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3D Finite Element Drift-Diffusion Simulation of Semiconductor Devices

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Chapter 1

Resolution of the system

In this chapter we introduce geometry and boundary conditions for the stationary form of system (1.53) and we discuss the iteration algorithms used to decouple the same system.

1.1 Geometry and boundary conditions

In order to close the *Poisson equation* and the *Drift Diffusion equation* for electrons and holes of the the stationary form of problem (1.53), suitable boundary conditions must be considered.

Let us consider the device domain as the union of two open disjoint subsets, Ω_{Si} (doped silicon part), and Ω_{ox} (oxide part), such that their intersection $\partial\Omega_{Si} \cap \partial\Omega_{ox} = \Gamma_{int}$ is the interface. The oxide region Ω_{ox} is assumed to be a perfect insulator so that:

$$\begin{aligned} n = p = 0 \\ \mathbf{J}_n = \mathbf{J}_p = \mathbf{0} \end{aligned} \tag{1.1}$$

The device boundary $\partial\Omega$ is divided into two disjoint subsets: $\partial\Omega_c$ and $\partial\Omega_a$. The subset $\partial\Omega_c$ includes the so called *ohmic contacts* (with ohmic contacts we define every electrical terminal of the device on which the external input voltages are applied). Ohmic contacts are assumed to be *ideal*, they are equipotential surfaces and no voltage drop occurs at the interface between the contact and the neighbouring domain. This is well performed by suitable Dirichlet boundary conditions, therefore in the follow we indicate $\partial\Omega_c = \Gamma_D$.

$$\begin{aligned} &\varphi = \varphi_D \\ &n = n_D \qquad on\, \Gamma_D. \\ &p = p_D \end{aligned} \tag{1.2}$$

we point that in the case of a perfect insulator domain, (**??**) reduces to the only condition on the electrostatical potential.

Artificial boundaries ($\partial\Omega_a$) are needed in order to obtain a self-contained simulation domain. On these boundaries no electric and current flux is exchanged with the surrounding environment, this fact is well performed by homogeneous Neumann boundary condition ($\partial\Omega_a = \Gamma_N$)

$$\begin{aligned} \mathbf{D}\cdot\mathbf{n} &= 0 \\ \mathbf{J}_n\cdot\mathbf{n} &= 0 \qquad on\,\Gamma_N \\ \mathbf{J}_p\cdot\mathbf{n} &= 0 \end{aligned} \tag{1.3}$$

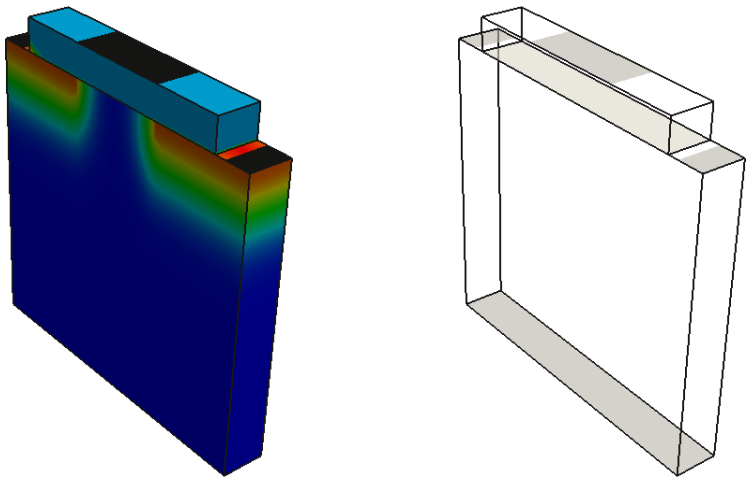
where $\mathbf{n}$ is the outward unit normal vector defined over $\partial\Omega$. As we noted before on $\partial\Omega_{ox}\cap\Gamma_N$ condition (**??**) is reduced to the first equation.

When oxide is present the silicon boundaries for continuity equations become

$$\begin{aligned} \Gamma_{D,Si} &= \Gamma_D\cap\partial\Omega_{Si} \\ \Gamma_{N,Si} &= \Gamma_N\cap\partial\Omega_{Si}\cup\Gamma_{int}. \end{aligned} \tag{1.4}$$

Fig.**??** shows an example of boundary setting for a MOS device: in Fig.**??** contacts are colored in black and in Fig.**??** with light gray we indicate the interface between oxide and silicon.

Thermodynamical equilibrium and charge neutrality are the condition of an ideal contact. These conditions correspond to the follow algebraic system



(a) **(b)**

Figure 1.1: (a) MOS device with net dopant concentration distributed accordingly to a gaussian profile and Γ_D colored in black. The oxide layer is colored in light blue. (b) Outline of the MOS device with Γ_{int} in light gray.

for n_D and p_D

$$\begin{cases} p_D n_D & = & n_i^2 \\ p_D - n_D + N_D - N_A & = & 0 \end{cases} . \tag{1.5}$$

Solving (**??**) on $\Gamma_{D,Si}$ we have:

$$n_D = \frac{D + \sqrt{D^2 + 4n_i^2}}{2} \tag{1.6}$$

$$p_D = \frac{-D + \sqrt{D^2 + 4n_i^2}}{2} \tag{1.7}$$

where $D := N_D - N_A$ is the net doping concentration. Furthermore at contact quasi fermi potential levels of silicon at contact are aligend with the external applyed voltage. As a consequence we can easily calculate potential condition on $\Gamma_{D,Si}$ using (1.10) and (1.11)

$$\varphi_D = \varphi_f + V_{th} ln\left(\frac{n_D}{n_i}\right) = \varphi_f - V_{th} ln\left(\frac{p_D}{n_i}\right) \tag{1.8}$$

where $\varphi_f = -E_f/q$ is the unique quasi fermi potential level defined on contacts. When $\Omega_{ox} \neq \varnothing$ we set φ_D equal to the external applyed voltage on $\Gamma_D/\Gamma_{D,Si}$.

The stationary form of (1.53) can be now written in a closed form as:

$$\begin{array}{rcll} -\Delta\epsilon\varphi - q(p-n) & = & qD & in\,\Omega = \Omega_{ox} \cup \Omega_{Si} \\ \varphi & = & \varphi_D & on\,\Gamma_D \\ \nabla\varphi \cdot \mathbf{n} & = & 0 & on\,\Gamma_N \\ & & & \\ \nabla \cdot (q\mu_n n\nabla\varphi - qD_n\nabla n) & = & -qR & in\,\Omega_{Si} \\ n & = & n_D & on\,\Gamma_{D,Si} \\ \nabla n \cdot \mathbf{n} & = & 0 & on\,\Gamma_{N,Si} \\ & & & \\ \nabla \cdot (-q\mu_p p\nabla\varphi - qD_p\nabla p) & = & -qR & in\,\Omega_{Si} \\ p & = & p_D & on\,\Gamma_{D,Si} \\ \nabla p \cdot \mathbf{n} & = & 0 & on\,\Gamma_{N,Si} \end{array} \tag{1.9}$$

The high coupled nonlinear nature of system (**??**) makes an analytical treatment very difficult, if not even impossible. For this reason, numerical schemes must be used to compute an approximate solution.

1.2 Iteration algorithms

The most used algorithms are *the fully coupled Newton's method* and *the decoupled Gummel map*. System (**??**) can be written in a compact form as:

$$\mathbf{F}(\mathbf{U}) = \mathbf{0} \tag{1.10}$$

where:

$$\mathbf{U} := [\varphi, n, p]^T \qquad \mathbf{F}(\mathbf{U}) := \begin{bmatrix} F_1(\mathbf{U}) \\ F_2(\mathbf{U}) \\ F_3(\mathbf{U}) \end{bmatrix} \tag{1.11}$$

and having set:

$$\begin{aligned} F_1(\mathbf{U}) &= \nabla \cdot (-\epsilon \nabla \varphi) - q(p - n + D) \\ F_2(\mathbf{U}) &= \nabla \cdot (q\mu_n n \nabla \varphi - qD_n \nabla n) + qR \\ F_3(\mathbf{U}) &= \nabla \cdot (-q\mu_p p \nabla \varphi - qD_p \nabla p) + qR \end{aligned}$$

Problem (**??**) is the generalization of the zero search for a real function $f : \mathbb{R} \to \mathbb{R}$. Because the vector function $\mathbf{F}$ is a nonlinear differential operator, the associated problem which we intend to resolve is: given a functional space V and the operator $\mathbf{F} : V \to V$, find $\mathbf{U} \in V$ such that (**??**) is satisfied.

In our application, the function space V is typically a subset of the Sobolev space $[H^1(\Omega)]^d$ (where d is the number of component of $\mathbf{F}$). The general form of a Sobolev space for an integer $m \geq 0$ is

$$H^m(\Omega) := \left\{ v : D^\alpha v \in L^2(\Omega), \forall |\alpha| \leq m \right\}. \tag{1.12}$$

where $L^2(\Omega)$ is the space of square integrable functions on Ω

$$L^2(\Omega) := \left\{ v : \int_\Omega |v|^2 d\,\Omega = ||v||^2_{L^2(\Omega)} < +\infty \right\}. \tag{1.13}$$

On these space, we shall use the semi-norm

$$|v|^2_{m,\Omega} = \sum_{|\alpha|=m} ||D^\alpha v||^2_{L^2(\Omega)} \tag{1.14}$$

and the norm

$$||v||^2_{m,\Omega} = \sum_{k \leq m} |D^\alpha v|^2_{k,\Omega} \tag{1.15}$$

We shall also need to consider functions that vanish on either the entire or a part of the boundary

$$H_0^1 := \left\{ v : v \in H^1(\Omega), v|_{\partial\Omega} = 0 \right\} \tag{1.16}$$
$$H_{0,\Gamma_D}^1 := \left\{ v : v \in H^1(\Omega), v|_{\Gamma_D} = 0 \right\} \tag{1.17}$$

For $v \in H_0^1(\Omega)$ we have the *Poincaré inequality*

$$|v|_{0,\Omega} \leq C(\Omega)|v|_{1,\Omega} \tag{1.18}$$

and the seminorm $|\cdot|_\Omega$ is therefore a norm in $H^1(\Omega)$, equivalent to $||\cdot||_{1,\Omega}$.

The above function spaces are used widely in the proceeding of this work, especially during the well-posedness analysis as reported in chapter **??**.

1.2.1 Newton's method

Definition 1.1 (Frechèt differentiable)**.** Let be X and Y two vector spaces. Given $f, g \in X$ and a functional $F : X \to Y$, the functional F is Frechét differentiable if it exists a linear bounded operator $A_f : X \to Y$ such that:

$$\lim_{||g||\to 0} \frac{||F(f+g) - F(f) - A_f(g)||_Y}{||g||_X} = 0 \tag{1.19}$$

If the limit exists, we write $DF(f) = A_f$ and call it the Frechét derivative of F at f.

Considering the functional operator (**??**) we can easily compute the relative *Jacobian matrix* $\mathbf{F}'$, whose $(i,j)-th$ entry represents the Frechét derivative of the $i-th$ row of the non linear operator with respect to the $j-th$ variable.

$$\mathbf{F}'_{ij}(\mathbf{U})[\mathbf{V}]_j := \lim_{\eta\to 0} \frac{F_i(\mathbf{U} + \eta[\mathbf{V}]_j) - F_i(\mathbf{U})}{\eta} \qquad \mathbf{V} \in V \tag{1.20}$$

where $[\mathbf{V}]_j \in V$ is the projection of $\mathbf{V}$ in the $j-th$ direction.

$\mathbf{F}'_{ij}(\cdot)$ is a linear operator from V into $L(V,V)$, while $\mathbf{F}'_{ij}(\mathbf{U})$ is the Frechét derivative of the functional F_i respect the variable $[\mathbf{U}]_j$.

Accordingly with the above definitions the Newton's method reads as follows:

Newton's method

Let be X, Y two vector spaces and $\mathbf{F} : X \to Y$ a function operator Frechèt differentiable, given an intial step $\mathbf{U}^0 \in X$ and $toll > 0$, for all $k \geq 0$ solve the following linear problem

$$\begin{aligned} \mathbf{F}'(\mathbf{U}^k)\delta\mathbf{U}^k &= -\mathbf{F}(\mathbf{U}^k) \\ \mathbf{U}^{k+1} &= \mathbf{U}^k + \delta\mathbf{U}^k \end{aligned} \tag{1.21}$$

until $||\mathbf{F}(\mathbf{U}^{k+1})||_Y < toll$, where $||\cdot||_Y$ is a suitable norm on the space Y.

The application of Newton's method has transformed the original problem (**??**) into the *fixed-point problem* of finding $\mathbf{U} \in V$ such that

$$\mathbf{U} = T_{\mathbf{F}}(\mathbf{U}) \tag{1.22}$$

where

$$T_{\mathbf{F}}(\mathbf{U}) = \mathbf{F}'(\mathbf{U})^{-1}(\mathbf{F}'(\mathbf{U})\mathbf{U} - F(\mathbf{U})) \tag{1.23}$$

is the *iteration function* associated with the Newton method. The main result about the convergence of this method.

Theorem 1.1. *Let $\mathbf{U} \in V$ be a solution of problem (**??**). Assume that $\mathbf{F}'$ is Lipschitz continuos in the ball $\mathcal{B}(\mathbf{U}, \delta)$, i.e., that there exists $K > 0$ such that:*

$$||\mathbf{F}'(\mathbf{v}) - \mathbf{F}'(\mathbf{z})||_{L(V,V)} \leq K||\mathbf{v} - \mathbf{z}||_V \qquad \forall \mathbf{v}, \mathbf{z} \in \mathcal{B}(\mathbf{U}, \delta),\ \mathbf{v} \neq \mathbf{z} \tag{1.24}$$

*Then there exists in correspondence $\delta' > 0$, with $\delta' \leq \delta$, such that for all $\mathbf{U}^0 \in \mathcal{B}(\mathbf{U}, \delta')$ the sequence $\{\mathbf{U}^k\}$ generated by (**??**) converges quadratically to $\mathbf{U}$, i.e., there exists $C > 0$ such that, for a suitable $k_0 \geq 0$ we have:*

$$||\mathbf{U} - \mathbf{U}^{k+1}||_V \leq C||\mathbf{U} - \mathbf{U}^k||_V^2 \qquad \forall k \geq k_0 \tag{1.25}$$

1.2.2 Fully coupled Newthon's method

If we consider the linearization of the entire system (**??**) the relative Jacobian matrix is a 3x3 matrix and the problem reads as

$$\begin{bmatrix} F_{1,\varphi} & F_{1,n} & F_{1,p} \\ F_{2,\varphi} & F_{2,n} & F_{2,p} \\ F_{3,\varphi} & F_{3,n} & F_{3,p} \end{bmatrix} \begin{bmatrix} \delta\varphi \\ \delta n \\ \delta p \end{bmatrix} = \begin{bmatrix} -F_1(\varphi, n, p) \\ -F_2(\varphi, n, p) \\ -F_3(\varphi, n, p) \end{bmatrix}. \tag{1.26}$$

Each row of the above matrix is a PDE's equation which we can discretize with suitable numerical proceedings (i.e. finite element method). If we spent for example N_{dof} degrees of freedom to represent $\delta\varphi$, δn and δp we note that the structure of the relative discretizated matrix is a 3x3 block matrix system where every block is a $N_{dof} \times N_{dof}$ matrix:

$$\begin{bmatrix} \mathbf{K}_{1,\varphi} & \mathbf{K}_{1,n} & \mathbf{K}_{1,p} \\ \mathbf{K}_{2,\varphi} & \mathbf{K}_{2,n} & \mathbf{K}_{2,p} \\ \mathbf{K}_{3,\varphi} & \mathbf{K}_{3,n} & \mathbf{K}_{3,p} \end{bmatrix} \begin{bmatrix} \delta\varphi \\ \delta n \\ \delta p \end{bmatrix} = \begin{bmatrix} -\mathbf{F}_1(\varphi, n, p) \\ -\mathbf{F}_2(\varphi, n, p) \\ -\mathbf{F}_3(\varphi, n, p) \end{bmatrix}. \tag{1.27}$$

This implies that at every iteration step we have to solve a linear problem of $3 \times N_{dof}$ variables.

Moreover to ensure convergence of the Newton iterative process, it is important to provide a very good initial guess vector $[\varphi_0, n_0, p_0]$. Because the variable in play have different order of magnitude and the jacobian matrix is often quite ill-conditioned, appropriate scaling and balancing are needed in order to avoid problems associated with round-off error.

This method is widely used in commercial software especially for the strong result of convergence.

1.2.3 Gummel map algorithm

In 1964 H. K. Gummel proposed an orginal and alternative to (**??**) in order to solve the system (**??**) in a semiconductor device in one spatial dimension [Gum64].

The main idea of the algorithm is to move the nonlinearity to the Poisson equation only, and once obtained the electric potential profile, both continuity equations are linearized. This is possible if we consider the Maxwell-Boltzmann approximation for electrons (1.10) and holes (1.11) obtaining

$$F_1(\varphi) = \nabla \cdot (-\epsilon \nabla \varphi) - q(n_i(e^{((\varphi_p - \varphi)/V_{th})} - e^{((\varphi - \varphi_n)/V_{th})}) + D). \tag{1.28}$$

The Gummel algorithm is

Decoupled Gummel map.

0. Give a suitable initial condition for φ^0 and set a positive parameter $toll_{GM} > 0$ (Gummel Map tollerance)

1. Fix a positive parameter $toll_{NLP} > 0$ (Non Linear Poisson tollerance), solve the linearized Non Linear Poisson equation (NLP) in Ω using the Newton's method untill $||F_1(\varphi^{k+1})|| > toll_{NLP}$:

$$\begin{cases} \nabla \cdot (-\epsilon_{Si} \nabla \delta\varphi^k) + \dfrac{1}{V_{th}} \sigma_{Si}^k \delta\varphi^k = f_{Si}^k & in\ \ \Omega_{Si} \\ \nabla \cdot (-\epsilon_{ox} \nabla \delta\varphi^k) = f_{ox}^k & in\ \ \Omega_{ox} \\ \delta\varphi^k = 0 & on\ \ \Gamma_D \\ \nabla \delta\varphi^k \cdot \mathbf{n} = 0 & on\ \ \Gamma_N \\ \varphi^{k+1} = \varphi^k + \delta\varphi^k \end{cases} \tag{1.29}$$

having set,

$$\begin{aligned} \sigma_{Si}^k(\varphi^k) &= q n_i \left[e^{((\varphi_p - \varphi^k)/V_{th})} - e^{((\varphi^k - \varphi_n)/V_{th})} \right] \\ f_{Si}^k(\varphi^k) &= \nabla \cdot (-\epsilon \nabla \varphi^k) + q n_i \left[e^{((\varphi_p - \varphi^k)/V_{th})} - e^{((\varphi^k - \varphi_n)/V_{th})} + D \right] \\ f_{ox}^k(\varphi^k) &= \nabla \cdot (-\epsilon \nabla \varphi^k) \end{aligned}$$

computed accordingly to the definition of the Frechét derivate.

2. Solve the Linear Electron Contintuity Equation (LEC):

$$\begin{cases} \nabla \cdot (q\mu_n n \nabla \varphi^i - q D_n \nabla n) = -qR(n^{i-1}, p^{i-1}) & in\ \ \Omega_{Si} \\ n = n_D & on\ \ \Gamma_{D,Si} \\ \nabla n \cdot \mathbf{n} = 0 & on\ \ \Gamma_{N,Si} \end{cases} \tag{1.30}$$

3. Solve the Linear Hole Contintuity Equation (LHC):

$$\begin{cases} \nabla \cdot (-q\mu_p p \nabla \varphi^i - q D_p \nabla p) = -qR(n^{i-1}, p^{i-1}) & in\ \ \Omega_{Si} \\ p = p_D & on\ \ \Gamma_{D,Si} \\ \nabla p \cdot \mathbf{n} = 0 & on\ \ \Gamma_{N,Si} \end{cases} \tag{1.31}$$

4. If $max\{||\varphi^i - \varphi^{i-1}||_{L^\infty}, ||p^i - p^{i-1}||_{L^\infty}, ||n^i - n^{i-1}||_{L^\infty}\} > toll_{GM}$ restart from step (1).

We shall note with k the iteration step of the inner loop, while with i the iteration step of the Gummel Map: Fig.**??** shows a concisely scheme. Unfortunately there isn't any convergence result for this method like (**??**), although there are several advantages which make Gummel map algorithm to the Fully Coupled Newton's Method. In fact simulations experience shows that the Gummel process is much more insesitive to the choice of the initial guess than Newton's method. This is particularly important in multidimensional problems where it is far from trivial to design a good starting point for initializing.

Another attractive feature is the reduced computational and memory cost: at each iteration step the Gummel algorithm requires the successive solution of three problems, each one of size equal to $N_{dof} \times N_{dof}$.

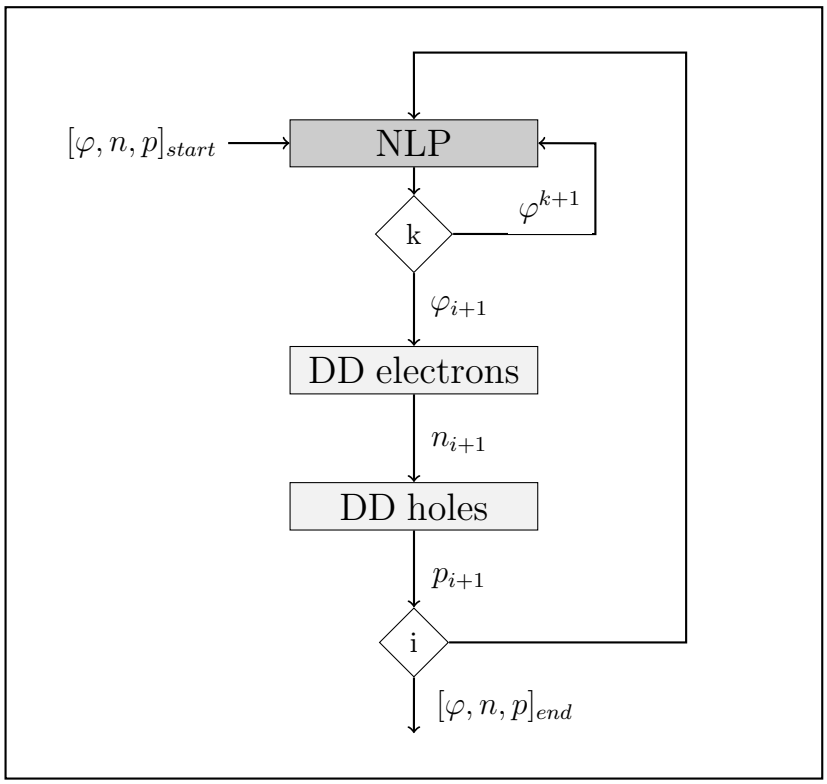


Figure 1.2: Gummel map algorithm

Let us discuss again on step 2-3 of *Decoupled Gummel map*. Accordingly with (1.54) the general R/G phenomenon can be separated in a reaction term and a force term (except for the II which is only a force term contribution). Considering

$$\begin{aligned} R_n^{i-1}(n) &= \sigma_n^{i-1} n - f^{i-1} \\ R_p^{i-1}(p) &= \sigma_p^{i-1} p - f^{i-1} \end{aligned} \tag{1.32}$$

where

$$\begin{gathered} \sigma_n = \frac{p^{i-1}}{F(p^{i-1}, n^{i-1})} \qquad \sigma_p = \frac{n^{i-1}}{F(p^{i-1}, n^{i-1})} \\ f = \frac{n_i^2}{F(p^{i-1}, n^{i-1})}. \end{gathered} \tag{1.33}$$

we can rewrite systems (**??**) and (**??**) as

$$\begin{cases} \nabla \cdot (q\mu_n n \nabla \varphi^i - qD_n \nabla n) + q\sigma_n^{i-1} n = q f^{i-1} & in \ \Omega_{Si} \\ n = n_D & on \ \Gamma_{D,Si} \\ \nabla n \cdot \mathbf{n} = 0 & on \ \Gamma_{N,Si} \end{cases} \tag{1.34}$$

$$\begin{cases} \nabla \cdot (-q\mu_p p \nabla \varphi^i - qD_p \nabla p) + q\sigma_p^{i-1} p = q f^{i-1} & in \ \Omega_{Si} \\ p = p_D & on \ \Gamma_{D,Si} \\ \nabla p \cdot \mathbf{n} = 0 & on \ \Gamma_{N,Si} \end{cases} \tag{1.35}$$

This splitting of R/G term is called *lagging approach* and corresponds to extending to the non-linear case the classical *Jacobi* method for the iterative solution of linear algbraic systems. Thus equations are sequentially solved, it's possible take advantage of the knowing a solution. Indeed an alternative approach would be use the solution of the first solved equation to compute the R/G contribute in the second equation. In such case the lagging method corresponds to extending to the nonlinear case tha classical *Gauss-Seidel* method for the iterative solution in linear algebraic systems.

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