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Hexahedral Mesh Untangling *

Patrick M. Knupp

Parallel Computing Sciences Department
Sandia National Laboratories
M/S 0847, P.O. Box 5800
Albuquerque, NM 87185-0847
pknupp@sandia.gov

Abstract

We investigate a well-motivated mesh untangling objective function whose optimization automatically produces non-inverted elements when possible. Examples show the proceedure is highly effective on simplicial meshes and on non-simplicial (e.g., hexahedral) meshes constructed via mapping or sweeping algorithms. The current whisker-weaving (WW) algorithm in CUBIT usually produces hexahedral meshes that are unsuitable for analyses due to inverted elements. The majority of these meshes cannot be untangled using the new objective function. The most likely source of the difficulty is poor mesh topology.

Keywords: mesh untangling, mesh optimization, hexahedral meshing, whisker weaving

1. Introduction

Automatic meshing of complex geometries into unstructured hexahedral elements remains an active area of research. Many algorithms such as sweeping [11], whisker weaving [3], H-Morph [15], and hex-tet plastering [13] have been devised to create hex-dominant meshes. Unfortunately, none of these algorithms guarantees that the resulting mesh will not contain inverted elements that render the mesh unsuitable for computer simulations. When meshes with inverted elements are created some type of user intervention such as geometry decomposition, changing of element sizes, interval counts, or meshing schemes is necessary.

A direct but not always reliable way to fix meshes with inverted elements is to apply smoothing or optimization algorithms. Ideally, such methods would possess a guarantee that the final mesh is non-inverted, even if the initial mesh is inverted. For two-dimensional structured meshes one has such a guarantee using a smoother based on solving the Winslow partial differential equations. Unfortunately, for unstructured hexahedral meshes such a guarantee is presently lacking. A promising approach for achieving a guarantee is mesh optimization of objective functions

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containing barriers [9]. Barrier methods generally require that the initial mesh to be optimized is non-inverted. Thus, what is needed to achieve full automation is an optimization technique which untangles unstructured hexahedral meshes. Automatic smoothing would thus consist of two stages: untangling to remove inverted elements followed by optimization of a barrier objective function to improve element shape [4].

Untangling algorithms can also be used to determine if an untangled mesh exists for a given mesh connectivity. There is no known à priori test to determine if a given mesh can be untangled. A computer 'proof-by-construction' that an untangled mesh exists is offered by mesh untangling optimizers. If an untangled mesh exists for a given mesh connectivity, it is usually non-unique.

The term 'tangled' mesh refers to meshes which contain inverted elements (equivalent terms are 'invalid' or 'folded' meshes). A mesh which contains no inverted elements is called 'untangled', 'valid', or 'unfolded'. Usually, tangled meshes cannot be used for physical analyses because unphysical results will be produced. Tangled meshes rarely occur when simplicial elements are used but are not uncommon when non-simplicial elements are employed in either structured or unstructured meshes.

The definition of an inverted simplicial element is straightforward; it is any element whose volume (with respect to the given node numbering scheme) is non-positive. Definitions for non-simplicial elements are considered in section 3.

A mesh untangling objective function for simplicial meshes was indirectly suggested in reference [2] but was not developed within the framework of mesh optimization. The objective function proposed in this paper uses a similar idea, namely, that the total volume of the ball of elements associated with a mesh node is independent of the position of the node. However, our method applies to both simplicial and non-simplicial meshes and is posed within the framework of mesh optimization.

Recently, another mesh untangling objective function was devised at Sandia National Laboratories during the 1998 summer collaboration between the present author and L. Freitag. The approach has been developed for simplicial meshes by Freitag and Plassman [5]. The objective function maximizes the minimum volume of all elements containing the node to be moved. A series of optimization problems is performed for each interior node of the mesh until node-movement is less than some tolerance. This approach is generally referred to as a **local** optimization problem because the objective function depends on only one node at a time. The 'local' objective function has the nice feature of having convex level sets [5], thus a unique maximum is assured [1]. Unfortunately, there is no guarantee that looping over all the interior nodes in a sequence of local optimizations converges or, if it does, that the final mesh is non-inverted.

In contrast, the method proposed in this paper optimizes a single 'global' objective function that depends on all of the interior nodes simultaneously. All of the nodes are moved at once for each iteration of the optimization proceedure. A single objective function is optimized, thus the value of the objective function can be used to monitor progress during the optimization proceedure. Although we use a global objective function (i.e., one that depends on all of the mesh nodes), we do not attempt to find a global minimum but rather to locate a stationary point.

The present algorithm performs mesh untangling by optimization of an objective function via a node movement procedure involving the interior nodes of the mesh. Mesh topology is fixed. A parameter in the objective function can be used to bound the worst elements of the mesh away from the set of inverted elements. Elements far from the set of inverted elements are left untouched. The objective function is constructed so that its value is non-negative; when the parameter is positive the objective function equals zero if and only if the mesh is untangled.

We show that, *for a single free node*, the proposed objective function is convex. This property ensures that every minimum is a global minimum. Optimization of the single-node objective function always results in an untangled mesh provided such a mesh exists for the given mesh topology. This theoretical property has been checked computationally using both tetrahedral and hexahedral meshes with inverted elements.

2. Tetrahedral Mesh Untangling

Although our main goal is to untangle hexahedral meshes, it is worthwhile to begin with the simpler case of tetrahedral mesh untangling.[1] Let T_m be the m-th tetrahedral element of the mesh ($m = 1, 2, ..., M$), with corresponding volume $\alpha_m/6$. It is well-known that the volume is related to the determinant of a 3×3 matrix [6] and can also be written as a triple product:

$$\alpha_m = (x_m^{(1)} - x_m^{(0)}) \cdot (x_m^{(2)} - x_m^{(0)}) \times (x_m^{(3)} - x_m^{(0)})$$

where $x_m^{(k)}$ is the vector coordinate of the k-th node of the m-th tetrahedral element. Since $\sum_{m=1}^{M} \alpha_m/6$ is the total volume V of the mesh, it must be independent of the positions of the interior nodes of the mesh.[2] It is assumed that the total volume of the mesh is positive, $V > 0$.

[1]The approach to be presented applies equally well to triangles in two-dimensions.

[2]The volume of the geometric object to be meshed is not necessarily the same as the total volume V of the mesh elements due to surface curvature.

Recall that a tetrahedral mesh is untangled if $\alpha_m > 0$ for all m. This suggests the following global objective function for mesh untangling

$$f_0 = \frac{1}{2} \sum_{m=1}^{M} \{ | \alpha_m | - \alpha_m \} .$$

f_0 is non-negative and is one-half the ℓ_1 norm of the vector of $\{\alpha_m\}$'s minus 3 times the volume of the mesh. f_0 is a function of the coordinates of the interior mesh nodes (boundary node positions are assumed to be fixed). The domain of the objective function consists of points in R^{3p}, where p is the number of interior nodes in the mesh. $f_0 = 0$ for any untangled mesh because then $\alpha_m > 0$ for all m. Thus any untangled mesh forms a global minimum of f_0. $f_0 \geq 0$ for any tangled mesh. This can be seen by re-writing the objective function as

$$f_0 = - \sum_{n \in \mathcal{N}_0} \alpha_n \geq 0$$

where $\mathcal{N}_0 = \{n \mid \alpha_n < 0\}$, i.e., sum includes only elements with negative volume.

A defficiency of this objective function is that if its value is zero, it can still contain an inverted element (with zero volume).[3] We can address this defficiency in the following manner. Let $0 < \beta$ be a user parameter and modify the untangle objective function to read

$$\begin{aligned} f_\beta &= \frac{1}{2} \sum_{m=1}^{M} \{ | \alpha_m - 6\beta\bar{V} | - (\alpha_m - 6\beta\bar{V}) \} \\ &= - \sum_{n \in \mathcal{N}_\beta} (\alpha_n - 6\beta\bar{V}) \end{aligned}$$

where $\mathcal{N}_\beta = \{n \mid \alpha_n < 6\beta\bar{V}\}$ and $\bar{V} = V/M$ ($\bar{V}$ is thus the average element volume). The objective function is then globally minimized when the Jacobian determinants are all greater than or equal to $6\beta\bar{V}$. For $\beta > 0$, $f_\beta = 0$ if and only if the mesh is untangled.

[3]In this case $\mathcal{N}_0$ is empty.

Define the *feasible* set $\mathcal{F}_\beta$ to be the set of points in R^{3p} at which $\alpha_m > 6\beta\bar{V}$ for all m. Then $\mathcal{F}_0$ is the set of points for which the mesh is untangled. $\mathcal{F}_\beta$ is a subset of $\mathcal{F}_0$. The feasible region is an open set and its closure $\bar{\mathcal{F}}_\beta$ is the set of points which make the objective function zero.

Let us use the notation $f_\beta^{(p)}$ to denote that the objective function depends on p free interior nodes. The 'local' objective function with one free node is then $f_\beta^{(1)}$.

Figure 1 shows level sets of $f_0^{(1)}$ for a triangular mesh with one free node and five boundary points. Note how the objective function is flat and equals zero in the feasible region; the minimum is non-unique. Figure 2 shows levels sets of $f_\beta^{(1)}$ for the same boundary points, with $\beta = 0.2$. Note how the set on which the objective function is zero has contracted. Figure 3 shows level sets of $f_0^{(1)}$ for boundary points which do not permit an untangled mesh to exist. In this case the feasible region is empty; the value of the objective function inside the smallest contour is a constant (approximately 1). The level sets in Figures 1, 2, and 3 are convex, even though the feasible region may be empty.

Lemma 1
Let $\alpha(x) = (x_1 - x) \cdot [(x_2 - x) \times (x_3 - x)]$ be six times the volume of a tetrahedral element. Then for any scalar λ and any points $x = x_a$, $x = x_b$,

$$\alpha[\lambda x_a + (1-\lambda)x_b] = \lambda\alpha[x_a] + (1-\lambda)\alpha[x_b]$$

i.e., α is a linear function in x.
Proof
Expand the triple product to find that $\alpha(x) = c + x \cdot v$ for some constant c and some constant vector v. §

Proposition 1
The objective function $f_\beta^{(1)}$ is convex and thus

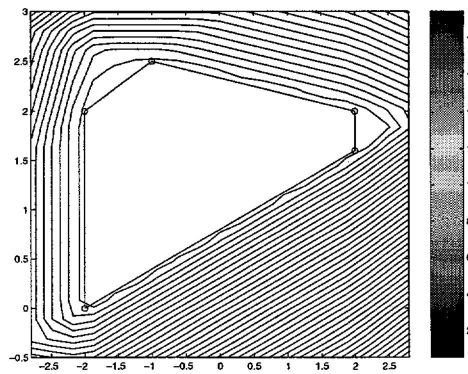

Figure 1: *Level Sets of* $f_0^{(1)}$ *for Triangle Mesh - NonEmpty Feasible Region*

every minimum is a global minimum.
Proof
Let $0 \le \lambda \le 1$. Using the triangle inequality and Lemma 1, one can show

$$f_\beta^{(1)}[\lambda x_a + (1-\lambda)x_b] \le \lambda f_\beta^{(1)}[x_a] + (1-\lambda) f_\beta^{(1)}[x_b]$$

§

For the m-th tetrahedral element, there exists a constant c_m and a vector v_m such that $\alpha_m = c_m + x \cdot v_m$. This leads to

Lemma 2 For $f_\beta^{(1)}$,

$$\sum_{m=1}^{M} v_m = 0$$

Proof
Since $V = \sum_{m=1}^{M} \alpha_m = \sum_{m=1}^{M} c_m + x \cdot v_m$, $\sum_{m=1}^{M} v_m = \partial V / \partial x = 0$. §

Consider the *gradient*, $\nabla f_\beta^{(1)}$, of the objective function $f_\beta^{(1)}$. The gradient exists for any node configuration for which $\alpha_m \neq 6\beta\bar{V}$ for

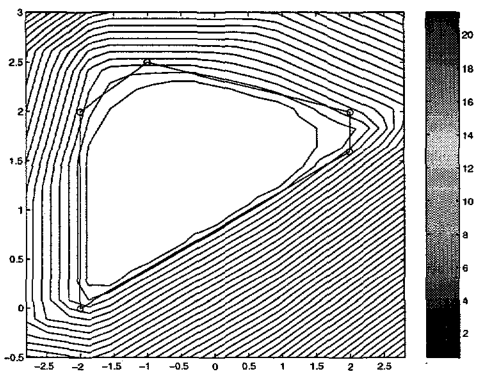

Figure 2: *Level Sets of $f_\beta^{(1)}$ for Triangle Mesh - NonEmpty Feasible Region, $\beta = 0.2$*

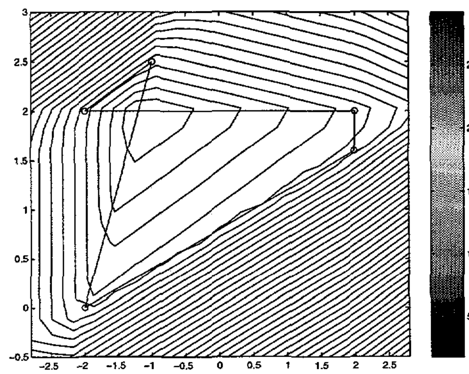

Figure 3: *Level Sets of $f_0^{(1)}$ for Triangle Mesh - Empty Feasible Region*

all m. The gradient does not exist for any node configuration for which there exists m such that $\alpha_m = 6\beta\bar{V}$. We call node configurations of the latter type degenerate. Thus the gradient exists for any tetrahedral mesh with a non-degenerate node configuration. Stationary points are points at which the gradient exists and $\nabla f_\beta^{(1)} = 0$. Because $f_\beta^{(1)} \geq 0$ is convex, any stationary point must be a global minimum. It is easy to show that for non-degenerate configurations

$$\nabla f_\beta^{(1)} = -\sum_{n \in \mathcal{N}_\beta} v_n$$

If $\mathcal{N}_\beta$ is empty for some non-degenerate node configuration, then that node configuration forms a stationary point. Hence, every point in the feasible region is a stationary point. However, every stationary point need not lie in the feasible region because $\sum_{n \in \mathcal{N}_\beta} v_n$ can be zero if the vectors are not linearly independent. This situation occurs when the feasible region is empty. Figure 4 provides an example; the feasible region is empty because β is large. Stationary points exist inside the smallest contour but the value of the objective function there is approximately 5. Note that the stationary points in this example result in an untangled mesh.

Now consider meshes with more than one free node. If there is more than one free node, the global triangle objective function is evidently non-convex. Figure 5 shows a slice through the objective function $f_0^{(3)}$ of a triangle mesh having three free nodes. Two curves are shown giving values of $f_0^{(3)}[(1-\lambda)x_a + \lambda x_b]$ and $(1-\lambda) f_0^{(3)}[x_a] + \lambda f_0^{(3)}[x_b]$ vs. λ where x_a and x_b are two configurations of the free nodes. The first curve should lie below the straight line given by the second curve if the objective function were convex. It is near-certain that the global tetrahedral objective function is also non-conex since there is no fundamental difference between the triangular and tetrahedral objective functions.

To minimize the objective function we implemented a Polack-Ribiere conjugate gradient algorithm and line search based on the discussion in [14]. The algorithm was tailored to the mesh generation setting (optimization of

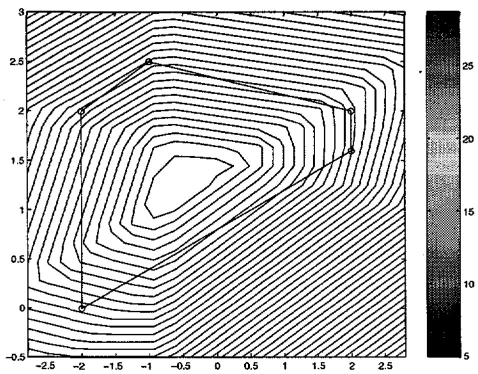

Figure 4: *Level Sets of $f_\beta^{(1)}$ for Triangle Mesh - Empty Feasible Region, $\beta = 1$*

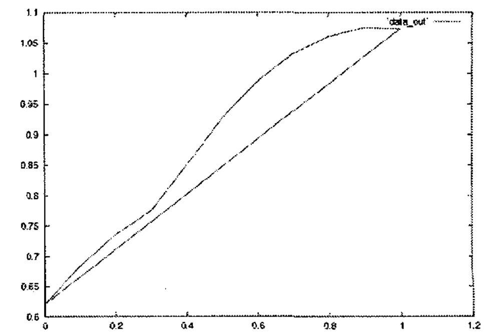

Figure 5: *Slice through $f_0^{(3)}$ vs. λ for Triangle Mesh Showing Non-convexity*

3p unknowns) and to the data structures of CUBIT. We compute the gradient of the objective function numerically. Technically, since the untangling objective function is continuous but non-differentible at certain locations in the nodal coordinate domain, the gradient does not exist everywhere. Our line search proceedure ensures that the optimization halts if the minimum occurs at a non-differentiable point. If a non-differentiable point is encountered elsewhere this delays but does not prevent convergence to the minimum.

The untangling algorithm presented in this section was tried successfully on tetrahedral meshes like those given in Figure 6 and in Figure 3 of [4]. Since the meshes were untangled to begin with, we invoked CUBIT's 'randomize' algorithm which perturbs node locations randomly to create non-smooth, possibly inverted meshes for testing of smoothing and optimization schemes such as untangling. The optimal meshes resulting from the untangling algorithm were non-inverted *regardless of the starting point.* This is unexpected in light of the fact that the objective function is non-convex, yet one must keep in mind that lack of convexity does not necessarily preclude the possibility that all minimae are global minimae. Further work is needed to resolve this question. From a practical standpoint, the untangler works often enough to make it a useful tool.

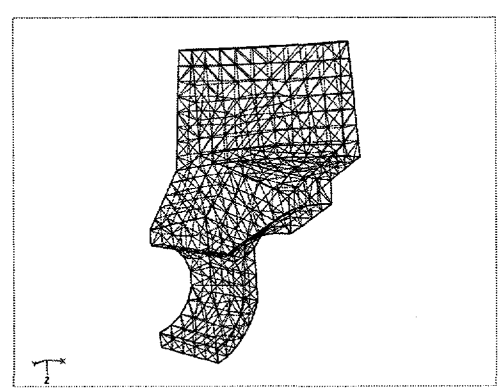

Figure 6: *Tetrahedral Mesh on Hook Geometry*

3. Hexahedral Mesh Untangling

For non-simplicial elements, the definition of an inverted element is less straightforward. For an arbitary quadrilateral or hexahedral element one generally makes use in finite elements of a mapping from a uniform master element to the given physical element. The determinant of the Jacobian of the mapping measures the local volume at any point of the element. Several definitions are possible: an element could be considered inverted if (a) the integral of the local volume over the element is non-positive, (b) it has a non-positive local volume at any of its Gaussian integration points, (c) it has a non-positive local volume at any of its corners, or (d) it has a non-positive local volume at some other point or points inside the element. Because we desire to use untangling as a pre-processor to optimization of a barrier-based shape metric, the definition of inverted must also permit good element shape. Thus, for example, if one adopts (b) as the definition of an inverted element, then untangling will produce elements with positive volume at the gauss points, but not necessarily at the element corners. The barrier-based shape objective function would then only guarantee that the shape-optimized mesh is non-inverted at the element gauss points. In our experience, positive volume at the element corners is a necessary, but not at all sufficient condition for achieving well-shaped hexahedral elements. We thus we adopt (c) as the definition of an inverted non-simplicial element. We note in passing that quadrilateral elements that are non-inverted according to definition (c) are non-inverted according to definitions (a) and (b). Hexahedral elements that are non-inverted according to definition (c) almost always are non-inverted according to definition (b). In rare cases a hexahedral element may be non-inverted according to (c), but inverted according to (b) (see [12]).

Given definition (c) for an inverted non-simplicial element we define for each hexahedral element H_m, eight volumes $\alpha_{k,m}$, $k = 1, 2, ..., 8$, which correspond to the triple products derived from three edge vectors emanating from the k-th node of the m-th hex.[4] Then our untangling objective function is

$$f_\beta = \frac{1}{2} \sum_{m=1}^{M} \sum_{k=1}^{8} \{ \mid \alpha_{k,m} - \beta \bar{V} \mid - (\alpha_{k,m} - \beta \bar{V}) \}$$

At the global minimum the mesh satisfies $\alpha_{k,m} \geq \beta \bar{V} > 0$. The comments in the previous section analyzing the tetrahedral objective function apply also to the hexahedral objective function.

Level sets for the objective function with a single free node attached to quadrilateral elements are shown in Figures 7 and 8. Much the same behavior is observed: there is still a flat region containing the minimizing points. If the mesh cannot be untangled, the objective function is non-zero in the flat region. The open circles in figures 3 and 4 denote boundary nodes that are adjacent to the free node while crosses denote boundary nodes that are opposite to the free node. Thus it is evident in Figure 8 that an untangled mesh cannot be created due to the boundary point configuration. The level sets are convex. The proof of this fact goes much like the tetrahedral case: the only difference is that in the quadrilateral case the free node is attached to 3 'triangles' per element instead of just one (and four in the hexahedral case). Though no example was sought, it is believed that the objective function with $p > 1$ free nodes is non-convex.

Results with this objective function for quadrilateral meshes was investigated in [7] and in [10]. We turn here to the untangling of 3D hexahedral meshes. The untangler readily untangled CUBIT mapped, submapped, and

[4] For quadrilateral elements, $\sum_{m=1}^{M} \sum_{k=1}^{4} \alpha_{m,k} = 4V$, while for hexahedral elements there is no simple relationship unless all the elements are parallelopipeds.

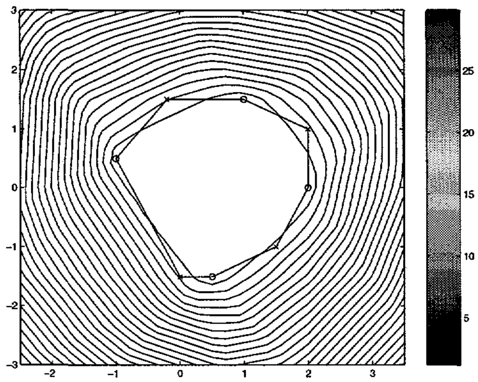

Figure 7: *Level Sets of* $f_0^{(1)}$ *for Quadrilateral Mesh - Non-Empty Feasible Region*

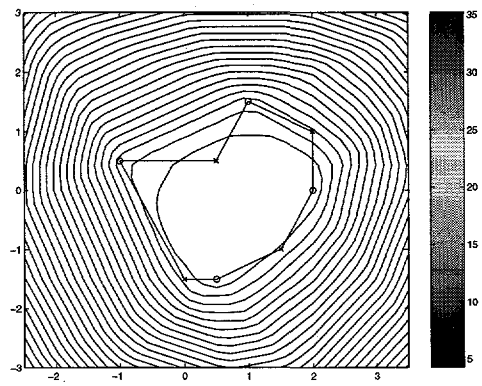

Figure 8: *Level Sets of* $f_0^{(1)}$ *for Quadrilateral Mesh - Empty Feasible Region*

swept meshes where it was clear that an untangled mesh existed. Figures 9 and 10 illustrate the success of the untangler on a hexahedral mesh; the mesh was successfully untangled using a variety of initially tangled meshes. On other geometries, a few badly tangled swept meshes were not successfully untangled, but it was not known if an untangled mesh existed in these cases. The method was also tried with success on the CUBIT HexTet algorithm with Geode transistion elements [13].

A major disappointment was the inability of the untangler to eliminate inverted elements in many CUBIT Whisker-Weaved meshes. Weaving generates connectivity for all-hexahedral meshes given arbitrary quadrilateral surface meshes, but often fails to generate a mesh with positive Jacobians at the element corners [3]. Although the untangler often improved the minimum scaled-Jacobians of weaved meshes from -0.90 to -0.010, there were cases where little improvement could be made. For example, the minimimum scaled jacobian for a whisker-weaved mesh of the 'hook' geometry of Figure 6 was -0.93; the untangler could only improve this to -0.8. A variety of initial meshes was created from the whisker-weaved mesh of the hook by randomizing the node locations. None of these initial starting points permitted the untangler to succeed. We also tried various schemes involving the choice of the parameter β; for example, an increasing sequence of values of β starting from -1.0 and a decreasing sequence of values starting from +1.0. Visual inspection of some of the whisker-weaved meshes gave the impression that an untangled mesh did not exist. Because of the success of the untangler in untangling meshes generated by methods other than weaving, and the fact that untangle consistently fails on a wide variety of weaved meshes, we conclude that the difficulty lies with the mesh connectivities generated by the current CUBIT weaving algorithm. Since there is no à priori test for whether or not a mesh can be untangled, there is at present no way to conclusively settle the question of existence of an untangled mesh for the weave examples tried.

In conclusion, we have shown that a

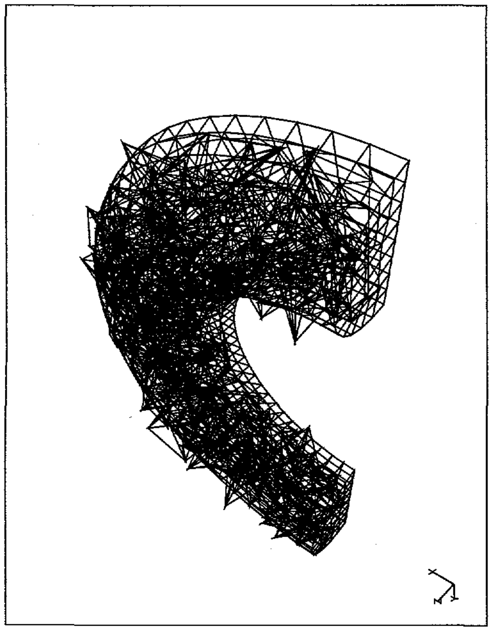

Figure 9: *Hexahedral Mesh on Half-Torus Geometry - Before Untangle*

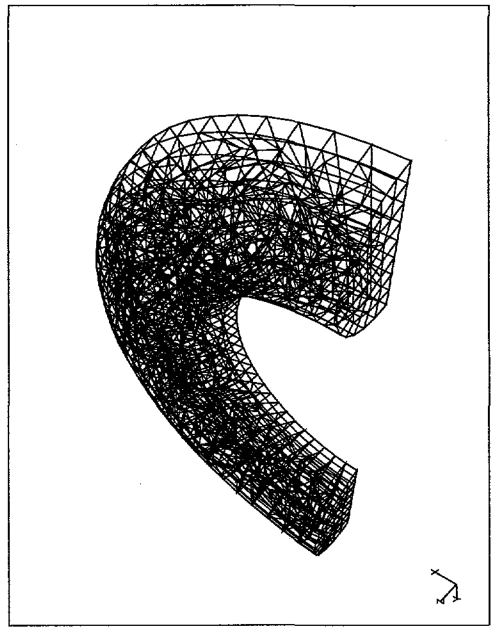

Figure 10: *Hexahedral Mesh on Half-Torus Geometry - After Untangle*

global, well-motivated mesh untangling objective function exists that can be used to automatically untangle 3D meshes. The objective function is convex for a single free node, but non-convex in general. In spite of this, we are able to untangle a wide variety of tetrahedral and hexahedral meshes, except those created by the whisker-weaving algorithm. The untangler has been used effectively on Swept meshes as a pre-processor to mesh smoothing via shape optimization.

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