Precession axis modification to a semianalytical Landau–Lifshitz solution technique

D. G. Porter[1,a)] and M. J. Donahue[1]
[1]*National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA*

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A recent article [Van de Wiele *et al.*, IEEE Trans. Magn. **43**, 2917 (2007)] presents a semianalytical method to solve the Landau–Lifshitz (LL) equation. Spin motion is computed analytically as precession about the effective field H, where H is assumed fixed over the time step. However, the exchange field dominates at short range and varies at the time scale of neighbor spin precessions, undermining the fixed field assumption. We present an axis corrected version of this algorithm. We add a scalar multiple of m to H (preserving torque and hence the LL solution) to produce a more stable precession axis parallel to the cross product of the torques $m \times H$ at two closely spaced time steps. We build a predictor-corrector solver on this foundation. The second order convergence of the solver enables calculation of adjustable time steps to meet a desired error magnitude.
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I. INTRODUCTION

At the heart of many micromagnetic simulation tasks is the computation of magnetization dynamics via numerical integration of the Landau–Lifshitz equation,

$$\frac{dm}{dt} = \frac{\gamma}{1+\alpha^2} m \times H - \frac{\alpha\gamma}{1+\alpha^2} m \times H \times m, \tag{1}$$

where $\gamma = -221$ kHz/(A/m) is the gyromagnetic constant, α is a dimensionless phenomenological damping parameter, m is a unit vector in the magnetization direction, and H is the effective field representing the effect of all energies included in the simulation. Solution schemes of increased efficiency are sought to permit simulations of larger objects over longer time intervals.

Some properties of Eq. (1) are noteworthy. Magnetization trajectories that solve the equation are norm preserving. The equation computes varying magnetization direction with time, while the magnetization magnitude remains fixed. Also, the change in magnetization direction m in response to the effective field H is entirely a function of $m \times H$. That is, the trajectory is determined by the torque, not by the field itself. Consequently, so long as we preserve torque, we are free to modify the value of H as needed to pursue other goals. Finally, we note that each of the two terms of Eq. (1) can be described by its effect on the trajectory. When the damping parameter α is near zero, the influence of the damping term fades and the precession term dominates.

Many general numerical integration algorithms are not tailored to computing norm-preserving trajectories. When these algorithms are applied to Eq. (1) in micromagnetic simulation work, it is common practice to augment them with renormalization from time to time during the computation. Different renormalization schemes combined with various numerical integration algorithms give rise to different systematic computational errors.

Motivated by these factors, alternative numerical integration schemes have been proposed[1–4] that directly account for the norm-preserving nature of Eq. (1). Some of these schemes take simulation steps made up of rotations rather than straight-line increments. Such schemes are expected to better track trajectories when precession dominates, offering the hope of acceptably accurate results even when employing larger time steps. The result is increased simulation efficiency. In this paper, we examine the scheme of Ref. 1 and offer improvements to it.

II. ANALYSIS

The fast semianalytical scheme presented in Ref. 1 begins with the observation that so long as H remains fixed, the trajectory of m can be computed analytically. Because H is a function of m, we cannot expect it to truly remain fixed, but so long as time steps are kept small enough, the error created by this approximation can be kept acceptably low. For a typical simulation, it was reported that compared to solver schemes such as the Euler and Heun methods, full trajectory simulations to equilibrium could be completed using longer time steps, and consequently fewer total calculations.

In simulations where exchange energy plays a leading role, we expect the assumptions of the semianalytical scheme to be undermined. With a significant portion of H arising from the other spins in the simulation, and each of those spins also in motion, we expect an assumption of fixed H over a time step to become invalid for shorter time steps. To illustrate this effect, we simulated a two-spin system with exchange energy as the only contributor to H. Permalloy parameters (exchange energy constant $A = 13$ nJ/m, magnetization magnitude $M = 800$ kA/m, and $\alpha = 0.01$) and spins a distance $\Delta = 5$ nm apart were assumed. The initial spin direc-

a)Electronic mail: donald.porter@nist.gov.

tions were oriented 20° apart. We find that the simple single step semianalytic scheme[1] fails to converge with time steps of 0.2 ps or longer.

For this simple two-spin, exchange-only system, we can analytically demonstrate an alternative scheme that performs better. The exchange field at spin 1 H_1 due to the magnetization of spin 2 m_2 is conventionally expressed as

$$H_1 = \frac{2A}{\mu_0 M \Delta^2} m_2. \tag{2}$$

Recall that the dynamics of spin 1 are determined only by the torque $m_1 \times H_1$, however. This means we may add any scalar multiple of m_1 to H_1 without changing the dynamics. With this in mind, let

$$\tilde{H} = H_1 = H_2 = \frac{2A}{\mu_0 M \Delta^2}(m_1 + m_2), \tag{3}$$

and we see that both spins in the system may have their dynamics computed as in response to a common field value. We may further examine how a common field value defined in this manner evolves in time.

$$\frac{d\tilde{H}}{dt} = \frac{2A}{\mu_0 M \Delta^2}\left(\frac{dm_1}{dt} + \frac{dm_2}{dt}\right) \tag{4}$$

$$= \frac{4A^2 \alpha |\gamma|}{(\mu_0 M \Delta^2)^2} \sin(\theta) \tan\left(\frac{\theta}{2}\right) \frac{m_1 + m_2}{2}, \tag{5}$$

where θ is the angle between m_1 and m_2. The derivation comes from substituting Eq. (1) for the dm/dt terms. Note that both $\tilde{H}$ and $d\tilde{H}/dt$ are in the direction of m_1+m_2, so we conclude the value $\tilde{H}$ increases in magnitude, but has fixed direction. Its maximum value is reached as θ reaches 0, corresponding to a maximum precession frequency of

$$f_{\max} = \frac{2A|\gamma|}{\pi \mu_0 M \Delta^2}. \tag{6}$$

Computing dynamics according to the common field value $\tilde{H}$ more closely fulfills the fixed field assumption and permits larger time steps without divergence, or loss of accuracy beyond specified bounds. In effect, we have replaced the effective field with a different one directed along a corrected axis, for which the efficiency gains are greater. We find that when we apply our axis-corrected semianalytic scheme to our example problem, solutions continue to converge to the proper equilibrium state for time steps up to 6 ps, a significant increase over the 0.2 ps achieved by the uncorrected scheme.

For other two-spin simulations with other energies in addition to exchange, such a common field value does not arise, but the same strategy of adding a scalar multiple of m to H to get an effective field that changes direction less rapidly is still effective. At each time step, we are computing the torque $m \times H$. Given the value of $m \times H$ at time $t=-\tau$ and at time $t=0$, an axis is determined by

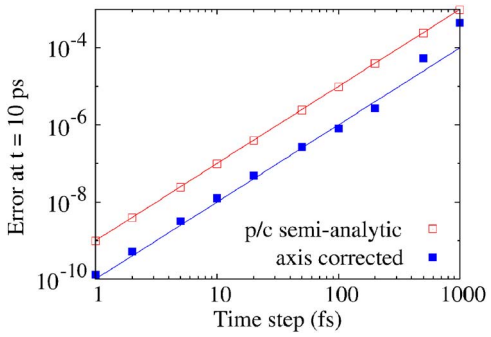

FIG. 1. (Color online) Comparison of relative error vs time step length for the original semianalytic predictor-corrector solver and the proposed axis-corrected alternative.

$$a = (m \times H)(-\tau) \times (m \times H)(0). \tag{7}$$

At $t=0$, we add the appropriate scalar multiple of m to the effective field H to produce a corrected $\tilde{H}$ that is parallel to that axis. That is, we solve

$$\tilde{H} = (H + \lambda m)(0) = \beta a \tag{8}$$

for suitable scalar values of λ and β. Consider the inner product

$$\tilde{H} \cdot (m \times H \times m). \tag{9}$$

Make the substitutions $\tilde{H}=H+\lambda m$ and $\tilde{H}=\beta a$ in turn, simplify, and compare to see that

$$H \cdot (m \times H \times m) = \beta a \cdot (m \times H \times m). \tag{10}$$

Solving for β,

$$\beta = \frac{H \cdot (m \times H \times m)}{a \cdot (m \times H \times m)}, \tag{11}$$

we have all we need to determine λ and $\tilde{H}$. The analytic LL solution assuming the fixed value $\tilde{H}$ over the next time interval then yields the value of m at time $t=\tau$. When we employ this scheme to the exchange only case, we compute the common $\tilde{H}$ field detailed above. This strategy applies when other energies are represented as well.

III. PREDICTOR-CORRECTOR SOLVERS

In Ref. 1, the semianalytic step was used as a foundation to construct a predictor-corrector solver. The axis-corrected semianalytic scheme also supports a predictor-corrector extension. To determine the effectiveness of our axis correction, we simulated a two-spin system with exchange, demagnetization, and cubic anisotropy energies. First, we used several runs of a 5(4) Runge–Kutta–Fehlberg solver[5] at various time steps to compute a converged base-line solution over a 10 ps interval. Then, the predictor-corrector solver from Ref. 1 and our axis corrected predictor-corrector solver were used to compute solutions over the same interval using a variety of time steps for both. The error at $t=10$ ps relative to the base-line solution was taken as a figure of merit. Figure 1 displays the results. The axis-corrected solver yields about an order of magnitude less error compared to the ref-

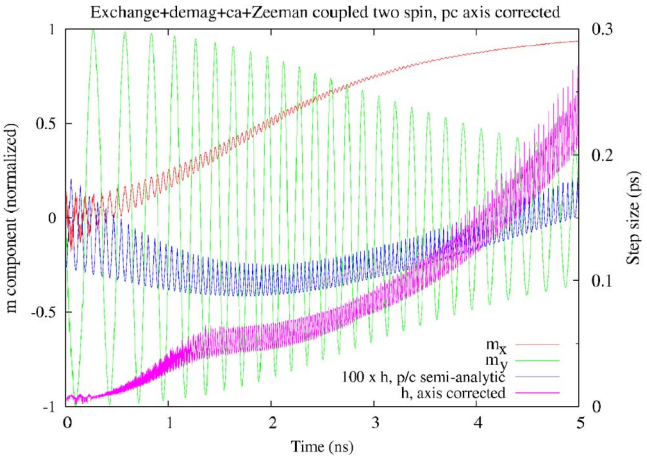

FIG. 2. (Color online) Comparison of effectiveness of adjustable time step determination applied to the original semi-analytic predictor-corrector solver and to the proposed axis-corrected alternative. Magnetization components m_x and m_y as a function of time are plotted against the scale on the left. Time step lengths as a function of time are plotted against the scale on the right. Note the scaling of the third curve for sake of visibility makes values appear 100 times greater than they are.

erenced predictor-corrector scheme. Equivalently, the axis-corrected solver achieves the same magnitude of error with three times larger time steps.

IV. ADJUSTABLE TIME STEP SOLVERS

Figure 1 clearly demonstrates that both solution algorithms exhibit second order convergence. This means they are suitable foundations for the construction of adjustable time step algorithms that dynamically grow and shrink the time step duration to keep the overall calculation within a desired error magnitude.

Figure 2 illustrates the results of the adjustable time step solvers based on the two predictor-corrector solvers. Again, a two-spin system is simulated, this time with exchange, demagnetization, cubic anisotropy, and Zeeman energies in the simulation. The x and y components of m for one of the spins are displayed, showing its precession and approach to convergence to an equilibrium direction after 5 ns of simulated time. The same system was simulated using the Runge–Kutta–Fehlberg solver with a fixed time step of 1 fs to produce a base-line solution. In Fig. 2, both solvers compute results with errors less than 2×10^{-6} relative to the base-line solution. However, the required time steps to achieve that error level are quite distinct.

Note that the time step duration as a function of time for the original semianalytic predictor-corrector solver is displayed with a magnification of 100 times. In this case, the time step adjustments never produce a time step even as long as 2 fs. In contrast, the time step adjustments applied to the axis-corrected version of the semianalytic predictor-corrector solver are able to reach time steps of more than 200 fs by the end of the 5 ns simulation interval, and the time steps appear to still be lengthening at that point.

Because the axis corrected solver over time takes longer and longer time steps while maintaining the same error level, it is able to achieve the same computational results with thirty times fewer calculations.

V. SUMMARY

In this article, three new developments have been presented. First, we have described an axis correction that improves on a previously published Landau–Lifshitz solution technique and demonstrated its benefits. Second, we have analyzed the convergence of these solution techniques and demonstrated that they exhibit second order convergence. Third, we have taken advantage of the second order convergence property of these solution techniques to implement adjustable time step algorithms that permit even more striking demonstration of the advantage of axis correction.

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