Improved Objective Functions for Tetrahedral Mesh Optimisation*

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Abstract. The quality improvement in mesh optimisation techniques that preserve its connectivity are obtained by an iterative process in which each node of the mesh is moved to a new position that minimises a certain objective function. In general, objective functions are derived from some quality measure of the *local submesh*, that is, the set of tetrahedra connected to the adjustable or *free node*. Although these objective functions are suitable to improve the quality of a mesh in which there are non *inverted* elements, they are not when the mesh is tangled. This is due to the fact that usual objective functions are not defined on all $\mathbb{R}^3$ and they present several discontinuities and local minima that prevent the use of conventional optimisation procedures. Otherwise, when the mesh is tangled, there are local submeshes for which the free node is out of the *feasible region*, or this does not exist. In this paper we propose the substitution of objective functions having barriers by modified versions that are defined and regular on all $\mathbb{R}^3$. With these modifications, the optimisation process is also directly applicable to meshes with inverted elements, making a previous untangling procedure unnecessary.

1 Introduction

In finite element simulation the mesh quality is a crucial aspect for good numerical behaviour of the method. In a first stage, some automatic 3-D mesh generator constructs meshes with poor quality and, in special cases, for example when node movement is required, inverted elements may appear. So, it is necessary to develop a procedure that optimises the pre-existing mesh. This process must be able to smooth and untangle the mesh.

The most usual techniques to improve the quality of a *valid* mesh, that is, one that does not have inverted elements, are based upon local smoothing. In short, these techniques consist of finding the new positions that the mesh

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nodes must hold, in such a way that they optimise an objective function. Such a function is based on a certain measurement of the quality of the *local submesh,* $N(v)$, formed by the set of tetrahedra connected to the *free node* v. As it is a local optimisation process, we can not guarantee that the final mesh is globally optimum. Nevertheless, after repeating this process several times for all the nodes of the current mesh, quite satisfactory results can be achieved. Usually, objective functions are appropriate to improve the quality of a valid mesh, but they do not work properly when there are inverted elements. This is because they present singularities (barriers) when any tetrahedron of $N(v)$ changes the sign of its Jacobian determinant. To avoid this problem we can proceed as Freitag et al in [7,9,10], where an optimisation method consisting of two stages is proposed. In the first one, the possible inverted elements are untangled by an algorithm that maximises their negative Jacobian determinants [9]; in the second, the resulting mesh from the first stage is smoothed using another objective function based on a quality metric of the tetrahedra of $N(v)$ [10]. One of these objective functions are present in Section 2. After the untangling procedure, the mesh has a very poor quality because the technique has no motivation to create good-quality elements. As remarked in [7], it is not possible to apply a gradient-based algorithm to optimise the objective function because it is not continuous all over $\mathbb{R}^3$, making it necessary to use other non-standard approaches.

In Section 3 we propose an alternative to this procedure, such that the untangling and smoothing are carried out in the same stage. For this purpose, we use a suitable modification of the objective function such that it is regular all over $\mathbb{R}^3$. When a feasible region (subset of $\mathbb{R}^3$ where v could be placed, being $N(v)$ a valid submesh) exists, the minima of the original and modified objective functions are very close and, when this region does not exist, the minimum of the modified objective function is located in such a way that it tends to untangle $N(v)$. The latter occurs, for example, when the fixed boundary of $N(v)$ is tangled. With this approach, we can use any standard and efficient unconstrained optimisation method to find the minimum of the modified objective function, see for example [2].

In this work we have applied the proposed modification to one objective function derived from an *algebraic mesh quality metric* studied in [11], but it would also be possible to apply it to other objective functions which have barriers like those presented in [12]. The results for two test problems are shown in Section 4. Finally, conclusions and future research are presented in Section 5.

2 Objective Functions

Several *tetrahedron shape measures* [4] could be used to construct an objective function. Nevertheless those obtained by algebraic operations are specially indicated for our purpose because they can be computed very efficiently. The above mentioned algebraic mesh quality metric and the corresponding objective function are shown in this Section.

Let T be a tetrahedral element in the physical space whose vertices are given by $\mathbf{x}_k = (x_k, y_k, z_k)^T \in \mathbb{R}^3$, $k = 0, 1, 2, 3$ and T_R be the reference tetrahedron with vertices $\mathbf{u}_0 = (0,0,0)^T$, $\mathbf{u}_1 = (1,0,0)^T$, $\mathbf{u}_2 = (0,1,0)^T$ and $\mathbf{u}_3 = (0,0,1)^T$. If we choose $\mathbf{x}_0$ as the translation vector, the affine map that takes T_R to T is $\mathbf{x} = A\mathbf{u} + \mathbf{x}_0$, where A is the Jacobian matrix of the affine map referenced to node $\mathbf{x}_0$, and expressed as $A = (\mathbf{x}_1 - \mathbf{x}_0, \mathbf{x}_2 - \mathbf{x}_0, \mathbf{x}_3 - \mathbf{x}_0)$.

Let now T_I be an equilateral tetrahedron with all its edges of length one and vertices located at $\mathbf{v}_0 = (0,0,0)^T$, $\mathbf{v}_1 = (1,0,0)^T$, $\mathbf{v}_2 = (1/2, \sqrt{3}/2, 0)^T$, $\mathbf{v}_3 = \left(1/2, \sqrt{3}/6, \sqrt{2}/\sqrt{3}\right)^T$. Let $\mathbf{v} = W\mathbf{u}$ be the linear map that takes T_R to T_I, being $W = (\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)$ its Jacobian matrix.

Therefore, the affine map that takes T_I to T is given by $\mathbf{x} = AW^{-1}\mathbf{v} + \mathbf{x}_0$, and its Jacobian matrix is $S = AW^{-1}$. This weighted matrix S is independent of the node chosen as reference; it is said to be *node invariant* [11]. We can use matrix norms, determinant or trace of S to construct algebraic quality measures of T. For example, the Frobenius norm of S, defined by $|S| = \sqrt{\operatorname{tr}(S^T S)}$, is specially indicated because it is easily computable. Thus, it is shown in [11] that $q = \frac{3\sigma^{\frac{2}{3}}}{|S|^2}$ is an algebraic quality measure of T, where $\sigma = \det(S)$. The maximum value of these quality measures is the unity and it corresponds to equilateral tetrahedron. Besides, any flat tetrahedron has quality measure zero. We can derive an optimisation function from this quality measure. Thus, let $\mathbf{x} = (x, y, z)^T$ be the free node position of v, and let S_m be the weighted Jacobian matrix of the m-th tetrahedron of $N(v)$. We define the objective function of $\mathbf{x}$, associated to an m-th tetrahedron as

$$\eta_m = \frac{|S_m|^2}{3\sigma_m^{\frac{2}{3}}} \tag{1}$$

Then, the corresponding objective function for $N(v)$ can be constructed by using the p-norm of $(\eta_1, \eta_2, \ldots, \eta_M)$ as

$$|K_\eta|_p(\mathbf{x}) = \left[\sum_{m=1}^{M} \eta_m^p(\mathbf{x})\right]^{\frac{1}{p}} \tag{2}$$

where M is the number of tetrahedra in $N(v)$. The objective function $|K_\eta|_1$ was deduced and used in [1] for smoothing and adapting of 2-D meshes. The same function was introduced in [3], for both 2 and 3-D mesh smoothing, as a result of a force-directed method. Finally, this function, among others, is studied and compared in [12]. We note that the cited authors only use this objective function for smoothing valid meshes.

Although this optimisation function is smooth in those points where $N(v)$ is a valid submesh, it becomes discontinuous when the volume of any tetrahedron of $N(v)$ goes to zero. It is due to the fact that η_m approaches infinity when σ_m tends to zero and its numerator is bounded below. In fact, it is possible to prove that $|S_m|$ reaches its minimum, with strictly positive value, when v is placed in the geometric centre of the fixed face of the m-th tetrahedron. The positions where v must be located to get $N(v)$ to be valid, i.e., the feasible region, is the interior of the polyhedral set P defined as $P = \bigcap_{m=1}^{M} H_m$, where H_m are the half-spaces defined by $\sigma_m(\mathbf{x}) \geqslant 0$. This set can occasionally be empty, for example, when the fixed boundary of $N(v)$ is tangled. In this situation, function $|K_\eta|_p$ stops being useful as optimisation function. On the other hand, when the feasible region exists, that is $int\ P \neq \emptyset$, the objective function tends to infinity as v approaches the boundary of P. Due to these singularities, a barrier is formed which avoids reaching the appropriate minimum by using gradient-based algorithms, when these start from a free node outside the feasible region. In other words, with these algorithms we can not optimise a tangled mesh $N(v)$ with the above objective function.

3 Modified Objective Functions

We propose a modification in the previous objective function (2), so that the barrier associated with its singularities will be eliminated and the new function will be smooth all over $\mathbb{R}^3$. An essential requirement is that the minima of the original and modified functions are nearly identical when $int\ P \neq \emptyset$. Our modification consists of substituting σ in (2) by the positive and increasing function

$$h(\sigma) = \frac{1}{2}(\sigma + \sqrt{\sigma^2 + 4\delta^2}) \tag{3}$$

being the parameter $\delta = h(0)$. We represent in Fig. 1 the function $h(\sigma)$. Thus, the new objective function here proposed is given by

$$\left|K_\eta^*\right|_p(\mathbf{x}) = \left[\sum_{m=1}^{M} (\eta_m^*)^p(\mathbf{x})\right]^{\frac{1}{p}} \tag{4}$$

where

$$\eta_m^* = \frac{|S_m|^2}{3h^{\frac{2}{3}}(\sigma_m)} \tag{5}$$

is the modified objective function for the m-th tetrahedron.

The behaviour of $h(\sigma)$ in function of δ parameter is such that, $\lim_{\delta \to 0} h(\sigma) = \sigma$, $\forall \sigma \geq 0$ and $\lim_{\delta \to 0} h(\sigma) = 0$, $\forall \sigma \leq 0$. Thus, if $int\ P \neq \emptyset$, then $\forall \mathbf{x} \in int\ P$ we have $\sigma_m(\mathbf{x}) > 0$, for $m = 1, 2, \ldots, M$ and, as smaller values of δ are chosen, $h(\sigma_m)$ behaves very much as σ_m, so that, the original objective function and its corresponding modified version are very close in the feasible region. Particularly, in the feasible region, as $\delta \to 0$, function $\left|K_\eta^*\right|_p$ converges pointwise to $|K_\eta|_p$. Besides, by considering that $\forall \sigma > 0$, $\lim_{\delta \to 0} h'(\sigma) = 1$ and $\lim_{\delta \to 0} h^{(n)}(\sigma) = 0$, for $n \geq 2$, it is easy to prove that the derivatives of this objective function verify the same property of convergence. As a result of these considerations, it may be concluded that the positions of v that minimise original and modified objective functions are nearly identical when δ is *small.* Actually, the value of δ is selected in terms of point v under consideration, making it as small as possible and in such a way that the evaluation of the minimum of modified functions does not present any computational problem. Suppose that $int\ P = \emptyset$, then the

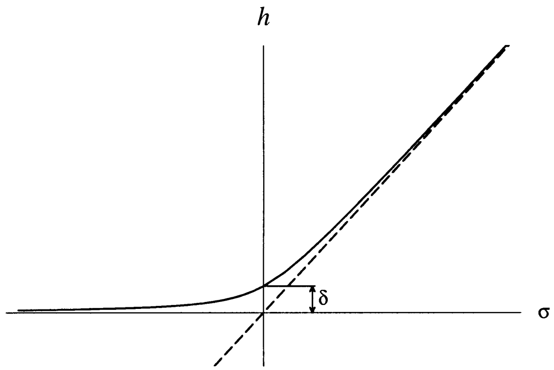
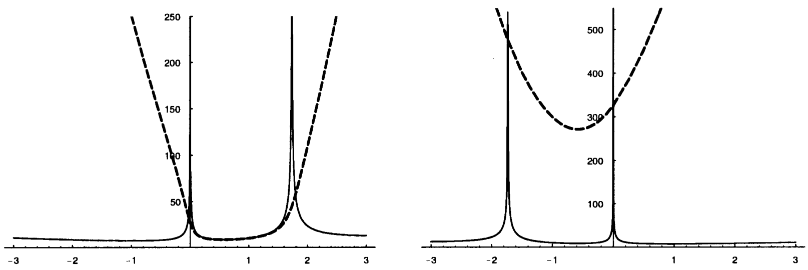


Fig. 1. Representation of function $h\left(\sigma\right)$.

original objective function, $\left|K_\eta\right|_p$, is not suitable for our purpose because it is not correctly defined. Nevertheless, modified function is well defined and tends to solve the tangle. We can reason it from a qualitative point of view by considering that the dominant terms in $\left|K^*_\eta\right|_p$ are those associated to the tetrahedra with more negative values of σ and, therefore, the minimisation of these terms imply the increase of these values. It must be remarked that $h\left(\sigma\right)$ is an increasing function and $\left|K^*_\eta\right|_p$ tends to ∞ when the volume of any tetrahedron of $N\left(v\right)$ tends to $-\infty$, since $\lim\limits_{\sigma\to-\infty} h\left(\sigma\right) = 0$.

In conclusion, by using the modified objective function, we can untangle the mesh and, at the same time, improve its quality. Obviously, the modification here proposed can be easily applied to other objective functions.

For a better understanding of the behaviour of the objective function and its modification, we propose the following 2-D test example. Let us consider a simple 2-D mesh formed by three triangles, vBC, vCA and vAB, where we have fixed $A(0,-1)$, $B(\sqrt{3},0)$, $C(0,1)$ and $v(x,y)$ is the free node. In this case, the feasible region is the interior of the equilateral triangle ABC. In Fig. 2(a) we show $\left|K_\eta\right|_2$ (solid line) and $\left|K^*_\eta\right|_2$ (dashed line) as a function of x for a fixed value $y=0$ (the y-coordinate of the optimal solution). The chosen parameter δ is 0.1. We can see that original objective function presents several local minima and discontinuities, opposite to the modified one. Besides, the original function reach their absolute minimum outside the feasible region. Vertical asymptotes in original objective function correspond to positions of the free node for which $\sigma = 0$ for any tetrahedra of the local mesh. As might be expected, the optimal solution for the modified function results in $v(\sqrt{3}/3, 0)$. The original and modified functions are nearly identical in the proximity of this point, see Fig. 2(a).



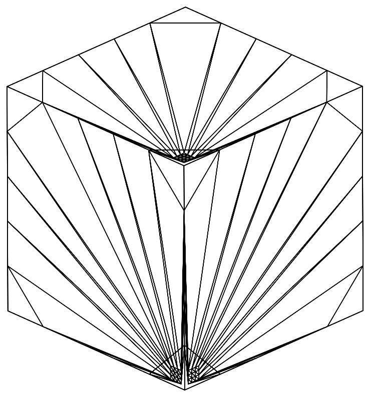
(a) (b)

Fig. 2. (a) Transversal cut of $|K_\eta|_2$ (solid line) and $|K_\eta^*|_2$ (dashed line) for the 2-D test example; (b) the same objective functions for the tangled mesh.

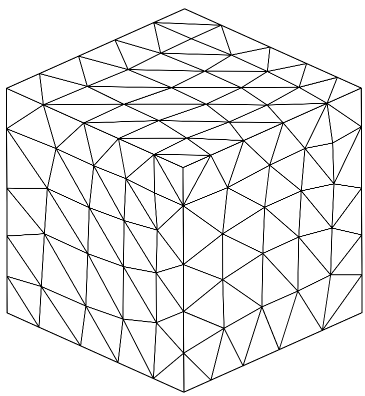
Let us now consider the tangled mesh obtained by changing the position of point $B(\sqrt{3}, 0)$ to $B'(-\sqrt{3}, 0)$. Here, the mesh is constituted by the triangles $vB'C$, vCA and vAB', where $vB'C$ and vAB' are inverted. The feasible region does not exist in this new situation. The graphics of functions $|K_\eta|_2$ and $|K_\eta^*|_2$ are represented in Fig. 2(b). Although the mesh can not be untangled, we get $v(-\sqrt{3}/3, 0)$ as the optimal position of the free node by using our modified objective function. For this position the three triangles are "equally inverted" (same negative values of σ). In this example the same result could be achieved by maximising the minimum value of σ in the mesh, as proposed in [9].

4 Applications

To check the efficiency of the proposed techniques we first consider a regular mesh of a unit cube with 750 tetrahedra, 216 nodes uniformly distributed and a maximum valence of 16. In order to get a tangled test mesh, we transform the unit cube into a greater one $(10 \times 10 \times 10)$ changing the positions of some nodes and preserving their connectivities. The inner nodes remains in their original positions, the nodes sited on the edges of the unit cube are replaced on the edges of new cube and, finally, the interior nodes of each face of the unit cube are projected on the corresponding face of the new cube. The initial tangled mesh, shown in Fig. 3(a), has 10 inverted tetrahedra and an average quality measure of $q_{avg} = 0.384$ (the average quality of the regular mesh is 0.749).



(a)



(b)

Fig. 3. (a) Initial tangled mesh of a cube and (b) the resulting mesh after twenty four steps of the optimisation process.

Besides, approximately the 50% of tetrahedra has a very poor quality (less than 0.04). Here we have chosen the quality measure proposed in [7], $q = \frac{3}{|S_m|\left|S_m^{-1}\right|}$, for valid tetrahedra and $q = 0$ for inverted ones. The result after twenty four sweeps of the mesh optimisation process with $\left|K_\eta^*\right|_2$ is shown in Fig. 3(b). In this case, the steepest descent algorithm was used for the optimisation of the objective

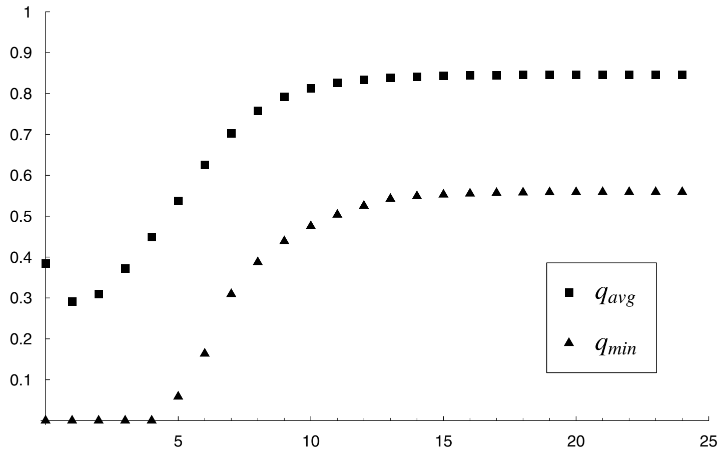
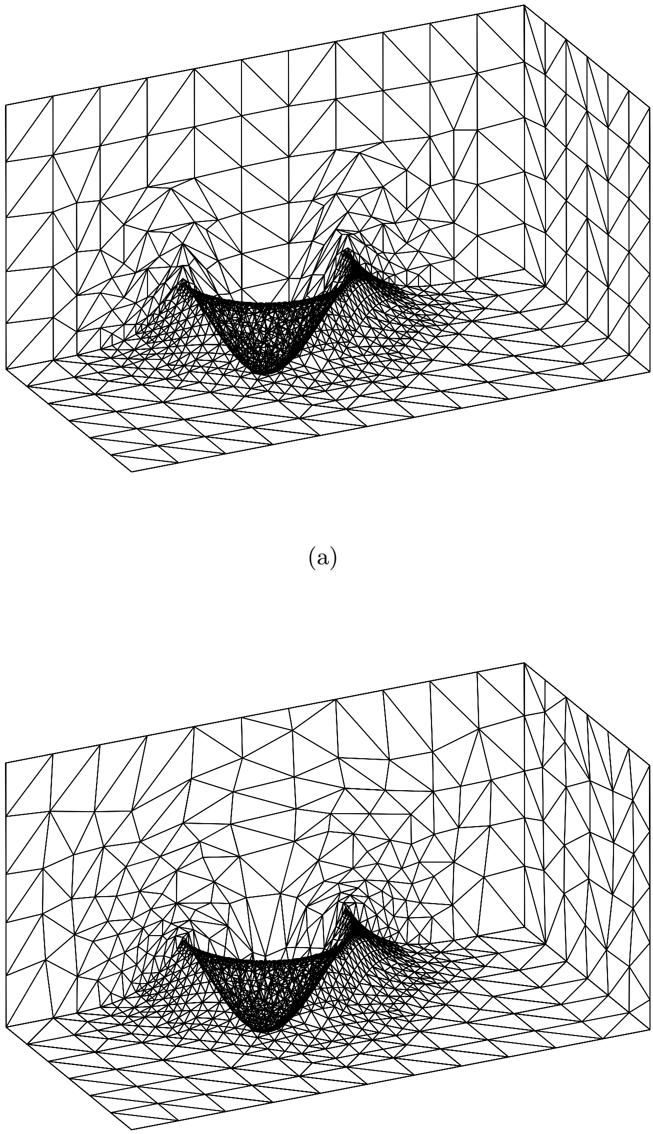


Fig. 4. Values of the average quality q_{avg} and the minimal quality q_{min} in terms of the number of iterations of the mesh optimisation process for the cube test.

function. In Fig. 4 we present the evolution of the average quality measure, q_{avg}, and the minimal quality, q_{min}, in terms of the number of iterations of the mesh optimisation process. Note that the average quality initially decreases because the number of inverted tetrahedra increases in former iterations. The mesh has 22 inverted tetrahedra after the first iteration, 33 after the second, 16 after the third, 11 after the fourth and 0 after the fifth.

We have also used these optimisation techniques to construct 3-D meshes adapted to complex surfaces as those defined by irregular terrains [13] and [14]. A version of the refinement/derefinement algorithm presented in [6] and the 3-D Delaunay triangulation analysed in [5] are implemented in this mesh generator. In the resulting mesh there can be occasional low quality elements, or even inverted elements, thus making it necessary to apply any untangling and smoothing procedure. As application of the mesh generator and the optimisation procedure we have taken under consideration the “volcano” test problem shown in Fig. 5. The meshes have 20038 tetrahedra and 4013 nodes, with a maximum valence of 31. The initial tangled mesh has 576 inverted tetrahedra with an average quality measure $q_{avg} = 0.529$. The node distribution is modified during the optimisation process in such a way that all the inverted elements disappear in the fourth step of this process and the average quality measure increases to $q_{avg} = 0.615$ in the sixth step. We remark that only a few seconds of CPU time on an XEON were necessary to obtain the optimised mesh applying six steps of this latter procedure and using BFGS method [2] to minimise the objective function.



(a)

(b)

Fig. 5. “Volcano” test problem: (a) initial mesh with 576 inverted tetrahedra and (b) resulting valid mesh after six steps of the optimisation process.

5 Conclusions and Future Research

In this paper we present a way to avoid the singularities of common objective functions used to optimise tetrahedral meshes. To do so, we propose a modification of these functions in such a way that it makes them regular all over $\mathbb{R}^3$. Thus, the modified objective functions can be used to smooth and untangle the mesh simultaneously. The regularity shown by the modified objective functions allows the use of standard optimisation algorithms as steepest descent, conjugate gradient, quasi-Newton, etc. In principle, a similar modification could be also applicable to other objective functions having the same behaviour as that studied here. These techniques can be implemented in a parallel algorithm, as reported in [8], in order to reduce the computational time of the process.

We have efficiently used these techniques in the generation of 3-D meshes adapted to complex surfaces [13] and [14], and in other applications [15]. A promising field of study would combine the 3-D refinement/derefinement of nested meshes with node movement, where the ideas presented here could be introduced. Good recent results have been obtained in [16] and [17] using these techniques, for determining the shape and size of the elements in anisotropic problems.

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