On the Interplay Between Meshing and Discretization in Three-Dimensional Diffusion Simulation

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***Abstract*—The maximum principle is the most important property of solutions to diffusion equations. Violation of the maximum principle by the applied discretization scheme is the cause for severe numerical instabilities: the emergence of negative concentrations and, in the nonlinear case, the deterioration of the convergence of the Newton iteration. We compare finite volumes (FV) and finite elements (FE) in three dimensions with respect to the constraints they impose on the mesh to achieve a discrete maximum principle. Distinctive mesh examples and simulations are presented to clarify the mutual relationship of the resulting constraints: Delaunay meshes guarantee a maximum principle for FV, while the recently introduced dihedral angle criterion is the natural constraint for FE. By constructing a mesh which fulfills the dihedral angle criterion but is not Delaunay we illustrate the different scope of both criteria. Due to the lack of meshing strategies tuned for the dihedral angle criterion we argue for the use of FV schemes in three-dimensional diffusion modeling.**

***Index Terms*—Delaunay, diffusion, dihedral angle criterion, finite element, finite volume, M-matrix, maximum principle, meshing, positive transmissibility, negative concentration.**

I. Motivation

CONTINUUM-based diffusion and dopant activation models are among the dominant tools used to investigate and understand integrated circuit process development.

A major part of model development and simulation are still done in one and two dimensions. This is due to metrological reasons and the enormous numerical costs for a complex three-dimensional (3-D) model. Besides this, an additional factor makes simulation in three dimensions very difficult, namely strong constraints on meshing. The purpose of our article is a fundamental one: To clarify the nature of the proper constraints on the mesh which will ensure a good quality of the solution.

II. Diffusion

The well-known model equation for diffusion is

$$\frac{\partial C}{\partial t} = \nabla \cdot D \nabla C \tag{1}$$

where C denotes the concentration and D is called diffusion coefficient or diffusivity.

In general, the diffusion models used in semiconductor process simulation are strongly nonlinear because the diffusion coefficients depend, e.g., on the impurity and point defect concentrations. These dependences also couple the equations for multiple impurities and point defects. Additionally, more complex models include chemical reactions and contain convection terms.

The actual physical diffusion mechanisms in semiconductor manufacturing processes are a topic of active research (see [1] for a special example or [2, Chapter on "Modeling and Simulation"], for wishful thinking). As a basis there is the entropy principle, universally valid for any assumed physical model: The flow must always go from regions of high concentrations to regions where the concentration is low. Evolving in time, the concentration must smooth out to an equilibrium distribution. It is desirable that the simulation mirrors this physical behavior. However, this is far from being a trivial task.

III. Physical Soundness

A. The Maximum Principle

In the case of diffusion, physical soundness of the solution finds its concise expression in the maximum principle for parabolic differential operators.

Let D denote a finite open domain in $\mathbb{R}^m$ with smooth boundary $\partial D, \bar{D}$ its closure. Let $D_T = (0,T] \times D, S_T = (0,T] \times \partial D$ for each $T > 0$. Let $C^0(\overline{D_T})$ denote the set of all functions continuous on $\overline{D_T}, C^{1,2}(D_T)$ the set of all functions which are once continuously differentiable in t and twice continuously differentiable in x for all $(t,x) \in D_T$.

Then, the maximum principle for parabolic differential operators can be stated as follows [3], [4]: Let u be a nonconstant function

$$u \in C^{1,2}(D_T) \cap C^0(\overline{D_T}) \tag{2}$$

which satisfies

$$\frac{\partial u}{\partial t} - Lu \leq 0 \quad \text{in } D_T \tag{3}$$

where L is a uniformly elliptic operator with bounded coefficients (e.g., the Laplace operator). Then, u can attain its maximum only for $t = 0$ or on the boundary ∂D of D. Furthermore, if u attains its maximum m at some point (t_m, x_m) of S_T then

$$\frac{\partial u}{\partial \nu}(t_m, x_m) > 0 \tag{4}$$

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where $\partial/\partial\nu$ denotes the outward normal derivative.

Physically, this means that the maximum occurs at the initial time or at the boundary. In the latter case, some flow from outside must exist at the point of maximum.

The dual minimum principle states that the minimum occurs at the initial time or at the boundary. In the latter case, some flow to the outside must exist.

If homogeneous Neumann boundary conditions

$$\frac{\partial u}{\partial \nu} = 0 \quad (\text{on } S_T) \tag{5}$$

and a continuous initial distribution $u_0(0,x)$ are prescribed to the partial differential equation (PDE)

$$\frac{\partial u}{\partial t} - Lu = 0 \quad (\text{on } D_T) \tag{6}$$

the combined minimax principle guarantees that the concentration will stay below the initial maximum value and above the initial minimum value for all times, as extrema can only occur for $t = 0$.

B. Positive Transmissibility Condition

The parameters of the discretization of a PDE have to be chosen in a way that the most characteristic physical properties are maintained.

Assuming a suitable mass conserving node-based discretization (e.g., finite differences, finite elements (FE) with lumping mass, finite boxes), the discretized diffusion equation can be written as a system of equations of the form

$$w_i \frac{\Delta C^i}{\Delta t} + \sum_j \gamma_{ij} C_n^j = 0 \tag{7}$$

where $w_i > 0$ and γ_{ij} denote real coefficients, C_n^i is the concentration value on node i after timestep n and (using backward Euler)

$$\frac{\Delta C^i}{\Delta t} = \frac{C_n^i - C_{n-1}^i}{t_n - t_{n-1}}. \tag{8}$$

Then, it follows that the discrete solution will satisfy a minimax principle if the matrix γ resulting from the discretization is an M-matrix [5], i.e., a real, nonsingular $n \times n$ matrix A where

$$a_{ij} \le 0 \quad \forall i \ne j \tag{9}$$

and

$$A^{-1} \ge 0 \tag{10}$$

which means that all elements of A^{-1} are greater or equal to zero.

Constraint (9) has a physical interpretation in terms of a positive transmissibility condition [6]: Rewriting (7) gives

$$w_i \frac{\Delta C^i}{\Delta t} = \sum_{j \ne i} \gamma_{ij} \left(C_n^i - C_n^j\right) - \left(\sum_j \gamma_{ij}\right) C_n^i. \tag{11}$$

Here, $\gamma_{ij}(C_n^i - C_n^j)$ can be interpreted as the amount of mass transfered from node j to node i per time unit. The physical flow has to be directed from higher to lower concentrations, which requires

$$\gamma_{ij} \le 0 \quad \forall i \ne j \tag{12}$$

and this corresponds to Condition (9).

The violation of the maximum principle in simulation results can be detected by the emergence of negative concentrations and spurious oscillations which are caused by negative transmissibilities and the resulting nonphysical flows.

IV. Finite Volumes versus Finite Elements

The popular discretization schemes for PDEs in complicated domains can be divided into two species: FE and finite volume (FV) (finite box) methods.

We compare FV and FE with respect to the constraints they impose on the mesh to achieve positive transmissibilities and, hence, a discrete minimax principle.

For the theoretical analysis of the possible discretization schemes, we concentrate on the model case (1) with constant diffusivity D.

For both FV and FE we use the standard approaches with backward Euler time discretization [7]. In the case of FE, we use the Galerkin approach with linear shape functions and lumping mass.

In two dimensions, FE and finite boxes give exactly the same discretization, if in the case of FE the mass matrix is lumped [8]. Therefore, the usage of a customary Delaunay mesh guarantees that the solution does not contain any nonphysical negative concentrations [9].

In three dimensions, the situation changes drastically, since the good properties of FE on a Delaunay mesh are lost. We will analyze and explain the meaning of this in practical and theoretical terms. In this section, we will make the beginning and show simulation results demonstrating what "loss of good properties" means in purely practical terms. Section V contains a theoretical analysis and gives the abstract theory behind the problem. Finally, Section VI analyzes in detail the examples of this section using the machinery developed in Section V.

The simulations were done using $\mathcal{A}$MIGOS [10], a general purpose PDE solver and integrated model development environment. All simulations are done on one and the same 3-D Delaunay mesh. The rather coarse mesh is derived from an ortho-product point distribution ($21 \times 21 \times 21$ points) on a cubic simulation domain, whereby every sub-cube is tetrahedralized into six tetrahedra. The mesh is depicted in Fig. 9 (see also Fig. 7), its theoretical properties are analyzed in Section VI.

The initial distribution exhibits radial symmetry (Fig. 1) given by a two-dimensional (2-D) Gaussian profile (offset 10^{12}). Homogeneous Neumann boundary conditions are prescribed on the whole boundary.

The example is chosen to illustrate the fundamental qualitative difference between two and three dimensions for FE diffusion simulations.

A good discretization should approximately conserve the independence of z and the symmetry of the initial distribution

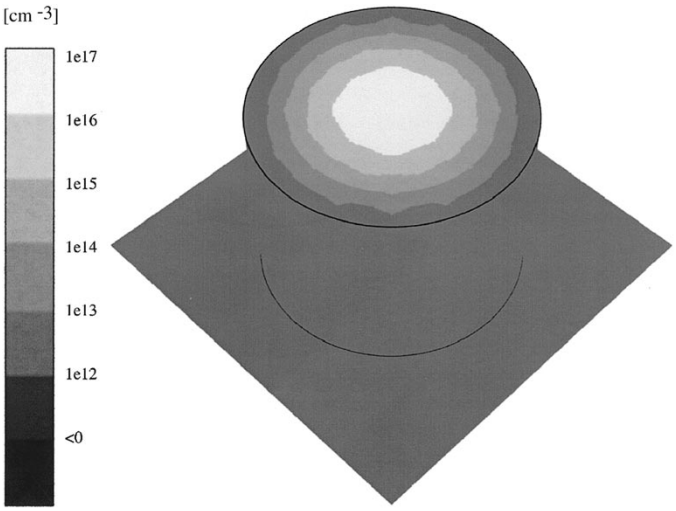


Fig. 1. Initial cylinder symmetrical distribution.

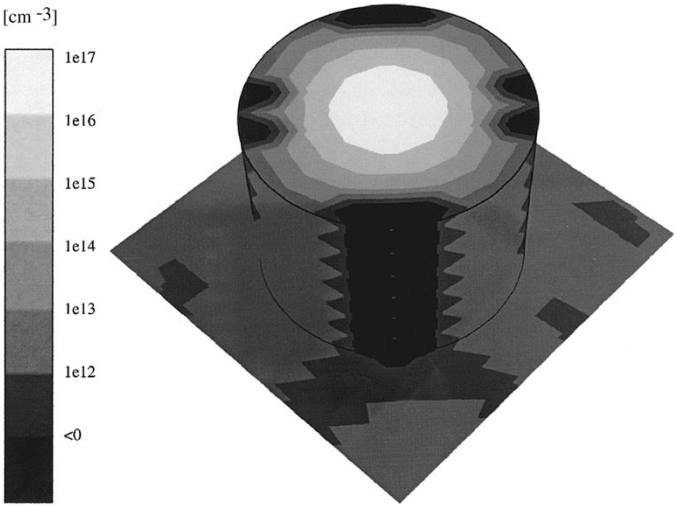


Fig. 2. FE solution after 3000 s. Concentration is negative on black areas.

when it evolves in time. Note that even in the continuous case the rotational symmetry is broken by the cubic boundary.

The visualization of the 3-D concentration distribution is accommodated to the symmetry by use of a planar cut in the xy plane combined with a cylindrical cut in z direction.

Fig. 2 shows the FE solution after 3000 s. The concentration has fallen below the initial minimum value on large areas. The emergence of negative concentrations is demonstrated by the black patterns on the figure. All symmetries are lost, most remarkably the independence of z is not preserved. The latter is shown on Fig. 3 where the viewpoint is rotated 90°. The negative areas spread out in time as seen when comparing Figs. 3 and 4.

The solution produced by FE is qualitatively not satisfactory and even incorrect on a macroscopic scale. This is opposed by the FV solution (Fig. 5) which preserves the symmetry and fulfills the critical minimax principle. Marginal violation of the independence of the solution of z is due to rounding and interpolation errors.

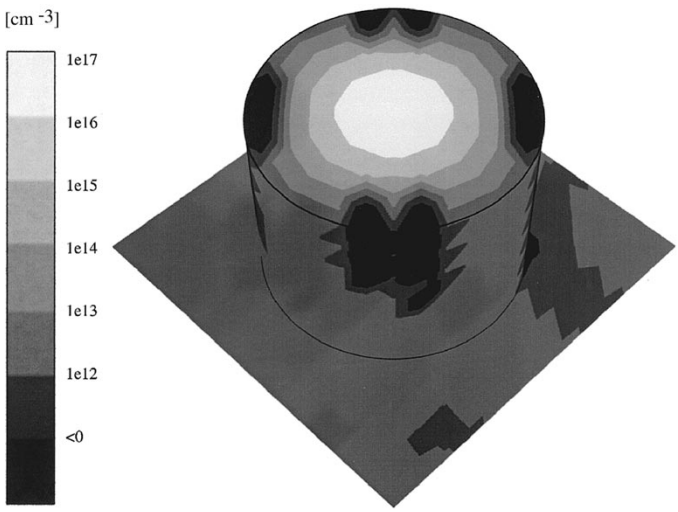


Fig. 3. FE after 3000 s. Independence of z is lost.

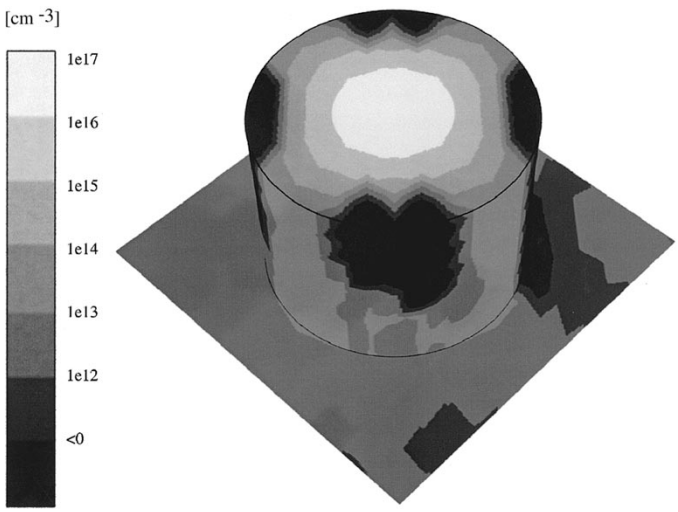


Fig. 4. FE after 10 000 s. The FE disaster. Negative Concentrations have spread out.

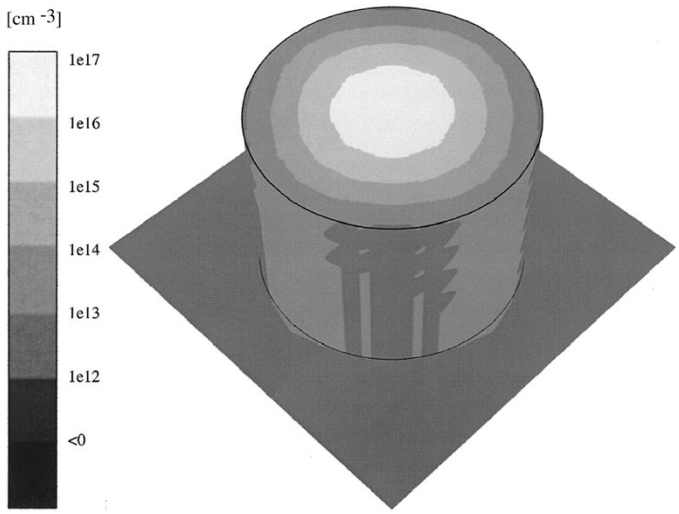


Fig. 5. FV after 10 000 s. Preservation of the symmetry.

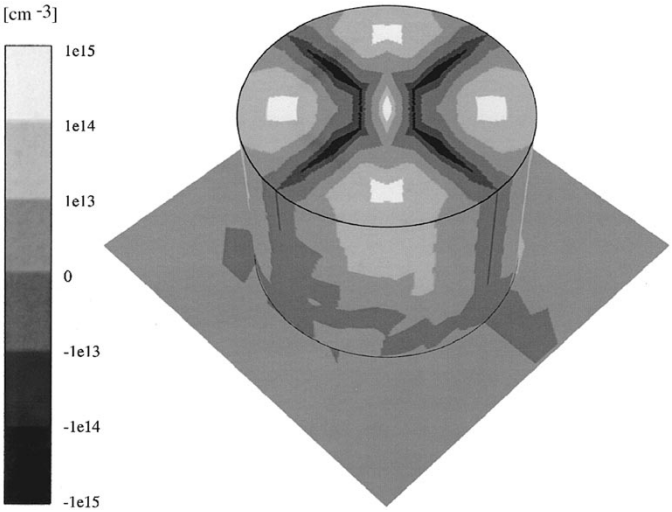


Fig. 6. Absolute error between FE and FV. Global anisotropy.

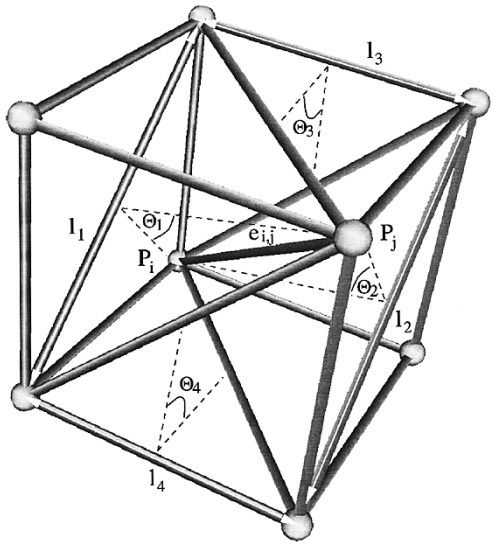


Fig. 7. T_6 tessellation and the dihedral angle criterion (16).

Finally, Fig. 6 displays the absolute error (FV solution minus FE solution) between FE and FV and depicts a global anisotropy.

In a 2-D FE simulation of the same problem, none of the effects described above can be observed when a Delaunay mesh is used. The examples in this section were based on an ortho-grid for ease of theoretical analysis in Section VI. As a side effect they also show that naive use (choice of a "bad" Delaunay triangulation) of a mesh based on a structured grid can lead to large discretization errors.

V. Natural Meshing Constraints

The experiments above demonstrate a puzzling dependence of the quality of FE solutions on the dimension of the Delaunay mesh. While in two dimensions FE solutions exhibit good qualitative properties, in three dimensions the produced solutions can be a disaster. The aim of this section is to investigate the observed effects in terms of mesh requirements.

Already in two dimensions, careless discretization (e.g., FE without lumping mass) and/or bad meshing (e.g., use of a non-Delaunay mesh) will result in nonphysical flows and the emergence of negative concentrations, see [6] and [11].

In three dimensions, the interplay between meshing and discretization is still more complicated. In many cases, the discretizations rely on heavy constraints on the meshing strategy applied in order to achieve the desired properties.

In the simulations above, we used the standard Galerkin approach for FE with linear shape functions and backward Euler time discretization.

In this case, the system matrix $\mathbf{K}$ is of the form

$$\mathbf{K} = \frac{1}{\mathbf{\Delta t}}\mathbf{M} + \mathbf{DS} \tag{13}$$

where $\mathbf{M}$ denotes the mass matrix, $\mathbf{S}$ is the stiffness matrix, and D is the diffusion constant.

The discrete solution fulfills a maximum principle if the mass matrix is lumped and $\mathbf{S}$ is an M-matrix. The coefficients s_{ij} of $\mathbf{S}$ are given by

$$s_{ij} = \sum_{\text{elements}} \int_e \nabla N_i \cdot \nabla N_j \, dA \tag{14}$$

where N_i and N_j denote the shape functions and A is the area (volume) of element e. The sum runs over all elements e containing the edge e_{ij}. To make $\mathbf{S}$ an M-matrix, the off-diagonal entries must not be positive

$$s_{ij} \leq 0, \quad i \neq j. \tag{15}$$

If the mesh has no obtuse angles, every term in the sum is negative and Condition (9) is trivially fulfilled. However, this is too strict.

The scalar product $(\nabla N_i \cdot \nabla N_j)$ has a simple geometrical meaning and allows a reinterpretation of the constraint (15) in basic geometrical terms using only the dihedral angles and the length of the edges.

Xu and Zikatanov [12] derive the following equivalent criterion which we name the (weighted) dihedral angle criterion: Let e_{ij} be the edge connecting two vertices v_i and v_j in a 3-D mesh. In every tetrahedra t_k containing e_{ij}, there exists a face opposite to v_i and a face opposite to v_j. The two faces span a dihedral angle θ_k and their intersection has length l_k. $\mathbf{S}$ is an M-matrix if and only if, for any fixed edge e_{ij} the following inequality is satisfied:

$$\sum_{k=1}^{n} l_k \cot \theta_k \geq 0 \tag{16}$$

where n is the number of tetrahedra adjacent to e_{ij}.

Fig. 7 displays the dihedral angles linked to the cube diagonal in a tessellation consisting of six tetrahedra.

The 2-D variant of (16) is

$$\cot \theta_1 + \cot \theta_2 \geq 0 \tag{17}$$

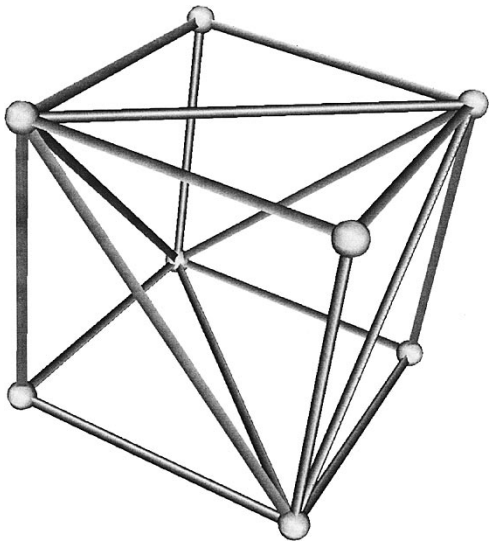


Fig. 8. T_5 tessellation, no obtuse dihedral angles.

where θ_1 and θ_2 are the angles opposite to an edge e_{ij} which is shared by two triangles. This is equivalent to the Delaunay criterion [9] and explains the good properties of FE in two dimensions on Delaunay meshes.

VI. Distinctive Mesh Examples

In three dimensions, the dihedral angle and the Delaunay criterion are of quite diverse nature. Both constraints form the interesting case of two natural quality criteria, which are equivalent in two dimensions but split into different notions in three dimensions.

Our analysis is based on three specific mesh examples.

Mesh Example 1: A Delaunay mesh which is not suitable as a FE mesh for diffusion applications. This kind of mesh was used in the simulations above.

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

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

The combination of these examples proves that in three dimensions the Delaunay criterion is neither sufficient nor necessary to achieve a maximum principle in FE diffusion simulations.

A. Basic Mesh Construction

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

T_6 *Tessellation:* A cube is composed of six tetrahedra (Fig. 7).

T_5 *Tessellation:* A cube is composed of five tetrahedra (Fig. 8).

For the purpose of demonstration a specific tessellation T_6 (Fig. 7) is used which contains sliver elements with obtuse dihedral angles. (Note that also T_6 tessellations exist which do not contain obtuse angles.) The tessellation T_5 (Fig. 8), on the other hand, does not contain such elements.

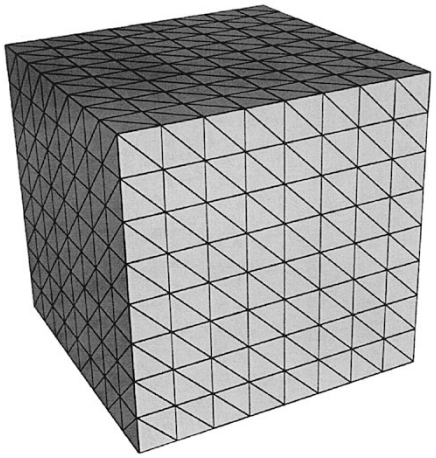


Fig. 9. Delaunay mesh built from T_6-tessellated cubes, dihedral angle criterion is not fulfilled.

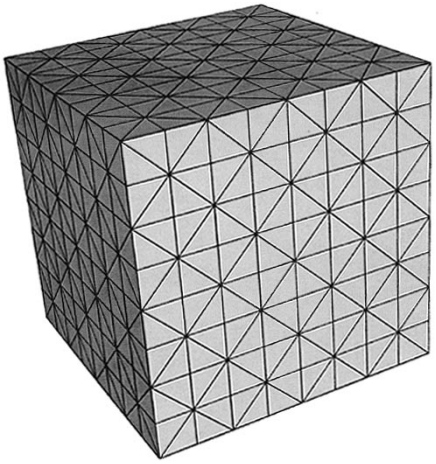


Fig. 10. Delaunay mesh built from T_5-tessellated cubes, dihedral angle criterion is satisfied.

Meshes suitable for simulation are then built by stacking a large number of identically tessellated cubes (see Figs. 9 and 10). The typical characteristics of each tessellation type are thereby conserved.

All elements of both tessellations fulfill the empty circumsphere Delaunay criterion, because all points lie on the perimeter of the cube's circumsphere.

Because of the total absence of obtuse dihedral angles, the T_5 tessellation fulfills the dihedral angle criterion.

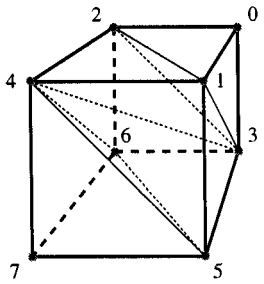
To test if this result is valid for the T_6 tessellation, we use AMIGOS to display the stiffness matrix and directly check the sign of the matrix entries. The stiffness matrix corresponding to a T_6-tessellated cube is shown in Fig. 11 where the entries for the edge (3, 4) of the mesh are underlined. The global coupling coefficient has positive sign, which proves that the dihedral angle criterion is violated in this case.

Hence, both meshes are global Delaunay meshes and yet only one satisfies the dihedral angle criterion.

B. A Non-Delaunay Mesh Suitable for FE

We try to construct a mesh, which is not Delaunay, but still fulfills the dihedral angle criterion. The key idea to its construc-

$$\begin{pmatrix} 5.0 & -1.6 & -1.6 & -1.6 & & & & \\ -1.6 & 8.3 & 1.6 & -1.6 & -5.0 & -1.6 & & \\ -1.6 & 1.6 & 8.3 & -1.6 & -5.0 & & -1.6 & \\ -1.6 & -1.6 & -1.6 & 11.6 & \underline{3.3} & -5.0 & -5.0 & \\ & -5.0 & -5.0 & \underline{3.3} & 11.6 & -1.6 & -1.6 & -1.6 \\ & -1.6 & & -5.0 & -1.6 & 8.3 & 1.6 & -1.6 \\ & & -1.6 & -5.0 & -1.6 & 1.6 & 8.3 & -1.6 \\ & & & & -1.6 & -1.6 & -1.6 & 4.9 \end{pmatrix}$$



TET: 4 5 6 3

$$\begin{pmatrix} 1.6 & -1.6 & -1.6 & \underline{1.6} \\ -1.6 & 3.3 & 1.6 & -3.3 \\ -1.6 & 1.6 & 3.3 & -3.3 \\ \underline{1.6} & -3.3 & -3.3 & 5 \end{pmatrix}$$

TET: 6 4 3 2

$$\begin{pmatrix} 3.3 & 0 & -1.6 & -1.6 \\ 0 & 1.6 & \underline{0} & -1.6 \\ -1.6 & \underline{0} & 1.6 & 0 \\ -1.6 & -1.6 & 0 & 3.3 \end{pmatrix}$$

TET: 3 4 1 2

$$\begin{pmatrix} 1.6 & \underline{1.6} & -1.6 & -1.6 \\ \underline{1.6} & 5 & -3.3 & -3.3 \\ -1.6 & -3.3 & 3.3 & 1.6 \\ -1.6 & -3.3 & 1.6 & 3.3 \end{pmatrix}$$

TET: 4 5 3 1

$$\begin{pmatrix} 1.6 & 0 & \underline{0} & -1.6 \\ 0 & 3.3 & -1.6 & -1.6 \\ \underline{0} & -1.6 & 1.6 & 0 \\ -1.6 & -1.6 & 0 & 3.3 \end{pmatrix}$$

Fig. 11. Global stiffness matrix for a T_6 tessellation and local matrices of those four elements which are adjacent to edge (3, 4).

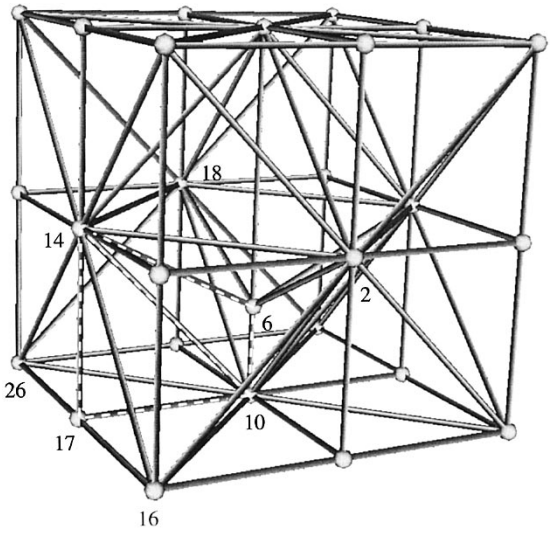


Fig. 12. T_5 type tessellation with a shifted point. Building block for mesh in Fig. 13.

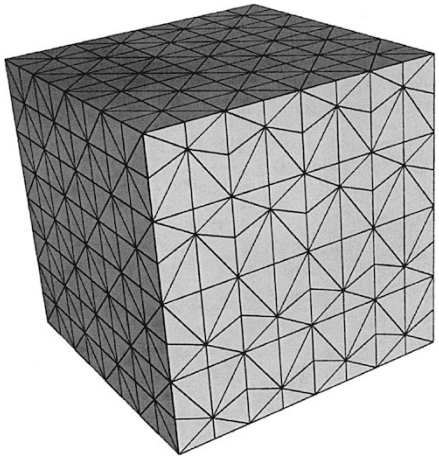


Fig. 13. Non-Delaunay mesh fulfilling the dihedral angle criterion.

tion is to take the "good" T_5 mesh (which fulfills both the angle and the Delaunay criterion) and to modify it in such a way, that Delaunay is violated but the angle criterion is preserved [13].

As the T_5 mesh is a degenerate case with eight cospherical points, violation of Delaunay is easily achieved by shifting points slightly (e.g., infinitesimally) in certain locations. This results in a non-Delaunay mesh which (by a simple continuity argument) still satisfies (16).

Fig. 12 shows a submesh consisting of eight cubes, which form the building blocks of the mesh in Fig. 13. The point in the middle (numbered "6"), which belongs to all eight cubes has been shifted downwards. The Delaunay criterion is violated, because the circumspheres of several unmodified tetrahedra contain the shifted point in its interior. The dashed lines in the figure mark two of the non-Delaunay triangles.

The calculation for the entire mesh (Fig. 13) verifies, that the FE 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, criterion (14) is satisfied and the global stiffness matrix remains an M-matrix.

C. Heuristics

Our examples show that Delaunay neither implies nor is it implied by the dihedral angle criterion.

The former result was discussed in [9] where a Delaunay mesh unsuitable for FE simulation was presented. The construction of a simple mesh which fulfills the dihedral angle criterion

but not the Delaunay criterion complements this previous research.

Heuristically, the latter result was motivated by Putti's discovery (see Section VII-A) that FE gives the same discretization as gravity boxes in three dimensions. Gravity boxes and Voronoi boxes are distinct notions. There is no sense in which a gravity box is a Voronoi box or vice versa. By this analogy, there is no reason why Delaunay should imply the dihedral angle criterion and vice versa.

Our examples also point out another weakness of combining FE and the Delaunay criterion: If the Delaunay tetrahedralization is not unique, FE gives different results depending on the choice of tetrahedralization. The FV schemes, however, only rely on the Voronoi boxes. In degenerate cases, the result does not depend on the choice of tetrahedralization.

In this respect, the dihedral angle criterion cannot achieve for FE what Delaunay achieves for FV. There may be several or no tetrahedralizations which fulfill the dihedral angle criterion and they will produce different solutions.

VII. Discussion

A. The Abstract Viewpoint

Stemming from the equivalence of FE and FV in two dimensions there is a widely spread belief that this equivalence is also valid in higher dimensions, in other words that FE can be reduced to some kind of FV and vice versa. However, FE and FV are different with respect to the heuristical basis on which they are derived. Finite elements are a very general and flexible approach for which a sophisticated mathematical theory exists. On the other hand, there are FV schemes which are motivated more physically. Usually, the latter employ a conservation law or balance equations for control volumes using an integral theorem. [14] compares FE and FV schemes using concepts from algebraic topology and the theory of differential forms. It explains why FE and FV are different on a fundamental level and why "the charge brought against FE of reducing all to nodes must be reconsidered" [14].

In the special case of the Laplace operator, it is still possible to interpret FE as a FV scheme in three dimensions, but in contrast to the 2-D case the corresponding FV scheme is based on gravity boxes instead of the Voronoi boxes [7].

B. Practical Strategies

In the attempt to avoid numerical instabilities, the most important strategic decision is the proper choice of discretization. With respect to diffusion problems the decision is an easy one: use a variant of FV. Many meshing tools construct their basic meshes relying on the Delaunay criterion, then possibly doing some kind of quality improvement. In any case, many available meshers are Delaunay-based. Finite elements on a conventional Delaunay mesh, however, can be a disaster and are much more vulnerable and sensitive to the meshing quality.

If one wants or has to use a FE solver a practical meshing strategy will 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 enforce the dihedral angle criterion directly. Existing meshing techniques often try to avoid any obtuse dihedral angles. This is not necessary if techniques can be developed to generate FE meshes which satisfy the dihedral angle criterion. However, such a technique remains open to further research.

In many practical cases, one cannot rely on a very good quality of the FE mesh. Then, additional strategies are pursued: e.g., mesh refinement combined with a time step reduction. According to standard FE theory, the discretized solution (using backward Euler) will converge to the exact solution if meshing granularity and time step size tend to zero. The main obstacle to make successful use of this property is the lack of a smart refinement strategy. There is no way to exclude global anisotropic effects as in Fig. 6. In cases like this, getting rid of negative concentrations by h-refinement is not feasible.

Alternative strategies like the use of higher order shape functions (p-refinement) or a simplistic cutting off of negative concentrations are even less promising from a theoretical as well as from an empirical point of view.

C. Nonlinear Case

In the linear case, the emergence of negative concentrations can be simply considered as an annoyance as long as the precision is high enough. In the nonlinear case, the consequences of insufficient meshing quality are much more serious: (1) is then solved by a Newton method. Exemplary simulations reveal that negative transmissibilities cause a deterioration of the convergence of the Newton iteration. For a physical explanation, see [6].

The negative concentrations are particularly severe in diffusion problems for semiconductor process simulation, because in typical applications the concentration varies in many orders of magnitude within a small area. If the Newton iteration does not converge, the time step is usually reduced. This can lead to convergence, but has no diminishing effect on the emerging negative concentrations. Therefore, appropriate meshing quality is of utmost importance for the solution of nonlinear transient problems with high concentration gradients like, e.g., the pair diffusion model [15].

VIII. Resume

We presented a case study on the interplay between meshing and discretization in diffusion simulation. Finding meshing algorithms specially tuned for the discretization in use is a strong challenge to the TCAD community. From a mathematical point of view, FE schemes are often easier to analyze than FV schemes for the same problem. However, with regard to easy fulfillment of the corresponding meshing requirements, FV is the superior discretization. Progress in the development of robust PDE solvers can only be achieved by a point of view which regards discretization and meshing not as two distinct tasks but as one problem with an analytic and a more algorithmic part. One instance for a solution is the perfect interplay between the FV discretization and Delaunay meshes. This symmetry is broken when FE is combined with the Delaunay criterion and it is restored only incompletely when Delaunay is replaced by the dihedral angle criterion.

Based on a vast series of numerical experiments conducted using AMIGOS and theoretical investigations, we advocate the use of FV schemes in 3-D diffusion modeling.

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