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SIMULATION OF 3D SPIN CHAINS WITH GEOMETRY-DRIVEN ANISOTROPY

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We develop a C-code based spin-lattice simulator SLaSi for magnetization dynamics in ferro- and antiferromagnets. It solves discrete dynamical Landau-Lifshitz-Gilbert equations taking into account exchange and coordinate-dependent anisotropy defined in terms of local discrete Frenet-Serret reference frame calculated on fly. Runge-Kutta-Fehlberg integration scheme of 4-5 order is used for description of time evolution. A user-friendly interface for sample and integrator parameters is developed.

Introduction

Exploration of modern ways for development of nanoelectronics devices actively utilizes phenomena in magnetic nanostructures. Extension of planar structures into the third dimension uncovers new phenomena based on an interplay between sample’s shape and magnetic sub-system through geometry-driven interactions like anisotropy and dipole-dipole interaction [1, 2]. One of the most simple and practically important case study of such systems are thin ferromagnetic wires where dipolar interaction results in a geometry-driven uni- and biaxial anisotropy respectively [3]. Their intensive study requires corresponding simulation tools, supporting different geometries and coordinate-dependent material parameters. Popular micromagnetic frameworks do not allow simulation of curvilinear systems due to finite differences discretization methods or do not support coordinate-dependent magnetic interactions [4]. To overcome these limitations we develop an extended version of spin-lattice simulator SLaSi with an embed calculation of geometrical parameters crucial for arbitrary shape spin chains [5].

Model

SLaSi solves the Landau-Lifshitz-Gilbert equation to determine the time evolution of ferromagnetic spin chain, written in terms of magnetic moments per lattice site

$$\frac{d\mathbf{m}_n}{dt} = -\gamma m_n \times \mathbf{H}_n^{\text{eff}} + \alpha_n \mathbf{m}_n \times \frac{d\mathbf{m}_n}{dt}, \quad n = 1, N, \quad (1)$$

where $\gamma > 0$ is the gyromagnetic ratio, $\alpha_n$ is Gilbert damping coefficient, $N$ is the number of spins, and $\mathbf{H}_n^{\text{eff}} = \frac{1}{M_S} \frac{dH}{dn} \mathbf{m}_n$ is the effective field for n-th magnetic moment with $M_S$ being the saturation magnetization and Heisenberg Hamiltonian

$$H = -S^2 \sum_{i=1}^{N-1} J_{i,i+1} (\mathbf{m}_i \cdot \mathbf{m}_{i+1}) - \frac{S^2}{2} \sum_{i=1}^{N} \sum_{k=1}^{3} K^k_i (\mathbf{m}_i \cdot \mathbf{e}_k^i)^2, \quad (2)$$

where $S$ is spin length, $J_{i,i+1}$ represents exchange integral between neighboring sites, $K^k_i$ is the anisotropy coefficient and $\mathbf{e}_k^i$, with $k = 1, 3$ is the direction of the axis of single-ion anisotropy in the i-th site (three axes are supported). Model (2) is appropriate for description of spin chains in a quasi-classical limit, quasi-one-dimensional systems like ferromagnetic wires and thin ferromagnetic ribbons.

Due to physical background of appearance of anisotropy in spin chains, the most natural definition of anisotropy in (2) is based on a local reference frame defined according to spin chain shape. The key feature of the new version of SLaSi software module is the on-fly calculation of discrete Frenet-Serret local reference frame [6] with tangential, normal and binormal unit vectors: $\mathbf{T}, \mathbf{N}$ and $\mathbf{B}$, respectively, using sites coordinates only. In the laboratory reference frame local anisotropy direction is

$$\left(\mathbf{e}_i^k\right)_{\text{Cartesian}} = (\mathbf{T} \quad \mathbf{N} \quad \mathbf{B}) \cdot \mathbf{e}_i^k, \quad \text{with} \quad \mathbf{e}_i^k = \begin{pmatrix} e_{it}^k \\ e_{in}^k \\ e_{ib}^k \end{pmatrix}, \quad i = 1,N, \quad k = 1,3. \quad (3)$$

Here index $i$ enumerates lattice site, $k$ enumerates anisotropy term in (2) and $e_{iq}^k$ with $q = t, n, b$ give the direction of anisotropy axis relative to the local basis. For example, the easy-tangential anisotropy induced
by a dipole-dipole interaction in a ferromagnetic wire is defined by $\mathbf{e}_i = (1 \ 0 \ 0)^T$ from the user side. While tangential, normal and binormal directions are not defined for straight wires, Cartesian reference frame is used with the spin chain direction along an abscissa.

**Testing**

SLaSi is developed using C language. Runge-Kutta-Fehlberg scheme of 4-5 order (RKF45) is used for the integration of (1) for a flexible time step correction. Dependence of parameters of precision to the value of error was calculated as absolute difference between the theoretical and the experimental modeled result, see Fig. 1. The initial magnetization distribution in the laboratory reference frame is $\mathbf{m}_0 = \left( \frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}, 0 \right)$, with uniform exchange $J = J_{i,i+1}$ for all $i = 1,N$, magnetic length $\ell = a\sqrt{J/K_1} = 5a$ measured in lattice constant $a$ units and Gilbert damping $\alpha = 10^{-2}$ for 100 spins.

**Conclusion**

We have developed a new version of spin-lattice simulator SLaSi for modeling curved spin chains using the Heisenberg Hamiltonian with geometry-determined anisotropy. It is tested using known exact analytical solutions for straight and 3D curved samples (helix). Implemented on-fly determination of geometrical parameters in terms of tangential, normal and binormal unit vectors opens a way for studying a wider range of magnetic samples.

**References**


