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Numerical Solutions of Some Semiconductor Devices by a Domain Decomposition Method

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Abstract

In this report we examine a domain decomposition technique for the numerical solution of some semiconductor devices. The domain decomposition method employed here is non-overlapped and is based on a variant of the simple shooting method. A number of different one-dimensional examples are given. The study reported here can be easily extended to two and three-dimensional semiconductor simulations.

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1 Introduction

Although the numerical simulation of semiconductor devices in two dimensions is well established, many of the numerical techniques used are not suited to implementation on parallel computers. Divide-and-conquer algorithms have been demonstrated most suitable for such simulations on coarse-grain parallel computers. Ideally, one would require that the computational domain split into a number of subdomains, yielding a family of independent subproblems of lower computational complexity. These independent subproblems are then combined to generate the solution for the whole computational domain. In a parallel implementation this combination will result in data communication between subproblems. This takes place only when the family of independent subproblems has been solved. The nature of domain decomposition [2] dictates that this communication is only between neighbouring subproblems. This has the advantage of reducing the total communication time within a network of processors, assuming each subproblem is being solved in one processor. The consistency of the subproblem solutions with the original problem is ensured by imposing interface conditions between these subproblems.

The current domain decomposition method is based on the concept of simple shooting method [4], and we employ a fixed point iteration technique developed in [2] to solve the discretised interface operator equation. The interface operator equation represents the interface problem. Its discrete version is usually represented by a full matrix but is not constructed in our approach. Some preliminary results for p-n junctions were reported in [3]. In this report, the algorithm is tested using a series of one-dimensional semiconductor devices. The study also provides some insight into the extension of the method to two-dimensional and three-dimensional simulations.

2 The Mathematical Model

The classical drift-diffusion differential equations governing the electrical behaviour of semiconductor devices [1] are given by

$$\nabla^2\psi = -\frac{q}{\epsilon}(\Gamma + p - n) \tag{1}$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla\cdot\mathbf{J}_p - R \tag{2}$$

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla\cdot\mathbf{J}_n - R \tag{3}$$

where ψ denotes the electrostatic potential, $\mathbf{J}_p$ and $\mathbf{J}_n$ the hole and electron current concentrations respectively, R the net recombination rate, q the electronic charge, ϵ the permitivity of the device material, Γ the doping function, p the hole concentration and n the electron concentration.

The currents are derived from the Boltzmann transport equation and are given by

$$\mathbf{J}_p = -qD_p\nabla p - q\mu_p p\nabla\psi \tag{4}$$

$$\mathbf{J}_n = qD_n\nabla n - q\mu_n n\nabla\psi \tag{5}$$

where D_p and D_n are the diffusion constants for holes and electrons respectively, and μ_p and μ_n are the mobilities for holes and electrons. Introducing the quasi-Fermi potentials ϕ_p and ϕ_n defined by

$$p = n_i e^{(\phi_p - \psi)/V_T} \tag{6}$$

$$n = n_i e^{(\psi - \phi_n)/V_T} \tag{7}$$

where V_T is the thermal voltage ($V_T = KT/q$), K is the Boltzmann's constant, T is the absolute temperature, and n_i is the intrinsic concentration of electrons in the device. Substituting (6) and (7) into the current equations (4) and (5) yields

$$\mathbf{J}_p = -q\mu_p p \nabla \phi_p \tag{8}$$

$$\mathbf{J}_n = -q\mu_n n \nabla \phi_n \tag{9}$$

For a junction in an *off state*, there is *no* current flowing through the contacts and it is sufficient to model this situation with Poisson's equation (1). For computational reasons the equations and variables are scaled to obtain dimensionless quantities. The symbols of the above unscaled variables are adopted as the symbols of the scaled variables in the subsequent scaled equations. Therefore for one-dimensional devices in the off state, we require the solution of the following scaled two-point boundary value problem:

$$\frac{d^2\psi}{dx^2} + Q(x,\psi) = 0 \qquad \in \qquad \Omega = \{x : 0 \leq x \leq w\} \tag{10}$$

subject to the Dirichlet boundary conditions $\psi(0) = V_0$ and $\psi(w) = V_w$. Here we have measured ψ in units of thermal volts, x in units of the Debye length ($L^2 = \epsilon KT/q^2 n_i$), $Q(x,\phi)$ in units of n_i. The source term is given by

$$Q(x,\psi) = \Gamma(x) + e^{(\phi_p - \psi)} - e^{(\psi - \phi_n)}$$

where $\Gamma(x)$ is measured in units of n_i. Assuming Boltzmann statistics and suppose the scaled thermal equilibrium condition $pn = 1$ holds at the contacts, we obtain the scaled quasi-Fermi potential boundary values [1] as

$$\phi_p(0) = V_0 + \ln\left[-\Gamma(0)/2 + \sqrt{(\Gamma(0)/2)^2 + 1}\right] \tag{11}$$

and

$$\phi_n(w) = V_w - \ln\left[\Gamma(w)/2 + \sqrt{(\Gamma(w)/2)^2 + 1}\right] \tag{12}$$

As the device is in the off state (11) and (12) fix the values of the quasi-Fermi potentials throughout the device.

3 The Numerical Scheme

3.1 The Domain Decomposition Method

We adopted a non-overlapped domain decomposition at the level of the physical problem. The subdomains are joined only at the interfaces to form the global domain. Hence each of the subproblems can be completely decoupled from the others. This is particularly suitable for the coarse-grained parallel computational environment. In this report, we concentrate on

the nonlinear elliptic boundary value problem (10). The domain Ω is subdivided into $s+1$ subdomains with the following $s+1$ related nonlinear elliptic boundary value subproblems,

$$\frac{d^2u_k}{dx^2} + Q(x, u_k) = 0, \qquad u_k(x_{k-1}) = \lambda_{k-1}, \quad u_k(x_k) = \lambda_k \tag{13}$$

with $x_0 = 0$ and $x_{s+1} = w$, $u_1(0) = \psi(0)$ and $u_{s+1}(w) = \psi(w)$. Suppose $u_k = u_k(x; \boldsymbol{\lambda})$ denotes the solution of (13) in $x_{k-1} < x < x_k$, where $\boldsymbol{\lambda} = [\lambda_1 \ \lambda_2 \ \cdots \ \lambda_s]$. In order to have unique values of $\psi'(x_k)$, $k = 1, 2, \cdots, s$, we require a vector $\boldsymbol{\lambda}$ such that the following vector defect equation is satisfied,

$$\mathbf{D}(\boldsymbol{\lambda}) = [D_k(\boldsymbol{\lambda})] \equiv [\frac{\partial}{\partial x} u_k(x_k; \boldsymbol{\lambda}) - \frac{\partial}{\partial x} u_{k+1}(x_k; \boldsymbol{\lambda})] = 0 \tag{14}$$

The continuity of the function ψ across the interfaces is implicit in (13). The vector defect equation represents the reduced interface problem and guarantees the continuity of ψ' across the interfaces. If $\boldsymbol{\lambda} = \boldsymbol{\lambda}^*$ is a root of $\mathbf{D}(\boldsymbol{\lambda}) = 0$, then the function

$$\psi(x) = \begin{cases} \lambda^*_{k-1} & x = x_{k-1} \\ u_k(x; \boldsymbol{\lambda}^*) & x_{k-1} < x < x_k, \\ \lambda^*_k & x = x_k \end{cases} \qquad k = 1, 2, \cdots, s+1 \tag{15}$$

where $\lambda^*_0 = V_0$ and $\lambda^*_{s+1} = V_w$, is a solution of (10). The method can be considered as a variant of the shooting method [4]. In the two subdomain case, the defect equation is a scalar equation involving one interface and thus only one unknown. In the multidimensional case, the Jacobian matrix $\mathbf{J}(\boldsymbol{\lambda}) = \mathbf{D}'(\boldsymbol{\lambda})$ is a symmetric tridiagonal matrix [2].

3.2 Solution of the Interface Problem

In order to solve the interface problem, i.e. the defect equation, without computing the matrix coefficients of the Jacobian matrix, a fixed point iteration technique is applied. The vector defect equation is rewritten as

$$\boldsymbol{\lambda} = \mathbf{G}(\boldsymbol{\lambda}) \equiv \boldsymbol{\lambda} - \alpha \mathbf{D}(\boldsymbol{\lambda}) \quad \alpha \neq 0 \tag{16}$$

and we employ the scheme

$$\boldsymbol{\lambda}^{(m+1)} = \boldsymbol{\lambda}^{(m)} - \alpha_m \mathbf{D}(\boldsymbol{\lambda}^{(m)}) \quad m = 0, 1, 2, \cdots \tag{17}$$

Here α_m is an adaptive parameter [2] given by

$$\alpha_m := \alpha_{m-1} \frac{\|\mathbf{D}(\boldsymbol{\lambda}^{(m-1)})\|_2}{\|\mathbf{D}(\boldsymbol{\lambda}^{(m)}) - \mathbf{D}(\boldsymbol{\lambda}^{(m-1)})\|_2} \tag{18}$$

In order to evaluate $\mathbf{D}(\boldsymbol{\lambda}^{(m)})$, we need to solve the $s+1$ subproblems as given by (13). Since the subproblems are nonlinear, applying Newton's iteration scheme to (13) leads to

$$\left(\frac{d^2}{dx^2} + \frac{\partial Q}{\partial u_k}\right)(u_k^{(\nu)} - u_k^{(\nu-1)}) = -\frac{d^2 u_k}{dx^2}^{(\nu-1)} - Q(x, u_k^{(\nu-1)}) \tag{19}$$

Here ν denotes the number of the Newton iteration loops for the solution of a subproblem, and clearly $\nu = \nu(m, k)$. A second order finite difference technique is used to discretise (19) leading to a set of tridiagonal equations and we use U_k to denote the discrete approximation of u_k. We take $U_k^{(0)} = U_k(x; \boldsymbol{\lambda}^{(m-1)})$ and iterate until $\|U_k^{(\nu)} - U_k^{(\nu-1)}\|_1 < \delta$. Our experience shows that ν is usually 1 except when $m = 1$ if δ is chosen as 0.01. In choosing this δ, one can minimise the computational work involved in the Newton iterations.

3.3 Performance Monitor

Let N denote the total number of nodes in the entire computational domain. One work unit is defined as the computational work required to perform one Newton iteration on a mesh with $N-2$ unknowns. Also, let N_k be the number of nodes in k-th subdomain, $k = 1, 2, \cdots, s+1$ and M be the number of updates in order to obtain a converged solution $\boldsymbol{\lambda}^{(M)}$ along the interfaces by using the fixed point iteration scheme given by (17). Suppose there is a set of $s+1$ concurrent processors and that the connectivity is the same as the layout of the subdomains, then it is possible to estimate the total computing time by using the following total work unit count

$$\tau = \sum_{m=1}^{M} \max_{1 \le k \le s+1} \left\{ \frac{N_k - 2}{N-2} \nu(m,k) \right\} \tag{20}$$

where $\nu(m,k)$ is the number of Newton iterations required to solve the k-th subproblem during the m-th update of the interfaces. Clearly, when $s = 0$, i.e. no interface, we have $\tau = \sum_{m=1}^{M} \nu(m,1)$ in which case the number of Newton iterations is the total work unit count.

4 Some Basic Devices

In the following numerical tests, we have used silicon as the semiconductor material of which the permitivity is $\epsilon = 1.1 \times 10^{-16}\mathrm{F}(\mu\mathrm{m})^{-1}$. The ambient temperature is assumed constant at 300°K and thus $n_i = 1.48 \times 10^{-2}(\mu\mathrm{m})^{-3}$. Taking $K = 1.38 \times 10^{-23}\mathrm{J°K}^{-1}$ and $q = 1.6 \times 10^{-19}\mathrm{C}$, we can evaluate the normalisation constants.

A series of different sizes of devices with different doping functions are described in this section. We look at basic devices, including p-n junctions, p-i-n junctions and thyristors, but excluding transistors. The reason being that an extra Dirichlet boundary condition applied at the emitter immediately decouples the problem into two independent p-n junctions [1].

4.1 p-n Junctions

A p-n junction consists of a p-layer and an n-layer with a transition region between the two. It is the basic structure found within all more complex semiconductor devices. It also has a variety of functions on its own, such as current rectification, amplification, switching, and oscillation. A linearly graded junction can be defined by the doping function

$$\Gamma_{10}(x) = \begin{cases} -N_a & 0 \le x \le w_1 \\ -N_a + \dfrac{(N_a + N_d)}{(w_2 - w_1)}(x - w_1) & w_1 < x < w_2 \\ N_d & w_2 \le x \le w \end{cases} \tag{21}$$

where N_a is the acceptor concentration and N_d is the donor concentration. By taking $N_a = N_d$ and $w = w_1 + w_2$, the doping profile is symmetric about $x = w/2$, otherwise the profile is non-symmetric.

In order to understand more about the present numerical scheme, we have constructed two other doping profiles such that the acceptor and donor concentrations are equal to $\mathcal{N}$. These two doping profiles which result in p-n junctions, are given by

$$\Gamma_{11}(x) = -\mathcal{N}e^{-x^2/w^2} + \mathcal{N}e^{-(w-x)^2/w^2} \tag{22}$$

$$\Gamma_{12}(x) = -\mathcal{N}e^{-m_1 x^2} + \mathcal{N}e^{-m_2(w-x)^2} \tag{23}$$

where $m_1 = \frac{1}{w_a^2}\ln\mathcal{N}$, $m_2 = \frac{1}{w_d^2}\ln\mathcal{N}$, and the width of the device is $w = w_a + w_d$. Both of the diffused layers in (22) and in (23) have Gaussian-type distribution. $\Gamma_{11}(x)$ gives a symmetric doping profile about $x = w/2$ and $\Gamma_{12}(x)$ gives a symmetric doping profile only when $w_a = w_d$.

4.2 *p-i-n* Junctions

A typical *p-i-n* junction is the microwave power limiter. It consists of a *p*-type diffused layer with an acceptor concentration of N_a, width w_a, at one end, and an *n*-type region with a donor concentration of N_d, width w_d, at the other end. In between the two regions, there is a central *n*-type with a donor concentration of N_b of width w_b. The total width of the device is $w = w_a + w_b + w_d$. The doping function of a typical *p-i-n* junction is given by

$$\Gamma_{20}(x) = -N_a e^{-m_1 x^2} + N_b + N_d e^{-m_2(w-x)^2} \tag{24}$$

where $m_1 = \frac{1}{w_a^2}\ln(N_a/N_b)$, and $m_2 = \frac{1}{w_d^2}\ln(N_d/N_b)$. Both diffused layers have Gaussian-type distributions.

4.3 Thyristors

Thyristors are high-power switching devices that are widely applied in power controlling and conversion equipment in the field of power electronics. A thyristor has a *p-n-p-n* four layer structure with two main electrodes connected to outer *p* and *n* layers and a control gate connected to either of the intermediate layers. In transient calculations [1], the following hypothetical diode is always used to prepare initial data to the thyristor calculation,

$$\Gamma_{30}(x) = N_{ne}e^{-m_1 x^2} + N_{pb}e^{-m_2(x+w_{off})^2} + N_{nb} - N_{pe}e^{-m_3(w-x)^2} \tag{25}$$

whereas the actual thyristor has the following doping function which only differs in one sign

$$\Gamma_{31}(x) = N_{ne}e^{-m_1 x^2} - N_{pb}e^{-m_2(x+w_{off})^2} + N_{nb} - N_{pe}e^{-m_3(w-x)^2} \tag{26}$$

Here

$$m_2 = \frac{1}{(w_{pb}+w_{ne}+w_{off})^2}\ln(N_{pb}/N_{nb})$$

$$m_1 = m_2\left(1 + \frac{w_{off}}{w_{ne}}\right)^2 + \frac{1}{w_{ne}^2}\ln(N_{ne}/N_{pb})$$

$$m_3 = \frac{1}{w_{pe}^2}\ln(N_{pe}/N_{nb})$$

The total width of the device is $w = w_{ne} + w_{pb} + w_{nb} + w_{pe}$. All diffused layers have Gaussian-type distribution.

5 Numerical Examples

In the following section we present the results from a number of numerical experiments using the techniques and test problems described above.

Table 1 shows the series of examples to be tested. The various dimensionless quantities are multiplied by their respective normalisation constants to give the corresponding physical values. All tests were performed using double precision and solved on the entire domain without decomposition as a standard set of results for comparison with the subsequent domain decomposition results. We use superscript S to denote a symmetric doping profile. Table 2 shows the total number of grid points N and the corresponding mesh size h used in each tests.

Where the computations performed on the entire domain, the stopping criterion used was $\|\Psi^{(\nu)} - \Psi^{(\nu-1)}\|_2 < \eta$, where Ψ is the discrete approximation of ψ. In the case of domain decomposition, the stopping criterion was $\|\lambda^{(m)} - \lambda^{(m-1)}\|_2 < \eta$. Here η is chosen as 0.5×10^{-10} to avoid getting too close to the machine accuracy of double precision arithmetic which is usually around 12 digits.

The initial approximation, i.e. $\lambda^{(0)}$ was $\Psi(c) = (\psi(0) + \psi(w))/2$ where c satisfies $\Gamma(c) = 0$, otherwise it was taken as either $\min\{\psi(0), \psi(w)\}$ when $\Gamma < 0$ or $\max\{\psi(0), \psi(w)\}$ when $\Gamma > 0$.

$\Gamma(x)$	$\psi(0)$ $\times V_T$	$\psi(w)$	wL (μm)	other widths (μm)	acceptor/donor concentration $(\mu\text{m})^{-3}$
Γ_{10}^S	0	10	180	$w_1 L = 30$, $w_2 L = 150$	$N_a n_i = N_d n_i = 1480$
Γ_{10}	0	10	180	$w_1 L = 10$, $w_2 L = 130$	$N_a n_i = N_d n_i = 1480$
Γ_{11}^S	0	10	180	None	$\mathcal{N} n_i = 1480/(1 - e^{-1})$
Γ_{12}^S	0	10	180	$w_a L = w_d L = 90$	$N_a n_i = N_d n_i = 1480$
Γ_{12}	0	10	180	$w_a L = 70$, $w_d L = 110$	$N_a n_i = N_d n_i = 1480$
Γ_{20}	0	10	3.5	$w_a L = 2$, $w_b L = 1$ $w_d = 0.5$	$N_a n_i = 10^9$, $N_b n_i = 10^3$ $N_d n_i = 4 \times 10^7$
Γ_{30}	10	0	700	$w_{ne} L = 27.5$, $w_{pb} L = 37.5$ $w_{nb} L = 510$, $w_{pe} L = 125$ $w_{off} L = 60$	$N_{ne} n_i = 10^9$, $N_{pb} n_i = 2 \times 10^7$ $N_{nb} n_i = 40$, $N_{pe} n_i = 2 \times 10^7$
Γ_{31}	10	0	700	Same as Problem Γ_{30}	Same as Problem Γ_{30}

Table 1: Definitions of the test problems.

Doping	Mesh					
$\Gamma_{10}(x)$	$N =$	91	181	361	721	1441
$\Gamma_{11}(x)$	$h =$	2.000	1.000	0.500	0.250	0.125
$\Gamma_{12}(x)$						
$\Gamma_{20}(x)$	$N =$	141	281	561	1121	2241
	$h =$	0.025	0.0125	0.00625	0.003125	0.0015625
$\Gamma_{30}(x)$	$N =$	701	1401	2801	5601	
$\Gamma_{31}(x)$	$h =$	1.000	0.500	0.250	0.125	

Table 2: Meshes used for the test problems.

We examine the convergence of each test by recording the total work unit τ and the number

of iterations M to update the interfaces assuming a constant mesh size in each subdomain. τ is only compared with the standard results because M only records the number of iterations to update the interfaces. This number of iterations can be reduced or increased with a different type of fixed point iterations. In the following tables "N.A." means *not applicable* the given number of grid points cannot be shared equally among the subdomains and "oscillation" means the error $\|\lambda^{(m)} - \lambda^{(m-1)}\|_2$ is oscillating instead of decreasing.

5.1 p-n Junctions

We first present the results of the simple $p-n$ junction using profiles Γ_{10}^S, Γ_{11}^S and Γ_{10}^S. These are the symmetric forms of the profiles with the junctions at $x = w/2$.

The results for Problem Γ_{10}^S are shown in Tables 3 and 4. For $s+1 = 2,4,6,10,20,30$, the subdomains are evenly distributed with the restriction that $x = w/2$ is an interface. For $s+1 = 3,5,9,15$, the subdomains are evenly distributed with no interface lying inside the depletion layer.

$s+1$	N				
	91	181	361	721	1441
2	1	1	1	1	1
4	N.A.	8	7	7	7
6	11	11	10	11	11
10	17	17	16	16	15
20	N.A.	29	30	26	22
30	oscillation	130	108	87	69
3	8	8	7	8	8
5	15	15	14	14	12
9	29	30	24	24	20
15	358	124	100	81	75

Table 3: M for Problem Γ_{10}^S.

The results for Problem Γ_{11}^S are shown in Tables 5 and 6. Again for $s+1 = 2,4,6,10,20,30$, the subdomains are evenly distributed with the restriction that $x = w/2$ is an interface. For $s+1 = 3,5,9,15$, the subdomains are evenly distributed with no interface lying inside the depletion layer.

Finally the results for Problem Γ_{12}^S are shown in Tables 7 and 8. For $s+1 = 2,4,6,10$, the subdomains are evenly distributed with the restriction that $x = w/2$ is an interface. For $s+1 = 3$, the subdomains are evenly distributed with no interface lying inside the depletion layer.

The initial approximations of the above three problems at the point $x = w/2$ are the exact solutions at that point. Therefore it is expected to have $M = 1$ for two subdomain cases with the interface chosen at $x = w/2$.

For a given number of subdomains one would expect that the number of iterations M will be independent of the number of mesh points N. This is borne out in Tables 3,5 and 7.

$s+1$	N				
	91	181	361	721	1441
1	11	13	13	13	13
2	4.449	4.475	4.986	4.993	4.997
4	N.A.	3.933	3.967	3.983	3.992
6	2.989	3.078	3.123	3.310	3.322
10	2.038	2.374	2.437	2.469	2.385
20	N.A.	1.654	1.847	1.704	1.530
30	oscillation	4.162	3.799	3.231	2.776
3	5.213	5.274	5.304	5.651	5.659
5	4.393	4.497	4.549	4.549	4.188
9	3.742	4.034	3.585	3.585	3.204
15	20.787	8.480	7.432	6.275	6.074

Table 4: τ for Problem Γ_{10}^S.

However one should note that M appears to become more variable as s increases. As expected M increases as the number of subdomains increases.

The total work unit τ is intedned to be independent of the number of mesh points N and this is demonstrated in Tables 4, 6 and 8. As the number of subdomains increases τ decreases. This continues until a certain number of subdomains is reached whereby τ begins to increase again. A possible reason is that there is at least one subdomain lies entirely inside the depletion layer. Since the change in ψ' from outside the depletion layer to inside the depletion is very rapid it is difficult to solve the vector defect equation. The depletion layer for problem Γ_{10}^S is approximately $80 < xL < 100$. Hence for $s+1 = 30$, there are six subdomains inside the depletion layer. The depletion layers for problems Γ_{11}^S and Γ_{12}^S are larger than that for problem Γ_{10}^S. In these examples we see that the maximum number of subdomains required to achieve a minimum τ decreases.

These results seem to confirm the analysis of the method for symmetric junctions. The second set of tests performed were on the unsymmetric form of the junctions.

The results for the unsymmetric form of Problem Γ_{10} are shown in Tables 9 and 10. For the upper parts of the tables, the subdomains are evenly distributed without any interface restriction. For the lower parts of the tables, the interfaces are chosen at $xL = 70$ when $s+1 = 2$, at $xL = 70$ and 125 when $s+1 = 3$, at $xL = 35$, 70, 97.5, 125, and 152.5 when $s+1 = 6$, and at $xL = 35$, 70, 92, 114, 136, 158 when $s+1 = 7$.

The coordinate at $xL = 70$ has $\Gamma_{10}(70/L) = 0$ and $\psi(70/L) = (\psi(0) + \psi(180/L))/2$. With the choice of initial approximation at $xL = 70$ as described previously, we have actually obtained the exact solution at that point. Therefore one would expect $M = 1$ for a two subdomain case with its interface chosen at $xL = 70$. The depletion layer for Problem Γ_{10} approximately satisfies $60 < xL < 80$. For thoses cases where the depletion layer contains an interface, e.g. $s+1 = 5, 10$, no converged solution is obtained unless a very accurate inital approximation is used at the interface, e.g. $s+1 = 3$. From Table 10, minimum values of τ occur at $s+1 = 6$. In order to avoid any subdomain lying entirely inside the depletion layer,

$s+1$	N				
	91	181	361	721	1441
2	1	1	1	1	1
4	N.A.	8	7	7	8
6	11	11	11	10	12
10	24	24	21	18	15
20	N.A.	31	31	28	24
30	oscillation	oscillation	364	221	173
3	7	7	7	8	8
5	13	13	13	13	13
9	30	34	31	23	23
15	259	115	94	84	60

Table 5: M for Problem Γ_{11}^{S}.

$s+1$	N				
	91	181	361	721	1441
1	11	13	13	13	13
2	4.449	4.972	4.986	4.993	5.496
4	N.A.	4.179	3.976	3.983	4.491
6	2.989	3.240	3.278	3.145	3.654
10	2.876	3.134	2.925	2.656	2.484
20	N.A.	1.788	1.894	1.801	1.727
30	oscillation	oscillation	12.256	8.573	7.088
3	4.888	5.274	5.304	5.651	5.992
5	4.011	4.302	4.351	4.376	4.578
9	3.843	4.564	4.345	3.516	3.867
15	15.449	8.112	7.240	6.602	5.281

Table 6: τ for Problem Γ_{11}^{S}.

$s+1$	N				
	91	181	361	721	1441
2	1	1	1	1	1
4	N.A.	9	9	9	10
6	22	20	19	19	17
10	293	167	133	99	125
3	22	11	11	11	12

Table 7: M for Problem Γ_{12}^{S}.

$s+1$	N				
	91	181	361	721	1441
1	15	15	15	15	15
2	5.933	5.966	5.983	5.992	5.996
4	N.A.	4.916	4.958	4.979	5.239
6	5.191	5.022	4.930	5.296	5.149
10	28.135	17.950	15.209	11.949	15.006
3	7.269	7.251	7.292	8.310	8.655

Table 8: τ for Problem Γ_{12}^S.

$s+1$	N				
	91	181	361	721	1441
2	7	7	7	8	9
4	N.A.	12	11	11	11
5	oscillation	oscillation	oscillation	oscillation	oscillation
6	26	26	24	19	20
8	N.A.	N.A.	243	222	119
10	oscillation	oscillation	oscillation	oscillation	oscillation
2	1	1	1	1	1
3	N.A.	7	6	6	7
6	N.A.	N.A.	14	13	12
7	N.A.	15	13	14	13

Table 9: M for Problem Γ_{10}.

we can only have a maximum of nine subdomains.

The convergence results for Problem Γ_{12} are shown in Tables 11 and 12. The lower blocks of the tables are divided into three parts. In the top part, the subdomains are evenly distributed without any interface restriction. In the middle part, the interface is chosen at $xL = 70$ when $s+1 = 2$, and at $xL = 70$ and 126 when $s+1 = 3$. The depletion layer is isolated in the bottom part such that for $s+1 = 3$, the interfaces are chosen at $xL = 50$ and 100 and for $s+1 = 4$, the interfaces are chosen at $xL = 50$, 100, and 140.

The coordinate at $xL = 70$ has $\Gamma_{12}(70/L) = 0$ but does not imply $\psi(70/L) = (\psi(0) + \psi(180/L))/2$. Therefore $M \neq 1$ for a two subdomain case with its interface chosen at $xL = 70$. The general discussion on the relations between M, N, and $s+1$ applies here. The depletion layer for Problem Γ_{12} approximately satisfies $50 < xL < 100$ and the maximum number of subdomains as shown in the tables is three. Finally, from the results for Problems Γ_{10} and Γ_{12} we observe that if there is an interface inside the depletion layer, e.g. Table 9, then we need a good initial approximation or the exact value of ψ at that point in order to obtain a converged result. Usually one can provide a good approximation but not the exact value based on the doping profile. On the other hand, if a good initial approximation cannot be

$s+1$	N				
	91	181	361	721	1441
1	11	13	13	13	13
2	7.416	7.458	7.978	8.488	8.994
4	N.A.	4.916	4.958	4.979	4.990
5	oscillation	oscillation	oscillation	oscillation	oscillation
6	5.348	5.508	5.423	4.634	4.817
8	N.A.	N.A.	36.279	36.650	22.515
10	oscillation	oscillation	oscillation	oscillation	oscillation
2	5.461	5.480	6.100	6.100	6.108
3	N.A.	5.782	5.808	5.821	6.215
6	N.A.	N.A.	4.421	4.253	4.072
7	N.A.	4.369	4.613	4.446	4.265

Table 10: τ for Problem Γ_{10}.

$s+1$	N				
	91	181	361	721	1441
2	16	15	14	13	13
3	70	56	78	76	62
4	oscillation	oscillation	oscillation	oscillation	oscillation
2	7	8	8	7	7
3	117	72	61	77	101
3	16	15	13	16	15
4	36	31	28	26	26

Table 11: M for Problem Γ_{12}.

provided, then converged solution cannot be achieved, e.g. Tables 9 and 11.

5.2 *p-i-n* Junction

The convergence results for Problem Γ_{20} are shown in Tables 13 and 14. The doping profile of this problem is non-symmetric. For the upper parts of the tables, interface restriction is applied. For the lower parts of the tables, the depletion layer is isolated. The interface denoted as N.A. is the standard test result, i.e no domain decomposition. The general discussion on the relations between M, N, and $s+1$ applies here. This problem has a very large depletion layer, $1.6 < xL < 3.2$, which occupies almost half of the entire device. The maximum number of subdomains as shown in the tables is two. Furthermore the convergence result is not convencing compare with the standard result. Therefore the present algorithm is not suitable for devices which have a depletion layer of width equal to or larger than half of the width of the device.

$s+1$	N				
	91	181	361	721	1441
1	16	16	16	16	16
2	19.281	18.397	17.950	16.976	17.488
3	33.236	30.983	44.086	45.540	39.944
2	12.742	13.397	12.811	12.822	12.828
3	53.865	36.464	33.526	39.730	52.594
4	oscillation	oscillation	oscillation	oscillation	oscillation
3	10.079	9.737	9.451	12.028	11.598
4	12.944	11.777	11.306	11.624	10.259

Table 12: τ for Problem Γ_{12}.

$s+1$	Interfaces	N				
		141	281	561	1121	2241
2	1.5	18	18	18	17	17
2	1.6	19	19	19	21	18
2	1.7	23	23	22	21	20
3	1.0, 2.2	oscillation	oscillation	oscillation	oscillation	oscillate
3	1.6, 3.2	28	25	24	23	22

Table 13: M for Problem Γ_{20}.

5.3 Thyristor

The convergence results for Problems Γ_{30} are shown in Tables 15 and 16. In the upper parts of the tables, the subdomains are evenly distributed without any interface restriction. The lower parts of the tables have the depletion layers being isolated, i.e. the interfaces are chosen at 130, 270, 400, and 540. The general discussion on the relations between M, N, and $s+1$ applies here. The depletion layer approximately satisfies $560 < xL < 640$. Previous discussion on the location of interfaces and depletion layers applies here. The numerical results show that the maximum number of subdomains is around seven.

The convergence results for Problem Γ_{31} are shown in Tables 17 and 18. The subdomains are evenly distributed without any interface restriction. It has two depletion layers situated at a large distance and approximately satisfy $0 < xL < 90$ and $560 < xL < 660$. The maximum number of subdomains as shown in the tables is around seven.

The results suggest that there should be no subdomain within a depletion layer. It is obvious that in order to avoid any subdomain lying inside a depletion layer, the maximum number of subdomains must be less than w/w_l where w_l is the width of the depletion layer. For simple junctions such as those given above, it is possible to estimate w_l and its location based on the doping profile.

$s+1$	Interfaces	N				
		141	281	561	1121	2241
1	N.A.	19	20	20	20	20
2	1.5	18.755	19.376	19.402	19.987	21.136
2	1.6	18.345	18.943	19.971	21.155	21.163
2	1.7	22.986	22.552	22.077	22.096	22.105
3	1.0, 2.2	oscillation	oscillation	oscillation	oscillation	oscillate
3	1.6, 3.2	19.489	18.633	18.247	19.636	19.647

Table 14: τ for Problem Γ_{20}.

$s+1$	N			
	701	1401	2801	5601
2	31	31	30	30
4	31	31	31	30
5	37	36	37	36
7	66	56	52	48
10	oscillation	oscillation	oscillation	oscillation
5	31	31	31	30

Table 15: M for Problem Γ_{30}.

6 Conclusion

A non-overlapped domain decomposition method has been applied to the numerical solutions of some semiconductor devices in one dimension. The physical domain has been decomposed into a number of disjoint subdomains and we have examined the behaviour of the number of iterations M and the total work unit τ with respect to the number of subdomains. We have also examined the relation between the subdomains and the depletion layers. The work suggests that the current numerical scheme does not allow any subdomain to fall into a depletion layer. We have the following two major properties based on the numerical results :

- Suppose a p-n junction has a depletion layer of width w_l and a total width of w, and suppose there is no interface inside the depletion layer, then the maximum number of subdomains to be used in the current non-overlapped domain decomposition method must be less than w/w_l.

- Suppose there are $\mathcal{L}$ depletion layers in a junction, each of width w_l, $l = 1, 2, \cdots, \mathcal{L}$ situated at sufficiently large distance from each other, and suppose there is no interface inside the depletion layers, then the maximum number of subdomains to be used in the current non-overlapped domain decomposition method must be less than $w/\max_{1\le l\le \mathcal{L}}\{w_l\}$.

It is also suggested that should there be an interface within a depletion layer, the initial approximation at that interface must be very close to the exact solution at that point for

$s+1$	N			
	701	1401	2801	5601
1	29	29	29	29
2	27.960	27.980	28.990	29.495
4	13.940	13.970	14.734	14.742
5	12.528	12.564	13.181	13.191
7	12.888	11.522	11.262	10.988
10	oscillation	oscillation	oscillation	oscillation
5	12.731	12.769	13.469	13.478

Table 16: τ for Problem Γ_{30}.

$s+1$	N			
	701	1401	2801	5601
2	31	30	30	30
4	31	31	31	30
5	37	36	37	36
7	61	55	52	48
10	oscillation	oscillation	oscillation	oscillation

Table 17: M for Problem Γ_{31}.

the algorithm to converge. The depletion layer governs the splitting of the physical domain. In order to overcome the current problem, we propose to examine the use of a fixed point iteration method with a preconditoner.

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$s+1$	N			
	701	1401	2801	5601
1	29	29	29	29
2	27.960	27.980	28.990	29.495
4	13.940	13.970	14.734	14.742
5	12.727	12.763	13.181	13.191
7	12.180	11.380	11.262	10.988
10	oscillation	oscillation	oscillation	oscillation

Table 18: τ for Problem Γ_{31}.

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