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Domain Decomposition Algorithms for PDE Problems with Large Scale Variations

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Abstract

We consider a Schur complement BPS-like domain decomposition algorithm for the 2D drift-diffusion equations arising from semiconductor modeling. In particular, we focus on two problems: anisotropic phenomena and large changes in the PDE coefficients as one moves spatially within the domain. The preconditioners that we discuss are essentially BPS preconditioners [2] where the interface coupling is approximated using band matrices generated by the probing technique [3]. To cope with anisotropic phenomena, we introduce additional band matrices (in the context of the probe preconditioner) to approximate the coupling between neighboring interfaces. To address coefficient variations over the domain, we make use of the close connection between domain decomposition and multigrid and introduce specialized interpolation, projection, and averaging techniques to develop an accurate coarse grid approximation. We demonstrate the benefits of the new approach using computational experiments.

1 Introduction

We consider algorithms for the solution of the drift-diffusion equations in two dimensions. The solution of these equations is of great importance for semiconductor device modeling. In this paper, we focus on efficiently solving the linear systems that arise from Gummel's method [8] via Schur complement domain decomposition algorithms. The principal difficulties presented by our formulation of the drift-diffusion equations are anisotropic behavior introduced by the discretization and large variations in the PDE coefficients. To solve the resulting linear systems, the conjugate gradient method is used in conjunction with a BPS-like [2] preconditioner:

$$M^{-1} = M_E^{-1} + I_H^h A_H^{-1} I_h^H,$$

where M_E^{-1} is the interface approximation, $I_H^h A_H^{-1} I_h^H$ is the coarse grid problem, A_H corresponds to the discretization matrix of the original problem on

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a coarse grid whose elements are defined by the non-overlapping subdomains, and $I_h^H = [I_H^h]^T$ denotes the transfer operator between the original fine grid and the coarse grid. In Section 2, we describe briefly the drift-diffusion equations and show how anisotropic behavior and large variations in the PDE coefficients arise from our formulation. Next in Section 3, we present new methods for M_E^{-1} suitable for anisotropic problems and specifically designed for situations when the coupling between neighboring interfaces is stronger than the coupling within an interface [6]. Then, in Section 4 we propose grid transfer operators suitable for highly variable coefficient problems. These operator-dependent transfers correspond to extensions of operator-dependent prolongation and restriction operators used in standard multigrid methods [7]. Lastly, in Section 5 computational results are given to illustrate the different approaches.

2 The Drift-Diffusion Equations

A drift-diffusion model is used to approximate the behavior of a single semiconductor device [9]. This model consists of a potential equation

$$\varepsilon \nabla^2 \psi + q[n_{ie} e^{-q\psi/kT} v - n_{ie} e^{q\psi/kT} u + N_D - N_A] = 0,$$

and two continuity equations

$$\nabla \cdot [\frac{kT}{q} \mu_n n_{ie} e^{q\psi/kT} \nabla u] + R = 0 \quad \text{and} \quad \nabla \cdot [\frac{kT}{q} \mu_p n_{ie} e^{-q\psi/kT} \nabla v] - R = 0,$$

where ε is the scalar permittivity of the semiconductor, n_{ie} is the effective intrinsic carrier concentration, q is the elementary charge, k is the Boltzmann constant, T is the temperature in Kelvin, N_D is the density of donor impurities, N_A is the density of acceptors, and μ_n and μ_p are the electron and hole mobilities respectively. The dependent variables are the electric potential, ψ, and the two Slotboom variables u and v. The density of free electrons, n, and free holes, p, can be recovered using

$$n = n_{ie} e^{q\psi/kT} u \qquad p = n_{ie} e^{-q\psi/kT} v.$$

Notice that the drift-diffusion equations are nonlinear and that the individual equations are symmetric self-adjoint operators with highly variable coefficients (due to the exponential operators).

A discrete approximation to the drift-diffusion equations is obtained by approximating each of the derivative terms with central differences on a highly stretched grid. Unfortunately, a significant degree of anisotropic behavior is introduced as a consequence of this highly stretched grid. The resulting system of three discrete nonlinear equations is then solved using a nonlinear Gauss-Seidel method known as the Gummel iterative technique [8]. This nonlinear technique requires the solution of three symmetric linear systems (corresponding to the three discrete PDEs) within each Gummel

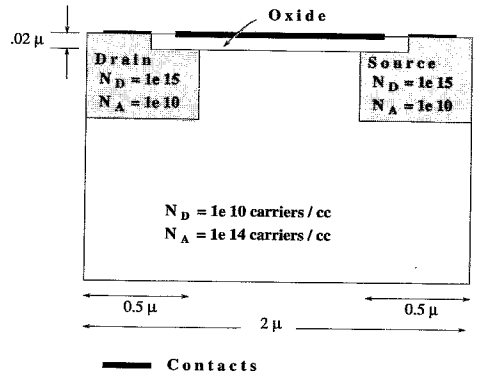

FIG. 1. *MOSFET Device*

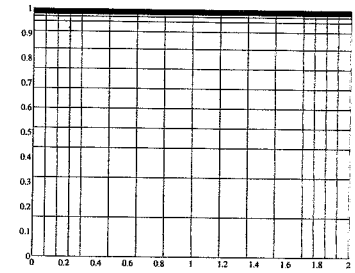

FIG. 2. *Example of a stretched grid*

iteration. To solve these linear systems, we use a conjugate gradient algorithm in conjunction with the BPS-like preconditioner

$$M^{-1} = M_E^{-1} + I_H^h A_H^{-1} I_h^H.$$

The remainder of this paper discusses the development of the two components of this preconditioner.

3 Interface Component

To construct the interface component M_E^{-1}, we follow [3]. That is, the diagonal blocks of the Schur complement that correspond to the coupling between fine grid points on the same subdomain edge are approximated by band matrices. This choice is motivated by the following observations for a two subdomain decomposition. First, the Schur complement matrix is "close" to a band matrix. That is, the entries decay rapidly from the diagonal. Second, all entries of a band matrix having upper and lower bandwidth d can be computed by the action of this matrix on $2d+1$ carefully chosen probe vectors p^k (e.g. , $p^k = (..,0,0,1,0,0,1,0,0,1,...)^T$ for $d = 1$). In the rest of the paper, d denotes the upper and lower bandwidth of the approximation matrices. To generalize the probing technique to multiple domains, we must generate one band matrix for each edge. One possibility is to build all the band approximations on the vertical edges at the same time and then on the horizontal edges. That is, a composite probe vector is defined first over all the vertical edges by combining individual probe vectors for each edge. Then the same process is performed for the horizontal edges. This variant gives rise to the preconditioner referred to as $M_E^{vh(d)}$. The second variant further subdivides both horizontal and vertical edges into 'red' and 'black' sets to minimize the approximation errors arising from coupling between vertical (or horizontal) interfaces. The resulting preconditioner is denoted by $M_E^{rb(d)}$.

TABLE 1
# of iterations for $u_{xx} + \epsilon u_{yy} = f$ *on a* 128×128 *grid*

$\varepsilon = 1.0$					
	# domains				
M^{-1}	2×2	4×4	8×8	16×16	32×32
$M_E^{sim(1)}$	15	24	32	48	81
$M_E^{rb(1)}$	15	24	31	48	81
$M_E^{full(1)}$	-	21	32	50	69
$\varepsilon = 10^{-3}$					
	# domains				
M^{-1}	2×2	4×4	8×8	16×16	32×32
$M_E^{sim(1)}$	9	56	200	485	–
$M_E^{rb(1)}$	9	26	54	71	120
$M_E^{rb(2)}$	8	26	54	71	120
$M_E^{full(1)}$	-	14	16	17	17

For anisotropic problems, the off-diagonal blocks of the Schur complement can have large entries. In such situation, the previous block Jacobi type preconditioners can be inefficient. In order to capture the off-diagonal block coupling, we consider a new preconditioner which approximates the Schur complement coupling along each line of the original grid by a separate band matrix. The band matrix for each line differs depending on whether a line is aligned with an interface or not. On a uniform grid with $n_x \times n_y$ grid points partitioned among $N_x \times N_y$ equi-sized rectangles, the $N_y - 1$ horizontal grid lines that are aligned with the interfaces have n_x points in the Schur complement operator and those lines between the interfaces have $N_x - 1$ points. The probe idea can be applied to compute an approximation of the Schur complement restricted to the lines. For detailed information on these full probing approximations, we refer to [6] and simply state that the new preconditioner looks like an additive version of alternating line relaxation method or an additive ADI method applied on the Schur complement operator. In this paper the resulting preconditioner is referred to as $M_E^{full(d)}$.

In Table 1 we display the number of iterations required using various interface preconditioners without a coarse grid preconditioner for a Poisson problem defined on the unit square with Dirichlet boundary conditions. Convergence is attained when the Euclidean norm of the residual is reduced by a factor 10^5. These results show that while all the preconditioners are equivalent for the nonanisotropic case, there is a great deal of variation

for anisotropic problems. In the anisotropic case, the red-black probing improves the convergence noticeably and with full probing we obtain very fast convergence for the anisotropic case. When the problem is very anisotropic and constant coefficient, a coarse grid preconditioner is not needed as the problem is essentially one dimensional and thus preconditioned accurately by the band solves.

4 Coarse Grid Component

The coarse grid component of the preconditioner is defined by $I_H^h A_H^{-1} I_h^H$ where the restriction operator I_h^H is the transpose of the prolongation operator I_H^h. The definition of the grid transfer operators is crucial to develop an accurate coarse grid approximation. When the coefficients are highly variable, the close relationship between the BPS-type preconditioner and multigrid can be exploited. In the context of multigrid for regular meshes, where the fine grid contains one point in between all adjacent coarse grid points, the definition of those operators is relatively well understood [1], and [4]. In our work we have generalized these results to the case when the number of fine grid points between two adjacent coarse grid points is greater than one and not necessarily constant. These operator dependent transfers correspond to an extension of standard operator dependent prolongation and restriction operators used in standard multigrid methods. It can be shown that for certain coarse grids the 1D version of this prolongation is equivalent to recursive use of standard operator dependent prolongation on a hierarchy of grids in a multigrid method where a harmonic average is used to average the PDE coefficients [7]. For a detailed description of this grid transfer operator in the context of multigrid, we refer to [7] where averaging techniques and Galerkin formulations are also discussed for obtaining the operator A_H.

5 Experimental results

Results are given corresponding to a simple MOSFET device simulation. In Fig. 1, we illustrate the characteristics of this device. The contacts correspond to Dirichlet boundary conditions while the other boundaries are Neumman conditions. For the potential equation the solution is solved over the whole domain. For the u and v equations, we solve on the whole domain excluding the oxide where Neumman conditions are used on the oxide interface. A scaled down version of the grid used in this paper is given in Fig. 2. Table 2 displays the average number of conjugate gradient iterations for each linear solve corresponding to the two continuity equations for a MOSFET simulation discretized on a 129×129 grid. In the table, we show only the results using the full probing technique as the other probing techniques required many more iterations. From the table, we can see the importance of the coarse grid component in the preconditioner. That is,

TABLE 2
average # of iterations for the n and p equations.

	# domains			
Preconditioner	4×4	8×8	16×16	32×32
without coarse grid	33	58	103	156
standard grid transfers	41	58	65	60
op. dep. transfers	38	45	40	31

without the coarse grid the number of iterations grows significantly as the number of domains is increased. Further, we can see the effect of using carefully chosen operator-dependent grid transfers, compared with using simple bilinear interpolation. In particular, for the problem using 32×32 domains there is a factor of two difference in the number of iterations between the two while the work per iteration is approximately the same. For more details on the probing and anisotropic phenomena we refer the reader to [6]. For more details on the grid transfers we refer the reader to [7]. Finally, more extensive numerical experiments for several semiconductor devices using a few different domain decomposition algorithms will be presented in [5].

References

[1] R. Alcouffe, A. Brandt, J. Dendy, and J. Painter, *The multigrid method for diffusion equations with strongly discontinuous coefficients*, SIAM J. Sci. Stat. Comput., 2 (1981), pp. 430–454.

[2] J. Bramble, J. Pasciak, and J. Schatz, *The construction of preconditioners for elliptic problems by substructuring I.*, Math. Comp., 47 (1986), pp. 103–134.

[3] T. F. Chan and T. P. Mathew, *The interface probing technique in domain decomposition*, SIAM J. Matrix Anal. Appl., 13 (1992), pp. 212–238.

[4] J. Dendy, *Black box multigrid*, J. Comp. Phys., 48 (1982), pp. 366–386.

[5] L. Giraud and R. Tuminaro, *A domain decomposition method for the drift-diffusion equations*, Tech. Rep. in preparation, CERFACS, Toulouse, France.

[6] ——, *A domain decomposition probing variant suitable for anisotropic problems*, Tech. Rep. TR/PA/93/36, CERFACS, Toulouse, France, 1993.

[7] ——, *Grid transfer operators for highly variable coefficient problems*, Tech. Rep. TR/PA/93/37, CERFACS, Toulouse, France, 1993.

[8] H.K.Gummel, *A self-consistent iterative scheme for one-dimensional steady state transistor calculations*, IEEE Transactions on Electron Devices, ED-11 (1964), pp. 455–465.

[9] S. Selberherr, *Analysis and Simulation of Semiconductor Devices*, Springer-Verlag, New York, 1984.

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