Laurea magistrale
in ingegneria matematica

Elaborato di Tesi ...

Titolo progetto di tesi ...

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Indice

Capitolo 1

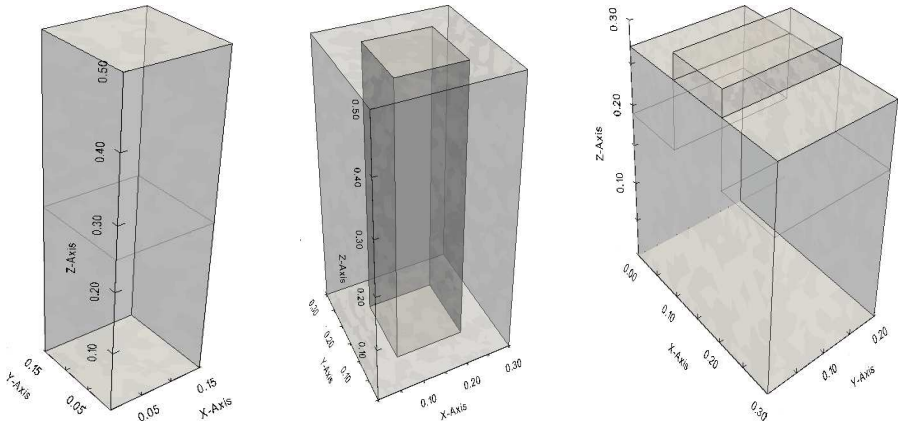
Introduction

1.1 General Introduction

In questa sezione una breve panoramica su FEMOS su cosa è già stato implementato su cosa si vuole fare...

1.2 Case tests presentation

In questa invece andiamo più nello specifico di questo lavoro presentando i casi test che verranno studiati...non penso sia il caso di trattare le equazioni qui dato che c'è tutto un capitolo sul modello e le equazioni usate



(a) (b) (c)

Capitolo 2

Semiconductor model

O forse prima parte...dipende da quello che riusciamo a fare...nel caso la divisione fra il primo ed il secondo capitolo sarebbe approccio formulazione agli spostamenti e duale mista

2.1 DD Model

In this work we deal with mathematical modeling and numerical simulation of different semiconductor devices.

There are several methods to model integrated devices, this project is based on a semi-classical model, in particular we work with the classical Drift-Diffusion model (DD). Maybe this kind of model is the most used for industrial simulation, due to an excellent trade-off between machine time cost and physical accuracy. Nevertheless to describe the propagation of any electromagnetic signal in a medium, we have to start from the system of Maxwell equations, which reads as follows:

$$\begin{cases} \nabla \times \mathbf{H} &= \mathbf{J} + \dfrac{\partial \mathbf{D}}{\partial t} \\ \nabla \times \mathbf{E} &= -\dfrac{\partial \mathbf{B}}{\partial t} \\ \nabla \cdot \mathbf{D} &= \rho \\ \nabla \mathbf{B} &= 0 \end{cases} \tag{2.1}$$

We are able to complete the system with the following set of constitutive laws that characterize the electromagnetic properties of the medium:

$$\begin{aligned} \mathbf{D} &= \epsilon \mathbf{E} \\ \mathbf{B} &= \mu_m \mathbf{H} \end{aligned} \tag{2.2}$$

From (2.1) we elaborate the DD model, through some interesting hypostesis which are:

- Lorentz-Gauge for the vector potential of $\mathbf{B}$.
- Quasi static approximation.

The second one is related with the IC component sizes and characteristics and it is a reasonable hypotesis for our simulations. The system obtained after this suitable approximation looks as follows:

$$\begin{cases} \nabla \cdot (-\epsilon \nabla \varphi) &= \rho & \textit{Poisson equation} \\ \dfrac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} &= 0 & \textit{Continuity equation} \end{cases} \tag{2.3}$$

To close the above system we need to specify the mathematical form of the electric charge density and the electric conduction current density.

It's well known that intrinsic semiconductor does not appreciably allow current flow, for this reason it's usual introducing impurities (called dopants) in the periodic structure. Dopant impurities are divided into two types:

- acceptor type, wich provide positive carriers (holes);
- donor type, wich provide negative carriers (electron).

It is usual point out acceptor concentration with N_A while donor concentration with N_D. However for the electric charge density formulation we are interested only in ionized impurities, thus we obtain the sequent costitutive law:

$$\rho = \underbrace{q(p-n)}_{\rho_{free}} + \underbrace{q(N_D^+ - N_A^-)}_{\rho_{fixed}} \tag{2.4}$$

We emphasize the two kind of charge present in the device: ρ_{fixed} related to ionized impurities and ρ_{free} related to free carriers in band (p and n are the concentration of holes and electron respectively). Notice that we assume N_D^+ and N_A^- time invariant.

In this work we consider only the transport of these two charge carriers in the device. Consistently with this hypotesis the conduction current density can be written as:

$$\mathbf{J} = \mathbf{J_n} + \mathbf{J_p} \tag{2.5}$$

where J_n and J_p are respectively the electric conduction current density of electrons and holes. To model charge current flow we consider two principal mechanisms:

- Diffusion current, according to Fick's law.
- Drift current, according to Ohm's law.

The form of these current densities is expressed by the following relations:

$$\begin{aligned} \mathbf{J_n} &= \overbrace{q\mu_n n\mathbf{E}}^{Drift} + \overbrace{(-qD_n(-\nabla n))}^{Diffusion} \\ \mathbf{J_p} &= q\mu_p p\mathbf{E} + (-qD_p\nabla p) \end{aligned} \tag{2.6}$$

According with the preview hypotesis and replacing the costitutive laws, we obtain the seguent DD model forumulation:

$$\begin{cases} \nabla\cdot(-\epsilon\nabla\varphi) = q(p-n+N_D^+-N_A^-) & \textit{Poisson equation} \\ -q\dfrac{\partial n}{\partial t}+\nabla\cdot(-q\mu_n n\nabla\varphi+qD_n\nabla n) = qR & \textit{Electron Continuity equaiton} \\ q\dfrac{\partial p}{\partial t}+\nabla\cdot(-q\mu_p p\nabla\varphi-qD_p\nabla p) = -qR & \textit{Hole Continuity equaiton} \end{cases} \tag{2.7}$$

The system is an incompletely parbolic initial value/boundary problem in three scalar unkown dependent variables $\varphi(\mathbf{x},t)$, $n(\mathbf{x},t)$ and $p(\mathbf{x},t)$. Notice that the problem is a nonlinearly coupled system of PDE's, because of the presence of the drift terms $n\nabla\varphi$ and $p\nabla\varphi$.

From Maxwell equations we are able to guarantee only that $\mathbf{J}$ is a solenoidal field, we can't say nothing about the properties of $\mathbf{J_n}$ and $\mathbf{J_p}$. For this reason there is a new term in the right hand side. We can interpret $R(\mathbf{x},t)$ as the net rate of generation and recombination.

We consider also the stationary form for our purpose.

$$\begin{cases} \nabla\cdot(-\epsilon\nabla\varphi) = q(p-n+N_D^+-N_A^-) \\ \nabla\cdot(-q\mu_n n\nabla\varphi+qD_n\nabla n) = qR \\ \nabla\cdot(-q\mu_p p\nabla\varphi-qD_p\nabla p) = -qR \end{cases} \tag{2.8}$$

2.2 Resolution of the system

2.2.1 Drawbacks of the Box Methods

While the box method has become the standard technique for the discretization of the continuity equations, it suffers from several drawbacks arising from geometrical considerations. Satisfactory results can be obtained only for acute triangulations. Even one obtuse triangle can lead to a large spike in the solution of the equation.

In this form we can approach to the resolution of the problem only with a completely coupled Newton method. It's well known that there are several issues adopting this way of resolution:

- the jacobian matrix is often quite ill-conditioned and needs appropriate scaling and balancing in order to avoid problems associated with round-off error;
- to ensure convergence of the Newton iterative process, it is particularly important to ensure a very good initial guess for the unknown variables;
- dimension of the linearized problem is of the order of N_{dofs}^3 (N_{dofs} is the number of degree of freedom used for the numerical approximation).

These considerations urges us to pursue an alternative approach: the decoupled Gummel Map. First of all we have to introduce the Maxwell-Boltzamann approximation for the carriers:

$$\begin{aligned} n &= n_i exp\left(\frac{\varphi - \varphi_n}{V_{th}}\right) \\ p &= n_i exp\left(\frac{\varphi_p - \varphi}{V_{th}}\right) \end{aligned} \tag{2.9}$$

Thanks to these expressions we are able to shift the nonlinearity on the poisson equation. Finally we obtain the following system:

$$\begin{cases} \nabla \cdot (-\epsilon \nabla \varphi) + n_i \left(exp\left(\frac{\varphi - \varphi_n}{V_{th}}\right) - exp\left(\frac{\varphi_p - \varphi}{V_{th}}\right)\right) &= q(N_D^+ - N_A^-) \\ -q\frac{\partial n}{\partial t} + \nabla \cdot (-q\mu_n n \nabla \varphi + qD_n \nabla n) &= qR \\ q\frac{\partial p}{\partial t} + \nabla \cdot (-q\mu_p p \nabla \varphi - qD_p \nabla p) &= -qR \end{cases} \tag{2.10}$$

Referring on system (2.10) it's trivial introduce the Gummel Map algorithm:

Gummel Map

Given $\varphi_n^{(0)}$ and $\varphi_p^{(0)}$, $\forall k$ until convergence:

- Solve the Nonlinear Poisson Equation (NLP):

$$\nabla \cdot (-\epsilon \nabla \varphi) + n_i \left(exp\left(\frac{\varphi - \varphi_n^{(k)}}{V_{th}} \right) - exp\left(\frac{\varphi_p^{(k)} - \varphi}{V_{th}} \right) \right) = q(N_D^+ - N_A^-)$$

  Set $\varphi^{(k)} = \varphi$.

- Solve the Linear Electron Contintuity Equation (LEC):

$$-q\frac{\partial n}{\partial t} + \nabla \cdot (-q\mu_n n \nabla \varphi^{(k)} + qD_n \nabla n) = qR$$

  Set $n^{(k)} = n$.

- Solve the Linear Hole Contintuity Equation (LHC):

$$q\frac{\partial p}{\partial t} + \nabla \cdot (-q\mu_p p \nabla \varphi^{(k)} - qD_p \nabla p) = -qR$$

  Set $p^{(k)} = p$.

Actually there are several methods to set up this algorithm and basically they depends on how we represent the conduction current density. Take for example this well-known change of variables proposed by the physicist Jan Slotboom:

$$\begin{aligned} u_n &:= n_i exp\left(-\frac{\varphi_n}{V_{th}} \right) \\ u_p &:= n_i exp\left(\frac{\varphi_p}{V_{th}} \right) \end{aligned} \tag{2.11}$$

As a consequence we can reformulate (2.7) taking into account this interesting series of equivalences:

$$\begin{aligned} \mathbf{J_n} = q\mu_n \left(-n\nabla\varphi + V_{th}\nabla\left(u_n exp\left(\frac{\varphi}{V_{th}} \right) \right) \right) \\ = q\mu_n \left(-n\nabla\varphi + V_{th}\nabla u_n exp\left(\frac{\varphi}{V_{th}} \right) + n\nabla\varphi \right) \\ = qD_n exp\left(\frac{\varphi}{V_{th}} \right) \nabla u_n \end{aligned}$$

The new Gummel Map algorithm read as follows:

Gummel Map

Given $u_n^{(0)}$ and $u_p^{(0)}$, $\forall k$ until convergence:

- Solve the Nonlinear Poisson Equation (NLP):

$$\nabla \cdot (-\epsilon \nabla \varphi) + u_n^{(k)} exp\left(\frac{\varphi}{V_{th}}\right) - u_p^{(k)} exp\left(\frac{-\varphi}{V_{th}}\right) = q(N_D^+ - N_A^-)$$

  Set $\varphi^{(k)} = \varphi$.

- Solve the Linear Electron Contintuity Equation (LEC):

$$-q\frac{\partial u_n exp\left(\frac{\varphi^{(k)}}{V_{th}}\right)}{\partial t} + \nabla \cdot (qD_n exp\left(\frac{\varphi^{(k)}}{V_{th}}\right) \nabla u_n) = qR$$

  Set $u_n^{(k)} = u_n$.

- Solve the Linear Hole Contintuity Equation (LHC):

$$q\frac{\partial u_p exp\left(\frac{-\varphi^{(k)}}{V_{th}}\right)}{\partial t} + \nabla \cdot (qD_n exp\left(\frac{-\varphi}{V_{th}}\right) \nabla u_p) = -qR$$

  Set $u_p^{(k)} = u_p$.

2.3 Nonlinear Poisson Equation

In this section we'll show how the NLP is resolved in the code. Many decisions have been taken on the management of the interface. Note that the electrostatic problem must be resolved on the whole domain and the right hand side changes from region to region.

Qui dipende da come vogliamo introdurre FEMOS...sarebbe carino far capire la scelta che stata fatta di porre nei nodi di frontiera del silicio il valore della forzante e della reazione del silicio.Ma ovviamente questo discorso necessita una introduzione sui casi test.

2.3.1 Weak formulation

Let us consider the linearized problem (qua ci vuole la referenza a quella linearizzata) in a more generalized form which reads as follows:

$$\begin{cases} \nabla \cdot (-\epsilon \nabla \varphi) + \sigma^{(k)}(\mathbf{x})\varphi &= f^{(k)}(\mathbf{x}) & in\ \Omega \\ \varphi &= \varphi_D & on\ \Gamma_D \\ \nabla \varphi \cdot \mathbf{n} &= 0 & on\ \Gamma_N \end{cases} \tag{2.12}$$

For the sake of simplicity we summerize the reaction and force term in σ and f, but we kept visible the iteration dependence. The well-posedness of such problem is ensured by several (and reasonable) hypotesis:

- $\epsilon \in L^\infty(\Omega)$ and $\exists m$ s.t. $0 < m \leq \epsilon$ (a.e.) in Ω;
- $\sigma \in L^\infty(\Omega)$ and $\exists m$ s.t. $0 < m \leq \sigma$ (a.e.) in Ω.

We proceed with the classical displacement weak formulation. Given $\varphi_D \in H^{1/2}(\Gamma_D)$ and $f \in L^2(\Omega)$ find $\varphi \in H^1(\Omega)$ such that

$$\int_\Omega \epsilon \nabla\varphi \nabla v \, d\Omega + \int_\Omega \sigma^{(k)} \varphi v \, d\Omega = \int_\Omega f^{(k)} v \, d\Omega \qquad \forall v \in H^1_{\Gamma_D}(\Omega) \tag{2.13}$$

2.3.2 Numerical approximation

2.3.3 Damping

Interessante fare vedere qualche grafico con qualche controllo della convergenza...

2.4 Continuity Equation

2.4.1 Weak formulation

Without loss of generality we consider only the electron continuity equation (similar reasoning could be make for the hole continuity equation). Problem referenza al problema is a classical diffusion-advection-reaction (DAR) problem written in conservative form. We will treat this PDE's equation likewise Poisson equation with the standard displacement weak formulation.

Be carefull about the right hand side: in the operation of many devices this term generates mass; this implies that a new reaction term is usually added in the left side of the equation:

$$R_n = \sigma n - f \tag{2.14}$$

$$\begin{cases} \dfrac{\partial n}{\partial t} + \nabla \cdot (-D_n \nabla n) + \nabla \cdot (\mu_n \nabla \varphi^{(k)} n) + \sigma n &= f & \text{in } \Omega \\ n &= n_D & \text{on } \Gamma_D \\ \nabla n \cdot \mathbf{n} &= 0 & \text{on } \Gamma_N \end{cases} \tag{2.15}$$

Given $n_D \in H^{1/2}(\Gamma_D)$ and $f \in L^2(\Omega)$ find $n \in H^1(\Omega)$ such that:

$$\begin{cases} \dfrac{\partial n}{\partial t} + \nabla \cdot (-D_n \nabla n) + \mu_n \nabla \varphi^{(k)} \nabla n + (\mu_n \Delta \varphi^{(k)} + \sigma) n &= f & \text{in } \Omega \\ n &= n_D & \text{on } \Gamma_D \\ \nabla n \cdot \mathbf{n} &= 0 & \text{on } \Gamma_N \end{cases} \tag{2.16}$$

with $\Gamma_D \cap \Gamma_N = \varnothing$, $\Gamma_D \cup \Gamma_N = \partial\Omega$ and where $\mathbf{n}$ is the outward normal vector on Ω. We respect the standard hypotesti for the wellposdness of the problem:

- $D_n \in L^\infty(\Omega)$ and $\exists\, m$ s.t. $0 < m \leq D_n$ a.e. in Ω;
- $\sigma \in L^\infty(\Omega)$ and $\exists\, m$ s.t. $0 < m \leq \sigma$ a.e. in Ω;
- $\mu_n \nabla \varphi \in (W^{1,\infty}(\Omega))^d$.

formulazione con tempo?

2.4.2 Numerical approximation

Partiamo con una semidiscretizzazione spaziale e poi trattiamo anche quella temporale?

Descrizione dettagliata (o meno?) del metodo implementato FVSG

2.5 Maximum discrete principle

Scriviamo qualcosa in merito?Quanto approfondito?

2.6 The current calculation problem

In many physical and engineering problems the real interesting variable of the conservation law is the flux in the domain or on specific surfaces and boundaries. The study of micro and nano electronics devices doesn't except this observation, in fact most of all models are oriented to obtain a satisfactory description of the current density. We know that the primal and not mixed formulation for the continuity equation doesn't resolved the flux density. The conseguence of this fact is a binding post-processing of the quantities computed in order to reconstruct the current density of electrons and holes. It's evident which this part covers a lead role in the device simulation: as we are satisfied of the impressive results of the finite element scheme, it will be reather regrettable to lost the accuracy of our simulation during the computation of the current density. About this question many academics propose different solutions and the relative literature is boundless. Nevertheless the problem shows various aspects to take into account, among these there are some which every good method should be respect:

- reduced computational cost;
- easy extension to 3D simulation;
- detains some useful properties like orthogonal conservation across a generic surface of the domain;
- preserve consistency with the numerical scheme adopted.

It's not trivial ensure everyone of these points, thus move on toward a unique choice of a method is a delicate matter. Luckily there's some *main stone* which offers ever a good start point whence achieve new results. Probably the most known and recognized by the inherent literature is the *Sharfetter-Gummel formula*.

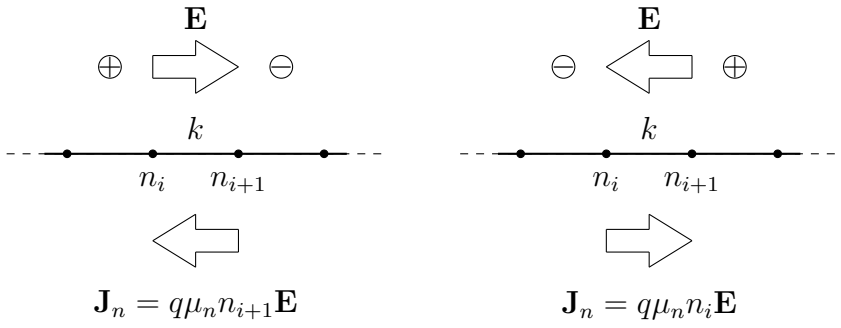
2.6.1 Scharfetter-Gummel formula

Consider the resolution of the continuity equation along a monodimensional domain. For the sake of simiplicity we contemplate a uniform partition (this hypotesis is not necessary for a more generic analysis). Moreover on every nodes is defined the electrostatic potential φ, and on every elements the relative electrostatic field $\mathbf{E}$. In order to avoid redundant considerations and calculuses, we proceed with our analysis considering only the current density of electrons ($\mathbf{J}_n$).

In 1969 D. Scharfetter and H.K. Gummel (two scientists of Bell Labs), introduced a formula to compute the current density in this case, given φ and the density solution (n) on every nodes. This innovative approach led

for the twenty years to follow every simulation which contemplates electric-devices. Morover many mathematics discover important properties about this method questa parte la vorrei fare meglio.

La potenza di questo metodo riesiede nella possibilità di gestire le varie situazioni di upwinding. Considerando la figura la formula recita:



$$J_n^k = -q\frac{D_n}{h}\left[n_{i+1}\mathcal{B}\left(\frac{\Delta\varphi^k}{V_{th}}\right) - n_i\mathcal{B}\left(-\frac{\Delta\varphi^k}{V_{th}}\right)\right] \qquad \forall k = 1 \dots N_{elements} \tag{2.17}$$

where $\Delta\varphi^k = \varphi_{i+1} - \varphi_i$

2.6.2 Extension for the 3D case

The extension of this formula for the 3D case is not trivial. We show the method for the computation of the current density of electrons (the extension for the current density of holes is quite similar). We remark the quasi fermi formula for current density:

$$\mathbf{J}_n = -q\mu_n n\nabla\varphi_n \tag{2.18}$$

where φ_n is the quasi fermi potential level. Let us write (2.18) in function of potential and in a canonic form:

$$\mathbf{J}_n\frac{exp\left(\frac{\varphi_n - \varphi}{V_{th}}\right)}{q\mu_n n_i} + \nabla\varphi_n = 0 \tag{2.19}$$

Now consider a generic discretization for $\mathbf{J}_n$ and φ_n, for example finite element with $\mathbb{P}_1$ functions as bases (vero che si puo scegliere qualsiasi discretizzazione con una qualsiasi base?), we'll call these spaces $[V_h]^d$ and V_h (with h we intend the step of discretization and d is the dimension of simulation). We are able to test (2.19) against $\mathbf{q}^h \in [V_h]^d$, we choose three different $\mathbf{q}^h$:

$$\mathbf{q}^h_{1,2,3} = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\} \tag{2.20}$$

We show the variational form for a generic element K of the discretization:

$$\int_K \frac{exp\left(\frac{\varphi_n - \varphi}{V_{th}}\right)}{q\mu_n n_i} \mathbf{J}^h_n \cdot \mathbf{q}^h_i \, dK + \int_K \nabla\varphi^h_n \cdot \mathbf{q}^h_i \, dK = 0 \qquad \forall i = 1,2,3 \tag{2.21}$$

La questione è: $\nabla\varphi^h_n \in [V_h]^d$??. Possiamo dirlo sapendo che $\varphi^h_n \in V_h$??

We know that $\nabla\varphi_n \in \mathbb{P}_0$ and without any approximation (except for the discretization) we obtain the sequent formula for the current density components:

$$[\mathbf{J_n}]_i = -\mathbb{H}_K \left(q\mu_n n_i exp\left(\frac{\varphi - \varphi_n}{V_{th}}\right)\right) \frac{\partial\varphi^h_n}{\partial x_i} \quad i = 1...d \quad \forall K \in \tau_h \tag{2.22}$$

where $\mathbb{H}_K(f)$ is the armonic average on the elment K of the function f.

Although resolve the armonic average with a comlete 3D integration may be expensive in calculation time and propably not necessary. One approximation of this integral would be pass from a 3D integration to 1D integration along one edge of the element K.

$$\left(\frac{\int_K f^{-1}\, dK}{|K|}\right)^{-1} \simeq \left(\frac{\int_{e*} f^{-1}\, de}{|e^*|}\right)^{-1} \tag{2.23}$$

The approximation (2.23) is valid if we consider the correct edge.

Consider a quantity defined on the verteces:

$$\Phi := \varphi - \varphi_n \tag{2.24}$$

which is the difference between the electrostatic potential and the quasi fermi potential level. Now for every element consider two vertices: $\mathbf{x}_m$ s.t. $\Phi(\mathbf{x}_m) = \Phi_m := min_K(\Phi)$ and $\mathbf{x}_M$ s.t. $\Phi(\mathbf{x}_M) = \Phi_M := max_K(\Phi)$. Obviously it exists only one edge which connects these two points and on this one we perform the 1D integration (2.23). First of all as we reduce the dimension is feasible to represent $\sigma(\mathbf{x})$ in a easier mode as follows:

$$\sigma_n(s) = q\mu_n n_i exp\left(\Phi_m + (\Phi_M - \Phi_m)\frac{s - s_m}{|e^*|}\right) \tag{2.25}$$

where $s \in [s_m, s_M]$ is the parameter refered to the edge e^* s.t. $\sigma_n(s_m) = \sigma_n(\mathbf{x}_m)$ and $\sigma_n(s_M) = \sigma_n(\mathbf{x}_M)$. We can easily resolve (2.23) with the substitution of variable:

$$\eta := \frac{s - s_m}{|e^*|}$$

this lead us to the sequent steps of integration:

$$\begin{aligned}\int_{e^*} \sigma_n^{-1}\, de &= |e^*| \int_0^1 \frac{exp\left(-\Phi_m - (\Phi_M - \Phi_m)\eta\right)}{q\mu_n n_i}\, d\eta \\ &= |e^*| \frac{exp(-\Phi_m)}{q\mu_n n_i} \frac{exp(\Phi_m - \Phi_M) - 1}{\Phi_m - \Phi_M} \\ &= |e^*| \frac{exp(-\Phi_m)}{q\mu_n n_i} \frac{1}{\mathbf{B}(\Phi_m - \Phi_M)}\end{aligned}$$

finally we obtain:

$$\int_K \sigma_n^{-1}\, dK \simeq q\mu_n n_i exp(\Phi_m)\mathbf{B}(\Phi_m - \Phi_M) \tag{2.26}$$

Similar results may be obtained repeating the integration and considering s_M as start point:

$$\int_K \sigma_n^{-1}\, dK \simeq q\mu_n n_i exp(\Phi_M)\mathbf{B}(\Phi_M - \Phi_m) \tag{2.27}$$

Numerical results (qua sarebbe carino fare un po' di test con una parte o l'altra della formula per mettere in crisi) shows that the best choice is e linea combination of these approzimations as follows:

$$\mathbf{J_n}^K = -q\mu_n \left[\frac{n_{min}\mathbf{B}(-\Delta\Phi_{max}) + n_{max}\mathbf{B}(\Delta\Phi_{max})}{2}\right] \nabla\varphi_n^h \tag{2.28}$$

This approach is the natrual extension of (2.17).

2.6.3 Residue Method

Contact method

In the following we present an accurate method for the evaluation of boundary integrals in semiconductor device based on the work . It's well known that the evaluation of boundary integrals is a difficult task occuring routinely in electron device simulations. In general, given a contact Γ_i, fluxes of current density to be calculated assume the following form:

$$\mathcal{I}_i^\nu = \int_{\Gamma_i} \mathbf{J}_\nu(\nu) \cdot \mathbf{n}\, d\Gamma_i \qquad \nu = \{n, p\} \tag{2.29}$$

where as usual $\mathbf{n}$ is the unit outward normal of the domain boundary. Difficulties in the numerical evalutaion of (2.29) arise from singularities in spatial derivatives of the approximate solution n^h or p^h near the contact edges, due to a change in the boundary condition type (from Dirichlet to

Neumann) at the contact ends. In this work we extend the residue method on the 3D case and we confirm the optimal results obtained previously, matching them with SDEVICE (come bisogna scirvere il software che politica usare?). Moreover we remark that the method can be succesfully applied to a wide spread of applications, including contact charges, carrier quantum probability fluxes and heat fluxes.

Before go further with the presentation of the results, it's useful look up the anlysis made in Citazione and adapt it to our case. Before applying boudnary conditions, the discretized form of referenza equazione reads:

$$\sum_{j\in\eta} A_{ij}\nu_j\psi_j(x_j) = b_i \qquad \forall i \in \eta \tag{2.30}$$

A_{ij} is the K_{FVSG} global matrix but it's possibile use every discretization scheme. We can split the set of total nodes in contact node η_g and the complementary part η_n. The values of ν_j are known on the contacts and (2.30) can be rewritten as follows:

$$\begin{cases} \sum_{j\in\eta_n} A_{ij}\nu_j\psi_j(x_j) = b_i - \sum_{j\in\eta_g} A_{ij}\nu_j\psi_j(x_j) & \forall i \in \eta_n \\ \\ \sum_{j\in\eta_n} A_{ij}\nu_j\psi_j(x_j) = b_i - \sum_{j\in\eta_g} A_{ij}\nu_j\psi_j(x_j) & \forall i \in \eta_g \end{cases} \tag{2.31}$$

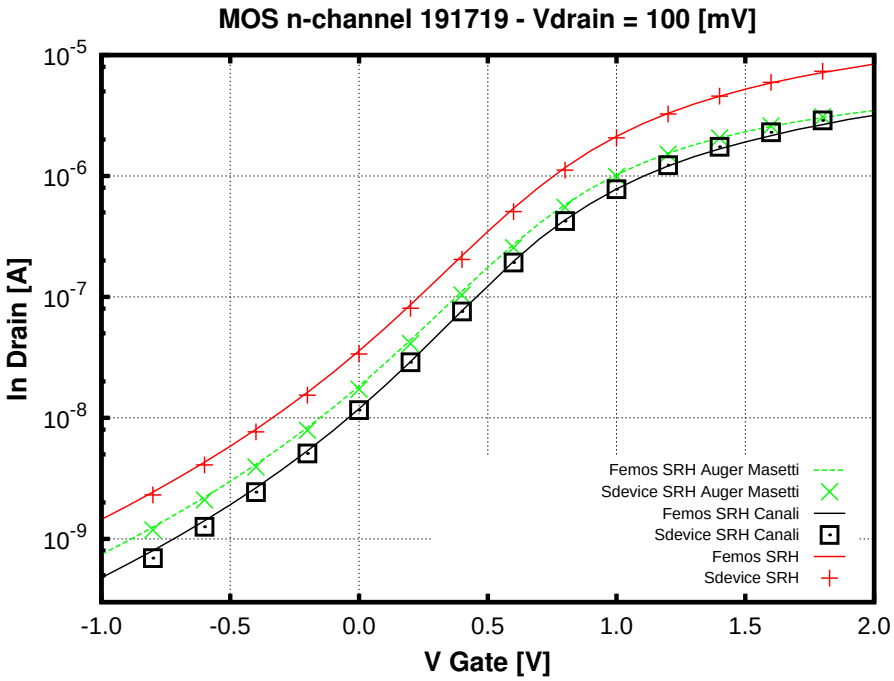
The first set of equations is then solved for the problem unknowns ν_j (carrier density) while the second can be used for boundary flux estimation as described in the folowing. Consider a different test function v_i^h defined as:

$$v_i^h = \sum_{j\in\eta_{gi}} \psi_j \tag{2.32}$$

where η_{gi} is the set of nedes lying on contact Γ_i. We can rewrite (2.29) as follows:

$$\begin{aligned} \mathcal{I}_i^\nu &= \int_{\Gamma_i} \mathbf{J}_\nu(\nu)\cdot\mathbf{n}\, d\Gamma_i = \sum_{j=1}^{n_d} \int_{\Gamma_j} \mathbf{J}_\nu(\nu)\cdot\mathbf{n}\, v_i^h\, d\Gamma_j \\ &= \sum_{i\in\eta_{gi}} \sum_{j=1}^{n_d} \int_{\Gamma_j} \mathbf{J}_\nu(\nu)\cdot\mathbf{n}\,\psi_i\, d\Gamma_j = \sum_{i\in\eta_{gi}} \int_{\partial\Omega} \mathbf{J}_\nu(\nu)\cdot\mathbf{n}\,\psi_i\, d\partial\Omega \\ &= \sum_{i\in\eta_{gi}} \left[\int_\Omega \nabla\cdot\mathbf{J}_\nu(\nu)\psi_i\, d\Omega + \int_\Omega \mathbf{J}_\nu(\nu)\cdot\nabla\psi_i\, d\Omega\right] \\ &= \sum_{m\in\eta_{gi}} \left[\sum_{j\in\eta} A_{ij}\nu_j\psi_i - b_i\right] \end{aligned} \tag{2.33}$$

Results


MOS n-channel 191719 - Vdrain = 100 [mV]
ln Drain [A]
10-5
10-6
10-7
10-8
10-9
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
V Gate [V]
Femos SRH Auger Masetti
Sdevice SRH Auger Masetti
Femos SRH Canali
Sdevice SRH Canali
Femos SRH
Sdevice SRH

Bulk method

Now the question is: it's possible extend the residue technique at the calculation of current inside the domain? The answer at this question is not trivial. A good start point is the work of J.R. Hughes and Larson in the article The Continuous Galerikin Method Is Locally Conservative.The aim of their work is well exposed in the title and the conclusion is that this important property (locally conservation) is ensured less than the existence of an **auxiliary flux** denoted as $H(\omega)$ (with $\omega \subseteq \Omega$). To extract the statement of global and local conservation from the variational formulation, thay need to be able to set the weighting function to one. Obviously this is possible if $\Gamma_g = \varnothing$. In order to include every case an extended weak formulation is presented: consider η the set of all verteces of the discrete domain and η_g the subset of verteces on Dirichlet boundaries. Now we are able to define the discrete space $\mathcal{V}^h := span\{\psi_i\}_{i\in\eta-\eta_g}$ and $V^h := \mathcal{V}^h \oplus span\{\psi_i\}_{i\in\eta_g}$, where ψ_i is the basis function assiociated with the node i. The last space is the completion of the usual finite element space ($\mathcal{V}^h$). Note that the constant function having value 1 is contained in V^h. The modified form of Galerkin's method is given by:

Find $u^h \in \mathcal{S}^h$ and $H^h(\Omega) \in V^h - \mathcal{V}^h$ such that

$$(W^h, H^h(\Omega))_{\Gamma_g} = B(W^h, u^h) - L(W^h) \qquad \forall W^h \in V^h \tag{2.34}$$

Note that (2.34) splits into two subproblems:

$$0 = B(w^h, u^h) - L(w^h) \qquad \forall w^h \in \mathcal{V}^h \tag{2.35}$$

$$(W^h, H^h(\Omega))_{\Gamma_g} = B(W^h, u^h) - L(W^h) \qquad \forall W^h \in V^h - \mathcal{V}^h \tag{2.36}$$

Equation (2.36) is a problem which determines $H^h(\Omega)$. In it we assume u^h is already determined by (2.35). The coefficient matrix for (2.36) is the mass matrix associated with Γ_g

$$\sum_{j\in\eta_g} (\psi_i, \psi_j) H^h_j(\Omega) = B(\psi_i, u^h) - L(\psi_i) \qquad \forall i \in \eta_g \tag{2.37}$$

Il prodotto sul bordo genera la medesima matrice di massa?E cosa succede nei punti che non sono di Dirichlet?Non pu essere formulato in questo modo il problema?

In ogni caso noi abbiamo provato ad estendere il secondo problema ad ogni elemento interno che intersechi o meno i bordi di Dirichlet. Questo a cosa corrsiponde?

Abbiamo interpretato la costruzione per elemento come se in ogni elemento il problema avesse delle condizioni di dirichlet che si affacciano con gli altri elementi adiacenti. Se assumiamo che questa procedura sia corretta allora penso che i successivi ragionamenti stiano in piedi.

Sempre nell'articolo viene testata la formulazione estesa contro la funzione test costante e si ottiene la seguente equivalenza:

$$\int_{\Gamma_g} H^h(\Omega)\, d\Gamma = \int_{\Gamma_h^+} (a_n u^h - h^+)\, d\Gamma - \int_{\Gamma_h^-} h^-\, d\Gamma - \int_{\Omega} f\, d\Omega \tag{2.38}$$

avendo assunto ogni nodo come Dirichlet allora valgono le seguenti affermazioni:

- $\Gamma_g = \partial\Omega$
- $\Gamma_h = \varnothing$

quindi possiamo affermare che per ogni elemento vale:

$$\int_{\partial\Omega} H^h(\Omega)\, d\Gamma = -\int_{\Omega} f\, d\Omega \tag{2.39}$$

Ora vorrei ripartire dal problema di partenza:

$$\begin{aligned} -\nabla \cdot \mathbf{J} &= f \\ \textstyle\int_\Omega -\nabla \cdot \mathbf{J} \Psi_k\, d\Omega &= \textstyle\int_\Omega f \Psi_k\, d\Omega \qquad \forall k = 1...N_{elements} \\ \textstyle\int_K -\nabla \cdot \mathbf{J}\, d\Omega &= \textstyle\int_K f\, d\Omega \qquad \forall k = 1...N_{elements} \\ \textstyle\int_{\partial K} -\mathbf{J} \cdot \mathbf{n}\, d\Omega &= \textstyle\int_K f\, d\Omega \qquad \forall k = 1...N_{elements} \end{aligned} \tag{2.40}$$

La domanda quindi è possiamo in qualche modo dire che:

$$H^h(K) = \mathbf{J} \cdot \mathbf{n} \tag{2.41}$$

Entrambe le quantità sono definite sul bordo dell'elemento, inoltre la ricostruzione dalle componenti normali al vettore densità di corrente non è impossibile. Tuttavia occorre passare prima a definire la grandezza sulle facce del tetraedro:

- Calcolo delle quantità nodali $H_j^h(\Omega)$
- Redistribuzione dei valori sulle facce (metodo percentuale proporzionalmente alle aree) $\bar{H}_j^h(\Omega)$
- Ortogonalizzazione dei contributi normali alle facce $\bar{H}_j^h(\Omega)\mathbf{n}_j$ tramite procedura alla Grand-Shmidt $H_j^* \mathbf{n}_j^*$
- Calcolo del vettore densità di corrente nell'elemento $\mathbf{J} = \sum_{i=1}^{4} H_j^* \mathbf{n}_j^*$

2.7 First results

Capitolo 3

Dual mixed method (or thermo electric system?)