T_{n+1} W^{-1} = T_n F W^{-1} = A_n (W F W^{-1}) \tag{7}$$

It can be shown that $U = WFW^{-1}$ is an orthogonal matrix, from which it follows that $|||A_{n+1}||| = |||A_n|||$ for any matrix norm that is unitarily invariant. This result appears in reference [3] as theorem 3. Although reference [3] considers only the Frobenius norm,

$$|||A||| \equiv \|A\|_2 = (trace\, A^T A)^{\frac{1}{2}} \tag{8}$$

their proof applies to any unitarily invariant norm. A unitarily invariant norm $|||A|||$ is a matrix norm such that $|||UA||| = |||AV||| = |||A|||$ for any unitary (orthogonal) matrices U and V.

To verify that $U = WFW^{-1}$ is orthogonal we may choose any convenient representation for the reference equilateral element since an edge matrix is obviously invariant under translation, and U is clearly invariant under a uniform scaling of W. Consider a cube of side length 1 and centered at the origin. The inscribed tetrahedron defined by the vertex positions, $\mathbf{x}_0^T = (\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$, $\mathbf{x}_1^T = (-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})$, $\mathbf{x}_2^T = (\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})$, and $\mathbf{x}_3^T = (-\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ is evidently a regular tetrahedron with edge length $\sqrt{2}$. With the corner vertex at $n = 0$ we obtain the edge matrix,

$$W = \begin{pmatrix} -1 & 0 & -1 \\ -1 & -1 & 0 \\ 0 & 1 & 1 \end{pmatrix} \tag{9}$$

whence we obtain

$$W^{-1} = \frac{1}{2} \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \end{pmatrix} \tag{10}$$

and

$$U = WFW^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \tag{11}$$

It follows that $UU^T = I$ and $|U| = 1$.

We now define a shape measure for the element T to be a scalar variable $\tau(T)$ with the following properties:

1. $0 < \tau(T) \leq 1$,
2. $\tau(T) = 1 \Longleftrightarrow T$ is an equilateral element,
3. $\tau(T)$ is invariant under translation, uniform scaling and rotation of T.

A unitarily invariant norm of a deformation matrix A is invariant under translation and rotation but not under a uniform scaling. This can be remedied by constructing the condition number $\kappa(A) = |||A|||\,|||A^{-1}|||$. If we choose the spectral norm,

$$|||A|||_2 = max\{\sigma;\ \sigma^2 \text{ is an eigenvalue of } A^T A\} \tag{12}$$

we see that $|||A|||_2 = \sigma_{max}$ and $|||A^{-1}|||_2 = \sigma_{min}^{-1}$ where σ_{max} and σ_{min} are the maximum and minimum singular values introduced in the previous section. The condition number $\kappa_\infty(A)$ based on the spectral norm is therefore

$$\kappa_\infty(A) = \frac{\sigma_{max}}{\sigma_{min}} \tag{13}$$

Evidently $\kappa_\infty(A) \geq 1$ with equality when $\sigma_{min} = \sigma_{max}$ which can only occur if the matrix A represents a uniform scaling and/or a rotation of the reference equilateral element. Using the spectral norm we can thus define the following shape measure for the element T,

$$\tau_\infty(T) = \frac{1}{\kappa_\infty(A)} = \frac{\sigma_{min}}{\sigma_{max}} \tag{14}$$

An alternative shape measure based on the Frobenius norm (eqn. (8)) was proposed by Freitag and Knupp [3]. The Frobenius norm of A is given by

$$\|A\|_2 = \left(\sum_{i=1}^{d} \sigma_i^2\right)^{\frac{1}{2}} \tag{15}$$

where $\sigma_{max} \equiv \sigma_1 \geq \cdots \geq \sigma_d \equiv \sigma_{min}$ and the condition number $\kappa_2(A)$ based on the Frobenius norm is given by

$$\kappa_2(A)^2 = \left(\sum_{i=1}^{d} \sigma_i^2\right)\left(\sum_{j=1}^{d} \sigma_j^{-2}\right) \tag{16}$$

It is known that a scalar function $N(A)$ of the matrix A is a unitarily invariant norm if and only if $N(A)$ is a symmetric gauge function of the singular values of A [5]. One example of a family of symmetric gauge functions is the family of ℓ^p norms. When applied to the singular values of a matrix they generate unitarily invariant norms known as the Schatten p norms [5],

$$N_p(A) = \left(\sum_{i=1}^{d} \sigma_i^p\right)^{\frac{1}{p}}, \quad 1 \leq p < \infty \tag{17}$$

The case $p = 2$ is the Frobenius norm, the limiting case $p \to \infty$ is the spectral norm and the case $p = 1$ is the trace norm,

$$|||A|||_{tr} = \sum_{i=1}^{d} \sigma_i(A) \tag{18}$$

The condition number $\kappa_p(A)$ based on the p norm is given by

$$\kappa_p(A)^p = \left(\sum_{i=1}^{d} \sigma_i^p\right)\left(\sum_{j=1}^{d} \sigma_j^{-p}\right) \tag{19}$$

Now

$$\frac{\partial \kappa_p(A)^p}{\partial \sigma_i} = p\sigma_i^{p-1}\left(\sum_{j=1}^{d} \sigma_j^{-p}\right) - p\sigma_i^{-p-1}\left(\sum_{j=1}^{d} \sigma_j^{p}\right) \tag{20}$$

Hence the minmum value of $\kappa_p(A)$ is attained when

$$\frac{\partial \kappa_p(A)^p}{\partial \sigma_i} = 0 \implies \sigma_i^2 = \kappa_p(A), \quad i = 1, \ldots, d \tag{21}$$

and hence

$$min\, \kappa_p(A) = d^{\frac{2}{p}} \tag{22}$$

We can therefore define a family of ℓ^p shape measures by

$$\tau_p(T) = \frac{d^{\frac{2}{p}}}{\kappa_p(A)} \tag{23}$$

From the inequalities

$$\sigma_{max} \leq \left(\sum_{i=1}^{d} \sigma_i^p\right)^{\frac{1}{p}} \leq d^{\frac{1}{p}}\, \sigma_{max} \tag{24}$$

it follows that

$$\sigma_{max} \leq N_p(A) \leq d^{\frac{1}{p}}\, \sigma_{max} \tag{25}$$

Similarly,

$$\sigma_{min}^{-1} \leq N_p(A^{-1}) \leq d^{\frac{1}{p}}\, \sigma_{min}^{-1} \tag{26}$$

Hence

$$\frac{\sigma_{max}}{\sigma_{min}} \leq N_p(A) N_p(A^{-1}) \leq d^{\frac{2}{p}}\, \frac{\sigma_{max}}{\sigma_{min}} \tag{27}$$

It follows that the condition numbers and the shape measures derived from the ℓ^p norms satisfy the following inequalities,

$$\kappa_\infty(A) \leq \kappa_p(A) \leq d^{\frac{2}{p}}\, \kappa_\infty(A) \tag{28}$$

and

$$\tau_\infty(T) \leq \tau_p(T) \leq d^{\frac{2}{p}}\, \tau_\infty(T) \tag{29}$$

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