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3D Finite Element Drift-Diffusion Simulation of Semiconductor Devices

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Chapter 1

Finite element discretization

In this chapter we present the weak formulation of problems (**??**), (**??**) and (**??**). For each weak problem we discuss the well-posedness analysis and describe the finite element discretization.

1.1 Non Linear Poisson Equation: weak form

Let us write problem (**??**) in compact form:

$$\begin{cases} \nabla \cdot (-\epsilon \nabla \delta\varphi^k) + \sigma^k \delta\varphi^k &= f^k & in\ \Omega \\ \delta\varphi^k &= 0 & on\ \Gamma_D \\ \nabla \delta\varphi^k \cdot \mathbf{n} &= 0 & on\ \Gamma_N \\ \varphi^{k+1} &= \varphi^k + \delta\varphi^k & \end{cases} \tag{1.1}$$

having set:

$$\begin{aligned} \epsilon &= \epsilon_s \mathcal{I}_{\Omega_{Si}} + \epsilon_{ox} \mathcal{I}_{\Omega_{ox}} \\ f &= f_s \mathcal{I}_{\Omega_{Si}} + f_{ox} \mathcal{I}_{\Omega_{ox}} \\ \sigma &= \sigma_s \mathcal{I}_{\Omega_{Si}} \end{aligned}$$

where $\mathcal{I}_A(\mathbf{x})$ is equal to 1 if $\mathbf{x} \in A$ and 0 otherwise. System (1.1) is a Diffusion-Reaction (DR) problem in Ω, with respect to the dependent variable $\delta\varphi^k$. Now we multiply the first equation in (1.1) by a test function $v \in H^1_{\Gamma_D}(\Omega)$ and integrating over all the domain we obtain

$$-\int_\Omega \nabla \cdot (-\epsilon \nabla \delta\varphi^k) v \, d\Omega + \int_\Omega \sigma^k \delta\varphi^k v \, d\Omega = \int_\Omega f^k v \, d\Omega \qquad \forall v \in H^1_{\Gamma_D}(\Omega). \tag{1.2}$$

Applying the Green formula and considering the boundary conditions, we obtain the weak formulation of (1.1) which reads: find $\delta\varphi^k \in H^1_{\Gamma_D}(\Omega)$ such that

$$\int_\Omega \epsilon \nabla \delta\varphi^k \nabla v \, d\Omega + \int_\Omega \sigma^k \delta\varphi^k v \, d\Omega = \int_\Omega f^k v \, d\Omega \qquad \forall v \in H^1_{\Gamma_D}(\Omega). \tag{1.3}$$

We are able to define the following bilinear form

$$a : H^1_{\Gamma_D}(\Omega) \times H^1_{\Gamma_D}(\Omega) \to \mathbb{R}, \qquad a(u,v) = \int_\Omega \epsilon \nabla u \nabla v \, d\Omega + \int_\Omega \sigma^k uv \, d\Omega. \tag{1.4}$$

and the linear and bounded functional

$$F : H^1_{\Gamma_D}(\Omega) \to \mathbb{R}, \qquad F(v) = \int_\Omega f^k v \, d\Omega \tag{1.5}$$

In order to prove the existence and uniqueness of the solution of (1.3), we apply the *Lax-Milgram theorem* [Sal10]. Well-posedness is ensured by several physical hypotheses:

- $\epsilon \in L^\infty(\Omega)$ and $\epsilon(\mathbf{x}) > 0$ a.e. in Ω;
- $\forall k \geq 0$ $\sigma^k \in L^\infty(\Omega)$ and $\sigma^k(\mathbf{x}) > 0$ a.e. in Ω_{Si}.

We define some useful quantities:

$$\begin{aligned} \epsilon_M &= \max_\Omega \epsilon \quad & \epsilon_m &= \min_\Omega \epsilon \\ \sigma_M &= \max_\Omega \sigma \quad & \sigma_m &= \min_\Omega \sigma = 0 \end{aligned}$$

Take into account the above hypotheses it's possible to demonstrate:

- **Continuity of the bilinear form:**

  $\forall u, v \in H^1_{\Gamma_D}$

  $$\begin{aligned} |\textstyle\int_\Omega \epsilon \nabla u \nabla v + \int_\Omega \sigma^k uv| &\leq \epsilon_M ||\nabla u||_{L^2} ||\nabla v||_{L^2} + \sigma_M ||u||_{L^2} ||v||_{L^2} \\ &\leq \max\{\epsilon_M, \sigma_M\} \left(||\nabla u||_{L^2} ||\nabla v||_{L^2} + ||u||_{L^2} ||v||_{L^2} \right) \\ &\leq \max\{\epsilon_M, \sigma_M\} ||u||_{H^1_{\Gamma_D}} ||v||_{H^1_{\Gamma_D}}. \end{aligned}$$

- **Coercivity of the bilinear form:**

  $\forall u \in H^1_{\Gamma_D}$

  $$\begin{aligned} |\textstyle\int_\Omega \epsilon \nabla u \nabla u + \int_\Omega \sigma^k u^2| &\geq \epsilon_m ||\nabla u||^2_{L^2} + \sigma_m ||u||^2_{L^2} \\ &= \epsilon_m ||\nabla u||^2_{L^2} \\ &= \epsilon_m |\nabla u|^2_{H^1_{\Gamma_D}} \equiv \epsilon_m ||u||^2_{H^1_{\Gamma_D}}. \end{aligned}$$

- **Continuity of the functional:**

$$|\int_\Omega f^k v| \quad \leq ||f^k||_{L^2}||v||_{H^1_{\Gamma_D}} \qquad \forall v \in H^1_{\Gamma_D}.$$

Then we can state that $\forall k \geq 0$ there exists a unique weak solution of the linearized Non Linear Poisson equation.

1.2 Continuity Equations: weak form

Without loss of generality we consider only the electron continuity equation. System (**??**) is a diffusion-advection-reaction (DAR) problem in conservative form. With a suitable change of variables we are able to treat these PDE likewise the linearized Non Linear Poisson equation in the previous section. Consider the Slotboom variable (**??**), we can rewrite system (**??**) as:

$$\begin{cases} \nabla \cdot \left(-qD_n e^{\varphi^i/V_{th}} \nabla u_n\right) + \sigma_n^{i-1} e^{\varphi^i/V_{th}} u_n &= f^{i-1} & in\ \Omega_{Si} \\ u_n &= n_D e^{-\varphi^i/V_{th}} & on\ \Gamma_{D,Si} \\ \nabla u_n \cdot \mathbf{n} &= 0 & on\ \Gamma_{N,Si}\,. \end{cases} \tag{1.6}$$

Proceeding as in Section 1.1, the weak formulation of the Electron Continuity equation is:

find $u_n \in H^1_{\Gamma_{D,Si}}(\Omega)$ such that

$$\int_{\Omega_{Si}} qD_n e^{\varphi^i/V_{th}} \nabla u_n \nabla v \, d\Omega + \int_{\Omega_{Si}} \sigma_n^{i-1} e^{\varphi^i/V_{th}} u_n v \, d\Omega = \int_{\Omega_{Si}} f^{i-1} v \, d\Omega \qquad \forall v \in H^1_{\Gamma_{D,Si}}. \tag{1.7}$$

Existence and uniqueness of the unknown variable u_n ensures the same properties on n, thanks to the relation (**??**) between u_n and n. Further hypotheses on the coefficients $\forall i \geq 0$:

- $qD_n e^{\varphi^i/V_{th}} \in L^\infty(\Omega_{Si})$ and $D_n(\mathbf{x}) > 0$ a.e. in Ω_{Si};
- $\sigma_n^{i-1} e^{\varphi^i/V_{th}} \in L^\infty(\Omega_{Si})$ and $\sigma_n^{i-1}(\mathbf{x}) > 0$ a.e. in Ω_{Si}.

We define the bilinear form

$$a(u,v) = \int_{\Omega_{Si}} qD_n e^{\varphi^i/V_{th}} \nabla u_n \nabla v \, d\Omega + \int_{\Omega_{Si}} \sigma_n^{i-1} e^{\varphi^i/V_{th}} u_n v \, d\Omega \tag{1.8}$$

and the linear and bounded functional

$$F(v) = \int_{\Omega_{Si}} f^{i-1} v \, d\Omega \tag{1.9}$$

Well-posedness of problem (1.7) is verified using the same arguments as in Section 1.1.

1.3 Numerical approximation

In this section we introduce the Galerkin method to approximate the weak formulations (1.3) and (1.7) (see [QV08]). Each of them can be represented in compact form as:

find $u \in V$ such that

$$a(u, v) = F(v) \qquad \forall v \in V \tag{1.10}$$

where V is the space of admissible functions, e.g. $H^1_{\Gamma_D}(\Omega)$ or $H^1_{\Gamma_{D,Si}}(\Omega_{Si})$. Let us introduce V_h which is a family of finite-dimensional subspaces of V, depending on a positive parameter h, such that

$$V_h \subset V, \quad \dim V_h < \infty \qquad \forall h > 0 \tag{1.11}$$

The *Galerkin problem* reads:

find $u_h \in V_h$ such that

$$a(u_h, v_h) = F(v_h) \qquad \forall v_h \in V_h. \tag{1.12}$$

Unique solvability of (1.12) is an immediate consequence of the analysis carried out in Sections 1.1 and 1.2.

Let $\mathcal{T}_h$ be a partition of Ω, and K a generic element of $\mathcal{T}_h$ such that $\bar{\Omega} = \bigcup \bar{K}$. In this case the parameter h represents the characteristic dimension of each element K. For $n \geq 1$ let us introduce the general finite element spaces of the polynomial element wise functions

$$X^r_h(\Omega) := \{v_h \in C^0(\bar{\Omega}) : v_h|_K \in \mathbb{P}_r(K), \forall K \in \mathcal{T}_h\} \tag{1.13}$$

and the associated space where functions vanish on boundaries

$$X^r_{h,\Gamma_D}(\Omega) := \{v_h \in X^r_h : v_h|_{\Gamma_D} = 0\}. \tag{1.14}$$

If $\Omega \subset \mathbb{R}^3$ we have

$$\dim \mathbb{P}_r(K) := \binom{3+r}{r} \tag{1.15}$$

We approximate $H^1_{\Gamma_D}(\Omega)$ with $X^1_{h,\Gamma_D}(\Omega)$ and $H^1_{\Gamma_{D,Si}}(\Omega_{Si})$ with $X^1_{h,\Gamma_{D,Si}}(\Omega_{Si})$. Therefore according to (1.15) we have:

$$\begin{aligned} \dim\mathbb{P}_1(K) &= 4 \\ \dim X^1_h &= N_h \\ \dim X^1_{h,\Gamma_D} &= N_h - N_g \end{aligned}$$

where N_h is the number of vertices of the partition $\mathcal{T}_h$ and N_g is the number of vertices that belong to the Dirichlet boundary.

We denote by $\{\psi_j\}_{j=1}^{N_h}$ the Lagrangian basis of the space X^1_h in such a way that

$$u_h(\mathbf{x}) = \sum_{j=1}^{N_h} u_j \psi_j(\mathbf{x}). \tag{1.16}$$

Since each function of V_h is a linear combination of ψ_i for $i = 1, \ldots, N_h$, the Galerkin problem (1.12) becomes:

find $[u_1, u_2, ..., u_{N_h}]^T \in \mathbb{R}^{N_h}$ such that

$$\sum_{j=1}^{N_h} u_j a(\psi_j, \psi_i) = F(\psi_i) \qquad \forall i = 1, \ldots, N_h. \tag{1.17}$$

In order to implement problem (1.17) it's convenient to express the bilinear form $a(\cdot,\cdot)$ and the linear functional $F(\cdot)$ with respect to each element of the partition $\mathcal{T}_h$ as

$$\sum_{j=1}^{N_h} u_j \sum_{K\in\mathcal{T}_h} a_K(\psi_j, \psi_i) = \sum_{K\in\mathcal{T}_h} F_K(\psi_i) \qquad \forall i = 1, \ldots, N_h. \tag{1.18}$$

1.3.1 Geometrical discretization

Each element $K \in \mathcal{T}_h$ is a tetrahedron of volume $|K|$. From now on, we assume that there exists a constant $\delta > 0$ such that

$$\frac{h_K}{\rho_K} \leq \delta \qquad \forall K \in \mathcal{T}_h \tag{1.19}$$

where $h_k = \mathrm{diam}(K) = \max_{x,y\in K} |x - y|$ and ρ_K is the diameter of the sphere inscribed in the tetrahedral K. Condition (1.19) is the so called *mesh regularity condition* [Qua08] [QV08]. We denote with $\mathcal{E}_h$, $\mathcal{V}_h$ and $\mathcal{F}_h$ the set

of all the edges, vertices and faces of $\mathcal{T}_h$ respectively, and for each $K \in \mathcal{T}_h$ we denote by ∂K and $\mathbf{n}_{\partial K}$ the boundary of the element and its outward unit normal.

We notice that $\mathcal{T}_h$ is built in such a way that every K belongs to a single region, while it is possible that vertices belong to different regions.

1.3.2 Linearized Non Linear Poisson equation

Concerning with the linearized NLP equation we have

$$a(\psi_j, \psi_i) = \int_\Omega \epsilon \nabla\psi_j \nabla\psi_i \, d\Omega + \int_\Omega \sigma^k \psi_j \psi_i \, d\Omega \tag{1.20}$$

and the restriction on each element K is

$$a_K(\psi_j, \psi_i) = \int_K \epsilon \nabla\psi_j \nabla\psi_i \, dK + \int_K \sigma^k \psi_j \psi_i \, dK. \tag{1.21}$$

Equation (1.21) contains two distinct contributions: the first one identifies the diffusive contribution and generates the so-called *stiffness matrix*, while the second refers to the reaction term and generates the *mass matrix*.

The coefficient ϵ is a piece wise constant function, which changes on different material regions. Therefore ϵ is constant over each element and the first integral in (1.21) become easier to compute.

As a consequence of choosing the discrete space X_h^1, we can not expect a better convergence rate than the first order in $||\cdot||_{1,\Omega}$ with respect to h [QV08]. This implies that is not necessary to make use of an high-order quadrature rule, so that the trapezoidal rule is enough accurate. The main consequence of the using trapezoidal quadrature rule is that the mass-matrix becomes diagonal. This technique is well known as *lumping procedure* applied on the mass-matrix.

The contributions of the local system matrix A_K^k is

$$[A_K^k]_{ij} = \epsilon_K L_{ij} + \frac{|K|}{4} \sigma_i^k \tag{1.22}$$

having set

$$\begin{aligned} L_{ij} &= \textstyle\int_K \nabla\psi_i \nabla\psi_j \, d\Omega \\ \sigma_i^k &= \sigma^k(\mathbf{x}_i). \end{aligned} \tag{1.23}$$

The construction of the right hand side of (1.18) using the trapezoidal rule yields:

$$[F_K]_i^k = f_i^k \frac{|K|}{4} \simeq \int_\Omega f^k \psi_i \, d\Omega. \tag{1.24}$$

The local contributions of each element K are assembled in the global matrix A as follows. Let I be the global index of a generic vertex belonging to the partition $\mathcal{T}_h$. We denote by $\mathcal{J}_K : \mathcal{V}_{\mathcal{T}_h} \to \mathcal{V}_K$ the map which connects I to its corresponding local index $i = 1, \ldots, 4$ in the element K. Then we have

$$A_{IJ}^k = \sum_{\substack{\forall K \in \mathcal{T}_h s.t. \\ \mathcal{J}_K(I), \mathcal{J}_K(J) \subset \mathcal{V}_K}} [A_K]_{ij}^k. \tag{1.25}$$

Analogously for the force term $\mathbf{b}^k$

$$b_I^k = \sum_{\substack{\forall K \in \mathcal{T}_h s.t. \\ \mathcal{J}_K(I) \subset \mathcal{V}_K}} [F_K]_i^k. \tag{1.26}$$

Once we have built the global matrix A^k and the global vector $\mathbf{b}^k$ we need to take into account the essential boundary conditions. In fact the displacement formulation is a primal method which enforces Dirichlet boundary condition in a strong manner. Therefore we have to modify the algebraic system. We choose the *diagonalization* technique which does not alter the matrix pattern nor introduce ill-conditioning in the linear system. Let i_D be the generic index of a Dirichlet node, we denote by $[\delta\varphi_D]_i$ (which in this case is equal to zero) the known value of the solution $\delta\varphi$ at the node. We consider the Dirichlet condition as an equation of the form $\beta[\delta\varphi]_i = \beta[\delta\varphi_D]_i$, where $\beta \neq 0$ is a suitable coefficient. In order to avoid degradation of the global matrix condition number, we take β equal to the diagonal element of the matrix at row i_D.

Finally, the discretization of step 1 in the Gummel algorithm, reads:

$$\left\{ \begin{array}{rcl} A^k \delta\varphi^k & = & \mathbf{b}^k \\ \varphi^{k+1} & = & \varphi^k + \delta\varphi^k. \end{array} \right. \tag{1.27}$$

As every iteration procedure, problem (1.27) needs a suitable convergence break criterion. A good approach is based on checking the satisfaction of the fixed point equation (**??**) by the k-th solution. In this case the inner loop of the Gummel Map reads as: given a tolerance $toll > 0$ solve problem (1.27) until

$$||\mathbf{b}(\varphi^{k+1})||_2 > toll \tag{1.28}$$

where $||\cdot||_2$ is the usual Euclideian norm for a vector.

Damping

Despite the validity of Thm.**??**, the use of the Newton's method may be affected by numerical difficulties. The main problem is the tendency of the method to overestimate the length of the correction step. This phenomenon is frequently indicated as *overshoot*. In the case of the semiconductor equations this overshoot problem can be treated by simply limiting the size of the correction vector ($\delta\varphi$) determined by Newton's method. The usual established modifications to avoid overshoot are given by the following formulation:

$$\tilde{A}(\varphi_k) = \frac{1}{t_k} A(\varphi_k) \tag{1.29}$$

where t_k is a positive parameter to be properly chosen, with $t_k = 1$ the modified Newton method reduces to the classical Newton method. For the case (1.29) a simple criterion suggested by Deuflhard [Deu74], prescirbes that t_k is taken in $(0, 1]$ in such a way that for any norm, we have

$$||A(\varphi_k)^{-1}\mathbf{b}(\varphi_k - t_k A(\varphi_k)^{-1}\mathbf{b}(\varphi_k))|| < ||A(\varphi_k)^{-1}\mathbf{b}(\varphi_k)||. \tag{1.30}$$

Satisfying condition (1.30) guarantees that the norm of the residual is decreasing with k. This condition is hardly to be evaluated because the presence of the inverse of A. If the solution is accomplished using a direct method like the LU factorization, the evaluation of the argument of the norm on the left hand side of (1.30) is reduced to a forward and backward substitution and the evaluation of $\mathbf{b}(\varphi)$. However we use an iterative method (BCG solver based on [PTVF07]) and this implies serious difficulties to the application of the criterion (1.30). In order to overcome this problem we consider another valid possibility, replacing A in (1.30) with the main diagonal $D(\varphi_k)$:

$$||D(\varphi_k)^{-1}\mathbf{b}(\varphi_k - t_k D(\varphi_k)^{-1}\mathbf{b}(\varphi_k))|| < ||D(\varphi_k)^{-1}\mathbf{b}(\varphi_k)||. \tag{1.31}$$

This criterion has been adopted in our code. However the value to use for t_k is a question of trial and error. Frequently the following sequences are used:

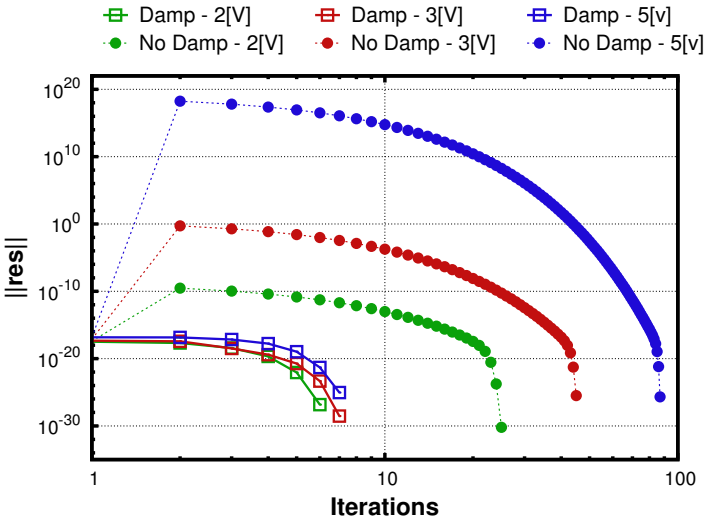
$$t_k = \frac{1}{2^i} \tag{1.32}$$

$$t_k = \frac{1}{2^{\frac{i(i+1)}{2}}} \tag{1.33}$$

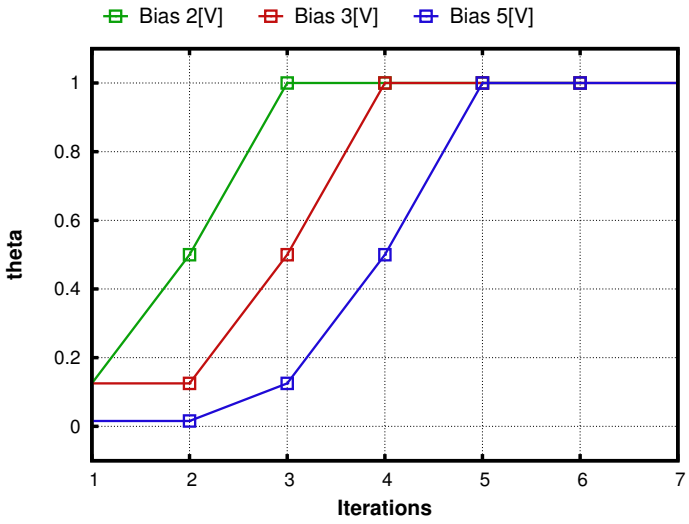
where i is the number of subiterations of the damping procedure needed to satisfy (1.31). Close to the solution, (1.30) (and so (1.31)) will be satisfied with $t_k = 1$ so that the quadratic convergence properties of the classical Newton method are recovered.

The benefits due to the damping techinque are visible in Fig.1.1a, where for different voltages applied to a p-n junction, the evolution of the residual, for the first Gummel map iteration, is shown. When damping is switched-off first iterations are critical, because the solution found is very far from the real one. When damping is switched-on this problem is solved and the scheme converges with fewer iterations. In some heuristic sense this procedure guarantees a progressive approaching of the solution to the ball mentioned in Thm.**??**, where the convergence rate is quadratical. In Fig.1.1b the evolution of the coefficient t_k is depicted. The curves are monotonic from 0 to 1 below and this means that damping procedure is more relevant in the first iterations than in the last, where the standard Newton method is recovered.

Finally, we notice that for high voltages the scheme needs more iterations to converge. This phenomena is strictly related to the shape of the initial guess and we see it in detailed in Section **??**.



(a) *Non Linear Poisson residual: damping benefit prodedure.*



(b) t_k *parameter.*

Figure 1.1: (a) Number of iteration against residual for different voltages in a diode test case. (b) Magnitude of the damping parameter t_k.

1.3.3 Continuity equations

Concerning with equation (1.6) we can write the bilinear form as

$$a(u,v) = \int_{\Omega_{Si}} qD_n e^{\varphi^i/V_{th}} \nabla\psi_j \nabla\psi_i \, d\Omega + \int_{\Omega_{Si}} \sigma_n^{i-1} e^{\varphi^i/V_{th}} \psi_j \psi_i \, d\Omega. \qquad (1.34)$$

Even if this form allows an immediate analysis of well-posedness, the choice of using Slotboom variables u_n and u_p causes the onset of overflow problems due to the evaluation of $\exp(\varphi/V_{th})$, which can be a rapidly varying function according to the behaviour of the potential φ.

Therefore special care has to be taken in the treatment of the diffusion coefficient. In view of further discussion we introduce some useful notation. For each set $S \subset \Omega$ having measure $|S|$, we introduce the following averages of a given function g that is integrable on S:

$$\mathcal{M}_S(g) = \frac{\int_S g \, dS}{|S|}, \qquad \mathcal{H}_S = (\mathcal{M}_S(g^{-1}))^{-1}.$$

Notice that $\mathcal{M}_S$ is the usual integral average, while $\mathcal{H}_S$ is the *harmonic average*. It is well-known that the use of the harmonic average provides a superior approximation performance in one spatial dimension [IE83].

The weak form (1.34) is the result of a standard displacement approach, although different variational formulations and therefore different finite element approximations may be used, like a primal mixed approach (PM). First of all it is convenient to reformulate problem (**??**) by using relations (**??**) and (**??**) in a more generical form as:

$$\begin{cases} \nabla \cdot \mathbf{J}_n(n) + \sigma n = f & in \ \Omega_{Si} \\ \mathbf{J}_n = qD_n e^{\varphi/V_{th}} \nabla(e^{-\varphi/V_{th}} n) & in \ \Omega_{Si} \\ n = n_D & on \ \Gamma_{D,Si} \\ \mathbf{J}_n \cdot \mathbf{n} = 0 & on \ \Gamma_{N,Si}. \end{cases} \qquad (1.35)$$

Problem (1.35) can be discretized considering the *Edge Averaged Finite Elements* (EAFE). The complete derivation of this scheme can be found in [XZ99] [ZL12].

The EAFE scheme is particularly suited for problems with a highly variable diffusion coefficient. Furthermore this approach has several good properties, i.e. in 2D simulation if $\mathcal{T}_h$ is a Delaunay partition the system matrix is an M-matrix [BCC98]. The main consequence of this statement is that the solution satisfying the *Discrete Maximum Principle*. This is a notable

property which implies that no negative concentrations are admitted. Unfortunately this property is not anymore valid in 3D framework, because the Delaunay condition on the mesh is not sufficient to guarantee that the system matrix is an M-matrix. A more general condition is presented in [XZ99].

Theorem 1.1 (Zikatanov condition)**.** *The system matrix of the EAFE scheme is an M-matrix if and only if for any fixed edge E of the partition $\mathcal{T}_h$ the following inequality holds*

$$\omega_E = \frac{1}{d(d-1)} \sum_{K \supset E} |k_E^K| cot\theta_E^K \geq 0, \tag{1.36}$$

where $\sum_{K\supset E}$ means summation over all simplexes K containing E, θ_E^K is tha angle between the faces f_i, $f_j \in \mathcal{T}_h$ such that $f_i \bigcap f_j = E$ and k_E^K is the edge in K which does not share any verticies with E.

Observation 1.1. For $d = 2$, condition (1.36) means that the sum of the angles opposite to any edge is less than or equal to π, which implies that the partition is a Delaunay triangulation.

Observation 1.2. Condition (1.36) highlights that in order to satisfy the discrete maximum principle, a partition without obtuse angles is preferable.

We remark that presently meshing algorithm are oriented to care about the minimum angle of the elements, rather than the maximum, this implying that to obtain a mesh which satisfies condition (1.36) is a really difficult task.

Fig.1.2 shows a simple partition of a cube performed with the Synopsis tool SNMESH. For every element we evaluated how many edges do not satisfy condition (1.36). It is clear that there are a lot of edges which do not fulfil the condition and a precise pattern cannot be signed out. When several bad edges belong to a single element we can identify the presence of many obtuse angles.

In order to avoid this problem some alternative solutions are proposed in the literature, like the *Orthogonal Subdomain Collocation method* [PC98], but also this approach is not a definite solution.

Therefore in presence of a negative concentration the most used technique in 3D numerical simulation is to local mesh refinement in the regions where trouble occurs, which often are the ones where the carrier density decreases.

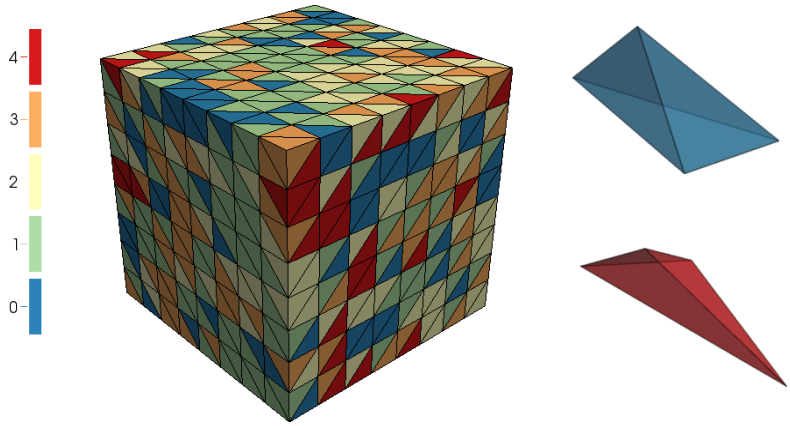


Figure 1.2: Evaluation of the Zikatanov condition over a simple partition. Red elements do not satisfy condition (1.36) over four edges while blue elements fully satisfy the criterion.

Bibliography

[BCC98] R. E. Bank, W. Coughran, and L. C. Cowsar. The finite volume sharfetter-gummel method for steady convection diffusion equations. *Computing and Visualization in Science*, 1:123–136, 1998.

[Deu74] P. Deuflhard. A modified newton method for the solution of ill-conditioned system of nonlinear equations with application to multiple shooting. *Numer. Math*, 22:289–315, 1974.

[IE83] Babuška I. and Osborn J. E. Generlized finite element methods: Their performance and their relation to mixed methods. *Numer. Anal.*, 20:510–536, 1983.

[PC98] M. Putti and C. Cordes. Finite element approximation of the diffusion operator on tetrahedra. *Society for Industrial and Applied Mathematics*, 19:1154–1168, 1998.

[PTVF07] William H. Press, Saul A. Teukoisky, William T. Vetterling, and Brian P. Flannery. *Numerical Recipes, The Art of Scientific Computing*. Cambridge University Press, New York, 2007.

[Qua08] Alfio Quarteroni. *Modellistica Numerica per Problemi Differenziali*. Springer Italia, Milan, 2008.

[QV08] Alfio Quarteroni and Alberto Valli. *Numerical Approximation of Partial Differential Equations*. Springer, 2008.

[Sal10] Sandro Salsa. *Equazioni a Derivate Parziali, metodi, modelli e applicazioni*. Springer Italia, Milan, 2010.

[XZ99] Jinchao Xu and Ludmil Zikatanov. A monotone finite element scheme for convection-diffusion equations. *Mathematics of Computation*, 68:1429–1446, 1999.

[ZL12] L. T. Zikatanov and R. D. Lazarov. An exponential fitting scheme for general convection-diffusion equations on tetrahedral meshes. *math*, pages 455–465, 2012.