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Convergent geometric integrator for the Landau-Lifshitz-Gilbert equation in micromagnetics

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We consider a lowest-order finite element scheme for the Landau-Lifshitz-Gilbert equation (LLG) which describes the dynamics of micromagnetism. In contrast to previous works, we examine LLG with a total magnetic field which is induced by several physical phenomena described in terms of exchange energy, anisotropy energy, magnetostatic energy, and Zeeman energy. In our numerical scheme, the highest-order term which stems from the exchange energy, is treated implicitly, whereas the remaining energy contributions are computed explicitly. Therefore, only one sparse linear system has to be solved per time-step. The proposed scheme is unconditionally convergent to a global weak solution of LLG.

1 Introduction

In physics, the Landau-Lifshitz-Gilbert equation (LLG) is a well-accepted approach to model the dynamics of micromagnetism. Numerical simulations of LLG provide a fundamental insight into the understanding and development of magnetic materials which is of utter relevance e.g. in magneto-resistive storage devices.

The micromagnetic body is denoted by a polyhedral bounded Lipschitz domain $\Omega \subset \mathbb{R}^3$. The magnetic behavior of the micromagnetic body is characterized by the (unknown) magnetization $\mathbf{m} : (0,\tau) \times \Omega \to \mathbb{S}^2 = \{\mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| = 1\}$, where $(0,\tau)$ denotes the time interval. Then, LLG reads in non-dimensional form

$$\mathbf{m}_t = -\frac{\alpha}{1+\alpha^2}\mathbf{m} \times (\mathbf{m} \times \mathbf{h}_{\rm eff}) - \frac{1}{1+\alpha^2}\mathbf{m} \times \mathbf{h}_{\rm eff} \tag{1}$$

$$\mathbf{m}(0) = \mathbf{m}_0 \quad \text{in } H^1(\Omega;\mathbb{S}^2), \qquad \partial_n \mathbf{m} = 0 \quad \text{on } (0,\tau) \times \partial\Omega, \tag{2}$$

with $\alpha > 0$ the Gilbert damping parameter which depends only on the material. As a consequence of (1), the magnetization satisfies a non-convex side constraint $|\mathbf{m}| = 1$ a.e. in $\Omega_\tau := (0,\tau) \times \Omega$. Moreover, $\mathbf{h}_{\rm eff} = \mathbf{h}_{\rm eff}(\mathbf{m},\mathbf{f})$ indicates the total magnetic field and is given by the negative variation of the Gibbs free energy

$$\mathbf{h}_{\rm eff} = -\frac{\delta e(\mathbf{m})}{\delta \mathbf{m}} \quad \text{with } e(\mathbf{m}) = \int_\Omega |\nabla \mathbf{m}|^2 \, d\mathbf{x} + \int_\Omega \Phi(\mathbf{m}) \, d\mathbf{x} + \frac{1}{2}\int_{\mathbb{R}^3} |\mathcal{P}(\mathbf{m})|^2 \, d\mathbf{x} - \int_\Omega \mathbf{f} \cdot \mathbf{m} \, d\mathbf{x}. \tag{3}$$

Here, Φ refers to the anisotropy density, $\mathcal{P}(\mathbf{m})$ is related to the demagnetization field which is induced by the magnetostatic Maxwell's equations, and $\mathbf{f}$ denotes an applied field. The contributions of the bulk energy $e(\mathbf{m})$ are called exchange energy, anisotropy energy, stray-field energy, and Zeeman energy, respectively.

Supplemented by the same initial and boundary conditions (2), LLG (1) can equivalently be stated as

$$\alpha\, \mathbf{m}_t + \mathbf{m} \times \mathbf{m}_t = \mathbf{h}_{\rm eff} - \big(\mathbf{m} \cdot \mathbf{h}_{\rm eff}\big)\mathbf{m}, \tag{4}$$

cf. e.g. [4] for a detailed proof. This alternative formulation serves as basis for our FE scheme to solve LLG numerically, where we approximate $\mathbf{m}_h \approx \mathbf{m}$ and $\mathbf{v}_h \approx \mathbf{m}_t$. Note that, due to $|\mathbf{m}| = 1$ a.e., the time derivative $\mathbf{m}_t$ belongs to the tangential space of $\mathbf{m}$, i.e. $\mathbf{m} \cdot \mathbf{m}_t = 0$ a.e. in Ω_τ.

2 Numerical algorithm

Let $\mathcal{T}_h = \{T_1, \dots, T_n\}$ denote a quasi-uniform and regular triangulation of Ω into tetrahedra and $\mathcal{N}_h = \{\mathbf{z}_1, \dots, \mathbf{z}_N\}$ be the set of its nodes. To discretize the magnetization $\mathbf{m}$ in the spatial variable, we use the vector-valued Courant FE space $\mathcal{V}_h = \mathcal{S}^1(\mathcal{T}_h)^3$ of piecewise linear and globally continuous functions. Let

$$\mathcal{M}_h = \big\{\boldsymbol{\phi}_h \in \mathcal{V}_h : |\boldsymbol{\phi}_h(\mathbf{z})| = 1 \text{ for all } \mathbf{z} \in \mathcal{N}_h\big\} \tag{5}$$

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be the restricted finite element set, where $\mathbf{m}_h^j \approx \mathbf{m}(\tau_j)$ is sought due to the constraint $|\mathbf{m}| = 1$. Furthermore, let

$$\mathcal{K}_{\boldsymbol{\phi}_h} = \{\boldsymbol{\psi}_h \in \mathcal{V}_h : \boldsymbol{\psi}_h(\mathbf{z}) \cdot \boldsymbol{\phi}_h(\mathbf{z}) = 0 \text{ for all } \mathbf{z} \in \mathcal{N}_h\} \tag{6}$$

be the discrete tangential space associated with some $\boldsymbol{\phi}_h \in \mathcal{M}_h$, where the discrete time derivative $\mathbf{v}_h^j \approx \mathbf{m}_t(\tau_j)$ is sought.

To obtain a time-splitting scheme to solve LLG numerically, we follow the idea of [1], where the small particle limit $\mathbf{h}_{\text{eff}} = \Delta\mathbf{m}$ is considered. Therefore, we proceed by setting $\mathbf{v} = \mathbf{m}_t$ in (4) and by discretizing the weak form. The term of highest order, i.e. the exchange contribution, is treated implicitly by means of a θ-scheme, whereas the remaining three terms of the effective magnetic field $\mathbf{h}_{\text{eff}}$ are computed explicitly.

Algorithm 2.1. *Input: Initial data $\mathbf{m}_h^0 \in \mathcal{M}_h$, damping parameter α, parameter $0 < \theta \leq 1$, counter $j = 0$.*

(i) *Find $\mathbf{v}_h^j \in \mathcal{K}_{\mathbf{m}_h^j}$, such that for all test functions $\boldsymbol{\psi}_h \in \mathcal{K}_{\mathbf{m}_h^j}$ it holds that*

$$\begin{aligned} &\alpha \int_\Omega \mathbf{v}_h^j \cdot \boldsymbol{\psi}_h \, d\mathbf{x} + \int_\Omega (\mathbf{m}_h^j \times \mathbf{v}_h^j) \cdot \boldsymbol{\psi}_h \, d\mathbf{x} \\ &\quad = -\int_\Omega \nabla(\mathbf{m}_h^j + \theta k \mathbf{v}_h^j) \cdot \nabla \boldsymbol{\psi}_h \, d\mathbf{x} - \int_\Omega \Big(D\Phi(\mathbf{m}_h^j) + \mathcal{P}_h(\mathbf{m}_h^j) - \mathbf{f}^j \Big) \cdot \boldsymbol{\psi}_h \, d\mathbf{x}. \end{aligned} \tag{7}$$

(ii) *Set $\mathbf{m}_h^{j+1}(\mathbf{z}) = \frac{\mathbf{m}_h^j(\mathbf{z}) + k\mathbf{v}_h^j(\mathbf{z})}{|\mathbf{m}_h^j(\mathbf{z}) + k\mathbf{v}_h^j(\mathbf{z})|}$ for all nodes $\mathbf{z} \in \mathcal{N}_h$, increase counter $j \mapsto j+1$, and go to (i).*

Output: Sequence of functions $\mathbf{v}_h^j \in \mathcal{K}_{\mathbf{m}_h^j}$ as well as $\mathbf{m}_h^j \in \mathcal{M}_h$ for $j \geq 0$. □

According to the Lemma of Lax-Milgram, (7) admits a unique solution $\mathbf{v}_h^j \in \mathcal{K}_{\mathbf{m}_h^j}$. As a consequence of $\mathbf{m}_h^j(\mathbf{z}) \cdot \mathbf{v}_h^j(\mathbf{z}) = 0$, the discretized magnetization $\mathbf{m}_h^{j+1} \in \mathcal{M}_h$ for $j \geq 0$ is thus well-defined. We stress that only one (sparse) linear system (7) has to be solved per time-step and that the non-convex side constraint $|\mathbf{m}| = 1$ is nodewise fulfilled.

Remark 2.2 The implementation of the non-local energy contribution, i.e. the magnetostatic potential $\mathcal{P}(\mathbf{m})$, is related to the solution of a transmission problem in $\mathbb{R}^3$ and thus involves certain boundary integral operators. Therefore, the computation of the demagnetization field is the most time and memory consuming part in numerical simulations and has to be realized effectively. Comments on the numerical treatment of the magnetostatic potential $\mathcal{P}$ are found in [5]. Therein, several approaches are considered and analyzed to conclude convergence including an approximate computation $\mathcal{P}_h$ of this energy contribution.

3 Convergence result

The definition of a weak solution to LLG is stated in [4] and is based on the idea of [2]. To prove weak convergence to a global weak solution, the discrete solutions $\mathbf{m}_h^j$ and $\mathbf{m}_h^{j+1}$ are affinely interpolated in time. For all $\mathbf{x} \in \Omega$ and all times $t \in [0, \tau]$ with $j = \{0, \dots, J-1\}$ and $t \in [jk, (j+1)k)$, we define $\mathbf{m}_{hk}(t, \mathbf{x}) := \frac{t - jk}{k} \mathbf{m}_h^{j+1}(\mathbf{x}) + \frac{(j+1)k - t}{k} \mathbf{m}_h^j(\mathbf{x})$. The following convergence theorem generalizes the result of [1], yields reliability of the proposed algorithm, and even proves existence of global weak solutions. A rigorous proof is given in [4]. We stress that no coupling of the time-step size k and space-mesh size h is imposed.

Theorem 3.1 *Fix $\theta \in (1/2, 1]$. Suppose that $\mathcal{T}_h$ is a family of regular triangulations with mesh-sizes $h \searrow 0$ such that all occurring dihedral angles are smaller than $\pi/2$. Assume that $\mathbf{m}_h^0 \to \mathbf{m}_0$ in $H^1(\Omega; \mathbb{R}^3)$ as $h \searrow 0$ and that the stray-field approximation $\mathcal{P}_h$ satisfies*

$$\|\mathcal{P}_h \mathbf{m}_h^j\|_{L^2(\Omega)} \leq C \, \|\mathbf{m}_h^j\|_{L^2(\Omega)} \quad \textit{as well as} \quad \|\mathcal{P}\mathbf{m} - \mathcal{P}_h \mathbf{m}\|_{L^2(\Omega_\tau)} \xrightarrow{h \to 0} 0 \tag{8}$$

with some h-independent constant $C > 0$. Then, as $h, k \searrow 0$, the approximate magnetization $\mathbf{m}_{hk}$ admits a subsequence which converges weakly in $H^1(\Omega_\tau; \mathbb{R}^3)$ to a weak solution $\mathbf{m}$ of LLG. □

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References

[1] F. Alouges, Discrete Contin. Dyn. Syst. Ser. S, **1**, 187–196 (2008).
[2] F. Alouges and A. Soyeur, Nonlinear Anal. **18**, 1071–1084, (1992).
[3] S. Bartels, SIAM J. Numer. Anal. **43**, 220–238 (2005).
[4] P. Goldenits, Phd-Thesis, Institute for Analysis and Scientific Computing, Vienna University of Technology.
[5] P. Goldenits and D. Praetorius, work in progress, Institute for Analysis and Scientific Computing, Vienna University of Technology.
[6] R. Verfürth, A review of a posteriori error estimation and adaptive mesh-refinement techniques (Wiley-Teubner, 1996).