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Review

Numerical methods for the stray-field calculation: A comparison of recently developed algorithms

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ABSTRACT

Different numerical approaches for the stray-field calculation in the context of micromagnetic simulations are investigated. We compare *finite difference based fast Fourier transform methods*, *tensor-grid methods* and the *finite-element method with shell transformation* in terms of computational complexity, storage requirements and accuracy tested on several benchmark problems. These methods can be subdivided into integral methods (fast Fourier transform methods, tensor-grid method) which solve the stray field directly and in differential equation methods (finite-element method) which compute the stray field as the solution of a partial differential equation. It turns out that for cuboid structures the integral methods, which work on cuboid grids (fast Fourier transform methods and tensor-grid methods), outperform the finite-element method in terms of the ratio of computational effort to accuracy. Among these three methods the tensor-grid method is the fastest for a given spatial discretization. However, the use of the tensor-grid method in the context of full micromagnetic codes is not well investigated yet. The finite-element method performs best for computations on curved structures.

1. Introduction

Micromagnetic simulations nowadays are highly important for the investigation of ferromagnetic materials which are used in storage systems and electric motors and generators. In these simulations the magnetic state of the ferromagnet is represented by a classical magnetization vector field.

The computation of the non-local magnetostatic interactions is the most time-consuming part of micromagnetic simulations. Naive implementation of the superposition-based integral operators (5) or solvers for the underlying differential equation (Poisson equation (3)) yield computational costs proportional to the square of the number of grid points, i.e. $\mathcal{O}(N^2)$. Several methods have been introduced in the literature in order to reduce these costs.

The magnetic scalar potential can be computed by solving the Poisson equation. The solution of the Poisson equation with the finite-element method (FEM) has a complexity of $\mathcal{O}(N)$ if boundary conditions are given at the boundary of the sample and a multigrid preconditioner is used [1]. However, the stray-field problem has open boundary conditions, where the potential is known at infinity. Two possible solutions for the open boundary problem are the coupling of the boundary element method (BEM) with the finite-element method [2] and the application of a shell transformation [3]. BEM gives an additional complexity of $\mathcal{O}(M^2)$ where M is the number of boundary nodes. This complexity can be reduced to $\mathcal{O}(M \log M)$ by application of the $\mathcal{H}$-matrix approximation for the dense and unstructured boundary element matrices [4–6]. The storage requirements and computational complexity of the FEM with shell transformation will be described in the forthcoming text.

Another class of methods rely on the evaluation of volume and/or surface integrals for the direct computation of the magnetostatic potential or the field, e.g. fast multipole methods [7,8], nonuniform grid methods [9] and fast Fourier transform (FFT) methods [10,11], scaling from $\mathcal{O}(N)$ to $\mathcal{O}(N \log N)$. The more recent tensor-grid method (TG), which also belongs to this class scales even better under certain assumptions.

In this paper we compare recently developed algorithms, namely the FFT-based methods for the computation of the field via the scalar potential (SP) and directly (DM) [10,12], a recently developed approach from numerical tensor-structured methods (TG) [14], and the finite-element method with shell transformation (FES), which is a FEM method that does not rely on BEM approaches and thus only introduces sparse matrices.

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2. Stray-field problem

Consider a magnetization configuration $\boldsymbol{M}$ that is defined on a finite region $\Omega = \{\boldsymbol{r} : \boldsymbol{M}(\boldsymbol{r}) \neq 0\}$. In order to perform minimization of the full micromagnetic energy functional or solve the Landau–Lifshitz–Gilbert (LLG) equation it is necessary to compute the stray field within the finite region Ω. The stray-field energy is given by

$$e_d = -M_s \frac{1}{2} \int_\Omega \boldsymbol{M} \cdot \boldsymbol{H} \, \mathrm{d}^3\boldsymbol{r}. \tag{1}$$

The Landau–Lifshitz–Gilbert equation reads

$$\boldsymbol{M}_t = -\frac{\gamma}{1+\alpha^2} \boldsymbol{M} \times \boldsymbol{H}_{\mathrm{eff}} + \frac{\alpha\gamma}{M_s(1+\alpha^2)} \boldsymbol{M} \times (\boldsymbol{M} \times \boldsymbol{H}_{\mathrm{eff}}), \tag{2}$$

where α is the Gilbert damping constant and $\boldsymbol{H}_{\mathrm{eff}}$ is the effective field given by the variational derivative of the energy w.r.t. the magnetization [15,16]. In both cases the stray field is only required to be known within Ω. The stray field $\boldsymbol{H}$ has a scalar potential ϕ, which is the solution of a Poisson equation [17]

$$\boldsymbol{H} = -\nabla\phi, \tag{3}$$

$$\Delta\phi = \nabla \cdot \boldsymbol{M}. \tag{4}$$

The stray field $\boldsymbol{H}$ and thus also the scalar potential ϕ are required to vanish at infinity. This boundary condition is often referred to as open boundary condition [18].

3. Methods

3.1. FFT Methods (SP and DM)

One way to reduce the computational complexity is to employ the fast Fourier transform (FFT). FFT methods solve an integral solution of the Poisson equation by applying the convolution theorem. The solution to the Poisson equation (3) is given by the integral, see [17],

$$\phi(\boldsymbol{r}) = -\frac{1}{4\pi} \int_\Omega \frac{\nabla' \cdot \boldsymbol{M}(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} \, \mathrm{d}^3\boldsymbol{r}' + \frac{1}{4\pi} \int_{\partial\Omega} \frac{\boldsymbol{n}' \cdot \boldsymbol{M}(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} \, \mathrm{d}A', \tag{5}$$

which directly fulfills the required open boundary condition. Performing integration by parts yields

$$\phi(\boldsymbol{r}) = \frac{1}{4\pi} \int_\Omega \boldsymbol{M}(\boldsymbol{r}') \cdot \nabla' \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} \mathrm{d}^3\boldsymbol{r}' \tag{6}$$

$$\phi(\boldsymbol{r}) = \boldsymbol{S}(\boldsymbol{r}-\boldsymbol{r}') * \boldsymbol{M}(\boldsymbol{r}'). \tag{7}$$

By employing the convolution theorem

$$\phi = \boldsymbol{S} * \boldsymbol{M} = \mathcal{F}^{-1}(\mathcal{F}(\boldsymbol{S}) \cdot \mathcal{F}(\boldsymbol{M})), \tag{8}$$

this convolution can be discretized and solved with the fast Fourier transform. A prerequisite for this procedure is the usage of an equidistant grid, which is required for a discrete convolution. The stray field

$$\boldsymbol{H}(\boldsymbol{r}) = -\nabla\phi(\boldsymbol{r}), \tag{9}$$

can be obtained by applying finite differences. This method is referred to as the scalar-potential method (SP) in the following. It is described in detail in [10].

It is also possible to compute the stray field $\boldsymbol{H}$ directly as a result of a matrix–vector convolution.

$$\boldsymbol{H}(\boldsymbol{r}) = -\frac{1}{4\pi} \int \left(\nabla\nabla' \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} \right) \boldsymbol{M}(\boldsymbol{r}') \, \mathrm{d}^3\boldsymbol{r}' \tag{10}$$

$$\boldsymbol{H}(\boldsymbol{r}) = \boldsymbol{N}(\boldsymbol{r}-\boldsymbol{r}') * \boldsymbol{M}(\boldsymbol{r}'). \tag{11}$$

Here $\boldsymbol{N}$ denotes the demagnetization tensor. Similar to (8) the convolution can be solved as an element-wise matrix–vector multiplication in Fourier space. This method is referred to as the demagnetization-tensor method (DM) in the following and is implemented by different finite-difference codes [19,20,12]. For the numerical experiments we use MicroMagnum [12] which implements both the SP and the DM method.

3.2. Tensor grid methods (TG)

Tensor grid methods (TG) for micromagnetic stray-field computation were recently introduced in [14,21]. They were developed for the purpose of handling so called low-rank tensor or compressed tensor magnetization, see [22] for a survey, in order to accelerate the computations and relieve storage requirements, see [14]. In the following we give a brief introduction into the ideas behind this method, also see [14] for a detailed description.

3.2.1. Analytical preparations

The computation of the stray field within the magnetic body is based on the explicit integral formula for the scalar potential (6). The main idea is the usage of a representation for the integral kernel in (6) as an integral of a *Gaussian function* by the formula

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|^3} = \frac{2}{\sqrt{\pi}} \int_{\mathbb{R}} \tau^2 e^{-\tau^2|\boldsymbol{r}-\boldsymbol{r}'|^2} \, \mathrm{d}\tau, \tag{12}$$

which leads from (6) to

$$\phi(\boldsymbol{r}) = \frac{1}{2\pi^{3/2}} \int_{\mathbb{R}} \tau^2 \int_\Omega e^{-\tau^2|\boldsymbol{r}-\boldsymbol{r}'|^2} \boldsymbol{M}(\boldsymbol{r}') \cdot (\boldsymbol{r}-\boldsymbol{r}') \, \mathrm{d}^3\boldsymbol{r}' \, \mathrm{d}\tau. \tag{13}$$

Eq. (13) reduces the computation to independent spatial integrals along each principal direction (the part of the Ω integral without the magnetization is now a product of independent 1D integrals). This analytical preparation directly results in a reduction of the computational effort from $\mathcal{O}(N^2)$ to $\mathcal{O}(N^{4/3})$ if discretized on a *tensor-product grid* before even using compressed/low-rank tensor formats for the discretized magnetization components. A similar method was introduced for the computation of the electrostatic scalar potential [24].

The additional τ-integration is carried out by the exponentially convergent *Sinc quadrature* [25], the spatial integrals are computed by *Gauss–Legendre quadrature*, both resulting in a numerical error of about the machine epsilon.

3.2.2. Discretization on a tensor-product grid

The magnetic body Ω is discretized on a *tensor-product grid* arising from the tensor outer product of three vectors $h_p \in \mathbb{R}^{N_p}$, $p = 1 \ldots 3$ related to the grid spacings along each axis (see Fig. 1). This results in a not necessarily uniform *Cartesian grid* but in contrast to methods like DM/SP described before, tensor-grid methods make use of the tensor-product interpretation of such grids.

The magnetization on the center points of the cells is given as a 3-tensor [22] for each component, i.e.

$$\mathcal{M}^{(p)} \in \mathbb{R}^{N_1 \times N_2 \times N_3}, \quad p = 1 \ldots 3 \tag{14}$$

where N_1, N_2, N_3 are the number of cells in the principal directions. Thus it is possible to use *low-rank* representation for the magnetization like *Canonical/Parallel Factors Decomposition* (CP) or *Tucker formats*, see Appendix A or [22]. We obtain the potential on the center points of the computational cells, as the discrete