Numerical Methods for the Landau-Lifshitz-Gilbert Equation

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Abstract. In this paper we give an overview of the numerical methods for the solution of the Landau-Lifshitz-Gilbert equation. We discuss advantages of the presented methods and perform numerical experiments to demonstrate their performance. We also discuss the coupling with Maxwell's equations.

1 Introduction

Numerical simulations based on Landau-Lifshitz-Gilbert (LLG) equation are widely used in the magnetic recording applications. The LLG equation, describing the time evolution of magnetization in a ferromagnetic material, can be written in a normalized form

$$\partial_t \boldsymbol{m} = \gamma M_s \left(\boldsymbol{h}_T \times \boldsymbol{m} + \alpha \boldsymbol{m} \times (\boldsymbol{h}_T \times \boldsymbol{m}) \right) \quad \text{in} \quad \Omega \times (0,T), \tag{1}$$

where $\boldsymbol{h}_T = -\dfrac{1}{\mu_0 M_s^2} \dfrac{\partial \boldsymbol{E}}{\partial \boldsymbol{m}}$ is the total field, $\boldsymbol{E}$ is the total free energy in the ferromagnet, M_s is the saturation magnetization, α is the damping constant, γ is the gyromagnetic ratio and μ_0 is the permeability of vacuum. The first term on the right-hand side causes the precession of $\boldsymbol{m}$ around $\boldsymbol{h}_T$ and the second term is the damping term. The magnetization $\boldsymbol{m}$ satisfies an initial condition $\boldsymbol{m}(0) = \boldsymbol{m}_0$ and Neumann boundary condition

$$\frac{\partial \boldsymbol{m}}{\partial \boldsymbol{\nu}} = \boldsymbol{0} \quad \text{on} \quad \partial\Omega, \tag{2}$$

where $\boldsymbol{\nu}$ is the outward unit vector to the boundary.

We take $\boldsymbol{h}_T = \boldsymbol{H}/M_s + \boldsymbol{H}_a + \boldsymbol{H}_{ex}$, where $\boldsymbol{H}$ is the magnetic field usually obtained from the Maxwell's equations. Since we are only concerned with the numerical methods for LLG equation, we will assume $\boldsymbol{H}$ to be a known function. The term $\boldsymbol{H}_a$ is the anisotropy field which, in the case of uniaxial anisotropy in the direction of unit vector $\boldsymbol{p}$, takes the form $\boldsymbol{H}_a = \dfrac{K}{\mu_0 M_s^2} (\boldsymbol{p} \cdot \boldsymbol{m}) \boldsymbol{p}$; the exchange field $\boldsymbol{H}_{ex} = \dfrac{A}{\mu_0 M_s^2} \Delta \boldsymbol{m}$ arises due to the exchange interaction between the spins (K, A are the anisotropy and exchange constants).

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A scalar multiplication of (1) by $\boldsymbol{m}$ gives $\partial_t \boldsymbol{m} \cdot \boldsymbol{m} = \frac{1}{2}\partial_t |\boldsymbol{m}|^2 = 0$. This directly implies the conservation of magnitude of magnetization $|\boldsymbol{m}(t)| = |\boldsymbol{m}(0)| = 1$, which is a crucial conservation property of the LLG equation. A typical way for solving LLG equations is to first discretize it in space by finite elements or finite differences and than to solve numerically the resulting system of ODE's in time by an appropriate method. It's not difficult to argue that standard time-discretization methods fail to preserve the magnitude of magnetization.

2 Overview of Numerical Methods for LLG

2.1 Projection Methods

The idea of projection methods is simple: first solve LLG by a standard method and then project the solution onto a unit sphere to enforce the constraint $|\boldsymbol{m}| = 1$.

For simplicity we consider LLG in a dimensionless form

$$\boldsymbol{m}_t = -\boldsymbol{m} \times \Delta \boldsymbol{m} - \alpha\, \boldsymbol{m} \times (\boldsymbol{m} \times \Delta \boldsymbol{m}). \tag{3}$$

We took $\boldsymbol{h}_T = \Delta \boldsymbol{m}$, but the extension to the general case is straightforward. From the vector cross product formula $\boldsymbol{a} \times (\boldsymbol{b} \times \boldsymbol{c}) = (\boldsymbol{a} \cdot \boldsymbol{c})\boldsymbol{b} - (\boldsymbol{a} \cdot \boldsymbol{b})\boldsymbol{c}$ and from the fact that $\nabla |\boldsymbol{m}|^2 = 0$ we can rewrite the damping term entering (3),

$$\boldsymbol{m} \times (\boldsymbol{m} \times \Delta \boldsymbol{m}) = -\Delta \boldsymbol{m} - |\nabla \boldsymbol{m}|^2 \boldsymbol{m}.$$

Then (3) can be rewritten in an equivalent form

$$\boldsymbol{m}_t - \alpha \Delta \boldsymbol{m} = \alpha |\nabla \boldsymbol{m}|^2 \boldsymbol{m} - \boldsymbol{m} \times \Delta \boldsymbol{m}. \tag{4}$$

The variational formulation of the equation (4) along with the boundary condition (2) reads as

$$(\boldsymbol{m}_t, \boldsymbol{\varphi}) + \alpha(\nabla \boldsymbol{m}, \nabla \boldsymbol{\varphi}) = \alpha(|\nabla \boldsymbol{m}|^2 \boldsymbol{m}, \boldsymbol{\varphi}) + (\boldsymbol{m} \times \nabla \boldsymbol{m}, \nabla \boldsymbol{\varphi}) \quad \forall \boldsymbol{\varphi} \in V. \tag{5}$$

This problem is nonlinear. However it is possible to avoid solving the nonlinear system by a suitable linearization, while maintaining the accuracy.

Let us denote by $\boldsymbol{m}_j$ the approximation of the solution of (5) at the time t_j. Then, starting from given $\boldsymbol{m}_{j-1}$, $\boldsymbol{m}^*_{j-1}$ we compute $\boldsymbol{m}_j$, $\boldsymbol{m}^*_j$ by the following algorithm [1]:

1. Obtain $\boldsymbol{m}_j$ from backward Euler approximation of (5), viz.

$$\left(\frac{\boldsymbol{m}_j - \boldsymbol{m}^*_{j-1}}{\tau}, \boldsymbol{\varphi}\right) + \alpha(\nabla \boldsymbol{m}_j, \nabla \boldsymbol{\varphi}) = \alpha(|\nabla \boldsymbol{m}_{j-1}|^2 \boldsymbol{m}_j, \boldsymbol{\varphi}) + (\boldsymbol{m}^*_{j-1} \times \nabla \boldsymbol{m}_j, \nabla \boldsymbol{\varphi}). \tag{6}$$

2. Project $\boldsymbol{m}_j$ onto a unit sphere to get $\boldsymbol{m}^*_j$ as

$$\boldsymbol{m}^*_j = \frac{\boldsymbol{m}_j}{|\boldsymbol{m}_j|}. \tag{7}$$

The previous semi-implicit scheme is linear and first order accurate.

Another method for the LLG equation, introduced in [2], is based on a splitting procedure. At a time point $t = t_j$, we first obtain the solution of the gyromagnetic part and this is combined with the projection scheme from [3] for the damping part. The gyromagnetic part of (4) reads

$$\boldsymbol{m}_t = -\boldsymbol{m} \times \Delta \boldsymbol{m}, \tag{8}$$

while the damping part is

$$\boldsymbol{m}_t - \alpha \Delta \boldsymbol{m} = \alpha |\nabla \boldsymbol{m}|^2 \boldsymbol{m}.$$

The splitting method consists of two steps:

1. Given the solution $\boldsymbol{m}_{j-1}$ of (4) from the previous time level we discretize (8) by the backward Euler method. The resulting nonlinear system is solved by a Gauss-Seidel based technique (for more details see [2]) in order obtain the approximate solution $\boldsymbol{m}_j^*$ of (8).
2. Having $\boldsymbol{m}_j^*$, we can use the projection method from [3], consisting of

$$\left(\frac{\boldsymbol{m}_j^{**} - \boldsymbol{m}_j^*}{\tau}, \boldsymbol{\varphi} \right) + \alpha (\nabla \boldsymbol{m}_j^{**}, \nabla \boldsymbol{\varphi}) = \boldsymbol{0},$$

and

$$\boldsymbol{m}_j = \frac{\boldsymbol{m}_j^{**}}{|\boldsymbol{m}_j^{**}|}.$$

The computations in [2] show that the method is stable and faster than a 4-th order Runge-Kutta method.

In [4] the authors propose a backward Euler finite element scheme for the LLG equation, which also uses a projection to conserve $|\boldsymbol{m}|$. The system of nonlinear equations resulting from the implicit discretization of the LLG equations is solved by a GMRES-based method. It is shown in [5] that this method can use larger time steps than an Adams method.

Since the projection type methods don't conserve the norm of magnetization $|\boldsymbol{m}|$ in an implicit way, it can be used as an error indicator during the computations.

2.2 Norm-Conservative Methods

In this section we present another type of methods, where $|\boldsymbol{m}|$ is automatically conserved. These methods are also able to conserve some other physical properties of the micromagnetic systems (cf. [6], [7], [8]).

The LLG equation can be rewritten in the form

$$\boldsymbol{m}_t = \boldsymbol{a}(\boldsymbol{m}) \times \boldsymbol{m}, \tag{9}$$

where $\boldsymbol{a}(\boldsymbol{m}) = \gamma M_s \left(\boldsymbol{h}_T - \alpha \boldsymbol{h}_T \times \boldsymbol{m} \right)$.

We can discretize the previous equation at $t = t_j$ using the midpoint rule

$$\frac{\boldsymbol{m}_j - \boldsymbol{m}_{j-1}}{\tau} = \boldsymbol{a}_{j-1/2} \times \frac{\boldsymbol{m}_j + \boldsymbol{m}_{j-1}}{2}, \tag{10}$$

where $\boldsymbol{a}_{j-1/2}$ denotes the approximation of vector $\boldsymbol{a}(\boldsymbol{m})$ at the time $t_j - \tau/2$.

After scalar multiplication of (10) by $(\boldsymbol{m}_j + \boldsymbol{m}_{j-1})$ we obtain that

$$\frac{|\boldsymbol{m}_j| - |\boldsymbol{m}_{j-1}|}{\tau} = 0,$$

from which we see that the midpoint rule conserves $|\boldsymbol{m}|$.

A possible choice could be $\boldsymbol{a}_{j-1/2} = \dfrac{\boldsymbol{a}(\boldsymbol{m}_j) + \boldsymbol{a}(\boldsymbol{m}_{j-1})}{2}$. The resulting scheme reads as follows

$$\frac{\boldsymbol{m}_j - \boldsymbol{m}_{j-1}}{\tau} = \frac{\boldsymbol{a}(\boldsymbol{m}_j) + \boldsymbol{a}(\boldsymbol{m}_{j-1})}{2} \times \frac{\boldsymbol{m}_j + \boldsymbol{m}_{j-1}}{2}, \tag{11}$$

and we have to solve a nonlinear system. In [9] a scheme based on the idea of midpoint rule was introduced. The authors constructed an explicit solution for the nonlinear system for materials with uniaxial anisotropy in the absence of exchange field. When the exchange field is included, an explicit solution to the scheme presented in [9] no longer exists and the system has to be solved for instance by Newton's method [6].

In [10] the value of $\boldsymbol{a}_{j-1/2}$ is extrapolated form the values on the previous time levels by the formula $\boldsymbol{a}_{j-1/2} = \frac{3}{2}\boldsymbol{a}(\boldsymbol{m}_{j-1}) - \frac{1}{2}\boldsymbol{a}(\boldsymbol{m}_{j-2}) + O(\tau^2)$. The resulting 2nd order scheme is explicit

$$\frac{\boldsymbol{m}_j - \boldsymbol{m}_{j-1}}{\tau} = \left(\frac{3}{2}\boldsymbol{a}(\boldsymbol{m}_{j-1}) - \frac{1}{2}\boldsymbol{a}(\boldsymbol{m}_{j-2})\right) \times \frac{\boldsymbol{m}_j + \boldsymbol{m}_{j-1}}{2}. \tag{12}$$

We only have to solve a linear system of dimension 3×3 at every spatial mesh point to obtain the values of $\boldsymbol{m}_j$. In [8], the previous method is compared with implicit and explicit Euler methods, and is shown to be more accurate.

In [11] the authors present two explicit first order schemes for LLG equation which conserve $|\boldsymbol{m}|$. They use the fact that for a constant vector $\boldsymbol{a}$ the following linear ODE along with initial data $\boldsymbol{m}(0) = \boldsymbol{m}_0$

$$\boldsymbol{m}_t = \boldsymbol{a} \times \boldsymbol{m},$$

can be solved analytically:

$$\boldsymbol{m} = \boldsymbol{m}_0^{\parallel} + \boldsymbol{m}_0^{\perp} \cos(|\boldsymbol{a}|t) + \frac{\boldsymbol{a}}{|\boldsymbol{a}|} \times \boldsymbol{m}_0^{\perp} \sin(|\boldsymbol{a}|t), \tag{13}$$

where $\boldsymbol{m}_0 = \boldsymbol{m}_0^{\parallel} + \boldsymbol{m}_0^{\perp}$, $\boldsymbol{m}_0^{\parallel}$ is parallel to $\boldsymbol{a}$ and $\boldsymbol{m}_0^{\perp}$ is perpendicular to $\boldsymbol{a}$.

Having the solution $\boldsymbol{m}_{j-1}$ at time level $t = t_{j-1}$ we set $\boldsymbol{a} = \boldsymbol{a}(\boldsymbol{m}_{j-1})$ in (9)

$$\boldsymbol{m}_t = \boldsymbol{a}(\boldsymbol{m}_{j-1}) \times \boldsymbol{m}. \tag{14}$$

We obtain $\boldsymbol{m}_j$ by means of (13) in the time interval (t_{j-1}, t_j), taking $\boldsymbol{m}_{j-1}$ as the initial data.

The second method is based on the analytical solution of the nonlinear ODE (when $\boldsymbol{h}$ is constant): $\boldsymbol{m}_t = \boldsymbol{h} \times \boldsymbol{m} + \alpha \boldsymbol{m} \times (\boldsymbol{h} \times \boldsymbol{m})$. We set $\boldsymbol{h} = \gamma M_s \boldsymbol{h}_T(\boldsymbol{m}_{j-1})$

on the time interval (t_{j-1}, t_j) and proceed analogously as in the first method (for more details see [11]).

In [12], [7] the authors use the Lie Group formalism to develop methods which conserve the modulus of magnetization. Formally, a numerical method of order k for the equation (9) can be written as follow

$$\boldsymbol{m}_j = \mathrm{Exp}(\boldsymbol{A})\boldsymbol{m}_{j-1}, \tag{15}$$

where $\boldsymbol{A}$ is an update determined by $\boldsymbol{a}(\boldsymbol{m})$. By a suitable choice of this update $\boldsymbol{A}$ we can construct explicit or implicit methods of desired order.

The function Exp is an algorithmic exponential of the Lie group $SO(3)$ (for more details and different constructions of the update, see [12], [7]). With the exact matrix exponential we have

$$\exp(\boldsymbol{A})\boldsymbol{m}_{j-1} = \boldsymbol{m}_{j-1} + \frac{\sin(|\boldsymbol{A}|)}{|\boldsymbol{A}|}\boldsymbol{A}\times\boldsymbol{m}_{j-1} + \frac{1-\cos(|\boldsymbol{A}|)}{|\boldsymbol{A}|^2}\boldsymbol{A}\times(\boldsymbol{A}\times\boldsymbol{m}_{j-1}).$$

When we take $\boldsymbol{A} = \tau\boldsymbol{a}(\boldsymbol{m}_{j-1})$ in the previous equation we arrive at a method which is equivalent to method (13). Algorithms of arbitrary order can also be constructed using the Cayley transform, which is a second order approximation of the exact exponential, viz

$$\mathrm{cay}(\boldsymbol{A}) = \left(I - \tfrac{1}{2}\mathrm{skew}[\boldsymbol{A}]\right)^{-1}\left(I + \tfrac{1}{2}\mathrm{skew}[\boldsymbol{A}]\right),$$

where I is the identity matrix and

$$\mathrm{skew}[\boldsymbol{x} = (x_1, x_2, x_3)] = \begin{pmatrix} 0 & -x_3 & x_2 \\ x_3 & 0 & -x_1 \\ -x_2 & x_1 & 0 \end{pmatrix}.$$

When we put $\boldsymbol{A} = \frac{\tau}{2}(\boldsymbol{a}(\boldsymbol{m}_j) + \boldsymbol{a}(\boldsymbol{m}_{j-1}))$, we get a method equivalent to the implicit midpoint rule (11).

With the schemes from this section we can no longer use $|\boldsymbol{m}|$ as an error indicator. A self consistency error control scheme which can be used along with norm-conservative methods was suggested in [13].

3 Numerical Experiments

We will consider a numerical example of a conducting thin film subjected to an in-plane circularly polarized magnetic field, which was suggested in [14]. This problem can be reduced to a 1D problem on the interval $(0, \delta)$, where δ is the thickness of the film. In order to obtain the magnetic field $\boldsymbol{H} = (H_1, H_2, H_3)$, the LLG equation has to be coupled with the eddy current equation. This, in the 1D case takes the form

$$\mu_0\partial_t H_i - \frac{1}{\sigma}\frac{\partial^2 H_i}{\partial z^2} = -\mu_0\partial_t M_i \quad i = 1, 2, \tag{16}$$

and $H_3 = -M_3$. We take the vector $\boldsymbol{M} = (M_1, M_2, M_3) = M_s\boldsymbol{m}$.

We solve (16) along with with the boundary condition

$$\boldsymbol{H}(t) = H_s\,(\cos(\omega t), \sin(\omega t), 0) \quad z = 0,\ z = \delta. \tag{17}$$

The total field in the LLG equation takes the form $\boldsymbol{h}_T = \dfrac{\boldsymbol{H}}{M_s} + \dfrac{2A}{\mu_0 M_s^2}\dfrac{\partial^2 \boldsymbol{m}}{\partial z^2}$.

The calculations were performed with the following parameters: $\gamma = 2.211 \times 10^5$, $\alpha = 0.01$, $M_s = 8 \times 10^5$, $\sigma = 4 \times 10^6$, $\delta = 1.5 \times 10^{-6}$, $A = 1.05 \times 10^{-11}$, $\omega = 2\pi \times 10^9$, $H_s = 4.5 \times 10^3$, $\mu_0 = 4\pi \times 10^{-7}$. Moreover a uniform initial condition for the LLG equation was used: $\boldsymbol{m}_0 = (1, 0, 0)$. It is expected that the solution of the system (1), (16) with the boundary conditions (2), (17) is periodic in time (Fig. 1).

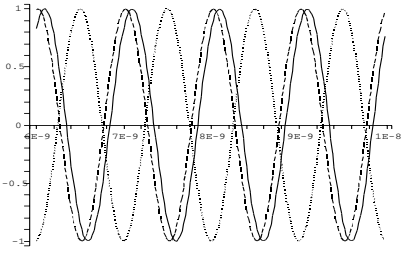

Fig. 1. x-component of $\boldsymbol{H}$ on the boundary (dashed line) and x-component of the magnetization in the points at distance $\delta/6$ (solid line) and $\delta/2$ (dotted line) from the boundary, respectively

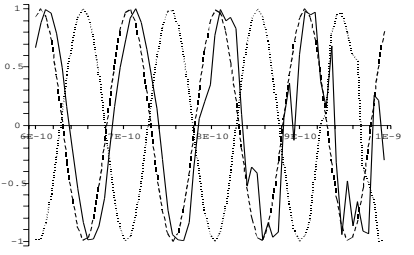

Fig. 2. Unstable solution

The time discretization of the example was performed with the methods described by (6)-(7), (10), (12), (14), and with the classical 4-th order Runge-Kutta method. We will refer to this methods as PR_1, MP_{im}, MP_{ex}, EXP_1, RK_4, respectively. For the time discretization of (16) we used the Crank-Nicholson scheme. which allowed us to use larger time steps for some of the methods. The space discretization was done by standard finite-differences. The nonlinear system in MP_{im} was solved by the Broyden's method.

Although the performance of the methods for the LLG equation is influenced by the coupling with (16), we observed that the errors induced by the discretization of (16) had minor influence on the computation, when compared to the effect of the discretization of the LLG equation. However, some methods were able to use slightly larger time steps when we discretized (16) by the Crank-Nicholson scheme, compared to the situation where we used backward Euler approximation of (16). In practice the magnetic field $\boldsymbol{H}$ is not known and the LLG equation has to be coupled with Maxwell's equations in an appropriate form.

In our experiments we first fixed the mesh parameter $h = \delta/50$ and looked for the largest time step (τ_{max}) for which we could obtain an acceptable numerical solution without oscillations. Then, we decreased the value of h to see if the stability of the method was sensitive to the mesh refinement. An example of an unstable solution computed with MP_{ex} ($h = \delta/60$, $\tau = 6 \times 10^{-12}$) is depicted in Fig. 2. The results of the numerical experiments can be found in Table 1 (by h-sensitive we denote the methods, for which we needed to decrease τ, when we decreased h in order to avoid big changes of the modulus or oscillations). In some cases, the computation of the magnetic field from Maxwell's equation at every time level is a more computationally intensive task than the approximation of the LLG equation. In such a case, the possibility of using larger times steps, gives an obvious advantage. Schemes, which are h-insensitive, can be useful when we want to use adaptive strategies.

The methods MP_{ex} and EXP_1 conserved $|\boldsymbol{m}|$ with an error of order 10^{-15}. The method MP_{im} conserved $|\boldsymbol{m}|$ up to the truncation error of the Broyden's iterations. With the residue of the Broyden's iteration about 10^{-10}, the resulting magnitude drift was of order 10^{-9} and it decreased when we increased Boryden's precision. The method MP_{im} allowed us to use larger time steps than the explicit methods. We expect that more sophisticated nonlinear strategies could speed up the method and give better results.

The projection method PR_1 was the only method for which the choice of the time step was independent of the mesh parameter h. The error in the magnitude, when $\tau = \tau_{max}$, was of order 10^{-3} and decreased with smaller values of τ. Without the projection step (7) the method would blow-up for greater values of τ. From the explicit methods, the RK_4 method could use the largest time-steps, however the magnitude drift was of order 10^{-7}.

Table 1. Performance of the methods

method	τ_{max}	h-sensitive
EXP_1	9×10^{-13}	yes
MP_{ex}	6×10^{-12}	yes
RK_4	1×10^{-11}	yes
MP_{im}	1×10^{-11}	yes
PR_1	1.4×10^{-11}	no

4 Summary

In this paper we have given a comparative overview of various methods for solving the LLG equation of micromagnetics. One of principal goals in micromagnetic computations is to maintain the constraint $|\boldsymbol{m}| = 1$. The projection methods enforce this constraint explicitly at every time level by projecting the solution onto a unit sphere. They seem to be stable with respect to the space discretization and allow us to use large time steps. They might be a good choice

when mesh adaptivity is involved. The explicit norm-conservative schemes need to use smaller time steps than the projection methods, but they satisfy the constraint $|\boldsymbol{m}| = 1$ nearly precisely. Because of their fast implementation they have been explored and used in practice. The implicit norm-conservative methods can use larger time steps than explicit methods for the cost of non-linearity of the resulting discrete system. Although the classical RK_4 performed quite well in our numerical example, in more complex problems, we still need to use the projection or small time steps to satisfy the norm constraint. The explicit norm-conservative methods of higher order should be a better choice for their capability of maintaining the physical constraints.

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