Using Scalar Algebraic Multigrid Solvers for Efficient 3-D Stress Analysis of Microfabricated Structures

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ABSTRACT

A methodology to improve the performance of iterative solvers in 3-D stress analysis using scalar algebraic multigrid (AMG) solvers has been presented. The principle idea is to split the global system of coupled stress governing discrete equations into a sequence of local matrix problems suitable for application of scalar AMG solvers. The proposed methodology have been implemented as a preconditioner for Krylov iterative methods. The effectiveness of the global solving procedure has been tested practically in 3D stress analysis of microfabricated structures. Numerical experiments have shown nearly optimal and stable convergence properties of the resulting iterative solvers in applications related to microfabrication technology.

Keywords: algebraic multigrid, Krylov iterative solvers, stress analysis, microfabrication

1 INTRODUCTION

There is an increasing interest for the stress analysis of microfabricated structures. The principle aims are to predict and eliminate the harmful effects that stress can impose on the produced microelectronics and micromechanical devices, and to provide guidelines for the development of new technologies that may take advantage of the stress presence [1].

The complex geometry of the microfabricated structures typically requires finite element stress analysis based on general unstructured grids. The continuing increase of the computational resources enables finite element stress analysis of larger and more complex 3-D industrial applications [2]. However, with the increase of the problem size, the performance of the solvers for the corresponding discrete problems becomes much poorer. A non-optimal number of floating operations is encountered both with direct and iterative solvers. While direct solvers have inherent difficulties in achieving the linear scaling with the problem size, iterative solvers are facing the problems of bad conditioning.

It is well known that the multigrid methods offer the prospect of optimal scaling with problem size. The essential idea of multigrid methods is to employ a hierarchy of discrete representation of the problem in order to efficiently eliminate the solution error in different subspaces [3]. However, multigrid methods require grid hierarchy which is not readily available for unstructured grids. In order to overcome this problem, the idea of *algebraic multigrid* (AMG) has been introduced [4] where the required discrete hierarchy is generated in the automatic coarsening process, based exclusively on the algebraic relationships between the discrete variables. However, the coarsening heuristics of the standard AMG algorithm has been essentially developed in the context of a stiffness matrix corresponding to scalar problems and it is generally not directly applicable to the systems of stress governing equations.

In this paper, an effective methodology to improve the performance of iterative solution of stress governing equations by scalar AMG solvers have been demonstrated. The principle idea is to apply a scalar AMG solver in a segregated way to the series of scalar block-diagonal matrix problems corresponding to the individual displacement vector components. It is demonstrated that the local block-diagonal matrices are quite suitable for the scalar AMG coarsening and solving process. The methodology is practically employed as a preconditioner for standard Krylov subspace iterative methods.

2 PROBLEM FORMULATION

Let us consider multilayer material structure occupying bounded domain $\Omega \in R^3$. The deformation of the multilayer material structure is generally governed by the second Newton law in the form

$$\nabla \cdot \sigma(u) = 0 \quad \text{in} \quad \Omega, \tag{1}$$

where $\sigma(u)$ is the Cauchy stress tensor being a function of the displacement vector $u = [u_i]_{i=1,2,3}$. Notice that in the stress analysis of microfabricated structures we can neglect the acceleration term in the Newton law as well as body forces.

Without losing generality we will restrict our analysis to the constitutive equations of linear elasticity. In that case, the stress tensor is related to the displacement vector as

$$\sigma(u) = \mu \left(\nabla u + \nabla u^T\right) + \lambda \left(\nabla \cdot u\right) I + \sigma^0 \tag{2}$$

where $\mu > 0$ and $\lambda > 0$ are Lamé's coefficients, I is the identity tensor and σ^0 is the term that takes into account the previous stress history. In the stress analysis of microfabricated structures σ^0 can be used to specify the intrinsic stress in the deposited material layers or to account for the intrinsic strain due to the variation of processing temperature. The interfaces between different material layers, including the free external boundaries of Ω, are characterized by the interface condition

$$[\sigma(u) \cdot n] = 0 \tag{3}$$

where n is the unit normal vector to the interface.

Multiplying (1) by an arbitrary test function ψ and integrating by parts in Ω, one can also obtain a weak formulation of (1) which is: find $u \in V(\Omega)$ such that

$$\int_{\Omega} \sigma(u) \cdot \nabla\psi \, d\Omega = 0 \tag{4}$$

where $V(\Omega)$ is the space of admissible displacement fields in Ω that also satisfy $u = 0$ on the fixed external boundaries of Ω. In order to formulate the corresponding discrete finite element stress analysis problem, we consider u as a discrete displacement vector $u \in V_h(\Omega)$, where $V_h(\Omega) \in V(\Omega)$ consists of piecewise polynomial functions. Introducing $\phi^1, \ldots, \phi^N$, $N = \dim V_h(\Omega)$, as a basis for $V_h(\Omega)$, the discrete displacement vector components are defined as

$$u_i = \sum_{r=1}^{N} u_i^r \phi^r, \quad i = 1, 2, 3 \tag{5}$$

where u_i^r, are unknown discrete solution coefficients. Substituting (2) with (5) in (4) and evaluating (4) using $\psi = \phi^r$ as a test function, we obtain for $i = 1, 2, 3$ and $r = 1, \ldots, N$ a system of $3N$ algebraic equations

$$\sum_{j=1}^{3} \sum_{s=1}^{N} A_{ij}^{rs} u_j^s = b_i^r \tag{6}$$

where

$$\begin{aligned} A_{ij}^{rs} =& \delta_{ij} \int_{\Omega} \mu \nabla\phi_r \nabla\phi_s \, d\Omega + \\ &+ \int_{\Omega} \left(\mu \partial_j \phi^r \partial_i \phi^s + \lambda \partial_j \phi^s \partial_i \phi^r\right) d\Omega \end{aligned} \tag{7}$$

and

$$b_i^r = -\int_{\Omega} \sigma^0 \cdot \nabla\phi_r \, d\Omega. \tag{8}$$

We can also formulate (6) as a matrix problem

$$\mathbf{A}\mathbf{u} = \mathbf{b} \tag{9}$$

where $\mathbf{A} = \{\{A_{ij}^{rs}\}_{i,j=1}^{3}\}_{r,s=1}^{N}$ is the $3N \times 3N$ global stiffness matrix, $\mathbf{b} = \{\{b_j^s\}_{j=1}^{3}\}_{s=1}^{N}$ is the corresponding right hand side and the nodal values of discrete displacement will be obtained in $\mathbf{u} = \{\{u_j^s\}_{j=1}^{3}\}_{s=1}^{N}$ after solving the system (9).

3 A SOLVING METHODOLOGY

In order to solve the sparse linear system (9) we can apply a host of iterative and direct methods that are currently available. However, since direct methods have inherent difficulties in achieving the linear scaling with the problem size, we constrain ourselves to the Krylov subspace iterative methods. These methods are based on the minimisation of the error in the subspaces involving orthogonal projections of the form

$$\mathcal{K}(\mathbf{A}, \mathbf{b}) = \text{span}\{\mathbf{b}, \mathbf{A}\mathbf{b}, \mathbf{A}^2\mathbf{b}, \ldots\}. \tag{10}$$

When applied to obtaining the solution of the linear system (9), the solution is found in at most $3N$ iterations (providing that an exact arithmetic is used). However, this limit could be quite impractical for large systems of equations which characterize real engineering applications.

The situation can be radically improved by introducing preconditioning of the original system (9). Instead of applying Krylov iterative methods directly to system (9), we solve mathematically equivalent system

$$\mathbf{M}^{-1}\mathbf{A}\mathbf{u} = \mathbf{M}^{-1}\mathbf{b}, \tag{11}$$

where $\mathbf{M}$ is nonsingular matrix which is spectrally close to $\mathbf{A}$ but simple to assemble, and to compute an action of its inverse. The main idea behind preconditioning is to obtain more favourable spectral properties of the preconditioned matrix $\mathbf{M}^{-1}\mathbf{A}$ which enables us to solve the system (9) within some tolerance in a substantially lower number of iterations than $3N$. Optimal convergence rate is obtained if $\mathbf{M}^{-1}\mathbf{A}$ equals the identity matrix $\mathbf{I}$.

Instead of explicitly assembling and inverting the preconditioning matrix $\mathbf{M}$, it often convenient to replace the action of $\mathbf{M}^{-1}$ through the application of an auxiliary iterative method. However, classical iterative methods are very slow to remove smooth error components in the discrete solution and produce quite inefficient preconditioning. A widely accepted approach towards nearly optimal Krylov iterative method, with convergence rate independent of N, is to employ multigrid methods as preconditioners. The essential idea of multigrid methods is to employ a hierarchy of discrete representation of the problem in order to efficiently eliminate the solution error in different subspaces [3], [5]. The most straightforward approach to construct such a hierarchy is to coarsen or refine the original grid. However, complex unstructured grids are usually not coarse

enough to serve as the coarsest multigrid level when grid refinements is used. On the other hand, the construction of coarse grid structures is not readily available for general unstructured grids.

In order to free the solver from the dependence on domain and grid geometry the idea of algebraic multigrid (AMG) method has been introduced [4]. The AMG approach provides a purely algebraic means to construct the coarser representations of the discrete problem as well as interpolation and restriction operators which are required for the multigrid algorithm. The coarsening heuristics of the AMG algorithm is formulated exclusively on the algebraic relationships between the discrete variables using *strength of dependence* principle [4]. It is essentially developed by having in mind a stiffness matrix corresponding to a scalar elliptic PDE and has appeared to be quite inadequate for stiffness matrices of general non-scalar PDE systems. Although important progress has been achieved in applying the AMG algorithm directly to some systems of PDEs, there is not yet the well-established approach showing the robustness and efficiency of the scalar AMG solvers [5].

An appealing idea to still employ the scalar AMG solvers in the preconditioning process is to decompose the global matrix problem into a sequence of scalar problems suitable for the standard AMG algorithm. To this end, we consider (9) in the form

$$\begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} & \mathbf{A}_{13} \\ \mathbf{A}_{21} & \mathbf{A}_{22} & \mathbf{A}_{23} \\ \mathbf{A}_{31} & \mathbf{A}_{32} & \mathbf{A}_{33} \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \mathbf{u}_3 \end{pmatrix} = \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \end{pmatrix} \tag{12}$$

where

$$\mathbf{A}_{ij} = \begin{pmatrix} A_{ij}^{11} & \cdots & A_{ij}^{1N} \\ \vdots & \ddots & \vdots \\ A_{ij}^{N1} & \cdots & A_{ij}^{NN} \end{pmatrix} \tag{13}$$

are block stiffness matrices, while

$$\mathbf{u}_i = (u_i^1, \ldots, u_i^N)^T \quad \text{and} \quad \mathbf{b}_i = (b_i^1, \ldots, b_i^N)^T \tag{14}$$

are vectors of nodal displacement and right-hand side corresponding to the ith Cartesian coordinate. The sequence of scalar problems can be formulated introducing the preconditioning matrix $\mathbf{M}$ in the form of lower triangular matrix

$$\mathbf{M} = \begin{pmatrix} \mathbf{A}_{11} & & \\ \mathbf{A}_{21} & \mathbf{A}_{22} & \\ \mathbf{A}_{31} & \mathbf{A}_{32} & \mathbf{A}_{33} \end{pmatrix}. \tag{15}$$

Notice that the inversion of the preconditioning matrix (15) could be implemented in a segregated way solving the sequence of matrix problems

$$\mathbf{A}_{ii}\mathbf{u}_i = \mathbf{b}_i - \sum_{j=1}^{i-1} \mathbf{A}_{ij}\mathbf{u}_j \tag{16}$$

for $i = 1, 2, 3$. It is equivalent to the application of single block Gauss-Seidel iteration.

Each individual step of (16) could be interpreted as the scalar algebraic problem for the solution of nodal displacements along the i-th Cartesian coordinate provided that the displacements in other directions are kept fixed. Since the block diagonal matrices $\mathbf{A}_{ii}$ are quite suitable for the standard AMG coarsening methodology, the segregated problem could be effectively inverted using scalar AMG solvers. Notice that the AMG setup procedure, in which the coarse level multigrid components are assembled, can be performed for each block separately at the beginning of the iterative solving procedure. Moreover, in practical implementations it is sufficient to solve the scalar displacement problems only approximately applying only $1 - 2$ multigrid cycles.

4 CASE STUDY

The efficiency of the scalar AMG solving methodology has been practically tested in 3-D stress analysis problems from microfabrication. Figure 1 shows an example of the grid and geometry for a nitride-oxide-silicon structure used in numerical experiments. The source of the stress is the deposition induced intrinsic stress in the top nitride layer.

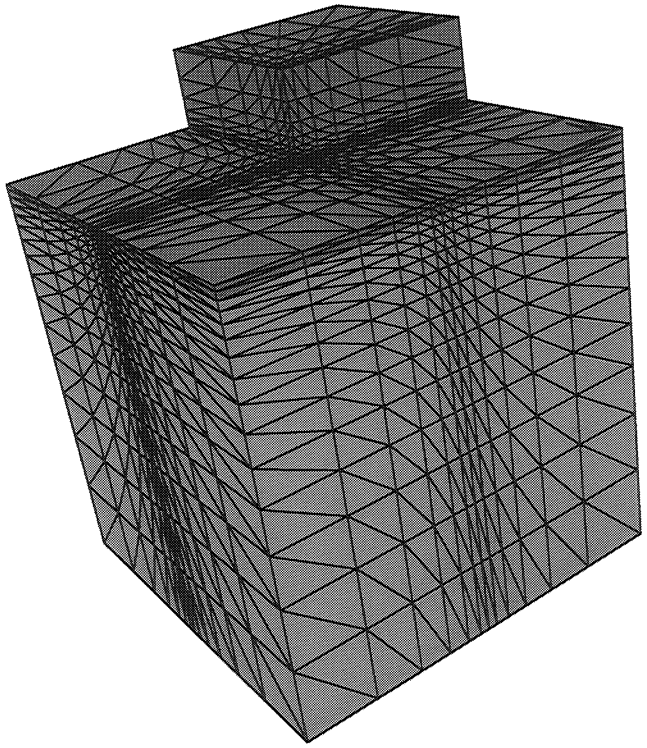

Figure 1: An example of the geometry and grid used in stress analysis of the nitride-oxide-silicon structure having deposition induced intrinsic stress in top nitride layer.

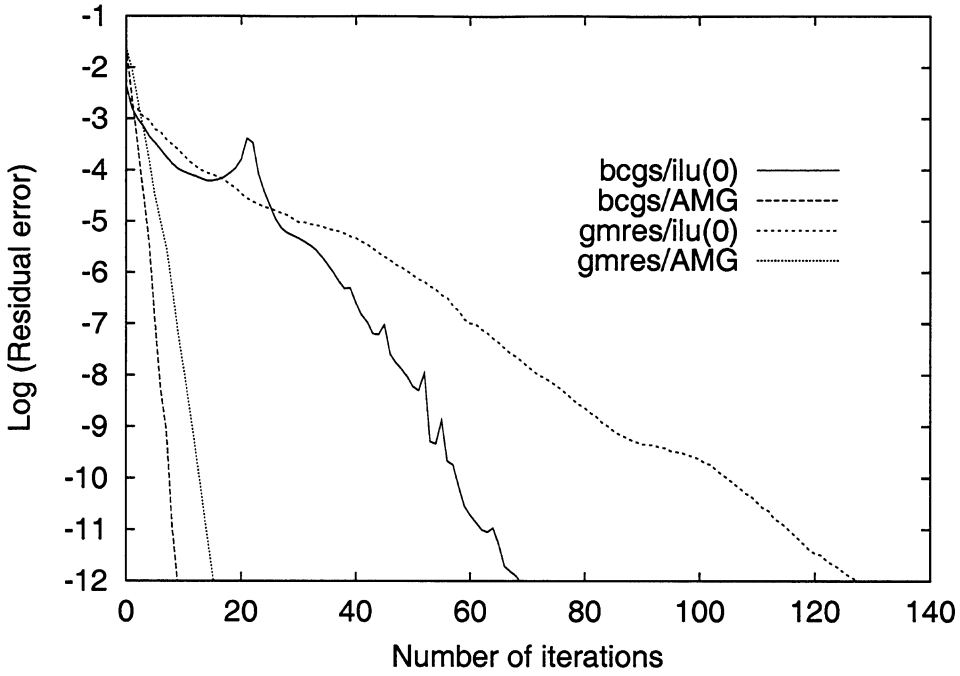

Figure 2: Comparison of the convergence histories for standard and scalar AMG preconditioned iterative solvers applied to the solution of the problem from Figure 1.

The discrete stress governing equations are solved using *biconjugate gradient* (bcgs) and *generalised minimal residual* (gmres) Krylov subspace iterative methods [6]. Both iterative methods have been implemented with standard *incomplete LU factorization* (ilu(0)) or a new AMG based preconditioning described in Section 3. The well established and publicly available code AMG1R5 [4] have been used as a scalar AMG solver.

The convergence histories shown in Figure 2 clearly demonstrate the superiority of the proposed AMG based preconditioning methodology which significantly reduces the number of iteration for both Krylov iterative solvers.

5 CONCLUSIONS

A methodology to improve the performance of iterative solvers in stress analysis using robust scalar AMG solvers have been presented. The principal idea lies in the sequential application of scalar AMG solvers to block diagonal matrices corresponding to locally one-dimensional discrete stress analysis problems along each of the Cartesian coordinates.

The method is essentially implemented as preconditioner for Krylov iterative methods. Numerical experiments have shown robust and stable convergence properties of the proposed AMG based preconditioning methodology which gives significantly faster convergence comparing to standard incomplete LU preconditioners.

It should be emphasised that the present implementation, based on scalar AMG solvers, could be considered as one particular realization within a global framework of component decomposition preconditioning. Namely, some other effective factorisations for scalar problems could be implemented in component-wise fashion instead of AMG. Finally, it could be important to also justify the method through more rigorous theoretical analysis.

REFERENCES

[1] S.M. Hu, "Stress related problems in silicon technology," Int. J. Appl. Phys, 15, R53–R80, 1991.

[2] W. Joppich and S. Mijalković, "Semiconductor Process Modeling" in "Wiley Encyclopedia of Electrical and Electronics Engineering" (J.G. Webster, ed.), John Wiley & Sons, Inc., 19, 127–139, New York, 1999.

[3] W. Joppich and S. Mijalković, "Multigrid Methods for Process Simulation," Springer-Verlag, Wien New York, 1993.

[4] K. Stüben, "Algebraic multigrid (AMG): experiences and comparisons," Appl. Math. Comp., 13, 419–452, 1983.

[5] U. Trottenberg, C.W. Oosterlee and A. Schüller, Multigrid Methods, Academic Press, 2000.

[6] S. Balay, W. Gropp, L.C. McInnes, B. Smith, "PETSc 2.0 Users Manual," ANL-95/11–Revision 2.0.29, Argonne National Laboratory, 2000.