A LOCAL CELL QUALITY METRIC AND VARIATIONAL
GRID SMOOTHING ALGORITHM

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ABSTRACT

A local cell quality metric is introduced as a function of Jacobian matrix and used to construct a variational functional
for a grid smoothing algorithm. The properties of the local quality measure which combines element shape and size
control metrics are examined and the effectiveness of the algorithm is tested on several representative grids. The
approach can be applied to different cell types and dimensions.

Keywords: mesh generation, smoothing, mesh quality measures

1. INTRODUCTION

Generating quality meshes that permit reliable accurate simulations remains a major technical and theoretical problem. The need to solve more complex applications for multi-material domains with irregular geometry and varying spatial scales exacerbates the difficulty. For example, large scale simulations now involve meshes with millions of cells and feature sizes that vary by orders of magnitude. Generated meshes are often mathematically incorrect (e.g. contain folded cells) or unreliable, so generating, remeshing, and improving the mesh have become time consuming but pressing tasks. This adversely impacts our ability to do efficient simulation and design. In simulations where moving boundaries arise, the situation can be much worse since the mesh deteriorates as cells deform degrading accuracy, conditioning, and computational effectiveness (more iterations and shorter timesteps). Periodic remeshing and frequent grid smoothing are needed, as well as other corrective actions.

The present work examines this issue from the standpoint of local cell quality and a novel scalar cell quality indicator is introduced. This indicator is used to construct a global functional for mesh optimization that we use here as a mesh smoothing and correction strategy that is investigated numerically in several test problems.

Algorithms based on such optimization strategies have been utilized previously, one of the earliest studies being that of Winslow [1]. More recent works [2] - [7] develop related ideas. The outline of the present treatment is as follows: we first summarize some basic ideas underlying harmonic maps and Laplace-type grid smoothing in a variational setting. This leads us to introduce a local “distortion measure” and its reciprocal defines the local mesh quality indicator. The global functional is constructed as an accumulation of the element contributions. The optimization descent problem is solved using a damped Newton scheme. Several case studies are provided in the results.

2. MAPPING AND VARIATIONAL
STATEMENT

A popular strategy in structured grid generation is to map a uniform Cartesian grid in a reference domain Ω to a curvilinear grid of well-shaped cells in the physi-
cal domain $\Omega$. The properties of conformal maps can be exploited to ensure a good mesh. The associated properties of analytic functions of a complex variable have led to the use of harmonic functions from complex analysis and, indirectly, to schemes based on solving the associated Laplace equation. Since the potential and stream function solutions to Laplace’s equation form a suitable coordinate family for a mesh, this idea has motivated PDE solver strategies for mesh generation. In particular, the Laplace problems

$$\Delta \xi = 0, \quad \Delta \eta = 0 \quad (1)$$

in the physical domain $\Omega$ can be mapped to quasilinear PDEs in the reference domain $\Omega$ and solved for untangled meshes in $\Omega$.

Alternatively, variational formulations for these PDE problems can be easily constructed and an equivalent optimization problem is obtained. For (1), the variational functional is the classical Dirichlet integral for the Laplacian and we have

$$I = \int_\Omega \left[ (\nabla \xi)^2 + (\nabla \eta)^2 \right] d\xi d\eta . \quad (2)$$

The pair of Laplace problems (1) follow as the associated Euler-Lagrange equations. Mapping the variational problems to the reference domain we have

$$I = \int_\Omega \frac{\text{tr}(S^T S)}{\det S} d\xi d\eta \quad (3)$$

which can be expressed compactly as

$$I = \int_\Omega \text{tr}(S^T S) \frac{d\xi d\eta}{\det S}$$

where $\text{tr}$ denotes the trace and $S$ is the Jacobian matrix of the map between the two frames. From this, following the idea of describing grid quality by metric-tensor invariants [8, 5] or functions of Jacobian matrix [9], we define the local distortion measure

$$\beta(S) = \frac{1}{4} \frac{\text{tr}(S^T S)}{\det S} \quad (4)$$

and local mesh quality as $Q_0 = \beta^{-1}$. In fact, this distortion measure generalizes to any dimension directly [10] as

$$\beta(S) = \left( \frac{\text{tr}(S^T S)}{\det S} \right)^{n/2} . \quad (5)$$

The size of the cell can be controlled by introducing a second local measure which we term the “dilation” measure. Let $v$ be a “desired” element size measure (related to area in 2D and volume in 3D). For the “desired” uniform grid, $v$ is taken to be the average cell area

$$v = \frac{\int_\Omega \det S d\xi d\eta}{\int_\Omega d\xi d\eta} .$$

Then the ratios $\det S/v$ and $v/\det S$ indicate the departure of $\det S$ from $v$. Since $\det S$ can be above or below $v$ we introduce the symmetric dilation measure [7]

$$\mu(S) = \frac{1}{2} \left( \frac{\det S}{v} + \frac{v}{\det S} \right) . \quad (6)$$

Then $\mu = 1$ when $v = \det S$ and $\mu \to \infty$ as $\det S \to \infty$ or 0. Following the ideas of multi-objective functions [2, 6], we introduce an additive distortion-dilation measure (other forms are clearly possible)

$$E_\theta = (1 - \theta)\beta(S) + \theta \mu(S) , \quad (6)$$

where coefficient $0 \leq \theta < 1$ in linear combination can be adjusted to emphasize the respective distortion and dilation terms.

Now the variational grid smoothing formulation can be stated as follows: minimize the functional

$$I = \int_\Omega E_\theta(S) d\xi d\eta \quad (7)$$

subject to relative boundary (or other) constraints. In order to obtain the discretized problem formulation (7), contributions to the functional from each cell $c$ are approximated using some numerical integration rule as

$$I_h = \sum_{c=1}^{N_c} \sum_{q=1}^{N_q} \sigma_{q(c)} E_\theta(S_{q(c)}), \quad (8)$$

where $\{q(c)\}$ identify the quadrature points and $\sigma_{q(c)}$ are the corresponding quadrature weights for cell $c$.

Remarks: 1. The formulation can be applied to any unstructured grid containing different types of cells, using appropriate quadrature rules; 2. Unstructured grids will have varying nodal valence and this effect will also be investigated in the numerical work of section 6.

### 3. LOCAL QUALITY MEASURE

Let us first mention some general properties of the local distortion measures (5) and (6) and then focus on their behavior for meshes using the basic triangle and quadrilateral cells since they are most widely used in grid generation.

The function $\beta(S)$, reformulated in terms of invariants of the metric tensor of coordinate transformation $G = S^T S$, was considered in [5]. It was shown that $\beta(S)$ controls the cell angles and cell aspect ratio in the 2D case and has similar properties in 3D. The estimates for the angle $\alpha$ between two cell edges and cell aspect ratio $F$ (ratio of the lengths of the edges) for 2D quadrilateral cells are

$$\sin^2 \alpha \geq (1/\beta)^2, \quad 2 \leq F + 1/F \leq 4/\beta^2 - 2.$$
Thus $\beta \to 1$ enforce $\alpha \to \pi/2$ and $F \to 1$; i.e. a square cell.

The modified distortion measure $E_\theta$ retains these properties of $\beta(S)$. It is an indicator for quasi-isometry of the mapping $[7, 10]$ - analog of mapping conformality characterization, in the sense that

$$\gamma^2 I \leq S^T S \leq \Gamma^2 I,$$

where $\gamma$ and $\Gamma$ can be estimated from $E_\theta$.

In the following sections we will examine the local measure $E_\theta(S)$ or corresponding local quality measure $Q_\theta(S) = 1/E_\theta(S)$ ($Q_\theta(S) = 1/\beta(S)$ ) on linear mapped simplex elements and bilinear isoparametric elements in more detail.

### 3.1 Simplex elements

Let us first consider the 2D triangular element, which has been most extensively analyzed in the literature (see [5, 11] for references). Taking the reference element to be the equilateral triangle with sides of length 1 and computing the constant Jacobian matrix of the linear map onto an arbitrary triangular element with area $A$ and edges of lengths $l_1, l_2, l_3$, we get

$$\det S = \frac{4}{\sqrt{3}} A, \quad \text{tr}(S^T S) = \frac{2}{3} (l_1^2 + l_2^2 + l_3^2).$$

Thus

$$\beta = \frac{l_1^2 + l_2^2 + l_3^2}{4\sqrt{3} A},$$

and quality measure $Q_\theta$ is equal to

$$Q_\theta = \frac{4\sqrt{3} A}{l_1^2 + l_2^2 + l_3^2}.$$ 

This is a well known example [12, 13] of a “fair” geometric measure in the sense that it is equal to 0 on any type of degenerate triangle. It is also normalized (takes values from the interval $[0, 1]$).

The corresponding additive measure from (6) is

$$E_\theta = (1 - \theta) \frac{l_1^2 + l_2^2 + l_3^2}{4\sqrt{3} A} + \frac{\theta}{2} \left( \frac{\sqrt{3}}{4A} + \frac{4A}{\sqrt{3}} \right).$$

The level sets of the corresponding modified quality measure $Q_\theta = E_\theta^{-1}$ for a triangle with fixed edge $(0, 0) - (0, 1)$ as a function of the coordinates $(x, y)$ of the opposite vertex are shown in Figure 1 for different values of parameter $\theta$. As $\theta$ increases, the quality measure becomes less restrictive in the sense that it admits more points in the regions $Q_\theta > \text{const}$, but it remains a “fair” measure.

For the mapping of an arbitrary tetrahedron onto the regular tetrahedral reference element with edges of

$$\theta = 0 \quad \theta = 0.4 \quad \theta = 0.8$$

length 1 we have

$$\det S = 6\sqrt{2} V, \quad \text{tr}(S^T S) = \frac{1}{7} \sum_{i=1}^{6} t_i^2,$$

where $V$ is the volume of the tetrahedron and $t_1, \ldots, t_6$ are its edge lengths. Thus for the quality and additive distortion-dilation measures respectively we get

$$Q_\theta = \frac{72\sqrt{3}V}{(\sum_{i=1}^{6} t_i^2)^{3/2}},$$

$$E_\theta = (1 - \theta) \frac{(\sum_{i=1}^{6} t_i^2)^{3/2}}{72\sqrt{3}V} + \frac{\theta}{2} \left( \frac{1}{6\sqrt{2}V} + 6\sqrt{2}V \right),$$

and $Q_\theta = E_\theta^{-1}$ which are also “fair” measures in the sense given above. A similar tetrahedron shape measure

$$\eta = \frac{12(3V)^{2/3}}{\sum_{i=1}^{6} t_i^2} = (Q_\theta)^{2/3}$$

was derived in [14] from the singular values of transformation $S$. Geometrically $\eta$ reflects the shape of the inscribed ellipsoid.

### 3.2 Tensor product linear elements

The case of the mapped tensor product linear cell in $n$ dimensions is more complex, since the Jacobian matrix is not constant on the cell. Nevertheless, $E_\theta$ satisfies a “maximum principle” [10], in the sense that it is bounded from above by a finite linear convex combination of its values on certain bases (matrices). Thus an upper bound for the additive measure (lower bound for quality measure) can always be computed. Matrices for this bound are a full set of constant matrices arising from a representation of the Jacobian matrix on the tensor product cell. For example, the bilinear map of unit square $0 \leq \xi_1, \xi_2 \leq 1$ onto the cell with vertices $r_{j,k}$, $j, k = 0, 1$ can be written as

$$r = \sum_{j,k=0}^{1} (1 - \xi_1)^{(1-j)} (1 - \xi_2)^{(1-k)} \xi_1^j \xi_2^k r_{j,k}$$

**Figure 1**: Level sets of $Q_\theta(x, y)$ on triangle with vertices $(0, 0), (0, 1), (x, y)$.
and its Jacobian matrix is

$$S = \sum_{j, k=0}^{1} (1-\xi_1)^{(1-j)}\xi_1^j (1-\xi_2)^{(1-k)}\xi_2^k (r_{1k} - r_{0k}, r_{j1} - r_{j0})$$

(10)

$$= \sum_{j, k=0}^{1} c_{jk}\hat{S}_{jk}, \text{ where } \sum_{j, k=0}^{1} c_{jk} = 1,$$

where $c_{jk} = (1-\xi_1)^{(1-j)}\xi_1^j (1-\xi_2)^{(1-k)}\xi_2^k$ are the scalar coefficients in (10) and the corresponding pairs of vectors are the columns of matrices $\hat{S}_{jk} = (r_{1k} - r_{0k}, r_{j1} - r_{j0})$.

Thus for the bilinear cell, the bound is 1/4 of the sum of additive measures computed at vertices of the quadrilateral cell. That is

$$E_\theta \leq \sum_{j, k=0}^{1} \frac{1}{4} E_\theta(\hat{S}_{jk}).$$

For a trilinear cell this type of representation of the Jacobian matrix contains 64 different constant matrices. They can be obtained from trilinear images of the basis triples in reference space. All 64 such basis triples can be obtained from the four distinct vector triples shown in Figure 2 by rotation and reflection (after reflection the orientation should be changed to preserve right basis).

The level sets for the lower bound of the quality measure $Q_\theta$ for the bilinear cell are shown in Figure 3, where quality contours are graphed as functions of the position $(x, y)$ of one vertex of the quadrilateral with the other vertices fixed at points $(0, 0), (0, 1)$ and $(1, 0)$.

The existence of the upper bound on the local additive measure $E_\theta$ implies that in order to control cell quality it is sufficient to control the bound; that is, the values of the additive measure on a finite number of combinations of cell vertex basis vectors. Thus the choice of these combinations as quadrature points for approximating the discrete functional (8) will guarantee the improvement in mesh quality as the result of solving minimization problem (7).

$$\theta = 0 \quad \theta = 0.4 \quad \theta = 0.8$$

Figure 3: Level sets of lower bound for $Q_\theta(x, y)$ on quadrilateral element with vertices (0,0), (0,1), (1,0), (x,y)

4. NUMERICAL IMPLEMENTATION

The gradient of the smoothing functional (8) is nonlinear so an iterative optimization algorithm, such as Newton’s method or another gradient descent method, should be applied to the associated algebraic problem. In this work, the damped Newton method is used. After each iteration the global minimum quality measure

$$(Q_\theta)_{\text{min}} = \min_{q(c)} \frac{1}{E_\theta(S_{q(c)})}$$

(11)

is computed in order to monitor the optimization process. Iterations cease when the difference between the minimum quality (11) of two subsequent grids is less than a given tolerance (other criteria are possible).

5. MODIFICATIONS OF THE METHOD

If the initial grid is folded or has nonconvex cells, the functional can be modified by adding penalty terms (see, for example, [6]). The original functional (8) has an infinite barrier on the set of grids with convex cells which is due to the presence of det $S$ in the denominator of the integrand. A penalty formulation can be developed by replacing this factor det $S$ by an exterior penalty function $\chi_v(\det S)$, such that the new integrand will be a finite approximation of the original infinite barrier. This modification allows the minimization procedure to start from a folded grid and, since the value of the functional $I_h$ is significantly increased when folded cells are present in the grid, the final grid will not contain nonconvex cells (assuming there exists such a mesh solution for the given connectivity and boundary conditions).

Since the distortion measure $\beta(S)$ provides control over element shape, one can define a priori the desired element shape by introducing a metric in reference coordinates. These metrics essentially use different reference elements for different cells in the grid. Minimization of the correspondingly modified functional will result in a grid with cells having the shape as close as possible (under given connectivity of the grid and imposed boundary conditions) to the target shapes.
6. NUMERICAL EXAMPLES

6.1 Smoothing of a triangular grid in non-convex domain

The Laplace smoother may produce overlapping grids in nonconvex domains, so it is important to check the behavior of the present type of smoother for such domains. Consider the nonconvex (V-shaped) domain with triangular grid and fixed boundary nodes shown on the left in Figure 4. Smoothing with the presented additive functional using $\theta = 0.8$ produces the grid on the right in Figure 4. There is no overlap and the mesh lines are well behaved. Cells at the peak on the symmetry line are slightly dilated and those at the reentrant corner are slightly compressed.

6.2 2D meshes with points of changing valence

The following numerical test demonstrates the advantages of the described smoothing algorithm, when operating on a grid with varying valence. Some algorithms will produce significant local dilation effects in the regions where valence changes [15].

Figure 5 demonstrates the smoother behavior on triangular grids with changing valence. All boundary nodes are fixed in this example. There is some disparity in dilation effects but the behavior is satisfactory.

The effect of smoothing on a mesh of quadrilateral cells is shown in Figure 6. The initial grid consists of two block-generated subgrids corresponding to a trapezoidal subdomain and its continuation to the annular region. Boundary nodes on the exterior circular boundary are fixed and nodes on the vertical diameter boundary of the semicircle are allowed to “slide” along this line. The initial mesh and the “evolving” mesh at iterations 1, 2, 3 are shown.

6.3 Mesh unfolding in nonconvex domain

Barrier formulations of variational smoothing algorithms facilitate mesh unfolding as well as smoothing.
As an example let us consider the unfolding of a folded quadrilateral mesh for an annular cylindrical domain. For the initial grid we relocate the nodes interior to a cylindrical polar mesh for a semicircular annulus and place them at the origin as indicated by the mesh on the left in Figure 7. After applying the smoothing algorithm for 5 iterations, the grid is close to equidistributed as seen on the right in Figure 7.

6.4 Initially adaptive quadrilateral grid with folded cells

In the next example the smoothing procedure is applied to a more elaborate grid, generated to adaptively fit a multi-airfoil domain. This grid has many nodes with irregular valence and it initially had several folded cells. The most relevant part of this grid before and after smoothing is shown in Figure 8. This example indicates the importance of cell size control (via $\mu(S)$), since without it the smoothing procedure "undoes" desired clustering near the airfoils and tends to promote a uniform grid, which is unacceptable because boundary layers need to be resolved. Initially, the volumetric factors $v$ were computed for each cell, and then the smoothing algorithm was run using these values. The improvement in the grid details can be seen in Figure 9.

It can also be observed from Figure 9 that smoothing may not retain enough clustering in the boundary layers. Thus, in order to have a grid that retains the initial mesh density in the boundary layer, a block smoothing strategy may be utilized.
7. CONCLUDING REMARKS

The variational smoothing algorithm developed here yields satisfactory results for triangular and quadrilateral meshes. In particular, it handles several of the difficulties that have been troublesome for other smoothers. It is applicable to general element types and hybrid grids as well as 3D (the 3D case is currently being tested). We have also carried out tests on higher resolution grids and explored the effect of varying $\theta$. Other issues related to the effect of different local valence are also being investigated.

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References


