Performance of various algebraic multigrid based preconditioners for the drift-diffusion equations for semiconductor devices

*Paul T. Lin¹, John N. Shadid² and Robert J. Hoekstra³

¹ Sandia National Labs PO Box 5800 MS 0316 Albuquerque NM 87185 ptlin@sandia.gov ² Sandia National Labs PO Box 5800 MS 0316 Albuquerque NM 87185 jnshadi@sandia.gov

³ Sandia National Labs PO Box 5800 MS 0316 Albuquerque NM 87185 rjhoeks@sandia.gov

Key Words: *Preconditioning, algebraic multigrid, drift-diffusion, semiconductor devices, finite element method.*

ABSTRACT

In this work we apply various algebraic multigrid (AMG) based preconditioners to the drift-diffusion equations for modeling semiconductor devices. This will include AMG preconditioners applied to the full Jacobian, as well as approximate block factorization The and physics-based preconditioners. motivation behind physics-based preconditioners is to use legacy algorithms that were developed with some insight into the physics of the problem [1]. After application of the block factorization preconditioners, the resulting scalar subsystems are solved by various iterative methods including AMG-type techniques. The AMG-type techniques used in this work are a nonsmoothed aggregation technique [2] as well as a smoothed aggregation technique for nonsymmetric linear systems [3]. Both of these aggregation techniques employ an aggressive coarsening algorithm.

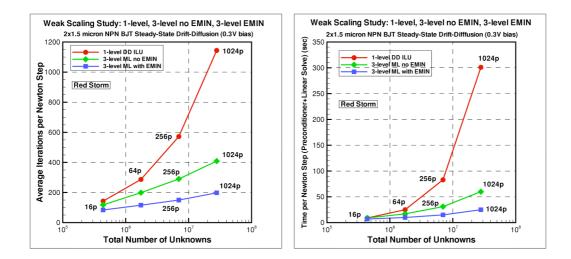
We employ a stabilized finite element method (FEM) discretization of the driftdiffusion equations on unstructured meshes. The nonlinear coupled system is solved with a parallel preconditioned Newton-Krylov method.

Block preconditioners can use used to produce sub-block systems that are more amenable to optimal multilevel methods. A block Jacobi, block Gauss-Seidel, and block SOR preconditioner has already been implemented. More advanced preconditioners such as use of the Gummel iteration [4] as a preconditioner as well as use of operatorsplitting techniques are presently under consideration.

Results will be presented demonstrating the performance of the various preconditioners for an NPN bipolar junction transistor (BJT). The following two figures show a comparison among three preconditioners applied to the full Jacobian: a 1-level Schwarz domain decomposition (DD) preconditioner based on an incomplete LU factorization (ILU), the 3-level nonsmoothed aggregation preconditioner, and the 3-level smoothed aggregation preconditioner for nonsymmetric linear systems. These three preconditioners are denoted as "1-level DD ILU", "3-level ML no EMIN" and "3-level ML with EMIN" respectively in the table legend. The left figure compares the average iterations per Newton step while the right figure compares the solve time per Newton step for a two-dimensional steady-state drift-diffusion calculation of a 2x1.5 micron BJT at voltage bias of 0.3V. This weak scaling study was performed on up to 1024 processors of the Sandia Red Storm machine.

Additional results will be presented that will show a comparison between application of AMG-type preconditioners on the full Jacobian versus the application of AMG-type preconditioners on the sub-blocks produced by the block preconditioners.

This work was funded by the DOE NNSA's ASC Program and the DOE Office of Science AMR Program, and was carried out at Sandia National Laboratories operated for the U.S. Department of Energy under contract no. DE-ACO4-94AL85000.



REFERENCES

- [1] D.A. Knoll and D.E. Keyes, "Jacobian free Newton-Krylov methods: a survey of approaches and applications," Journal of Computational Physics, Vol. 193, pp. 357-397 (2004).
- [2] M. Gee, C. Siefert, J. Hu, R. Tuminaro, and M. Sala, "ML 5.0 smoothed aggregation user's guide," Sandia National Labs Report SAND2006-2649, 2006.
- [3] M. Sala and R. Tuminaro, "A new Petrov-Galerkin smoothed aggregation preconditioner for nonsymmetric linear systems", submitted for publication at SIAM Journal on Scientific Computing.
- [4] H.K. Gummel, "A self-consistent iterative scheme for one-dimensional steady state transistor calculations," IEEE Transactions on Electron Devices, pp. 455-465,1964.