Algebraic Multigrid and Element Preconditioning I

Stefan Reitzinger[1]
Johannes Kepler University Linz, SFB F013
"Numerical and Symbolic Scientific Computing"
Freistädter Str. 313, 4040 Linz, Austria
phone: ++43 732 2468 7178
fax: ++43 732 2468 7179
email: reitz@numa.uni-linz.ac.at

Abstract

This paper presents a solution strategy for poor conditioned, large linear systems with a sparse matrix arising from an FE-discretization. Especially robustness has to be gained, if anisotropic elements are used.
To achieve this, the algebraic multigrid (AMG) method of Ruge/Stüben is used. This algorithm is robust for M-matrices, but unfortunately the 'region of robustness' between s.p.d. M-matrices and general s.p.d. matrices is very fuzzy. For this reason the so called element preconditioning technique is introduced to obtain a spectral equivalent M-matrix with respect to the original stiffness matrix. AMG, with the spectral equivalent M-matrix instead of the original stiffness matrix, is then applied as preconditioner to the conjugate gradient method.
Numerical studies are done for a magnetic shielding, a sandwich and a boundary layer problem in 2D (and 3D) which show the numerical robustness of the new preconditioning method.

Keywords algebraic multigrid, anisotropic elements, element preconditioning, robust solvers, preconditioned conjugate gradient method

AMS Subject Classification 65N22, 65F10

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1 Introduction

In order to solve a poor conditioned, large linear system with a sparse matrix arising from an finite element (FE) discretization of an elliptic partial differential equation (PDE), an efficient solution strategy is required. Multigrid methods (MGM) have proven to be an optimal solver for such kind of problems, see [3, 11, 12, 13, 14, 15, 20, 25, 30]. MGMs are known to be asymptotically optimal, but they require a hierarchical grid structure which may not always be available. Algebraic multigrid (AMG) is a technique which preserves the most advantages of multigrid methods and needs no hierarchical grid structure. Actually, AMG just needs the matrix and the right hand side. This makes AMG very attractive as black-box solver with the features of multigrid cycling processes.

The first serious approach to AMG was made in 1982 and an improved version can be found in [5]. The algorithm described therein behaves robust against parameter jumps, geometry of the domain, etc., if the underlying matrix is an M-matrix or if it is at least very close to an M-matrix (i.e. there are just few relatively small positive off-diagonal entries). For such kind of problem setting a lot of numerical studies were done and can be found in [10, 28, 29].

Other 'pure' AMG methods with quite interesting approaches can be found in [8, 20, 27, 32]; these authors are just vicarious for those working on this topic.

Additionally, the methods described in [7, 33] are also called 'algebraic', due to the matrix dependent prolongation and restriction. Anyway, they need some hierarchical grid structure.

In this paper, the AMG method of Ruge-Stüben (denoted by RSAMG) is applied as a preconditioner for the conjugate gradient method. For theory on RSAMG we refer to [5, 28, 29, 4]. On one hand we know that RSAMG is robust for s.p.d. M-matrices. On the other hand we need in a preconditioning step of PCCG only a matrix B_h which is spectrally equivalent to the original matrix A_h. In order to achieve robustness for anisotropic elements (especially rectangles in 2D and pentahedra in 3D) the element preconditioning method (EP) is suggested to obtain a spectrally equivalent M-matrix B_h, so that RSAMG can be applied to it. Putting these three methods together (i.e. EP, RSAMG and PCCG) will result in a robust solution strategy, i.e. RSAMG with B_h instead of A_h is applied as a preconditioner to PCCG. This technique can always be used if the element stiffness matrices of the original stiffness matrix A_h are available.

The paper is organized as follows: First, the main points of RSAMG and PCCG are given. Next we present a method to achieve a matrix with M-matrix property which is spectrally equivalent to the original stiffness matrix, with small spectral constants. This method is called element preconditioning. For the element preconditioning technique, numerical examples are shown which prove the numerical robustness of the method. At the end some conclusions and further remarks are given.

Notation Throughout the paper s.p.d. is the abbreviation for symmetric positive definite. Moreover an element matrix $A^{(r)}$ is called M-matrix even if it is just symmetric positive semidefinite. Spectral equivalence of matrices, i.e. $c_1(Au, u) \leq (Bu, u) \leq c_2(Au, u)$, is abbreviated by $A \sim B$. And finally, the null-space of a matrix A is denoted by $N(A)$.

2 RSAMG and PCCG

We use the AMG method of Ruge and Stüben as our basic tool. This technique has proven to be robust for M-matrices or nearly M-matrices (small positive off diagonal entries are admissible) and for special classes of symmetric matrices (for a more exact explanation see [4]).
AMG is in principle very simple. In order to solve the equation

$$A_h u_h = f_h \tag{1}$$

by means of a multigrid cycle the interpolation, restriction, coarse grid and smoothing operator has to be defined in an algebraic way. We explain this methodology by means of a two grid method, where h and H describe the fine and coarse grid, respectively. First of all, the smoothing operator is fixed and usually the simplest one is taken, i.e. Gauß-Seidel. Next the coarse grid operator A_H is defined via the Galerkin-approach, i.e. $A_H = I_h^H A_h I_H^h$. In the last formula, the restriction and interpolation operator are denoted by I_h^H and I_H^h, respectively. The additional assumption $I_h^H = (I_H^h)^T$ means that only the interpolation operator I_H^h has to be defined. An appropriate method for computing the interpolation weights is given in [28, 26]. If the operators are set up, a multigrid cycle can be constructed in the usual way (see [13]).
Besides the fact that RSAMG can be used as a solver itself, it can also be interpreted as a preconditioner (for CG). It is well known that the combination of PCCG and RSAMG results in an efficient solution strategy. Before we proceed, the main preliminaries for PCCG are presented. For more details we refer to [16]. The essential and sufficient assumptions for PCCG are:

- the original stiffness matrix A_h is s.p.d.
- the preconditioner for PCCG will be derived from a matrix B_h by applying RSAMG to it
- $B_h \sim A_h$ with B_h s.p.d.; clearly, $B_h = A_h$ would be the best choice for the preconditioning step in PCCG but it is not necessary
- Gauß-Seidel is used as a smoother in the MG preconditioner
- the coarse grid systems are derived via the Galerkin-approach

3 Element Preconditioning

3.1 The idea

Here we propose a technique to produce a spectrally equivalent M-matrix B_h out of A_h, which is s.p.d. This is very important because the M-matrix property of A_h can be lost if

- quadratic FE-functions are used instead of linear ones
- the triangulation is not regular
- long thin rectangles are used
- etc.

Now, if the non-negative values in the matrix get too big, RSAMG will break down; i.e. it loses the robustness. How can we omit this leak?
Notice that RSAMG will be used as a preconditioner and therefore only a spectrally equivalent matrix is needed on the finest grid; and as mentioned in the last section, this is sufficient for PCCG. Hence we are looking for a matrix B_h which is spectrally equivalent to the original stiffness matrix A_h and B_h is M-matrix. A sophisticated method to get a spectrally equivalent M-matrix is to extract more information out of the element-matrices.

Theorem 3.1. *Let $A_h \in \mathbb{R}_n^n$ be an s.p.d. matrix arising from an FE-discretization. Moreover let $A^{(r)}$ be the corresponding element matrices and assume*

$$B^{(r)} \sim A^{(r)} \qquad \forall r \in \mathbb{R}_h \tag{2}$$

with $B^{(r)}$ M-matrix. Moreover let $c_1^{(r)}$ and $c_2^{(r)}$ be the lower and upper spectral constants of (2), respectively. (Notice: $A^{(r)}$ could be positive semidefinite and thus we have to require $N(B^{(r)}) = N(A^{(r)})$.) Then we get

$$B_h \sim A_h \tag{3}$$

where B_h is the assembled matrix of $B^{(r)}$. The lower and upper spectral constants of (3) are $\min_{r\in\mathbb{R}_h} c_1^{(r)}$ and $\max_{r\in\mathbb{R}_h} c_2^{(r)}$, respectively. Additionally, B_h has M-matrix property.

Proof. The proof follows immediately by using the connectivity matrices. □

To use the above theorem for each element δ_r, $r \in \mathbb{R}_h$, a spectrally equivalent element matrix has to be computed; but how could this be done?
From a practical point of view we have to check the element matrix before we assemble it. If the element-matrix $A^{(r)}$ is no M-matrix it will be replaced by $B^{(r)}$.

3.2 Practical usage, general algorithm and special cases

In the following discussion we restrict ourself to $\Omega \subset \mathbb{R}^2, \mathbb{R}^3$ and the potential equation, i.e.

$$-\operatorname{div}(\mu(x)\operatorname{grad} u(x)) = f(x) \qquad x \in \Omega \tag{4}$$

Besides the spectral equivalence property of the element matrix $B^{(r)}$ to $A^{(r)}$ there are two more objectives:

- $B^{(r)}$ is an M-matrix
- the generalized eigenvalue problem $A^{(r)}u = \lambda B^{(r)}u$ has a constant spectrum, independent from 'bad' parameters

A general technique to find the best possible M-matrix for a given element matrix $A^{(r)}$ is described in Algorithm 1.

PROCEDURE GeneralSpectralMatrix($A^{(r)}$)
BEGIN

get the element matrix for element r, i.e.$A^{(r)}$
IF *element matrix* $A^{(r)}$ *is no M-matrix* **THEN**
BEGIN
calculate $B^{(r)}$ *with*
$\frac{\lambda_{max}}{\lambda_{min}} \to \min$
such that $B^{(r)}$ *is an M-matrix, symmetric, positive semidefinite*
END

END

Algorithm 1: General technique to get an M-matrix

This procedure is general and useful for all arising element matrices, which are positive semidefinite. Note, that this technique can also be applied in 3D and for any elliptic operator of second order.

Next we are going to compute such spectrally equivalent element matrices for two special elements; namely the rectangle in 2D and the prismatic pentahedron in 3D. Fortunately in these cases a pure algebraic approach can be given to attain a spectrally equivalent M-matrix.

First, we consider a long thin rectangle as in Figure 1 with bilinear FE-functions. By calculating the element stiffness matrix we attain

$$A^{(r)} = \frac{1}{6pq}\begin{pmatrix} 2(p^2+q^2) & p^2-2q^2 & -2p^2+q^2 & -(p^2+q^2) \\ p^2-2q^2 & 2(p^2+q^2) & -(p^2+q^2) & -2p^2+q^2 \\ -2p^2+q^2 & -(p^2+q^2) & 2(p^2+q^2) & p^2-2q^2 \\ -(p^2+q^2) & -2p^2+q^2 & p^2-2q^2 & 2(p^2+q^2) \end{pmatrix} \tag{5}$$

Notice, that for $q < \frac{p}{\sqrt{2}}$ positive off-diagonal elements will occur and thus the M-matrix property is lost.

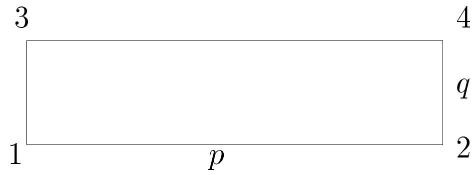

Figure 1: A long thin rectangle

A method to get a spectrally equivalent M-matrix is suggested in Algorithm 2. Therefore let us assume the numbering of the unknowns as in Figure 1 and the original element stiffness matrix (5).

PROCEDURE SpectralMatrixRec$(A^{(r)})$
BEGIN

  IF $a_{12} > 0$ *or* $a_{34} > 0$ **THEN**
  BEGIN
    $s_x = 2(a_{12} + a_{14} + a_{23} + a_{34})$
    $s_y = 2(a_{13} + a_{24})$
  END
  IF $a_{13} > 0$ *or* $a_{24} > 0$ **THEN**
  BEGIN
    $s_x = 2(a_{12} + a_{34})$
    $s_y = 2(a_{13} + a_{24} + a_{14} + a_{23})$
  END
  calculate the elements of $B^{(r)}$
  $b_{11} = b_{22} = b_{33} = b_{44} = -\frac{s_x + s_y}{2}$
  $b_{12} = b_{34} = \frac{s_x}{2}$
  $b_{13} = b_{24} = \frac{s_y}{2}$
  $b_{14} = b_{23} = 0$
END

Algorithm 2: Algebraic technique to attain an M-matrix for a rectangle

With Algorithm 2 we obtain the spectrally equivalent matrix (6).

$$\tilde{A}^{(r)} = \frac{1}{6pq} \begin{pmatrix} 2(p^2+q^2) & -3q^2 & -2p^2+q^2 & 0 \\ -3q^2 & 2(p^2+q^2) & 0 & -2p^2+q^2 \\ -2p^2+q^2 & 0 & 2(p^2+q^2) & -3q^2 \\ 0 & -2p^2+q^2 & -3q^2 & 2(p^2+q^2) \end{pmatrix} \quad (6)$$

This matrix is symmetric, positive semidefinite and an M-matrix for $q < \frac{p}{\sqrt{2}}$; i.e. the height of the rectangle is much smaller than the length. Finally it is shown that (6) is spectrally equivalent to (5).

Theorem 3.2. *Let (5) be an element matrix. Then (6) is a spectrally equivalent matrix to (5). The eigenvalues λ of the generalized eigenvalue problem*

$$A^{(r)}u = \lambda B^{(r)}u \tag{7}$$

are in the interval $\{0\} \cup [\frac{1}{2}, \frac{3p^2}{2p^2-q^2}]$.

Proof. The proof was done by calculating the eigenvalues of the generalized eigenvalue problem (7) with the program package Mathematica. □

Second, an anisotropic prismatic pentahedron as in Figure 2 is under consideration with the following basis functions on the reference element.

$$\psi_1 = x_1 \cdot x_3 \tag{8}$$
$$\psi_2 = x_1 \cdot (1 - x_3) \tag{9}$$
$$\psi_3 = x_2 \cdot x_3 \tag{10}$$
$$\psi_4 = x_2 \cdot (1 - x_3) \tag{11}$$
$$\psi_5 = (1 - x_1 - x_2) \cdot x_3 \tag{12}$$
$$\psi_6 = (1 - x_1 - x_2) \cdot (1 - x_3) \tag{13}$$

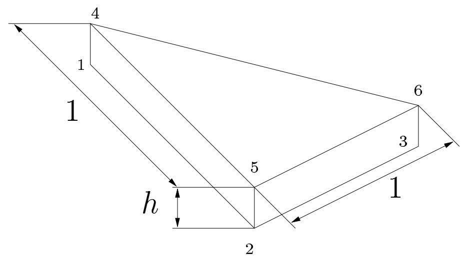

Figure 2: An anisotropic pentahedron

Similar to the method for the rectangle the Algorithm 3 produces a spectrally equivalent M-matrix for a prismatic pentahedron.

PROCEDURE SpectralMatrixPent$(A^{(r)})$
BEGIN

IF $A^{(r)}$ *is no M-matrix* **THEN**
BEGIN
$s_x^1 = a_{12} + a_{15} + a_{24} + a_{45}$
$s_y^1 = a_{14} + a_{25}$
$s_x^2 = a_{13} + a_{16} + a_{34} + a_{46}$
$s_y^2 = a_{14} + a_{36}$
$s_x^3 = a_{23} + a_{65} + a_{35} + a_{26}$
$s_y^3 = a_{25} + a_{36}$
$s_z^{i,j} = s_z^i + s_z^j$

END
calculate the elements of $B^{(r)}$
$b_{11} = b_{44} = -(s_x^{1,2} + \frac{s_y^{1,2}}{2})$
$b_{22} = b_{55} = -(s_x^{1,3} + \frac{s_y^{1,3}}{2})$
$b_{33} = b_{66} = -(s_x^{2,3} + \frac{s_y^{2,3}}{2})$
$b_{12} = b_{45} = s_x^1$
$b_{13} = b_{46} = s_x^2$
$b_{23} = b_{56} = s_x^3$
$b_{14} = \frac{s_y^{1,2}}{2}$
$b_{25} = \frac{s_y^{1,3}}{2}$
$b_{36} = \frac{s_y^{2,3}}{2}$
$b_{ij} = 0$ *for all remaining i,j*
END

Algorithm 3: Algebraic technique to attain an M-matrix for a prismatic pentahedron

Theorem 3.3. *Let* $A^{(r)}$ *be an element matrix of a prismatic pentahedron. Then* $B^{(r)}$ *produced by Algorithm 3 is a spectrally equivalent matrix to* $A^{(r)}$*. The eigenvalues* λ *of (7) are in the interval* $\{0\} \cup [0.25, 1.25]$.

Proof. The proof was done by calculating the eigenvalues of (7) with the program package Mathematica. $\square$

Remark 3.4. *Until now, rectangles and prismatic pentahedra were considered. Other elements which are also very important and very similar to the previous ones are quadrilaterals and pentahedra with two parallel surfaces (see Figure 3).*

In these cases Algorithm 2 and Algorithm 3 can also be applied and deliver an M-matrix. Obviously the eigenvalues of the generalized eigenvalue problem depend on the smallest angle α of such an element. But the $B^{(r)}$ are acceptable if $\frac{\pi}{4} \le \alpha \le \frac{\pi}{2}$.

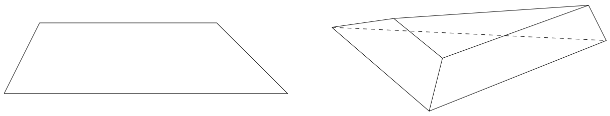

Figure 3: An anisotropic quadrilateral and pentahedron with two parallel surfaces

4 Numerical Studies

In this section the effectivity and robustness of EP+RSAMG+PCCG is shown. Therefore the code was included in the program package FEPP, see [31]. Therein RSAMG is used as a preconditioner for PCCG.
The potential equation, typically arising in magnetic field problems, a sandwich problem and a boundary layer problems are treated as examples.
The overall abbreviations are listed in Table 1 for this section.

PCAMG	PCCG with RSAMG
ModPCAMG	PCCG with EP and RSAMG
N	number of unknowns
level	number of levels used in the calculation
κ	condition number of $C^{-1}A$
	where C is the preconditioner, i.e. RSAMG
iter	number of iterations of the PCCG

Table 1: Abbreviations for the numerical studies

We used in RSAMG a generalized V-cycle. For all examples the iteration was terminated after an error reduction in preconditioner energy norm by a factor of 10^{-8}. All calculations were done on a SUN Ultra 1 workstation, 170 MHz.

4.1 Shielding problem in 2D

Let us consider the following problem

$$
\begin{aligned}
-\operatorname{div}(\mu_i \operatorname{grad} u(x)) &= 0 \qquad \forall x \in \Omega_i \qquad i = 1,2 && (14)\\
u(x) &= -\mu_1 \cdot (B_x x_1 + B_y x_2) \qquad \forall x \in \partial\Omega_1 \setminus \partial\Omega_2 && (15)\\
-\mu_1 \frac{\partial u_1(x)}{\partial n} &= -\mu_2 \frac{\partial u_2(x)}{\partial n} \qquad \forall x \in \partial\Omega_2 && (16)
\end{aligned}
$$

with parameter setting $\mu_1 = 1$, $\mu_2 = 1000$, $B_x = 21$, $B_y = 45$ and domain Ω as shown in Figure 4.

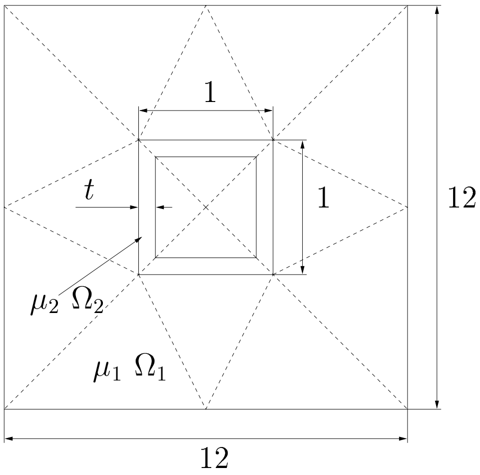

Figure 4: Shielding problem with two materials

In Table 2, the condition numbers and the number of iterations are shown for 2D problem if element preconditioning is used. For comparison the non robust PCAMG method is listed for $t = 10^{-3}$ in Table 3.

	ModPCAMG			
t	N	level	κ	iter
10^{-2}			5.59	25
10^{-3}	2369	3	5.42	24
10^{-4}			4.93	22
10^{-5}			4.31	20
10^{-2}			6.58	29
10^{-3}	9345	4	6.57	28
10^{-4}			6.05	27
10^{-5}			5.14	24
10^{-2}			8.91	33
10^{-3}	37121	6	9.26	34
10^{-4}			7.96	31
10^{-5}			6.60	28

Table 2: Shielding problem in 2D

	PCAMG			
t	N	level	κ	iter
10^{-3}	2369	3	1401	>100
	9345	4	927	>100
	37121	6	625	>100

Table 3: Shielding problem in 2D

4.2 Sandwich problem in 3D

Second, a so called sandwich problem is considered, with the same PDE and boundary condition as in the shielding example. The geometry of the problem can be seen in Figure 5.

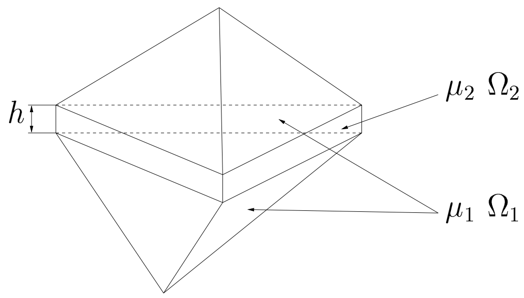

Figure 5: Sandwich problem in 3D

	ModPCAMG			
h	N	level	κ	iter
10^{-2}	645	2	4.08	40
10^{-3}			4.04	39
10^{-4}			4.09	37
10^{-5}			4.53	39
10^{-2}	4233	4	9.28	45
10^{-3}			4.26	41
10^{-4}			4.43	40
10^{-5}			4.12	40

Table 4: Sandwich problem in 3D

In Table 4 the robustness of ModPCAMG is stated if the element preconditioning method is applied to the prismatic pentahedra. If this technique is not used, then the condition number κ is increasing with the number of unknowns (e.g. $\kappa \sim 10^6$ for the case $N = 4233$, $h = 10^{-5}$).

4.3 Boundary layer problem in 2D

Third, we consider a boundary layer problem of the following kind

$$\begin{aligned} -\epsilon^2 \Delta u + u &= 1 \qquad \forall x \in \Omega \qquad (17) \\ u &= 0 \qquad \forall x \in \Gamma \qquad (18) \end{aligned}$$

and with an appropriate discretization presented in Figure 6 (bilinear FE-functions).

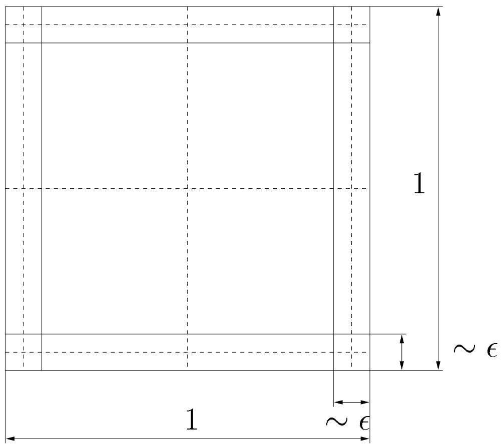

Figure 6: Boundary layer problem

	ModPCAMG			
ϵ	N	level	κ	iter
10^{-2}			2.98	13
10^{-3}	625	2	3.05	12
10^{-4}			2.94	11
10^{-5}			2.92	11
10^{-2}			3.08	13
10^{-3}	2401	4	4.61	23
10^{-4}			3.11	12
10^{-5}			3.14	12
10^{-2}		5	3.18	13
10^{-3}	9409	8	3.17	13
10^{-4}		8	4.24	15
10^{-5}		8	3.25	11

Table 5: Boundary layer problem

In Table, 5 the robustness of the ModPCAMG can be seen again. Further more we can emphasize that ModPCAMG is robust; not so PCAMG.

5 Conclusions and further Remarks

The numerical results show the robustness of the suggested technique if anisotropic elements are used for discretization. First it is clear that this strategy can be applied to all kinds of positive definite problems if we have access to the element stiffness matrices. But it should also be mentioned that the spectral equivalence constants could be large. Moreover it might be a big numerical effort to produce an M-matrix in the general case.
Second, this method was introduced for scalar elliptic equations. A straight forward approach to systems is not obvious but a generalization is under current research.
Another way to overcome the 'M-matrix property' is to seek for a new interpolation method and/or for a new coarsening strategy. This means, if the interpolation could be improved, we should end up with a better convergence rate (even if just s.p.d. matrices are considered). Of course this is closely related to the coarsening strategy because positive off-diagonal entries have to be treated in the right way.

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