

# A Comparison of Various Accelerators for the Iterative Solution of Large Nonsymmetric Systems

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Our device simulator MINIMOS 5, capable of 3D MOSFET/MESFET simulation, uses Gummel's algorithm to solve the nonlinear system of discretized semiconductor equations. Using finite difference discretization matrix ranks of order  $10^5$  of the sparse linear systems are produced. In this paper we compare the convergence properties of various accelerators for the iterative solution of the discretized carrier continuity equations, the coefficient matrices of which are nonsymmetric but symmetrizable by a diagonal matrix  $W$ . All algorithms are preconditioned by incomplete LU factorization.

We begin with the CGNR-algorithm, which solves the symmetric, positive definite (SPD) problem  $A^T A x = A^T b$ . The convergence of this algorithm is governed by the singular values of the preconditioned matrix  $A$  [3], is strictly monotonic but cannot satisfy our requirements (Fig. 1).

For the symmetrized CG-method the symmetrization matrix  $W$  is required for the computation of the inner products in order to calculate the iteration parameters [2]. As  $w_{i,n} = \exp\left(\frac{\psi_i}{2U_i}\right)$  for the continuity equation for electrons and  $w_{i,p} = \exp\left(-\frac{\psi_i}{2U_i}\right)$  for that of holes, the  $w_i$  can have an enormous number range, so that scaling of the inner products is necessary. Nevertheless, we found this method only applicable for low voltage simulations, as scaling very often causes loss of significance (underflow) when computing the iteration parameters. Explicit symmetrization of the coefficient matrix  $A$  is possible as well, but restricts applicability of the CG-algorithm to even lower voltages, because scaling cannot be performed as efficiently as in our implementation.

ORTHOMIN [4] minimizes the 2-norm of the residual at each iteration step. Full orthogonalization at iteration  $n$  requires the storage of  $n$  vectors, which is not

possible in practice, so that a truncated version  $\text{ORTHOMIN}(m)$  is used, where only  $m$  backvectors have to be stored. Losing optimal convergence speed is the price.

GMRES [5] has the same minimization property as  $\text{ORTHOMIN}$ , but an orthonormal basis is built by an Arnoldi process. We also use a truncated version  $\text{GMRES}(m)$ , for which above mentioned restrictions are valid also.

Squaring classical Lanczos methods leads to  $\text{BIOMIN}^2$  (CGS),  $\text{BIORES}^2$ , and  $\text{BIODIR}^2$  [1][6]. The Lanczos methods use a biorthogonality condition to the transposed system instead of an orthogonality condition to backvectors in order to build a basis. The residual decreases not monotonically, hence subtle stopping criteria are required. Breakdown by vanishing of certain inner products, which cannot be excluded totally, never occurred in our applications. These three squared Lanczos methods produce the same iterates in exact arithmetic, but in practice  $\text{BIOMIN}^2$  (CGS) is the numerically most stable.

We found that for our applications  $\text{BIOMIN}^2$  (CGS) minimizes both overall arithmetic work and storage consumption. CPU time per iteration times the average number of iteration is much lower than for the other algorithms.

Figure 1 shows a comparison of the convergence behavior of the above mentioned methods. The test problem is from  $\text{MINIMOS}$  (n-channel silicon MOSFET with  $1.5\mu\text{m}$  channel length,  $U_S = U_B = 0V$ ,  $U_G = 1V$ ,  $U_D = 3V$ , mesh size:  $29 \times 31 \times 35$ ).  $e_n = \|\bar{x} - x_n\|_\infty$  is the infinity norm of the difference of the iterates  $x_n$  and the “true” solution  $\bar{x}$  which was obtained by Gaussian elimination.

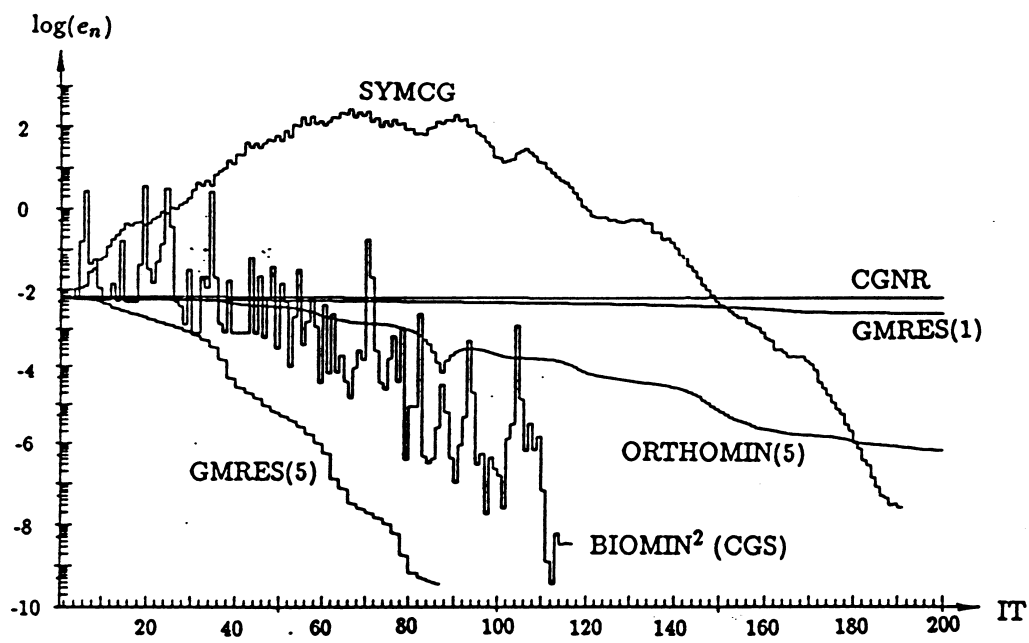


Figure 1  
Convergence properties of accelerators

## References

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