A Variable Preconditioning of Krylov Subspace Methods for Hierarchical Matrices with Adaptive Cross Approximation

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Krylov subspace methods to solve linear systems whose coefficient matrix is represented by an hierarchical matrix are discussed. We propose a precondition technique using a part of the original hierarchical matrix in order to accelerate the convergence of the Krylov subspace methods. The proposed precondition technique is based on the assumption that sub-matrices on the original hierarchical matrix are approximated by using the adaptive cross approximation or variants thereof. The performance of Krylov subspace methods with the proposed precondition technique are examined through numerical experiments on an electrostatic field analysis.

***Index Terms*— Approximation algorithms, Linear systems, Iterative algorithms, Numerical analysis, Electrostatic processes.**

I. Introduction

Hierarchical matrices (H-matrices) [1]-[2], as well as the fast multipole method (FMM) [3]-[4], is one of approximation techniques which can be applied to dense matrices appeared on boundary element method (BEM). Although it is inconvenience of BEM to have to handle dense matrices when conducting large scale analyses, these approximation techniques enable us to conduct them. Furthermore, if we use distributed memory parallel computer systems besides the approximation techniques, we could perform huge size simulation. The authors have proposed parallel algorithms for H-matrices [5], and the HACApK library based on the algorithms is released [6].

When we consider the use of a Krylov subspace method for solving a linear system with an H-matrix derived from a BEM analysis, some preconditioner will be needed to handle huge size problems. However, because of the special structure of H-matrices, it is not straight forward to apply well-known preconditioners. An LU decomposition-based preconditioner for H-matrices is proposed in [7]. In this paper, a different approach is presented. We consider a kind of variable preconditioner [8]-[9], and propose a simple method to reduce the computational cost of the preconditioner with possessing the acceleration effect of the Arnoldi types of the Krylov subspace methods. We also examine its analogical algorithm to the BiCGSTAB method though the method is not based on the Arnoldi process. This is because it is reported in [4] that a variant of the BiCGSTAB method employing the method itself as the preconditioner is effective to solve the approximated linear system in the case of FMM application.

II. Proposed precondition technique

For $N \in \mathbb{N}$, an H-matrix $\tilde{A}_H^K$, the approximation of $A \in \mathbb{R}^{N\times N}$, is characterized by a partition H of $N \times N$ with blocks $h = s_h \times t_h \in H$ and block-wise rank K. Then, sub-matrices corresponded to some of the blocks are dense matrices, and the sub-matrices corresponded to most of the blocks are low-rank matrices represented by $\tilde{A}_H^K|^h := \sum_{\nu=1}^{k_h} v^\nu (w^\nu)^T$, where $v^\nu \in \mathbb{R}^{s_h}$, $w^\nu \in \mathbb{R}^{t_h}$ and $k_h \le K$. The number K is determined such that $||A - \tilde{A}_H^K||_F \le \varepsilon$ for a given tolerance ε.

For $x, b \in \mathbb{R}^N$, we consider the following equation:

$$\tilde{A}_H^K \, x = b. \qquad (1)$$

To solve (1), we consider a Krylov subspace method employing the Krylov subspace method itself as a preconditioner. It means that the method consists of a main solver to solve (1) and a preconditioner solver to solve roughly $Pz = r$, where $r \in \mathbb{R}^N$ is determined in the main solver and $P \in \mathbb{R}^{N\times N}$ is the so-called precondition matrix. The matrix P should be an approximation of $\tilde{A}_H^K$. The trivial case is $P := \tilde{A}_H^K$.

Our proposal is as follows: making low-rank sub-matrices $\tilde{A}_H^K|^h$ by the adaptive cross approximation (ACA) [10] and applying the restricted H-matrix as $K = 1$ for the precondition matrix, i.e., $P := \tilde{A}_H^1$. This is based on a heuristic that the approximation accuracy of low-rank matrices asymptotically becomes higher as the rank of the low-rank matrices k_h increases when the low-rank matrices are made by ACA. The arithmetic necessary for the proposed precondition technique is only the multiplication of the restricted H-matrix $\tilde{A}_H^1$ and a vector. It can be calculated by using the original H-matrix $\tilde{A}_H^K$ and the vector. Thus, we do not need any extra memory for storing the restricted the H-matrix $\tilde{A}_H^1$.

III. Numerical Experiments

A. Test problem

As a benchmark, we have selected an electrostatic field problem. It is assumed that perfect conductors, which have the shape of humanoids, are standing on the ground in a uniform electric field (Fig. 1). By using the surface charge method which is one of the indirect BEMs based on a single layer potential formulation, the induced electrical charge on the surface of humanoids is calculated. We divided the surface of humanoids into 2,359,680 triangular elements, and used step functions as the base function of BEM. We applied H-matrices with ACA by setting $\varepsilon = 10^{-4}$ to the coefficient matrices of the linear systems derived from the above formulation and get (1). In this case, the maximum rank $K = 27$ and the average of ranks of low-rank matrices was about 8.

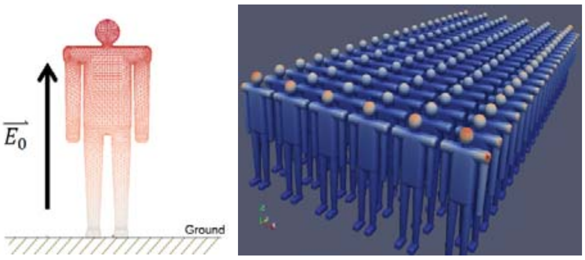

Fig. 1. Analytical condition (left) and the result (right). The analytical objects in the shape of humanoid is discretized by triangular elements, and they are arrayed on the grid of 6×20.

B. *Examined algorithms*

In order to investigate the applicability of our proposed precondition technique, we have examined six algorithms summarized in Table I by solving (1). As represented Krylov subspace methods, the GCR(m) and the BiCGSTAB methods are selected. Cases 1-1 and 2-1 are standard algorithms without any preconditioner. The case 1-2 is so-called GCR(m) with the trivial variable preconditioner, and the case 2-2 is its analogical algorithm to BiCGSTAB. Cases 1-3 and 2-3 are algorithms used our proposed precondition technique, which are derived from cases 1-2 and 2-2 by replacing the coefficient matrix in preconditioner by $\tilde{A}_H^1$. The case 1-3 is corresponded to the algorithm concluded effective in the case of an electrostatic field calculation by FMM in [4].

TABLE I
EXAMINED ALGORITHMS

Case	Main solver	Preconditioner solver	Matrix used in preconditioner
1-1	GCR(m)	Not used	-
1-2	GCR(m)	GCR(m)	$\tilde{A}_H^{27}$
1-3	GCR(m)	GCR(m)	$\tilde{A}_H^{1}$
2-1	BiCGSTAB	Not used	-
2-2	BiCGSTAB	BiCGSTAB	$\tilde{A}_H^{27}$
2-3	BiCGSTAB	BiCGSTAB	$\tilde{A}_H^{1}$

C. *Calculation results*

All the algorithms in Table 1 are implemented by using the Fortran95 programming language and integrated with the HACApk library. We judge the convergence of the main solvers and preconditioner solvers by relative residual norms to be less than 10^{-6} and 10^{-1}, respectively. Moreover, maximum number of iteration for preconditioner solvers is restricted to 8 times. Furthermore, we set the parameter $m = 8$ for the restart of the GCR(m) method. All the calculations are carried out by using 2 cores on 2 computational nodes of CRAY XC30 at Kyoto University, which is equipped with Xeon E5™ and 64GB memory per a node.

In Fig. 2, convergence curves of the main solver are plotted when solving the problem above. In the first place, we focus on the difference of GCR(m) and BiCGSTAB methods. The convergence curve of the case 1-1 goes along with one of the case 2-1. Thus we conclude the application of GCR(m) or BiCGSTAB method without a preconditioner makes no large difference in the case of our test problem. Second, in the cases of BiCGSTAB method with preconditioner (cases 2-2, 2-3), they are slower than methods without a preconditioner. In our opinion, this is partially because the algorithms of cases 2-2 and 2-3 are out of theorem of Krylov subspace methods with the variable preconditioner. Finally, we examine the GCR(m) methods with preconditioner. The case 1-2 reduces the number of iterations of the main solver from the case 1-1, but it results in the same as the case 1-1 in terms of calculation time. On the other hand, the GCR(m) with our proposed precondition technique (case 1-3) is significantly faster than normal GCR(m) and BiCGSTAB methods. The calculation time of the case 1-3 is about 2-thirds of cases 1-1 and 2-1. In terms of the number of iterations of the main solver, the difference of case 1-2 and 1-3 is slight in spite of the large difference in computational costs.

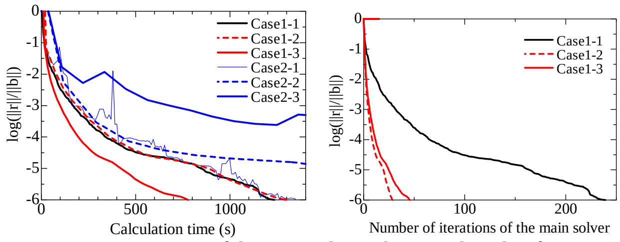

Fig. 2. Convergence curves of the main solver. They are plotted as functions of calculation time (left) and the number of iterations of the main solver (right).

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