3D Biconjugate Gradient-Multi Grid Coupling Schemes for Field Equations in Semiconductor Device Simulation

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ABSTRACT

A significant portion of the time required for simulating full three-dimensional (3D) charge transport in semiconductor devices using particle-based methods is spent solving the necessary field equations. Two highly effective, iterative techniques available for solving large-sparse systems of equations are the conjugate gradient (CG) method and the multigrid (MG) method. In this work, variants of the CG and MG methods are self-consistently coupled to a particle-based full-band simulator and are applied to model small, 3D structures. Detailed analyses of both performance and solver robustness are presented for different algorithmic configurations. Hybrid strategies using various coupling schemes for improving overall performance behavior of the Poisson solver are also discussed.

Keywords: *conjugate gradient, multigrid, Bi-CGSTAB, Poisson solver, particle-based simulation.*

1 Introduction

In particle-based[1] device simulations the spatial distribution of the electric field is generally computed through the frequent solution of Poisson's equation. The Laplace operator is typically discretized in 3D using an inhomogeneous, 7-point, finite-difference scheme. The result is a large set of linear equations which are best solved through iterative techniques because a good initial guess is available through the self-consistent framework of particle-based simulation algorithms. Both CG [2] and MG[3] methods have been used recently in device simulations with considerable success [4][5][6]. Their applicability to solving large systems of linear equations can be quite useful considering the need of frequent solution of the field equations in self-consistent device simulations. Indeed, the field equations are solved tens of thousands of times in a typical simulation. Each of the mentioned methods is unique in terms of the manner in which the numerical algorithm is utilized to achieve the desired convergence threshold. The next section is devoted to a discussion of the numerical methods used in our simulations. Results are then presented and discussed in detail. Finally, we conclude with some brief remarks about the effectiveness of each method.

2 Numerical Methods

Three of the most commonly used iterative techniques in device simulations today include the successive over-relaxation (SOR)[1] method, the multigrid method (MG), and variants of the method of conjugate gradients (CG). Each of these methods has its own inherent advantages and disadvantages when used for solving Poisson's equation in device simulations.

Among the mentioned approaches, the simpler technique for solving systems of linear equations is the SOR method. This method is easy to implement and can quickly be incorporated into a device simulation code. Although this method can be robust for solving a system of linear equations, its effectiveness is limited to smaller convergence threshold values (typically less than $1x10^{-4}$ for homogeneous systems and even less for inhomogeneous ones) due to its increasingly small error reduction rate as the error decreases. This behavior is typical of standard iterative solvers, and depends on the fact that different Fourier components of the error are not equally reduced on a given discretization grid. Thus, this method can be

costly at lower convergence values resulting in unpractical convergence times.

A more efficient method is the multigrid method. Even if it has a highly algorithmic complexity when compared to the SOR approach, the multigrid is a highly effective method for simultaneously reducing different spectral components of the error. This is accomplished by recursively solving the linear system on a hierarchy of differently spaced grids, by interpolating quantities from a series of fine to course grids through projection and restriction operators that conserve integrals [6]. Besides the algorithmic complexity, the multigrid approach has been proved to be capable of efficiently handling the irregular grids used in device simulations [7].

Conjugate gradient solvers have become popular in recent years due to their relatively easy implementation and the efficiency with which they can quickly solve large systems of linear equations assuming that a good initial guess is provided. This type of solver is typically classified as an error projection method in that a set of linearly independent basis vectors is generated to determine the solution update. Because of their dependence on the initial guess, the convergence behavior of this approach has been shown to improve through use of an appropriate preconditioner that can effectively reduce the spectral radius of the system thus decreasing the convergence time.

In this work, we compare the three methods mentioned above in application to a particle-based simulator[8]. We also investigate the effectiveness of the multigrid method when used as a preconditioner for the conjugate gradient method. The CG variant chosen is the biconjugate gradient stabilized method (Bi-CGSTAB) due to its improved convergence behavior as discussed in [9].

3 Simulations

The device chosen to perform the tests is a three-dimensional silicon diode with uniform doping on both sides of the junction ($N_A=N_D=10^{17}cm^{-3}$). Two sets of simulations are performed. The first one is discretized on a 50x50x60 homogeneous grid with 5 nm mesh spacing. The second simulation grid is still 50x50x60 but is slightly inhomogeneous in the z direction with cell dimensions of 5 nm within the depletion region and 5nmx5nmx7.5nm in the bulk regions. Due to the diffusion time of minority carriers in the diode structure, the simulation time is 10ps. Timing data was recorded for 0.1 ps. Therefore the results graphed represent only a fraction of the total simulation time required for convergence. The total time required for a simulation time of 0.1 is approximately 1-2 hours. These results represent the transient behavior of the simulation where the SOR and CG methods are the most inefficient. Steady-state results can be seen at the end of the simulation at 0.1 ps. The number of carriers used for all simulations are 150000 electrons and holes and correspond to 4 particles per cell. To compensate for the fluctuations in plasma density due to the small number of particles per cell, a Poisson time step of 2fs was used.

Timing data are shown in Figs. 1 and 2 for a convergence threshold of $1x10^{-5}$. Figure 1 shows the results obtained for the homogeneous device. The timing results for the inhomogeneous device are presented in Fig. 2 and indicate an average increase in the required cpu time over the homogeneous case of 4-5s per iteration for the multigrid preconditioned conjugate gradient method and 8-10s per iteration for the SOR-preconditioned Bi-CGSTAB method. The results shown in Fig. 2 are obtained during the initial transient phase of the device. Timing data is taken in the steady state region near the end of this plot. These results are consistent with that expected for a slightly non-symmetric system.

In both sets of simulation results, the parameters used for each iterative method were identical. A relaxation coefficient (ù) of 1.2 was used in the SOR preconditioner to minimize the time spent per iteration within the Bi-CGSTAB routine.

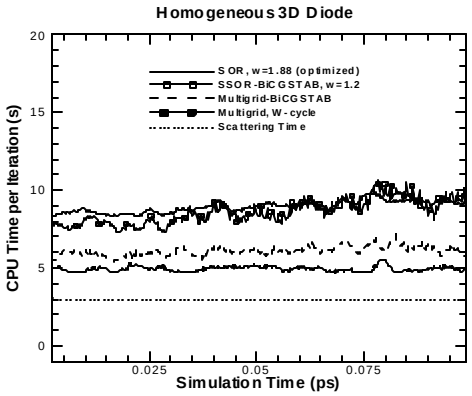

Figure 1: Timing results for a homogeneous device.

The MG algorithm uses the W-cycle to loop through the grid levels and an alternating line relaxation routine [1]. The optimal relaxation scheme is highly dependent on device geometry and in these simulations the most efficient method is to relax in both the x- and y-directions on each grid [7].

The multigrid preconditioned Bi-CGSTAB method (MGCG) uses a V-cycle for the MG preconditioner.This particular cycle, representing the algorithmic path of smoothing, is the most efficient cycle for coupling the two iterative methods.

The basic SOR solver used in both sets of simulations employs a relaxation coefficient determined by using the optimized 2D relaxation coefficient discussed in [3]. For the device simulated, the value of this coefficient is 1.88.

A brief comparison of the results shows that an increase in Poisson solver times for both the SSOR-BiCGSTAB and MGCG methods occurs in the inhomogeneous case. The MG method, on the other hand, appears to have increased only slightly (less than 0.5s per iteration). Despite the large computational implementation required results indicate that the MG method is faster than both the SSOR preconditioned Bi-CGSTAB method by 6-10 seconds per iteration and the multigrid preconditioned Bi-CGSTAB method by 3-5 seconds per iteration on average.

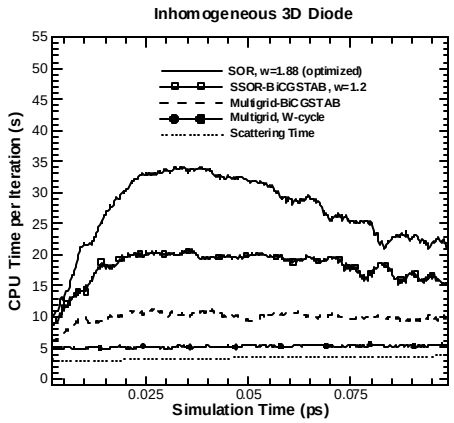

Figure 2: Timing results for an inhomogeneous device.

This is due in large part to the number of internal device loops that must be completed during each iteration of the Bi-CGSTAB method. Although the latter method effectively reduces the total number of Poisson solver iterations required for convergence, the total time spent in the solver itself is larger than that achieved using just the MG method. There appears to be a definite tradeoff between solver iterations and the cpu time expended per iteration within this comparison tilting the scale in favor of using multigrid techniques over CG methods in future simulations.

In both Figs. 1 and 2, it is clear that the Poisson solver time in 3D simulations is significantly larger than the average scattering time. When compared with 2D simulation results however, the scattering time is the dominant contribution to the total simulation time. Thus the importance of faster Poisson solvers becomes clear as the complexity and dimensionality of simulated device structures increases.

4 Future Work/Conclusions

Although, the use of MG method appears to be the most efficient and effective method for solving large systems of linear field equations in device simulations particularly in inhomogeneous systems, we have demonstrated the improved performance of the Bi-CGSTAB method using a MG preconditioner.

Results have only been shown for the first 1/100 time steps necessary to reach the full steady-state results and therefore only represent the performance of the presented Poisson solvers in the transient regime. Although the time-per-iteration is not thought to decrease dramatically after 0.1 ps.

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