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Multigrid Becomes a Competitive Algorithm for some 3D Device Simulation Problems

J. Fuhrmann and K. Gärtner†

Institute for Applied Analysis and Stochastics
Hausvogteiplatz 5-7, D-10117 Berlin, GERMANY
†Interdisciplinary Project Center for Supercomputing, ETH-Zürich
ETH-Zentrum, CH-8092 Zürich, SWITZERLAND

Abstract

For situations where Gummel's decoupling scheme is applicable a multigrid algorithm for the continuity equations fully consistent with the usual Scharfetter-Gummel discretization can be used to solve the van Roosbroeck equations. The main problems for applying a multigrid algorithm are that discrete spaces are not nested in the usual sense for the refined grids because of the Scharfetter-Gummel discretization and that problem coefficients vary strongly. Transforming the equations to symmetric form and applying a block MILU decomposition based on the coarse-fine splitting of the discrete spaces with a perturbed Schur complement defines the prolongation and restriction operators. The transformation back to the original variables is possible. Coarse grid matrices are M-matrices.

Let $\mathcal{M}_0, \ldots \mathcal{M}_j$ be a sequence of Euclidean vector spaces with growing dimension. In order to define a standard multigrid algorithm to solve the continuity equation of the van-Roosbroeck system $A_j u = f$ on the j-th level there need to be the following components (in the terminology of [2]):

- scalar products $((\cdot,\cdot))_k : \mathcal{M}_k \times \mathcal{M}_k \to R$
- symmetric, positive definite with respect to $((\cdot,\cdot))_k$ operators $A_k : \mathcal{M}_k \to \mathcal{M}_k$,
- interpolations $I_k : \mathcal{M}_{k-1} \to \mathcal{M}_k$
- restrictions $P_k^0 : \mathcal{M}_k \to \mathcal{M}_{k-1}$.
- smoothers $R_k : \mathcal{M}_k \to \mathcal{M}_k$

While the smoothers R_k are provided by one or more steps of a classical iteration method (Jacobi, Gauß-Seidel, ILU), the design of other components in cases of strongly varying coefficients or missing standard finite element background is unclear. Here, we try a 'semi-algebraic' method as described in previous stages in [4, 5, 6]. Rather similar ideas of constructing multigrid or multilevel preconditioners have been used in [1, 3, 9, 10].

In what follows, we abbreviate the level-k-indices, to mean a fine grid corresponds to space $\mathcal{M}_k$, a coarse grid then corresponds to $\mathcal{M}_{k-1}$.

On a three-dimensional grid with quadrilateral cells generated by standard refinement from a coarser one, we have the splitting of the grid vertex set $V(A) = V_C \cup V_F \cup V_E \cup V_N$ into sets of coarse grid cell midpoints, coarse grid cell face midpoints, coarse grid

cell edge midpoints and coarse grid node points, respectively. We get the matrix partitioning

$$A = \begin{pmatrix} \begin{pmatrix} A_C & B_{CF} & 0 \\ B_{FC} & A_F & B_{FE} \\ 0 & B_{EF} & A_E \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \\ B_{EN} \end{pmatrix} \\ \begin{pmatrix} 0 & 0 & B_{NE} \end{pmatrix} & A_N \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix},$$

where the off diagonal blocks are nonpositive and the diagonal blocks $A_C = A_{CF} + M_C$, $A_F = A_{FC} + A_{FE} + M_F$, $A_E = A_{EF} + A_{EN} + M_E$ and $A_N = A_{NE} + M_N$, are positive diagonal matrices which consist of sums of off diagonal row entries and a nonnegative "mass" term. The assumptions made on A imply at least one entry of the "mass" M_* is positive.

Let $\tilde{A}_F = A_{FE} + M_F$, $\tilde{A}_E = A_{EN} + M_E$, and choose

$$F = \begin{pmatrix} A_C & B_{CF} & 0 \\ 0 & \tilde{A}_F & B_{FE} \\ 0 & 0 & \tilde{A}_E \end{pmatrix}, \qquad G = A_{12}, \qquad U = \begin{pmatrix} F & G \\ 0 & I \end{pmatrix}.$$

U can be seen as a transformation matrix to an approximate harmonic basis [7]. Then for $\cdot^T$ being the transposition with respect to the $((\cdot,\cdot))$-scalar product we have

$$A = U^T \begin{pmatrix} F^{-T} A_{11} F^{-1} & \Delta \\ \Delta^T & S \end{pmatrix} U, \tag{1}$$

with $\Delta = F^{-T}(A_{12} - A_{11}F^{-1}G)$ and $S = \hat{S} + \Delta^T (F^{-T} A_{11} F^{-1})^{-1} \Delta$, and $\hat{S} = A_{22} - A_{21}(A_{11})^{-1} A_{12}$ is the Schur complement. To create a block diagonal preconditioner for A in the new basis, one takes the decomposition (1) and omits the off diagonal blocks Δ. Omitting the error correction in the fine grid part, too, yields a coarse grid correction by projecting the error vector onto the fine grid space in the new basis. It has the form

$$B = U^{-1} \begin{pmatrix} 0 & 0 \\ 0 & S^{-1} \end{pmatrix} U^{-T} = I_k S^{-1} P_k^0$$

with

$$I_k = \begin{pmatrix} -F^{-1}G \\ I \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} -A_C^{-1} B_{CF} \tilde{A}_F^{-1} B_{FE} \tilde{A}_E^{-1} B_{EN} \\ \tilde{A}_F^{-1} B_{FE} \tilde{A}_E^{-1} B_{EN} \\ -\tilde{A}_E^{-1} B_{EN} \end{pmatrix} \\ I \end{pmatrix}$$

and P_k^0 being its $((\cdot,\cdot))$-adjoint. S is the Galerkin coarse grid operator corresponding to the given choice of the intergrid transfer operators:

$$\begin{aligned} S = P_k^0 A I_k \;=\; & (A_N - B_{NE}\tilde{A}_E^{-1} B_{EN}) + B_{NE}\tilde{A}_E^{-1}(A_{EF} - B_{EF}\tilde{A}_F^{-1} B_{FE})\tilde{A}_E^{-1} B_{EN} \\ & + B_{NE}\tilde{A}_E^{-1} B_{EF}\tilde{A}_F^{-1}(A_{FC} - B_{FC}A_C^{-1} B_{CF})\tilde{A}_F^{-1} B_{FE}\tilde{A}_E^{-1} B_{EN}. \end{aligned}$$

Some geometrical considerations and numerical experiments suggest that in the sense of spectral equivalences, it should hold that $S \approx 4(A_N - B_{NE}\tilde{A}_E^{-1} B_{EN}) =: A_{k-1}$, when the coefficients are not too strongly varying. This suggests replacing S by A_{k-1} in B. At the other hand, A_{k-1} is the Schur complement of the positive definite matrix

$$4 \begin{pmatrix} A_{EN} + M_E & B_{EN} \\ B_{NE} & A_N \end{pmatrix}$$

and inherits the $((\cdot,\cdot))$-symmetry, the M-property, and the seven-diagonal structure of A, so the process described above can be continued recursively. To ensure the preservation of the M-property in a floating point representation, one has to choose a matrix data structure where, on all the levels, instead of the main diagonal entries of A, the difference between these entries and the sum of the remaining entries of the same column is stored.

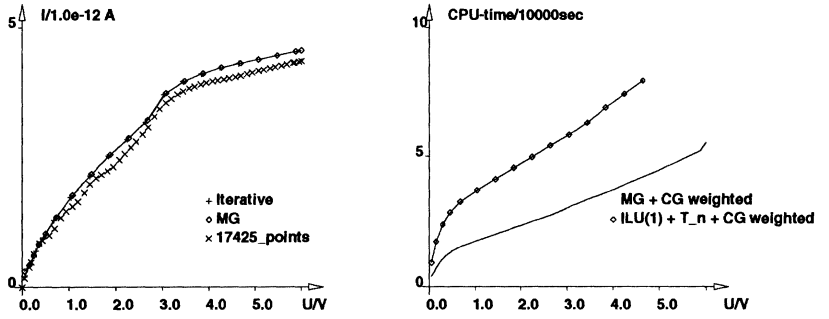
It can be shown [4] that for $((\cdot,\cdot))$-symmetric, positive definite operators, the convergence of a multigrid method with components defined this way depends on a number of reasonable factors:

- the spectral equivalence of A_{11} and F, and of A_{11} and its diagonal;
- the cosines of the angles between coarse grid and fine grid spaces in the A-energy scalar product;
- the spectral equivalence of S and A_{k-1};
- a smoothing property for R_k, which for Jacobi and Gauß-Seidel smoothers is valid for any symmetric M-matrix [11]

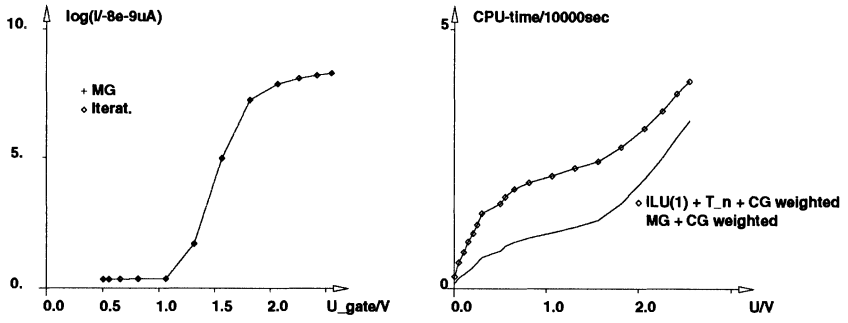
The whole multigrid operator described above is selfadjoint in the $((\cdot,\cdot))$-scalar product provided the smoothers are selfadjoint. Without smoothing, the MG-operator has a special recursively defined MILU decomposition interpretation. One can use it as a preconditioner for conjugated gradients in this scalar product. If one considers the Scharfetter-Gummel discretization of carrier transport equations in semiconductors, the discrete operators are selfadjoint with respect to a scalar product using a weight $e^{\pm\psi}$ where ψ is the electrostatic potential.

Here, we compare the algorithm above with a classical iterative one — ILU(1) preconditioning using Chebyshev polynomials and CG with weighted inner product.

The pictures show results for a photo diode with multiple differently doped horizontal layers. The aim is to deplete the whole diode and to compute the recombination current. The kink at 3.5V in the I-U-curve is what the designers are looking for. The Gummel iteration has been stopped at 10^{-7} U_T to fulfill the current balance better then 10^{-4}. A second example shows the results for a MOSFET at the 1MBit DRAM design level.



MEDEA, photo diode, Multigrid versus iterative method, 3 grids:
130977 = 49 × 33 × 81, 17425 = 25 × 17 × 41, 2457 = 13 × 9 × 21 points, CONVEX C220



MEDEA, 'half-MOSFET', 1MBit DRAM design level, $U_{\text{bulk}} = -2V$, $U_{\text{drain}} = 0.1V$, $156849 = 97 \times 33 \times 49$, $20825 = 49 \times 17 \times 25$, $2925 = 25 \times 9 \times 13$, $455 = 13 \times 5 \times 7$, $84 = 7 \times 3 \times 4$ points, DEC ALPHA (3000/500, 64MB)

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