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An Angular Method with Position Control for Block Mesh Squareness Improvement

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Abstract

We optimize a target function defined by angular properties with a position control term for a basic stencil with a block-structured mesh, to improve element squareness in 2D and 3D. Comparison with the condition number method shows that besides a similar mesh quality regarding orthogonality can be achieved as the former does, the new method converges faster and provides a more uniform global mesh spacing in our numerical tests.

1 Introduction

Mesh orthogonality, if achieved, reduces computational errors by eliminating the cross-terms in the truncation error therefore a more accurate result can be obtained in a numerical simulation. There are various way to approach mesh orthogonality and the condition-number [1] mesh smoothing is among the most widely employed in practices. It minimizes a target function defined by the ratio between the sum of element edge length squared and a power of the volume consistent with the dimension of length squared, defined for a corner for each corner in an element. When orthogonality is achieved, the volume of a quad (or hex) element takes its maximum possible value thus the target function is minimized. In general, the condition-number method often provides good element shapes and it also works in the case of an arbitrary mesh.

The condition-number method provides square elements when the boundary of mesh is consistent with orthogonality. However it also provides relatively small sizes around a reduced-connectivity point. This is not desired and may limit the time step in a simulation in which the Courant-Friedrichs-Levy (CFL) condition is used to control instability. We have also observed a relatively slow convergence with the conditional number method, especially when the initial mesh is twisted.

A new mesh-smoothing approach is proposed. The method is almost parallel to the condition-number method in the two-dimensional case, except with a difference target function to minimize. In three-dimensions the new method sums up target functions similar to the 2D one, defined on the three logically 2D stencils shared by a given center node. Therefore the new method is easier to implement than the condition-number method in 3D.

Besides providing element squareness as the condition-number method does, the new method converges much faster and provides globally more uniform mesh sizes.

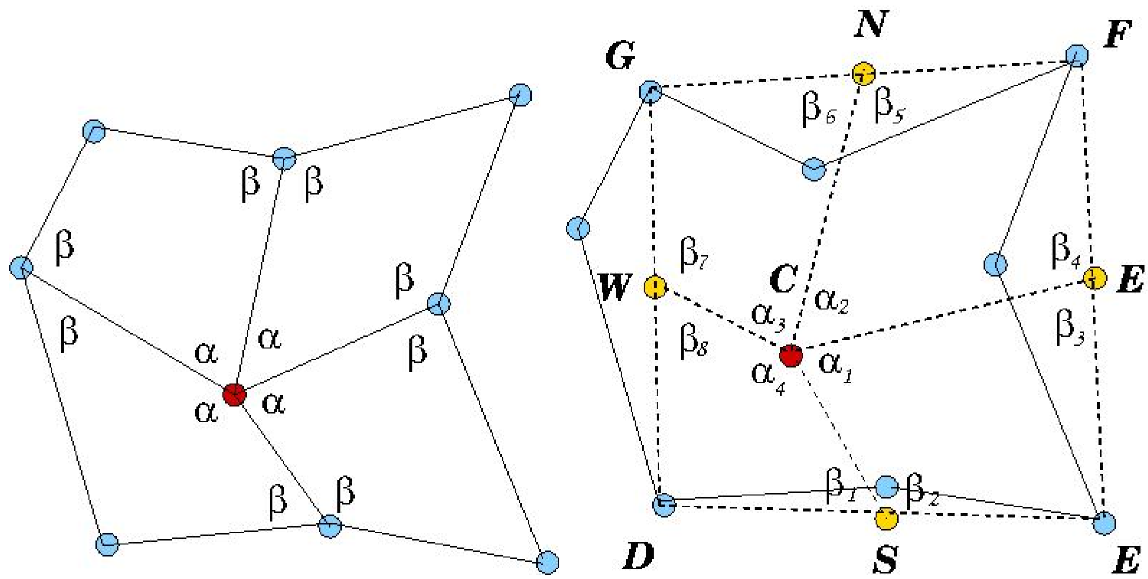

Figure 1: Left: A normal stencil in 2D; right: a simple stencil modified from the left. Yellow points are mid-points on faces of the simplified stencil (a quad defined by dashed lines).

2 A quartic target function

In (fig. 1) a basic two-dimensional stencil is shown on the left. The red node at the center is to move and one may attempt to make the sum of squared angle cosines as small as possible for orthogonality. In the ideal case, the α angles (with the center node as the tip) and the β angles (with middle nodes on each wall of a regular stencil) would all be $\pi/2$ and the sum of their cosines is *zero*. However, with an initially much twisted mesh such a direct approach dose not always smooth the mesh and a Newton's method for minimizing the sum of cosine squared often diverges or finds undesired solutions.

To simplify the problem we consider that a mesh would have nearly straight mesh lines after smoothing. Thus, we modify the basic stencil in fig. 1 left by ignoring the middle nodes on the four walls of the stencil. To provide some position control we take the four midpoints on the faces of the resulting quad and call them S(south), E(east), N(north), and W(west) (fig. 1, right). Then we link the node at the center C to S, E, N, and W (as desired node positions). Then 12 angles are formed with $\alpha_i (i = 1, 2, 3, 4)$ stand for the corners with C as their tip and $\beta_i (i = 1, 2, 3, ...8)$ with the $four$ mid-points (S, E, N, and W) on faces as corner tips. Since in the ideal case with orthogonality all the α and β are right angles. We write a target function as the follows

$$T = \frac{1}{2} \left(\sum_{i=1}^{4} \cos^2(\alpha_i) + \sum_{i=1}^{8} \cos^2(\beta_i) \right). \tag{1}$$

For each angle contained in the above function, the square of cosine is computed by the square of the $inner - product$ of the two vectors defined by corner tip and face middle points or some corner-nodes of the stencil. For examples (in fig. 1)

$$\cos^2(\alpha_1) \equiv \frac{(\vec{CS} \cdot \vec{CE})^2}{|CS|^2 \cdot |CE|^2},$$

and

$$\cos^2(\beta_1) \equiv \frac{(\vec{SC} \cdot \vec{SD})^2}{|SC|^2 \cdot |SD|^2}.$$

The target-function defined above, when being minimized by a Newton's method, still sometimes diverges or finds spurious roots. To achieve stability we simplify the target function further by fixing the denominators in the Newton's iterations. This is to say the the leg-lengths in a smoothing iteration are taken to their values at the previous iteration. As the smoothing converges, the length of a given leg gradually reaches its limiting value. Thus, if the proposed method converges, the above approximation of target function in eq. 1 will not change the solution, however, it simplifies the mathematics quite a bit.

Then we are left with a positively definite quartic function to minimize. This is a well defined algebraic problem and the target function behaves well in an optimization by the Newton's method.

3 A local optimization with the Newton's method

In a smoothing step of the proposed method we loop over all internal nodes (boundary nodes are assumed fixed) and for each internal node, the simplified target function can be written as

$$T = \frac{1}{2}\sum_{i=1}^{12} c_i \left((x - a_{1i})(x - a_{2i}) + (y - b_{1i})(y - b_{2i})\right)^2. \tag{2}$$

The subscript 'i' stands for the contribution of angle 'i' and there are 12 angles in total. However when a corner-node is also a reduced connectivity point in a regular stencil, because the mesh-line there is not expected to be straightened, we ignore contributions of corners with the reduced-connectivity as their tip. The constants a_{1i}, a_{2i}, b_{1i}, b_{2i}, and c_i are all in terms of coordinates of the simplified stencil (fig. 1 right). The iterator 'i' counts α angles then β ones. For example the first term in the sum would be

$$\cos^2(\alpha_1) = \frac{((x - x_S)(x - x_E) + (y - x_S)(y - y_E))^2}{[(x_C - x_S)^2 + (y_C - y_S)^2][(x_C - x_E)^2 + (y_C - y_E)^2]}$$

which is in the format of eq.2 with

$$a_{11} = x_S, a_{21} = x_E; b_{11} = y_S, b_{21} = y_E; \text{ and}$$

$$c_1 = \omega_i[(x_C - x_S)^2 + (y_C - y_S)^2]^{-1}[(x_C - x_E)^2 + (y_C - y_E)^2]^{-1}.$$

In the above expression x, y are the coordinates to be updated of the center node C. x_C, y_C are the coordinates of C at the last smoothing iteration, similar with x_E, y_E and x_S, y_S. ω_i are weights. In this paper we have taken $\omega_i = 1$ an constant unless with a reduced connectivity corner-tip, for which ω_i is taken to 0.

At a minimizer one must have $\partial T/\partial x = 0$ and $\partial T/\partial y = 0$ where

$$\frac{\partial T}{\partial x} = \sum_{i=1}^{12} c_i(2x + a_{1i} + a_{2i})\left((x + a_{1i})(x + a_{2i}) + (y + b_{1i})(y + b_{2i})\right)$$

$$\frac{\partial T}{\partial y} = \sum_{i=1}^{12} c_i(2y + b_{1i} + b_{2i})\left((x + a_{1i})(x + a_{2i}) + (y + b_{1i})(y + b_{2i})\right) \tag{3}$$

With the Newton's method for optimization the second derivatives of the target function are also needed

$$\frac{\partial^2 T}{\partial x^2} = \sum_{i=1}^{12} c_i[(2x + a_{1i} + a_{2i})^2 + 2\left((x + a_{1i})(x + a_{2i}) + (y + b_{1i})(y + b_{2i})\right)]$$

$$\frac{\partial^2 T}{\partial y^2} = \sum_{i=1}^{12} c_i[(2y + b_{1i} + b_{2i})^2 + 2\left((x + a_{1i})(x + a_{2i}) + (y + b_{1i})(y + b_{2i})\right)]$$

$$\frac{\partial^2 T}{\partial xy} = \sum_{i=1}^{12} c_i[(2x + a_{1i} + a_{2i})(2y + b_{1i} + b_{2i})] \tag{4}$$

Because the target function is a sum of squares, a minimizer must exists. The position of the minimizer is not related to the original position of a given node. To start with, the initial guess of the minimizer is taken to the geometrical center of a quad formed by S, E, N, and W

$$x_0 = \frac{1}{4}(x_S + x_E + x_N + x_W),$$

$$y_0 = \frac{1}{4}(y_S + y_E + y_N + y_W).$$

This can be justified by considering that when mesh orthogonality and even mesh-spacing are achieved, this initial guess would be exactly the solution point.

A Newton's iteration is then carried out with

$$x_1 = x_0 - \left[\frac{\partial^2 T}{\partial x \partial y}\frac{\partial T}{\partial y} - \frac{\partial^2 T}{\partial y^2}\frac{\partial T}{\partial x}\right] / \left[\frac{\partial^2 T}{\partial x^2}\frac{\partial^2 T}{\partial y^2} - (\frac{\partial^2 T}{\partial x \partial y})^2\right]$$

$$y_1 = y_0 - \left[\frac{\partial^2 T}{\partial x \partial y}\frac{\partial T}{\partial x} - \frac{\partial^2 T}{\partial x^2}\frac{\partial T}{\partial y}\right] / \left[\frac{\partial^2 T}{\partial x^2}\frac{\partial^2 T}{\partial y^2} - (\frac{\partial^2 T}{\partial x \partial y})^2\right]. \tag{5}$$

We perform the above Newton's iteration eq. 5 only once in a smoothing step for each internal node to obtain its improved position (x_1, y_1). Then a loop over all the nodes moves each node to its improved position. There maybe nodes at singular connectivity points that do not own a normal stencil. In this case we simply take the geometrical average of the three nodes directly linked to the center node by simple legs. We stop the smoothing when the global L_2 difference between the results of two consecutive smoothing steps is smaller than a preset threshold, or a preset limit of the number of steps is reached.

4 An additional position control term

Minimizing the target function defined in the last section usually give good mesh quality that is comparable to the condition-number method with fewer steps and better mesh-spacing around singular points. However, when the element aspect ratio is big, the contribution from corners that have short sides cannot balance contributions from other corners. As a result the minimizer maybe located exterior to the stencil while the mesh squareness is reasonably achieved locally. To avoid this situation, we add a position control term to the target function proposed in (eq.1) defined by the distances from center node to the mid-face points squared

$$U = \frac{1}{2}[(x-x_S)^2+(y-y_S)^2+(x-x_E)^2+(y-y_E)^2+(x-x_N)^2+(y-y_N)^2+(x-x_W)^2+(y-y_W)^2], \quad (6)$$

and the target function to minimize is then becoming

$$T + \sigma U. \quad (7)$$

The factor σ is an aspect ratio defined by $|NS|^2/|WE|^2$ and if it is less than unity, its reverse is taken. If minimizing T alone takes a node out of its stencil, the term σU will move the node back in the stencil. There are other possibilities for a position control function. We use the current one because it works well in all the cases we have tested.

It should be pointed out that simply taking the geometric average of S, E, N and W (the initial guess chosen above) also smooths the mesh (which can be seen as a Laplacian smoothing [7] about element face centers) but does not privide a more uniform mesh spacing. An example about this will be showed in a later section.

5 The target function in three-dimensions

In three-dimensions, a given regular interior node (i.e., not at a singular point) is shared by three logically two-dimensional regular stencils (fig. 2), one in each logical direction. To achieve three-dimensional mesh orthogonality (and hopefully even mesh-spacing), it is necessary that the two-dimensional mesh orthogonality is obtained in each of the logically 2D spatial normal stencil.

Thus, we propose to sum the three two-dimensional target functions associated with a given node for a three-dimensional target function to minimize. The two

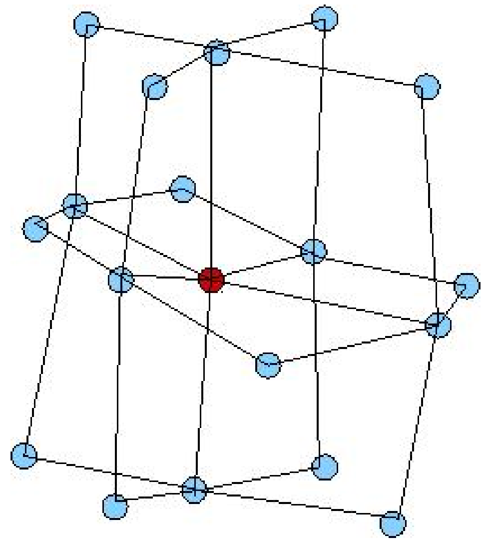

Figure 2: A regular node in three-dimensions is shared by three logically two-dimensional regular stencils.

vectors involved in an inner product (to compute cosine of an angle) are both three-dimensional in this case. The target function has *three* independent variables x, y, z instead of only *two* in the previously described two-dimensional case.

A Newton's iterative scheme can again be used to minimize the quartic target function. Although it is a common practice, we still write down the standard procedure to minimize a general function $F(x, y, z)$ for reference. Let the initial guess of the minimizer be (x_0, y_0, z_0). Because the condition $\nabla F = 0$ must be satisfied at a minimizer, therefore we expand the gradient of F around (x_0, y_0, z_0) (where k is the current number of iterations) and keep only the linear terms and solve the following 3 by 3 linear system

$$\begin{bmatrix} \partial^2 F/\partial x^2 & \partial^2 F/\partial x\partial y & \partial^2 F/\partial x\partial z \\ \partial^2 F/\partial x\partial y & \partial^2 F/\partial y^2 & \partial^2 F/\partial y\partial z \\ \partial^2 F/\partial x\partial z & \partial^2 F/\partial y\partial z & \partial^2 F/\partial z^2 \end{bmatrix} \cdot \begin{bmatrix} \delta x \\ \delta y \\ \delta z \end{bmatrix} = - \begin{bmatrix} \partial F/\partial x \\ \partial F/\partial y \\ \partial F/\partial z \end{bmatrix}. \qquad (8)$$

Then the position of the solution gets updated by $x_1 = x_0 + \delta x$, $y_1 = y_0 + \delta y$, and $x_1 = x_0 + \delta z$.

For the proposed orthogonality method with even mesh spacing, the initial guess (x_0, y_0, z_0) is taken as the geometric average of the three initial guesses with each logically 2D stencil (fig.2). The above Newton's scheme is performed for a single time in

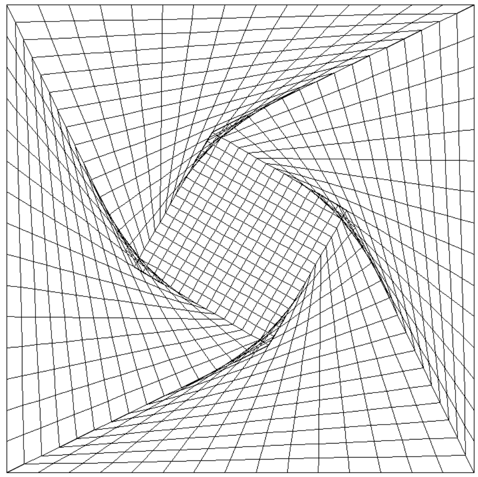

Figure 3: A butterfly mesh on a 6 by 6 square with the center block twisted counter-close-wise by $\pi/3$.

each smoothing step. The three-dimensional target function taken for minimization is defined as the follows

$$F = (P_I + \sigma_I U_I) + (P_J + \sigma_J U_J) + (P_K + \sigma_K U_K), \tag{9}$$

where I, J, and K stand for the three logical directions, P, σ, and U have the same definitions as in the two-dimensional case except that the position of a point has three components x, y, and z in this case.

6 Comparison with the condition-number method

The proposed method can somehow be seen as a condition-number method with its target function replaced by (eq. 1) or (eq. 9). Therefore it should be easy to modify an existing condition number implementation to perform the proposed method.

In all numerical tests we have tested, the proposed method provides a faster convergence and a globally more uniform mesh with better spacing around reduced connectivity points. The mesh-squareness provided by the proposed method is comparable to the condition number method in all the cases.

In the following test problems we compare the results obtained with the proposed method the condition-number method. Results obtained with an angle-based

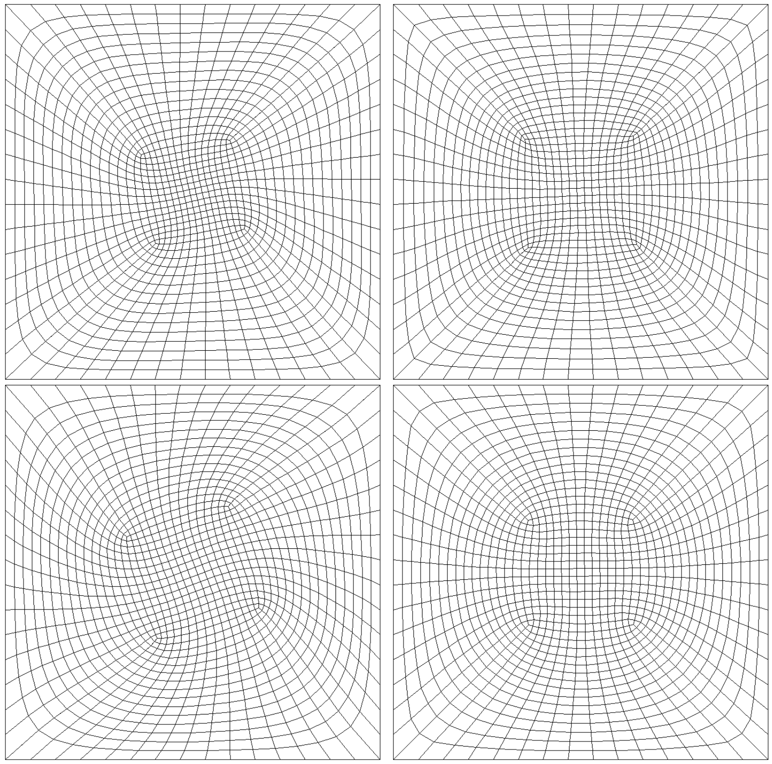

Figure 4: The initial mesh in fig.3 smoothed with 160 iterations: upper left: with the angle-based method; upper right: with the Winslow-Crowley method; lower left: with the condition-number method; lower right: with the proposed method.

method [2], the equi-potential method [3], and an equal-distance method [6] are also provided for references.

The treatment for nodes at reduced connectivity points is the same with all the methods, by taking the geometrical center of the triangle formed by the nodes directly linked to a reduced-connectivity point.

6.1 A deformed butterfly mesh

The two-dimensional five-block butterfly configuration we tested is contained in a perfect 6 by 6 square. Each block are assigned an algebraic mesh by a bi-linear mapping from an ideal mesh in the parametric space to physical space.

In the first case the center block is twisted counter-clock-wise by 60 degrees (fig.

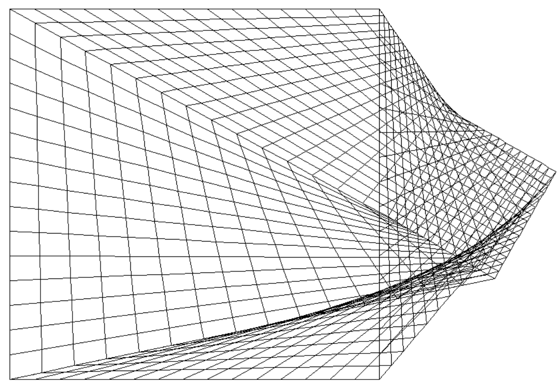

Figure 5: A butterfly mesh on a 6 by 6 square with the center block twisted by 60 degree and shifted by 9 units in the x-direction.

3). Each block is assigned a 15 by 15 mesh. Fig. 4 shows the comparison between the proposed method and other well known methods.

Clearly, with a fixed smoothing steps, the proposed method produced symmetry and the largest mesh size around a reduced connectivity point. The condition number method and the angle-based method converge slower. The Winslow-Crowley method, although converges not as slow (but slower than the proposed method), produces undesirably small elements around the reduced connectivity points.

In the second case the twisted center then is shifted in the x-direction with a distance of 9 units (fig. 5).

Fig. 6 shows the comparison between the proposed method and other well known methods. In this the condition-number method did no converge. The proposed method not only converges, but also provides the best mesh quality among all the methods.

To demonstrate the contribution of the target function that include the angular terms, we compare the results between simply taking the geometric average of S, E, N, and W in fig. 1 (the initial guess), against with the Newton's step for minimizing the target function. Fig. 7 show their difference. The result with minimizing the target function clearly has a bigger center box which is consistent with globally more uniform mesh sizes.

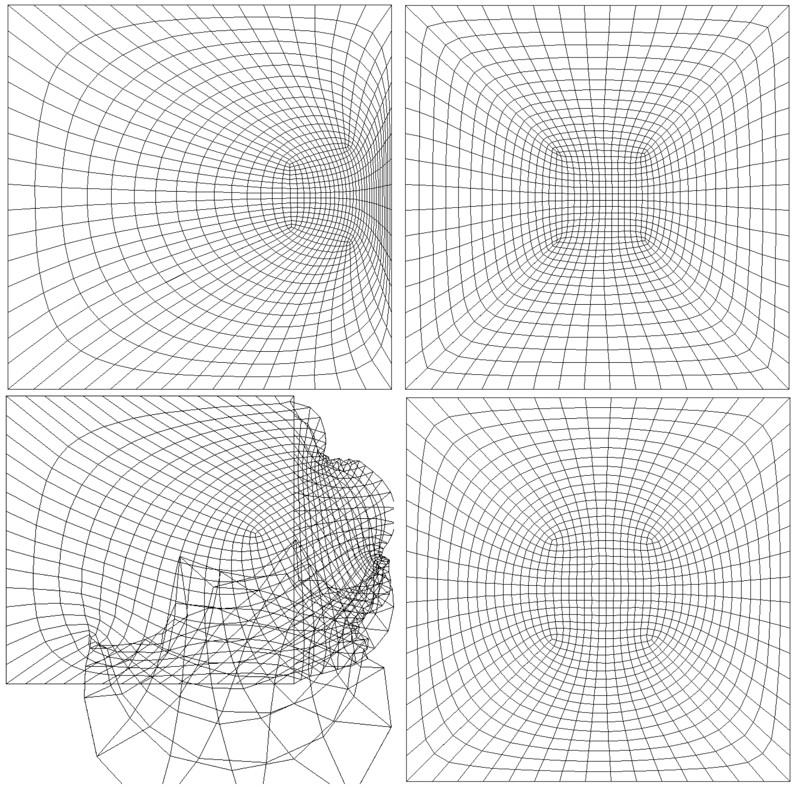

Figure 6: The initial mesh in fig. 5 smoothed with 800 iterations: upper left: with the angle-based method; upper right: with the Winslow-Crowley method lower left: with the condition-number method; lower right: with the proposed method.

6.2 On a curved surface

Fig. 8 shows a three-block initial mesh which is on the inner side of a 1/8 spherical surface with a radius of 15 units centered at the origin. We perform smoothing with four approaches: the condition number; the equipotential; the equal-distance [6]; and the proposed orthogonality method with position control. Each smoothing method is applied for 500 times. The stencil associated with each node is projected on a plane tangential to the sphere $r = 15$ at the given point to allow a 2D smoothing step, then the improved node position is projected back to the original surface at the end of each iteration for updating the node with another loop over all nodes.

The results of smoothing are shown in fig. 9. The original equi-potential method (upper left figure) does a fair job foe mesh squareness, however also produces rela-

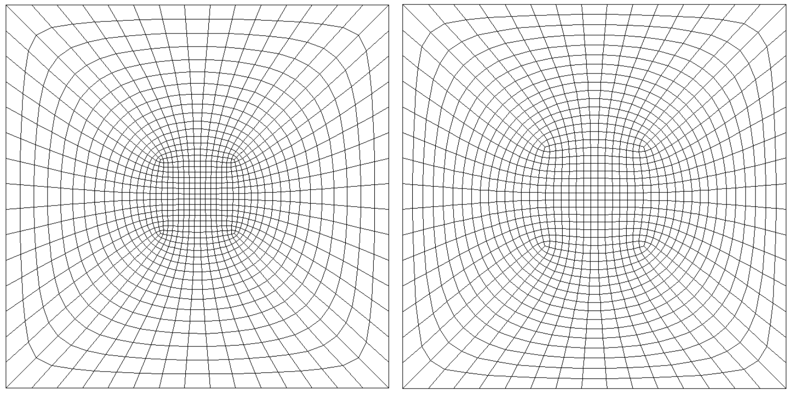

Figure 7: The initial mesh in fig. 5 smoothed with 2000 iterations for convergence: left: without the Newton's step for minimizing the target function (taking the geometric average of S, E, N, and W in fig. 1); right: with the Newton's step (the proposed method).

tively small mesh-sizes around the reduced-connectivity point. The equal-distance method (upper-right figure), which is aimed at producing a globally uniform mesh size, produces the largest mesh sizes around the reduced-connectivity point. It does not produce the best squareness of elements because orthogonality is not a condition of the method. The condition-number method (lower left figure) does provide mesh-squareness, but still generates small mesh-sized around the reduced-connectivity point. The proposed orthogonality method also provide mesh-squareness, nevertheless, its smallest mesh-size is larger than produced by the condition-number method, consistent with the previous examples.

6.3 A three-dimensional block mesh with center twisted

We show here the comparison between various smoothing methods with three mesh-quality metrics for a three-dimensional test problem. They are chosen to be: a) the minimum element size; b) the smallest angle; and c) the aspect ratio.

The minimum element size is computed with the volume of a given element divided by the maximum face area of the same element. The smallest angle is computed by finding the largest inner product of a pair of element-edges that share the common tip, divided by the products of the two edge-lengths, then taking its inverse cosine. The aspect ratio is computed with the longest diagonal divided by the smallest edge size for each element, then taking the maximum among them.

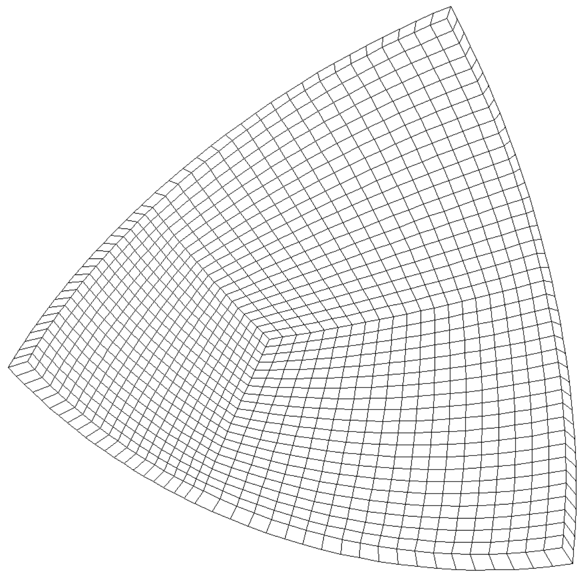

Figure 8: The initial three-block mesh on the inner side of a 1/8 spherical shell. The smaller block has element dimensions nearly half of the dimensions of elements in rest of the blocks.

We take a cubic block structure with *3 by 3 by 3 = 27* blocks centered at the origin. Each block is a cube with an edge-length of 2. Initially, the block at the center is rotated by $5\pi/6$ around the x-axis, then rotated another $5\pi/6$ around the y-axis, finally the center is again rotated by $5\pi/6$ around the z-axis. Each block is then assigned a *10 by 10 by 10* algebraic mesh.

The ideal metrics for a perfectly smoothed cubic mesh would be the smallest relative element size, the smallest angle, and the largest aspect ratio equal to $(1, \pi/2, \sqrt{3})$. The initial mesh metric is given by $(0.0000188721, 3.214596, 1505562)$. Among the $27,000$ elements in total, 490 of them are flipped (fig. 10).

The table below shows comparison between mesh metrics for four different smoothing methods including the condition-number method and the proposed orthogonality method. The other two are the equal-potential method and the angle-based method.

Clearly, the proposed method provides the best mesh metrics with fixed numbers of the smoothing steps. The equi-potential comes the second, followed by the angle-based method. The condition-number method converges the slowest. Further computation shows that for smallest mesh size to get within a relative threshold of

10^{-3} to the ideal case, 180 smoothing steps is sufficient with the proposed method, in contrast, about 1000 steps with the condition-number method are necessary to achieve the same accuracy.

$Iters$	CND	OTR	ANG	EQP
2^2	(0.001, 1.10, 9088)	(0.24, 24.3, 11.9)	(0.001, 3.52, 8395)	(0.09, 6.02, 36.5)
2^3	(0.045, 7.89, 23.2)	(0.60, 52.7, 3.39)	(0.16, 12.9, 16.9)	(0.37, 27.9, 6.24)
2^4	0.417, 37.0, 4.77)	(0.76, 69.6, 2.42)	(0.42, 35.4, 5.07)	(0.63, 50.1, 3.33)
2^5	(0.670, 62.3, 2.83)	(0.89, 80.9, 1.99)	(0.65, 58.0, 3.02)	(0.81, 68.0, 2.38
2^6	(0.805, 76.5, 2.20)	(0.97, 87.2, 1.80)	(0.816, 74.7, 2.24)	(0.924, 80.6, 1.96)
2^7	(0.890, 84.2, 1.92)	(0.997, 89.6, 1.74)	(0.912, 84.5, 1.89)	(0.979, 87.4, 1.78)

Table 1: Mesh metrics against number of iterations regarding the initial mesh in fig. 10. 'CND' stands for condition number; 'OTR' for proposed orthogonality; 'ANG' for angle-based; and 'EQP' for equi-potential (Winslow-Crowley). The first number in the metrics is the smallest relative side length, the second number is the minimum 2D angle in degrees, the last one is the aspect ratio defined by the longest diagonal divided by the shortest side-length. The ideal metrics is $(1.0, 90.0, 1.732)$.

7 Conclusion

We propose a mesh smoothing algorithm which is parallel to the condition-number method, with the target function replaced by the sum of an asymptotic expression of cosine squares of angles defined in a simplified regular stencil, plus a position control function similar to used in the Laplacian smoothing. Numerical results show that while achieving a similar quality of element squareness, the proposed method converges much quicker, and provide globally more uniform mesh size than the condition-number method. In addition, the proposed method also behaves better than the angle-based method and the Winslow-Crowley method in our numerical tests.

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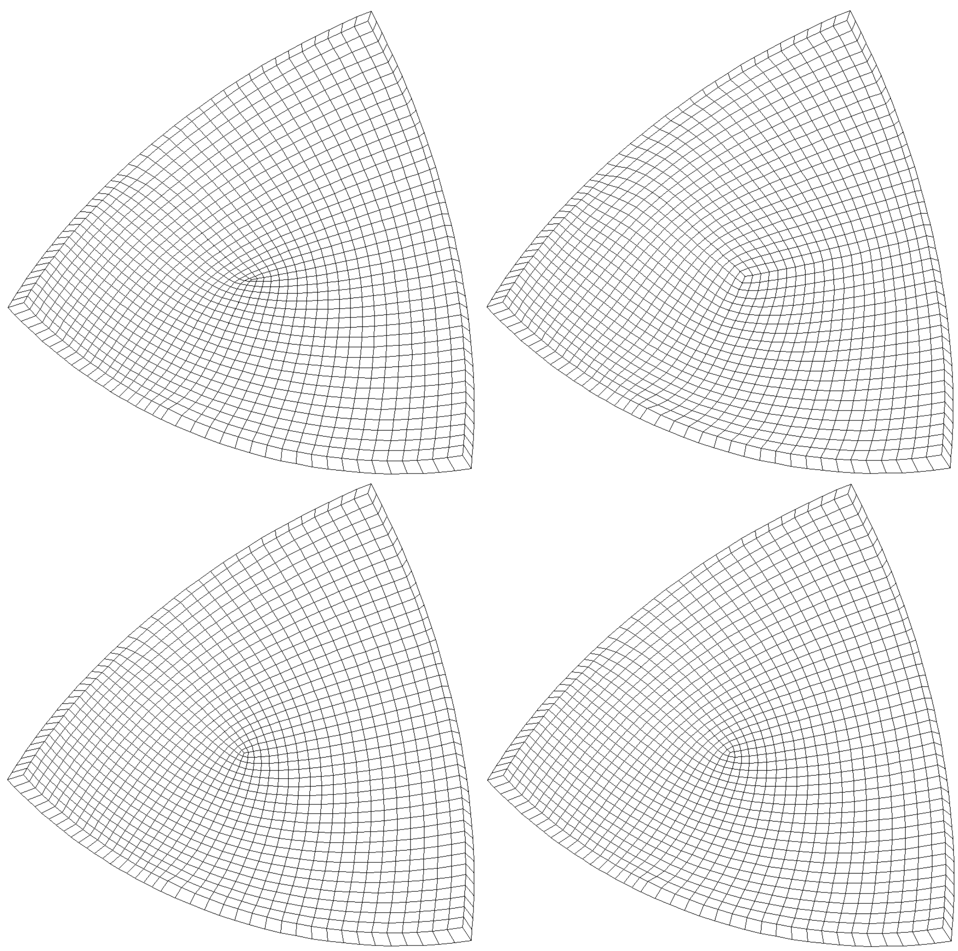

Figure 9: The initial mesh in fig. 8 smoothed with 500 iterations: upper left: with the original equi-potenial method; upper right: with the equal-distance method. lower left: with the condition-number method; lower right: with the proposed method;

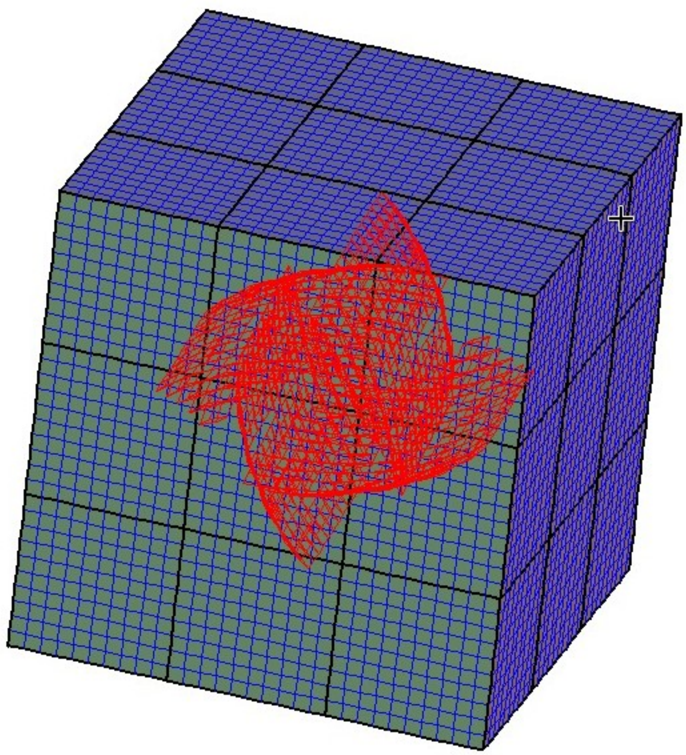

Figure 10: The elements marked by red color are flipped because of the three consecutive 75 degree rotations applied to the center block of a 3 by 3 by 3 perfect cubic block-mesh.