ON SCALING AND NORMS FOR SEMICONDUCTOR DEVICE SIMULATION

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We review and judge the various approaches for scaling the fundamental semiconductor equations. These scalings are the classical scaling after de Mari, the scaling with respect to maxima which leads to a singular perturbation problem in one parameter and a novel strategy which is based on the local magnitude of the doping concentration.
For devices where the doping concentration is of different orders of magnitude in different regions, this local scaling differs markedly from the scaling with respect to maxima and leads to a structure related to singular perturbation with more than one small parameter.
Furthermore, we demonstrate the relations between scaling and appropriate termination criteria for Newton-like iterative methods applicable for the solution of the semiconductor equations.

1. Introduction and scalings

In this paper we want to discuss the effects of different ways of scaling the fundamental semiconductor device equations. It will be shown that proper scaling yields both an a priori information about the solution structure as well as a cheap and effective way to improve certain iterative methods.
We will concentrate on Poisson's equation and for simplicity treat a device in thermal equilibrium. Thus, the potential $\tilde{\psi}$ satisfies

$$(1.1) \quad \operatorname{div}(\varepsilon \operatorname{grad} \tilde{\psi}) = q(2n_i \sinh(\frac{\tilde{\psi}}{U_T}) - D(\tilde{x}))$$

where $D(\tilde{x})$ denotes the doping profile. We assume the permittivity ε and the intrinsic number n_i to be constants.
A scaling is performed where the potential is scaled by the thermal voltage U_T and length is scaled by the Debye length $l = \sqrt{\frac{\varepsilon U_T}{q n_i}}$ of the impurity-free semiconductor which is an upper bound for the actual Debye length.

$$(1.2) \qquad \tilde{\psi} = U_T \psi \ , \quad \tilde{x} = lx \ , \quad D(\tilde{x}) = \frac{n_i}{\lambda^2(x)} C(x)$$

The factor $\lambda^2(x)$ used for scaling the doping concentration is as yet unspecified. It is the subject of this paper to compare the effects of different choices for $\lambda^2(x)$. The scaled Poisson's equation reads

$$(1.3) \qquad \lambda^2(x)\Delta\psi = 2\lambda^2(x)\sinh(\psi) - C(x)$$

In the classical scaling after de Mari (1968) and in the standard singular perturbation scaling (see Vasileva et al. (1976)) λ^2 is taken to be position independent. Singular perturbation theory (see Markowich et al. (1983)) tells us that λ represents a characteristic length of the device if it is chosen appropriately. It is well known, however, that realistic devices (e.g. n^+p-junction diodes) may possess different characteristic lengthes in different regions which suggests a position dependent choice of $\lambda^2(x)$.

In section 2 we give an outline of some results on a damped Newton procedure which are due to Deuflhard (1974). The classical Newton method being invariant under affine transformations is not affected by different choices of $\lambda^2(x)$ which only mean different factors in front of Poisson's equation. The efficiency of the damped Newton method, however, may rely heavily on a choice of $\lambda^2(x)$ which yields moderate bounds for the condition number of the linearized problem. Besides, a moderate condition number means that the norm of the residual is a good measure for the error in the approximate solution and, thus, can be used in termination criteria for the iteration process.

Table 1.1 contains the choices of $\lambda^2(x)$ in the de Mari scaling, the singular perturbation scaling and our suggestion of a local scaling. In section 3 we will discuss the conditioning of the corresponding linearized problems using a one dimensional model for an n^+p-junction for simplicity. Opposite to the traditional scalings, the local scaling allows for bounds of the condition number which are essentially independent of the doping profile.

Finally we want to stress that the use of the local scaling in a numerical method does not cause additional cost since it only amounts in using a different norm for the computed residual. Our points are demonstrated by some numerical results contained in section 4.

	de Mari	Vasileva	local scaling
$\lambda^2(x)$	1	$\lambda_o^2 := \frac{n_i}{\max\|D\|}$	$\lambda_D^2(x) := \frac{n_i}{\sqrt{D^2(x)+4n_i^2}}$
physical meaning of $\lambda(x)$	maximal scaled Debye length	minimal scaled Debye length	local scaled Debye length

Table 1.1

2. The modified Newton method

We consider the damped Newton method

$$(2.1) \qquad x_{k+1} = x_k - \mu_k DF^{-1}(x_k)F(x_k)$$

for the problem $F(x) = 0$. Here $DF(x)$ denotes the Frechet derivative of the operator $F(x)$. Under assumptions which essentially guarantee the existence of a solution x^* which can be connected to x_o by a path on which the norm of F decreases Deuflhard (1974) showed

Theorem 2.1: Let μ_k be selected so that

$$0 < \mu_k \leq \bar{\mu}_k \quad \text{where} \quad \bar{\mu}_k := \min\{1, \frac{1}{h_k(1+h_k)\,\mathrm{cond}(DF(x_k))}\}$$

with $h_k = \alpha \| F(x_k) \|$, where the constant α contains bounds on the Lipschitz constant and the inverse of $DF(x)$.

Then $\lim_{k\to\infty} x_k = x^*$ with $F(x^*) = 0$ and $\| F(x_{k+1}) \| < \| F(x_k) \|$

Obviously bad conditioning of the linear problems arising in the iteration procedure implies small steps which slows down the convergence. Besides, Taylor's formula

$$(2.2) \qquad F(x_k) = DF(x_k)(x^*-x_k) + O(\| x^*-x_k \|^2)$$

implies that the norm of the residual $F(x_k)$ can be used as a measure for $\| x^*-x_k \|$ if $DF(x_k)$ is well-conditioned.

3. Conditioning of the linearized problem

An abrupt n^+p-junction in thermal equilibrium can be described by the one dimensional model

$$(3.1a) \qquad \lambda_o^2 \psi'' = 2\lambda_o^2 \sinh(\psi) - C(x), \quad x\in[-1,1] \quad \text{with} \quad C(x) = \begin{cases} 1 & x<0 \\ -\delta^2 & x>0 \end{cases}$$

subject to the boundary conditions

(3.1b) $\psi(\pm 1) = \ln \frac{C(\pm 1)+\sqrt{C^2(\pm 1)+4\lambda_o^4}}{2\lambda_o^2}$

which represent Ohmic contacts. We assume $\lambda_o^2 \ll \delta^2 \ll 1$.
We analyse the linearization of problem (3.1)

(3.2a) $\lambda^2(x)\rho'' - 2\lambda^2(x)\cosh(\psi)\rho = f$

(3.2b) $\rho(-1) = a \ , \quad \rho(1) = b$

at the solution. For simplicity we use the fact that

$\psi(x) \sim \bar{\psi}(x) = \ln \frac{C(x)+\sqrt{C^2(x)+4\lambda^4(x)}}{2\lambda^2(x)}$ for x away from the junction x=0,

which follows from singular perturbation theory (see e.g. Markowich et al. (1983)). Besides we neglect the effect of the boundary conditions treating the case a = b = 0. Thus we replace (3.2) by

(3.3) $A_\lambda \rho := \lambda^2(x)(\rho'' - 2\cosh(\bar{\psi})\rho) = f$

with $A_\lambda : C^{2*} \to C^*$ where C^* is the space of functions which are continuous on $[-1,0)$ $(0,1]$ and have a jump discontinuity at x=0. C^{2*} is defined by $C^{2*} = \{\rho \varepsilon C^1[-1,1], \ \rho'' \varepsilon C^* , \ \rho(-1) = \rho(1) = 0\}$.
The spaces C^* and C^{2*} are equipped with the L^∞-norm $\|f\|_\infty := \sup_{[-1,1]} |f(x)|$ and the norm $\|\rho\|_* := \|\lambda_D^2 \rho''\|_\infty + \|\rho\|_\infty$ respectively. The condition number of A_λ is defined by

$$\mathrm{cond}(A_\lambda) := \|A_\lambda\|_{C^{2*}\to C^*} \ \|A_\lambda^{-1}\|_{C^*\to C^{2*}}$$

Now we can prove

Lemma 3.1: $\mathrm{cond}(A_\lambda) \leq 3 \left\| \frac{\lambda^2}{\lambda_D^2} \right\|_\infty \cdot \left\| \frac{\lambda_D^2}{\lambda^2} \right\|_\infty$

Proof: Using that $\frac{1}{\lambda_D^2(x)} = 2\cosh(\bar{\psi}(x))$ holds (3.3) can be written as

$$\frac{\lambda^2(\lambda)}{\lambda_D^2(\lambda)}(\lambda_D^2\rho'' - \rho) = f$$

which immediately implies

$$\|f\|_\infty \leq \left\| \frac{\lambda^2}{\lambda_D^2} \right\|_\infty \|\rho\|_* \ .$$

An application of the maximum principle yields $\|\rho\|_\infty \leq \left\| \frac{\lambda_D^2}{\lambda^2} \right\|_\infty \|f\|_\infty$,

which together with the estimate $\|\lambda_D^2\rho''\|_\infty = \left\| \rho + \frac{\lambda_D^2}{\lambda^2} f \right\|_\infty \leq 2 \left\| \frac{\lambda_D^2}{\lambda^2} \right\|_\infty \|f\|_\infty$

implies

$$\|\rho\|_* \leq 3 \left\| \frac{\lambda_D^2}{\lambda^2} \right\|_\infty \|f\|_\infty \cdot \square$$

With a doping profile as given in (3.1a) we obtain for any scaling with constant λ the estimate $\frac{3}{\delta^2}$ for the condition number. For the local scaling $\lambda(x) = \lambda_D(x)$ the bound for the condition number is independent of the doping profile.

4. Numerical example

We want to demonstrate the difference between the choices for $\lambda(x)$ on a realistic problem. A two dimensional model of a MOSFET was solved given a starting solution and a fixed grid. Table 4.1 is a comparison between two runs whith $\lambda(x) = \lambda_o$ and $\lambda^2(x) = \frac{n_i}{N_D(\tilde{x}) + N_A(\tilde{x})}$ where the doping concentration is given by $D(\tilde{x}) = N_D(\tilde{x}) - N_A(\tilde{x})$. In practical situations this choice of $\lambda(x)$ differs from $\lambda_D(x)$ only at the junction. In table 4.1 the number of iterations, the norms of the residuals and the damping factors different from 1 are depicted. The typical convergence behavior of Newton's method can only be observed for the local scaling which demonstrates that it is close to the "natural scaling" in the sense of Deuflhard (1974).

$\lambda^2(x) = n_i/(N_D+N_A)$			$\lambda(x) = \lambda_o$		
k	|| residual ||	μ_k	k	|| residual ||	μ_k
1	2,52 E3		1	2,04 E0	
2	2,43 E3	2^{-5}	2	1,91 E0	2^{-4}
3	2,05 E3	2^{-4}	3	9,54 E-1	2^{-1}
4	1,18 E3	2^{-2}	4	2,18 E-1	
5	4,36 E2	2^{-1}	5	8,04 E-2	
6	7,20 E2		6	2,96 E-2	
7	2,56 E1		7	1,09 E-2	
8	8,38 E0		8	4,00 E-3	
9	2,05 E0		9	1,47 E-3	
10	2,16 E-1		10	5,37 E-4	
11	2,96 E-3		11	1,93 E-4	
12	5,60 E-7		12	6,48 E-5	
13	3,57 E-11		13	2,08 E-6	
			14	4,21 E-8	
			15	1,81 E-11	

Table 4.1

References :

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