Quaternion-based algorithm for micromagnetics

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We describe an algorithm for the integration of the Landau-Lifshitz equation for the precession of a magnetic moment in the presence of dissipation. The algorithm describes the rotation of the magnetization vector in terms of rotation matrices (implemented using quaternions). Its major advantage is that it separates precessional and dissipational rotations, which allows the former to be computed analytically over long time intervals. This allows the use of a much longer time increment Δt than is possible with conventional algorithms, especially for problems with low anisotropy and weak exchange coupling. The spirit of the method is similar to that of the exact solution of the single-particle problem by Kikuchi [J. Appl. Phys. **27**, 1352 (1956)], who also separated the precessional and dissipational motions.

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I. INTRODUCTION

In this paper we consider the problem of micromagnetic simulation, i.e., the evolution of a collection of magnetic moments (representing finite volume elements in a magnetic material).[1–4] The evolution of this system is normally computed from the Landau-Lifshitz (LL) equation.[5] One of the most serious limitations of most micromagnetics algorithms is that the time increment Δt must be chosen to be small enough that the fractional change in magnetization (essentially the angle $\gamma H \Delta t$ through which the magnetization precesses during Δt) is very small; the error in a simple first-order Euler algorithm [such as Eq. (3) below] is proportional to this angle. The error can be decreased, at the expense of complicating the code, by adopting a higher-order method such as a Runge-Kutta algorithm. However, it is highly desirable to be able to include thermal noise[6]— for example, to study the thermal stability of magnetic media. This is very difficult in higher-order algorithms, so in the present paper we restrict our consideration to first-order algorithms.

We will recast the LL equation in the form of an evolution equation for a rotation matrix $R(t)$ (for each volume element) that gives the magnetization $\mathbf{M}(t)=R(t)\mathbf{M}(0)$ of that volume element in terms of some reference vector $\mathbf{M}(0)$. This rotation matrix transforms from a rotating ''local'' reference frame in which $\mathbf{M}$ is stationary (this rotating reference frame is related to the one that is familiar in the field of magnetic resonance[7]) to the lab frame. The matrix-rotation approach was originally motivated by a consideration unrelated to efficiency, namely, the desire to study coarse-grained dynamics[9] in a rotating reference frame in which $\mathbf{M}$ is slowly varying. However, the approach also has the advantage that it separates the precessional motion from the damping motion, in a way that is explained below; the precessional motion can be calculated exactly if the external field is constant (and nearly exactly if the external field is slowly varying). Thus the time increment can be much larger than in a conventional algorithm, without incurring unacceptable errors.

II. DERIVATION OF THE EVOLUTION EQUATION FOR THE ROTATION MATRIX

The basic equation for the time evolution of the magnetization $\mathbf{M}$ of a finite element of magnetic material is the Landau-Lifshitz equation, which can be written in the form

$$\frac{d\mathbf{M}}{dt}=\gamma\mathbf{H}\times\mathbf{M}+\frac{\alpha\gamma}{M_s}(\mathbf{M}\times\mathbf{H})\times\mathbf{M}. \tag{1}$$

Here $\mathbf{H}$ is the total magnetic field acting on the element (which can include magnetostatic fields of external sources or other elements, crystalline anisotropy, exchange, and Brownian random fields), M_s is the saturation magnetization, γ is the gyromagnetic ratio, and α is a dimensionless dissipation coefficient. In the absence of dissipation ($\alpha=0$) the equation can be solved analytically; we will obtain this solution below. The magnetization precesses in a cone around the field vector $\mathbf{H}$ (let us assume for now that this includes only a constant external field) as shown in Fig. 1(a).

First let us establish some notation: for any vector θ, let $R_A(\theta)$ be the matrix that rotates by an angle $|\theta|$ about the direction of the vector θ. For infinitesimal θ, the action of $R_A(\theta)$ on an arbitrary vector $\mathbf{v}$ is given by $R_A(\theta)\mathbf{v}=\mathbf{v}+\theta\times\mathbf{v}=(1+\theta\times)\mathbf{v}$, so we may formally write

$$R_A(\theta)=(1+\theta\times). \tag{2}$$

Then the LL equation may be written

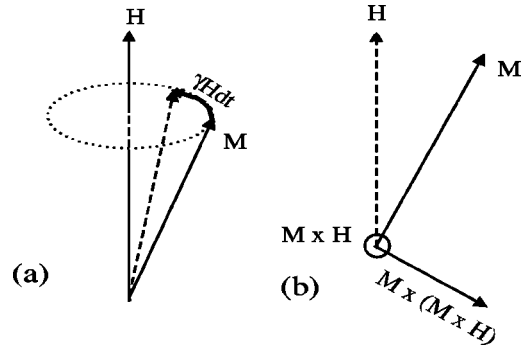

FIG. 1. (a) Precession of the magnetization about the magnetic field. (b) The coordinate axes in the local rotating reference frame; $\mathbf{M}\times\mathbf{H}$ points out of the paper.

$$\mathbf{M}(t+dt)=\left[1+\gamma dt\mathbf{H}\times+\frac{\alpha\gamma dt}{M_s}(\mathbf{M}\times\mathbf{H})\times\right]\mathbf{M}(t), \quad (3)$$

where the right-hand side has a rotation matrix $[\cdots]$ applied to $\mathbf{M}(t)$. We write dt instead of Δt to emphasize that it is infinitesimal here. This rotation matrix can be written as the product of two matrices (ignoring terms of order dt^2),

$$\left[1+\gamma dt\mathbf{H}\times\right]\left[1+\frac{\alpha\gamma dt}{M_s}(\mathbf{M}\times\mathbf{H})\times\right]$$
$$=R_A(\gamma dt\mathbf{H})R_A\left(\frac{\alpha\gamma dt}{M_s}(\mathbf{M}\times\mathbf{H})\right), \quad (4)$$

in terms of the axis rotation matrix defined above, leading to an evolution equation for $\mathbf{M}$:

$$\mathbf{M}(t+dt)=R_A(\gamma\mathbf{H}dt)R_A\left(\frac{\alpha\gamma dt}{M_s}\mathbf{M}\times\mathbf{H}\right)\mathbf{M}(t). \quad (5)$$

Equation (5) has a simple physical interpretation. The rightmost axis rotation factor $\mathbf{R}_A[(\alpha\gamma dt/M_s)\mathbf{M}\times\mathbf{H}]$ rotates $\mathbf{M}(t)$ about the vector $\mathbf{M}\times\mathbf{H}$, a rotation in the plane of the paper in Fig. 1(b) that moves $\mathbf{M}$ toward $\mathbf{H}$. This is a dissipation effect that will eventually cause $\mathbf{M}$ to be parallel to $\mathbf{H}$. The leftmost axis rotation $\mathbf{R}_A(\gamma\mathbf{H}dt)$ is the precession about the magnetic field $\mathbf{H}$.

We are looking for a rotation matrix $R(t)$ which gives $\mathbf{M}(t)=R(t)\mathbf{M}(0)$, where $\mathbf{M}(0)$ points in some reference direction that may as well be taken to be $(0,0,M_s)$. Then Eq. (5) becomes an equation for $R(t+dt)$:

$$R(t+dt)\mathbf{M}(0)=R_{\mathbf{A}}(\gamma\mathbf{H}dt)R_A\left(\frac{\alpha\gamma dt}{M_s}\mathbf{M}\times\mathbf{H}\right)R(t)\mathbf{M}(0). \quad (6)$$

There is still some arbitrariness in the choice of $R(t)$; multiplying it on the right by any rotation about $\mathbf{M}(0)$ gives another acceptable $R(t)$. Clearly the simplest choice of an equation for $R(t)$ is

$$R(t+dt)=R_{\mathrm{A}}(\gamma\mathbf{H}dt)R_A\left(\frac{\alpha\gamma dt}{M_s}\mathbf{M}\times\mathbf{H}\right)R(t). \quad (7)$$

We can show that this choice is the unique one that keeps $\mathbf{H}$ in a fixed plane in the local rotating reference frame [the plane of the paper in Fig. 1(b)] in the case that $\mathbf{H}$ is constant; this seems as good a choice as any.

At this point, we can see the exact solution in the undamped $\alpha=0$ case. If we evolve the system over a finite time interval T by applying the rotation $R_{\mathbf{A}}(\gamma\mathbf{H}dt)$ repeatedly (T/dt times), the product of these rotations about $\mathbf{H}$ is exactly $R_{\mathbf{A}}(\gamma\mathbf{H}T)$. This rotation, applied to the initial $\mathbf{M}(0)$, gives a magnetization vector that precesses around $\mathbf{H}$.

If we now allow α to be nonzero and again evolve the system T/dt times, this consolidation of rotations into a single large rotation does not work because there are rotations about a different axis mixed in, and (finite) rotations do not commute. However, there is a trick for separating the precession rotations from the dissipation rotations: move the dissipation rotations to the right of $R(t)$ in Eq. (7). Although these two rotations do not commute, this can be done if we replace the cross product (which is now in the lab frame) by its value $(\mathbf{M}\times\mathbf{H})_{\mathrm{local}}=R(t)^{-1}(\mathbf{M}\times\mathbf{H})$ rotated to the local frame:

$$R_A\left(\frac{\alpha\gamma dt}{M_s}\mathbf{M}\times\mathbf{H}\right)R(t)=R(t)R_A\left(\frac{\alpha\gamma dt}{M_s}(\mathbf{M}\times\mathbf{H})_{\mathrm{local}}\right). \quad (8)$$

(This is easiest to prove formally in terms of quaternions; see the Appendix.) We are now left with

$$R(t+dt)=R_A(\gamma\mathbf{H}dt)R(t)R_A\left(\frac{\alpha\gamma dt}{M_s}(\mathbf{M}\times\mathbf{H})_{\mathrm{local}}\right). \quad (9)$$

Now note that if we apply these two infinitesimal rotations repeatedly, this time one on the right and one on the left, the ones on the left can again be multiplied exactly to give $R_{\mathbf{A}}(\gamma\mathbf{H}T)$. This only works exactly if $\mathbf{H}$ is constant, but the error will be small if $\mathbf{H}$ is slowly varying. Thus the algorithm defined by Eq. (9) does not require the precession angle $\gamma\mathbf{H}dt$ to be small; it can even be of order 1 without loss of accuracy. This argument does not apply to the other axis rotation, representing dissipation, because $(\mathbf{M}\times\mathbf{H})_{\mathrm{local}}$ is not constant. Thus we must require the argument of the second rotation, of order $\alpha\gamma Hdt$, to be small, but this is not restrictive since usually α will be small. In general, the error is of order $\alpha\Delta\theta$, where $\Delta\theta$ is the angle of rotation, in this case γHdt. In the case of constant $\mathbf{H}$, Eq. (9) can be turned into a simple differential equation for the angle θ between $\mathbf{H}$ and $\mathbf{M}$ (namely, $d\theta/dt=\gamma\alpha M_s H\sin\theta$) which gives immediately the exact solution found by Kikuchi[10] in 1956.

The reader will note that we have so far not included an exchange field. However, the basic idea of the above derivation can be applied in the presence of an exchange field—the basic idea is that we separate the total magnetic field $\mathbf{H}$ into two parts,

$$\mathbf{H}=\mathbf{H}_{s\_\mathrm{lab}}+\mathbf{H}_{s\_\mathrm{loc}} \quad (10)$$

where $\mathbf{H}_{s\_\mathrm{lab}}$ is slowly varying in the lab frame (this includes only the external field, above) and $\mathbf{H}_{s\_\mathrm{loc}}$ is slowly varying in the local (rotating) frame. The axis rotation $R_{\mathbf{A}}(\gamma\mathbf{H}_{s\_\mathrm{lab}}dt)$ induced by $\mathbf{H}_{s\_\mathrm{lab}}$ is applied to the left of $R(t)$ whereas $R_{\mathbf{A}}(\gamma\mathbf{H}_{s\_\mathrm{loc}}dt)$ is applied (along with the dissipation term as above) on the right:

$$R(t+dt)$$
$$=R_A(\gamma\mathbf{H}_{s\_\mathrm{lab}}dt)R(t)R_A\left(\gamma\mathbf{H}_{s\_\mathrm{loc}}dt+\frac{\alpha\gamma dt}{M_s}(\mathbf{M}\times\mathbf{H})_{\mathrm{local}}\right). \quad (11)$$

Assuming that the neighboring magnetizations $\mathbf{M}_n$ (n indexes the neighbors) precess similarly to $\mathbf{M}$ itself, the exchange field $\mathbf{H}_{\mathrm{exch}}=\Sigma_n J\mathbf{M}_n$ (J is an exchange constant) is slowly varying in the local frame in which $\mathbf{M}$ is constant. Thus it should be included in $\mathbf{H}_{s\_\mathrm{loc}}$, in the right-hand R_A factor in the evolution equation [Eq. (11)].

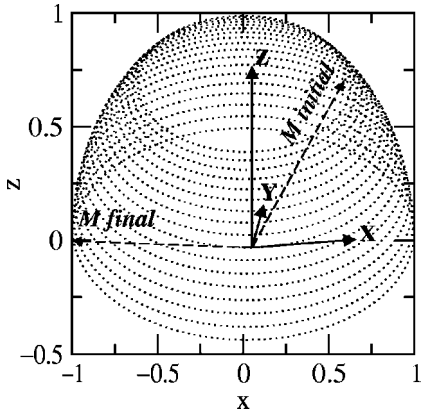

FIG. 2. Trajectory of the magnetization of a single particle, showing the initial magnetization vector and the subsequent path of its head.

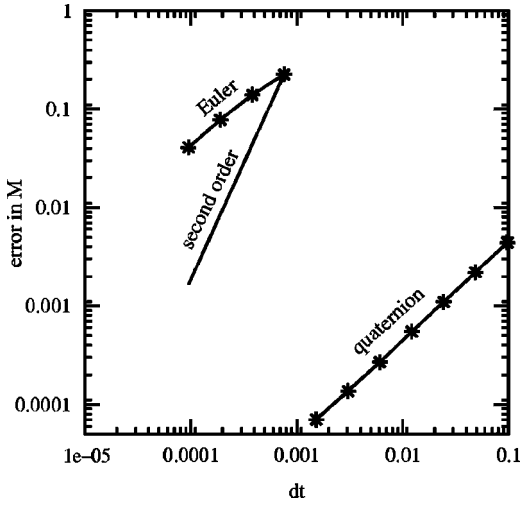

FIG. 3. Convergence of the final magnetization shown in Fig. 2: lines labeled ''Euler'' and ''quaternion'' give errors in the final vector magnetization as a function of time increment dt. The line for second-order algorithm was not actually calculated, but is drawn to indicate its scaling with dt.

In this paper we have dealt only with the case of an isotropic material. In a real micromagnetic simulation we would need to deal with anisotropic materials in which there is an additional effective anisotropy field $\mathbf{H}_{\text{anis}}$ which points along a fixed easy axis. The easy axis rotates in the local frame, so clearly $\mathbf{H}_{\text{anis}}$ is most slowly varying in the lab frame, and should be included with the external field in computing $\mathbf{H}_{s\_\text{lab}}$. This limits the time increments dt to values over which the variation in $\mathbf{H}_{\text{anis}}$ can be neglected—effectively the error becomes proportional to $\gamma H_K dt$ instead of $\gamma H dt$, where H_K is the conventional anisotropy field. For soft low-anisotropy materials this is a significant improvement; in a highly isotropic system this error can be improved if we are willing to tabulate or parameterize the single-particle magnetization trajectories and replace $R_{\mathbf{A}}(\gamma \mathbf{H}_{s\_\text{lab}} dt)$ by a table lookup.

We have implemented the algorithm described above; instead of rotation matrices it is most efficient to deal with quaternions (see the Appendix), although these are entirely equivalent and do not change any of the considerations described above. As a test of the convergence with respect to the time increment dt, we have integrated a test trajectory for a single particle (Fig. 2) over about 17 precession periods.

We plot the magnitude of the error in the final vector magnetization in Fig. 3. It is true that a higher-order (e.g., Runge-Kutta) method is more efficient if an extremely high accuracy is demanded (because it treats the damping term more accurately) but in the accuracy range that makes sense for comparison to experiment, such as the range shown in Fig. 3, the matrix method is much more efficient.

In addition to the above simple test, we have checked that this algorithm gives correct spin-wave frequencies, which can be calculated analytically for periodic square arrays. We have also used this algorithm for calculations on a thermal equilibium ensemble.[9]

The results above are for a one-cell system in which there is no exchange interaction. We have also done simulations in a periodic cubic array (up to $8\times8\times8$ cells) to verify that the algorithm treats exchange correctly. The spin-wave frequencies can be calculated analytically for this case,[11] and agree with the results of the quaternion algorithm. We have also compared Lyapunov exponents (growth rates of the instability due to time-step error) for spin waves to those of the Euler algorithm; the Euler algorithm is about twice as unstable (i.e., requires twice as small a Δt to show the same instability) as the quaternion algorithm.[11]

It might appear that a rotation-matrix-based algorithm is significantly less efficient than one in which only the three components M_x, M_y, and M_z need to be updated. However, quaternion multiplication is faster than matrix multiplication. Also, in a practical case the calculation of the magnetostatic interaction (which we have not included here) is much more time consuming, so the time required to update the rotation matrix is negligible.

III. CONCLUSION

We have described an algorithm for micromagnetic computation, based on rotation matrices or quaternions. It is based on the observation that some of the fields are slowly varying in the lab frame and some are slowly varying in the local rotating frame; the matrix method allows us to separate these effects and do an exact or nearly exact treatment of the precession in the lab frame, while treating damping in the local rotating frame. We have implemented this algorithm initially for an isotropic system, but this idea generalizes to the case of anisotropic systems, and work is in progress on an anisotropic implementation.

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APPENDIX: QUATERNIONS

A quaternion is a quadruple of real numbers $q=(q_0,q_1,q_2,q_3)$. They were introduced by Hamilton in 1853, and their properties were described in detail by Katz.[8] The components q_i are sometimes referred to as ''Euler parameters'' (not to be confused with the related Euler angles). Here we will summarize only the most critical facts that are needed to compute rotations using quaternions.

The last three components can be thought of as a space vector $\mathbf{q}$, so $q=(q_0,\mathbf{q})$. The multiplication rule is $(q_0,\mathbf{q})(p_0,\mathbf{p})=(q_0p_0-\mathbf{q}\cdot\mathbf{p},\mathbf{q}\times\mathbf{p}+q_0\mathbf{p}+\mathbf{q}p_0)$. We define the conjugate quaternion by $(q_0,\mathbf{q})^\dagger\equiv(q_0,-\mathbf{q})$; the magnitude is defined by $|q|^2\equiv q_0^2+\mathbf{q}\cdot\mathbf{q}$, which is also equal to $q^\dagger q$ and $qq^\dagger$. There are two important subsets of quaternions.

(i) Vectors: if $p_0=0$, the quaternion $(0,\mathbf{p})$ is essentially an ordinary vector; when a boldface symbol $\mathbf{v}$ appears in a quaternion expression it should be interpreted as $(0,\mathbf{v})$.

(ii) Unit quaternions (rotations): If $|q|^2=1$, the operation $\mathbf{v}\rightarrow q\mathbf{v}q^\dagger$ is a rotation of the vector $\mathbf{v}$. [You can see this by showing that the resulting quaternion is a vector (i.e., has no zeroth component) and has the same length as $\mathbf{v}$.]

Useful facts about quaternions are as follows.

(i) A rotation by the infinitesimal angle θ about the unit vector $\hat{\mathbf{n}}$ is given by

$$q=1+\frac{1}{2}\theta\hat{\mathbf{n}}, \tag{A1}$$

as you can verify by checking that it changes $\mathbf{v}$ by $\theta\mathbf{v}\times\hat{\mathbf{n}}$. It can then be shown that a rotation by a finite angle θ is given by $e^{1/2\,\theta\hat{\mathbf{n}}}$.

(ii) Associativity: $(qp)r=q(pr)$.

(iii) The relation of the quaternion product to dot and cross products is

$$\mathbf{vw}\equiv(0,\mathbf{v})(0,\mathbf{w})=(-\mathbf{v}\cdot\mathbf{w},\mathbf{v}\times\mathbf{w}), \tag{A2}$$

so that

$$\mathbf{v}\times\mathbf{w}=\frac{1}{2}(\mathbf{vw}-\mathbf{wv}). \tag{A3}$$

(iv) Conjugate of product: $(pq)^\dagger=q^\dagger p^\dagger$.

Using these facts, we can show that the quaternion corresponding to the axis rotation R_A [Eq. (2)] is

$$e^{i\theta/2}. \tag{A4}$$

The quaternion form of Eq. (6) is

$$\begin{aligned} q(t+dt)\mathbf{M}(0)q^\dagger(t+dt) &= q_{\mathbf{A}}(\gamma\mathbf{H}dt)\mathbf{q}_{\mathbf{A}}\left(\frac{\alpha\gamma dt}{M_s}\mathbf{M}\times\mathbf{H}\right)q(t)\mathbf{M}(0) \\ &\times q^\dagger(t)\mathbf{q}_{\mathbf{A}}^\dagger\left(\frac{\alpha\gamma dt}{M_s}\mathbf{M}\times\mathbf{H}\right)q_{\mathbf{A}}^\dagger(\gamma\mathbf{H}dt). \end{aligned} \tag{A5}$$

The quaternion form of Eq. (9) is identical to Eq. (9) with R replaced by q.

In addition to having fewer components than a rotation matrix, the quaternion makes it easier to interface with computer graphics. Most computer graphics programs specify rotations using quaternions, at least internally, so the quaternion can be passed directly to the graphics functions in a package such as Open Inventor.

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