

LAUREA MAGISTRALE
IN INGEGNERIA MATEMATICA

Elaborato di Tesi ...



Titolo progetto di tesi ...

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Capitolo 1

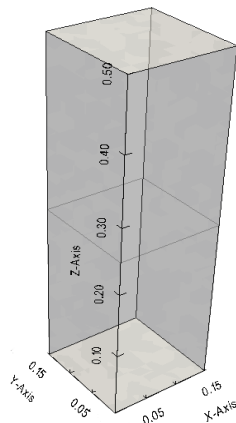
Introduction

1.1 General Introduction

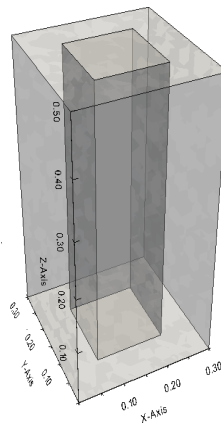
In questa sezione una breve panoramica su FEMOS su cosa è già stato implementato su cosa si vuole fare...

1.2 Case tests presentation

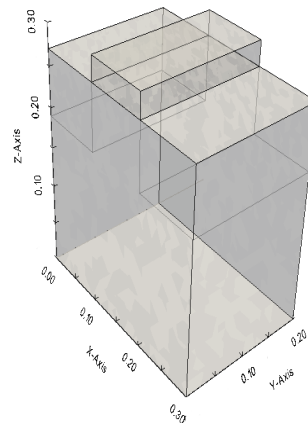
In questa invece andiamo più nello specifico di questo lavoro presentando i casi test che verranno studiati...non penso sia il caso di trattare le equazioni qui dato che c'è tutto un capitolo sul modello e le equazioni usate



(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:

$$\left\{ \begin{array}{l} \nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \\ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \\ \nabla \cdot \mathbf{D} = \rho \\ \nabla \mathbf{B} = 0 \end{array} \right. \quad (2.1)$$

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

$$\begin{array}{l} \mathbf{D} = \epsilon \mathbf{E} \\ \mathbf{B} = \mu_m \mathbf{H} \end{array} \quad (2.2)$$

From (2.1) we elaborate the DD model, through some interesting hypothesis 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 hypothesis for our simulations. The system obtained after this suitable approximation looks as follows:

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

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, which provide positive carriers (holes);
- donor type, which 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 constitutive law:

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

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 hypothesis the conduction current density can be written as:

$$\mathbf{J} = \mathbf{J}_n + \mathbf{J}_p \quad (2.5)$$

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 constitutive laws, we obtain the seguent DD model formulation:

$$\left\{ \begin{array}{ll} \nabla \cdot (-\epsilon \nabla \varphi) &= q(p - n + N_D^+ - N_A^-) & \text{Poisson equation} \\ -q \frac{\partial n}{\partial t} + \nabla \cdot (-q\mu_n n \nabla \varphi + qD_n \nabla n) &= qR & \text{Electron Continuity equation} \\ q \frac{\partial p}{\partial t} + \nabla \cdot (-q\mu_p p \nabla \varphi - qD_p \nabla p) &= -qR & \text{Hole Continuity equation} \end{array} \right. \tag{2.7}$$

The system is an incompletely parabolic initial value/boundary problem in three scalar unknown 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.

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

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-Boltzmann approximation for the carriers:

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

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

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

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 Continuity Equation (LEC):

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

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

- Solve the Linear Hole Continuity Equation (LHC):

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

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:

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

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

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

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 Continuity Equation (LEC):

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

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

- Solve the Linear Hole Continuity Equation (LHC):

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

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:

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

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

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

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:

$$R_n = \sigma n - f \quad (2.14)$$

$$\left\{ \begin{array}{ll} \frac{\partial n}{\partial t} + \nabla \cdot (-D_n \nabla n) + \nabla \cdot (\mu_n \nabla \varphi^{(k)} n) + \sigma n & = f \quad \text{in } \Omega \\ n & = n_D \quad \text{on } \Gamma_D \\ \nabla n \cdot \mathbf{n} & = 0 \quad \text{on } \Gamma_N \end{array} \right. \quad (2.15)$$

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

$$\left\{ \begin{array}{ll} \frac{\partial n}{\partial t} + \nabla \cdot (-D_n \nabla n) + \mu_n \nabla \varphi^{(k)} \nabla n + (\mu_n \Delta \varphi^{(k)} + \sigma)n & = f \quad \text{in } \Omega \\ n & = n_D \quad \text{on } \Gamma_D \\ \nabla n \cdot \mathbf{n} & = 0 \quad \text{on } \Gamma_N \end{array} \right. \quad (2.16)$$

with $\Gamma_D \cap \Gamma_N = \emptyset$, $\Gamma_D \cup \Gamma_N = \partial\Omega$ 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

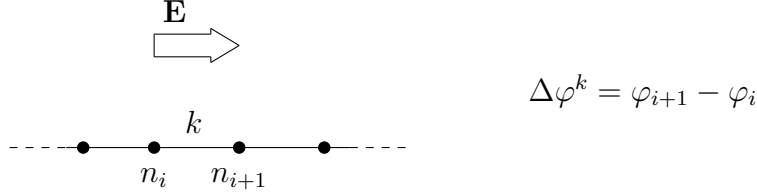
Scriviamo qualcosa in merito? Quanto approfondito?

2.6 The current calculation problem

Qua dobbiamo trovare un'introduzione che mette in luce i problemi di conto che escono fuori nel postprocessing del calcolo della corrente. Se davvero il problema fosse la non ottimale risoluzione del potenziale si potrebbero fare delle prove con il modulo mechanical (di fondo lo sforzo è assimilabile alla densità di corre potrebbero fare delle probe con float (occorre generalizzare il codice al tipo voluto lavoro lungo ma si può fare))

2.6.1 Scharfetter Gummel

We remark the well known *Scharfetter Gummel* equation for the carriers current density over the k^{th} 1D element. It was proposed in 1969 by D. Scharfetter and H.K. Gummel (two scientists of Bell Labs). We point out some specific notation for the 1D case:



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

$$J_p^k = -q \frac{D_p}{h} \left[p_{i+1} \mathcal{B} \left(-\frac{\Delta \varphi^k}{V_{th}} \right) - p_i \mathcal{B} \left(\frac{\Delta \varphi^k}{V_{th}} \right) \right] \quad (2.18)$$

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:

$$\mathbf{J}_n = -q \mu_n n \nabla \varphi_n \quad (2.19)$$

where φ_n is the quasi fermi potential level. Let us write (2.19) in function of potential and in a canonic form:

$$\mathbf{J}_n \frac{\exp \left(\frac{\varphi_n - \varphi}{V_{th}} \right)}{q \mu_n n_i} + \nabla \varphi_n = 0 \quad (2.20)$$

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 (2.20) against $\mathbf{q}^h \in [V_h]^d$, we choose three different \mathbf{q}^h :

$$\mathbf{q}_{1,2,3}^h = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\} \quad (2.21)$$

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

$$\int_K \frac{\exp \left(\frac{\varphi_n - \varphi}{V_{th}} \right)}{q \mu_n n_i} \mathbf{J}_n^h \cdot \mathbf{q}_i^h dK + \int_K \nabla \varphi_n^h \cdot \mathbf{q}_i^h dK = 0 \quad \forall i = 1, 2, 3 \quad (2.22)$$

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

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:

$$[\mathbf{J}_n]_i = -\mathbb{H}_K \left(q\mu_n n_i \exp \left(\frac{\varphi - \varphi_n}{V_{th}} \right) \right) \frac{\partial \varphi_n^h}{\partial x_i} \quad i = 1 \dots d \quad \forall K \in \tau_h \quad (2.23)$$

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 .

$$\left(\frac{\int_K f^{-1} dK}{|K|} \right)^{-1} \simeq \left(\frac{\int_{e^*} f^{-1} de}{|e^*|} \right)^{-1} \quad (2.24)$$

The approximation (2.24) is valid if we consider the correct edge.

This approach is the natrual extension of (2.17), indeed if we consider $d = 1$ and resolve the integrals we obatin **aggiungere i passaggi per dimostrare l'equivalenza con il caso 1D**.

$$\mathbf{J}_n^k = -\frac{q}{2}\mu_n \left[n_{min}^k \mathcal{B} \left(-\frac{\Delta \Phi_{max}}{V_{th}} \right) + n_{max}^k \mathcal{B} \left(\frac{\Delta \Phi_{max}}{V_{th}} \right) \right] \nabla \varphi_n^h \quad (2.25)$$

$$\mathcal{M}(n^h) = \frac{\int_k n^h}{|k|} \quad \mathcal{H}(n^h) = \left(\frac{\int_k (n^h)^{-1}}{|k|} \right)^{-1}$$

$$\Phi^h = \varphi_i^h - \varphi_n^h \quad \Phi_M^k = \max_{i \in K} (\Phi^h / V_{th}) \quad \Phi_m^k = \min_{i \in K} (\Phi^h / V_{th})$$

$$n_{min}^k = n_i \exp(\Phi_m^k / V_{th}) \quad n_{max}^k = n_i \exp(\Phi_M^k / V_{th}) \quad \Delta \Phi_{max}^k = \Phi_M^k - \Phi_m^k$$

2.6.2 Residue Method

- η are all vertexes, η^e are the vertexes of the element e
- $V^h = \text{span}\{\psi_i\}_{i \in \eta - \eta_g} \oplus \text{span}\{\psi_i\}_{i \in \eta_g}$ (η_g are the vertexes on Dirichlet boundary)
- $H^h(\Omega^e)$ is the **auxiliary flux** denoted as $H(\Omega^e) : \gamma^e \rightarrow \mathbb{R}$ ($\gamma^e = \partial \Omega^e$)

$$(W^h, H^h(\Omega^e))_{\gamma^e} = B_\Omega^e(W^h, u^h) - L_\Omega^e(W^h) - (W^h, H^h(\Omega))_{\Gamma_g \cap \Gamma_e} \quad \forall W^h \in V^h$$

$$\sum_{j \in \eta^e} (\psi_i, \psi_j)_{\gamma^e} H_j^h(\Omega^e) = \sum_{j \in \eta^e} B(\psi_i, \psi_j)_{\Omega^e} u_j - L(\psi_i)_{\Omega^e} - \sum_{j \in \eta^e} (\psi_i, \psi_j)_{\Gamma_g \cap \Gamma_e} H_j^h(\Omega) \quad \forall i \in \eta^e$$

The residue method reads as follows:

$$\mathbf{J} \text{ in } \Omega \quad \mathbf{H}_e = K_{FSGV}^e \mathbf{u}_e - \mathbf{F}_e \quad \mathbf{J}_e(\vec{x}) = \sum_{j \in \eta^e} [\mathbf{H}_e]_j \vec{\tau}_j^e(\vec{x}) \quad \vec{\tau}_j^e(\vec{x}) = \frac{\vec{x} - \vec{x}_j}{|e|}$$

$$\Phi \text{ on } \Gamma_g \quad \mathbf{H} = K_{FSGV} \mathbf{u} - \mathbf{F} \quad \Phi_g = \mathbf{H} \cdot \boldsymbol{\Upsilon}_{\eta_g} \quad [\boldsymbol{\Upsilon}_{\eta_g}]_i = (i \in \eta_g)$$

2.7 First results

Capitolo 3

Dual mixed method (or thermo electric system?)