On the Use of Concus-Golub Transformed Slotboom Variables in Semiconductor Device Simulations

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ABSTRACT

A new set of variables for semiconductor device simulation is obtained by applying the Concus-Golub transform¹ to the carrier continuity equations expressed in Slotboom variable form². Significant advantages are shown to result from use of the new variables.

- P. Concus and G. H. Golub, "Use of fast direct methods for the efficient numerical solution of non-separable elliptic equations," SIAM J. Numer. Anal., vol. 10, pp. 1103-1120, 1973.
- 2. J. W. Slotboom, "Iterative scheme for 1- and 2-Dimensional D. C. Transistor Simulation," El. Lett., vol. 5, pp. 677-678, 1969.

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INTRODUCTION

In considering numerical solution of equations of the form

$$-\nabla \left[a\left(x,y\right)\nabla u\right] = f\left(x,y\right) \tag{1}$$

Concus and Golub [1] introduced a change of variable

$$w(x,y) = [a(x,y)]^{\frac{1}{2}}u(x,y)$$
(2)

after which (1) becomes

$$-\Delta w + p(x,y)w = q(x,y) \tag{3}$$

where

$$p(x,y) = a^{-\frac{1}{2}} \nabla (a^{\frac{1}{2}})$$

and

$$q(x,y) = a^{-\frac{1}{2}f}.$$

The change of variable contained in equation (2) will be referred to as the Concus and Golub transform. It serves to convert an elliptic partial differential equation from self-adjoint form to Helmholtz form.

Equation (1) is the form of the dc continuity equations in the Slotboom variable formulation [2] of the equations of semiconductor device analysis. The basic idea of the work described in this presentation was to establish whether there are advantages in implementing semiconductor device simulations using Concus and Golub transformed Slotboom (CGS) variables with continuity equations in the form of equation (3), rather than using Slotboom variables with continuity equations in the form of equation (1).

The anticipated advantages were *simpler* discretization, *more accurate* discretization, and direct applicability of sophisticated numerical packages, which implement techniques such as conjugate gradient acceleration and multigrid. An anticipated *disadvantage* was the additional cost of performing the Concus and Golub transform each Gummel iteration.

In order to assess the overall usefulness of the CGS formulation one and twodimensional simulations using these variables were written. Ther performance was directly compared with that of existing programs using conventional Slotboom (S) and Scharfetter - Gummel (SG) discretizations of the current continuity equations.

SUMMARY OF RESULTS

The most interesting and useful result was unanticipated: use of CGS variables results in a major improvement of *convergence* properties. Convergence is maintained up to much higher injection levels than using the S and SG discretizations. At medium injection levels the CGS formulation requires fewer iterations for convergence. The anticipated properties of the CGS algorithm (simplicity and accuracy, but somewhat more work per Gummel iteration), were also observed.

DISCUSSION

This is a result of considerable significance, since it extends the use of simple Gummel-iteration based algorithms to injection levels where fully-coupled Newton iteration approaches have previously been considered necessary.

Some insight into the superior convergence properties of CGS based Gummel iteration will be provided by simple mathematical arguments, and also by specific examples of how CGS variables evolve between Gummel iterations, from initial conditions to convergence. More mathematically oriented colleagues are currently examining the convergence behavior from the viewpoint of the contractive behavior of the different methods' respective Gummel maps.