Algebraic Multigrid Method for Solving 3D Nonlinear Electrostatic and Magnetostatic Field Problems

M. Kaltenbacher, S. Reitzinger, J.Schöberl

***Abstract*— A recently developed robust Algebraic Multigrid (AMG) method for the efficient solution of 3D nonlinear electrostatic and magnetostatic field problems will be presented. The method is directed to large matrix equations which arise from finite element (FE) discretization where AMG is used as a preconditioner in the Preconditioned Conjugate Gradient (PCG) method. Numerical results will demonstrate the applicability of the developed AMG method.**

***Index Terms*— Multigrid, finite element methods, electrostatics, magnetostatics.**

I. Introduction

Often the FE-formulation of electrostatic and magnetostatic field problems results in a large system of equations. Therefore, the solution process is time consuming, especially for nonlinear or optimization problems, and there is a need for fast solvers.
In contrast to geometric multigrid AMG needs no FE-discretization with hierarchical grids. Still it preserves the most advantages of geometric multigrid, i.e., AMG is an iterative solver with optimal time and memory complexity which is especially suited for sparse linear systems with large condition number.

II. Physical Equations

The governing equation for the electrostatic field is given by

$$-\nabla \cdot \varepsilon(E) \nabla \phi = q \,. \tag{1}$$

In (1) ϕ denotes the scalar electric potential, E the absolute value of the electric field, q the volume charge and ε the permittivity of the material.
The total magnetic field strength $\vec{H}$ can be defined by

$$\vec{H} = \vec{H}_{\mathrm{s}} + \vec{H}_{\mathrm{m}} \,, \tag{2}$$

where $\vec{H}_{\mathrm{s}}$ describes the magnetic field due to current sources (calculated according to Biot-Savarts law) and $\vec{H}_{\mathrm{m}}$ the induced magnetism in ferromagnetic materials. Since $\nabla \times \vec{H}_{\mathrm{m}} = 0$ holds, (2) changes to

$$\vec{H} = \vec{H}_{\mathrm{s}} - \nabla \psi \tag{3}$$

by introducing the reduced scalar magnetic potential ψ. Using Maxwell's equations for the magnetostatic field results in [2]

$$\nabla \cdot \mu(H) \nabla \psi = \nabla \cdot \mu \vec{H}_{\mathrm{s}} \tag{4}$$

with $\mu(H)$ being the permeability of the material.

III. FE-Formulation

Applying the FE-formulation to (1) leads to the following matrix equation

$$\mathbf{K}_h^{\phi} \phi_h = Q_h \tag{5}$$

for the nodal vector ϕ_h of the scalar electric potential. The terms of the electric stiffness matrix $\mathbf{K}_h^{\phi}$ are computed by

$$K_h^{\phi} = \int_{\Omega_V} \mathbf{B}^T \varepsilon \mathbf{B} \, d\Omega \,; \quad \mathbf{B} = \left[\frac{\partial N}{\partial x} \; \frac{\partial N}{\partial y} \; \frac{\partial N}{\partial z} \right]^T \tag{6}$$

and the entries of the nodal source vector Q_h by

$$Q_h = \int_{\Omega_V} N q d\Omega \tag{7}$$

with N being the interpolation function.
The FE-formulation of the magnetostatic field problem yields the following matrix equation

$$\mathbf{K}_h^{\psi} \psi_h = R_h \tag{8}$$

with the magnetic stiffness matrix $\mathbf{K}_h^{\psi}$

$$K_h^{\psi} = \int_{\Omega_\phi} \mathbf{B}^T \mu \mathbf{B} \, d\Omega \tag{9}$$

and the nodal source vector R_h

$$R_h = -\int_{\Omega_\phi} N \left(\nabla \cdot (\mu \vec{H}_{\mathrm{s}}) \right) d\Omega + \int_{\Gamma_\phi} N \left(\vec{n} \cdot \mu \vec{H}_{\mathrm{s}} \right) d\Gamma \,. \tag{10}$$

IV. Algebraic Multigrid Method (AMG)

In order to outline the principles of solving a (sparse) linear system

$$\mathbf{K}_h u_h = f_h \tag{11}$$

with $\mathbf{K}_h = \{k_{ij}\}_{i,j=1,\ldots,n} \in \mathbb{R}^{n \times n}$ being symmetric positive definite (SPD), $u_h \in \mathbb{R}^n$ the solution vector and $f_h \in \mathbb{R}^n$ the right hand side, with the multigrid method we explain this by means of a two grid method. Therefore h and H

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describe the fine and coarse grids of a FE-discretization, respectively. The linear mappings (with $n > m$)

$$I_h^H : \mathbb{R}^n \to \mathbb{R}^m \qquad \text{and} \qquad I_H^h : \mathbb{R}^m \to \mathbb{R}^n \tag{12}$$

are called restriction and interpolation operators. Therewith, the two grid algorithm is performed as follows:

1. Relax ν_1 times on the fine grid $\mathbf{K}_h u_h = f_h$
(e.g. Gauß-Seidel forward)
2. Calculate the defect $d_h = f_h - \mathbf{K}_h u_h$
3. Project the defect d_h onto the coarse grid, i.e.

$$d_H = I_h^H d_h$$

4. Solve the coarse grid problem

$$\mathbf{K}_H v_H = d_H$$

5. Project the coarse grid correction v_H onto the fine grid, i.e.

$$v_h = I_H^h v_H$$

6. Update u_h by v_h, i.e. $u_h = u_h + v_h$
7. Relax ν_2 times on the fine grid $\mathbf{K}_h u_h = f_h$
(e.g. Gauß-Seidel backward)

Replacing the exact solution of the coarse grid problem in point 4 itself by a two grid approximation, we arrive at the recursive definition of a multigrid cycle. It is important to use Gauß-Seidel forward in the pre-smoothing step and Gauß-Seidel backward in the post-smoothing step to obtain a symmetric preconditioner, which can be used in the PCG-method ([3]).
In the case of AMG, the coarse grid matrix $\mathbf{K}_H$ has to be set up by the only knowledge of the fine grid matrix $\mathbf{K}_h$. Therefore, we have to introduce 'grids' as sets of unknowns, which are assumed to be nested, i.e.

$$\omega_h \supset \omega_H \tag{13}$$

where ω_h and ω_H is the 'grid' on the fine and coarse level, respectively; actually $\omega_h = \{1, \ldots, n\}$ and $|\omega_h| = n$, $|\omega_H| = m$. In terms of two consecutive levels h, H we assume that each coarse level variable u_k^H, $k \in \omega_H$ is used to directly correct a uniquely defined fine grid variable $u_{i(k)}^h$, $i(k) \in \omega_h$. Thus ω_h can be split into two disjoint subsets: the first contains the variables also presented on the coarser level (C-variables) and the second is the complementary subset (F-variables), i.e. $\omega_h = C \cup F$, $C \cap F = \emptyset$ and $\omega_H = C$. In order to define such a splitting the following definition is helpful

Definition 1: *An error $e \in \mathbb{R}^n$ that is not rapidly reduced by relaxation is called algebraic smooth and is characterized by*

$$\langle \mathbf{K}_h e, e \rangle \ll \langle e, e \rangle \,, \tag{14}$$

that is, the residual of the error is small compared to the error itself.
The essence of Definition 1 is that in general a smooth error component varies generally slowly in the direction of strong coupling. This result motivates the following definition:

Definition 2: *The neighborhood of a point i and the local sets of coarse and fine nodes are defined by*

$$N^i = \{j \,|\, k_{ij} \neq 0,\, i \neq j\} \,, \tag{15}$$
$$C^i = \{j \,|\, N^i \cap C\} \,, \tag{16}$$
$$F^i = \{j \,|\, N^i \cap F\} \,. \tag{17}$$

The distance between a fictitious point i and a set of fictitious points I is defined as

$$d(i, I) := \frac{\sum\limits_{j \in I} |k_{ij}|}{\max_{l \neq i} |k_{il}|} \tag{18}$$

The set of strongly coupled neighbours to i is defined as

$$S^i := \{j \in N_i : d(i, \{j\} \geq \alpha\} \,, \tag{19}$$

where in practice α takes the value of 0.25.
The set of points to which the point i has a strong coupling is defined as

$$S^{i,T} := \{j \in N_i : i \in S^j\} \,. \tag{20}$$

By help of this definition, we can set up the following coarsening algorithm [1]:
Phase I: Split N into C and F
1. $C = \emptyset$, $F = \emptyset$
2. While $C \cup F \neq N$ do

pick $i \in N \backslash \{C \cup F\}$ with
max. $|S^{i,T}| + |S^{i,T} \cap F|$
if $|S^{i,T}| + |S^{i,T} \cap F| = 0$ then
$F := V \backslash C$
else
$C := C \cup \{i\}$, $F := F \cup \{S^{i,T} \backslash C\}$
endif
end

Phase II: Check for each F-variable that it has a strong coupling with a C-variable or at least with a F-variable which itself has a strong coupling to a C-variable.

According to (14) we obtain for a smooth error $e \in \mathbb{R}^n$ the relation

$$k_{ii} e_i + \sum_{j \in N_i} k_{ij} e_j = 0 \quad \forall i \in \omega_h \,. \tag{21}$$

By using (21) we come up to the following interpolation weights α_{ij} [1]

$$\alpha_{ij} = \begin{cases} 1 & i = j \in C \\ -\frac{k_{ij} + c_{ij}}{k_{ii} + c_{ii}} & i \in F,\, j \in C \\ 0 & \text{else} \end{cases} \tag{22}$$

and

$$c_{ij} = \sum_{p \in F^i} \frac{k_{ip} k_{pj}}{\sum_{l \in C^i} k_{pl} + k_{pi}} \,. \tag{23}$$

Therewith, if $e_H \in \mathbb{R}^m$ represents a coarse grid correction, then the fine grid correction $e_h \in \mathbb{R}^n$ is computed via the interpolation operator by

$$(e_h)_i = (I_H^h e_H)_i = \sum_{j \in C} \alpha_{ij} e_j \qquad \forall i \in \omega_h \,. \tag{24}$$

The restriction operator I_h^H is defined by

$$I_h^H = (I_H^h)^T \tag{25}$$

and the coarse grid operator $\mathbf{K}_H \in \mathbb{R}^{m\times m}$ is calculated by the Galerkin-transformation

$$\mathbf{K}_H = I_h^H \mathbf{K}_h I_H^h \,. \tag{26}$$

By using an appropriate smoother (e.g. Gauß -Seidel) a multigrid cycle can be set up.
Before we describe the solution strategy we give a definition on spectrally equivalent matrices.

Definition 3: *Two positive semidefinite matrices $A, B \in \mathbb{R}^{n\times n}$ are called spectrally equivalent if there exist constants $c_1 > 0$ and $c_2 > 0$, $c_1 \le c_2$ such that*

$$c_1 \cdot \langle Bu, u\rangle \le \langle Au, u\rangle \le c_2 \cdot \langle Bu, u\rangle \qquad \forall u \in \mathbb{R}^n \,. \tag{27}$$

This is abbreviated by $A \sim B$. Especially it follows that the nullspace of A and B are equal.

For SPD M-matrices $\mathbf{K}_h$ (small positive off diagonal entries are admissible), the above AMG technique is known as a robust solver. But it inherently needs the M-matrix property. Unfortunately the M-matrix property is frequently lost by the FE-discretization (e.g. for long thin rectangles, flat hexahedra, quadratic FE-functions, etc.). To overcome this problem AMG is exclusively used as a preconditioner for the PCG method. Therefore, a spectrally equivalent M-matrix $\mathbf{B}_h$ to $\mathbf{K}_h$ is constructed and AMG applied to $\mathbf{B}_h$ yields a good preconditioner to the original matrix $\mathbf{K}_h$ for the PCG method ([4]). The basic idea of constructing such an M-matrix is given in the following corollary ([4]).

Corollary 1: *Let*

$$\mathbf{K}_h = \sum_{r\in\mathbb{R}_h} C_r^T K^{(r)} C_r \in \mathbb{R}^{n\times n} \tag{28}$$

be SPD with C_r connectivity matrices, $\mathbb{R}_h$ the set of elements and $K^{(r)}$ the element matrix for element $r \in \mathbb{R}_h$. If additionally $B^{(r)} \sim K^{(r)}$ for all $r \in \mathbb{R}_h$ and $B^{(r)}$ has the right sign condition then

$$\mathbf{B}_h \sim \mathbf{K}_h \tag{29}$$

with $\mathbf{B}_h = \sum_{r\in R_h} C_r^T B^{(r)} C_r$ M-matrix.

Thus the construction of a spectrally equivalent M-matrix $\mathbf{B}_h$ with respect to the original matrix $\mathbf{K}_h$ can be done on element basis. Therewith, the following PCG algorithm is performed:

1. Set:

$$g^0 = \mathbf{K}_h u_h^0 - f_h \tag{30}$$
$$\mathbf{B}_h d^0 = -g^0 \quad \textbf{(one AMG cycle)} \tag{31}$$
$$h^0 = -d^0 \tag{32}$$

2. Calculate for $k \ge 0$

$$u_h^{k+1} = u_h^k + \alpha^k d^k \tag{33}$$
$$\alpha^k = \frac{(g^k)^T h^k}{(d^k)^T \mathbf{K}_h d^k} \tag{34}$$
$$g^{k+1} = g^k + \alpha^k \mathbf{K}_h d^k \tag{35}$$
$$\mathbf{B}_h h^{k+1} = g^{k+1} \quad \textbf{(one AMG cycle)} \tag{36}$$
$$\beta^k = \frac{(g^{k+1})^T h^{k+1}}{(g^k)^T h^k} \tag{37}$$
$$d^{k+1} = -h^{k+1} + \beta^k d^k \tag{38}$$

In the case of nonlinear problems a series of linearized problems

$$\mathbf{K}_h(u_{h,i}) u_{h,i+1} = f_h \tag{39}$$

has to be solved; it can be expected that for the considered problems all $\mathbf{K}_h(u_{h,i})$ are spectrally equivalent with constants close to one. That means, the setup of AMG has to be done only once (e.g. for $\mathbf{B}_h$ which is spectrally equivalent to $\mathbf{K}_h(u_{h,1})$). The resulting preconditioner is then applied in the PCG method for all nonlinear steps. Additionally we use in the i^{th} nonlinear iteration $u_{h,i}^0 = u_{h,i-1}$ as an initial guess for the PCG method.

V. Numerical Results

A. Electrostatic

To study the computational complexity of the developed AMG solver, the numerical calculation of the electric field of a parallel plate capacitor filled with an ferroelectric material (PZT 5A) in the linear and nonlinear case is studied. The electrodes of the capacitor with a radius of 20 mm have a distance of 1 mm. The FE-discretization has been performed by brick elements (Fig. 1). Table I presents the

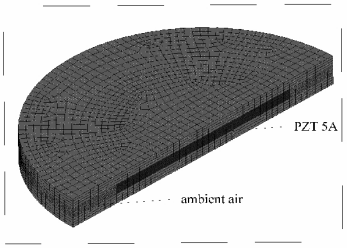

Fig. 1. FE-discretization of the capacitor

TABLE I
Elapsed time of AMG solver for setup and solution phase

number of unknowns	setup phase (seconds)	solution phase (seconds)
1765	2.8	0.3
6728	13.5	1.2
23535	98.6	5.8
70700	380.4	35.5

elapsed time of the AMG solver split into *setup phase* and *solution phase* as a function of unknowns, whereas Table

II shows the comparison of the total solution time of the AMG solver and a direct solver using a banded LU factorization. The extremely long simulation time for the direct solver in the case of 70700 unknowns is due to the large bandwidth of the system matrix which can be reduced just by a small amount by the profile optimization algorithm. In

TABLE II
ELAPSED TIME OF AMG SOLVER COMPARED TO A DIRECT SOLVER IN THE LINEAR CASE

number of unknowns	AMG solver (seconds)	direct solver (seconds)
1765	3.1	2.7
6728	14.8	63.2
23535	104.4	736.2
70700	415.9	22410.0

the nonlinear case a standard fixed point iteration scheme has been used, which took a total number of 12 nonlinear iterations. As described in the previous section, in the case of the AMG solver, the setup phase has been performed just once and the obtained preconditioner has been kept constant throughout all of the 12 iterations (Table III).

TABLE III
ELAPSED TIME OF AMG SOLVER COMPARED TO A DIRECT SOLVER IN THE NONLINEAR CASE

number of unknowns	AMG solver (seconds)	direct solver (seconds)
1765	9.7	27.4
6728	40.3	692.0
23535	224.4	10613.0

B. Magnetostatic

In the magnetostatic case a magnetic circuit with an air-gap, driven by a permanent magnet, has been considered (Fig. 2). The performance of the AMG solver is shown

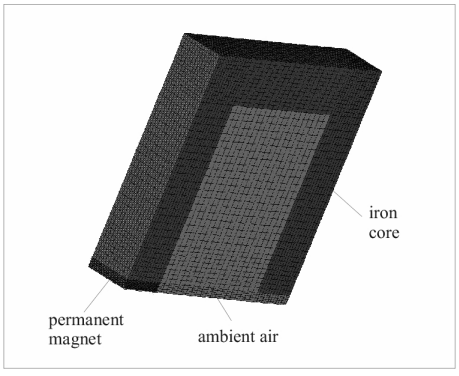

Fig. 2. FE-discretization of the magnetic circuit

in Table IV (solution time split into setup and solution phase).

TABLE IV
Elapsed time of AMG solver for setup and solution phase

number of unknowns	setup phase (seconds)	solution phase (seconds)
2646	1.35	0.36
9216	7.5	2.7
18942	19.3	7.8
68544	100.2	40.5

The comparison of the total elapsed CPU-time between the AMG solver and a direct solver with banded LU factorization is given in Table V.

TABLE V
Elapsed time of AMG solver compared to a direct solver in the linear case

number of unknowns	AMG solver (seconds)	direct solver (seconds)
2646	2.1	1.1
9216	10.2	7.6
18942	27.1	33.5
68544	140.7	2224.4

In the nonlinear case the fixed point iteration scheme took a total number of 19 iterations. In Table VI the comparison of AMG solver and a direct solver in the nonlinear case is given.

TABLE VI
Elapsed time of AMG solver compared to a direct solver in the nonlinear case

number of unknowns	AMG solver (seconds)	direct solver (seconds)
2646	12.2	26.7
9216	52.5	181.4
18942	245.9	863.6

VI. CONCLUSION

In this paper we have introduced a robust AMG method which is used as a preconditioner in the PCG method for the efficient solution of 3D nonlinear electrostatic and magnetostatic field problems. Especially in the nonlinear case, where the preconditioner is set up just in the first fixed point iteration and then held constant, the CPU time can be reduced tremendously compared to conventional direct solvers.

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