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A component decomposition preconditioning for 3D stress analysis problems

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SUMMARY

A preconditioning methodology for an iterative solution of discrete stress analysis problems based on a space decomposition and subspace correction framework is analysed in this paper. The principle idea of our approach is a decomposition of a global discrete system into the series of subproblems each of which correspond to the different Cartesian coordinates of the solution (displacement) vector. This enables us to treat the matrix subproblems in a segregated way. A host of well established scalar solvers can be employed for the solution of subproblems. In this paper we constrain ourselves to an approximate solution using the scalar algebraic multigrid (AMG) solver, while the subspace correction is performed either in block diagonal (Jacobi) or block lower triangular (Gauss-Seidel) fashion. The preconditioning methodology is justified theoretically for the case of the block-diagonal preconditioner using Korn's inequality for estimating the ratio between the extremal eigenvalues of a preconditioned matrix. The effectiveness of the AMG based preconditioner is tested on stress analysis 3D model problems that arise in microfabrication technology. The numerical results, which are in accordance with theoretical predictions, clearly demonstrate the superiority of a component decomposition AMG preconditioner over the standard ILU preconditioner, even for the problems with a relatively small number of degrees of freedom.
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KEY WORDS: preconditioning; stress analysis; 3D linear elasticity; algebraic multigrid; Krylov methods

1. INTRODUCTION

Stress analysis in 3D becomes essential for accurate design of complex physical and mechanical systems that utilise a variety of structural elements with differing mechanical properties and intrinsic built-in stress distributions. A standard approach to 3D stress analysis is to partition the multilayer material geometry using general unstructured grids and to discretize the governing stress equations by the finite element method. In multi-layer material domains with complex geometry this usually leads to the solution of large sparse matrix problems with a non-regular sparsity pattern and poor scaling of the equations. However, it is recognized that as the discrete problems size continues to increase,

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linear solvers performance becomes non-optimal. Namely, direct solvers have inherent difficulties in achieving the linear scaling with problem size, both in terms of execution time and of storage requirements, while iterative solvers face the problems of bad conditioning.

The problem of constructing efficient solution methods for the stress analysis problems, especially in the context of linear elasticity, have been studied by many authors. Some of this work covers specific topics, such as thin domain structures in 3D, like plates and shells (see, for example, [29],[30],[31],[32]), mixed and penalty methods for incompressible problems [18],[23] and the application of AMLI methods [1],[3],[33]. It is well known that multigrid methods offer the prospect of optimal scaling with problem size [36], either as stand-alone methods (in the case of well-structured grids), or as accelerators for the Krylov iterative methods (for the case of more general grids). However, multigrid methods require a hierarchical grid structure which is not readily available in unstructured grids. In order to overcome this problem, the idea of *algebraic multigrid* (AMG) has been introduced [36] (see also [37],[38] for more recent review). In AMG methods, the required grid hierarchy is generated in the automatic coarsening process based exclusively on the algebraic relationships between the discrete (nodal) variables. The coarsening heuristic in the standard AMG algorithm is based on the *strength of dependence* principle. It is essentially developed by having in mind a stiffness matrix corresponding to a scalar elliptic PDE (ideally an M-matrix), and has appeared to be quite inadequate for direct application to the matrices of general non-scalar PDE systems. Although important progress has been achieved in applying the AMG algorithm directly to some systems of PDEs (see, for example [14] for the linear elasticity equations), a well-established approach showing the robustness and efficiency of scalar AMG [36] does not yet exist.

The optimal (or nearly optimal) preconditioners for Krylov iterative methods are often constructed within a general framework of the *space decomposition and subspace correction* (SSC) methods [17]. The principle idea is to decompose, in a stable manner, the global finite dimensional space into a set of local subspaces. This introduces the corresponding restriction of the global problem into a set of local subspace problems. The global discrete solution is then obtained by the appropriate combinations of the solutions for the local subspace problems. Typical examples include *domain decomposition methods* with subspaces based on the geometrical partition of the domain, and *multigrid methods* where the hierarchy of coarser grids represents a basis for the space decomposition. The objective of this paper is to present another SSC preconditioning strategy which is particularly suitable for the system of equations in stress analysis problems. The idea is to consider the components of the material displacement vector as a base for additional space decomposition. In that case, the space decomposition is done in a way that local subspace problems actually control the material displacement along single Cartesian coordinate, provided that the the displacements in other directions are kept fixed (see [3]). As in any other SSC preconditioning methodology, the subspace correction can be performed either in parallel (Jacobi), or successive (Gauss-Seidel) fashion. In algebraic sense, the component decomposition preconditioning could be also interpreted as block diagonal preconditioning. Its effectiveness for linear elasticity problems has been also considered in [4]. Similar results can also be found in [3],[11].

The local subspace problems in component decomposition preconditioning have essentially the properties of the scalar PDE equations for which a variety of efficient preconditioning and solving procedures exist. In [4] the approximate factorisation is used for the solution of the individual block matrices. The preconditioner suggested in [33] has a block diagonal form and the author considers an approximation of the diagonal blocks by the additive AMLI method (for more detail on the approach used in [33], see Section 3). In this paper, we consider application of the standard algebraic multigrid (AMG) method for the preconditioning and subspace correction in the context of component

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decomposition preconditioning. For an AMG solver we employ the well-established publicly available code AMG1R5 [36].

The paper is organised as follows. In Section 2 we outline the problem and give details of the discretisation. We also explain the component-wise blocking strategy of the original coefficient matrix. In Section 3 we explain our preconditioning strategy, and in Section 4 a convergence analysis of the preconditioned discrete stress operator is presented. In particular, we give bounds for the spectrum which are independent of the mesh size, but depend upon the Poisson ratio and the domain shape. We also give some comparison of our spectral bounds with those reported in [33]. In Section 5 we demonstrate numerical efficiency of our approach on a realistic example from microfabrication technology. Finally, in Section 6 we give some concluding remarks.

2. PROBLEM FORMULATION

Deformation of a continuous material body occupying a bounded domain $\Omega \subset \mathbb{R}^3$ is governed by the boundary value problem

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

$$u = d \quad \text{on} \quad \Gamma_d, \tag{2}$$

$$\sigma(u) \cdot \hat{n} = g \quad \text{on} \quad \Gamma_g. \tag{3}$$

In the equations (1)–(3) σ is the Cauchy stress tensor which is a function of the displacement vector $u = [u_i]_{i=1,3}$, $f = [f_i]_{i=1,3}$ is a body force vector, d represents a prescribed displacement of the boundary segment $\Gamma_d \subset \partial\Omega$, and g is the surface traction of the boundary segment $\Gamma_g \subset \partial\Omega$ ($\Gamma_d \cap \Gamma_g = \emptyset$) with outward unit normal vector $\hat{n}$. In order to have a unique solution, the segment Γ_d has to be of a finite measure.

For linear elasticity problems, the stress tensor is related to the strain tensor $\epsilon(u)$ by Hooke's law as

$$\sigma(u) = 2\mu\epsilon(u) + \lambda\,(\nabla \cdot u)\,I, \tag{4}$$

where I is the identity tensor, and $\mu > 0$ and $\lambda > 0$ are Lamé's coefficients given by

$$\mu = \frac{E}{2(1+\nu)}, \qquad \lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}\,. \tag{5}$$

In (5) $E > 0$ is the Young's modulus and ν is the Poisson ratio ($0 < \nu < 0.5$). The elements of the strain tensor coefficient matrix can be expressed as

$$\epsilon_{ij}(u) = (\partial_j u_i + \partial_i u_j)\,/2, \tag{6}$$

where ∂_i denotes a partial derivative with respect to the ith Cartesian coordinate.

The generalised (variational) stress analysis problem can be formulated as follows: Find $u \in V(\Omega)$ such that

$$\mathcal{E}(u, v) = \mathcal{F}(v), \quad \forall v \in V_0(\Omega), \tag{7}$$

where $V_0(\Omega) = H_0^1(\Omega)$ is the standard Sobolev space with the homogeneous Dirichlet boundary conditions on a part of the boundary Γ_d, i.e.

$$V_0(\Omega) = \left\{ w : \int_\Omega (w^2 + |\nabla w|^2)\, d\Omega < \infty,\ w = 0 \text{ on } \Gamma_d \right\}. \tag{8}$$

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The bilinear form $\mathcal{E}(u, v)$ in (7) is symmetric and continuous in $V_0(\Omega)$. If the condition (2.3) from [29] holds for $\mathcal{E}(u, v)$, this implies, together with Korn's inequality [16], that $\mathcal{E}(u, v)$ is coercive in $V_0(\Omega)$. Therefore, the problem (7) has a unique solution (see [13]). The linear functional $\mathcal{F}(v)$, which is bounded in $V_0(\Omega)$, is given by

$$\mathcal{F}(v) = (f, v) + \int_{\Gamma_g} g \cdot v \, d\Gamma. \tag{9}$$

In (9) $(\cdot, \cdot)$ denotes a scalar product in $L^2(\Omega)$. Denote by $V(\Omega)$ the space of admissible displacement fields in Ω that satisfies the Dirichlet boundary conditions (2). In our case $V(\Omega) = H_d^1(\Omega)$, where

$$H_d^1(\Omega) = \left\{ w \; : \; \int_\Omega (w^2 + \mid \nabla w \mid^2) \, dx < \infty, \; w = d \text{ on } \Gamma_d \right\}. \tag{10}$$

The bilinear energy functional $\mathcal{E}(u, v)$ is given by

$$\mathcal{E}(u, v) = 2\mu \mathcal{S}(u, v) + \lambda(\nabla \cdot u, \nabla \cdot v), \tag{11}$$

where

$$\mathcal{S}(u, v) = \sum_{i,j=1}^{3} \epsilon_{ij}(u) \cdot \epsilon_{ij}(v). \tag{12}$$

In order to formulate a discrete stress analysis problem, we apply the Galerkin projection of $V(\Omega)$ onto $V_h(\Omega) \subset V(\Omega)$, thus getting a problem: Find $u^h \in V_h(\Omega)$ such that

$$\mathcal{E}(u^h, v^h) = \mathcal{F}(v^h), \quad \forall v^h \in V_{h_0}(\Omega). \tag{13}$$

In our case we adopt $V_h(\Omega)$ to be a space of piecewise linear polynomials that correspond to a given partitioning of the domain Ω into disjoint tetrahedra $\mathcal{T}_h = \bigcup T_i$, i.e.

$$V_h(\Omega) = \left\{ w^h \; : \; w^h(\mathbf{x}) = \sum_{0 \le i+j+k \le 1} c_{ijk} x^i y^j z^k \quad \text{for } \mathbf{x} = (x, y, z) \in T_i, \;\; c_{ijk} \in \mathbb{R} \right\}, \tag{14}$$

and $w^h(\mathbf{x}) = d(\mathbf{x})$ for $\mathbf{x} \in \Gamma_d$. Introducing a nodal basis set $\{\phi_r\}_{r=1}^N$, $N = \dim\{V_h(\Omega)\}$, we can define a discrete displacement vector component as

$$u_i = \sum_{r=1}^{N} u_i^r \phi_r, \quad i = 1, 2, 3 \tag{15}$$

where u_i^r are the unknown nodal coefficients for the displacement along ith Cartesian coordinate. If we substitute (15) into (7) and for the weighting functions we adopt $v^h \in V_{h_0} \subset V_0(\Omega)$, assuming the same basis set for $V_h(\Omega)$ and $V_{h_0}(\Omega)$, i.e. $\{\phi_r\}_{r=1}^N$ and $i = 1, 2, 3$, $(v^h = [\phi_r \delta_{ij}]_{j=1}^3)$, we obtain a linear algebraic system of $3N$ equations

$$\sum_{j=1}^{3} \sum_{s=1}^{N} A_{ij}^{rs} u_j^s = b_i^r, \qquad i = 1, 2, 3, \quad r = 1, \ldots, N \tag{16}$$

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where

$$A_{ij}^{rs} = \mu \sum_{k=1}^{3} \left(\partial_k \phi_r, \partial_k \phi_s\right) \delta_{ij} + \mu \left(\partial_j \phi_r, \partial_i \phi_s\right) + \lambda \left(\partial_j \phi_s, \partial_i \phi_r\right), \tag{17}$$

and

$$b_r^i = (f_i, \phi_r) + \int_{\Gamma_g} g_i \phi_r \, d\Gamma. \tag{18}$$

We can also formulate (16) as a matrix problem

$$A\mathbf{u} = \mathbf{b} \tag{19}$$

where

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}, \qquad A_{ij} = \begin{pmatrix} A_{ij}^{11} & \cdots & A_{ij}^{1N} \\ \vdots & \ddots & \vdots \\ A_{ij}^{N1} & \cdots & A_{ij}^{NN} \end{pmatrix} \quad i,j = 1,2,3 \tag{20}$$

are the global and component stiffness matrices, respectively, and

$$\mathbf{u} = \left(\mathbf{u}_1^T, \mathbf{u}_2^T, \mathbf{u}_3^T\right)^T, \qquad \mathbf{u}_i = (u_i^1, \ldots, u_i^N)^T, \quad i = 1,2,3, \tag{21}$$

$$\mathbf{b} = \left(\mathbf{b}_1^T, \mathbf{b}_2^T, \mathbf{b}_3^T\right)^T, \qquad \mathbf{b}_i = (b_i^1, \ldots, b_i^N)^T, \quad i = 1,2,3 \tag{22}$$

are correspondingly partitioned vectors of unknowns and right-hand sides.

3. PRECONDITIONING METHODOLOGY

In order to solve a large sparse linear system (19) we can apply a host of iterative and direct methods that are currently available (see, for example, [12],[15],[34]). However, in this paper we constrain ourselves to the Krylov subspace iterative methods. Given a linear algebraic system (19) and the initial guess of the solution vector $\mathbf{u}^{(0)}$ with the corresponding residual $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{u}^{(0)}$, one constructs a sequence of iterates $\mathbf{u}^{(k)}$ such that

$$\mathbf{u}^{(k)} = \mathbf{u}^{(0)} + \mathbf{p}^{(k)} \tag{23}$$

where $\mathbf{p}^{(k)} \in \mathcal{K}(A, \mathbf{r}^{(0)}) = \text{span}\{\mathbf{r}^{(0)}, A\mathbf{r}^{(0)}, \ldots, A^{k-1}\mathbf{r}^{(0)}\}$. By adding the corrections $\mathbf{p}^{(k)}$ to an initial guess $\mathbf{u}^{(0)}$, one minimises the error in solution $\mathbf{u}^{(k)}$ over the finite dimensional subspaces $\mathcal{K}(A, \mathbf{r}^{(0)})$.

When applied to the solution of the linear system (19), Krylov iterative solvers will converge to the solution $\mathbf{u}$ in at most $3N$ iterations (providing that an exact arithmetic is used). However, this limit could be quite impractical for large systems of equations. The situation can be radically improved by introducing preconditioning of the original system (19) as

$$M^{-1}A\mathbf{u} = M^{-1}\mathbf{b}, \tag{24}$$

where M is some matrix which is spectrally close to A, but simple to assemble and compute the action of its inverse. The main idea behind preconditioning is to obtain more favourable spectral properties of the preconditioned matrix $M^{-1}A$ which enables us to solve the system (19) within some tolerance in a substantially lower number of iterations than $3N$. The aim is to get the spectrum of a preconditioned

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matrix $M^{-1}A$ consisting of relatively few distinct eigenvalues with a large multiplicity. This goal is in practice quite often replaced by the requirement that the spectrum of $M^{-1}A$ is tightly clustered and bounded by the quantities that are independent (or very loosely dependent) upon the discretisation parameter h and the other parameters that figure in the problem formulation. For a symmetric positive definite matrices A and M, this goal can also be interpreted as a minimization of the condition number

$$\kappa(M^{-1}A) = \frac{\omega_{max}}{\omega_{min}}, \tag{25}$$

where ω_{max} and ω_{min} are the upper and the lower bound of ω in the the generalized eigenvalue problem

$$A\mathbf{x} = \omega M\mathbf{x}. \tag{26}$$

It is desirable to obtain a condition number (25) with an upper bound that is as small as possible and also independent on the mesh parameter h. This would give us an *optimal order* iterative method with the convergence rate independent of the problem size. In the case of a non-symmetric matrix A (or non-symmetric preconditioner M), in addition to the requirement that the ratio $\omega_{max}/\omega_{min}$ is small and independent of the mesh size h, one would also like to show that the condition number of the matrix of eigenvectors X of the preconditioned matrix can be bounded independently of h. Although there is no firm guarantee that the preconditioned Krylov method will converge in small number of steps if the boundedness condition of $\kappa(X)$ is violated, our experience is that if the first requirement is satisfied, then rapid convergence is usually observed (see also [34]).

In order to solve the discrete problem (19) by the SSC method, it is necessary to decompose the discrete finite element space $V_h(\Omega)$ into a sum

$$V_h(\Omega) = \sum_{i=1}^{m} V_h^{(i)}(\Omega) \tag{27}$$

The effective implementation of SSC methods require the efficient solution of the subspace problems. In practice, this can be done using the direct factorisation of the appropriate matrix blocks, however, this will give a non-optimal algorithm. The second option is to find an efficient way of preconditioning the subspace problems using optimal algorithms. In this sense, the intuition behind the construction of a preconditioner for the stress analysis system based on scalar AMG solvers is that the global finite dimensional space $V_h(\Omega)$ can be split into subspaces which could be suitable for an application of the scalar AMG methodology. To this end, it seems quite natural to introduce a component-wise space decomposition

$$V_h(\Omega) = \sum_{i=1}^{3} V_h^{(i)}(\Omega), \tag{28}$$

where for $\mathbf{u} \in V_h^{(i)}(\Omega)$ we have $u_j = 0$ if $i \neq j$ (see also [3]). The generalised restricted problems can be formulated as follows: Find $\mathbf{u}_i \in V_h^{(i)}(\Omega)$ such that

$$\mathcal{E}(\mathbf{u}_i, \mathbf{v}_i) = \mathcal{F}(\mathbf{v}_i) \quad \forall \mathbf{v}_i \in V_h^{(i)}(\Omega), \tag{29}$$

for $i = 1, 2, 3$. The restricted subspace problems can be expressed in the algebraic form as

$$Du = b, \tag{30}$$

with $D = \mathrm{diag}\,(A_{11}, A_{22}, A_{33})$.

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The subspace problems (29) are solved only approximately using a scalar AMG solver as the local subspace preconditioner, performing typically only a small fixed number of AMG cycles per local subproblem. The subspace correction of the global solution can be generally realised in parallel, which is similar to the block Jacobi method, or successively, resembling the block Gauss-Seidel method (see [39]). If we represent the effect of subspace scalar AMG solvers with preconditioning matrices $M_i^{AMG}, i = 1, 2, 3$, the global preconditioning matrix is given by

$$M_P = \text{diag}\left(M_1^{AMG}, M_2^{AMG}, M_3^{AMG}\right) \tag{31}$$

in the case of the parallel subspace correction, and

$$M_S = M_P + L \tag{32}$$

if the subspace correction is applied successively. Here L denotes the block lower triangular matrix in the splitting $A = D + L + U$, where U is the corresponding block upper triangular matrix.

We briefly comment on suitability of the AMG as a local problem solver. Local subspace operators

$$\mathcal{D}(u, v) = \mu \sum_i (\nabla u_i, \nabla v_i) + (\lambda + \mu) \sum_i (\partial_i u_i, \partial_i v_i) \tag{33}$$

are anisotropic (in the second and third term in (33) we have the first derivatives only in one direction). In [3] Axelsson discusses the implications of this fact on the efficiency and robustness of the AMLI methods when applied as the local subproblem solvers. In order to alleviate the effect of anisotropy, a modified block diagonal preconditioning strategy is introduced, where the blocks correspond to the discrete Laplacian operator for the i-th displacement variable (only the first term in (33)). Note that the same approach is adopted in [33]. This approach leads to the preconditioner that is variable, i.e. it varies at each CG iteration, due to the dependence of the CG method of the initial residual (see [3]). In our approach we apply a standard AMG as a "black-box" solver to the entire local subproblems (33). We expect an efficient and robust performance of the AMG with respect to anisotropies and discontinuities along the interfaces between the different materials in the local subproblems, since the AMG automatically performs the coarsening in the directions in which the error varies smoothly (which also match the directions of strong connectivity). Secondly, operator-based interpolation guarantees that the discontinuities are properly treated (see e.g. the example in [38]). As a conclusion, we expect a good performance as long as the coefficient λ is not very large, i.e. the material under consideration is not incompressible. We remark that our idea is similar to the ideas of domain decomposition and multigrid based preconditioners for the solution of elliptic problems whose natural setting is the Hilbert space $H(\text{div})$ (see [2]).

4. CONVERGENCE ANALYSIS

In this section we are concerned with an analysis of the preconditioning strategy that is proposed in Section 3. To this end we give an estimate for the rate of convergence of a Krylov solver preconditioned by the parallel (block diagonal) SSC preconditioner in terms of the upper bounds for the ratio $\omega_{max}/\omega_{min}$ of a preconditioned discrete stress operator (25). This analysis resembles the approach outlined in [3],[4],[11]. Let us consider the following generalised eigenvalue problem: Find $\omega \in R$ such that

$$\mathcal{E}(u, v) = \omega \mathcal{M}(u, v) \quad \forall v \in V(\Omega), \tag{34}$$

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where $\mathcal{M}(u,v)$ is a bilinear form corresponding to the preconditioning matrix M. Constraining our analysis to the Ritz method, we can then estimate ω_{min} and ω_{max} from the extremal values of the *Rayleigh quotient* as

$$\omega_{min} = \inf_{V(\Omega)} \frac{\mathcal{E}(u)}{\mathcal{M}(u)} \qquad \text{and} \qquad \omega_{max} = \sup_{V(\Omega)} \frac{\mathcal{E}(u)}{\mathcal{M}(u)}, \tag{35}$$

where $\mathcal{E}(u) = \mathcal{E}(u,u)$ and $\mathcal{M}(u) = \mathcal{M}(u,u)$. It is also convenient to introduce a splitting of the energy bilinear form

$$\mathcal{E}(u,v) = \mathcal{D}(u,v) + \mathcal{L}(u,v) + \mathcal{U}(u,v) \tag{36}$$

where

$$\mathcal{D}(u,v) = \mu \sum_i (\nabla u_i, \nabla v_i) + (\lambda + \mu) \sum_i (\partial_i u_i, \partial_i v_i), \tag{37}$$

$$\mathcal{L}(u,v) = \mu \sum_{i>j} (\partial_i u_j, \partial_j v_i) + \lambda \sum_{i>j} (\partial_i u_i, \partial_j v_j), \tag{38}$$

$$\mathcal{U}(u,v) = \mu \sum_{i<j} (\partial_i u_j, \partial_j v_i) + \lambda \sum_{i<j} (\partial_i u_i, \partial_j v_j), \tag{39}$$

are the bilinear forms that correspond to the matrices D, L and U, respectively. Also, denote $\mathcal{D}(u) = \mathcal{D}(u,u)$, $\mathcal{L}(u) = \mathcal{L}(u,u) = \mathcal{U}(u,u) = \mathcal{U}(u)$. Let us introduce a component-wise decomposition of the the space of admissible displacements $V(\Omega)$

$$V(\Omega) = \sum_{i=1}^{3} V_i(\Omega). \tag{40}$$

and let $\mathcal{M}_i^{AMG}(u_i) = \mathcal{M}_i^{AMG}(u_i,u_i)$ denote a functional formulation of the subspace algebraic multigrid preconditioning. Then the parallel and the successive subspace correction preconditioning methods can be described as

$$\mathcal{M}_P(u) = \sum_{i=1}^{3} \mathcal{M}_i^{AMG}(u_i), \tag{41}$$

$$\mathcal{M}_S(u) = \mathcal{M}_P(u) + \mathcal{L}(u), \tag{42}$$

where the quadratic functionals $\mathcal{M}_P(u)$ and $\mathcal{M}_S(u)$ correspond to the preconditioning matrices M_P and M_S, respectively. Since

$$\mathcal{D}(u) = \sum_{i=1}^{3} \mathcal{E}(u_i) \tag{43}$$

the following estimate may be derived

$$\omega_0 \mathcal{D}(u) \leq \mathcal{M}_P(u) \leq \omega_1 \mathcal{D}(u), \tag{44}$$

where

$$\omega_0 = \min_{1\leq i\leq 3} \inf_{V_i(\Omega)} \frac{\mathcal{E}(u_i)}{\mathcal{M}_i^{AMG}(u_i)} \qquad \text{and} \qquad \omega_1 = \max_{1\leq i\leq 3} \sup_{V_i(\Omega)} \frac{\mathcal{E}(u_i)}{\mathcal{M}_i^{AMG}(u_i)}. \tag{45}$$

It follows from (45) that the values ω_0 and ω_1 describe quality of the local subproblems solver/preconditioner. It is obvious that if one employs a direct sparse solver in this context, then

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$\omega_0 = \omega_1 = 1$, however this choice does not give an algorithm that exhibits a (nearly) optimal scaling with the problem size (in fact, the asymptotic complexity of such an implementation will be asymptotically the same as the complexity of a direct sparse solver applied to the original problem (19)). Applying an incomplete LU factorisation (with no fill-ins) as a subspace solver will give an algorithm in which scaling per iteration is optimal. However, in the case of the ILU preconditioner, the values of ω_0 and ω_1 depend on the mesh parameter h. This causes a significant increase in the number of iteration steps in the Krylov iterative algorithm (see the example in Section 5 and the examples from [25]). On the other hand, applying the scalar AMG algorithm [36] for an approximate solution (or preconditioning) of the local subproblems closely fulfills the requirement of asymptotic optimality for a solution algorithm. Indeed, in the case when the AMG is applied to the solution of the local subproblems $\mathcal{E}(u_i)$, the ratio between ω_1 and ω_0 can be estimated as

$$\frac{\omega_1}{\omega_0} \sim C_{AMG}, \tag{46}$$

where C_{AMG} is a constant that is not dependent (or very loosely dependent) upon the mesh parameter h, providing that ν is not close to 0.5. Convergence analysis of the AMG V-cycle for various classes of matrices can be found in [37]. In [37],[38] the author analyses and compare various aspects of MG and AMG and stresses that the computational cost of the AMG solution phase (ignoring the set-up) should be comparable to the computational cost of a robust MG solver when applied to standard elliptic problems.

Consequently, we can formulate an estimate for the condition number $\kappa\left(M_P^{-1}A\right)$ as

$$\kappa\left(M_P^{-1}A\right) \le \frac{\omega_1}{\omega_0}\frac{C_1}{C_0}, \tag{47}$$

with

$$C_0 = \inf_{V(\Omega)} \frac{\mathcal{E}(u)}{\mathcal{D}(u)} \qquad \text{and} \qquad C_1 = \sup_{V(\Omega)} \frac{\mathcal{E}(u)}{\mathcal{D}(u)}. \tag{48}$$

Using previously described analysis, which is based on Rayleigh quotients, we are unable to find estimates for the ratio $\omega_{max}/\omega_{min}$ for the case of discrete stress operator preconditioned by the successive SSC method (32). However, from the experimental results outlined in Table II we can assume that a Krylov solver preconditioned by the successive SSC method should converge in fewer steps than its parallel SSC counterpart. The arithmetic complexity of the successive SSC algorithm (per iteration) is somewhat larger than that of the parallel SSC algorithm, which has an effect on the overall execution time. We shall illustrate this in more detail in Section 5 (see also [25]). In addition, if one considers parallelism in the successive and the parallel SSC algorithm, the parallel SSC version is favourable (being inherently parallel). However, we shall not discuss parallel implementation issues in this paper.

The parameters C_0 and C_1 introduced in (48) are directly defined by the component-wise space decomposition methodology. We now estimate their values. If we define the bilinear forms

$$\mathcal{Q}(u) = \sum_i (\nabla u_i, \nabla u_i) \tag{49}$$

and

$$\mathcal{T}(u) = \sum_i (\partial_i u_i, \partial_i u_i) \tag{50}$$

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it is obvious that

$$\mathcal{T}(u) \leq \mathcal{Q}(u). \tag{51}$$

Note further that $\mathcal{D}(u)$ can be expressed as

$$\mathcal{D}(u) = \mu\mathcal{Q}(u) + (\lambda + \mu)\mathcal{T}(u). \tag{52}$$

¿From (51) and (52) we have

$$\mathcal{D}(u) \leq (2\mu + \lambda)\,\mathcal{Q}(u). \tag{53}$$

Using the *Korn's inequality* [16]

$$\mathcal{Q}(u) \leq K_\Omega \mathcal{S}(u), \tag{54}$$

where $\mathcal{S}(u) = \mathcal{S}(u, u)$ and K_Ω is a positive constant depending only on the shape of the domain Ω, we have from (11) that

$$\mathcal{E}(u) \geq 2\mu\mathcal{S}(u). \tag{55}$$

Finally, from (53), (54) and (55) we have

$$C_0 = \frac{1}{K_\Omega}\frac{2\mu}{2\mu + \lambda}. \tag{56}$$

Taking into account an estimate from [16] that $K_\Omega \geq 4$ for all 3D domains (we consider here the case when there are no free rotations, see [3],[16] and a particular choice of the boundary conditions (2)–(3)), and, on the other hand, that for thin domains $K_\Omega \to \infty$, we can derive the following bounds for C_0

$$0 \leq C_0 \leq \frac{\mu}{2(2\mu + \lambda)}. \tag{57}$$

Estimates for the values of the Korn's constant for some special domains in 2D and 3D are summarised in [16]. For a particular non-trivial domain in 2D, one may give sharper estimates for the value of K_Ω in terms of the eigenvalues of the Dirichlet and the Neumann Laplacian. Alternatively, one can choose to embrace a domain between the two simple domains for which the eigenvalues of the Laplace operator are explicitly known (e.g. the square) and to give an estimate using the monotonicity argument.

In order to give an estimate for the value of C_1, we start from the inequalities

$$\sum_{i \neq j} (\partial_i u_i, \partial_j u_j) \leq \mathcal{T}(u), \tag{58}$$

and

$$\sum_{i \neq j} (\partial_i u_j, \partial_j u_i) \leq \mathcal{Q}(u) - \mathcal{T}(u), \tag{59}$$

which give

$$\frac{\mathcal{E}(u)}{\mathcal{D}(u)} \leq \frac{3\mu\mathcal{Q}(u) + 3\lambda\mathcal{T}(u)}{\mu\mathcal{Q}(u) + (\lambda + \mu)\mathcal{T}(u)}. \tag{60}$$

From (60) we can derive an estimate

$$C_1 = 3. \tag{61}$$

From (56) and (61) it follows that the condition number estimate (47) is given by

$$\kappa(M_P^{-1}A) \leq \frac{K_\Omega(2\mu + \lambda)}{\mu} \tag{62}$$

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assuming that no approximation in the local subproblems is used (i.e. $\omega_0 = \omega_1 = 1$). Having in mind (5), the estimate (62) reduces to

$$\kappa(M_P^{-1}A) \leq K_\Omega \frac{2-2\nu}{1-2\nu}. \qquad (63)$$

This estimate can also be found in [3]. If we compare the estimate (63) with the one from [33], we can conclude that for the values $\nu \leq 1/3$ the approach to take only an elliptic part in (33) as a preconditioner gives slightly lower bound for the condition number (although the values from [33] and (63) are comparable and small in magnitude). For $\nu > 1/3$ a bound (63) is lower than the one from [33]. This can be explained by the fact that in [33] the author takes the approximation of the functional (33), while in our approach the whole functional is taken into consideration. When ν is sufficiently close to 0.5, the second term in (33) becomes dominant, and the approximation from [33] becomes less efficient.

Both condition number estimates (63) and from [33] reveal two potential situations when the effectiveness of the suggested block diagonal preconditioners can be diminished, as the condition number of a preconditioned operator tends to infinity. The first case is when the value of Korn's constant deteriorates to infinity. This happens in the case of 3D domains that are referred to as "thin", i.e. for which the dimension in one coordinate direction is much less than in the other two (the examples in 3D being plates and shells of a finite thickness t), providing that we have a case of non-homogeneous Dirichlet (or some more general) boundary conditions. As noted in [29], the poor coercivness of such problems, that is given by the classic Korn inequality [22], gives rise to slow convergence for iterative methods. In fact, the upper bound of the spectrum of a preconditioned discrete elasticity operator is limited by a constant, while the lower bound deteriorates to 0 as $O(t^2)$. Many authors have addressed this problem for particular domains (see [29] and the references contained therein). However, the recent work of Ovtchinnikov and Xanthis [29],[30],[31],[32] offers a general framework for dealing with this problem by suggesting a concept of a new Korn type inequality in subspaces. This concept, together with the EDRA algorithm, described in [28], provide a powerful methodology for the solution of elasticity problems for thin domains.

The second case, when the preconditioning strategy introduced in [33] and this paper can deteriorate, is when the Poisson ratio ν tends to the limit 0.5. This is the case of an isotropic linear elasticity problem of incompressible media, in which all motions preserve the volumes locally (that is, each small portion of the medium has the same volume as before the deformation, see [18]). In this case a more sophisticated formulation of the problem and discretisation techniques that are locking-free should be applied, rather than a straightforward application of the block AMG preconditioning (see [3],[18],[24]).

5. CASE STUDY

A component decomposition preconditioning methodology based on AMG is practically tested on a stress analysis problem that arises in microfabrication technology. One of the principal sources of stress fields in microfabrication technology is a mismatch between thermal expansion coefficients of different material layers [17].

As a practical model problem, we consider here a 3D structure consisting of two material layers: bulk silicon with a trench filled by oxide. The geometry and a typical grid structure for the selected test example are shown in Figure 1.

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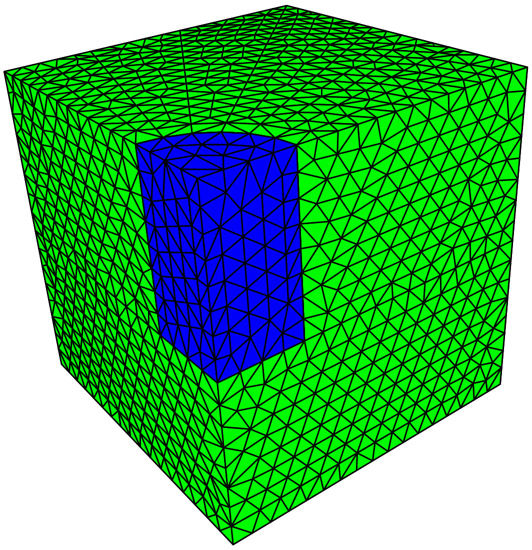

Figure 1. Material distribution and 3D grid structure with 5425 nodes

The discretization is performed using piecewise linear finite elements based on unstructured grids that are created by the grid generation software GEOMPACK [20]. Using GEOMPACK, grids of different sizes are independently generated. The Krylov iterative solvers that we have employed are Generalised Minimal Residual (GMRES) [35] and BiConjugate Gradient Stabilised (BCGS) [34] as provided by the PETSc library [8]. In [3] the author applies preconditioned CG method to solve discrete elasticity problems. This approach is justifiable in the case of Dirichlet boundary conditions, as both the coefficient matrix and the block-diagonal preconditioner are symmetric. Here we are studying a more general case of boundary conditions which gives rise to non-symmetric coefficient matrices. Moreover, our successive SSC preconditioner is non-symmetric. Our intention is to suggest a robust "black-box" solver for elasticity problems in microfabrication technology (which can potentially applied to elasticity problems in other areas). Therefore, robustness and wide applicability are our major motives behind adopting non-symmetric versions of Krylov solvers. The well established and publicly available code AMG1R5 [36] has been used as a scalar AMG solver. The approximate AMG solving procedure consists of 1 V(1,1) multigrid cycle. The component-wise AMG preconditioner, implemented in both parallel (AMG-P) and successive (AMG-S) versions, has been compared with the standard incomplete LU (ILU) preconditioner [19] from PETSc library.

Figure 2 gives convergence history for various Krylov solvers and various preconditioners for one particular discretisation that is presented in Figure 1 and consists of 5425 nodes. The Krylov solvers preconditioned by the AMG converge rapidly in a monotonic fashion, while the ILU preconditioned solvers exhibit much slower and less smooth convergence characteristics.

Table I presents convergence results for various sizes of the discrete problem. The results are given in terms of iteration counts needed for the two Krylov solvers (with various preconditioners) to reduce the initial ℓ_2 residual norm by the factor 10^{-10}. Note that the imposed tolerance is much higher than usually required by industrial applications (and that is needed from the point of view of discretisation errors). However in this way we demonstrate that our algorithm will perform in a robust manner and is

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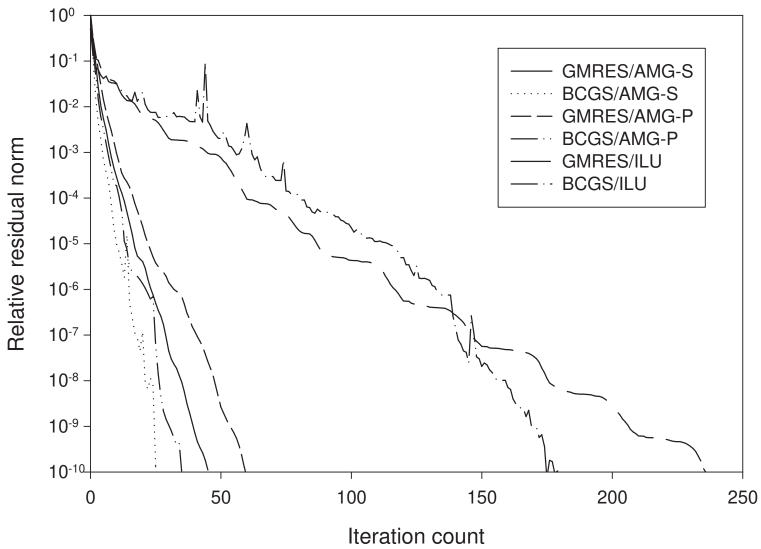

Figure 2. Convergence history for the case $N = 5425$ (16275 equations)

capable of accommodating various severe demands imposed by potential users from microfabrication technology. We would like to point the difference between the number of iteration steps for the 3D case reported in Table I and those for 2D problems reported in [25]. Larger number of iteration steps in 3D when the code AMG1R5 is used as the AMG solver is due to the fact that the AMG interpolation is realised as a compromise between the direct and the standard interpolation [38]. In complex 3D examples this approach generates excessive amount of fill-ins towards coarser levels. The more sophisticated code RAMG05 [37] can resolve this difficulty (see numerical examples in [38]).

Table I. Iteration counts for the 3D problem.

$3N$	GMRES/ AMG-S	BCGS/ AMG-S	GMRES/ AMG-P	BCGS/ AMG-P	GMRES/ ILU	BCGS/ ILU
16275	45	26	60	35	251	180
27120	53	26	68	35	1290	324
53412	55	28	77	36	8472	1404

The iteration counts for the AMG preconditioning are virtually independent of the problem size for the BCGS method, whilst in our example GMRES iteration counts slowly increase with the problem size. We hypothesise, however, that this number tends to a constant in the limit. This behaviour can be explained by the fact that the ratios $\omega_{max}/\omega_{min}$ of the preconditioned matrices $\mathbf{M}_P^{-1}\mathbf{A}$ and $\mathbf{M}_S^{-1}\mathbf{A}$ can be bounded independently of the problem size. Spectral bounds, however, depend upon the domain geometry.

For the illustration purposes we give spectral results that are obtained for 4 different discretisations

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of the problem presented in Fig. 1. We compute the spectrum using the NAG routine F02BJF [26]. The results are summarised in Table II. In the table, n denotes the total number of degrees of freedom.

Table II. Ratios $\omega_{max}/\omega_{min}$ for A, $M_P^{-1}A$ and $M_S^{-1}A$ as a function of the problem size.

n	A	$M_P^{-1}A$	$M_S^{-1}A$
426	$1.677 \cdot 10^6$	4.259	1.499
915	$3.327 \cdot 10^6$	4.592	1.554
1833	$5.546 \cdot 10^6$	4.742	1.597
3696	$1.029 \cdot 10^7$	4.864	1.613

In all cases we assume an exact factorisation of the local subproblems ($\omega_0 = \omega_1 = 1$). In order to put these spectral results into the context of an AMG approximation of the local subproblems, one has to take into the consideration the formula (46). From Table II it is obvious that, although $\omega_{max}/\omega_{min}(A) \sim O(h^{-2})$, the same quantities for preconditioned discrete operators $M_P^{-1}A$ and $M_S^{-1}A$ remain small and bounded as the mesh is refined.

Finally, Table III presents the total wall clock time in seconds for the preconditioned Krylov solvers for various problem sizes. All our numerical experiments are carried out on a single processor HP 9000/782 architecture. It should be emphasised that the AMG setup times and ILU factorisation time are also included in the execution times. Notice that for the smaller problems, ILU preconditioned iterative methods are the fastest. However, component-wise AMG preconditioned Krylov methods become faster than the ILU methods for sufficiently large discrete problems.

Table III. Execution times for the 3D problem.

$3N$	GMRES/ AMG-S	BCGS/ AMG-S	GMRES/ AMG-P	BCGS/ AMG-P	GMRES/ ILU	BCGS/ ILU
16275	17.91	18.47	21.72	22.99	17.81	21.08
27120	37.67	40.96	45.18	43.78	156.29	62.29
53412	92.75	89.39	116.40	111.88	2079.37	552.65

It can be concluded from Tables I and III that the AMG preconditioned Krylov solvers scale nearly linearly with problem size and are faster than their ILU preconditioned counterparts. In all numerical experiments the successive implementation of the component-wise AMG preconditioning is superior to the corresponding parallel version. It should be emphasised that the obtained results compare favourably, both in terms of the execution time and the memory requirements, with direct sparse solvers provided in the PETSc library (although, for clarity of presentation, we did not include these comparisons here). This makes the method that we propose a suitable choice for the class of problems under consideration in this paper.

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6. DISCUSSION

In this paper we present a preconditioned iterative algorithm for the solution of discrete problems in linear elasticity. We analyse the preconditioned strategy that is a special case of the global SSC concept suggested in [39]. Space decomposition in our case is based on decoupling different Cartesian components of a displacement vector. This idea was analysed in the context of linear elasticity in [3]. In this paper we suggest an alternative way of solving/preconditioning the local subspace problems using the standard scalar algebraic multigrid (AMG) solver [36]. Subspace correction is performed either in block diagonal or lower triangular fashion. Spectral analysis of a block diagonal preconditioner (similar to those in [3],[11]) reveals that the preconditioned discrete elasticity operator has a spectrum independent on the discretisation parameter h. The algorithm that we suggest was tested extensively on problems from microfabrication technology and exhibited a robust performance. Despite testing our methodology on problems from one particular application, we believe that it represents a suitable alternative for the solution of a wide class of stress analysis problems on complex geometries with multi-layer material properties, and that robust performance observed in our experiments would extend to elasticity problems arising in other areas (subject to the domain shape and compressibility restrictions outlined in the paper).

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