Computational Tool for Evaluating the Electromagnetic Response of Distributions of Magnetic Nano-particles

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1 Abstract

Analyzing effective electromagnetic properties of mixtures is a problem that dates back at least a century to explaining the origin of colors in stained glass windows. Since then literature is abundant with effective medium theories that have been used to design dielectric materials. The unsolved problem is the design of magnetic properties; this takes on new importance as having the ability to tailor both electric and magnetic properties simultaneously is critical to miniaturization. It is desirable to model nano-scale electromagnetic interactions to study these macroscopic magnetic properties. The physics involved will be accounted for via classical field propagators together with the Landau-Lifshitz-Gilbert (LLG) equation that parametrizes the response of a single particle.

2 Introduction

Magnetic nano-particles exist with a collection of intrinsic magnetic dipoles due to the spin of unpaired electrons known as magnetization. The objective of this simulation is to track the magnetizations of distributions of magnetic nano-particles in response to electromagnetic fields. There are four sources of electromagnetic fields in the system: scattered fields, exchange fields, anisotropy fields, and incident fields. The magnetization's response to these fields is modeled by the LLG equation which is solved self-consistently with the field equations in an integral equation framework.

3 Fields

The total magnetic field in the system is decomposed into four major components: scattered fields, anisotropy fields, exchange fields and incident fields, respectively [1]:

$$\boldsymbol{H}(\boldsymbol{r},t) = \boldsymbol{H}_s + \boldsymbol{H}_{ani} + \boldsymbol{H}_{exc} + \boldsymbol{H}_{inc} \tag{1}$$

The scattered fields come from radiation from the nano-particles in the simulated system and are given by:

$$\boldsymbol{H}_s(\boldsymbol{r},t) = \frac{4\pi\epsilon\omega^2}{c^2}\int_V [\bar{\boldsymbol{I}} + \frac{\nabla\nabla\cdot}{k^2}]\frac{e^{-jkR}}{4\pi R}\boldsymbol{M}(\boldsymbol{r}',t)dV' \tag{2}$$

We are required to do singularity extraction on this equation. This results in a term encapsulating the fields due to all particles not at $\boldsymbol{r}$ and a self-term encapsulating the fields due to the particle at $\boldsymbol{r}$. The scattered fields can then be written as:

$$\boldsymbol{H}_s(\boldsymbol{r},t) = 4\pi\epsilon k^2 \int_V [P.V.[\bar{\boldsymbol{I}} + \frac{\nabla\nabla\cdot}{k^2}]\frac{e^{-jkR}}{4\pi R} - \frac{\bar{I}\delta(\boldsymbol{r}-\boldsymbol{r}')}{3k^2}]\cdot\boldsymbol{M}(\boldsymbol{r}',t)dV' \tag{3}$$

where the principal volume simply excludes when $\boldsymbol{r} = \boldsymbol{r}'$. The anisotropy fields are given by:

$$\boldsymbol{H}_{ani}(\boldsymbol{r},t) = \frac{2K_u}{\mu_0 M_s^2}(\boldsymbol{M}(\boldsymbol{r}',t)\cdot\hat{\boldsymbol{k}})\hat{\boldsymbol{k}} \tag{4}$$

and the exchange fields are given by:

$$\boldsymbol{H}_{exc}(\boldsymbol{r},t) = \frac{2A}{\mu_0 M_s^2}\nabla^2\boldsymbol{M}(\boldsymbol{r}',t) \tag{5}$$

The incident field is any combination of a modulated gaussian pulse and a DC biasing field.

4 Magnetization Dynamics

The Landau-Lifshitz-Gilbert equation shown below is a differential equation parameterizing the electromagnetic response of magnetic nano-particles [6]. Shown below is the LLG equation with function dependencies omitted for succinctness.

$$\dot{\boldsymbol{M}} = \gamma_0 \boldsymbol{M} \times \boldsymbol{H} - \frac{\gamma_0 \alpha}{(1+\alpha^2) M_s} \boldsymbol{M} \times \boldsymbol{M} \times \boldsymbol{H} \tag{6}$$

where γ_0 is the gyromagnetic ratio of an unpaired electron, α is a dimensionless damping constant and M_s is the saturation magnetization. The two characteristics of a particles's temporal response are: precession about the magnetic field axis and alignment the magnetic field axis. Meanwhile, the total energy in the system remains constant (i.e. $|\boldsymbol{M}| = M_s$).

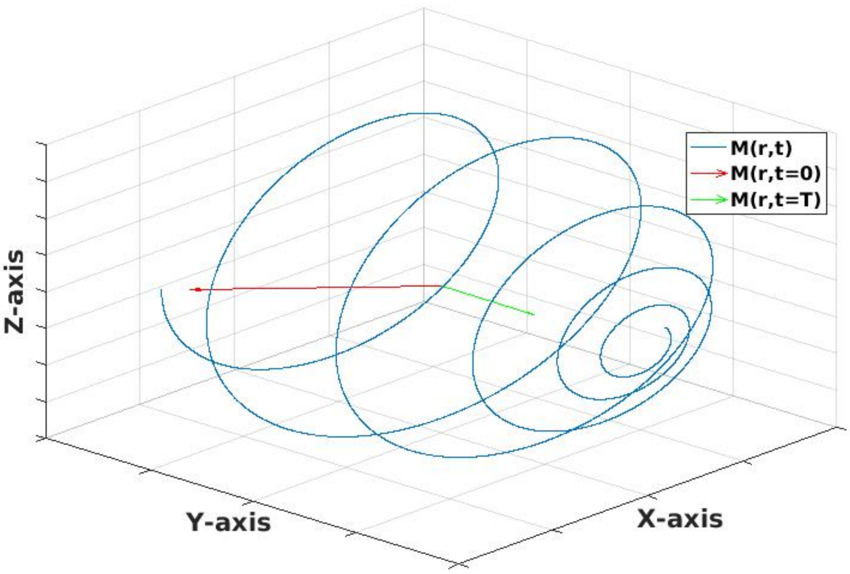

Figure 1: 3D plot showing the magnetization dynamics of a single particle as obtained from the simulation with the following inputs: total time $T = 20ps$, $\Delta t = 10^{-15}s$, damping constant $\alpha = 0.005$, saturation magnetization $M_s = 2 \times 10^6 \frac{A}{m}$, and a DC bias of $\boldsymbol{H}_{inc} = 10^3 \hat{\boldsymbol{y}} \frac{A}{m}$

5 Proposed Solution

The LLG equation is a highly nonlinear ODE making it impossible to solve analytically and difficult to solve numerically. In order to get a correct and stable solution, there are physical constraints placed on the systems that can be simulated. These will be discussed later, but a modification to temporarily alleviate them is to set the speed of light to infinity. This forces fields to travel instantaneously from one particle to another. Mathematically, it reduces the number of terms in $\boldsymbol{H}_s$. The solution also ignores the exchange and anisotropy fields at the moment.

Solving the LLG equation is done using a jacobian free Newton Krylov (JFNK) formulation. This refers to the fact that the solution to the LLG is set up as solving a matrix-vector product, $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$, for $\boldsymbol{x}$. Jacobian free refers to the fact that the matrix-vector product involved can be computed without explicitly forming the jacobian matrix. In this case, a matrix-vector product is derived from a Taylor expansion of $\dot{\boldsymbol{M}}_n^{m+1}$ about $\boldsymbol{M}_n^m$ in the backward Euler method and is shown below. [1][2]

$$[\bar{\boldsymbol{I}} + \Delta t \boldsymbol{J}_{\dot{\boldsymbol{M}}}(\boldsymbol{M}_n^m)] \boldsymbol{v}_n^{m+1} = \boldsymbol{M}_{n-1} - \boldsymbol{M}_n^m + \Delta t \dot{\boldsymbol{M}}_n^m \tag{7}$$

where m is the current iteration, $\bar{\boldsymbol{I}}$ is the identity matrix, $\boldsymbol{J}_{\dot{\boldsymbol{M}}}(\boldsymbol{M}_n^m)$ is the jacobian of $\dot{\boldsymbol{M}}$ and $\boldsymbol{v}_n^{m+1} = \boldsymbol{M}_n^{m+1} - \boldsymbol{M}_n^m$. Solving this system begins with guessing the current iteration then using an update routine each iteration thereafter. One way that $\boldsymbol{v}_n^{m+1}$ is updated is by using GMRES until a desired tolerance is met. The second way to update $\boldsymbol{v}_n^{m+1}$ is using Neumann iterations. The formulation changes slightly to:

$$\boldsymbol{v}_n^{m+1} = \boldsymbol{M}_{n-1} - \boldsymbol{M}_n^m + \Delta t \dot{\boldsymbol{M}}_n^m - \Delta t \boldsymbol{J}_{\dot{\boldsymbol{M}}}(\boldsymbol{M}_n^m)\boldsymbol{v}_n^m \tag{8}$$

6 Results

The following results demonstrate the accuracy of this solution methodology. Figure 2 shows the solver's error in solving an ODE with a known analytical solution [3]. As the number of timesteps increases (i.e. as timestep size decreases), the error decreases meaning the solver is accurate and controllable.

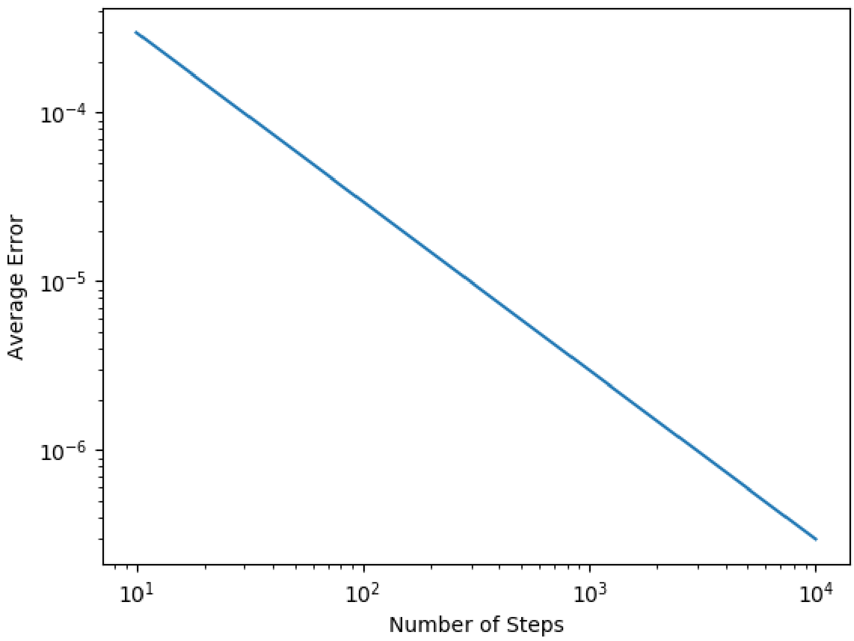

Figure 2: A plot showing the L2-norm error between the analytical solution to $\dot{\boldsymbol{u}} = \boldsymbol{u} \times \boldsymbol{\alpha}$ and the numerical solution using the JFNK formulation and Neumann iterations.

Figure 3 demonstrates the accuracy and controllability of the solution methodology when solving the LLG equation. As we increase the number of timesteps, error drops.

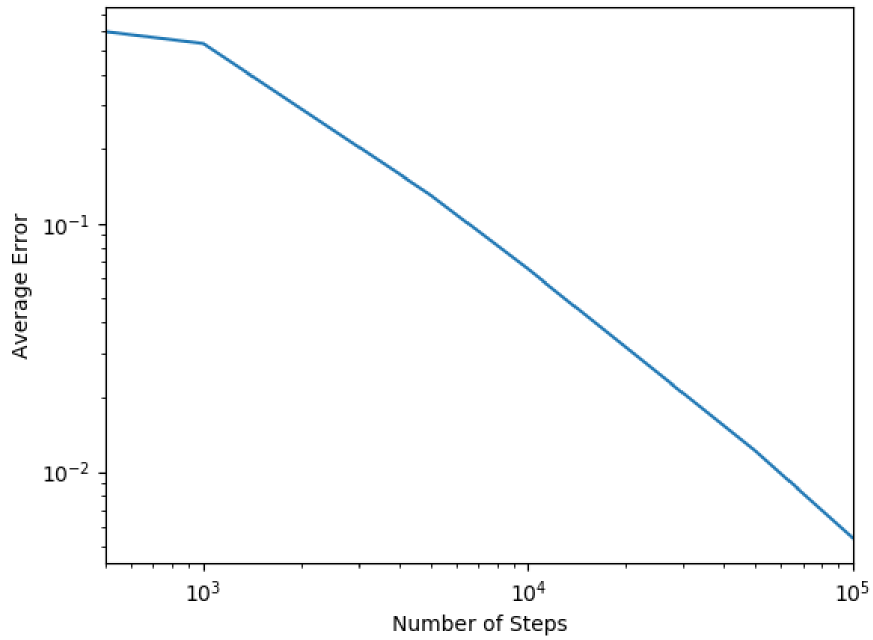

Figure 3: A plot showing the L2-norm error convergence of various numbers of timesteps taken to solve the full LLG equation for a one particle system compared with 5×10^5 timesteps using the JFNK formulation and Neumann iterations

The following two figures show the dynamics of magnetic nano-particles simulated in a single particle and multi-particle system.

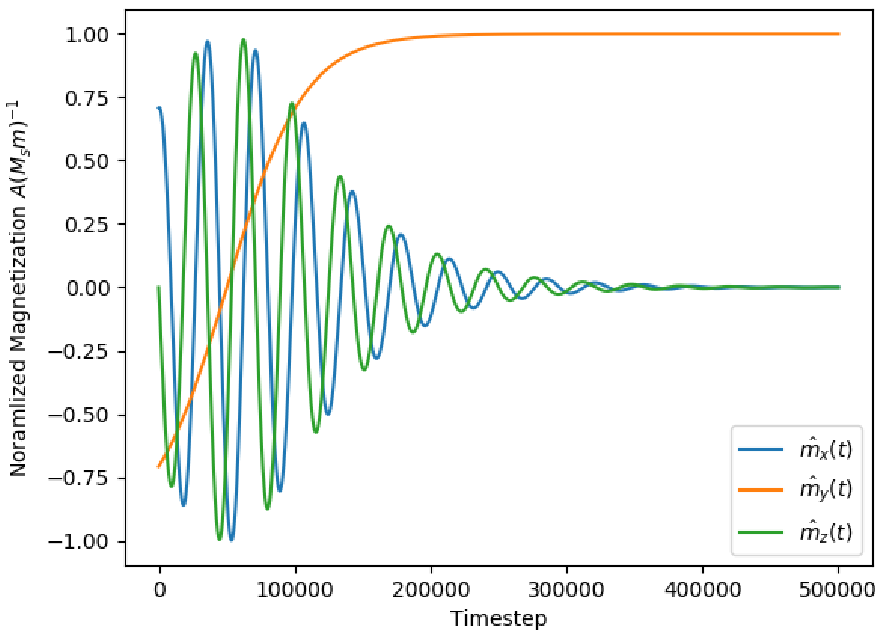

Figure 4: A plot showing the electromagnetic response of a single magnetic nano-particle reaching steady state in a DC biasing field. Obtained via JFNK formulation with Neumann iterations. Parameters: $T = 10^{-18}s$, $\alpha = 0.01$, $M_s = 10^6 \frac{A}{m}$, $\boldsymbol{H}_{inc} = 10^3 \hat{\boldsymbol{y}} \frac{A}{m}$

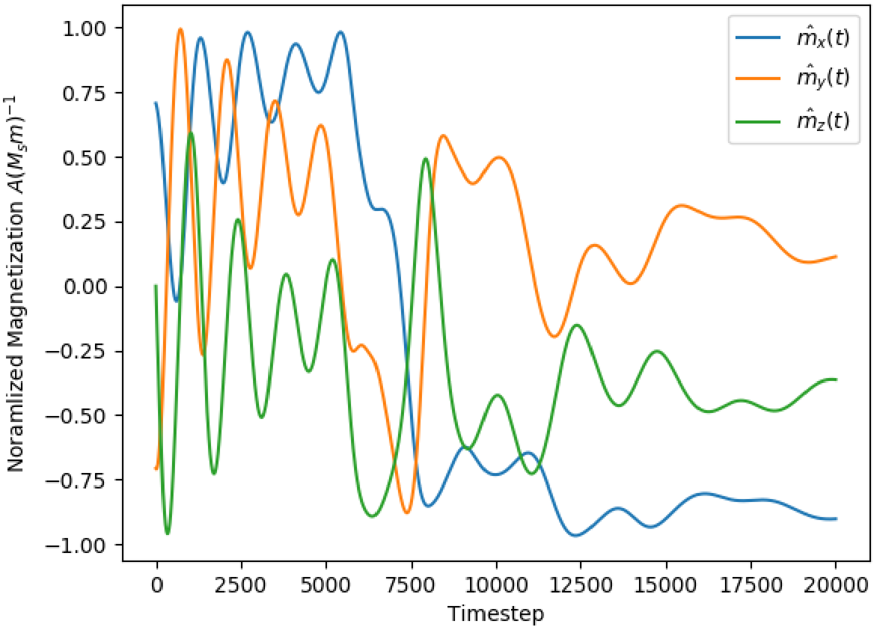

Figure 5: A plot showing a much more irregular response dominated by interactions between particles compared with Figure 4. The system consists of 4 magnetic nano-particles solved with the JFNK formulation and Neumann iterations. Parameters: $T = 10^{-19}s$, $\alpha = 0.01$, $M_s = 10^6 \frac{A}{m}$, $\boldsymbol{H}_{inc} = 10^3 \hat{\boldsymbol{y}} \frac{A}{m}$, $R \approx 10^{-2}m$

Figure 5 gives insight into the physical constraints this simulation faces. In order to obtain accurate results from the simulation with a multi-particle system, the particles need to be either sufficiently far apart or have a small enough timestep size. In the multi-particle system of figure 5, the particles are on the order of centimeters apart. If placed closer, the strength of the scattered fields grows thus decreasing the duration of the magnetization dynamics and forcing the simulation to become innacurate unless timestep size is decreased. One can infer that limitations eventually form on what can be simulated due to computer memory and run time constraints.

7 Future Work

The physical limitation of what can be simulated should be addressed next. Realistic materials cannot be handled as the simulation stands due to the physical constraints on particle separation and timestep size. We need to be able to simulate more particles with smaller separations without running up the compute time of the simulation than what is currently possible. The total time that interesting magnetization dynamics occurs is also worryingly low. For example, in a single particle system like shown in Figure 4, the electromagnetic response reaches a steady state within 10^{-18} seconds—an unrealistically small amount of time. There are two potential leading causes of this issue. By adding in the exchange and anisotropy fields, there may be a decrease in the total magnetic fields in the system, thus slowing down the magnetization dynamics. The second cause may be due to unrealistically high input parameters such as the strength of $\boldsymbol{H}_{inc}$ and M_s. Addressing this issue should allow the speed of light to be set to its physical value.

References

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