Simple Mesh Examples to Illustrate Specific Finite Element Mesh Requirements

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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 computation. Mesh requirements based on a recent condition given in literature are investigated to guarantee certain properties of the resulting stiffness matrix. The experiments are conducted using a general finite element and finite volume solver.

Keywords. Delaunay, finite element mesh, finite volume mesh, non-obtuse mesh elements, M-matrix.

1 Introduction

Two important discretization methods are the finite volume and the finite element method. Each method imposes certain requirements on the mesh. For the finite volume method Delaunay meshes are usually employed to utilize the Voronoi boxes as control volumes [1]. For the finite element method geometrical quality criteria suffice for most applications. However, strictly speaking further principles need to be investigated. This is especially important for transient simulations as for example diffusion problems.

2 Requirements for Finite Element Meshes

Well pronounced requirements can be formulated for a specific application of the finite element method. The basis is the *maximum principle* which is the most important property of solutions to convection-diffusion equations. In its simplest form it states that both the maximum and the minimum concentrations occur on the boundary or at the initial time. This implies that if the boundary and initial values are positive, the solution must be positive everywhere and concentrations may never reach negative values. It is desirable that the employed discretization also satisfies a maximum principle. As is well known, this is guaranteed, if the system matrix resulting from the discretization is an M-matrix[1] [2][4].
The system matrix $\mathbf{K}$ for a simple diffusion with a standard Galerkin weighted residual approach, linear elements, and backward Euler time discretization has the following form

$$\mathbf{K} = \frac{1}{\Delta t}\mathbf{M} + D\mathbf{S} \tag{1}$$

where $\mathbf{M}$ denotes the mass matrix, $\mathbf{S}$ is the stiffness matrix, and D is the diffusion constant. $\mathbf{K}$ becomes an M-matrix if the mass matrix is lumped and $\mathbf{S}$ is an M-matrix. Since $\mathbf{S}$ only depends on the mesh this condition translates to a constraint on the mesh. The

[1] A real, nonsingular $n \times n$ matrix A where $a_{i,j} \leq 0 \;\forall\; i \neq j$ and $A^{-1} > 0$.

off-diagonal entries $s_{ij}, i \neq j$ of **S** must not be positive. These coefficients can be generally expressed as

$$s_{ij} = \sum_{elements} \int_e \nabla N_i \cdot \nabla N_j \, dA \qquad (2)$$

where N_i, N_j denote the basis functions and A is the area (volume) of element e. The in-product $(\nabla N_i \cdot \nabla N_j)$ has a simple geometrical meaning and leads to an angle criterion for each edge in the mesh, which was recently introduced by [6]. It is an important consideration in three-dimensional finite element mesh generation for diffusion applications with a high concentration gradient.

Criterion 1 (sum of dihedral angles) *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 $k = 1 \ldots n$ of the cotangens of θ_k weighted by l_k must be greater or equal than zero.*

$$\sum_{k=1}^{n} l_k \cot \theta_k \geq 0 \qquad (3)$$

Fig. 2 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 $\cot \theta_1 = \cot \theta_2 = -\frac{1}{\sqrt{2}}$ (θ_1, θ_2 are obtuse, $\sim 125.3°$) and hence the total sum is negative.
In two dimensions (3) can be written as

$$\cot \theta_1 + \cot \theta_2 \geq 0 \qquad (4)$$

where θ_1 and θ_2 are the angles of two triangles sharing a common edge $e_{i,j}$ as shown in Fig. 1. It can be assumed that

$$0 < \theta_{1,2} < 180° \qquad (5)$$

and therefore

$$\sin \theta_1 \sin \theta_2 > 0 \qquad (6)$$

Hence, multiplying (4) with $\sin \theta_1 \sin \theta_2$ results in

$$\sin \theta_2 \cos \theta_1 + \sin \theta_1 \cos \theta_2 \geq 0 \qquad (7)$$

which is equivalent to

$$\sin(\theta_1 + \theta_2) \geq 0 \qquad (8)$$

Due to (5) and (8) the finite element mesh criterion (Crit. 1) can be expressed in two dimensions as

$$\theta_1 + \theta_2 \leq 180° \qquad (9)$$

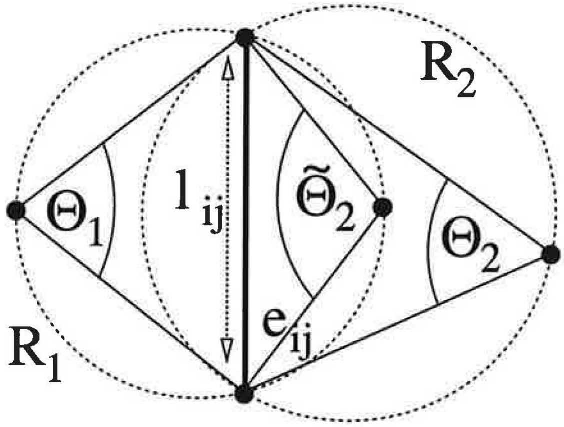

Figure 1: Finite element mesh criterion for two dimensions.

In two dimensions (10) describes the relation between the circumcircle radius, the edge length, and the opposite angle in a triangle.

$$\sin \theta_i = \frac{l_i}{2R} \qquad (10)$$

In three dimensions a relation for the circumsphere radius, the edge length, and the opposite dihedral angle θ_k (which is important for Crit. 1) in a tetrahedron does not exist as illustrated in Fig. 3. This leads to a very interesting conclusion. It can be shown due to the existing relation (10) that the finite element mesh requirement (Crit. 1) is in two dimensions identical to the finite volume mesh requirement which is based on the empty circumcircles Delaunay criterion. To see this equivalence of the angle condition (9) and the Delaunay criterion dependent on (10) consider the extreme case where (9) becomes

$$\theta_1 + \theta_2 = 180° \qquad (11)$$

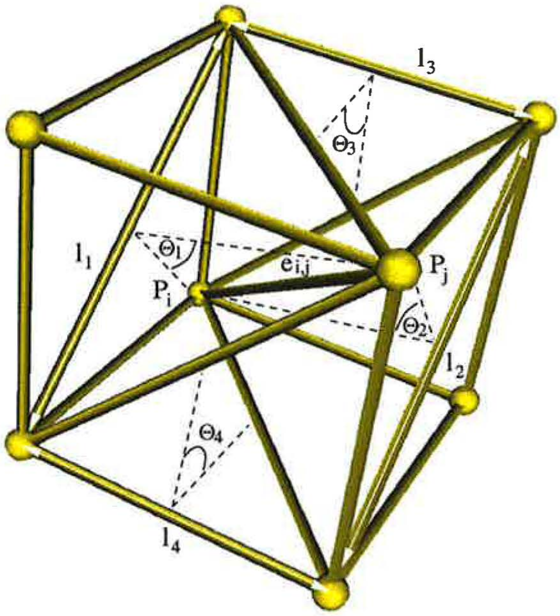

Figure 2: T_6 tessellation and Crit. 1.

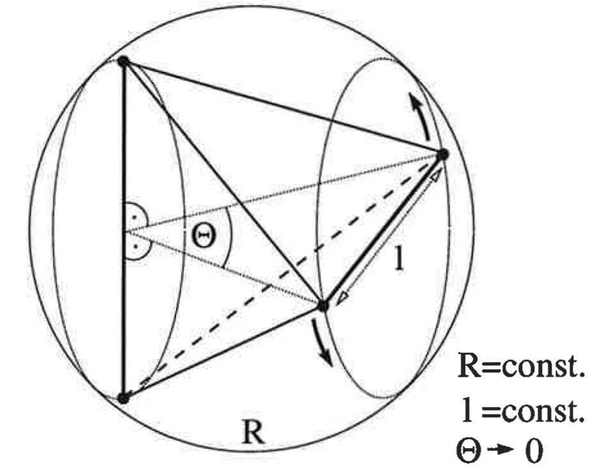

Figure 3: With constant edge length and circumsphere radius the opposite dihedral angle in a tetrahedron can have arbitrary values.

It follows that

$$\sin\theta_1 = \sin\theta_2 \tag{12}$$

and furthermore with Equation 10

$$\frac{l_{ij}}{2R_1} = \frac{l_{ij}}{2R_2} \tag{13}$$

The two triangles with the common edge $e_{i,j}$ (Fig. 1) must possess circumcircles with equally sized radii. Because of (11) the circumcircles must be in fact identical. Each circumcircle passes therefore through all four vertices of the two triangles and the Delaunay criterion is "just" fulfilled. With a decreasing sum $(\theta_1 + \theta_2)$ the distance between the two circumcenters (centers of the circumcircles) increases and the Delaunay criterion is definitely satisfied.
As expected, in two dimensions the finite volume and the finite element method lead to the same discretization with identical requirements. They both rely on Delaunay meshes to fulfill the maximum principle. For other finite element applications than diffusion, like stationary problems or problems with less high gradients, the use of Delaunay meshes can often be omitted. In three dimensions Crit. 1 and the Delaunay criterion are of quite different nature as will be shown with simple examples in the next section. In practice finite element mesh generators may generally try to avoid extremely obtuse (dihedral) angles and badly shaped elements without too much concern on the Delaunay property and without a technique to directly enforce Crit. 1. Such a technique remains open to further research.

3 Simple, Distinctive Mesh Examples

The pure diffusion equation is solved with the finite element and the finite volume method using AMIGOS [5]. This allows the comparison of the solutions on identical meshes with the same linear solver. A Gaussian profile is used as the initial distribution. In two dimensions correct and identical results are obtained with both methods on Delaunay meshes. In three dimensions the finite volume method still achieves qualitatively correct results on a Delaunay mesh as expected. However, the finite element method fails on the same three-dimensional Delaunay mesh. Even for such a simple test problem the finite element solution strongly violates the maximum principle. The resulting concentration reaches negative values in some areas. These areas spread out in time and the absolute value of the emerging negative concentrations is much larger than the minimal initial concentration. The relative error between the solutions of the two methods oscillates strongly and is large in regions where the concentration is negative. These negative concentrations are particularly annoying for diffusion applications in semiconductor process simulation where the concentration varies many orders of a magnitude within a small area. For a more complicated transient problem like the pair diffusion model the negative concentrations lead to severe instabilities.

The aim of this section is to investigate the observed effects in terms of mesh requirements and to construct simple mesh examples where the finite element method can be applied successfully to the diffusion problem.

Mesh Example 1: A Delaunay mesh which is not suitable as a finite element mesh for diffusion applications.

Mesh Example 2: A Delaunay mesh which is suitable for finite element diffusion simulation.

Mesh Example 3: A non-Delaunay mesh with obtuse dihedral angles which is still suitable as a finite element mesh.

The three presented meshes illustrate the different scope of the Delaunay criterion and Crit. 1. They prove that in three dimensions the Delaunay criterion is *neither sufficient nor necessary* to obtain a correct finite element mesh for diffusion so that the maximum principle is fulfilled. The examples also show that a strict adherence to a sole non-obtuse angle criterion is not necessary. This important insight complements previous research [3] where one example, a Delaunay mesh insufficient for such applications, was given.

The examples were constructed by exploiting an ortho-product point distribution. A cube defined by eight points can be tetrahedralized in two qualitatively different ways.

T_6 **Tessellation:** A cube is composed of six tetrahedra (Fig. 2).

T_5 **Tessellation:** A cube is composed of five tetrahedra (Fig. 4).

For comparison purposes a specific tessellation T_6 is used which contains sliver elements with obtuse dihedral angles. The tessellation T_5 on the other hand does not contain such elements. Note that also T_6 tessellations exist which do not contain obtuse angles. The Delaunay Triangulation is known to maximize the minimum angle in two dimensions only. However, in three dimensions Delaunay slivers may exist. 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. On the other hand Fig. 2 clearly shows that the finite element mesh requirement (Crit. 1) is not met by the chosen T_6 tessellation. It is only met by the T_5 tessellation, because of the total absence of obtuse dihedral angles.

Suitable meshes for simulation are then built by stacking a large number of such tessellated cubes. The typical characteristics of each tessellation type are thereby conserved. Hence, both meshes are global Delaunay meshes and yet only one satisfies Crit. 1. The two fundamentally different meshes based on an *identical* ortho-product point cloud are depicted in Fig. 5 and Fig. 6. The finite element simulation on the T_6 type Delaunay mesh results in negative concentrations as was previously pointed out. The T_5 type Delaunay mesh which fulfills Crit. 1 indeed succeeds to yield the required entries in the stiffness matrix and the concentrations remain positive at all times during the transient simulation.

The most important fact however is shown by the third example. Further exploiting the ortho-product point set and its T_5 type tessellation with slightly shifted points in certain locations results in a *non-Delaunay* mesh which still satisfies Crit. 1. Fig. 7 shows an instance of the mesh consisting of eight cubes. The point in the middle has been shifted. The Delaunay criterion must be violated, because the cir-

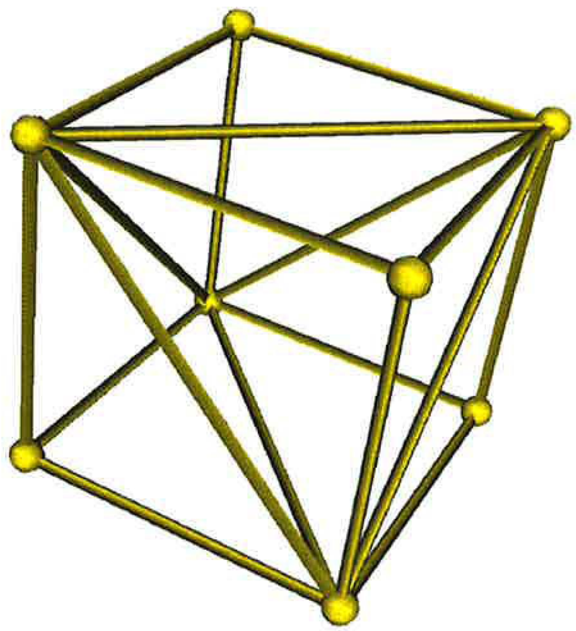

Figure 4: T_5 tessellation, no obtuse dihedral angles.

cumspheres of several unmodified tetrahedra contain the shifted point in its interior.
The simulation using AMIGOS for the entire mesh (Fig. 8) shows, that the requirements for the stiffness matrix are fulfilled. Again, the concentrations do not reach negative values at any time. 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, Crit. 1 is satisfied and the stiffness matrix remains an M-matrix.

4 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 satisfy Crit. 1.

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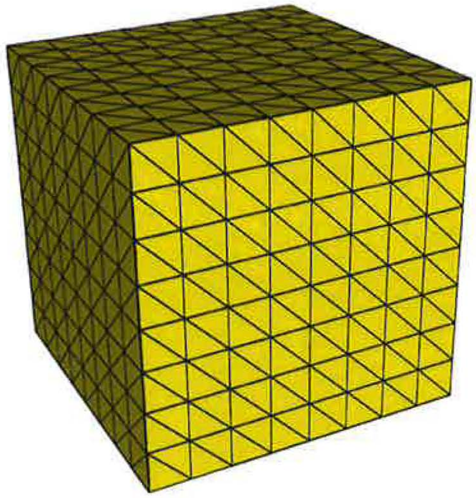

Figure 5: Delaunay mesh (T_6), 3072 tetrahedra.

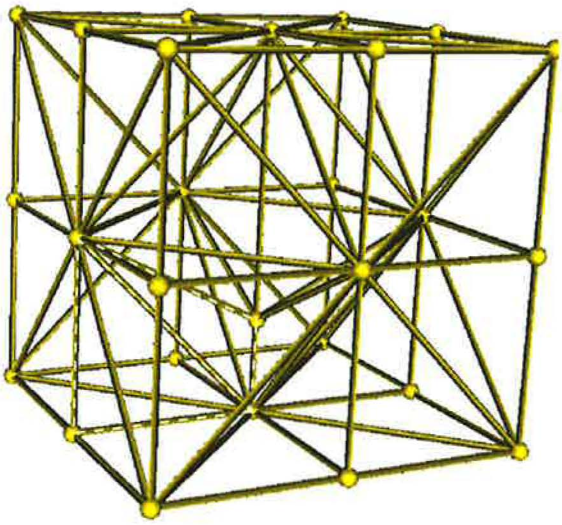

Figure 7: T_5 type tessellation with a shifted point.

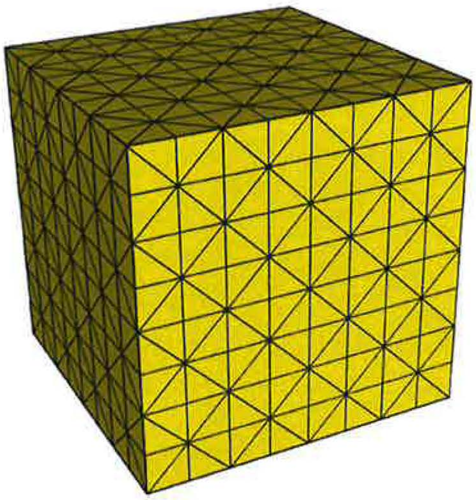

Figure 6: Delaunay mesh (T_5), 2560 tetrahedra.

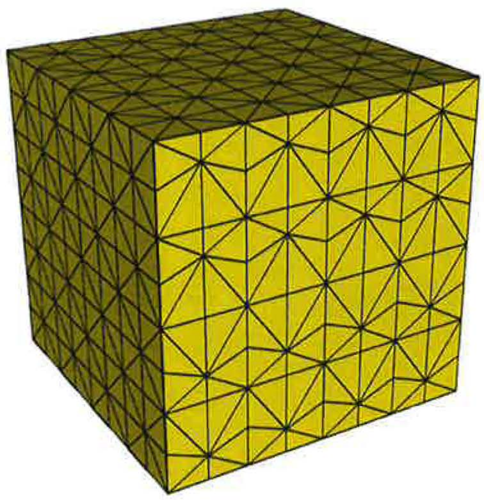

Figure 8: Non-Delaunay mesh, 2560 tetrahedra.