Parallel Domain Decomposition Applied to 3D Poisson Equation for Gradual HBT

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ABSTRACT

This paper presents the implementation of a parallel solver for the 3D Poisson equation applied to gradual HBT simulation in a memory distributed multiprocessor. The Poisson equation was discretized using a finite element method (FEM) on an unstructured tetrahedral mesh. Domain decomposition methods were used to solve the linear systems. We have simulated a gradual HBT, and we present electrical results and some measures of the efficiency of the parallel execution for several solvers. This code was implemented using a message–passing standard library MPI and was tested on a CRAY T3E.

Keywords: 3D Poisson equation, Gradual HBT, Domain Decomposition, Multiprocessors.

INTRODUCTION

Heterojunction bipolar transistors are nowadays an active area of research due to interest in their high–speed electronic circuit applications. For example InP/InGaAs HBT's have attained frequencies of over 200GHz [1].

Development of simulators for HBT's is essential in order to better understand their physical behaviour and for design optimization. In this work we have studied the implementation of a parallel solver for the 3D Poisson equation applied to gradual HBT simulation in a memory distributed multiprocessor. This solver is a first step in the development of a complete parallel 3D simulator for HBTs, based on the 1D simulator that we presented in [2]. We have used the finite element method in order to discretize the Poisson equation. The properties of the resulting linear systems and their high range make it necessary to find adequate solvers as classic methods, such as incomplete factorizations, are very inefficient. The majority of computer time is spent solving these linear systems, typically containing several thousand equations. We have studied various domain decomposition methods in order to solve these systems.

In the next section we introduce the formulation of the Poisson equation for gradual HBTs. The following section presents some domain decomposition methods. Then we compare time of execution and iteration numbers of these solvers as well as influence of Kirlov subspace in a gradual AlGaAs/GaAs HBT. In the last section, the main conclusions of this work are presented.

POISSON EQUATION

For studying electrical behaviour of a gradual heterojunction bipolar transistor such as the one in the Figure 2(a) Poisson equation has to be solved. In the bulk semiconductor region this equation can be written as:

$$div(\varepsilon \nabla \psi) \quad = \quad -q(p - n + N_D^+ - N_A^-) \tag{1}$$

where ψ is the electrostatic potential, q is the electron charge, ε is the dielectric constant of the material, n and p are the electron and hole densities, and N_D^+ and N_A^+ are the doping effective concentrations.

Assuming a single parabolic conduction band, the electron density can be expressed as:

$$n = N_c F_{1/2}(\eta_c) \tag{2}$$

where Nc is the effective density of states in the conduction band, $F_{1/2}$ is the Fermi–Dirac integral of order 1/2, and η_c is,

$$\eta_c = \frac{E_{fn} - E_c}{kT} \tag{3}$$

From the aforementioned equations it is easy to obtain the expression 4 for the electron concentration and, using a similar procedure, equation 5 for the hole concentration:

$$n = n_{\mathrm{ien}} \exp\left(\frac{q\psi - q\phi_n}{kT}\right) \tag{4}$$

$$p = n_{\mathrm{iep}} \exp\left(\frac{q\phi_p - q\psi}{kT}\right) \tag{5}$$

where n_{ien} and n_{iep} can be calculated as follows:

$$n_{\mathrm{ien}} = n_{\mathrm{i,ref}} \left(\frac{N_c}{N_{\mathrm{c,ref}}}\right) \exp\left(\frac{q\chi - q\chi_{\mathrm{ref}}}{kT}\right) \left(\frac{F_{1/2}(\eta_c)}{\exp(\eta_c)}\right) \tag{6}$$

$$n_{\mathrm{iep}} = n_{\mathrm{i,ref}} \left(\frac{N_v}{N_{\mathrm{v,ref}}}\right) \exp\left(-\frac{(q\chi - q\chi_{\mathrm{ref}}) + (E_g - E_{\mathrm{g,ref}})}{kT}\right) \left(\frac{F_{1/2}(\eta_v)}{\exp(\eta_v)}\right) \tag{7}$$

and η_c and η_v are:

$$\eta_c = \frac{q\psi - q\phi_n}{kT} + \frac{q\chi - q\chi_{\mathrm{ref}}}{kT} - \ln\left(\frac{N_{\mathrm{c,ref}}}{n_{\mathrm{i,ref}}}\right) \quad (8)$$

$$\eta_v = \frac{q\phi_p - q\psi}{kT} - \frac{(q\chi - q\chi_{\mathrm{ref}}) + (E_g - E_{\mathrm{g,ref}})}{kT} - \quad (9)$$
$$- \ln\left(\frac{N_{\mathrm{v,ref}}}{n_{\mathrm{i,ref}}}\right)$$

Note that η_c and η_v depend on the electrostatic potential and the quasi–Fermi potentials. Since these magnitudes are the unknowns in the numerical implementation of the model, an iterative solution process is established in order to guarantee coherent results.

The formulation given by 4 and 5 for carrier concentrations is simple and compact. Parameters n_{ien} and n_{iep} may include different phenomena that affect the concentrations at high doping levels: influence of Fermi–Dirac statistics, changes in the energy levels and variations in the effective densities of states.

Over the separation interface of two different semiconductor regions could exist some superficial charge which it is necessary to include in the equation of Poisson. If this superficial charge by area unit is expressed as Q_I we obtain the following modified Poisson equation:

$$div(\varepsilon \nabla \psi) = -q(p - n + N_D^+ - N_A^-) + Q_I \quad (10)$$

This equation is scaled using the scaling presented in [3]. Next, the finite element method should be applied in order to discretize the scaled equations, thus obtaining a system of nonlinear equations, with range N, where N is the number of nodes of the discretization [4].

DOMAIN DECOMPOSITION SOLVERS

In recent years domain decomposition has emerged as a fairly general paradigm for solving linear systems of equations on parallel computers [5]. A domain is partitioned into several sub–domains, and some techniques are used to recover the global solution by a succession of solutions of independent subproblems associated with the subdomain [6].

If we consider the problem of solving the Poisson Equation on a domain Ω partitioned into p subdomains Ω_i, then domain decomposition methods attempt to solve the problem on the entire domain by a problem solution on each subdomain Ω_i. This means that Ω_i's are such that

$$\Omega = \bigcup_{i=1}^{p} \Omega_i \quad (11)$$

Figure 1 is an illustration of a subdomain of the physical domain. Each node belonging to a subdomain is

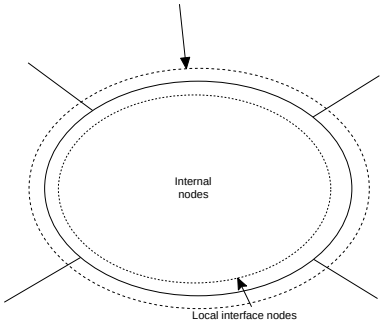

Figure 1: Nodes in a subdomain

an unknown of the problem. It is important to distinguish between three types of unknowns: interior nodes are those that are coupled only with local nodes, local interface nodes are those coupled with external nodes as well as local nodes, and external interface nodes are those nodes in other subdomains which are coupled with local nodes. We label the nodes by subdomains, first the internal nodes and last the interface nodes.

We have studied several types of domain decomposition preconditioners such as Additive Schwarz and others based on Schur complement techniques.

The Additive Schwarz procedure is similar to a block-Jacobi iteration and consists of updating all the new components from the same residual. The basic additive Schwarz iteration would therefore be as follows:

1.- Obtain $y_{i,ext}$

2.- Compute local residual $r_i = (b - Ax)_i$

3.- Solve $A_i \delta_i = r_i$

4.- Update solution $x_i = x_i + \delta_i$

In order to solve the linear system $A_i \delta_i = r_i$ a standard ILUT preconditioner combined with GMRES for the solver associated with the blocks is used [6].

The Schur complement techniques refer to methods which iterate on the interface unknowns only, implicitly using internal unknows as intermediate variables.

Consider the linear system for the subdomain Ω_i described as,

$$\begin{pmatrix} B_i & E_i \\ F_i & C_i \end{pmatrix} \begin{pmatrix} x_i \\ y_i \end{pmatrix} = \begin{pmatrix} f_i \\ g_i \end{pmatrix} \quad (12)$$

in which B is assumed to be non–singular. From the first equation of 12 the unknown x can be expressed as

$$x = B^{-1}(f - Ey) \quad (13)$$

Upon substituting this into the second equation of 12, the following reduced system is obtained

$$(C - FB^{-1}E)y = g - FB^{-1}f \quad (14)$$

Where the matrix $S = C - FB^{-1}E$ is called the Schur complement matrix associated with the y variable. If this system can be solved, all the interface variables

Table 1: Doping profile of gradual HBT

	$N_{eff}(\mathrm{cm}^{-3})$	Δ X	Δ Y	Δ Z
E (n–$Al_{0.3}Ga_{0.7}As$)	5.0 10^{17}	0.5	1.0	0.3
B (p–$GaAs$)	5.0 10^{19}	1.5	3.0	0.12
C(n–$GaAs$)	1.0 10^{17}	1.5	3.0	0.5
SC(n–$GaAs$)	2.0 10^{18}	3.0	6.0	0.3

y will become available, and thus it will be possible to compute the remaining unknowns by using 13. Due to the particular structure of B, observe that any linear system solution with it decouples into p separate systems. The parallelism in this situation arises from this natural decoupling.

EVALUATION

We have analyzed a gradual HBT device such as the one in Figure 2(a). It has four zones: the sub–collector (SC), the collector (C), the base (B), and the emitter (E). Some of the main parameters are the doping profile and the dimensions in μm of each zone, which are shown in table I.

In order to reduce the simulation time, the program was developed for distributed–memory multicomputers, using the MIMD strategy (*Multiple Instruction–Multiple Data*) under the SPMD paradigm (*Simple Pro-gram–Multiple Data*). These machines consist of a certain number of processors or nodes interconnected by a network with a certain topology. Our program was implemented using the MPI message passing standard library [7]. The main advantage of using this library is that it is presently implemented in many computers, and this guarantees the portability of the code [8], [9]. All results were obtained on a CRAY T3E multicomputer using the MPI communication library, hence portability to other parallel machines is guaranteed.

The voltage in thermal equilibrium for this device in a cross section (plane x z) of the HBT is showed in figure 2(b), for a mesh with 13856 nodes and 70699 elements.

All preconditioners converge, however there are significant differences in execution time. This simulator takes several minutes to solve the Poisson equation in equilibrium using the Newton method, as it needs to solve several linear systems.

Figure 3(a) shows the performance results using additive Schwarz preconditioner for different values of the fill–in parameter. In Figure 3(b) the influence of the size of Krylov subspace for the resolution of only a linear system is shown. For this preconditioner, using low levels of fill–in and a small size of Krylov subspace leads to lower execution time.

We have used a mesh with more nodes to compare the three solvers. Figure 4 shows the execution time

Table 2: Table II. Iterations for Additive Schwarz, Schur with FGMRES and Schur with ILU

	Additive Schwarz	Schur–FGMRES	(Schur–ILU)
2	465	808	22
4	371	710	18
6	423	808	23
8	628	1140	23

for Additive Schwarz and others based on Schur complement techniques. For the latter case the Schur Complement matrix is solved by using two different preconditioners, FGMRES and ILU. The best results were obtained using Schur combined with ILU preconditioner, because it has the least number of iterations, as is shown in table II.

CONCLUSIONS

In this work we have studied domain decomposition solvers applied to 3D Poisson Equation for a gradual AlGaAs/GaAs HBT. The code was implemented using the message passing interface library MPI. All the data were measured on a multicomputer CRAY T3E.

In order to solve systems of linear equations, which is the most CPU consuming part, we have tested different methods of domain decomposition, which present great advantages as opposed to the classic methods, as regards to speed and memory requirements.

ACKNOWLEDGEMENTS

The work described in this paper was supported in part by the Ministry of Education and Science (CICYT) of Spain under the project TIC96–1125–C03. We want to thank CIEMAT (Madrid) for providing us access to the Cray T3E multicomputer.

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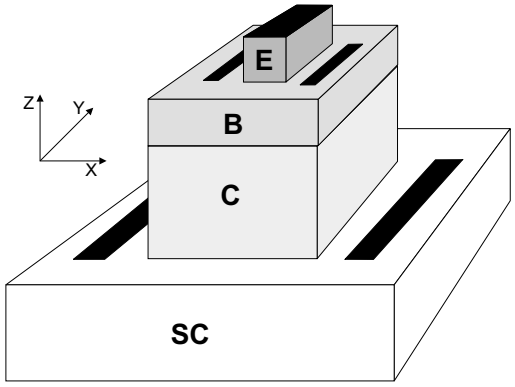
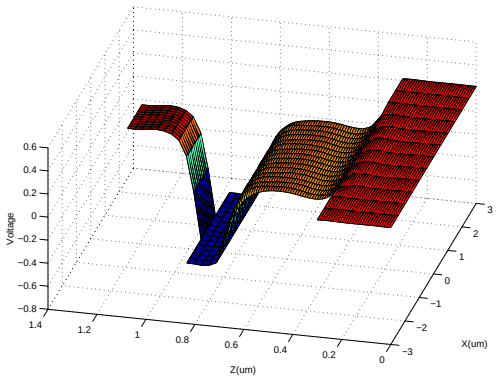


(a) Gradual HBT



(b) Voltage in thermal equilibrium

Figure 2: Bipolar Transistor

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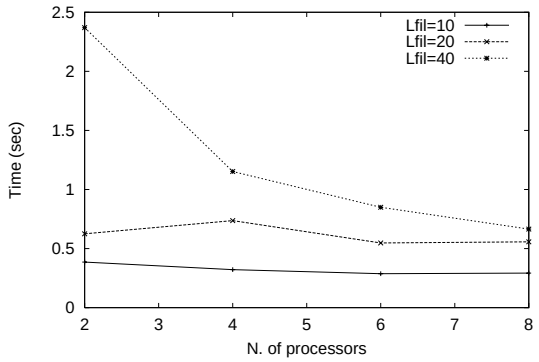
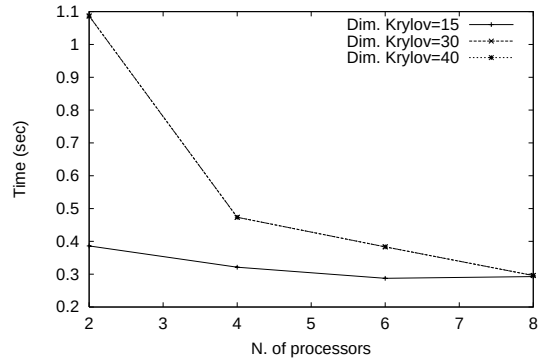


(a) Influence of fill–in parameter (dim. Krylov=15)



(b) Influence of size of Kirlov subspace (fill–in=10)

Figure 3: Time of execution to Additive Schwarz

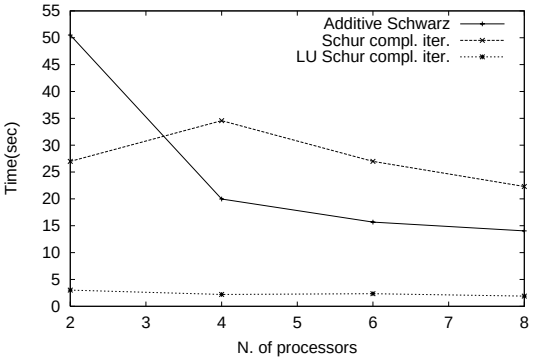


Figure 4: Time of execution for several solvers