Quality Improvement of 3D Meshes in ALE simulation of Gas Dynamics[1]

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Abstract

An important part of the Arbitrary Lagrangian-Eulerian method is the rezoning or mesh improvement step after completion of the Lagrangian step where the mesh is deformed according to the flow. A procedure is presented here to optimize the quality of elements in 3D solid meshes by node repositioning. The procedure aims to improve the quality of boundary mesh faces and interior mesh regions while keeping the nodes close to their original locations and preserving the essential characteristics of the boundary surfaces.

Keywords: ALE methods, mesh optimization, surface and solid meshes, Jacobian condition number, Reference Jacobian based Mesh Optimization

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1 Description

Arbitrary Lagrangian Eulerian methods (ALE) methods have become an important tool in the simulation of gas dynamics problems since they incorporate the best features of both Lagrangian and Eulerian methods. In ALE methods, a Lagrangian step is first performed where the flow is calculated and the mesh is deformed according to the fluid flow. At the end of a Lagrangian step, a mesh optimization or rezoning step is performed to improve the quality of the mesh. The solution is then transferred from the Lagrangian mesh to the improved mesh and the simulation continued.

In this research, a procedure has been developed for the optimization of 3D mesh quality by node repositioning after the completion of the Lagrangian step. The procedure, called Reference Jacobian based Mesh Optimization, is designed to improve the quality or geometric shape of mesh regions and boundary mesh faces while keeping the improved mesh as close as possible to the original mesh. The method has been found to improve the quality of elements on external boundaries, material interfaces and in the interior while preserving mesh features and surface characteristics.

The element quality measure improved in the mesh optimization process is the Jacobian Condition Number [1] measured at each element corner. The Jacobian matrix at a vertex of an element is defined as the the matrix whose columns are edge vectors of the element connected to the vertex. Therefore, the Jacobian condition numbers at the vertex of a element in 2D and 3D are given as

$$\kappa_{2D} = \frac{\mid \mathbf{e}_\xi \mid^2 + \mid \mathbf{e}_\eta \mid^2}{\mid \mathbf{e}_\xi \times \mathbf{e}_\eta \mid}, \qquad \text{and}$$

$$\kappa_{3D} = \frac{(\mid \mathbf{e}_\xi \mid^2 + \mid \mathbf{e}_\eta \mid^2 + \mid \mathbf{e}_\zeta \mid^2)^{\frac{1}{2}} (\mid \mathbf{e}_\xi \times \mathbf{e}_\eta \mid^2 + \mid \mathbf{e}_\eta \times \mathbf{e}_\zeta \mid^2 + \mid \mathbf{e}_\zeta \times \mathbf{e}_\xi \mid^2)^{\frac{1}{2}}}{\mid (\mathbf{e}_\xi \times \mathbf{e}_\eta) \bullet \mathbf{e}_\zeta \mid}$$

respectively, where $\mathbf{e}_\xi$, $\mathbf{e}_\eta$ (and $\mathbf{e}_\zeta$ in 3D) are edge vectors of the element connected to the vertex.

The Reference Jacobian based Mesh Optimization method for improving mesh quality consists of two stages. The first stage of the procedure is a local optimization in which the optimal (*reference*) position of each mesh vertex is calculated with respect to the fixed positions of its neighbors. The local objective function is based on Jacobian condition numbers computed in the elements connected to the particular vertex [2]. The reference positions of vertices are used to calculate two *reference edge vectors* for each edge in the mesh; each reference edge vector goes from the reference position of one vertex of the edge to the original position of the other. The reference edge vectors are then used to compute *Reference Jacobian Matrices*, $\mathbf{J}^R$, in the same way that Jacobian matrices were defined for the original mesh.

In the second stage of the procedure, a global objective function is formulated using the element and reference Jacobian matrices as shown below:

$$F = \sum_i \sum_j \frac{\mid \mathbf{J}_{ij} - \mathbf{J}^R_{ij} \mid_F}{\mid \mathbf{J}_{ij} \mid / \mid \mathbf{J}^R_{ij} \mid}$$

where J_{ij} is the Jacobian of element j at vertex i. The definition of this objective function directs the optimization to find a configuration for all the mesh edges such that a compromise is struck between the various pairs of reference edge vectors, the mesh remains valid and the element quality is improved. The optimization of this global function is performed by iterating over all the mesh vertices and optimizing a local part of the global function at each

vertex by a nonlinear conjugate gradient procedure.

In the optimization of a 3D mesh, separate consideration must be given to repositioning vertices on the boundary and in the interior. Interior vertices may be repositioned directly by optimizing an objective function with respect to its Cartesian coordinates. However, boundary vertices must be repositioned so that they remain on the original surface definition, and thereby maintain the essential characteristics of the surface.

A new technique [3] has been devised here to reposition boundary vertices so that they remain on the original discrete surface. Each vertex is moved in a local parametric space constructed by a barycentric or isoparametric mapping of the original mesh element it is moving in. If the vertex goes out of bounds in the local parametric space of one element, the procedure moves the vertex to the local parametric space of an adjacent element and continues the optimization. Use of a local parameterization for node movement allows the procedure to be independent of an underlying smooth surface for the surface mesh and avoids the construction of a global parametric space which can be expensive.

The procedure has been tested on a number of surface and solid meshes and has proved to be very effective in improving mesh quality while minimizing changes to mesh features and surface characteristics.

2 Results

Figure 1(a) shows a mixed triangular and quadrilateral surface mesh for the Igea artifact mesh (original triangulation courtesy Cyberware, Inc.). Figure 1(b) shows the result of optimization by the Reference Jacobian based procedure while figure 1(c) shows the result

of a direct condition number optimization. Table 1 shows the average element condition number histograms and the worst condition number for the three meshes. The table also shows the maximum Hausdorff distance (defined as the maximum of the minimum distance from each point of one mesh to another [4]) and the maximum node movement of the two optimized meshes relative to the original. From the results, it is clear that the Reference Jacobian based procedure improves the mesh but also keeps the mesh close to the original mesh while direct condition number optimization makes large changes to the mesh in order to achieve a higher mesh quality.

Figure 2 shows an example of 3D mesh optimization where the tetrahedral mesh of a pig (Figure 2a) has been optimized using Reference Jacobian based Optimization (Figure 2b) and Condition Number Optimization (Figure 2c).

3 Conclusions

A procedure was presented to improve the condition number quality measure of elements in a 3D mesh while keeping the mesh close to original configuration. Future work involves extending the method to optimize general polygonal and polyhedral meshes.

4 Acknowledgments

The authors would like to acknowledge the help of Patrick Knupp of the Parallel Computing Sciences Division, Sandia National Laboratories, Albuquerque, NM in developing the ideas described in this paper. This work was done at Los Alamos National Laboratory which is

operated by the University of California for the US Department of Energy under contract W-7405-ENG-36. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

The authors also acknowledge use of software tools from the Scientific Computation Research Center, Rensselaer Polytechnic Institute, Troy, NY that enabled testing of the ideas presented in this paper

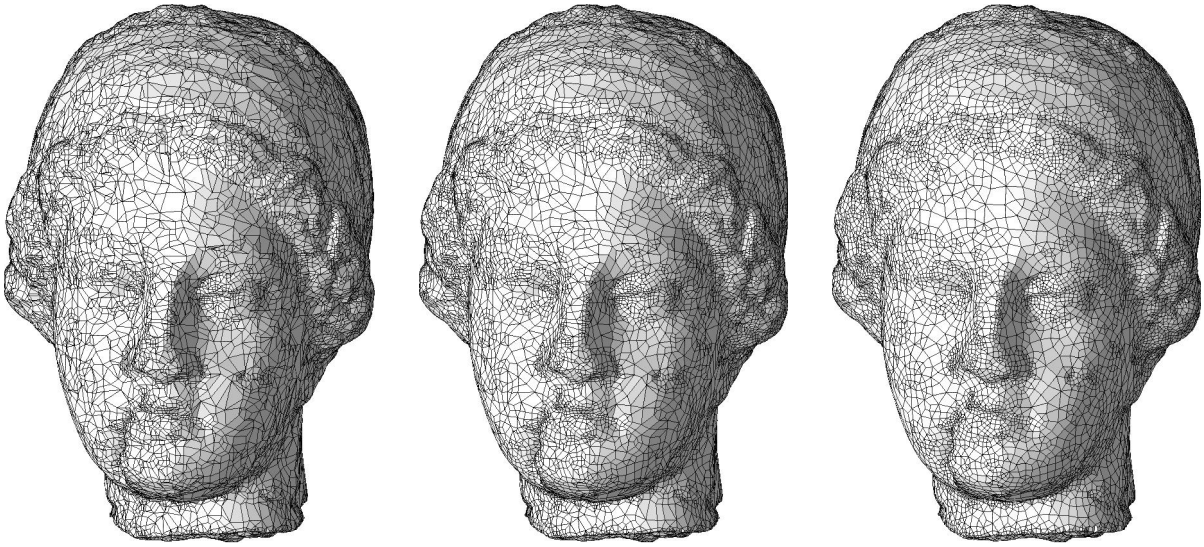
References

[1] P.M. Knupp. Achieving finite element mesh quality via optimization of the jacobian matrix norm and associated quantitites. Part I - a framework for surface mesh optimization. *International Journal for Numerical Methods in Engineering*, (48):401–420, 2000.

[2] M. Shashkov and P.M. Knupp. Optimization-based reference-matrix rezone strategies for arbitrary lagrangian-eulerian methods on unstructured grids. In *Proceedings of the 10th Anniversary International Meshing Roundtable*, pages 167–176, Newport Beach, CA, 2001. Sandia National Laboratories. `http://math.lanl.gov/~shashkov`.

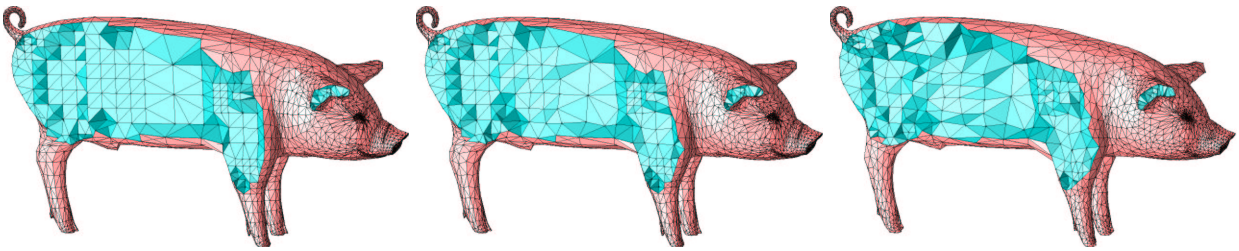
[3] R. V. Garimella, M. J. Shashkov, and P. M. Knupp. Optimization of surface mesh quality using local parameterization. In *Proceedings of the 11th International Meshing Roundtable*, pages 41–52, Ithaca, NY, Sep. 15-18 2002.

[4] P. Cignoni, C. Rocchini, and R. Scopigno. Metro: Measuring error on simplified surfaces. *Computer Graphics Forum*, 17(2):167–174, June 1998.



(a) (b) (c)

Figure 1: (a) Original surface mesh of Igea artifact (Cyberware, Inc.), (b) Mesh optimized with Reference Jacobian based objective function, (c) Mesh optimized with condition number objective function.



(a) (b) (c)

Figure 2: (a) Original 3D mesh for pig, (b) Mesh optimized with Reference Jacobian based objective function, (c) Mesh optimized with condition number objective function. Pictures show parts of the surface and interior meshes.

Avg. Condition Number for elements	Original Mesh	Reference Jacobian based Optimization	Condition Number based Optimization
1.0 – 1.5	15984	22021	23341
1.5 – 2.0	6071	1537	310
2.0 – 3.0	1370	88	1
3.0 – 4.0	142	5	0
4.0 – 5.0	33	1	0
5.0 – 7.5	40	0	0
7.5 – 10.0	8	0	0
10.0 – 15.0	3	0	0
15.0 –	1	0	0
Worst Condition No.	16.53	4.04	2.59
Max. Hausdorff Distance (% of Problem Size)		0.20	1.44
Max. Node Movement (% of Problem Size)		0.47	3.15

Table 1: Comparison of histograms of average condition numbers of elements for original and optimized meshes of Igea model