Comparison of Geometrical and Algebraic Multigrid Preconditioners for Data-Sparse Boundary Element Matrices

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Abstract. We present geometric (GMG) and algebraic multigrid (AMG) preconditioners for data-sparse boundary element matrices. Data-sparse approximation schemes such as adaptive cross approximation (ACA) yield an almost linear behavior in N_h , where N_h is the number of (boundary) unknowns. The treated system matrix represents the discretized single layer potential operator (SLP) resulting from the interior Dirichlet boundary value problem for the Laplace equation. It is well known, that the SLP has converse spectral properties compared to usual finite element matrices. Therefore, multigrid components have to be adapted properly. In the case of GMG we present convergence rate estimates for the data-sparse ACA version. Again, uniform convergence can be shown for the V-cycle.

Iterative solvers dramatically suffer from the ill-conditioness of the underlying system matrix for growing N_h . Our multigrid-preconditioners avoid the increase of the iteration numbers and result in almost optimal solvers with respect to the total complexity. The corresponding numerical 3D experiments are confirming the superior preconditioning properties for the GMG as well as for the AMG approach.

Keywords: integral equations of the first kind, single layer potential operator, boundary element method, adaptive cross approximation, algebraic multigrid, geometrical multigrid, preconditioners, iterative solvers.

1 Introduction

In this paper we are concerned with the fast solution of data-sparse boundary element equations by geometrical and algebraic multigrid methods.

The application of iterative solvers only will be reasonable, if the drawback of dense matrices can be overcome. In the last years different sparse approximation techniques for boundary element matrices have been developed. The multipole method [14], the panel clustering method [7], the \mathcal{H} -matrix approach [6] and wavelet techniques [9] are certainly now the most popular ones. In our paper we will consider the adaptive cross approximation (ACA) method suggested by M. Bebendorf and S. Rjasanow [1,2]. The basic idea is to decompose the system matrix into its near-field and far-field contributions. Finding an appropriate low-rank approximation for the far-field matrix yields a data-sparse BEM matrix approximating the original dense matrix in such a way that the discretization

error is not affected. In conclusion, the application of a sparse representation algorithm allows us to realize the matrix-by-vector multiplication in almost $O(N_h)$ operations.

Boundary element matrices originating from the discretization of the single layer potential lead to ill-conditioned system matrices with a condition number of order $O(h^{-1})$. Thus, it is obvious that we need appropriate preconditioning techniques in order to avoid the steady rise of the number of iterations for finer and finer discretizations. In [11,10] we introduced algebraic multigrid preconditioners for dense BEM matrices as well as for large-scaled data-sparse BEM matrices. In this paper we focus on the comparison between the GMG and AMG approach. Moreover, we give a convergence result for the geometric version of our multigrid approach.

The paper is organized as follows: Section 2 gives a brief overview on the considered single layer potential operator and its properties. In addition, the ACA-method is briefly described. In Section 3, we introduce the multigrid components designed for ACA-matrices and give convergence results for the geometrical variant. Some results of our numerical studies are presented in Section 4. Finally, we end up with some conclusions and discuss further investigations in Section 5.

2 Problem Formulation and the ACA-Method

Let $\Omega \subset \mathbb{R}^d$ (d=2,3) be a bounded, simply connected domain with one closed boundary piece $\Gamma = \partial \Omega$ that is supposed to be sufficiently smooth. We consider the boundary element technique by means of the interior Dirichlet problem for Laplace's equation:

$$-\Delta u(x) = 0 \qquad x \in \Omega$$

$$u(x) = g(x) \qquad x \in \Gamma$$
 (1)

Once the Neumann and Dirichlet data are available, it is possible to formulate the solution of the interior Dirichlet equation by the representation formula

$$\sigma(y)u(y) = \int_{\Gamma} \frac{\partial u}{\partial n_x}(x)E(x,y)ds_x - \int_{\Gamma} u(x)\frac{\partial E}{\partial n_x}(x,y)ds_x$$
(2)

where n_x denotes the unit outward normal vector and E(x, y) is the fundamental solution for the Laplace equation, i.e. in \mathbb{R}^3 we have $E(x, y) = \frac{1}{4\pi} \frac{1}{|x-y|}$. For $y \in \Omega$ we have $\sigma(y) = 1$, for $y \notin \overline{\Omega}$ it changes to $\sigma(y) = 0$. In the case of $y \in \Gamma$ and Γ is sufficiently smooth we will obtain $\sigma = 1/2$, that is still valid for applying Galerkin discretization on $C^{0,1}$ domains. In that case the first integral defines the single layer potential operator $V: H^{-1/2}(\Gamma) \mapsto H^{1/2}(\Gamma)$. In addition the second integral gives the double layer potential operator $K: H^{1/2}(\Gamma) \mapsto H^{1/2}(\Gamma)$. It can be shown that the single layer potential operator is symmetric and positive definite. These and other properties can be found in e.g. [15]. Applying Galerkin discretization with the use of piecewise constant trial functions leads to the matrix equation

$$V_h \underline{v}_h = \underline{f}_h = (\frac{1}{2}I_h + K_h)\underline{g}_h \tag{3}$$

where \underline{g}_h is the discrete Dirichlet data obtained by linear interpolation, $(V_h)_{ij} = \int_{\Gamma_j} \int_{\Gamma_i} E(x, y) ds_x ds_y$ and $(K_h)_{ij} = \int_{\Gamma_i} \int_{\Gamma} \frac{\partial E}{\partial n_x}(x, y) \psi_j(x) ds_x ds_y$ with the linear trial function ψ_j . At this point we have to notice that V_h is still fully populated and the condition number is of order $O(h^{-1})$. To overcome the drawback of dense matrices we replace the system matrix with some approximation matrix provided by the ACA-algorithm. On the contrary to other matrix approximation techniques, an explicit description of the integral kernel is not necessary. More precisely, only a procedure for evaluating selected matrix entries has to be available. The rest are simple algebraic operations.

The basic idea is to decompose the computational domain into smaller clusters \mathcal{D}_i and classify the interaction of two clusters into a near-field part and a far-field part of the generated matrix, respectively. Based on geometrical information we split the index set $I = \{1, ..., N_h\}$ into index clusters $t_i \subset I$ which corresponds to the partitioning of the domain $\Omega = \bigcup_i \mathcal{D}_i$. In order to select the blocks which can be approximated by low-rank matrices, we give an admissibility condition that classifies clusters-pairs into a near-field part and a far-field part.

Definition 1. Let $(\mathcal{D}_1, \mathcal{D}_2)$ be a cluster pair with $\mathcal{D}_1, \mathcal{D}_2 \subset \mathbb{R}^d$, then $(\mathcal{D}_1, \mathcal{D}_2)$ is called η - admissible if

$$\operatorname{diam} \mathcal{D}_2 \le \eta \operatorname{dist}(\mathcal{D}_1, \mathcal{D}_2).$$
(4)

As usual dist $(X, Y) = \inf\{|x - y|, x \in X, y \in Y\}.$

Both, the clustering procedure and the approximation algorithm will cause a overall complexity of $O(\epsilon^{-\alpha}N_h^{1+\alpha})$ with an arbitrarily small positive α . In [2] one can find the appropriate algorithms and more detailed information. Since the proposed adaptive cross approximation technique provides a low-rank approximation of V_h^{far} consisting of submatrices which are η -admissible we obtain the result

$$\widetilde{V}_h = V_h^{near} + \widetilde{V}_h^{far}.$$
(5)

Starting from this representation we are able to present an appropriate construction of multigrid methods in the next section. Finally, we refer to [1,2] for more detailed proofs and further remarks concerning the ACA-technique.

3 Multigrid Methods

In the previous section we showed, that our system matrix coincides with the approximated discretized single layer potential operator \widetilde{V}_h , which is the most interesting case concerning our multigrid approach. Hence, we have to solve $\widetilde{V}_h \underline{v}_h = \underline{f}_h$ in \mathbb{R}^{N_h} with \underline{v}_h are the unknown Neumann data and \underline{f}_h the corresponding right-hand side. In order to make multigrid methods really efficient,

it is necessary to adapt the multigrid components properly according to the underlying physical problem and variational formulation. In the following we are discussing the multigrid components by means of a twogrid algorithm. The indices h and H denote the fine grid and coarse grid quantities, respectively.

In fact, the efficiency of multigrid methods depends on a clever interaction of smoothing sweeps on the fine level and coarse grid correction on the coarse level. Once a grid hierarchy (GMG) or a matrix hierarchy (AMG) is available we can apply multigrid methods like the well-known V-cycle presented in Algorithm 1. The coarsest level is denoted by the variable COARSELEVEL therein.

Algorithm 1 Multigrid V-Cycle

$$\begin{split} & MG(\underline{u}_{\ell}, \underline{f}_{\ell}, \ell) \\ & \text{if } \ell = COARSELEVEL \\ & \text{calculate } \underline{u}_{\ell} = (V_{\ell})^{-1} \underline{f}_{\ell} \text{ by some coarse grid solver} \\ & \text{else} \\ & \text{smooth } \nu_{F} \text{ times on } V_{\ell} \underline{u}_{\ell} = \underline{f}_{\ell} \\ & \text{calculate the defect } \underline{d}_{\ell} = \underline{f}_{\ell} - V_{\ell} \underline{u}_{\ell} \\ & \text{restrict the defect to the next coarser level } \ell + 1 : \underline{d}_{\ell+1} = P_{\ell}^{\top} \underline{d}_{\ell} \\ & \text{set } \underline{u}_{\ell+1} \equiv 0 \\ & \text{call } MG(\underline{u}_{\ell+1}, \underline{d}_{\ell+1}, \ell + 1) \\ & \text{prolongate the correction } \underline{s}_{\ell} = P_{\ell} \underline{u}_{\ell+1} \\ & \text{update the solution } \underline{u}_{\ell} = \underline{u}_{\ell} + \underline{s}_{\ell} \\ & \text{smooth } \nu_{B} \text{ times on } V_{\ell} \underline{u}_{\ell} = \underline{f}_{\ell} \\ & \text{end if} \end{split}$$

Since the single layer operator represents a pseudo-differential operator of order minus one, the eigenvalues and eigenvectors act conversely compared to those of finite element matrices. Therefore, standard smoothing procedures like damped Jacobi or Gauß-Seidel does not provide a satisfying smoothing sweep. Bramble, Leyk and Pasciak [3] present an appropriate approach to this problem class of operators. In order to reduce the highly oscillating components of the error we introduce a matrix $A_h \in \mathbb{R}^{N_h \times N_h}$ being some discretization of the Laplace-Beltrami operator on the boundary Γ . Consequently, we obtain a smoothing iteration of the form

$$\underline{u}_h \leftarrow \underline{u}_h + \tau_h \cdot A_h(\underline{f}_h - \widetilde{V}_h \underline{u}_h) \tag{6}$$

with a well chosen damping parameter τ_h , see e.g. [10].

In the case of algebraic multigrid we need a matrix hierarchy which represents a 'virtual' grid on each level. Therefore, we first construct prolongation operators $P_h : \mathbb{R}^{N_H} \mapsto \mathbb{R}^{N_h}$ by exploiting a sparse auxiliary matrix B_h which includes geometrical information [11]. Then, we are applying Galerkin's method to obtain the system matrix $V_H = P_h^{-T} V_h P_h$ on the coarse level. In addition, the restriction of a fine ACA matrix \tilde{V}_h immediately leads to matrices on the coarse level

$$V_H^{near} = P_h^\top V_h^{near} P_h, \qquad \widetilde{V}_H^{far} = \sum_{i=1}^{N_B} \sum_{j=1}^{r_i} P_h^\top u_j^i \ (P_h^\top v_j^i)^\top \tag{7}$$

where N_B denotes the number of admissible blocks and r_i the rank of the i^{th} block. Due to the exact preserving of representation (5) on the coarse grid, we are able to use the same ACA-datastructures in our numerical realization.

On the other hand in the geometrical version of our multigrid approach a nested mesh-hierarchy is available. In this case we are calculating the discretized single layer potential on each grid separately. Strictly speaking, we apply the ACA-algorithm level by level to obtain the approximated single layer potential operators. Again we provide a set of data-sparse system matrices, which are used within the V-cycle.

In order to obtain results for convergence, we verify conditions on the approximated single layer potential operator \tilde{V}_h . Based on theoretical results in [4] which are weaker than the regularity and approximation conditions, we have to show the spectral equivalence inequalities

$$c_1(V_h\underline{v},\underline{v}) \le (\widetilde{V}_h\underline{v},\underline{v}) \le c_2(V_h\underline{v},\underline{v}) \quad \underline{v} \in \mathbb{R}^{N_h}$$
(8)

and an approximation result in the sense

$$|(V_h\underline{v},\underline{w}) - (\widetilde{V}_h\underline{v},\underline{w})| \le c_0\lambda_J^{-\beta/2}||\underline{v}_h||_{V_h}||\underline{w}_h||_{V_h} \quad \underline{v}_h,\underline{w}_h \in \mathbb{R}^{N_h}.$$
 (9)

In the last inequality λ_J denotes the largest eigenvalue of the induced operator \mathcal{V} defined by $(\mathcal{V}v_h, w_h)_{-1} = (V_h \underline{v}_h, \underline{w}_h)$ with the functions v_h, w_h described by the basis coefficients $\underline{v}_h, \underline{w}_h$. Moreover, β is a arbitrary small positive parameter. It can be proofed, that (8) holds with the spectral constants

$$c_1 = (1 - \epsilon \sqrt{N_h} \kappa(V_h)) c_2 = (1 + \epsilon \sqrt{N_h} \kappa(V_h)).$$
(10)

Furthermore, we can show that the estimate

$$|(V_h\underline{v}_h,\underline{w}_h) - (\widetilde{V}_h\underline{v}_h,\underline{w}_h)| \le c_0\epsilon h^{\gamma}\lambda_J^{-\beta/2}||\underline{v}_h||_{V_h}||\underline{u}_h||_{V_h} \quad \underline{v}_h,\underline{w}_h \in \mathbb{R}^{N_h}$$
(11)

is valid, where ϵ is the accuracy from the ACA-approximation. Nevertheless, the upper bound still depends on the typical mesh size h and whose exponent $\gamma = -(d + \beta + 4)/2$ additionally includes the dimension d of the boundary parameterization of $\partial \Omega$. With an appropriate choose of ϵ one can cancel out the h-dependency. However, in our numerical experiments we kept ϵ fix and cannot observe a negative influence anyway. From these estimates and the general convergence theory given in [4] we can immediately proof uniform convergence of the V-cycle.

4 Numerical Studies

In order to show the efficiency of the suggested multigrid approach we present some results in 3D for the interior Dirichlet boundary value problem for the Laplace equation. The Galerkin boundary element matrices are generated by



Fig. 1. 3D Geometries

Table 1. Assembling \widetilde{V}_h and Setup Times for L-Shape

	AMG (sec)		GMG (sec)	
Number of	Assembling	Galerkin	Assembling	Matrix-
Unknowns	\widetilde{V}_h	Projection	\widetilde{V}_h	hierarchy
7168	77	15	32.5	6.9
28672	158	30	158	40

the software package OSTBEM developed by O. Steinbach, cf. [16], the AMG-preconditioner is realized within the software package PEBBLES [8].

For our numerical comparison of the geometrical multigrid preconditioner and the algebraic multigrid preconditioner, we choose a few rather simple 3D geometries, see Figure 1. Nevertheless, these domains include a wide spectrum of problem classes, for e.g. edges, corners and non-convex domains. First of all, we compare the times for constructing the AMG matrix hierarchy by Galerkin projection and building up the ACA matrices for GMG on the coarser grids. These CPUtimes are almost of the same order, see Table 1. It is obvious, that most of the assembling time is needed for construction the system matrix \tilde{V}_h . Secondly, we compare the numbers of iterations, that are needed within the preconditioned conjugate gradient (PCG) method. Moreover, the CPU-time of one single PCGiteration for different numbers of unknowns are listed in Table 2. One can clearly observe the expected almost linear increase of the CPU-times for one iteration

Table 2. Key data for AMG/GMG Preconditioner

Number of	AMG		GMG				
Unknowns	PCG-Cycle (sec)	Iterations	PCG-Cycle (sec)	Iterations			
L-Shape							
1792	0.1	6	0.1	7			
7168	0.8	6	0.6	7			
28672	4.2	9	2.9	7			
Fichera-Corner							
1920	0.1	14	0.1	15			
7680	0.8	15	0.6	15			
30720	5.0	17	3.2	15			

with respect to the number of unknowns. Considering the time for one PCGiteration, we notice, that the GMG version is faster for larger problems.

Furthermore, we obtain constant iteration numbers for a wide range of problem sizes. That implies that our data-sparse multigrid preconditioner for the single layer potential operator is of high quality. In the case of AMG preconditioning we also have small iteration numbers, nevertheless they are slightly increasing. Because the coarser matrix levels are produced in a purely algebraic way, it is hardly possible to preserve corresponding 'virtual' coarse grids of the original geometry.

5 Conclusions and Further Remarks

In this paper we presented a geometrical multigrid and algebraic multigrid approach for the solution of large-scale boundary element equations. For that purpose an approximation of the boundary element matrices is absolutely essential. Our numerical experiments have been realized by the adaptive cross approximation technique which guarantees that the effort for storing the matrices and for a single matrix-by-vector multiplication can be reduced to almost $O(N_h)$. The discretized single layer potential operator yields symmetric positive definite matrices in the original dense version as well as in the ACA representation. Therefore, the system of boundary element equations can be solved by means of multigrid preconditioned CG-algorithms. Due to the sparse representation of our matrices, we had to adapt each component of our AMG-algorithm properly. In order to set up the matrix hierarchy and the corresponding transfer operators an auxiliary matrix was constructed for the AMG method. On the other hand the matrices were built accordingly to the grid hierarchy in the GMG method. The smoothing procedure was realized by the proposed BLP-smoother for pseudo-differential operators of order minus one.

The overall algorithm provides interesting numerical results. One can notice small constant iteration numbers for the GMG method and also small (but slightly increasing) iteration numbers for the AMG approach. That confirms the high quality of our multigrid preconditioners. In addition, the CPU time for a single iterative step almost grows like $O(N_h)$. As expected, the GMG variant is faster than the AMG version. We mention that efficient multigrid preconditioner for the discrete single layer potential operator are very important as building blocks in primal and dual domain decomposition preconditioners [5,12,13].

Last but not least we would like to acknowledge the Austrian Science Fund 'Fond zur Förderung der wissenschaftlichen Forschung (FWF)' for supporting this work under grant P14953 'Robust Algebraic Multigrid Methods and their Parallelization'.

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