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Numerical integration of Landau–Lifshitz–Gilbert equation based on the midpoint rule

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The midpoint rule time discretization technique is applied to Landau–Lifshitz–Gilbert (LLG) equation. The technique is unconditionally stable and second-order accurate. It has the important property of preserving the conservation of magnetization amplitude of LLG dynamics. In addition, for typical forms of the micromagnetic free energy, the midpoint rule preserves the main energy balance properties of LLG dynamics. In fact, it preserves LLG Lyapunov structure and, in the case of zero damping, the system free energy. All the above preservation properties are fulfilled unconditionally, namely, regardless of the choice of the time step. The proposed technique is then tested on the standard micromagnetic problem No. 4. In the numerical computations, the magnetostatic field is computed by the fast Fourier transform method, and the nonlinear system of equations connected to the implicit time-stepping algorithm is solved by special and reasonably fast quasi-Newton technique. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1858784]

Numerical integration of the Landau–Lifshitz–Gilbert (LLG) equation has been widely used in micromagnetics for the analysis of dynamical magnetization processes. In most studies, the time discretization is obtained by using "off-the-shelf" algorithms such as Euler, linear multistep (e.g., Adams, Crank–Nicholson, etc.), and Runge–Kutta methods.[1] These standard techniques usually corrupt intrinsic geometrical properties of LLG time evolution and may lead to inaccurate results especially when long-term behaviors of micromagnetic systems have to be investigated. In this respect, it is important to develop numerical schemes that have more appropriate geometrical properties (see, e.g., Refs. 2–5).

In this paper, the (implicit) midpoint rule is used for the numerical time integration of the LLG equation. This method leads to an unconditionally stable, second-order accurate scheme, which has very important geometric preservation properties.[6]

We start our discussion with a brief review of the LLG equation and its relevant properties. The equation can be written in the following normalized form:

$$\frac{\partial \mathbf{m}}{\partial t} = -\mathbf{m}\times\left(\mathbf{h}_{\text{eff}} - \alpha\frac{\partial \mathbf{m}}{\partial t}\right), \tag{1}$$

where $\mathbf{m}(t,\mathbf{r})=\mathbf{M}/M_s$ ($|\mathbf{m}|=1$), $\mathbf{M}$ is the magnetization vector field, M_s is the saturation magnetization, α is the dimensionless Gilbert damping constant, and the time is measured in units of $(|\gamma|M_s)^{-1}$ (γ is the gyromagnetic ratio). The vector field $\mathbf{m}(t,\mathbf{r})$ is nonzero for $\mathbf{r}\in\Omega$, where Ω is the region occupied by the magnetic body. The normalized effective field $\mathbf{h}_{\text{eff}}=\mathbf{H}_{\text{eff}}/M_s$ can be defined by the variational derivative of the micromagnetic free-energy functional $G(\mathbf{m})$, i.e., $\mathbf{h}_{\text{eff}}=-\delta G/\delta\mathbf{m}$.[7] The effective field is typically constituted by the sum of four terms: the applied field $\mathbf{h}_a(t)$, the exchange field $\mathbf{h}_{\text{ex}}=2A/(\mu_0 M_s^2)\nabla^2\mathbf{m}$ (A is the exchange constant), the anisotropy field $\mathbf{h}_{\text{an}}=[2K_1/(\mu_0 M_s^2)]\mathbf{e}_{\text{an}}(\mathbf{e}_{\text{an}}\cdot\mathbf{m})$ (K_1 is the uniaxial anisotropy constant and $\mathbf{e}_{\text{an}}$ is the easy axis unit vector), and the magnetostatic field $\mathbf{h}_m$, which can be expressed by the usual Coulomb convolution integral $\mathbf{h}_m=-\nabla_{\mathbf{r}}\int_\Omega \nabla_{\mathbf{r}'}[1/(4\pi|\mathbf{r}-\mathbf{r}'|)]\cdot\mathbf{m}(t,\mathbf{r}')dV_{\mathbf{r}'}$. The magnetization $\mathbf{m}(t,\mathbf{r})$ is also assumed to satisfy the Neumann condition $\partial\mathbf{m}/\partial\mathbf{n}=0$ at the body surface.

The first fundamental property of LLG dynamics is the time preservation of magnetization magnitude,

$$|\mathbf{m}(t,\mathbf{r})| = |\mathbf{m}(t_0,\mathbf{r})| \quad \forall\,\mathbf{r}\in\Omega, \tag{2}$$

which can be easily derived from Eq. (1) by dot multiplying both sides of the equation by $\mathbf{m}$. The second fundamental property can be derived, in the case of constant applied field, by scalar multiplying both sides of the equation by $(\mathbf{h}_{\text{eff}} - \alpha\partial\mathbf{m}/\partial t)$ and using the fact that $\mathbf{h}_{\text{eff}}=-\delta G/\delta\mathbf{m}$. This leads immediately to the following energy balance equation:

$$\frac{d}{dt}G(t) = -\int_\Omega \alpha\left|\frac{\partial \mathbf{m}}{\partial t}\right|^2 dV, \tag{3}$$

which has very important implications. First, we notice that, for constant applied field, the LLG dynamics has a Lyapunov structure, namely, the free energy is always a decreasing function of time. This property is very important because it guarantees that the system tends toward minima of free energy (i.e., metastable equilibrium points). Second, for $\alpha=0$,

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the free energy is preserved, and the LLG equation takes the Hamiltonian form $\partial \mathbf{m}/\partial t = -\mathbf{m}\times(\delta G/\delta \mathbf{m})$. Although the LLG dynamics is always dissipative, it is interesting to consider this special case since in most experimental situations the dissipative effect are quite small (typically $\alpha \ll 1$). In other terms, the LLG dynamics, on relatively short time scale, is a perturbation of the conservative precessional dynamics.

We want now to investigate the preservation properties of midpoint rule when it is applied to the LLG equation. To this end, let us assume that the magnetic body has been subdivided in N cells or finite elements. We denote the magnetization vector associated with the k-th cell or node by $\mathbf{m}_k(t) \in \mathbb{R}^3$, and the collection of all vectors $\mathbf{m}_k(t)$ by the vector $\underline{\mathbf{m}}(t) \in \mathbb{R}^{3N}$. Analogous notations are used for $\mathbf{h}_a$ and $\mathbf{h}_{\text{eff}}$. Let us notice that the mathematical form of the effective field is $\mathbf{h}_{\text{eff}}(\mathbf{m},t) = -\mathcal{C}\mathbf{m} + \mathbf{h}_a(t)$, where $\mathcal{C}$ is a linear integro-differential operator. Usual spatial discretization techniques (e.g., finite elements and finite difference) generally preserve this structure of the effective field, and the discretized version of $\mathbf{h}_{\text{eff}}$ is typically given by

$$\underline{\mathbf{h}}_{\text{eff}}(\underline{\mathbf{m}},t) = -\frac{\partial \underline{G}}{\partial \underline{\mathbf{m}}} = -\underline{C}\cdot\underline{\mathbf{m}} + \underline{\mathbf{h}}_a(t), \tag{4}$$

where $\underline{G}(\underline{\mathbf{m}}) = (1/2)\underline{\mathbf{m}}^T\cdot\underline{C}\cdot\underline{\mathbf{m}} - \underline{\mathbf{h}}_a^T\cdot\underline{\mathbf{m}}$ is the discretized free energy and $\underline{C}$ is a $3N\times 3N$ symmetric matrix. Using this notation, the spatially semidiscretized LLG equation can be written as follows:

$$\frac{d}{dt}\underline{\mathbf{m}} = -\underline{\Lambda}(\underline{\mathbf{m}})\cdot\left[\underline{\mathbf{h}}_{\text{eff}}(\underline{\mathbf{m}},t) - \alpha\frac{d}{dt}\underline{\mathbf{m}}\right], \tag{5}$$

where $\underline{\Lambda}(\underline{\mathbf{m}}) = \text{diag}[\Lambda(\mathbf{m}_1),\ldots,\Lambda(\mathbf{m}_N)]$ is a block-diagonal matrix with blocks $\Lambda(\cdot) \in \mathbb{R}^{3\times 3}$ such that $\Lambda(\mathbf{v})\cdot\mathbf{w} = \mathbf{v}\times\mathbf{w}$. Equation (5) can be numerically integrated by using the implicit midpoint rule which leads to the following implicit time-stepping algorithm:

$$\frac{\underline{\mathbf{m}}^{n+1} - \underline{\mathbf{m}}^n}{\Delta t} = -\underline{\Lambda}\left(\frac{\underline{\mathbf{m}}^{n+1} + \underline{\mathbf{m}}^n}{2}\right)\cdot \cdot\left[\underline{\mathbf{h}}_{\text{eff}}\left(\frac{\underline{\mathbf{m}}^{n+1} + \underline{\mathbf{m}}^n}{2}, t^n + \frac{\Delta t}{2}\right) - \alpha\frac{\underline{\mathbf{m}}^{n+1} - \underline{\mathbf{m}}^n}{\Delta t}\right], \tag{6}$$

which, for the generic k-th cell, can be written as

$$\frac{\mathbf{m}_k^{n+1} - \mathbf{m}_k^n}{\Delta t} = -\left(\frac{\mathbf{m}_k^{n+1} + \mathbf{m}_k^n}{2}\right) \times\left[\mathbf{h}_{\text{eff},k}\left(\frac{\underline{\mathbf{m}}^{n+1} + \underline{\mathbf{m}}^n}{2}, t^n + \frac{\Delta t}{2}\right) - \alpha\frac{\mathbf{m}_k^{n+1} - \mathbf{m}_k^n}{\Delta t}\right]. \tag{7}$$

Let us study the relevant properties of the midpoint discretized LLG equation. First, by dot multiplying both sides of Eq. (7) by $\mathbf{m}_k^{n+1} + \mathbf{m}_k^n$, it can be easily verified that $|\mathbf{m}_k^{n+1}| = |\mathbf{m}_k^n|$, i.e., at each cell the magnitude of the vector magnetization remains constant. Thus, the midpoint rule preserves exactly the LLG property (2). Next, let us assume constant applied field (i.e., that $\underline{\mathbf{h}}_{\text{eff}}$ does not depend on t) and let us multiply both sides of Eq. (6) by $[\underline{\mathbf{h}}_{\text{eff}}((\underline{\mathbf{m}}^{n+1} + \underline{\mathbf{m}}^n)/2) - \alpha(\underline{\mathbf{m}}^{n+1} - \underline{\mathbf{m}}^n)/\Delta t]$. By using the symmetry of the matrix $\underline{C}$ and the antisymmetry of the 3×3 blocks of the matrix $\underline{\Lambda}$ one can readily derive the following equation:

$$\frac{\underline{G}(\underline{\mathbf{m}}^{n+1}) - \underline{G}(\underline{\mathbf{m}}^n)}{\Delta t} = -\alpha\left|\frac{\underline{\mathbf{m}}^{n+1} - \underline{\mathbf{m}}^n}{\Delta t}\right|^2. \tag{8}$$

Notice that the proof of this equation is crucially connected with the fact that the free energy $\underline{G}(\underline{\mathbf{m}})$ is given by the sum of a quadratic form and a linear form in $\underline{\mathbf{m}}$. Equation (8) has very important consequences. First, independently from the time step, the discretized energy $\underline{G}(\underline{\mathbf{m}}^n)$ is decreasing. Second, for $\alpha = 0$, the energy is exactly preserved regardless of the time step. These two properties confirm the unconditional stability of the midpoint rule, but more importantly they indicate that, the midpoint rule will tend to correctly reproduce the most important part in the LLG dynamics, i.e., the precessional magnetization motion.

The properties we have just discussed are strongly related to the implicit nature of midpoint rule. As consequence of this implicit nature, we have to solve Eq. (6) for the unknown $\underline{\mathbf{m}}^{n+1}$ at each time step which amounts to solve a system of $3N$ nonlinear equations in the $3N$ unknowns $\underline{\mathbf{m}}^{n+1}$. The solution of this system of equations can be obtained by using Newton–Raphson (NR) algorithm for the equation $\mathbf{F}^n(\underline{\mathbf{m}}^{n+1}) = 0$, where

$$\mathbf{F}^n(\underline{\mathbf{y}}) = \left[I - \alpha\underline{\Lambda}\left(\frac{\underline{\mathbf{y}} + \underline{\mathbf{m}}^n}{2}\right)\right]\cdot(\underline{\mathbf{y}} - \underline{\mathbf{m}}^n) - \Delta t\,\mathbf{f}^n\left(\frac{\underline{\mathbf{y}} + \underline{\mathbf{m}}^n}{2}\right), \tag{9}$$

and $\mathbf{f}^n(\underline{\mathbf{m}}) = -\underline{\Lambda}(\underline{\mathbf{m}})\cdot\mathbf{h}_{\text{eff}}(\underline{\mathbf{m}}, t^n + \Delta t/2)$. The main difficulty in applying NR method is that the Jacobian $J^n(\underline{\mathbf{y}})$ of $\mathbf{F}^n(\underline{\mathbf{y}})$ is a full matrix, due to the long-range character of magnetostatic interactions. The inversion of the matrices $J^n(\underline{\mathbf{y}})$ at each NR iteration would lead to an exceedingly high computational cost. In this respect, as it is usual in solving field problems with implicit time stepping, we have used a quasi-Newton method by considering a reasonable approximation of the $J^n(\underline{\mathbf{y}})$. We have considered the approximated sparse Jacobian $\tilde{J}^n(\mathbf{y})$, obtained by neglecting in $J^n(\underline{\mathbf{y}})$ all the terms related to magnetostatic interactions. The inversion of the sparse matrix $\tilde{J}^n(\mathbf{y})$ can be then achieved by using fast iterative solvers. In particular, since the matrices $\tilde{J}^n(\mathbf{y})$ to be inverted are nonsymmetric, we have opted for the generalized minimal residual (GMRES) method.[8]

Up to this point, the considerations we have made about the properties and the implementation of midpoint rule were rather independent from the spatial discretization technique used. In the following, in order to test the method, we have chosen to perform the spatial discretization by using the finite difference method. The magnetic body is subdivided into a collection of rectangular prisms with edges parallel to the coordinate axes. The magnetization is uniform within each cell. The exchange field is computed by means of a (second-order accurate in space) seven-point finite difference Laplacian. The magnetostatic field is written as a discrete convolution by using analytical formula proposed in Ref. 9. The

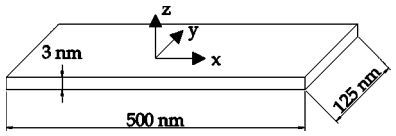

FIG. 1. Thin-film geometry for μ-mag standard problem No. 4.

discrete convolution is then computed by means of three-dimensional fast Fourier transform using the zero-padding algorithm.

We apply the above numerical technique to solve the μ-mag standard problem No. 4 (see Ref. 1). This problem concerns the study of magnetization reversal dynamics in a thin-film subject to a constant external field, applied almost antiparallel to the initial magnetization. The geometry of the medium is sketched in Fig. 1. The material parameters are $A=1.3\times10^{-11}$ J/m, $M_s=8.0\times10^5$ A/m, and $K_1=0$ J/m^3. The dimension of the cells are $3.125\ \text{nm}\times3.125\ \text{nm}\times3\ \text{nm}$. The total number of cells is $N=6400$. The external field is applied at an angle of 190° off the x axis, with x-y components such that $\mu_0 M_s h_{ax}=-35.5$ mT, $\mu_0 M_s h_{ay}=-6.3$ mT, and magnitude $\mu_0 M_s h_a=36$ mT.

In the following, we report the comparison between the numerical solution obtained by using the proposed implementation of the midpoint rule and the solutions submitted by other researchers to the μ-mag website.[1] The time step of the midpoint algorithm is constant and has been chosen such that $(\gamma M_s)^{-1}\Delta t=2.5$ ps. We observe that the time steps used in the algorithms developed by other authors[1] are considerably smaller (less than 0.2 ps). In Fig. 2 the plots of $\langle m_y\rangle$ ($\langle\cdot\rangle$ means spatial average) as a function of time are reported. In Fig. 3 the plot of magnetization vector field, when the first

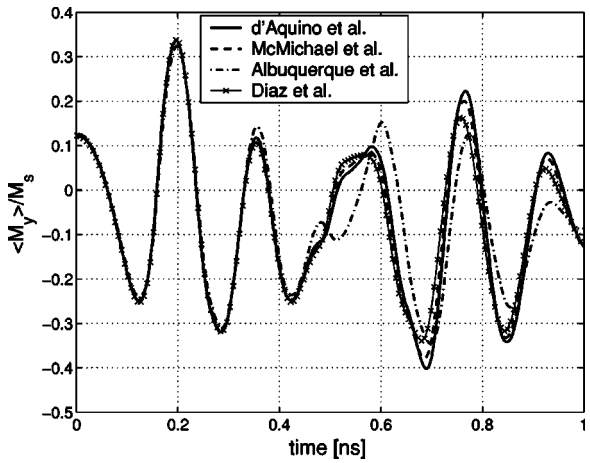

FIG. 2. Plots of $\langle m_y\rangle=\langle M_y\rangle/M_s$ vs time. The external field is applied 190° off the x axis.

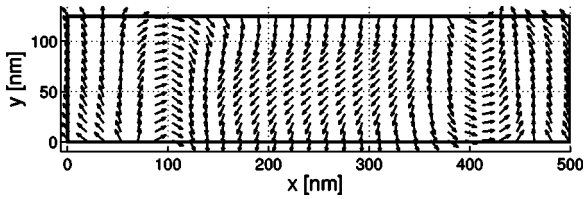

FIG. 3. Snapshot of magnetization vector field when the first zero crossing of $\langle m_x\rangle$ occurs. The external field is applied at an angle of 190° off the x axis.

zero crossing of $\langle m_x\rangle$ occurs, is reported. Numerical simulations of the same problem were performed with a smaller cell edge (2.5 nm), showing that the results do not depend on the mesh size.

Finally, we notice that the numerical implementation of the midpoint rule fulfills the preservation properties discussed above only within certain accuracy. This is a natural consequence of the fact that we solve the time-stepping equation $\mathbf{F}^n(\underline{\mathbf{m}}^{n+1})=0$ by an iterative procedure within a certain numerical tolerance. It is then important to verify a posteriori the accuracy in the preservation of magnetization magnitude and energy balance properties. To this end, we have verified the uniformity of the magnetization vector field by computing, at each time step, the average and the quadratic deviation of the values $|\mathbf{m}_k|$, with $k=1,\ldots,N$: $m_{\text{av}}=(\Sigma_{k=1}^N|\mathbf{m}_k|)/N$, $\sigma_m^2=\Sigma_{k=1}^N(m_{\text{av}}-|\mathbf{m}_k|)^2/N$. We have verified that $|m_{\text{av}}-1|\sim10^{-16}$ and $\sigma_m^2\sim10^{-30}$. To check also the accuracy of energy balance property preservation we have computed the sequence (according to a procedure proposed in Ref. 10) $\hat{\alpha}^n=-\{[\underline{G}(\underline{\mathbf{m}}^{n+1})-\underline{G}(\underline{\mathbf{m}}^n)]/\Delta t\}/|(\underline{\mathbf{m}}^{n+1}-\underline{\mathbf{m}}^n)/\Delta t|^2$ and we have verified that the relative deviation $e_\alpha^n=|\hat{\alpha}^n-\alpha|/\alpha$ is always less than 10^{-7}.

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