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Algebraic multigrid based on computational molecules, 2: Systems of elliptic partial differential equations

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Abstract

This paper deals with a new approach in algebraic multigrid (AMG) for self-adjoint and elliptic problems arising from finite-element (FE) discretization of systems of partial differential equations (PDEs).

Generalizing our approach for scalar problems [15], we propose an edge matrix concept regarding systems of PDEs. This gives a simple and reliable method for the evaluation of the strength of nodal dependence that can be applied to symmetric positive definite non-M matrices.

In the case of linear elasticity (2D as well as 3D problems) we consider approximate splittings of element matrices into symmetric positive semidefinite (SPSD) edge matrices of rank one. The reproduction of edge matrices on coarse levels offers the opportunity to combine classical coarsening techniques with robust (energy minimizing) interpolation schemes: the "computational molecules" involved in this process are assembled from edge matrices and thus allow for an efficient treatment of anisotropic problems as well. This yields a flexible new variant of AMG.

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Key words: edge matrices, algebraic multigrid, element preconditioning

1 Introduction

Algebraic multigrid (AMG) methods [4, 5, 17, 18] have become quite popular for the iterative solution of large sparse systems of linear algebraic equations. Mainly, this is due to their robust performance on various types of problems [2, 9, 10] achieving (geometric) multigrid-like convergence rates [11, 19].

The algorithm for the classical AMG method, originally proposed in [5], has been described in [17] almost 20 years ago. In the last couple of years various new AMG methods came up, most of which have been designed for

special applications. Especially, two classes of methods, namely AMG using element interpolation (AMGe) [6, 13, 14] and AMG based on smoothed aggregation [20, 21], considerably enhanced the range of applicability of classical AMG [17]. Whereas smoothed aggregation methods (applied to discretizations of elliptic problems) typically assume the knowledge of the near-nullspace that has to be preserved by the interpolation, AMGe methods capture this information implicitely by accessing the individual element stiffness matrices. Recent works on adaptive smoothed aggregation [7] and adaptive algebraic multigrid [8] try to remove the need of any assumptions on *algebraically smooth* error but, instead, use the method itself to determine near-nullspace components and adjust the coarsening process accordingly.

Our approach originates in so-called element preconditioning techniques first introduced in [12, 16]. The computation of edge matrices has already been considered in [15] for scalar problems. In the present paper we generalize this concept and describe its utilization in building efficient AMG preconditioners for problems arising in solid (or structural) mechanics. However, the general methodology, we propose, is not limited to linear elasticity equations at all.

Let us consider the following kind of large-scale sparse matrix problems: For a given vector $\mathbf{b} \in \mathrm{R}^N$ we seek the solution $\mathbf{x} \in \mathrm{R}^N$ to the linear system

$$A\mathbf{x} = \mathbf{b} \tag{1}$$

where $A \in \mathrm{R}^{N \times N}$ is a real, symmetric and positive definite (SPD) $N \times N$ matrix. In this presentation we focus on the case in which A and $\mathbf{b}$ stem from finite-element (FE) discretization of a boundary-value problem governed by a coupled system of second-order elliptic partial differential equations (PDEs). Additionally, we assume that the individual element (stiffness) matrices–without any essential boundary conditions imposed on them–are available. At the stage of global assembling this (additional) information can be retrieved with most of the common FE packages.

The primary objective of this paper is to present a new variant of algebraic multigrid for the solution of (1): A new definition of "strong" and "weak connections" (edges) provides the basis for adaptive and flexible coarsening. Local interpolation is desired to minimize the energy associated with so-called "computational molecules".[1]

Our approach lies in-between classical AMG–"strong" and "weak edges" affect the coarsening and formation of "interpolation molecules"–and AMGe–small-sized local matrices are used in order to compute the actual interpolation coefficients. The general goal is to achieve the improved robustness of AMGe-type methods at lower computational costs and storage requirements, which is mainly achieved by avoiding element agglomeration techniques. By

[1] We therefore refer to this method as algebraic multigrid based on computational molecules (AMGm).

balancing the computational costs of the set-up and the solution phase properly, the resulting method should also allow for a fast solution of *single right hand side systems*.

The remainder of the paper is organized as follows: In Section 2 we formulate the linear elasticity problem, which will serve for the presentation of the edge-matrix concept in Section 3. The major innovative aspects resulting in the proposed AMGm method are discussed in Section 4. In Section 5, we present numerical results for 2D and 3D elasticity problems using first-oder FE schemes. In the concluding remarks (in Section 6) we comment on an "element-free" version of AMGm for elasticity problems that is under current investigation.

2 The linear elasticity problem

Let Ω be a bounded open subset of R^d, $d = 2$ or $d = 3$, which is associated with the reference configuration of an elastic body. It is well known from linear elasticity theory (see, e.g., [3]) that the governing equations describing the deformation of the body under the influence of applied forces (taking into account only first order terms in the displacement $\mathbf{u}$) are given by

$$-\mathrm{div}\,\boldsymbol{\sigma} = \mathbf{f} \quad \text{in } \Omega, \tag{2}$$

$$\mathbf{u} = \mathbf{0} \quad \text{on } \Gamma_0, \tag{3}$$

$$\sum_{j=1}^{d} \sigma_{ij}\, n_j = g_i \quad \text{on } \Gamma_1, \quad 1 \le i \le d, \tag{4}$$

where $\boldsymbol{\sigma}$ denotes the stress tensor, $\mathbf{f}$ the body force, $\mathbf{u}$ the displacement field, and $\mathbf{n}$ is the outwards pointing unit normal vector on Γ_1. Writing stress and strain in vector form, i.e., $\boldsymbol{\sigma} = (\sigma_{11}, \sigma_{22}, \sigma_{12})^t$, $\boldsymbol{\varepsilon} = (\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{12})^t$ in the 2D model, and $\boldsymbol{\sigma} = (\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{12}, \sigma_{13}, \sigma_{23})^t$, $\boldsymbol{\varepsilon} = (\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, \varepsilon_{12}, \varepsilon_{13}, \varepsilon_{23})^t$ in the 3D model, the stress-strain relation (for St. Venant-Kirchhoff materials) is given by Hooke's law, i.e., $\boldsymbol{\sigma} = C \cdot \boldsymbol{\varepsilon}$, where $C{:=}\, C_{\mathrm{2D}}$ and $C{:=}\, C_{\mathrm{3D}}$ in two respectively three space dimensions (2D respectively 3D model):

$$C_{\mathrm{2D}}{:=} \frac{E}{(1+\nu)(1-2\nu)} \begin{pmatrix} 1-\nu & \nu & 0 \\ \nu & 1-\nu & 0 \\ 0 & 0 & \frac{1-2\nu}{2} \end{pmatrix},$$

$$C_{\mathrm{3D}}{:=} \frac{E}{(1+\nu)(1-2\nu)} \begin{pmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} \end{pmatrix}.$$

Here E denotes the modulus of elasticity and ν is the Poisson ratio. Introducing the share modulus of the material $\mu := E/[2(1+\nu)]$ and the Lamé constant $\lambda := (E\nu)/[(1+\nu)(1-2\nu)]$, equation (2) yields the classical Lamé differential equation

$$-2\,\mu\,\mathrm{div}\,\boldsymbol{\varepsilon} - \lambda\,\mathrm{grad}\,\mathrm{div}\,\mathbf{u} = \mathbf{f} \tag{5}$$

for the displacements u_i, $1 \le i \le d$.

Moreover, if we make use of the symmetric gradient $\nabla^{(s)}\mathbf{u} := \boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}(\mathbf{u})$,

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right),$$

the variational (weak) formulation of the boundary-value problem (2)–(4) is the following:

Find $\mathbf{u} \in V = V(\Omega) := \{\mathbf{v} \in [H^1(\Omega)]^d; \mathbf{v} = \mathbf{0} \text{ on } \Gamma_0\}$ such that

$$a(\mathbf{u},\mathbf{v}) = L(\mathbf{v}) \quad \forall \mathbf{v} \in V \tag{6}$$

where

$$a(\mathbf{u},\mathbf{v}) := 2\,\mu\,(\nabla^{(s)}\mathbf{u}, \nabla^{(s)}\mathbf{v}) + \lambda\,(\mathrm{div}\,\mathbf{u}, \mathrm{div}\,\mathbf{v}) \tag{7}$$

$$L(\mathbf{v}) := (\mathbf{f},\mathbf{v}) - \int_{\Gamma_1} \mathbf{g}^t\,\mathbf{v}\,d\Gamma_1 \tag{8}$$

and $\mathbf{f} \in [L_2(\Omega)]^d$, $\mathbf{g} \in [L_2(\Omega)]^d$, $d = 2$ or $d = 3$.

For finite element discretization we consider a triangulation $\mathcal{T} = \{T\}$ of the two- or three-dimensional domain Ω for which we make the usual assumptions. Mainly for the sake of a simple presentation of the proposed method we restrict considerations to first order finite-element schemes here. That is, we define the space V_h of piecewise linear (vector-valued) continuous functions by

$$V_h := \{\mathbf{v}_h = (v_1, v_2, v_3) \in [C^0(\bar{\Omega})]^3 : v_i|_T \in P_1(T),\ 1 \le i \le d,\ \forall T \in \mathcal{T}\} \tag{9}$$

and focus on linear systems (1) that stem from the following FE problem to which we will refer to as the 3D (or 2D) linear Elasticity Problem throughout this paper:

Problem 1 *Find $\mathbf{u}_h \in V_h$ defined by (9) such that*

$$a(\mathbf{u}_h,\mathbf{v}_h) = L(\mathbf{v}_h) \quad \forall \mathbf{v}_h \in V_h \tag{10}$$

where the bilinear form $a(\cdot,\cdot)$ and the linear form $L(\cdot)$ are defined by (7)-(8).

3 The edge matrix concept in linear elasticity

In this section, let $\mathcal{A} = \{A_T : T \in \mathcal{T}\}$ denote the set of element matrices arising from the 3D (2D) Elasticity Problem 1 where $\mathcal{T}$ is a triangulation of a 3D (2D) domain Ω. We note that the following lemma holds:

Lemma 3.1 *(Null space of element matrices) For any triangulation of a 3D domain Ω the element stiffness matrices A_T arising from the Elasticity Problem 1 are SPSD. Moreover, if (x_i, y_i, z_i), $i \in \{1, 2, 3, 4\}$ are the coordinates of the vertices of a non-degenerated tetraeder T then the null space of A_T has dimension six and is given by*

$$\begin{aligned}\ker(A_T) = \text{Span} \quad \{ & (1,0,0,1,0,0,1,0,0,1,0,0)^t, \\ & (0,1,0,0,1,0,0,1,0,0,1,0)^t, \\ & (0,0,1,0,0,1,0,0,1,0,0,1)^t, \\ & (y_1,-x_1,0,y_2,-x_2,0,y_3,-x_3,0,y_4,-x_4,0)^t, \\ & (z_1,0,-x_1,z_2,0,-x_2,z_3,0,-x_3,z_4,0,-x_4)^t, \\ & (0,z_1,-y_1,0,z_2,-y_2,0,z_3,-y_3,0,z_4,-y_4)^t\}.\end{aligned}$$

Proof. From the weak formulation of the Elasticity Problem 1 it follows that all the A_T's are SPSD. Moreover, it can easily be seen that there are positive constants c_1 and c_2 such that the following inequalities hold:

$$c_1\,\zeta(\boldsymbol{w}, \boldsymbol{w}) \leq \mathbf{w}^t A_T \mathbf{w} \leq c_2\,\zeta(\boldsymbol{w}, \boldsymbol{w}). \tag{11}$$

The linear function $\boldsymbol{w}$ on any element T is determined by the vector $\mathbf{w}$ and the function $\zeta(\cdot, \cdot)$ in (11) is defined by

$$\begin{aligned}\zeta(\boldsymbol{w}, \boldsymbol{w}) \;\coloneqq\; & \int_T \left[\left(\frac{\partial w_1}{\partial x}\right)^2 + \left(\frac{\partial w_2}{\partial y}\right)^2 + \left(\frac{\partial w_3}{\partial z}\right)^2 + \left(\frac{\partial w_1}{\partial y} + \frac{\partial w_2}{\partial x}\right)^2 \right. \\ & + \left. \left(\frac{\partial w_1}{\partial z} + \frac{\partial w_3}{\partial x}\right)^2 + \left(\frac{\partial w_2}{\partial z} + \frac{\partial w_3}{\partial y}\right)^2 \right] dT.\end{aligned}$$

Thus (for linaer $\boldsymbol{w}$) we get $A_T\mathbf{w} = 0$ if and only if

$$\boldsymbol{w} = (a_1 + by + cz, a_2 - bx + dz, a_3 - cx - dy)^t$$

for some vector $\mathbf{a} = (a_1, a_2, a_3, b, c, d)^t$. By choosing $\mathbf{a} = \mathbf{e}_i, 1 \leq i \leq 6$, and inserting the coordinates of the vertices of the tetraeder one obtains the desired basis for $\ker(A_T)$. ∎

Remark 3.1 *For the 2D Elasticity Problem a similar result holds. Here the element matrices have a three-dimensional kernel which is given by*

$$\begin{aligned}\ker(A_T) = \text{Span} \quad \{ & (1,0,1,0,1,0)^t, \\ & (0,1,0,1,0,1)^t, \\ & (y_1,-x_1,y_2,-x_2,y_3,-x_3)^t\}.\end{aligned}$$

Let A_T be an $(nd) \times (nd)$ SPSD element matrix where n denotes the number of nodes ($n = 3, 4$) of the element T, each of which accumulate d dofs ($d = 2, 3$ for 2D, 3D elasticity). Further, let e_{ij} denote the edge connecting nodes i and j, $1 \leq i < j \leq n$, and $\mathcal{E}_T = \{e_{ij} : i < j; i, j \in T\}$ the set of edges of the element T.

Definition 3.1 *(Edge matrix) An $(nd)\times(nd)$ matrix $E = E_{ij}$ whose entries are zero except for the $(2d)\times(2d)$ entries corresponding to nodes i, j is called an edge matrix.*

One can ask for the class of SPSD element matrices A_T that can be split exactly (disassembled) into SPSD edge matrices, i.e., for a characterization of SPSD matrices that allow for a *semipositive splitting*. For the scalar case $d = 1$ one can prove the following result, see Reference [15].

Theorem 3.1 *A symmetric (element) matrix A_T has a representation*

$$A_T = \sum_{e_{ij} \in \mathcal{E}_T} E_{ij} \tag{12}$$

with E_{ij} being SPSD ($E_{ij} \geq 0$) if and only if the L-ation of A_T is SPSD.

The L-ation B_T of a matrix A_T is the matrix that results by reversing the sign of all its positive off-diagonal entries.

Remark 3.2 *An immediate consequence of Theorem (3.1) is that an SPSD matrix $A_T = (a_{ij})_{i,j}$ with zero row sums has an exact semipositive splitting if and only if it is a singular M-matrix.*[2]

However, in case an exact semipositive splitting of A_T into edge matrices does not exist (the case of non-M matrices), one can relax the problem and admit general edge matrices. Alternatively, instead of requiring the exact splitting (12), let us consider the following Problem 2.

Problem 2 *Find a set of edge matrices $\mathcal{B}_T = \{E_{ij} : e_{ij} \in \mathcal{E}_T\}$ providing an approximate splitting*

$$A_T = B_T + R_T = \sum_{e_{ij} \in \mathcal{E}_T} E_{ij} + R_T \tag{13}$$

that minimizes the general condition number $\kappa_T = \kappa(A_T, B_T) := \frac{\lambda_{\max}}{\lambda_{\min}} \to \min$ subject to $E_{ij} \geq 0 \quad \forall e_{ij} \in \mathcal{E}_T$ where

$$\lambda_{\max} := \inf \{\lambda : \mathbf{x}^T A_T \mathbf{x} \leq \lambda \mathbf{x}^T B_T \mathbf{x} \quad \forall \mathbf{x}\} \tag{14}$$

$$\lambda_{\min} := \sup\{\lambda : \mathbf{x}^T A_T \mathbf{x} \geq \lambda \mathbf{x}^T B_T \mathbf{x} \quad \forall \mathbf{x}\}. \tag{15}$$

[2] According to Reference [1] a symmetric matrix C that has nonpositive offdiagonal entries is an M-matrix if and only if it is nonnegative definite.

Dealing with scalar second-order elliptic PDEs the individual element (stiffness) matrices throughout have a one-dimensional kernel (spanned by the constant vector $(1, 1, \ldots, 1)^T$). Thence, the solution of the constrained minimization Problem 2:(13)–(15) results in the *best approximation* of A_T by a singular M-matrix B_T in the sense of minimizing its (general) spectral condition number. From this viewpoint the above problem has already been considered in References [12, 16]. Symbolic methods can be used to speed up the (numerical) solution of this kind of (local) low-dimensional optimization problems (for $n = 3, 4$ and $d = 1$) [16]. The (global) M-matrix B, assembled from the B_T's, can serve as an approximation of A, and, in order to build a preconditioner, one can apply (classical) AMG to B instead of A [12].

Regarding (coupled) systems of second-order elliptic PDEs, e.g., the linear elasticity system (2)–(4), no symbolic solutions of Problem (P1) are available so far. Of course, one could easily solve this small-sized optimization problem numerically for every elemet matrix in $\mathcal{A} = \{A_T : T \in \mathcal{T}\}$. However, as a basis for constructing efficient AMG methods the set-up costs can be reduced significantly by using approximate splittings that in fact result in a larger condition number $\kappa_T = \kappa(A_T, B_T) < \infty$ but can be computed much faster.

The rest of this section is devoted to the characterization and construction of such approximate splittings. First we note that SPSD edge matrices always preserve the kernel of the element matrices.

Lemma 3.2 *(Kernel preservation) Let $\mathcal{B}_T = \{E_{ij} : E_{ij} \geq 0; e_{ij} \in \mathcal{E}_T\}$ be a set of SPSD edge matrices and $B_T := \sum_{E_{ij} \in \mathcal{B}_T} E_{ij}$ the corresponding splitting of an SPSD element matrix A_T such that $\kappa_T = \kappa(A_T, B_T) < \infty$. Then $\mathcal{B}_T$ is kernel preserving, i.e., $E\mathbf{v} = \mathbf{0} \quad \forall E \in \mathcal{B}_T \; \forall \mathbf{v} \in \ker(A_T)$.*

Proof. The case $A_T = 0$ is trivial. Further, if $A_T \neq 0$ it follows that $0 < \lambda_{\min} \leq \lambda_{\max} < \infty$. Assuming that there is an edge matrix $E \in \mathcal{B}_T$ and a vector $\mathbf{v} \in \ker(A_T)$ such that $E\mathbf{v} \neq \mathbf{0}$, and thence $\mathbf{v}^t E\mathbf{v} = c > 0$, one concludes $0 = \mathbf{v}^t A_T \mathbf{v} \geq \lambda_{\min} \mathbf{v}^t B_T \mathbf{v} \geq \lambda_{\min} \mathbf{v}^t E\mathbf{v} \geq \lambda_{\min} c > 0$ which contradicts $\lambda_{\min} > 0$. □

It is clear then that any solution $\mathcal{B}_T^\star = \{E_{ij}^\star\}$ of the Optimization Problem 2 is kernel preserving as well. The following lemma on the representation of rank-one matrices will help to characterize the approximate splittings of elasticity element matrices:

Lemma 3.3 *(Representation of rank-one matrices) Let E be a symmetric $k \times k$ matrix ($k = nd$ for edge matrices) and $\dim(\ker(E)) = k - 1$. Then for any vector $\mathbf{v} \in \mathrm{R}^k$, $\mathbf{v} \neq \mathbf{0}$, in the orthogonal complement of $\ker(E)$, i.e., $\langle \mathbf{v}, \mathbf{w} \rangle = 0 \quad \forall \mathbf{w} \in \ker(E)$, there is a constant $c \neq 0$ such that $E = c \cdot \mathbf{v}\,\mathbf{v}^t$.*

Proof. W.l.o.g. we may assume that $\|\mathbf{v}\| = 1$. Let $\{\mathbf{w}_2, \mathbf{w}_3, \ldots, \mathbf{w}_k\}$ be an orthonormal basis of $\ker(E)$ and $\mathbf{w}_1 := \mathbf{v}$.

Then there exists a $k\times k$ matrix $F = (f_{ij})_{i,j=1}^{k}$ s.t. $E = W\,F\,W^t$ and $W = (\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_k)$. Now, since

$$\mathbf{w}_i^t E \mathbf{w}_j = \mathbf{w}_i^t W\,F\,W^t \mathbf{w}_j = \mathbf{e}_i^t F \mathbf{e}_j = f_{ij} = 0$$

for all $i \neq j$ and $2 \leq i = j \leq k$ we have $F = c \cdot \mathbf{e}_1\mathbf{e}_1^t$, $c \neq 0$, and thus $E = c \cdot W\mathbf{e}_1\mathbf{e}_1^t W^t = c \cdot \mathbf{v}\,\mathbf{v}^t$. ∎

Theorem 3.2 *(Characterization of semipositive splittings) Let A_T be an SPSD element matrix arising from (first order) FE discretization of the 3D Elasticity Problem 1. Further, let $\mathcal{B}_T = \{E_{ij} \geq 0;\, 1 \leq i < j \leq 4\}$ be a set of SPSD edge matrices providing the splitting $B_T = \sum_{E_{ij}\in\mathcal{B}_T} E_{ij}$.*
Then $\kappa_T = \kappa(A_T, B_T) < \infty$ if and only if the $(2d)\times(2d)$ matrices E'_{ij} associated with the edge matrices E_{ij} (edges e_{ij}) have the form $E'_{ij} = c_{ij} \cdot \mathbf{v}_{ij}\,\mathbf{v}_{ij}^t$,

where $c_{ij} > 0$, $\mathbf{v}_{ij} = \begin{pmatrix} \pm\mathbf{v}'_{ij} \\ \mp\mathbf{v}'_{ij} \end{pmatrix}$, $\mathbf{v}'_{ij} = \begin{pmatrix} x_j - x_i \\ y_j - y_i \\ z_j - z_i \end{pmatrix}$ $\forall 1 \leq i < j \leq 4$,

and (x_k, y_k, z_k), $1 \leq k \leq 4$, are the vertices of the tetrahedron T.

Proof. Let $\kappa_T = \kappa(A_T, B_T) < \infty$. W.l.o.g. let us consider E_{12}. From Lemma 3.2 we have that $\mathcal{B}_T$ is kernel preserving. Thus Lemma 3.1 shows that $\ker(E'_{12})$ must contain the space

$$\begin{aligned} S &= \mathrm{Span}\{\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3, \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3\} \\ &\coloneqq \mathrm{Span}\{(1,0,0,1,0,0)^t, (0,1,0,0,1,0)^t, (0,0,1,0,0,1)^t, \\ &\quad (y_1, -x_1, 0, y_2, -x_2, 0)^t, (z_1, 0, -x_1, z_2, 0, -x_2)^t, \\ &\quad (0, z_1, -y_1, 0, z_2, -y_2)^t\}. \end{aligned} \tag{16}$$

For $(x_1, y_1, z_1) \neq (x_2, y_2, z_2)$ the dimension of S is 5 and thus $\dim(\ker(E'_{12}))$ is at least 5. Because E'_{12} is SPSD, Lemma 3.3 yields the representation $E'_{12} = c_{12}\mathbf{v}_{12}\,\mathbf{v}_{12}^t$, $c_{12} \geq 0$; $c_{12} = 0$ if and only if $\dim(\ker(E'_{12})) = 6$.

Moreover, the equations $E'_{12}\mathbf{t}_k = \mathbf{0}$ and $E'_{12}\mathbf{r}_k = \mathbf{0}$ for $k \in \{1,2,3\}$ imply $\mathbf{v}_{12} = \begin{pmatrix} \pm\mathbf{v}'_{12} \\ \mp\mathbf{v}'_{12} \end{pmatrix}$ and $\mathbf{v}'_{12} = c \cdot \begin{pmatrix} x_2 - x_1 \\ y_2 - y_1 \\ z_2 - z_1 \end{pmatrix}$, respectively.

Next we note that $\kappa(A_T, B_T) < \infty$ is equivalent to $\ker(A_T) = \ker(B_T)$. Assuming that one of the c_{ij}'s is zero, e.g., $c_{12} = 0$, we conclude, e.g.,

$$\begin{aligned} \ker(B_T) &= \ker(E_{13}) \cap \ker(E_{14}) \cap \ker(E_{23}) \cap \ker(E_{24}) \cap \ker(E_{34}) \\ &= \{\mathbf{v} \in \mathrm{R}^{12} :\, \mathbf{v} \perp \mathbf{w}_{13} \wedge \ldots \wedge \mathbf{v} \perp \mathbf{w}_{34}\} \end{aligned}$$

for some $\mathbf{w}_{13}, \ldots, \mathbf{w}_{34}$ and thus $\dim(\ker(B_T)) \geq 7 > \dim(\ker(A_T)) = 6$.

On the other hand it can easily be shown that if $c_{ij} > 0 \; \forall 1 \leq i < j \leq 4$ and $B_T := \sum_{E_{ij} \in \mathcal{B}_T} E_{ij}$ where E_{ij} is induced by

$$E'_{ij} = c_{ij} \cdot \begin{pmatrix} \pm \mathbf{v}'_{ij} \\ \mp \mathbf{v}'_{ij} \end{pmatrix} \begin{pmatrix} \pm \mathbf{v}'_{ij} \\ \mp \mathbf{v}'_{ij} \end{pmatrix}^t$$

then $\ker(A_T) = \ker(B_T)$. □

For the construction of edge matrices (from element matrices) different techniques can be used; we describe only one specific approach here: Let A_T be an arbitrary $(nd)\times(nd)$ SPSD element matrix arising from the 3D Elasticity Problem ($n = 4$ and $d = 3$) and let $e = e_{ij} := \{i, j\} \subset T$ be any edge of the element T. Further, let $\{k_1, k_2\} \subset T$ denote the opposite edge of e, i.e., $\{k_1, k_2\} \cap e = \emptyset$. An edge matrix for edge e can be computed using the following algorithm:

Algorithm 3.1 *(Computing (gen.) local Schur complements)*

1. *assign the local node numbers* $(k_1, k_2, i, j) \leftrightarrow (1, 2, 3, 4)$ *for* T*:* $A_T \leftrightarrow A'_T = (A_{pq})_{p,q=1}^{n} = (a_{rs})_{r,s=1}^{nd}$
2. *compute the (generalized) Schur complement:*

```
for k := 1 to (n − 2)d
  if a_kk ≠ 0
    for r := k + 1 to nd
      for s := k + 1 to nd
        a_rs := a_rs − (a_rk a_ks)/a_kk
```

3. $E'_{ij} := (a_{rs})_{r,s=(n-2)d+1}^{nd}$ *defines the edge matrix* E_{ij}

Finally, we observe that Algorithm 3.1 produces approximate semipositive splittings:

Corollary 3.1 *(Approximate splitting) Considering the Elasticity Problem 1 the generalized Schur complements computed according to Algorithm 3.1 yield approximate semipositive splittings of the element matrices* A_T*, i.e.,* $\kappa(A_T, B_T) < \infty \quad \forall T \in \mathcal{T}$.

Proof. Any Schur complement of an SPSD matrix A_T is SPSD. If a diagonal entry of an SPSD matrix vanishes the corresponding row and column have to be zero. Thus, the kernel of any generalized Schur complement computed via Algorithm 3.1 is given by the projection of the kernel of A_T onto the corresponding subspace (associated with the remaining degrees of freedom) which for non-degenerated tetrahedrons has dimension 5. Hence,

each edge matrix is an SPSD rank-one matrix generated by the respective edge vector. Theorem 3.2 therefore shows that $\kappa(A_T, B_T) < \infty$ holds. □

As an advantage over the element based AMG methods, which need to store all element matrices (and coarse versions of those) we note that the storage requirements are much less for the edge matrices (and coarse versions of those). For 3D unstructured tetrahedral meshes one has to store $12 \cdot 13/2 = 78$ floating point numbers per element whereas 3 values per edge suffice to keep the information of the edge matrices. Since the number of edges usually does not exceed two times the number of elements (for 3D triangulations), the amount of storage will be less than ten percent.

4 The AMGm framework

In a recent work [15], algebraic multigrid based on computational molecules (AMGm) has been introduced for scalar problems. In this section, we want to extend and generalize the major innovations from Reference [15] in such a way that the resulting method tackles problems governed by coupled systems of PDEs, e.g., the Elasticity Problem from Section 2.

We will mainly concentrate on those aspects that distinguish our approach from the classical AMG method described in [17]. First of all, the notion of "strong connections", herein after also referred to as "strong edges", will be explained.

4.1 "Strong edges"

Based on the knowledge of edge matrices the notion of "strong edges" can be developed:

Definition 4.1 *(Direct connections) Any two nodes i and j are said to be directly connected iff there is an edge $\{i, j\}$ connecting nodes i and j; let E_{ij} denote the corresponding edge matrix.*

Now for every loop of length 3 (triangle) in the *algebraic grid* with direct connections (edges) $\{i, j\}$, $\{j, k\}$, and $\{k, i\}$ we consider the molecule

$$M^{(i,j,k)} := E_{ij} + E_{jk} + E_{ki}, \tag{17}$$

which in general is a $(3d) \times (3d)$ matrix. Furthermore, for $d \geq 1$, let

$$\mathcal{M}^{\triangle} := \{M^{(i,j,k)} = (C_{pq})_{p,q} : C_{pp} \neq 0 \quad \forall p = 1, 2, 3\} \tag{18}$$

be the set of all such local matrices given as the sum of three edge contributions (for edges that form a triangle) for which the three $d \times d$ diagonal blocks (associated with the nodes i, j, k) are SPD. Then the following definition provides a (symmetric!) strong connectivity relation ("strong edges").

Definition 4.2 *(Strong edges) The strength of a (direct) connection* $\{i,j\}$ *is measured by*

$$s_{ij} := \min\{1, \min_{M^{(i,j,k)} \in \mathcal{M}^{\triangle}} \left\{ \frac{\|E_{ij}\|}{2 \cdot \sqrt{\|C_{p_i p_i}\| \cdot \|C_{p_j p_j}\|}} \right\}\} \tag{19}$$

where connections with $s_{ij} \geq \theta$ *are said to be strong,* $0 < \theta < 1$ *(e.g.,* $\theta = 1/4$*). Here* p_i *and* p_j *denote the local numbers associated with nodes* i *and* j*, i.e.,* $1 \leq p_i \equiv p(i), p_j \equiv p(j) \leq 3$*, and* $C_{p_i p_i}$ *and* $C_{p_j p_j}$ *are the corresponding* $d \times d$ *blocks in the diagonal of* $M^{(i,j,k)}$*.*

Remark 4.1 *For the scalar case* $d = 1$*, (regarding a triangular mesh) formula (19) reduces to*

$$s_{ij} := \min\{1, \min_{M^{(i,j,k)} \in \mathcal{M}^{\triangle}} \{|c_{p_i p_j}| / \sqrt{|c_{p_i p_i} c_{p_j p_j}|}\}\} \tag{20}$$

and essentially yields the energy cosine of the abstract angle between the i*-th and* j*-th (nodal) basis function.*

4.2 Interpolation based on molecules

The task is to define suitable computational molecules, assembled from edge matrices, for building interpolation. Assume that *strong* and *weak edges* have been identified, the coarse grid has been selected, and a set of edge matrices is available. For coarse-grid selection the algorithm(s) used with classical AMG [17] or slightly modified variants of these can be used [15].

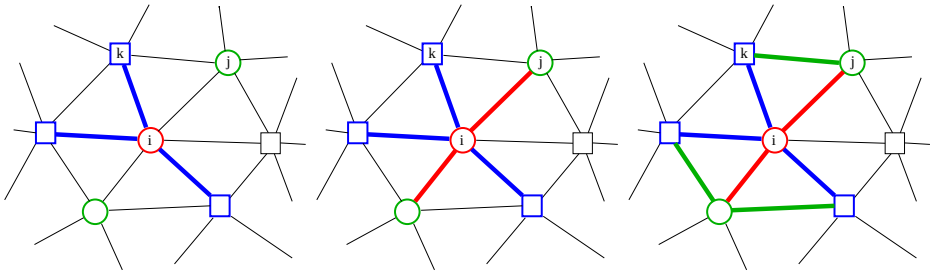
Then for any f-node i (to which interpolation is desired) we define a so-called interpolation molecule

$$M(i) := \sum_{k \in \mathcal{S}_i^c} E_{ik} + \sum_{j \in \mathcal{N}_i^f : \exists k \in \mathcal{S}_i^c \cap \mathcal{N}_j} E_{ij} + \sum_{k \in \mathcal{S}_i^c \cap \mathcal{N}_j : j \in \mathcal{N}_i^f} E_{jk}. \tag{21}$$

This molecule arises from assembling all edge matrices associated with three types of edges: The first sum corresponds to the strong edges connecting node i to some coarse direct neighbor k (*interpolatory edges*), i.e., $k \in \mathcal{S}_i^c$, cf., Figure 1(a). The second sum represents edges connecting the considered f-node i to any of its fine direct neighbors j being directly connected to at least one c-node $k \in \mathcal{S}_i^c$, i.e., $j \in \mathcal{N}_i^f : \exists k \in \mathcal{S}_i^c \cap \mathcal{N}_j$, cf., Figure 1(b). Finally, the last sum in (21) corresponds to these latter mentioned connections (edges) between fine direct neighbors j and strongly connected coarse direct neighbors k of node i, i.e., $k \in \mathcal{S}_i^c \cap \mathcal{N}_j : j \in \mathcal{N}_i^f$, cf., Figure 1(c). The formation of an interpolation molecule is illustrated in Figure 1.

In the numerical experiments in Section 5 we will compare two types of interpolation operators, the first one based on the "minimal molecules"

Figure 1: Formation of interpolation molecule



(a) minimal molecule (b) adding f-f edges (c) extended molecule

that are defined by the first sum in (21), cf., Figure 1(a), and the second one based on the "extended molecules" taking into account all three sums in (21), cf., Figure 1(c).

Now, let

$$M(i) = M = \begin{pmatrix} M_{ff} & M_{fc} \\ M_{cf} & M_{cc} \end{pmatrix} \tag{22}$$

be the interpolation molecule where the 2×2 block structure in (22) is associated with the partitioning into f-dofs and c-dofs. Assuming that $M(i)$ is SPSD and M_{ff} is SPD the interpolation coefficients (d×d matrices) for node i are given by the corresponding d rows of the matrix

$$P^{\star}_{fc} := -M_{ff}^{-1} M_{fc}. \tag{23}$$

Note that (similar to AMGe) this choice minimizes the following measure for the defect $\mathbf{d}_f := \mathbf{e}_f - P_{fc}\,\mathbf{e}_c$ of local interpolation:

$$\max_{\mathbf{e} \perp \ker(M)} \frac{(\mathbf{e}_f - P_{fc}\,\mathbf{e}_c)^t (\mathbf{e}_f - P_{fc}\,\mathbf{e}_c)}{\mathbf{e}^t M\,\mathbf{e}} \to \min$$

Hence, $P^{\star}_{fc}\,\mathbf{e}_c$ provides the minimum-energy extension (harmonic extension) with respect to $M(i)$. For a more detailed discussion, see [15].

4.3 Coarse edge matrices

Since interpolation rests on *strong edges*, the goal is to reduce the number of edges on coarser levels in order to end up with a low operator complexity. We therefore suggest the following practicable procedure for the computation of coarse-edge matrices:

1. Firstly, coarse edges are connecting (arbitrary) pairs of c-nodes (i, j) if and only if there is a path consisting of at most two (or three)

successive *strong* f-edges connecting nodes i and j via at most one (or two) f-nodes.

2. Secondly, the adjacency matrix (relation)

$$\mathcal{E}_c = \{(i,j) \in D_c \times D_c : \; i = j \; \vee \; e_{ij} \text{ defines a c-edge}\}$$

can be computed by evaluating the product of Boolean matrices

$$\mathcal{E}_c \coloneqq \mathcal{P}^t \times \mathcal{P} \quad \text{(or, alternatively,} \quad \mathcal{E}_c \coloneqq \mathcal{P}^t \times \bar{\mathcal{E}}_f \times \mathcal{P})$$

where $\mathcal{P}$ and $\bar{\mathcal{E}}_f$ define nodal adjacency relations for interpolation and *strong* f-edges, respectively.

3. Next, an auxiliary matrix B_f is assembled from f-edge matrices and the triple matrix product $B_c = P^t \, B_f \, P = (B_{ij})_{i,j=1}^{n_c}$ is evaluated for the off-diagonal blocks corresponding to $\mathcal{E}_c$.

4. Finally, for every coarse edge e_{ij}^c $(1 \le i < j \le n_c)$ the $(2d)\times(2d)$ coarse edge matrix E_{ij}^c is defined by

$$E_{ij}^c \coloneqq \begin{pmatrix} F_{ij} & -F_{ij} \\ -F_{ij} & F_{ij} \end{pmatrix} \quad \text{where} \quad F_{ij} \coloneqq \frac{G_{ij}}{\|G_{ij}\|} \quad \text{and} \quad G_{ij} = B_{ij}^t B_{ij}.$$

The additional costs for the *incomplete* triple matrix product we compute in step 3 of the above procedure incur due to the requirement of evaluating the (off-diagonal blocks of the) coarse-edge matrices. However, these costs in practice will be lower than those for computing the coarse-grid operator.

Remark 4.2 *Note that (by construction)* $\operatorname{rank}(E_{ij}^c) = 1 \; \forall e_{ij}^c$. *Moreover, for the 3D (2D) elasticity problem the c-edge matrices can be represented by a single vector of length 3 (2).*

4.4 Multilevel procedure

Regarding the multilevel algorithm, we notice that the AMGm method agrees with classical AMG, except for the coarse-grid selection and the interpolation component, which are controlled by edge matrices in case of AMGm. One can also view this as involving an auxiliary problem–the one determined by the edge matrices–in the coarsening process. Similar to AMGe, we use an interpolation rule that is based on local energy minimization (23) but now with respect to the molecules (21), which replace the local neighborhood matrices (assembled from certain element matrices) as used in AMGe.

The coarse-grid matrices are computed via the usual Galerkin approach, i.e., the triple matrix product $A_{k+1} = P_k^T A_k P_k$ at all levels $k = 0, 1, \ldots, l-1$.

5 Numerical results

The numerical experiments presented in this section refer to the following 2D and 3D Elasticity Problems, cf., (2)–(4).

2D Problem:

$$\begin{aligned} -\mathrm{div}\,\boldsymbol{\sigma} &= \mathbf{0} && \text{in } \Omega := (0,1)^2 \\ \mathbf{u} &= \mathbf{0} && \text{at the bottom} \\ \boldsymbol{\sigma}\cdot\mathbf{n} &= (\,0,\, f_y\,)^t && \text{at top line segment: } \overline{(\tfrac{1}{4},1)(\tfrac{3}{4},1)} \\ \boldsymbol{\sigma}\cdot\mathbf{n} &= \mathbf{0} && \text{on all other faces} \end{aligned}$$

3D Problem:

$$\begin{aligned} -\mathrm{div}\,\boldsymbol{\sigma} &= \mathbf{0} && \text{in } \Omega := (0,1)^3 \\ \mathbf{u} &= \mathbf{0} && \text{at the bottom} \\ \boldsymbol{\sigma}\cdot\mathbf{n} &= (\,0,\,0,\, f_z\,)^t && \text{at top circle: } \mathbf{m} = (\tfrac{1}{2},\tfrac{1}{2},1),\ r = \tfrac{1}{4} \\ \boldsymbol{\sigma}\cdot\mathbf{n} &= \mathbf{0} && \text{on all other faces} \end{aligned}$$

For both problems we consider the weak formulation (1) using the FE space (9) with increasing number of triangles (tetrahedrons) obtained by two levels of uniform refinement of an unstructured mesh. The triangulation of the domain and the corresponding FE solution are illustrated in Figures 2–3.

The arising linear systems were solved for different values of the Poisson ratio ν using either a V(2,2) or a W(2,2) cycle of AMGm with a symmetric (block) Gauß-Seidel smoother (complete inversion of the $d\times d$ diagonal pivot blocks) as a preconditioner for conjugate gradients. The iteration was initialized with the vector of all zeros in all experiments; the iteration count reported in Tables 1–2 refers to a reduction of the initial redidual norm by a factor 10^{-8}. Additionally, we report the avarage convergence rate ρ, as well as the grid and operator complexity σ^Ω and σ^A.[3]

The threshold parameter θ for strong edges was selected depending on the average strength of connections (average edge strength) $\bar{\theta}$, i.e., $\theta = \bar{\theta}/2$ for the 3D problems, and $\theta = \bar{\theta}/3$ for the 2D problems. The interpolation was either based on the minimal molecules (taking into account only the strong f-c edges), cf., Figure 1(a), or, alternatively, on the extended molecules, cf., Figure 1(c).

As we see from Tables 1–2 the usage of the extended molecules considerably improves the results based on the minimal molecules, which appear

[3] σ^Ω is the ratio of the total number of points on all grids to that on the fine grid, whereas σ^A is the ratio of the total number of nonzero entries in all matrices to that in the fine-grid matrix.

Figure 2: Solution of 2D Elasticity Problem

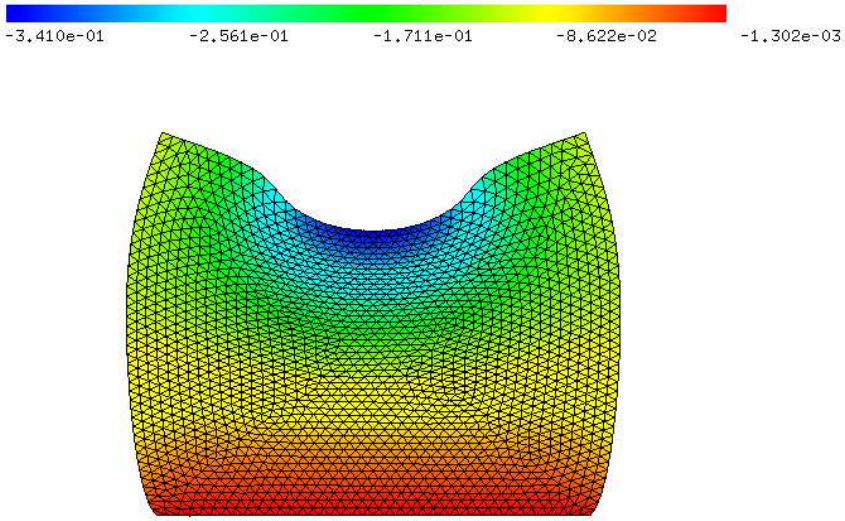
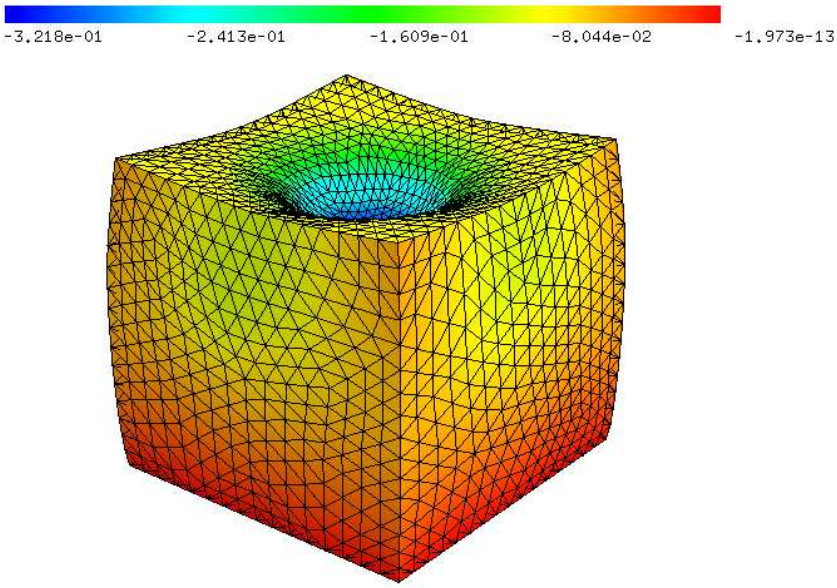


Figure 3: Solution of 3D Elasticity Problem



parenthesized in the respective second row. Whereas the AMGm preconditioner shows pefect robustness with respect to the Poisson ratio in the 2D problem, the iteration counts increase about fifty percent when increasing the parameter ν from 0.25 to 0.45 in the 3D problem. However, the linear elements we used for discretization are not accurate for almost incompressible materials anyway. Nevertheless, we used the first-order FE approximation since we are not interested in studying the limit case $\nu \to 1/2$ here.

The grid and operator complexity are very similar for the 2D and the 3D problems; the grid complexity is even slightly lower for the 3D problems if we apply the aforementioned rule for the threshold on strong connectivity (strong edges).

Table 1: AMGm results for 2D elasticity problem

#elements (dofs)		3760 (3922)		15040 (15362)		60160 (60802)	
#levels		2		4		6	
ext. (min.)	mols	#it.	ρ	#it.	ρ	#it.	ρ
$\nu = 0.25$:	V(2,2)	11	0.16	16	0.30	24	0.45
		(13)	(0.24)	(23)	(0.43)	(38)	(0.61)
	W(2,2)	-	-	13	0.22	14	0.24
		-	-	(16)	(0.30)	(17)	(0.33)
$\nu = 0.33$:	V(2,2)	11	0.17	16	0.31	24	0.45
		(14)	(0.25)	(23)	(0.44)	(39)	(0.61)
	W(2,2)	-	-	13	0.23	14	0.25
		-	-	(16)	(0.31)	(17)	(0.34)
$\nu = 0.4$:	V(2,2)	11	0.18	17	0.32	24	0.45
		(14)	(0.26)	(24)	(0.45)	(39)	(0.62)
	W(2,2)	-	-	14	0.23	15	0.25
		-	-	(17)	(0.32)	(18)	(0.36)
$\nu = 0.45$:	V(2,2)	12	0.19	17	0.33	24	0.46
		(15)	(0.27)	(24)	(0.45)	(40)	(0.63)
	W(2,2)	-	-	14	0.24	15	0.26
		-	-	(17)	(0.34)	(19)	(0.37)
	σ^{Ω}	1.44 (1.44)		1.71 (1.69)		1.74 (1.75)	
	σ^{A}	1.85 (1.84)		2.92 (2.80)		3.15 (3.39)	

6 Concluding remarks

We have generalized the edge-based algebraic multigrid methodology introduced in [15] in order to takle problems governed by systems of second-order elliptic PDEs, e.g., in solid (or structural) mechanics. The 3D and 2D linear

Table 2: AMGm results for 3D elasticity problem

#elements (dofs)		3024 (2355)		24192 (15291)		193536 (109203)	
#levels		2		4		6	
ext. (min.)	mols	#it.	ρ	#it.	ρ	#it.	ρ
$\nu = 0.25$:	V(2,2)	15	0.28	26	0.46	33	0.56
		(13)	(0.24)	(33)	(0.57)	(52)	(0.70)
	W(2,2)	-	-	18	0.35	19	0.36
		-	-	(23)	(0.44)	(28)	(0.52)
$\nu = 0.33$:	V(2,2)	17	0.30	27	0.50	34	0.58
		(14)	(0.26)	(36)	(0.59)	(55)	(0.71)
	W(2,2)	-	-	19	0.37	20	0.39
		-	-	(25)	(0.47)	(30)	(0.54)
$\nu = 0.4$:	V(2,2)	18	0.36	31	0.53	40	0.62
		(16)	(0.30)	(41)	(0.63)	(61)	(0.74)
	W(2,2)	-	-	22	0.42	23	0.44
		-	-	(28)	(0.52)	(34)	(0.58)
$\nu = 0.45$:	V(2,2)	22	0.42	37	0.60	49	0.68
		(19)	(0.36)	(51)	(0.69)	(77)	(0.78)
	W(2,2)	-	-	28	0.50	29	0.52
		-	-	(35)	(0.59)	(42)	(0.64)
	σ^Ω	1.50 (1.50)		1.59 (1.59)		1.54 (1.54)	
	σ^A	2.64 (2.63)		3.48 (3.45)		3.48 (3.47)	

elasticity problems considered in this paper could be solved in an efficient way regarding both, computational complexity, and storage requirements of the preconditioner. The investigation of symbolic methods that allow for a "cheap" computation of optimal (semipositive) splittings for different classes of element matrices is still an open question in the non-scalar case.

The transfer of the presented techniques to second- (or higher-) order FE schemes is under current investigation. This includes the development of an "element-free" version of AMGm; a construction of edge matrices from the global stiffness matrix makes the knowledge of element matrices dispensable. In case of the 3D (or 2D) elasticity problem herein before mentioned the edge matrices are generated by the "edge vectors" and thus determined up to a scalar constant each. Different ways of computing these constants are possible, proper algorithms are going to be explored.

A generalization of AMGm to non-symmetric problems will be subject of future research.

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