A Practical Approach for Solving Mesh Optimization Problems using Newton's Method

Jibum Kim[1], Rao V. Garimella[2], and Markus Berndt[3]

[1] Incheon National University, Incheon, South Korea, jibumkim@incheon.ac.kr
[2] Los Alamos National Laboratory, Los Alamos, NM, USA, rao@lanl.gov
[3] Los Alamos National Laboratory, Los Alamos, NM, USA, berndt@lanl.gov

1 Abstract

We present a practical approach for solving volume and surface mesh optimization problems. Our approach is based on Newton's method which uses both first-order (gradient) and second-order (Hessian) derivatives of the nonlinear objective function. The volume and surface optimization algorithms are modified such that surface constraints and mesh validity are satisfied. We also propose a simple and efficient Hessian modification method when the Hessian matrix is not positive definite. We demonstrate our approach by comparing our method with a popular nonlinear conjugate gradient method in terms of both efficiency and mesh quality.

2 Introduction

Mesh quality improvement and mesh untangling are important topics for partial differential equation (PDE)-based simulations, because elements with a poor quality can ruin accuracy and efficiency of the solution, and an inverted (tangled) element can result in failure to obtain a PDE solution. Mesh quality improvement and mesh untangling problems are often formulated as nonlinear optimization problems [1, 4]. In order to efficiently solve such nonlinear optimization problems, various nonlinear solvers have been developed. These solvers include steepest descent, conjugate gradient, feasible Newton, quasi Newton, and trust-region methods [2]. Previously, many researchers have used nonlinear conjugate gradient method (NLCG) for solving mesh optimization problems. However, it turns out that NLCG method is slow, prone to getting stuck in local minima and failing to converge due to surface mesh constraints.

In this paper, we employ Newton's method for solving various nonlinear mesh optimization problems. The use of Newton's method for solving nonlinear optimization problem is motivated by the observation that, if the nonlinear functional is sufficiently smooth, the optimal points are roots of the derivative function. Thus, a nonlinear optimization problem is transformed into a root finding problem. We choose Newton's method for solving the mesh optimization problem, because it provides both search direction and a step size using both first-order (gradient) and second-order (Hessian) information. In addition, its convergence is quadratic. We will demonstrate that Newton's method is successfully used to solve mesh optimization problems more accurately and efficiently.

3 Mesh Optimization and Untangling using Newton's Method

3.1 Volume Mesh Optimization

Let $F(x)$ be the nonlinear mesh optimization problem to minimize. Let q_i be the quality of i^{th} vertex and N be the number of vertices on the mesh. Then, $F(x)$ is formulated as $\sum_{i=1}^{N} q_i$. We use a condition number quality metric for mesh quality improvement. For a trivalent mesh corners in 3D, given by edge vectors e_1, e_2, and e_3, the quality of the vertex corner is given by [3]:

$$q_i = \frac{\sqrt{||\mathbf{e}_1 \times \mathbf{e}_2||^2 + ||\mathbf{e}_2 \times \mathbf{e}_3||^2 + ||\mathbf{e}_3 \times \mathbf{e}_1||^2}\sqrt{||\mathbf{e}_1||^2 + ||\mathbf{e}_2||^2 + ||\mathbf{e}_3||^2}}{(\mathbf{e}_1 \times \mathbf{e}_2) \cdot \mathbf{e}_3}. \tag{1}$$

The condition number quality metric is scale-invariant and prefers a right angle corner.

We minimize $F(x)$ using Newton's method by finding vertex coordinates x such that $\bigtriangledown F(x)$ is zero. We use finite difference approximations to compute these gradient $(\triangledown F(x))$ and Hessian matrix $(H_F(x))$ of $F(x)$. In the k^{th} iteration, we compute a Newton update, p_k , by solving, $p_k = -(H_F(x_k))^{-1} \bigtriangledown F(x_k)$. The k^{th} vertex position is updated as $x_{k+1} \leftarrow x_k + \alpha p_k$, where α is a constant. The α is determined by *Armijo condition* [2] dictating that the update should lead to a sufficient decrease in the objective function. In practice, we start with α=1 and cut it by 20% until the *Armijo condition* is satisfied. The Newton direction, p_k, reliably produces a decrease in function only if $H_F(x_k)$ matrix is positive definite. When $H_F(x_k)$ is not positive definite, we perform a Hessian modification step such that all eigenvalues of $H_F(x_k)$ are positive [2]. The Hessian modification step is performed by adding diagonal terms, $H_F(x_k) = H_F(x_k) + \beta I$, until $H_F(x_k)$ is positive definite, where β is a positive constant and I is an identity matrix.

For initially tangled meshes, we employ Escobar. et.al's [4] modification to the quality metric, which is able to simultaneously untangle and smoothe. The quality metric [4] is defined as

$$q_i = \frac{(A)(L)}{V + \sqrt{V^2 + \delta^2}}, \tag{2}$$

where $A = \sqrt{||\mathbf{e}_1 \times \mathbf{e}_2||^2 + ||\mathbf{e}_2 \times \mathbf{e}_3||^2 + ||\mathbf{e}_3 \times \mathbf{e}_2||^2}$, $L = \sqrt{\sum_{j=1}^{3} ||\mathbf{e}_j||^2}$, $V = (\mathbf{e}_1 \times \mathbf{e}_2) \cdot \mathbf{e}_3$, and δ is a constant value. If V is positive and δ is zero, the quality metric is same as the condition number quality metric. Introducing δ makes the objective function continuous across the zero volume. The choice of δ for different problem sizes is not well-defined in [4]. The δ value should be as small as possible (close to zero) in order to remain close to the original condition number quality metric, but bigger values of δ make the function less steep and ensure more robust gradient computations. In order to satisfy these requirements, we developed an adaptive and smooth δ function which satisfies above requirements using a sigmoid function.,

$$\delta = \frac{1}{1 + ce^{V/V_0}}, \tag{3}$$

where V_0 is a reference element volume for scale invariance which could be chosen as some average element volume around the element being untangled and c is a constant value. We observed that the c value between 10 and 100 works well.

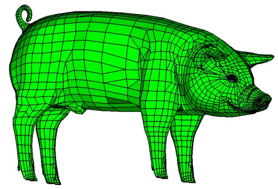
3.2 Surface Mesh Optimization

As described in [1], surface meshes are optimized by performing optimizations with respect to parametric coordinates. We use a condition number quality metric for mesh quality improvement. For surface meshes, the updated vertex coordinates should satisfy both surface constraints and the mesh validity. If the updated vertex coordinates are located beyond the parametric bound, we change the parametric space to the neighborhood parametric space. The Hessian modification step described in Section 3.1 is employed when the Hessian matrix is not positive definite.

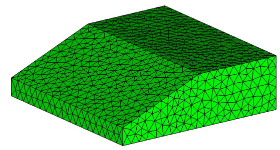
4 Numerical Experiments

We perform numerical experiments on both volume and surface meshes. For volume meshes, we consider an initially tangled mesh. We compare Newton's method with a popular nonlinear conjugate gradient (NLCG) method in terms of mesh quality and computational cost. Figure 1 shows the initial meshes that we tested. For the cube mesh, the initial mesh is randomly perturbed such that 60% of the elements are inverted.

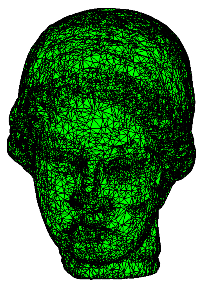
Table 1 shows timing results in seconds until various meshes are optimized. Our experimental results show that time to convergence for Newton's method is up to 4.8 times faster than for the NLCG method. Table 2 shows worst



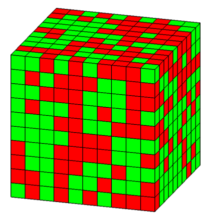
(a) Pig mesh (surface)



(b) Slope mesh (surface)



(c) Igea mesh (surface)



(d) Cube mesh (volume)

Fig. 1. The element types of the four initial meshes are (a) Pig: mixed elements, (b) Slope: polyhedral elements, (c) Igea: tetrahedral elements, and (d) Cube: hexahedral elements. Here, elements shown in red indicate inverted elements.

element qualities for various surface and volume meshes. A smaller value indicates a better mesh quality. For all these examples, Newton's method outperforms the NLCG method. For a cube mesh, we also observe that two elements fail to be valid and remain tangled after optimization when the NLCG is used. However, Newton's method is able to untangle all inverted elements. Table 3 shows surface mesh quality statistics of pig meshes. We observe that Newton's method outperforms the NLCG method in terms of both average element quality and worst element quality.

Mesh (Number of elements)	Newton	NLCG
Pig (surface, 3K)	61	226
Slope (surface, 3K)	504	1,810
Igea (surface, 40K)	297	1,422
Cube (volume, 3K)	77	335

Table 1. Time (sec) to optimize various meshes.

Mesh (Number of elements)	Initial	Optimized (Newton)	Optimized (NLCG)
Pig (surface, 3K)	45.07	6.89	11.34
Slope (surface, 3K)	48.30	1.75	2.06
Igea (surface, 40K)	19.08	3.68	3.91
Cube (volume, 3K)	1026.80	1.09	1.17

Table 2. Worst element quality computed by the condition number metric for surface and volume meshes.

Surface Element Quality	Initial	Optimized (Newton)	Optimized (NLCG)
1.0 - 1.5	2442	3727	3728
1.5 - 2.0	768	89	84
2.0 - 3.0	384	10	12
3.0 - 4.0	108	0	2
4.0 - 5.0	45	0	0
5.0 - 7.5	57	1	0
7.5 - 10.0	9	0	0
10.0 - 15.0	12	0	1
15.0 -	57	0	0

Table 3. Surface mesh quality statistics of pig meshes. We show the number of mesh elements whose average quality metric falls into a given range, for the initial mesh as well as the two optimized meshes (Newton and NLCG).

5 Acknowledgements

This work was performed under the auspices of the National Nuclear Security Administration of the US Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396 and supported by the DOE Advanced Simulation and Computing (ASC) program.

References

1. Garimella, R.V., Shashkov, M.J., Knupp, P.M., "Triangular and Quadrilateral Surface Mesh Quality Optimization using Local Parametrization," *Computer Methods in Applied Mechanics and Engineering*, vol. 193, no. 9-11, pp. 913-928, March 2004.
2. Nocedal, J. and Wright, S. *Numerical Optimization*, Springer, Berlin, 2006.
3. Dyadechko, V., Garimella, R.V. and Shashkov, M.J. "Reference Jacobian Rezoning Strategy for Arbitrary Lagrangian-Eulerian Methods on Polyhedral Grids", Proceedings, *13th International Meshing Roundtable*, Williamsburg, VA, Sandia National Laboratories report SAND #2004-3765C, pp. 459-470, Sep. 2004.
4. Escobar, J.M., et.al. "Simultaneous Untangling and Smoothing of Tetrahedral Meshes," *Computer Methods in Applied Mechanics and Engineering*, vol. 192, no. 25, pp. 2775-2787, June 2003.