TCAD Theory

Release 0.0.1

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CONTENTS:

CHAPTER

ONE

CHANGES

1.1 Version 0.0.2

Fix formula in equation (7.2). The notation in *Transient Method* has been updated and expanded.

1.2 Version 0.0.1

Fixed typo for b_1 in equation (7.1).

CHAPTER

TWO

EQUATION SYSTEM

2.1 Density of States

$$E_C = -\chi - q\psi$$
$$E_V = E_C - E_G$$

At equilibrium:

$$n = N_C \gamma_n(\eta_n) \exp(\eta_n)$$
$$\eta_n = \frac{E_F - E_C}{kT}$$
$$p = N_V \gamma_p(\eta_p) \exp(\eta_p)$$
$$\eta_p = \frac{E_V - E_F}{kT}$$

CHAPTER

THREE

SCHARFETTER-GUMMEL

3.1 Bernoulli Function

This derivation is partly based on [[Pin90]].

Starting with

$$J = \alpha n + \beta \nabla n$$

where β is a function of x

$$\int_{x_0}^{x_1} \frac{\partial x}{\beta} = \int_{n_0}^{n_1} \frac{\partial n}{J - \alpha n}$$

For the left side, we assume a linear function:

$$\int_{x_0}^{x_1} \frac{\partial x}{\beta_0 + \frac{\beta_1}{\beta_0} \frac{(x - x_0)}{(x_1 - x_0)}}$$

where

$$\beta_0 = \beta\left(x_0\right)$$

using (3.4)

$$\int_{x_0}^{x_1} \frac{\partial x}{\beta} = \frac{x_1 - x_0}{\beta_1 - \beta_0} \log \frac{\beta_1}{\beta_0}$$

$$\overline{\beta} = \frac{\beta_1 - \beta_0}{\log \frac{\beta_1}{\beta_0}} \tag{3.1}$$

$$L = x_1 - x_0$$

$$\frac{L}{\overline{\beta}} = \int_{n_0}^{n_1} \frac{\partial n}{J - \alpha n}$$

using (3.4)

$$\frac{L}{\overline{\beta}} = \frac{-1}{\alpha} \log \frac{J - \alpha n_1}{J - \alpha n_0}$$

Then solving for J

$$\frac{-\alpha L}{\overline{\beta}} = \log \frac{J - \alpha n_1}{J - \alpha n_0}$$
$$\exp\left(\frac{-\alpha L}{\overline{\beta}}\right) = \frac{J - \alpha n_1}{J - \alpha n_0}$$
$$\exp\left(\frac{-\alpha L}{\overline{\beta}}\right)(J - \alpha n_0) = J - \alpha n_1$$
$$J\left(\exp\left(\frac{-\alpha L}{\overline{\beta}}\right) - 1\right) = \exp\left(-\frac{\alpha L}{\overline{\beta}}\right)\alpha n_0 - \alpha n_1$$

We look for a form compatible with the Bernoulli function:

$$B(x) = \frac{x}{\exp(x) - 1}$$

$$J = \frac{\overline{\beta}}{L}\frac{\exp\left(\frac{-\alpha L}{\overline{\beta}}\right)\frac{\alpha L}{\overline{\beta}}n_0 - \frac{\alpha L}{\overline{\beta}}n_1}{\left(\exp\left(\frac{-\alpha L}{\overline{\beta}}\right) - 1\right)}$$
$$J = \frac{\overline{\beta}}{L}\left(\frac{\exp\left(\frac{-\alpha L}{\overline{\beta}}\right)\frac{\alpha L}{\overline{\beta}}n_0}{\left(\exp\left(\frac{-\alpha L}{\overline{\beta}}\right) - 1\right)} - \frac{\frac{\alpha L}{\overline{\beta}}n_1}{\left(\exp\left(\frac{-\alpha L}{\overline{\beta}}\right) - 1\right)}\right)$$
$$J = \frac{\overline{\beta}}{L}\left(\frac{\frac{\alpha L}{\overline{\beta}}n_0}{\left(1 - \exp\left(\frac{\alpha L}{\overline{\beta}}\right)\right)} - \frac{\frac{\alpha L}{\overline{\beta}}n_1}{\left(\exp\left(\frac{-\alpha L}{\overline{\beta}}\right) - 1\right)}\right)$$
$$J = \frac{\overline{\beta}}{L}\left(\frac{\frac{-\alpha L}{\overline{\beta}}n_1}{\left(\exp\left(\frac{-\alpha L}{\overline{\beta}}\right) - 1\right)} - \frac{\frac{\alpha L}{\overline{\beta}}n_0}{\left(\exp\left(\frac{\alpha L}{\overline{\beta}}\right) - 1\right)}\right)$$

Associated this to the case of electrons

$$J_n = \frac{\overline{\beta}}{L}\left(B\left(\frac{-\alpha_n L}{\overline{\beta}}\right)n_1 - B\left(\frac{\alpha_n L}{\overline{\beta}}\right)n_0\right) \tag{3.2}$$

For the case of holes

$$J_p = \alpha_p p - \beta \nabla p$$

and using the same definition for $\overline{\beta}$ in (3.1).

$$J_p = \frac{-\overline{\beta}}{L}\left(B\left(\frac{-\alpha_p L}{-\overline{\beta}}\right)p_1 - B\left(\frac{\alpha_p L}{-\overline{\beta}}\right)p_0\right)$$
$$J_p = \frac{-\overline{\beta}}{L}\left(B\left(\frac{\alpha_p L}{\overline{\beta}}\right)p_1 - B\left(\frac{-\alpha_p L}{\overline{\beta}}\right)p_0\right) \tag{3.3}$$

3.2 Testing Limits

Using L'Hopital's Rule.

$$B(x)\Big|_{x\to 0} = \frac{1}{\exp(0)} = 1$$

and as expected for diffusion

$$J_n\Big|_{\alpha\to 0} = \frac{\overline{\beta}}{L}\left(n_1 - n_0\right)$$
$$J_p\Big|_{\alpha\to 0} = -\frac{\overline{\beta}}{L}\left(p_1 - p_0\right)$$

For drift:

$$B\left(\frac{\alpha L}{\overline{\beta}}\right)\Big|_{\alpha\to\infty} = 0$$
$$B\left(\frac{-\alpha L}{\overline{\beta}}\right)\Big|_{\alpha\to\infty} = \frac{\alpha L}{\overline{\beta}}$$
$$B\left(\frac{\alpha L}{\overline{\beta}}\right)\Big|_{\alpha\to-\infty} = \frac{-\alpha L}{\overline{\beta}}$$
$$B\left(\frac{-\alpha L}{\overline{\beta}}\right)\Big|_{\alpha\to-\infty} = 0$$

$$J_n\Big|_{\alpha\to\infty} = \alpha n_1$$
$$J_n\Big|_{\alpha\to-\infty} = \alpha n_0$$

or

$$J_p\Big|_{\alpha\to\infty} = \alpha p_0$$
$$J_p\Big|_{\alpha\to-\infty} = \alpha p_1$$

3.3 Evaluate Bernoulli

This requires an expansion near 0 and use of (3.5).

$$\begin{cases} x < 0 & B\left(-x\right) = B\left(x\right) + x \\ x < \text{lim1} & B\left(x\right) = \left(\sum_{n=1}^{N} \frac{1}{(n+1)!} x^n\right)^{-1} \\ x < \text{lim2} & B\left(x\right) = \frac{x}{\exp(x)-1} \\ \text{else} & B\left(x\right) = x\exp\left(-x\right) \end{cases}$$

where lim1, lim2, and N are set appropriate for continuity and accuracy.

3.4 Helpful function

To perform the integrals in the derivations of (3.2)

$$\int_{x_0}^{x_1} \frac{\partial x}{a+bx}$$
$$y = a + bx$$
$$\partial y = b\partial x$$
$$\frac{1}{b}\int_{y_0}^{y_1} \frac{\partial y}{y}$$
$$\frac{1}{b}\log y\Big|_{y_0}^{y_1}$$
$$\frac{1}{b}\log\frac{y_1}{y_0}$$

$$\int_{x_0}^{x_1} \frac{\partial x}{a+bx} = \frac{1}{b}\log\frac{a+bx_1}{a+bx_0} \tag{3.4}$$

To reduce the number of computations for (3.2) and (3.3):

$$B(x) = \frac{x}{\exp(x)-1}$$
$$B(x)\exp(x) - B(x) = x$$
$$B(x) = B(x)\exp(x) - x$$
$$B(x) = \frac{x}{\exp(x)-1}\exp(x) - x$$
$$B(x) = \frac{x\exp(x)}{\exp(x)-1} - x$$
$$B(x) = \frac{x}{1-\exp(-x)} - x$$
$$B(x) = \frac{-x}{\exp(-x)-1} - x$$
$$B(x) = B(-x) - x$$

$$B(-x) = B(x) + x \tag{3.5}$$

3.5 Driving Force

3.5.1 For Electrons:

$$J_n = J_{drift} + J_{diffusion}$$
$$J_{diffusion} = q\nabla(D_n n)$$

At equilibrium:

$$J_n = 0 = J_{drift} + qD_n\nabla n + qn\nabla D_n$$
$$J_{drift} = -qD_n\nabla n - qn\nabla D_n$$

Assuming no temperature gradient:

$$
\begin{aligned}
J_{drift} &= -qD_n\nabla n \\
n &= N_c\gamma_n \exp\left(\frac{E_F - E_c}{kT}\right) \\
\nabla n &= n\left(\frac{\nabla N_c}{N_c} + \frac{\nabla\gamma_n}{\gamma_n} - \nabla\left(\frac{E_c}{kT}\right)\right) \\
\nabla n &= n\left(\nabla\log\left(N_c\right) + \nabla\log\left(\gamma_n\right) - \nabla\left(\frac{E_c}{kT}\right)\right) \\
J_{drift} &= -qD_n n\left(\nabla\log\left(N_c\right) + \nabla\log\left(\gamma_n\right) - \nabla\left(\frac{E_c}{kT}\right)\right) \\
J_{drift} &= qD_n n\left(\nabla\left(\frac{E_c}{kT}\right) - \nabla\log\left(N_c\gamma_n\right)\right)
\end{aligned}
$$

Then in general:

$$
\begin{aligned}
J_n &= qD_n n\left(\nabla\left(\frac{E_c}{kT}\right) - \nabla\log\left(N_c\gamma_n\right)\right) + qD_n\nabla n + qn\nabla D_n \\
J_n &= qD_n n\left(\nabla\left(\frac{E_c}{kT}\right) - \nabla\log\left(N_c\gamma_n\right) + \frac{\nabla D_n}{D_n}\right) + qD_n\nabla n \\
D_n &= \frac{kT\mu_n}{q} \\
J_n &= kT\mu_n n\left(\nabla\left(\frac{E_c}{kT}\right) - \nabla\log\left(N_c\gamma_n\right) + \frac{\nabla T}{T}\right) + kT\mu_n\nabla n \\
\frac{J_n}{k\mu_n} &= T\left(\nabla\left(\frac{E_c}{kT}\right) - \nabla\log\left(N_c\gamma_n\right) + \frac{\nabla T}{T}\right)n + T\nabla n
\end{aligned}
$$

Using:

$$
\alpha_n = T\left(\nabla\left(\frac{E_c}{kT}\right) - \nabla\log\left(N_c\gamma_n\right) + \frac{\nabla T}{T}\right)
$$

and assuming that the derivatives from x_0 to x_1 are constant:

$$
\alpha_n = \frac{\alpha_{n_1} - \alpha_{n_0}}{L}
$$

where

$$
\begin{aligned}
\alpha_{n_i} &= \overline{T}\left(\frac{E_{c_i}}{kT_i} - \log\left(N_{c_i}\gamma_{n_i}\right) + \frac{T_i}{\overline{T}}\right) \\
\overline{T} &= \frac{T_1 + T_0}{2} \\
\beta &= T
\end{aligned}
\tag{3.6}
$$

using (3.1)

$$
\overline{\beta} = \frac{T_1 - T_0}{\log\frac{T_1}{T_0}}
$$

can be shown to be

$$
\overline{\beta} = \frac{T_0}{B\left(\log\frac{T_1}{T_0}\right)}
\tag{3.7}
$$

3.5.2 For Holes:

$$
\begin{aligned}
J_{drift} &= qD_p\nabla p \\
p &= N_v\gamma_p \exp\left(\frac{E_v - E_F}{kT}\right) \\
\nabla p &= p\left(\frac{\nabla N_v}{N_v} + \frac{\nabla\gamma_p}{\gamma_p} + \nabla\left(\frac{E_v}{kT}\right)\right) \\
\nabla p &= p\left(\nabla\log\left(N_v\right) + \nabla\log\left(\gamma_p\right) + \nabla\left(\frac{E_v}{kT}\right)\right) \\
J_{drift} &= qD_p p\left(\nabla\log\left(N_v\right) + \nabla\log\left(\gamma_p\right) + \nabla\left(\frac{E_v}{kT}\right)\right) \\
J_{drift} &= qD_p p\left(\nabla\left(\frac{E_v}{kT}\right) + \nabla\log\left(N_v\gamma_p\right)\right)
\end{aligned}
$$

Then in general:

$$
\begin{aligned}
J_p &= qD_p p\left(\nabla\left(\frac{E_v}{kT}\right) + \nabla\log\left(N_v\gamma_p\right)\right) - qD_p\nabla p - qp\nabla D_p \\
J_p &= qD_p p\left(\nabla\left(\frac{E_v}{kT}\right) + \nabla\log\left(N_v\gamma_p\right) - \frac{\nabla D_p}{D_p}\right) - qD_p\nabla p \\
D_p &= \frac{kT\mu_p}{q} \\
J_p &= kT\mu_p p\left(\nabla\left(\frac{E_v}{kT}\right) + \nabla\log\left(N_v\gamma_p\right) - \frac{\nabla T}{T}\right) - kT\mu_p\nabla p \\
\frac{J_p}{k\mu_p} &= T\left(\nabla\left(\frac{E_v}{kT}\right) + \nabla\log\left(N_v\gamma_p\right) - \frac{\nabla T}{T}\right)p - T\nabla p
\end{aligned}
$$

Then (3.7) is used to calculate $\overline{\beta}$ and (3.6) is used to calculate $\overline{T}$.

$$
\alpha_{p_i} = \overline{T}\left(\frac{E_{v_i}}{kT_i} + \log\left(N_{v_i}\gamma_{p_i}\right) - \frac{T_i}{\overline{T}}\right)
$$

3.5.3 Temperature:

For the case of carrier temperatures, then T_n and T_p are substituted into $\overline{\beta}$ and T as appropriate.

CHAPTER

FOUR

DENSITY GRADIENT METHOD

4.1 DG Equation Discretization

The density gradient equations to be solved are of the following form:

$$\Lambda_e = -b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}}$$
$$\Lambda_h = -b_p \frac{\nabla^2 \sqrt{p}}{\sqrt{p}}$$

where b_n, b_p are coefficients relating the gradient in $\sqrt{n}$ with a quantum correction.

$$b_n = \frac{\gamma_n \hbar^2}{6 m_n}$$
$$b_p = \frac{\gamma_p \hbar^2}{6 m_p}$$

Using:

$$\frac{\nabla^2 \sqrt{n}}{\sqrt{n}} = \frac{1}{2}\left\{\nabla^2 \log n + \frac{1}{2}\left(\nabla \log n\right)^2\right\}$$

and

$$\Phi_e = \log n$$
$$\Phi_h = \log p$$

The equations become:

$$\Lambda_e + \frac{b_n}{2}\left(\nabla \cdot \nabla \Phi_e + \frac{1}{2}\left(\nabla \Phi_e\right)^2\right) = 0$$
$$\Lambda_h + \frac{b_p}{2}\left(\nabla \cdot \nabla \Phi_h + \frac{1}{2}\left(\nabla \Phi_h\right)^2\right) = 0$$

Considering the discretized equation along the edge between nodes i and j:

$$\Lambda_e \cdot \mathrm{NV}_i + \sum_j \frac{b_{n_{i,j}}}{2}\left(\mathrm{SA}_{i,j} \cdot \nabla_{i,j} \Phi_{e_{i,j}} - \frac{1}{2}\mathrm{EV}_{i,j}\left(\nabla_{i,j} \Phi_e\right)^2\right) - \mathrm{INT}_{i,k} \frac{b_{n_{ox}}}{x_n} = 0$$
$$\Lambda_h \cdot \mathrm{NV}_i + \sum_j \frac{b_{p_{i,j}}}{2}\left(\mathrm{SA}_{i,j} \cdot \nabla_{i,j} \Phi_{h_{i,j}} - \frac{1}{2}\mathrm{EV}_{i,j}\left(\nabla_{i,j} \Phi_h\right)^2\right) - \mathrm{INT}_{i,k} \frac{b_{p_{ox}}}{x_p} = 0$$

The gradient is then:

$$\nabla_{i,j}\Phi_x = \frac{\Phi_{x_j} - \Phi_{x_i}}{L_{i_j}}$$

The symbols have the following meaning:

NV_i	The total volume for node i in the semiconductor
$\mathrm{L}_{i,j}$	The distance between nodes i and j
$\mathrm{SA}_{i,j}$	The surface area of the perpendicular bisector between nodes i and j
$\mathrm{EV}_{i,j}$	The volume for the node attributed to the edge between nodes i and j
$\mathrm{INT}_{i,k}$	The surface area of the interface connecting node i and oxide interface k

Note that the sign on the EV *term depends on how the edge volume assembly is performed.*

4.2 Boundary Conditions

4.2.1 Semiconductor/Insulator interface

Wettstein [[WPL02]] solves the equations in both the insulator in semiconductor materials. For now, we consider the approach of other authors and assume that the carriers diminish quickly in the insulator [[GLSA+11]]. Solving the equations in the insulator would be important for resonant tunneling between adjacent semiconductor regions [[HohrSWF02]].

The calculations in the oxide are [[JPYJM04]]:

$$b_{n_{ox}} = \frac{\gamma_{n_{ox}}\hbar^2}{m_{ox}}$$
$$x_n = \frac{\hbar}{\sqrt{2m_{ox}\Phi_B}}$$

4.2.2 Ohmic Contacts

At ohmic contacts the following boundary conditions are required to meet the equilibrium boundary condition assumption:

$$\Lambda_e = 0 \tag{4.1}$$
$$\Lambda_h = 0 \tag{4.2}$$

4.3 Units

b_n, b_p, $b_{n_{ox}}$, $b_{p_{ox}}$	eV cm ^{2}
x_n, x_p	cm
Λ_e, Λ_h	eV

4.4 Calculation

The values of Φ_e and Φ_h are from the calculation of the electron and hole density from their respective Fermi levels.

$$\Phi_e = \frac{kT \log N_C + E_{F_n} - E_C - \Lambda_e}{kT} \tag{4.3}$$

$$\Phi_h = \frac{kT \log N_V - E_{F_p} + E_V - \Lambda_h}{kT} \tag{4.4}$$

4.5 Notes

4.5.1 Sign Conventions

The convention chosen in this description is the Λ_e and Λ_h act to reduce the electron and hole concentration.

$$n \propto \exp\left(-\Lambda_e\right) \tag{4.5}$$

$$p \propto \exp\left(-\Lambda_h\right) \tag{4.6}$$

4.5.2 Driving Force

The calculated values of Λ_e and Λ_h modify the driving force for current, as in other quantum correction models.

4.5.3 Recombination

In [[LMP+02]], the authors point out that n_i for recombination must be scaled, to prevent large recombination near the interface. This is since:

$$R \propto np - n_i^2$$

Therefore:

$$n_i^2 \propto \exp\left(\frac{-\Lambda_e - \Lambda_h}{kT}\right)$$

4.5.4 Preventing Floating Point Exceptions

In prototyping the DG equations, 2 points of numerical overflow where discovered. When calculating the edge volume contribution, a heuristic like:

$$\left(\nabla_{i,j}\Phi_x\right)^2 = \left(b_x 10^8\right)\left(10^{-4}\left(\frac{\Phi_{x_j} - \Phi_{x_i}}{L_{i_j}}\right)\right)^2$$

was used. In addition, it is important to make sure that updates in Λ_e and Λ_h are not too large to cause an overflow in the calculation of n and p.

$$n \propto \text{limexp}\left(\Phi_e\right) \tag{4.7}$$

$$p \propto \text{limexp}\left(\Phi_h\right) \tag{4.8}$$

where limiting the $\exp$ function is necessary to prevent overflow.

4.5.5 Ramping Strategies

Since the classical and density gradient solutions are different, it is necessary to ramp the parameters γ_n, and γ_p to improve convergence. A ramping strategy should be considered where the step change in γ_n and γ_p may be adjusted when a simulation fails to converge.

4.5.6 Meshing

To ensure accurate simulation results, it may be necessary to apply mesh refinements away from the interface, where the maximum in carrier concentrations occur.

4.5.7 Solving One DG Equation

For a MOS device, it makes sense to only solve the DG equation for the carrier in the channel of the device.

4.6 Derivation of log form of equation

4.6.1 The log form

$$\frac{\nabla^2\sqrt{n}}{\sqrt{n}} = u\nabla\cdot\vec{v} \tag{4.9}$$

$$S_n = \sqrt{n} \tag{4.10}$$

$$u = \frac{1}{S_n} \tag{4.11}$$

$$\nabla u = -\frac{\nabla S_n}{S_n^2} \tag{4.12}$$

$$\vec{v} = \nabla S_n \tag{4.13}$$

$$\nabla\cdot\vec{v} = \nabla\cdot\nabla S_n \tag{4.14}$$

$$\nabla\cdot(u\vec{v}) = u\nabla\cdot\vec{v} + \vec{v}\cdot\nabla u \tag{4.15}$$

$$u\nabla\cdot\vec{v} = \nabla\cdot(u\vec{v}) - \vec{v}\cdot\nabla u \tag{4.16}$$

$$u\vec{v} = \nabla\log S_n = \tfrac{1}{2}\nabla\log n \tag{4.17}$$

$$\vec{v}\cdot\nabla u = -\nabla S_n\cdot\frac{\nabla S_n}{S_n^2} = -\left(\nabla\log S_n\right)^2 = -\tfrac{1}{4}\left(\nabla\log n\right)^2 \tag{4.18}$$

$$\frac{\nabla^2\sqrt{n}}{\sqrt{n}} = \tfrac{1}{2}\nabla^2\log n + \tfrac{1}{4}\left(\nabla\log n\right)^2 \tag{4.19}$$

4.7 Wettstein

4.7.1 Introduction

We start with deriving the equations in [[WPL02]].

$$\Lambda_e = -b_n\frac{\nabla^2\sqrt{n}}{\sqrt{n}} \tag{4.20}$$

$$\Lambda_h = -b_p\frac{\nabla^2\sqrt{p}}{\sqrt{p}} \tag{4.21}$$

where

$$b_n = \frac{\gamma_n \hbar^2}{6 m_n} \tag{4.22}$$

$$b_p = \frac{\gamma_p \hbar^2}{6 m_p} \tag{4.23}$$

The effect is such that:

$$n = N_C \exp\left(\frac{E_F - E_C - \Lambda_e}{kT}\right) \tag{4.24}$$

$$p = N_V \exp\left(\frac{E_V - E_F - \Lambda_h}{kT}\right) \tag{4.25}$$

and the intrinsic carrier density is now:

$$n_i^2 \propto \exp\left(\frac{-\Lambda_e - \Lambda_h}{kT}\right)$$

This is especially important for recombination.

For convenience we define:

$$n = \exp\left(\frac{\Phi_e}{kT}\right) \tag{4.26}$$

$$p = \exp\left(\frac{\Phi_h}{kT}\right) \tag{4.27}$$

where

$$\Phi_e = E_F - E_C - \Phi_C - \Lambda_e \tag{4.28}$$

$$\Phi_h = E_V - E_F + \Phi_V - \Lambda_h \tag{4.29}$$

$$\tag{4.30}$$

where

$$\Phi_C = -kT \log(N_C) \tag{4.31}$$

$$\Phi_V = kT \log(N_V) \tag{4.32}$$

For current conduction, the effect is that:

$$J_n = n\mu\nabla\left(\Phi_e\right) + qD_n\nabla n \tag{4.33}$$

$$J_p = p\mu\nabla\left(\Phi_h\right) - qD_p\nabla p \tag{4.34}$$

where

$$\Phi_C = -kT \log(N_C) \tag{4.35}$$

$$\Phi_V = kT \log(N_V) \tag{4.36}$$

4.7.2 Method 1

In the derivation which follows, they exploit the following relation:

$$\frac{\nabla^2\sqrt{n}}{\sqrt{n}} = \frac{1}{2}\left\{\nabla^2 \log n + \frac{1}{2}\left(\nabla \log n\right)^2\right\}$$

For a volume integration:

$$\int \Lambda_e \partial v = -\frac{b_n}{2}\left\{\int \nabla \log n \cdot \partial s + \frac{1}{2}\int (\nabla \log n)^2 \, \partial v\right\} \tag{4.37}$$

$$\int \Lambda_h \partial v = -\frac{b_p}{2}\left\{\int \nabla \log p \cdot \partial s + \frac{1}{2}\int (\nabla \log p)^2 \, \partial v\right\} \tag{4.38}$$

When assembled onto node i with respect to nodes j.

$$\Lambda_{e,i}\Omega_i = \sum_j \frac{b_n \sigma_{i,j}}{2 l_{i,j}}\left\{\left(\frac{\Phi_{e,j}-\Phi_{e,i}}{kT}\right) - \frac{1}{4}\left(\frac{\Phi_{e,j}-\Phi_{e,i}}{kT}\right)^2\right\} \tag{4.39}$$

$$\Lambda_{h,i}\Omega_i = \sum_j \frac{b_p \sigma_{i,j}}{2 l_{i,j}}\left\{\left(\frac{\Phi_{h,j}-\Phi_{h,i}}{kT}\right) - \frac{1}{4}\left(\frac{\Phi_{h,j}-\Phi_{h,i}}{kT}\right)^2\right\} \tag{4.40}$$

4.7.3 Method 2

Following [[Wet00]] they discretize:

$$\int \Lambda_e \partial v = -b_n \int \frac{\nabla\sqrt{n}}{\sqrt{n}} \cdot \partial s \tag{4.41}$$

$$\int \Lambda_h \partial v = -b_p \int \frac{\nabla\sqrt{p}}{\sqrt{p}} \cdot \partial s \tag{4.42}$$

When assembled onto node i with respect to nodes j.

$$\Lambda_i \Omega_i = \sum_j \frac{b_n \sigma_{i,j}}{l_{i,j}}\left(\frac{\sqrt{n_i}-\sqrt{n_j}}{\sqrt{n_i}}\right) \tag{4.43}$$

$$\Lambda_i \Omega_i = \sum_j \frac{b_n \sigma_{i,j}}{l_{i,j}}\left(1-\frac{\sqrt{n_j}}{\sqrt{n_i}}\right) \tag{4.44}$$

Which then leads to:

$$\Lambda_{e,i}\Omega_i = \sum_j \frac{b_n \sigma_{i,j}}{l_{i,j}}\left\{1-\exp\left(\frac{\Phi_{e,i}}{2kT}-\frac{\Phi_{e,j}}{2kT}\right)\right\} \tag{4.45}$$

$$\Lambda_{h,i}\Omega_i = \sum_j \frac{b_n \sigma_{i,j}}{l_{i,j}}\left\{1-\exp\left(\frac{\Phi_{h,i}}{2kT}-\frac{\Phi_{h,j}}{2kT}\right)\right\} \tag{4.46}$$

CHAPTER

FIVE

IMPEDANCE FIELD METHOD

5.1 Derivation

The Impedance Field Method (IFM) is for performing a sensitivity analysis with respect to multiple perturbations [[BraninJr73]], [[BGPS98]].

Starting with

$$Ax = b$$

where A is the sensitivity matrix, and b is a vector containing a vector of fully correlated perturbations. The response is then

$$x = A^{-1}b$$

The disadvantage of this direct method is that one solve must be performed for each vector of source perturbations.

If we are interested in one output, we define an elementary vector e_i that selects the output as:

$$x_i = e_i^T x$$

where a 1 is placed in row i corresponding to the desired output variable.

The problem to be solved is then

$$x_i = e_i^T A^{-1} b$$

We recast the problem in the form

$$x_i = y^T b$$

where y is defined as

$$y^T = e_i^T A^{-1} \tag{5.1}$$

Then we can solve

$$A^T y = e_i \tag{5.2}$$

so that only one matrix factorization is required for a given simulation matrix and output. Then (5.1) is a dot product of y with any number of source perturbations.

From a statistical perspective, then:

$$\langle x_i, x_i^* \rangle = y^T \langle b, b^* \rangle y$$

which can be shown to be:

$$\overline{x_i x_i^*} = \sum_j y_j^* y_j \overline{b_j b_j^*} + \sum_j \sum_k 2Re\overline{y_j b_j b_k^* y_k^*}$$

where indexes j and k select the appropriate row in y corresponding to each perturbation. The correlations $b_j b_k^*$ must be known in order to account for any correlations which may exist.

5.2 Selecting the output

From (5.2), it was assumed that e_i was an elementary vector with a one in the row corresponding to the desired output variable. In principle, it can be any vector which calculates the desired output quantity.

If the output variable is a voltage, and a current is desired, it is possible to use a standard small signal analysis to get the output impedance of the device, and use that for conversion. Equivalently, it may be possible to use the impedance field entry in the row corresponding to the output.

5.3 The scalar impedance field

The impedance field couples a perturbation in an equation to the output. For the electron continuity equation, the effect would be

$$I = \int G_s \cdot R \partial r$$

where G_s is the scalar Green's function, R is the recombination rate and the integration is performed over each volume in the mesh.

Considering the device equations at each node, it is necessary to consider the desired perturbation unit.

Equation	Unit	Perturbation Unit
F_ψ	$V \cdot cm$	$1/cm^3$
F_n	$1/sec$	$1/(cm^3 \cdot sec)$
F_p	$1/sec$	$1/(cm^3 \cdot sec)$

The scalar impedance field for the Poisson equation is:

$$G_{\psi,i} = -\frac{\epsilon}{q \cdot vol} y_{\psi,i}$$

where $y_{\psi,i}$ is the entry in y which corresponds to the Poisson equation for node i. The vol is the volume of the node. The other parameters are material parameters, and the sign is based on how the dopant terms are entered into the system matrix.

The electron and hole scalar impedance field are then

$$G_{n,i} = -\frac{1}{vol} y_{n,i}$$
$$G_{p,i} = -\frac{1}{vol} y_{p,i}$$

5.4 Vector impedance field

The vector impedance field, $\overrightarrow{G}_v$, is used to calculate the device response to current density fluctuations in noise analysis. It is required to consider the effects of dopant fluctuations on moblity and bandgap narrowing.

If $\overrightarrow{j}$ is a fluctuation in the current density, then

$$I = \frac{1}{q} \int G_s \nabla \cdot \overrightarrow{j} \, \partial r$$

Using Green's identities

$$\int \left(G \nabla \cdot \overrightarrow{j} + \overrightarrow{j} \cdot \nabla G \right) \partial r = \int G \overrightarrow{j} \cdot \partial s$$

then

$$I = \frac{1}{q} \left[\int \overrightarrow{G}_v \cdot \overrightarrow{j} \, \partial r + \int G_s \overrightarrow{j} \, \partial s \right] \tag{5.3}$$

where

$$\overrightarrow{G}_v = -\nabla G_s$$

In the noise literature, (5.3) is replaced with

$$I = \frac{1}{q} \int \overrightarrow{G}_v \cdot \overrightarrow{j} \, \partial r$$

using the argument that the surface integral vanishes. For our purposes, it is unclear if the full form should (5.3) should be retained.

5.5 Density Gradient

To account for the Density Gradient, it is necessary to fully couple them into the system of equations being solved.

The Density Gradient equations are only dependent on n and p. However, in our implementation, the quasi-Fermi definitions for n and p are employed. This means that doping effects could enter through bandgap narrowing models.

Since n and p are fundamental solution variables, and are therefore constant, it seems that the impedance field is not required from the DG equations.

5.6 Boundary Conditions

For the case of ohmic contacts, the equations for ψ, n, p are replaced with other equations. Therefore nodes at the ohmic contacts should not be considered in the impedance fields with respect to the bulk equations.

For perturbations with respect to the work function, the contact impedance fields would be needed since they enter directly into the potential equation.

If it is necessary to transform output voltage to current, the impedance field with respect to voltage fluctuations in the potential equation could be considered.

CHAPTER

SIX

LOCALIZED GRADIENT MODELS

6.1 Single Element

6.1.1 Electric Field

Consider a vector field that we wish to ascribe to an edge or a node of a triangular or a tetrahedral element. We begin by calculating the components along each element edge. For the case of electric field, this is

$$E_{i,j} = \frac{\psi_i - \psi_j}{L_{i,j}}$$

where ψ_i is the potential at node i, and $L_{i,j}$ is the distance between the nodes i and j.

If the electric field on the element is known, this is equivalent to

$$E_{i,j} = \hat{s}_{i,j} \cdot \mathscr{E}$$

where $\hat{s}_{i,j}$ is the unit vector along the edge connecting nodes i and j. For a tetrahedron with nodes (i, j, k, l), we can then use the components of the unit vectors to calculate

$$\begin{pmatrix} \hat{s}^x_{i,j} & \hat{s}^y_{i,j} & \hat{s}^z_{i,j} \\ \hat{s}^x_{i,k} & \hat{s}^y_{i,k} & \hat{s}^z_{i,k} \\ \hat{s}^x_{i,l} & \hat{s}^y_{i,l} & \hat{s}^z_{i,l} \end{pmatrix} \begin{pmatrix} \mathscr{E}_x \\ \mathscr{E}_y \\ \mathscr{E}_z \end{pmatrix} = \begin{pmatrix} E_{i,j} \\ E_{i,k} \\ E_{i,l} \end{pmatrix}$$

or

$$S_i \times \mathscr{E} = \begin{pmatrix} E_{i,j} \\ E_{i,k} \\ E_{i,l} \end{pmatrix}$$

The derivatives are then

$$\frac{\partial \mathscr{E}}{\partial \psi_i} = S_i^{-1} \times \begin{pmatrix} \frac{\partial E_{i,j}}{\partial \psi_i} \\ \frac{\partial E_{i,k}}{\partial \psi_i} \\ \frac{\partial E_{i,l}}{\partial \psi_i} \end{pmatrix}$$

$$\frac{\partial \mathscr{E}}{\partial \psi_j} = S_i^{-1} \times \begin{pmatrix} \frac{\partial E_{i,j}}{\partial \psi_j} \\ 0 \\ 0 \end{pmatrix}$$

$$\frac{\partial \mathscr{E}}{\partial \psi_k} = S_i^{-1} \times \begin{pmatrix} 0 \\ \frac{\partial E_{i,k}}{\partial \psi_k} \\ 0 \end{pmatrix}$$

$$\frac{\partial \mathscr{E}}{\partial \psi_l} = S_i^{-1} \times \begin{pmatrix} 0 \\ 0 \\ \frac{\partial E_{i,l}}{\partial \psi_l} \end{pmatrix}$$

by storing these S^{-1} matrices, the electric field on each element and their derivatives may be stored. It can be shown that since

$$E_{i,l} L_{i,l} = E_{i,j} L_{i,j} + E_{j,k} L_{j,k} + E_{k,l} L_{k,l}$$

that only one S matrix would need to be formed for each tetrahedral element in the mesh.

6.1.2 Current Direction

What is needed

What is ultimately needed is the unit vector, j, which corresponds to the direction of current flow.

Since the current depends on the mobility, which depends on the current flow creates a cyclic dependency. Laux suggests breaking this cycle by

1. Calculating the current directions based on constant mobility
2. Calculating the electric field based on the the constant mobility current
3. Calculating the final current based on the electric field dependent mobility

Using edge currents

If we wanted to apply the same treatment for electron or hole current, we would then calculate the current components, by using 2 matrices for each edge to calculate the current. For the edge connecting nodes i and j, this would be

$$S_i \times J_i = \begin{pmatrix} J_{i,j} \\ J_{i,k} \\ J_{i,l} \end{pmatrix}$$

and

$$S_j \times J_j = \begin{pmatrix} J_{j,i} \\ J_{j,k} \\ J_{j,l} \end{pmatrix}$$

and these could be weighted as

$$J = 0.5 J_i + 0.5 J_j$$

Where the equal weighting is chosen for its relative ease of implementation. For a 2D implementation, the weighting of the triangle edges has been done by Laux based on the area of the perpendicular bisectors of the edges off of nodes i and j. In principle, this could be

$$J = \frac{\left(d_{i,k} + d_{i,l}\right) J_i + \left(d_{j,k} + d_{j,l}\right) J_j}{d_{i,k} + d_{i,l} + d_{j,k} + d_{j,l}}$$

Derivatives with respect to nodal quantities would then be done using the chain rule using a similar approach as shown for the electric field.

6.1.3 Using nearest interface

A more stable way of evaluating the mobility is to base the current directions based on the nearest interface. It is considered stable since the current directions are not iteration dependent.

To do this, a line is drawn from center of the edge to the nearest interface. The plane formed at the interface node is considered to be the direction parallel to current flow. The direction perpendicular to current flow is then the line normal to the plane.

6.2 Averaging the elements

6.3 Calculating electric field components

CHAPTER

SEVEN

TRANSIENT METHOD

7.1 Integration

7.1.1 General Integration

At each time step, the transient solver solves

$$0 = \boldsymbol{f}_0 = a_0\boldsymbol{q}_0 + a_{-1}\boldsymbol{q}_{-1} + a_{-2}\boldsymbol{q}_{-2} + b_0\boldsymbol{i}_0 + b_{-1}\boldsymbol{i}_{-1} + b_{-2}\boldsymbol{i}_{-2}$$

where $\boldsymbol{f}_0$ is the vector of net flux at each node in the mesh. The $\boldsymbol{i}_x$ represents the time independent part of the semiconductor equations and $\boldsymbol{q}_x$ represents the time derivatives terms. The subscript 0 denotes the current time step being solved. The subscripts -1 and -2 denote the previous two time steps.

At the beginning of each time step the components are copied in order so that:

$$\begin{aligned}\boldsymbol{i}_{-2} &= \boldsymbol{i}_{-1}\\ \boldsymbol{i}_{-1} &= \boldsymbol{i}_0\\ \boldsymbol{q}_{-2} &= \boldsymbol{q}_{-1}\\ \boldsymbol{q}_{-1} &= \boldsymbol{q}_0\end{aligned}$$

7.1.2 TRANSIENT_DC

This is a steady state solution with:

$$\begin{aligned}a_0 &= 1\\ a_1 &= 0\\ b_0 &= 1\\ b_1 &= 0\\ b_2 &= 0\end{aligned}$$

and represent the DC steady state. This step can be used to initialize the initial time step so that the other transient methods can begin.

7.1.3 BDF1

$$
\begin{aligned}
t_\Delta &= \gamma t_{step} \\
t_f &= \frac{1}{t_\Delta} \\
a_0 &= t_f \\
a_1 &= -t_f \\
b_0 &= 1 \\
b_1 &= 0 \\
b_2 &= 0 \\
\gamma &= 1
\end{aligned}
$$

7.1.4 BDF2

$$
\begin{aligned}
t_\Delta &= (1-\gamma) t_{step} \\
a_0 &= \frac{2-\gamma}{t_\Delta} \\
a_1 &= \frac{-1}{\gamma t_\Delta} \\
a_2 &= \frac{1-\gamma}{\gamma t_{step}} \\
b_0 &= 1 \\
b_1 &= 0 \\
b_2 &= 0 \\
\gamma &= 0.5
\end{aligned}
$$

7.1.5 TR

$$
\begin{aligned}
t_\Delta &= \gamma t_{step} \\
t_f &= \frac{2}{t_\Delta} \\
a_0 &= t_f \\
a_1 &= -t_f \\
b_0 &= 1 \\
b_1 &= 1 \\
b_2 &= 0
\end{aligned}
\tag{7.1}
$$

7.1.6 TRBDF2

Combination of 2 methods described in [[BCF+85]].

$$\gamma = 2 - \sqrt{2}$$

and use TR followed by BDF2

7.2 Projection

Calculate $\boldsymbol{q}_0$ as part of the solution process. Then compare with:

$$\begin{aligned} 0 &= i_1 + \frac{q_{proj} - q_1}{t_\Delta} \\ q_{proj} &= -i_1 t_\Delta + q_1 \end{aligned} \tag{7.2}$$

Calculate error between projection and actual charge solution

CHAPTER

EIGHT

MOBILITY

In its simplest form, mobility is a nodal quantity. For current density calculations, the mobility needs to be calculated on the edge connecting two nodes. Using an arithmetic average

$$\mu_{edge} = \frac{\mu_{node_0} + \mu_{node_1}}{2}$$

For the case of velocity saturation, mobility is dependent on the field parallel to current flow.

In addition, the electric field normal affects mobility components such as surface roughness, coulomb scattering, and acoustic phonon scattering.

Procedure

1. Nodal mobility components
2. Project onto Edge
3. Calculate Et on element edge
4. Calculate combined Element edge mobility
5. Apply Matthiessen's rule to get low field mobility
6. Calculate El on element edge
7. Apply velocity saturation to get high field mobility

CHAPTER

NINE

FERMI INTEGRALS

CHAPTER

TEN

REGIONS

10.1 Entities

- Device
- Region
- Interface
- Contact

Device contains Regions, Interfaces, Contacts

Circuit contains nodes attached to contacts and circuit elements.

The whole system contains all devices and circuit

Each contact is associated with 1 Region and possibly a circuit node.

Each interface is associated with 2 Regions

10.2 Assembly

10.2.1 Coordinates

Coordinates are global to the entire structure. They are essentially positions, and may be shared across multiple regions.

10.2.2 Nodes

Each region contains a list of nodes. These nodes are uniquely numbered and are associated with an underlying coordinate. Coordinates may be shared by different regions, however the node is distinct to the region. An interface governs how the equations at these coincident nodes interact.

10.2.3 Equation numbering

Each equation is assigned a unique number for each node in a region. The net flux of each equation is assembled into a sub matrix and RHS whose rows correspond to all of the interacting region nodes.

10.2.4 Permutation Vector

The permutation vector is used to manipulate the assembly of equations in the Jacobian matrix. If a contact boundary condition exists for an equation, the permutation entry for that node is set to -1, which means it is not loaded into the matrix. (The contact equation assembly routine will separately load the current density into the circuit nodes.)

For the "Type 1" interface boundary condition described below, the equation number entry for region 2 permutes into the equation number entry for region 1.

10.2.5 Final Assembly

Region Assembly

A sub matrix and RHS is evaluated for each node in a region. The permutation vector is used to avoid loading the bulk equation into the contact nodes. For "Type 1" interfaces, the bulk equation for the 2nd region at an interface is permuted into the equation row for the first region.

For most cases, it is not necessary for the region equation assembly to explicitly handle whether or not an interface or contact node is being assembled. These submatrix entries will be filtered out if they are not needed.

Interface Assembly

For the interface assembly, the permutation vector is ignored. Flux contributions across the interface has already been handled in the Region Assembly.

For interface equations, there are two types of boundary conditions.

Type 1

The bulk flux equation for Region 1 and Region 2 are assembled into the row corresponding to Region 1. An interface node model equation is evaluated and place into the row corresponding to Region 2.

This would be the natural boundary condition for the Poisson equation, as the interface model equation would enforce a continuous potential.

An example for this case would be having a continuous quasi-Fermi level between two similar material regions.

Type 2

The bulk flux equation for Region 1 and Region 2 are assembled into the rows corresponding to their respective regions. An additional interface node model is added to the flux for Region 1 and subtracted from Region 2. This additional flux term is integrated with respect to surface area of the interface between the nodes.

An example for this case would be tunneling at a heterojunction interface.

Contact Assembly

Contact assembly ignores the permutation vector. The contributions from the bulk equations are ignored during the Region assembly process.

The contact flux equation is then assembled in the bulk equation's place. In the presence of an external circuit on the contact, the equation for the external current flux and charge displacement is assembled into the circuit node equation. This is integration is with respect to the surface area of the contact node.

10.3 Caveats

10.3.1 Interface conflicts

It is entirely possible to have multiple regions to share a node or edge. In order to prevent issues with the equation assembly, it is important to make sure that these regions do not have conflicting permutations.

By definition, intersecting interfaces do not share surface area. If you have 3 regions:

1. interface 1: r1 r2
2. interface 2: r1 r3

Note that this should not occur

1. interface 3: r2 r3 (does not exist)

If the abutting interfaces are all "Type 1", you just need to ensure that the first region for both interfaces is the same. The permutation vector will then permute the bulk equations for the other regions into the bulk equation for the first region. The constraint equation for each interface will then properly handle the relationship between the connected regions.

This may be attained by prioritizing the interfaces, so they are always treated in the same order. Similarly for a mixture of "Type 1" and "Type 2" interfaces, it seems that this approach would work as well.

10.3.2 Contact conflicts

Overlapping contacts must be avoided. This is since the current coming out of overlapping nodes would be double counted. Contacts overlapping interfaces should be similarly avoided. The permutation vector could either get corrupted, or current could be double counted as going out of the contact, and across the interface.

10.3.3 Circuit Equations

For a single device solution, equation numbers for the terminal currents are not necessary. They are recovered after the dc solution has been obtained. For time dependent simulation, the circuit equations are important to sum up the particle and displacement current. They would also be important for small signal and impedance field simulation.

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