Investigation of a Mesh Criterion for Three-Dimensional Finite Element Diffusion Simulation

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Abstract

Three simple mesh examples are presented to show that neither Delaunay nor strictly non-obtuse mesh elements are required for a finite element diffusion computation. Mesh requirements based on a recently found condition are investigated to guarantee certain properties of the resulting stiffness matrix. The experiments are conducted using the general purpose solver AMIGOS.

1. Mesh Requirements

Certain conditions for the stiffness matrix of the Laplace operator are required during finite element diffusion simulation. We present three examples of a mesh to show the different scope of the Delaunay criterion and a newly introduced finite element mesh criterion by [2]. Our presented examples prove that the Delaunay criterion is *neither sufficient nor necessary* to fulfill the requirements. This is important insight and complements previous research [3]. It is also shown that a strict adherence to a sole non-obtuse angle criterion is not necessary.

Finite element (FE) mesh criterion: Let $e_{i,j}$ be an edge with n adjacent tetrahedra t_k . For each t_k two planes exist which do not contain $e_{i,j}$ and which span a dihedral angle Θ_k . The two planes share an edge with length l_k . The sum over $k = 1 \dots n$ of the cotangens of Θ_k weighted by l_k must be greater or equal than zero.

 $\sum_{k=1}^{n} l_k \cot \theta_k \ge 0$

Figure 1 depicts an example where this criterion is violated for the interior edge $e_{i,j}$. Four adjacent tetrahedra exist of which two span a 90° angle. Hence, $\cot \Theta_3 = 0$ and $\cot \Theta_4 = 0$. As one can see from the figure $\cot \Theta_1 = \cot \Theta_2 = -\frac{1}{\sqrt{2}} (\Theta_1, \Theta_2 \text{ are obtuse}, \sim 125.3^\circ)$ and hence the total sum is negative.

The two-dimensional empty-circumcircle Delaunay criterion is equivalent to the requirement that the sum of the two opposite angles of an adjacent pair of triangles is equal or smaller than 180°. While in two dimensions the FE criterion is equivalent to the Delaunay criterion, it evolves to an entirely different criterion in three dimensions. The Delaunay triangulation is known to maximize the minimum angle in two

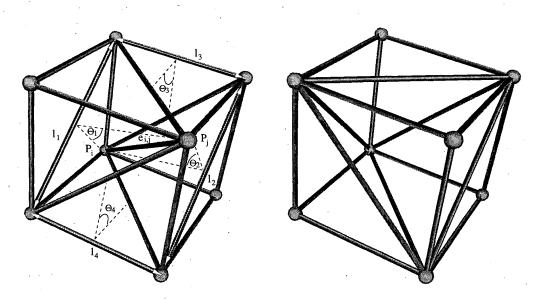


Figure 1: T_6 tessellation and FE criterion Figure 2: T_5 tessellation, no obtuse dihefor edge $e_{i,j}$.

dimensions [4]. This is not valid in three dimensions with respect to the dihedral angles. It rather minimizes the largest minimum-containment sphere [4]. This is also related to the fact that in three dimensions Delaunay slivers exist which do not have a two-dimensional anology. A Delaunay sliver contains obtuse dihedral angles but does not expose an extreme ratio between its edge lengths. The above mentioned FE criterion on the other hand is applied to dihedral angles in three dimensions.

2. Examples

The examples are (i) a Delaunay mesh which is not suitable as a finite element mesh for diffusion applications, (ii) a Delaunay mesh which is suitable, and (iii) a non-Delaunay mesh with obtuse dihedral angles which is still suitable as a finite element mesh. The examples were constructed by exploiting an ortho-product point distribution. A cube defined by eight points can be tetrahedralized into two qualitatively different ways.

 T_6 tessellation: A cube is composed of six tetrahedra (Fig. 1).

 T_5 tessellation: A cube is composed of five tetrahedra (Fig. 2).

For comparison purposes we used a specific tessellation T_6 which contains sliver elements with obtuse dihedral angles. The tessellation T_5 on the other hand does not contain such elements. (Note that there are also T_6 tessellations possible which do not contain obtuse angles.)

The key idea is that all elements of both tessellations fulfill the empty-circumsphere Delaunay criterion, because all points lie on the perimeter of a single sphere. Hence, both meshes satisfy the Delaunay criterion and yet only one satisfies the FE criterion. The two fundamentally different meshes based on an *identical* point cloud are depicted in Fig. 4 and Fig. 5. The mesh which fulfills the FE criterion (Fig. 2, Fig. 5) indeed succeeds to yield the required entries in the stiffness matrix as could be tested by diffusion simulation using AMIGOS [1]. The most important fact however

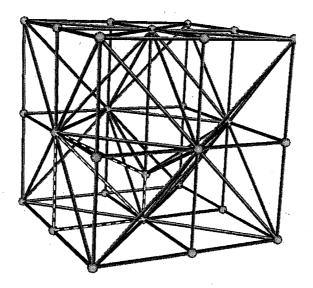


Figure 3: T_5 type tessellation with a shifted point.

is shown by the third example. Further exploiting the ortho-product point set and its type T_5 tessellation with slightly shifted points in certain locations results in a non-Delaunay mesh which still satisfies the *FE* criterion. Figure 3 shows an instance of the mesh consisting of eight cubes. The point in the middle has been shifted. The Delaunay criterion is violated, because the circumspheres of several unchanged tetrahedra contain the shifted point in its interior. Two non-Delaunay triangles are indicated in Fig. 3. Still, the simulation using AMIGOS for the entire mesh (Fig. 6) shows, that the requirements for the stiffness matrix are fulfilled. The shifting of a point introduces obtuse dihedral angles and positive contributions to off-diagonal elements of the stiffness matrix. However, in total due to the sum of the entries of the adjacent elements, the *FE* criterion is satisfied and the stiffness matrix remains correct.

3. Conclusion

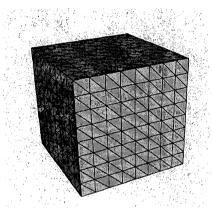
The investigated mesh requirements which depend on the employed discretization scheme, lead to the conclusion that in two dimensions Delaunay meshes are in all cases preferable. In three dimensions Delaunay meshes are neither sufficient nor necessary for a finite element simulation. In fact a non-Delaunay mesh with obtuse angles could be constructed for a successful finite element computation. Existing meshing techniques often try to avoid any obtuse dihedral angles. This is not necessary if techniques can be developed to generate finite element meshes which directly satisfy the FE criterion.

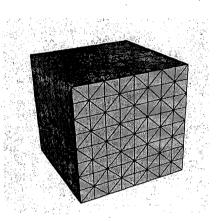
4. Acknowledgment

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References

- [1] M. Radi, E. Leitner, E. Hollensteiner, and S. Selberherr, "AMIGOS: Analytical Model Interface & General Object-Oriented Solver," in Simulation of Semiconductor Processes and Devices, pp. 331-334, 1997.
- [2] J. Xu and L. Zikatanov, "A Monotone Finite Element Scheme for Convection-Diffusion Equations." to be published in Mathematics of Computation.
- [3] F. Letniowski, "Three-Dimensional Delaunay Triangulations for Finite Element Approximations to a Second-Order Diffusion Operator," SIAM J.Sci.Stat.Comput., vol. 13, no. 3, pp. 765-770, 1992.
- [4] M. Bern and D. Eppstein, "Mesh Generation and Optimal Triangulation," in Computing in Euclidean Geometry (F. Hwang and D.-Z. Du, eds.), World Scientific, 1992.





hedra.

Figure 4: Delaunay mesh (T_6) , 3072 tetra- Figure 5: Delaunay mesh (T_5) , 2560 tetrahedra.

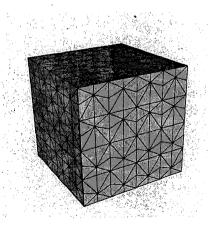


Figure 6: Non-Delaunay mesh, 2560 tetrahedra.