Application of Improved H-matrices in Micromagnetic Simulations

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This study examines the applicability of hierarchical-matrices (H-matrices) to the computation of the demagnetizing field that is the most-time consuming part in micromagnetic simulation. Given the fact that the kernel function of the convolution integral operator for the demagnetizing field has second order singularity, efficient approximation cannot be expected by using conventional H-matrices employing adaptive cross approximation (ACA) as the low-rank approximation. We introduce an improved H-matrices combined with a modified ACA to overcome this challenge. The efficiency of the method is confirmed through numerical experiments.

***Index Terms*— Approximation algorithms, Integral equations, Micromagnetics, Numerical analysis.**

I. Introduction

MICROMAGNETIC simulation is widely applied to devise designs as a physical model of magnetic domain structures for ferromagnetic materials. In recent years, large-scaled micromagnetic simulations have been conducted thanks to advanced computer technology. In order to perform fast computations needed during largescale micromagnetic simulation, one significant point to consider is the approach to be used to calculate the demagnetizing field. This is because direct calculation of it entails a computational cost of $O({N_V}^2)$ whereas, the cost for the other variables is $O(N_V)$, where N_V is the number of elements composing the magnetic material V in the numerical simulation.

Although a hybrid method of FEM and BEM [1] reduces the computational cost, it still requires $O({N_S}^2)$, where N_S is the number of elements on the surface of ∂V. In this study, we consider the application of hierarchical matrices (H-matrices) [2]-[4] to the BEM in order to reduce the complexity from $O({N_S}^2)$ to $O(N_S \log N_S)$.

II. Formulation for Micromagnetic Simulation

In a micromagnetic simulation, the distribution of magnetization $\boldsymbol{M}$ is calculated by using the Landau–Lifshitz–Gilbert equation.

$$(1+\alpha^2)\frac{\partial \boldsymbol{M}}{\partial t} = -\gamma(\boldsymbol{M}\times\boldsymbol{H}_{\text{eff}}) - \frac{\alpha\gamma}{M_s}\boldsymbol{M}\times(\boldsymbol{M}\times\boldsymbol{H}_{\text{eff}}), \quad (1)$$

where α, γ, and M_s are the damping constant, gyromagnetic ratio, and saturation magnetization, respectively. $\boldsymbol{H}_{\text{eff}}$ denotes the effective magnetic field obtained as follows:

$$\boldsymbol{H}_{\text{eff}} = \boldsymbol{H}^E + \boldsymbol{H}^D + \boldsymbol{H}^K + \boldsymbol{H}^A, \quad (2)$$

where $\boldsymbol{H}^E, \boldsymbol{H}^D, \boldsymbol{H}^K$, and $\boldsymbol{H}^A$ are the externally applied field, demagnetizing field, anisotropy field, and exchange field, respectively.

In order to compute $\boldsymbol{M}$ using (1) and (2), the magnetic material V is first discretized into elements. The computation of $\boldsymbol{M}$ by using (1) and the calculations of both $\boldsymbol{H}^E$ and $\boldsymbol{H}^K$ can be performed in each element, independently. The evaluation of $\boldsymbol{H}^A$ only needs an interaction between adjacent elements. Therefore, the computational cost for these variables is $O(N_V)$. However, the calculation of the demagnetizing field $\boldsymbol{H}^D$ in an element requires its interaction with all the other elements.

When we assume no free currents in the considered system, the demagnetizing field $\boldsymbol{H}^D$ can be calculated as the gradient of the magnetic scalar potential φ, i.e. $\boldsymbol{H}^D = -\nabla\varphi$. For a unit normal vector $\boldsymbol{n}$ on ∂V, it has to satisfy

$$\Delta\varphi(\boldsymbol{x}) = \begin{cases} \nabla\cdot\boldsymbol{M}(\boldsymbol{x}) & \text{for } \boldsymbol{x}\in V, \\ 0 & \text{for } \boldsymbol{x}\notin V \end{cases}$$
$$\varphi^{\text{ext}} = \varphi^{\text{int}} \text{ and } \frac{\partial\varphi^{\text{ext}}}{\partial\boldsymbol{n}} - \frac{\partial\varphi^{\text{int}}}{\partial\boldsymbol{n}} = -\boldsymbol{n}\cdot\boldsymbol{M} \text{ on } \partial V. \quad (3)$$

In accordance with how it is performed in [1], we split φ into two parts, $\varphi := \varphi_1 + \varphi_2$ such that $\Delta\varphi_1(\boldsymbol{x}) = \nabla\cdot\boldsymbol{M}$ for $\boldsymbol{x}\in V, \varphi_1(\boldsymbol{x}) = 0$ for $\boldsymbol{x}\notin V$ and $\frac{\partial\varphi_1(\boldsymbol{x})}{\partial\boldsymbol{n}} = \boldsymbol{n}\cdot\boldsymbol{M}$ on $\boldsymbol{x}\in\partial V$. As a result, we find $\Delta\varphi_2 = 0$ with $\varphi_2^{\text{ext}} - \varphi_2^{\text{int}} = \varphi_1$ and $\frac{\partial\varphi_2^{\text{ext}}}{\partial\boldsymbol{n}} = \frac{\partial\varphi_2^{\text{int}}}{\partial\boldsymbol{n}}$. Moreover, it is required that $\varphi_2 \to 0$ at infinity. According to potential theory, the boundary values of φ_2 on ∂V can be calculated by using φ_1; i.e., for $\boldsymbol{x}\in\partial V$,

$$\varphi_2(\boldsymbol{x}) = \frac{1}{4\pi}\int_{\partial V}\varphi_1(\boldsymbol{y})\nabla G(\boldsymbol{x},\boldsymbol{y})\cdot \mathrm{d}\boldsymbol{S} + \Omega(\boldsymbol{x})\varphi_1(\boldsymbol{x}), \quad (4)$$

where $G(\boldsymbol{x},\boldsymbol{y}) = 1/|\boldsymbol{x}-\boldsymbol{y}|$ is the Green function and $\Omega(\boldsymbol{x})$ is a coefficient in relation to the solid angle subtended by ∂V at $\boldsymbol{x}$. The second term of the right-hand side can be easily calculated if we have obtained the calculation result $\varphi_1(\boldsymbol{x})$ by using FEM. The first term in (4) is discretized on the boundary surface ∂V, and we get the linear equation

$$\boldsymbol{\varphi_2} = A\boldsymbol{\varphi_1}, \quad (5)$$

with the boundary matrix $A \in \mathbb{R}^{N_S\times N_S}$ and vectors $\boldsymbol{\varphi_1}, \boldsymbol{\varphi_2} \in \mathbb{R}^{N_S}$. The coefficient matrix A is usually almost dense matrix. Completing the calculation of the computational cost $O({N_s}^2)$ in (5) becomes the most time-consuming part in the micromagnetic simulation, if $N_S \cong N_V$.

III. H-MATRICES FOR MICROMAGNETIC SIMULATION

The first term in (4) has a form of the convolution integral. For remote interactions, the kernel functions of convolution integrals can be approximated by a degenerate kernel expressed by several terms of a series expansion. This implies that the submatrices of the coefficient matrix A in (5), which correspond to such remote interactions, can be approximated by the low-rank matrix approximation. We find these potential low-rank submatrices by H-matrices using clusters based on the geometrical information of surface elements.

A H-matrix $\tilde{A}_H^K$, the approximation of A, is characterized by a partition H of $N_S \times N_S$ with blocks $h = s_h \times t_h \in H$ and block-wise rank k_h. Most sub-matrices in $\tilde{A}_H^K$ are expected to be low-rank. A low-rank matrix $\tilde{A}_H^K|^h$, which approximates a sub-matrix $A_H|^h$ of the original matrix corresponding to block h, is represented by

$$\tilde{A}_H^K|^h := \sum_{v=1}^{k_h} v^v (w^v)^T, \quad (6)$$

where $v^v \in \mathbb{R}^{|s_h|}$, $w^v \in \mathbb{R}^{|t_h|}$, and $k_h \leq K$. The upper limit K of the ranks of sub-matrices is usually set such that $||A - \tilde{A}_H^K||_F / ||\tilde{A}_H^K||_F \leq \varepsilon$ for a given tolerance ε.

The adaptive cross approximation (ACA) [5] is known to be one of the most efficient algorithms for the low-rank approximation in the form of (6). An attempt to apply the conventional H-matrices with ACA to micromagnetic simulations is reported in [6]. The HACApK [7], our own H-matrices library, also adopts the ACA to approximate potential low-rank sub-matrices. However, if we apply the H-matrices with ACA to the calculation of the demagnetizing field as they exist, we will not be able to obtain an efficient approximation in some cases, due to the following two reasons.

The first reason is that the kernel function of the integral operator in (4) has second order singularity. The conventional H-matrices employing ACA work well for a first order singularity problem such as electrostatic field analysis [4]. However, we found with the earthquake cycle simulation that the maximum rank K of the H-matrix becomes larger when the kernel function has higher order singularity. To avoid this increase in the maximum rank K, we proposed the improved H-matrices with ACA in [3], which consists of a certain type of normalization and a new stopping criterion for the ACA.

The second reason is that the presence of zero entries in A may disturb the pivoting strategy employed with the ACA. Such creation of zero entries happens in the case of interactions between mutually perpendicular elements. As shown in Fig. 1, our target model has mutually perpendicular surfaces. Even if we were to use the improved H-matrices with ACA as discussed above, the ACA would fail to provide efficient approximation in our models. Instead of the ACA, we adopt the ACA+ algorithm [8], which is a variant of ACA that changes the pivoting strategy to improve convergence.

For the reasons discussed above, we have modified the HACApK library by adding a function of the improved H-matrices with ACA+.

IV. NUMERICAL EXPERIMENTS

For a benchmark, we have provided two types of mesh data, as shown in Fig. 1. In both the sets of data, the magnetic material V in the shape of a short cylinder was divided into hexahedron elements. It was confirmed from these sets of data that the conventional H-matrices with ACA present as part of the HACApK failed to construct efficient approximations.

We applied the improved H-matrices with ACA+ to (4) and obtained an approximation of (5). The number of surface elements $N_S$was 31,666 (left) and 770 (right). We observed the values for maximum rank, average rank, and memory usage of the H-matrices by setting the tolerance to be ε =1.0e-2, 1.0e-3, and 1.0e-4, respectively. The results are given in Table I, which also includes the memory compressibility of the H-matrices against the dense matrices of equivalent sizes. In all cases, the ACA+ algorithm successfully constructed the low rank approximation in the form of (6) for all potential low-rank sub-matrices. The ranks of the approximated sub-matrices were suppressed under 30 even for the case where $N_S = 31{,}666$ and ε =1.0e-4. Although the memory compressibility is not excellent in the case of $N_S = 770$, the memory usage of the improved H-matrices constitutes only about 4% of that of the original dense matrix for the case of $N_S = 31{,}666$. We can expect significant benefits from the use of H-matrices when N_S is larger than at least several thousands.

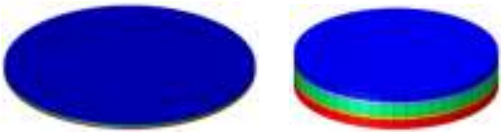

Fig. 1. Magnetic materials used for numerical experiments.

TABLE I
RANKS, MEMORY USAGE AND COMPRESSIBILITY OF H-MATRICES

ε	$N_S = 31{,}666$			$N_S = 770$		
	Rank Max/Ave.	Memory (MB)	Compress-ibility(%)	Rank Max/Ave.	Memory (MB)	Compress ibility(%)
1.0E-2	7/1	231	3.02	5/1	1.32	29.0
1.0E-3	13/3	258	3.37	9/4	1.63	35.9
1.0E-4	30/8	331	4.33	14/7	2.15	47.2

V. REFERENCES

[1] W. Scholz, J. Filder, T. Schrefl, D. Suess, R. Dittrich, H. Forster and V. Tsiantos, "Scalable parallel micromagnetic solvers for magnetic nanostructures," *Computational Materials Science*, Vol. 28, pp. 366–383, 2003.

[2] W. Hackbusch, "A Sparse Matrix Arithmetic Based on H-matrices. I. Introduction to H-matrices," *Computing*, Vol. 62(2), pp. 89-108, 1999.

[3] A. Ida, T. Iwashita, M. Ohtani and K. Hirahara, "Improvement of Hierarchical Matrices with Adaptive Cross Approximation for Large-scale Simulation", *Journal of Information Processing*, Vol. 23, No. 3 pp. 366-372, 2015.

[4] A. Ida, T. Iwashita, T. Mifune and Y. Takahashi, "Parallel Hierarchical Matrices with Adaptive Cross Approxima-tion on Symmetric Multiprocessing Clusters," *Journal of Information Processing* Vol. 22, pp.642-650, 2014.

[5] S. Kurtz, O. Rain and S. Rjasanow, "The Adaptive Cross-Approximation Technique for the 3-D Boundary-Element Method," *IEEE Trans. Magn.*, Vol.38(2), pp.421-424, 2002.

[6] H. Forster, T. Schrefl, R. Dittrich, W. Scholz, and J. Fidler, "Fast Boundary Methods for Magnetostatic Interactions in Micromagnetics", *IEEE Trans. Magn.*, vol. 39, no. 5, pp.2513-2515, 2003.

[7] http://ppopenhpc.cc.u-tokyo.ac.jp/

[8] S. Börm, L. Grasedyck and W. Hackbusch, *Hierarchical Matrices, Lecture Note*, Max-Planck-Institut fur Mathematik, 2006, pp.71-74.