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Computation of the magnetostatic interaction between linearly magnetized polyhedrons

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ABSTRACT

In this paper we present a method to accurately compute the energy of the magnetostatic interaction between linearly (or uniformly, as a special case) magnetized polyhedrons. The method has applications in finite element micromagnetics, or more generally in computing the magnetostatic interaction when the magnetization is represented using the finite element method (FEM).

The magnetostatic energy is described by a six-fold integral that is singular when the interaction regions overlap, making direct numerical evaluation problematic. To resolve the singularity, we evaluate four of the six iterated integrals analytically resulting in a 2d integral over the surface of a polyhedron, which is nonsingular and can be integrated numerically. This provides a more accurate and efficient way of computing the magnetostatic energy integral compared to existing approaches.

The method was developed to facilitate the evaluation of the demagnetizing interaction between neighbouring elements in finite-element micromagnetics and provides a possibility to compute the demagnetizing field using efficient fast multipole or tree code algorithms.

1. Introduction

In the continuum form of the Landau–Lifshitz–Gilbert equation, the effective field $\mathbf{H}_{\text{eff}}(\mathbf{r})$ is the functional derivative of the total energy functional $E(\mathbf{M})$ with respect to the magnetization $\mathbf{M}(\mathbf{r})$ [1]:

$$\mathbf{H}(\mathbf{r}) = -\frac{1}{\mu_0}\frac{\delta E}{\delta \mathbf{M}(\mathbf{r})} \tag{1}$$

$$E = E_{\text{Zeeman}} + E_{\text{demag}} + E_{\text{anisotropy}} + E_{\text{exchange}} + \cdots \tag{2}$$

In numerical micromagnetics, the dynamics of magnetization are described by the semi-discretized Landau–Lifshitz–Gilbert equation, in which the motion of magnetization is computed from the discretized effective field. It is desirable to preserve the relation (1) between effective field and total energy in the semi-discretized formulation [2] – if (1) holds for the discrete system, then the total energy will decrease in the simulation, simplifying the use of energy-based criteria for the control of the simulation or the search for an equilibrium.

In order to preserve (1), the effective field has to be computed from the discretized total energy function using the corresponding discrete counterpart to the functional derivative $\delta E/\delta \mathbf{M}(\mathbf{r})$. For the exchange, anisotropy, and Zeeman terms this is usually straightforward, however for the demagnetizing field it is more difficult. In finite difference (FD) micromagnetics, it can be achieved by computing the total demagnetizing energy of the system using the analytical expression [3–6] for the demagnetizing tensor, and then differentiating with respect to the degrees of freedom [7,2]. However, in finite element (FE) micromagnetics, the demagnetizing field is usually computed using the FEM/BEM method [8,9] where the field is derived from the magnetostatic potential, and the energy is not computed exactly.

It is therefore desirable to be able to accurately and efficiently compute the total magnetostatic energy of a system represented by a set of polyhedral elements, with magnetization linear inside each polyhedron (as in the FE method with linear Lagrange elements). The total energy of the system is the sum of pairwise interactions between the polyhedrons and in this paper we describe how to compute this pairwise interaction.

Given two interacting magnetized polyhedrons τ and τ' with arbitrary magnetizations $\mathbf{M}(\mathbf{r})$ and $\mathbf{M}'(\mathbf{r})$, the energy $E_{\tau\leftrightarrow\tau'}$ of the magnetostatic interaction between them is:

$$\begin{aligned} E_{\tau\leftrightarrow\tau'} &= -\mu_0 \int_{\tau} \mathbf{M}(\mathbf{r})\cdot\mathbf{H}'_{\text{demag}}(\mathbf{r})\, d\mathbf{r} \\ &= \frac{\mu_0}{4\pi}\int_{\tau}\int_{\tau'} \mathbf{M}(\mathbf{r})\cdot\left(\nabla_{\mathbf{r}}\nabla_{\mathbf{r}'}\frac{1}{|\mathbf{r}-\mathbf{r}'|}\right)\cdot\mathbf{M}'(\mathbf{r}')\, d\mathbf{r}\, d\mathbf{r}' \end{aligned} \tag{3}$$

where $\mathbf{H}'_{\text{demag}}(\mathbf{r}) = -\frac{1}{4\pi}\nabla_{\mathbf{r}}\int_{\tau'}\mathbf{M}'(\mathbf{r}')\cdot\nabla_{\mathbf{r}'}(1/|\mathbf{r}-\mathbf{r}'|)\, d\mathbf{r}'$ is the demagnetizing (stray) field produced by the polyhedron τ'.

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The straightforward approach of numerically computing the integral (3) is problematic because it requires explicit integration over a 6-dimensional region of space; additionally, when the polyhedrons overlap or coincide, the integrand is singular and regular integration methods cannot be applied. Many analytical results are available for similar 3-fold integrals arising during the calculation of the field [10–14]. However, none of the formulas can be easily adapted to this more complex 6d case. In [15] a method is developed for removing the singularity in (3) that can be applied to the uniform magnetization case but does not generalize easily to the linear magnetization case. A Fourier-transform method has been devised for the computation of magnetostatic energy [16,17], however for the case investigated in this paper, the required 3d numerical integration in the Fourier space is still somewhat impractical.

The rest of the paper describes the proposed method for the computation of this integral. The main approach is to analytically perform 4 out of 6 iterated integrals resulting in a 2d surface integral that is nonsingular and can be evaluated numerically using standard methods. This semi-analytical approach is similar to [18]; the use of notation and vector analysis in the analytical derivation is similar to the techniques in [13,14].

2. Formulation of the problem

For the purposes of computation, an arbitrary linear vector-valued function in space $\mathbf{M}(\mathbf{r})$ can be represented by a 3×4 matrix $\| M_{ij} \|$: $\mathbf{M}(\mathbf{r}) = \| M_{ij} \| \cdot (1, r_x, r_y, r_z)^T$. However, performing analytical calculations for this general case is quite inconvenient; instead we only consider vector-valued linear functions of the form $A(\mathbf{r})\mathbf{M}$ where $A(\mathbf{r})$ is a scalar linear function and $\mathbf{M}$ is a constant vector. For the common case of a tetrahedral element, an arbitrary linear vector-valued function $\mathbf{M}(\mathbf{r})$ can be reconstructed from the vertex values $\mathbf{M}_i$, $i = 1\ldots4$: $\mathbf{M}(\mathbf{r}) = \sum_{i=1}^{4} A_i(r)\mathbf{M}_i$, where $A_i(r)$ are the shape functions of the tetrahedron.

We perform the computations for a pair of interacting linearly magnetized polyhedrons τ and τ' with magnetizations $A(\mathbf{r})\mathbf{M}$ and $B(\mathbf{r})\mathbf{M}'$, where $\mathbf{M}$ and $\mathbf{M}'$ are constant magnetization vectors and $A(\mathbf{r})$, $B(\mathbf{r})$ are dimensionless linear functions in space (Fig. 1). From (3), the energy $E_{\tau\leftrightarrow\tau'}$ of the magnetostatic interaction between the polyhedrons is $E_{\tau\leftrightarrow\tau'} = \frac{\mu_0}{4\pi}\mathbf{M}\cdot\mathbf{N}\cdot\mathbf{M}'$, where $\mathbf{N}$ is the symmetric 3×3 "demagnetizing tensor"

$$\mathbf{N} = \mathbf{N}(A, B, \tau, \tau') = \int_{\tau}\int_{\tau'} A(\mathbf{r})B(\mathbf{r}')\nabla_{\mathbf{r}}\nabla_{\mathbf{r}'}\frac{1}{|\mathbf{r}-\mathbf{r}'|}\,d\mathbf{r}\,d\mathbf{r}' \tag{4}$$

The goal of this paper is to compute this sixfold integral given the coordinates of the vertices of τ and τ' and the coefficients of the linear functions $A(\mathbf{r})$ and $B(\mathbf{r})$. When the polyhedrons τ and τ' are separated, the integral can be computed numerically, however when the polyhedrons overlap or coincide, the integrand is singular and standard numerical integration is inaccurate.

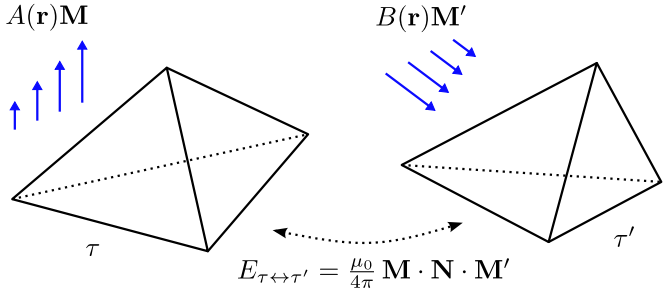

Fig. 1. The energy $E_{\tau\leftrightarrow\tau'}$ of the magnetostatic interaction between polyhedrons τ and τ' with magnetizations $A(\mathbf{r})\mathbf{M}$ and $B(\mathbf{r})\mathbf{M}'$, where $\mathbf{M}$ and $\mathbf{M}'$ are constant magnetization vectors and $A(\mathbf{r})$, $B(\mathbf{r})$ are dimensionless linear functions in space.

To deal with this issue, we analytically reduce the double volume integral (4) to a double surface integral, then evaluate the surface integral over $\mathbf{r}$ analytically, and the second surface integral over $\mathbf{r}'$ numerically. This procedure is similar to the one employed in [18] — the four analytical steps result in a surface integral with a bounded integrand that can be integrated numerically with reasonable accuracy and efficiency.

A short notice on units: the demagnetizing tensor commonly used in finite difference micromagnetics [4] is dimensionless, however the tensor $\mathbf{N}$ computed in this paper (4) has units of volume.

3. Method

The analytical derivation proceeds in the following three steps:

- transform the double volume integral (4) to a double surface integral using Gauss's theorem, removing linear factors via integration by parts (Section 4),
- express the integrand for the outer surface integral over $\mathbf{r}'$ as a linear combination of primitive terms (Section 5),

$$I_0(\tau;\,\mathbf{r}') = \int_{\partial\tau-\mathbf{r}'}\frac{1}{|\mathbf{R}|}\,ds \tag{5}$$

$$\mathbf{I}_1(\tau;\,\mathbf{r}') = \int_{\partial\tau-\mathbf{r}'}\frac{\mathbf{R}}{|\mathbf{R}|}\,ds \tag{6}$$

$$\mathbf{I}_2(\tau;\,\mathbf{r}') = \int_{\partial\tau-\mathbf{r}'}\frac{\mathbf{R}^{\otimes 2}}{|\mathbf{R}|}\,ds \tag{7}$$

  where $\partial\tau$ is the polygonal surface of the polyhedron τ, $\partial\tau-\mathbf{r}'$ is the same surface shifted by $\mathbf{r}'$ according to the substitution $\mathbf{R} = \mathbf{r}-\mathbf{r}'$, and $\otimes$ denotes tensor multiplication (i.e. $\mathbf{R}^{\otimes 2}$ is a symmetric tensor of rank 2).
- analytically integrate the primitive terms $\mathbf{I}_k$ over each polygonal surface, again by applying integration by parts, Stokes' theorem (for integration over a surface), and gradient theorem (for integration over a line), Section 5.1.

Eq. (16) derived in step 2 (see Section 5) together with the corresponding analytical formulas for the primitive terms $\mathbf{I}_k$ form the main result of the paper.

3.1. Auxiliary functions

The derivation of the analytical formulas for $\mathbf{I}_k$ requires the computation of a number of auxiliary functions:

$$J_0(\tau;\,\mathbf{r}') = \int_{\partial\tau-\mathbf{r}'}|\mathbf{R}|\,ds \tag{8}$$

$$\eta_0(\mathbf{R}_1,\,\mathbf{R}_2) = \int_{\mathbf{R}_1}^{\mathbf{R}_2}\frac{1}{|\mathbf{R}|}\,dl \tag{9}$$

$$\boldsymbol{\eta}_1(\mathbf{R}_1,\,\mathbf{R}_2) = \int_{\mathbf{R}_1}^{\mathbf{R}_2}\frac{\mathbf{R}}{|\mathbf{R}|}\,dl \tag{10}$$

$$\lambda_0(\mathbf{R}_1,\,\mathbf{R}_2) = \int_{\mathbf{R}_1}^{\mathbf{R}_2}|\mathbf{R}|\,dl \tag{11}$$

$$\boldsymbol{\lambda}_1(\mathbf{R}_1,\,\mathbf{R}_2) = \int_{\mathbf{R}_1}^{\mathbf{R}_2}\mathbf{R}|\mathbf{R}|\,dl \tag{12}$$

The relation between the formulas for these functions is shown below (an arrow indicates that the formula at the source depends on the formula at the target):