Journal of Computational Physics 229 (2010) 2544–2549

Contents lists available at ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

Kronecker product approximation of demagnetizing tensors for micromagnetics

A.V. Goncharov [a,*], G. Hrkac [a], J.S. Dean [a], T. Schrefl [a,b]

[a] Department of Engineering Materials, The University of Sheffield, Sheffield, UK
[b] Department of Computer Science, St. Poelten University of Applied Science, St. Poelten, Austria

ARTICLE INFO

Article history:
Received 18 June 2009
Received in revised form 26 November 2009
Accepted 2 December 2009
Available online 11 December 2009

Keywords:
Micromagnetics
Fast field
Low-rank

ABSTRACT

A comparison study of the asymptotic behavior between different compression techniques is reported. We show that by applying the Kronecker product approximation, the storage of a three-dimensional demagnetizing tensor with N^6 entries can be reduced to $O(N^2)$, showing a superlinear compression behavior. When magnetization and magnetostatic field vectors are stored in compressed forms, a superlinear speedup of a field evaluation is gained.

1. Introduction

The increasing industrial demand for large scale simulations leads to huge scale matrix equations, which require a high computational power. Various methods have been developed for data compression to treat such large matrices. Such techniques include Fast Multipole Method (FMM), *H*-matrices etc. [1,2]. Recently it has been shown that matrices, arising from the discretization of integral equations with fast decaying kernels, possess a good Kronecker product approximation [3–5]. Those matrices normally have a very small rank ($R \ll N$), which makes application of low-rank approximations feasible. More details on the Kronecker product approximation are given in Section 3. The advantage of this type of approximation compared to other techniques is its superlinear compression property. If in large scale three-dimensional simulations one space dimension is discretized by N cells, then a total number of cells is N^3. Direct integration algorithms will scale with a total number of cells squared giving N^6 for the full $N^3 \times N^3$ matrix. The Kronecker approximation allows us to store only $O(N^2)$ entries, which is less than the order of the original matrix. In the following we apply this type of approximation to the point-function demagnetizing tensor discretized on a tensor product grid, with N 1 nm cubic cells in each dimension. Using the demagnetizing tensor in the compressed form, the magnetostatic energy is calculated for problem sizes ranging from 10^3 cells to 8×10^6 cells. Corresponding problem sizes range from 13 Mb to approximately 500 Tb of RAM, for double precision numbers. Results of memory consumption are then compared with other common compression techniques. Magnetostatic energy and magnetization vectors are compressed using Kronecker format and evaluation times are also plotted versus problem sizes. All computations were performed using a 2 GHz processor with 3Mb L2 cache.

* Corresponding author. Tel.: +44 (0)1142226021.
E-mail addresses: a.goncharov@sheffield.ac.uk (A.V. Goncharov), g.hrkac@sheffield.ac.uk (G. Hrkac), j.dean@sheffield.ac.uk (J.S. Dean), t.schrefl@sheffield.ac.uk (T. Schrefl).

0021-9991/$ - see front matter © 2009 Elsevier Inc. All rights reserved.
doi:10.1016/j.jcp.2009.12.004

2. Discretization

The brief introduction of the problem being solved is given in this section. In following calculations the magnetostatic scalar potential formalism is used for the field evaluation inside the ferromagnetic body. The magnetic scalar potential at the position given by $\mathbf{r}$ and induced by the magnetization distributed over the domain Ω' is given by the following volume integral [6]:

$$\phi(\mathbf{r}) = \int_{\Omega'} \mathbf{M}(\mathbf{r}') \cdot \nabla' \left(\frac{\mathbf{1}}{|\mathbf{r} - \mathbf{r}'|} \right) d^3\mathbf{r}' \tag{1}$$

The magnetostatic field at location $\mathbf{r}$ is then given by

$$\mathbf{H}(\mathbf{r}) = -\nabla\phi = -\frac{\mathbf{1}}{\mathbf{4}\pi} \nabla \int_{\Omega'} \mathbf{M}(\mathbf{r}') \cdot \nabla' \left(\frac{\mathbf{1}}{|\mathbf{r} - \mathbf{r}'|} \right) d^3\mathbf{r}' \tag{2}$$

This integral can be quite difficult to solve analytically for the arbitrary shaped ferromagnetic body with a nonuniform magnetization distribution. The value of the field is found numerically using discretization. The computational domain Ω' is divided into computational cells. The integration over the domain with nonuniform magnetization is split into integrals over elements where magnetization is assumed to be constant. It is known that for a uniformly magnetized ferromagnetic body the demagnetizing field can be computed using the demagnetizing tensor [7]. In this case the new discretized equation is given by:

$$\mathbf{H}(\mathbf{r_i}) = \sum_{j=1}^{N^3} N(\mathbf{r_i})_\mathbf{j} \mathbf{M_j}, \tag{3}$$

where N^3 is the total number of cells and

$$N(\mathbf{r_i})_\mathbf{j} = -\frac{1}{4\pi} \int_{V_\mathbf{j}} \nabla\nabla' \left(\frac{1}{|\mathbf{r_i} - \mathbf{r}'|} \right) d^3\mathbf{r}' \tag{4}$$

is the point-function demagnetizing tensor for the **j**th cell. The field is evaluated at location $\mathbf{r_i}$, which is the centre of the **i**th cell. Integrals in (4) over cubic cells can be evaluated analytically as in [8]. The tensor has nine components and it is convenient to rewrite Eq. (3) in component form with $\mathbf{r_i}$ replaced by **i** index:

$$H^p_\mathbf{i} = \sum_{\mathbf{j}=\mathbf{1}}^{N^3} N^{pq}_\mathbf{ij} M^q_\mathbf{j} \tag{5}$$

Indices p and q in (5) run from 1 to 3 (for x, y and z, respectively) and same index implies summation over all components of the magnetization. Eq. (5) can be written in matrix form as:

$$H^p = N^{pq} M^q, \tag{6}$$

where N^{pq} is now a $N^3 \times N^3$ matrix with N^6 entries and H^p and M^q are vectors containing cartesian components of field and magnetization (both have length N^3).

3. Kronecker approximation

To show how the Kronecker approximation arises we shall start from the Eq. (6) for the magnetostatic field. Let us limit to the case where $p = q = 1$, i.e. $H^x(r) = N^{xx}(r, r')M^x(r')$. The procedure for all other cases is the same. On a cartesian grid, the indices $\mathbf{i}, \mathbf{j}$ in (3)–(6) are replaced with (i, j, k) and (i', j', k'), respectively. Then (5) can be written in tensor form:

$$H^x_{ijk} = \sum_{i'=1}^{N} \sum_{j'=1}^{N} \sum_{k'=1}^{N} N^{xx}_{ijki'j'k'} M^x_{i'j'k'} \tag{7}$$

where $H^x_{ijk} = H^x(x_i, y_j, z_k)$ is the x-component of the magnetostatic field in the centre of the (ijk) cell and $M^x_{i'j'k'}$ is the constant magnetization in the $(i'j'k')$ cell. The matrix N^{xx} can be viewed as a tensor:

$$N^{xx}_{ijki'j'k'} = \int_{V_{i'j'k'}} N^{xx}(x_i, y_j, z_k, x', y', z')\, dx'dy'dz' \tag{8}$$

If the kernel N^{xx} decays fast with the distance between the source and the field points, then the full tensor (8) has a small rank and can be approximated by a data sparse tensor [4,5]. If this is the case then the kernel allows a separable approximation with a small rank $R \ll N$:

$$N^{xx}(x, y, z, x', y', z') = \sum_{r=1}^{R} P^r(x, x') Q^r(y, y') R^r(z, z'), \tag{9}$$