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MNPDynamics: A computational toolbox for simulating magnetic moment behavior of ensembles of nanoparticles

H. Albers[1,*] · T. Kluth[1] · T. Knopp[2,3]

[1]Center for Industrial Mathematics, University of Bremen, Bremen, Germany
[2]Section for Biomedical Imaging, University Medical Center Hamburg-Eppendorf, Hamburg, Germany
[3]Institute for Biomedical Imaging, Hamburg University of Technology, Hamburg, Germany
[*]Corresponding author, email: halbers@math.uni-bremen.de

Abstract

In the context of system function modeling for magnetic particle imaging, computing fast and accurate approximations to the time evolution of magnetic nanoparticles' (MNPs) mean magnetic moment is a problem of interest. In a software toolbox we comprise algorithms and methods that can simulate Brownian and Néel relaxation of MNPs' magnetic moments that can be used to obtain more accurate model-based system matrices than those relying on the so-called equilibrium model. We present and discuss results obtained with these implementations which are made available in the software toolbox under github.com/MagneticParticleImaging/MNPDynamics.jl to inspire further research in these directions.

I Introduction

In magnetic particle imaging, a central problem of interest is the accurate modeling of the system function, reducing or even eliminating the need for "delta probe'" sampling, which is time-consuming and results in suboptimal spatial resolution. The system function $s_l : \mathbb{R}^3 \times I \to \mathbb{R}$ for the l'th receive coil in the scanner, describing the physical behavior of the system, is modeled as

$$s_l(x,t) := \int_I -a_l(t-t')\mu_0 p_l(x)^t \frac{\partial}{\partial t}\bar{m}(x,t)\,dt' \qquad (1)$$

where $I = [0,T]$ is the measurement time, $a_l : [-T,T] \to \mathbb{R}$ is the analog filter for the l'th receive coil, $p_l : \mathbb{R}^3 \to \mathbb{R}^3$ denotes the sensitivity profile of the receive coil unit, and $\bar{m}$ stands for the mean magnetic moment of the magnetic nanoparticles (MNPs) [1]. The dependence of the mean magnetic moment on the applied magnetic field $H_{app} : \mathbb{R}^3 \to \mathbb{R}^3$ and the physical properties of the MNPs is the crucial aspect of the system function modeling.

The most common approach to model $\bar{m}$ is to employ the so-called equilibrium model, i.e. introducing an appropriately parameterized Langevin function $L : \mathbb{R} \to \mathbb{R}$ and setting $\bar{m} := \mathcal{L}(|H_{app}|)H_{app}/|H_{app}|$ [2]. However, as the name suggests, this model is only a valid approximation for MNPs that are in or sufficiently close to thermodynamic equilibrium.

A more accurate way to model MNPs' behavior is to consider magnetization dynamics of the magnetic moments, i.e. Brownian (the whole particle rotates in a viscous fluid) and Néel relaxation (the particle's magnetic moment moves relative to the particle's position). In practice, one of each mechanisms is usually dominant [3]. Each case requires either the solution of many stochastic ordinary differential equations (ODEs) or that of a parabolic partial differential equation (PDE) on the sphere. For a detailed overview of the relaxation mech-

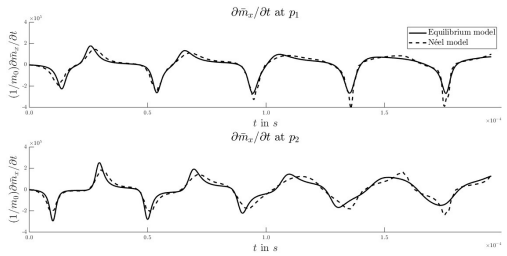

Figure 1: A numerical simulation for MNP relaxation in a field of view typical for MPI. Significant differences can be observed between the equilibrium model and the Néel model. For $\Omega = [-15,15]^2$ (in mm), we consider the points $p_1 = (-5,10)$, $p_2 = (0,2)$.

anisms and their mathematical description, see [1]. In this work, we introduce a computational toolbox for Julia and Matlab to numerically determine a solution of the mean magnetic moment of an ensemble of MNPs using the PDE approach and thus for modelling the system function. The toolbox is available at https://git.io/JertZ.

II Methods

In order to describe the behavior of an entire ensemble of MNPs one can consider the probability density function $f : S^2 \times I \to \mathbb{R}_+$ with respect to the orientation of the MNPs and time (S^2 being the unit sphere in $\mathbb{R}^3$). The computation of the mean magnetic moment $\bar{m}(x,t) = m_0 \int_{S^2} m f(m,x,t) dm$ for each position $x \in \Omega \subset \mathbb{R}^3$ is based on the solution f to the Fokker-Planck equation

$$\frac{\partial}{\partial t} f = \mathrm{div}_{S^2}\left(\frac{1}{2\tau}\nabla_{S^2} f\right) - \mathrm{div}_{S^2}(\vec{b} f). \tag{2}$$

The vector field $\vec{b} : S^2 \times \mathbb{R}^3 \times S^2 \to \mathbb{R}^3$ is given by

$$\begin{aligned}\vec{b}(m,H,n) = {} & p_1 H \times m + p_2 (m \times H) \times m + \\ & p_3 (n \cdot m) n \times m + p_4 (n \cdot m)(m \times n) \times m \end{aligned} \tag{3}$$

where $n \in S^2$ is the easy axis and we use for Néel relaxation $p_1 = \tilde{\gamma}\mu_0$, $p_2 = \tilde{\gamma}\alpha\mu_0$, $p_3 = 2\tilde{\gamma}\frac{K_{anis}}{M_S}$, $p_4 = 2\alpha\tilde{\gamma}\frac{K_{anis}}{M_S}$ and $\tau = \frac{V_C M_S}{2k_B T_B \tilde{\gamma}\alpha}$ ($\tilde{\gamma} = \frac{\gamma}{1+\alpha^2}$). The Brownian case is covered by an analogous parameterization where in particular $p_1 = p_3 = p_4 = 0$. Note that the parabolic PDE is parametric in $x \in \Omega$ enabling more efficient computations in parallel.

We include two methods to solve the Fokker-Planck equation numerically. The first one is a Galerkin method using spherical harmonics. The other one is a grid-based method which relies on a discretization of the unit sphere into spherical triangles. In both cases, the idea is to only discretize in the space variable m in order to approximate (2) by a system of ordinary differential equations, which can then be solved by a suitable numerical solver for ODEs.

II.I Expansion into spherical harmonics

The Galerkin method is derived as follows: Choose an appropriate Hilbert space $\mathscr{H}$ to search the solution f in, choose an orthogonal basis for this space, and insert the expansion of f in this basis into the PDE. Then, the PDE is multiplied with an arbitrary function from $\mathscr{H}$ and integrated. The discretization part is then simply choosing a finite-dimensional subspace of $\mathscr{H}$, or equivalently, truncating the expansion of f after a fixed index N. Expanding $f(m,t) = \sum_{k=1}^{\infty} C_{r_k}^{q_k}(t) Y_{r_k}^{q_k}(m)$, where $Y_{r_k}^{q_k}$ is the spherical harmonic function for indices q_k, r_k, $k \in \mathbb{N}$, we obtain with this method

$$\begin{aligned}\frac{\partial C_{r_k}^{q_k}}{\partial t} = {} & \frac{1}{2\tau} r_k (r_k + 1) \\ & - \frac{2r_k + 1}{4\pi(-1)^{q_k}} \sum_{i=1}^{\infty} \int_{S_2} (\vec{b} \cdot \nabla Y_{r_i}^{q_i})(Y_{r_k}^{q_k})^* d\sigma \end{aligned} \tag{4}$$

for each $k \in \mathbb{N}$. While the evaluation of the second term on the right-hand side of (4) generally requires computing N integrals numerically for each $k = 1,\dots,N$, it can be reduced to a small number of terms being calculated in advance for $\vec{b}$ as in (3) and a fixed easy axis n (see also [4]). We have extended this result to admit a time-dependent easy axis.

II.II Finite Volume method

For this grid-based method, we assume that we have a triangulation of the sphere that decomposes it into spherical triangles $T_i, i = 1,\dots,N$. For $x \in T_i$, we consider the discretization of f such that $f(x) \approx f_i := \frac{1}{|T_i|}\int_{T_i} f(x) dx$.

Thus, we obtain the equations

$$\frac{\partial}{\partial t} f_i = \frac{1}{|T_i|}\int_{T_i} \mathrm{div}(-\vec{b} f) dx + \frac{1}{|T_i|}\int_{T_i} \frac{1}{2\tau}\delta f dx \tag{5}$$

for $i = 1,\dots,N$. Then, we apply the divergence theorem and denote the edges of a triangle T_i by E_{i_1}, E_{i_2}, E_{i_3}, yielding

$$\frac{\partial f_i}{\partial t} = -\frac{1}{|T_i|}\sum_{j=1}^{3}\left[\int_{E_{i_j}} \vec{b} f \cdot \vec{e}_{i_j} d\sigma - \frac{1}{2\tau}\int_{E_{i_j}} \nabla f \cdot \vec{e}_{i_j} d\sigma\right] \tag{6}$$

where $\vec{e}_{i_j}$ is the outer surface normal on the j'th edge of the i'th triangle. These line integrals are then approximated using the midpoint rule, resulting in an ODE system for the values f_i.

III Results

With both proposed methods, a solution to the Fokker-Planck equation can usually be obtained within a few minutes. The calculation of a system function for a 30×30

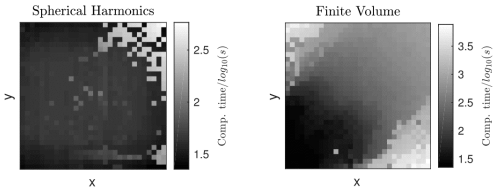

Figure 2: Computation times for each pixel for a 2D cosine excitation field. Three complete Langevin periods were computed for $K_{anis} = 625$ J/m^3 on a 30x30 grid. Plotted are the decadal logarithms of the computation times in seconds for the spherical harmonics as well as the Finite Volume approach.

pixel region of interest normally takes about two hours on 20 cores of two Intel Xeon E5-2687W v4 CPUs at 3 GHz. Since the 900 ODE systems that have to be integrated are not dependent on one another, parallelization is easy to achieve. However, the ODE system exhibit significant stiffness that appears to depend heavily on the physical parameters used, especially on the particle diameter and on the anisotropy coefficient K_{anis} but also on the static offset field as shown in Fig. 2.

Furthermore, the toolbox allows for an easy comparison of different models as can be seen in Fig. 1.

IV Discussion

As shown in [5], the particle dynamic models employed here yield promising results and constitute one step towards more accurate modeling of the MPI system function. With this toolbox, we hope to inspire more research in this direction, with respect to improving the proposed algorithms as well as their application to the magnetic particle imaging and calibration problem.

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