Constraint Preserving, Inexact Solution of Implicit Discretizations of Landau–Lifshitz–Gilbert Equations and Consequences for Convergence

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The Landau-Lifshitz-Gilbert equation describes dynamics of ferromagnetism. Nonlinearity of the equation and a non-convex side constraint make it difficult to design reliable approximation schemes. In this paper, we discuss the numerical solution of nonlinear systems of equations resulting from implicit, unconditionally convergent discretizations of the problem. Numerical experiments indicate that finite-time blow-up of weak solutions can occur and thereby underline the necessity of the design of reliable discretization schemes that approximate weak solutions.

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1 Introduction

The Landau-Lifshitz-Gilbert equation describes certain dynamics of ferromagnetism: Given a damping parameter $\alpha \geq 0$ the magnetization \( m : (0, T) \times \Omega \rightarrow S^2 \), where $T > 0$, $\Omega \subset \mathbb{R}^n$ is a Lipschitz domain, and $S^2 = \{ x \in \mathbb{R}^3 : |x| = 1 \}$, solves

$$ m_t = -\alpha \, m \times (m \times \Delta m) + m \times \Delta m, \tag{1} $$

subject to \( m(0) = m_0 \in W^{1,2}(\Omega; S^2) \) and $\partial_n m = 0$ on $(0, T) \times \partial \Omega$. Here, $n = 2$ or $n = 3$. The non-convex constraint $|m| = 1$ a.e. in $\Omega_T := (0, T) \times \Omega$ makes it difficult to design approximation schemes for (1) that (i) satisfy a discrete energy principle and (ii) produce approximations that converge to a weak solution of (1) under mild conditions on discretization parameters. Schemes that partially solve these two requirements have been proposed [5, 8, 7] and either satisfy the constraint by projection or approximately through penalization. The methods based on penalization seem unsatisfactory since they diverge singularities and lead to restrictive conditions on discretization parameters. We refer the reader to [6] for a detailed review of approximation schemes and further references. Recently, explicit discretizations of (1) which satisfy the unit-length constraint and thereby avoid any projection steps and that is unconditionally stable and convergent has been designed in [4]. It is based on the equivalent Gilbert form of (1),

$$ m_t + \alpha \, m \times m_t = (1 + \alpha^2) \, m \times \Delta m, \tag{2} $$

and reads: Given $\tilde{m}_h^0 \in V_h$, compute $\tilde{m}_h^{n+1} \in V_h$ such that for all $w \in V_h$

$$ (d_t \tilde{m}_h^{n+1}, w)_h + \alpha (\tilde{m}_h^{n+1/2} \cdot d_t \tilde{m}_h^{n+1}, w)_h = (1 + \alpha^2) (\tilde{m}_h^{n+1/2} \times \Delta_h \tilde{m}_h^{n+1/2}, w)_h, \tag{3} $$

see below for details on notation. A fixed-point iteration that converges to a solution of the nonlinear system of equations (3) provided that $k = O(h^2)$ is given in [4]. However, the analysis in [4] has two drawbacks: (i) the global convergence analysis towards a weak solution of (1) requires the exact solution of (3) and (ii) iterates in the fixed-point iteration do not satisfy the unit-length constraint at the nodes. In this paper we aim at improving these two points.

Notation. We let $V_h \subset W^{1,2}(\Omega; \mathbb{R}^3)$ be the lowest order finite element space subordinate to a regular triangulation $\mathcal{T}$ of the polygonal or polyhedral Lipschitz domain $\Omega$ into triangles or tetrahedra, respectively, of maximal and minimal diameter $h > 0$ and $h_{\text{min}} > 0$, respectively. A discrete version of the inner product in $L^2(\Omega; \mathbb{R}^3)$ satisfies for $v, w \in C(\overline{\Omega}; \mathbb{R}^3)$ and $v_h, w_h \in V_h$

$$ (v, w)_h = \sum_{z \in N} \beta_z v(z) \cdot w(z), \quad ||v_h||_{L^2} \leq ||v_h||_h = (v_h, v_h)_h^{1/2} \leq (n + 2)^{1/2} ||v_h||_{L^2}, $$

where $\beta_z = \int_{\Omega} \varphi_z \, dx$ for each node $z \in N$ if $\{ \varphi_z : z \in N \}$ denotes the nodal basis of the lowest order finite element space related to $\mathcal{T}$. The operator $\Delta_h : W^{1,2}(\Omega; \mathbb{R}^3) \rightarrow V_h$ satisfies for $w \in W^{1,2}(\Omega; \mathbb{R}^3)$ and all $w_h \in V_h$

$$ -(\Delta_h w, v_h)_h = (\nabla w, \nabla v_h), \quad ||\Delta_h w_h||_h \leq c_1 h_{\text{min}}^2 ||w_h||_2^2. \tag{4} $$

Given a time-step size $\kappa > 0$ and a sequence $(\varphi^j)_{j \geq 0}$ we write $d_t \varphi^j := k^{-1} (\varphi^j - \varphi^{j-1})$ for $j \geq 1$ and let $\varphi^{j+1/2} := \frac{1}{2} (\varphi^{j+1} + \varphi^j)$ for $j \geq 0$.

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2 Refined Convergence Analysis

Throughout this section we assume that we are given sequences \((m_h^j)_{j=0,1,...,J}, (r_h^j)_{j=0,1,...,J} \subset V_h\) such that for all \(j = 0, 1, ..., J - 1\) with \(T \leq J\) there holds \(||r_h^j||_h \leq \varepsilon\) and

\[
(d_t m_h^{j+1}, w_h)_h + \alpha (m_h^{j+1/2} \cdot d_t m_h^{j+1}, w_h)_h = (1 + \alpha^2) (m_h^{j+1/2} \cdot \Delta_h m_h^{j+1/2}, w_h)_h + (r_h^{j} \cdot m_h^{j+1/2}, w_h)_h. \quad (5)
\]

**Lemma 2.1** Suppose that \(|m_h^0(z)| = 1\) for all \(z \in \mathcal{N}\). Then the sequence \((m_h^j)_{j=0,1,...,J}\) satisfies \(|m_h^{j+1}(z)| = 1\) for \(j = 0, 1, ..., J - 1\) and all \(z \in \mathcal{N}\) and

\[
\frac{1}{2} d_t ||\nabla m_h^{j+1}||_2^2 + (1 - \varepsilon) \frac{\alpha}{1+\alpha^2} ||d_t m_h^{j+1}||_h^2 \leq \left( c_2 \varepsilon h^{-2} ||\mathcal{N}||^{1/2} + \alpha \varepsilon / (4(1+\alpha^2)) \right). \]

**Proof.** Choosing \(w_h = \varphi_{m_h^j}(z)\) in (5) implies \(\frac{1}{2} d_t |m_h^{j+1}(z)|^2 = d_t m_h^{j+1}(z) \cdot m_h^{j+1/2}(z) = 0\) and hence \(|m_h^{j+1}(z)| = 1\) provided \(|m_h^j(z)| = 1\). We choose \(w_h = -\Delta_h m_h^{j+1/2}\) in (5) to verify

\[
\frac{1}{2} d_t ||\nabla m_h^{j+1}||_2^2 - \alpha(m_h^{j+1/2} \cdot \Delta_h m_h^{j+1/2}, d_t m_h^{j+1}) \leq ||r_h'||_h ||m_h^{j+1/2}||_L^\infty ||\Delta_h m_h^{j+1/2}||_h \leq c_2^2 h^{-2} ||\mathcal{N}||^{1/2} \varepsilon,
\]

where we used \(||m_h^{j+1/2}||_L^\infty \leq 1\), (4), and \(||r_h'||_h \leq \varepsilon\). The choice \(w_h = d_t m_h^{j+1}\) gives

\[
\frac{\alpha}{1+\alpha^2} ||d_t m_h^{j+1}||_h^2 - \alpha(m_h^{j+1/2} \cdot \Delta_h m_h^{j+1/2}, d_t m_h^{j+1}) \leq \frac{\alpha}{4\varepsilon(1+\alpha^2)} ||r_h'||_h^2 + \frac{\alpha}{1+\alpha^2} ||d_t m_h^{j+1}||_h^2.
\]

A combination of the two estimates finishes the proof of the lemma. \(\square\)

**Definition 2.2** For \(j = 0, 1, ..., J - 1\) and \(t \in [j,k], (j+1,k)\) define

\[
M(t, \cdot) := \frac{t-j}{k} m_h^{j} + \frac{j+1-k}{k} m_h^{j+1}, \quad M^+(t, \cdot) := m_h^{j+1}, \quad M^-(t, \cdot) := m_h^{j+1/2}, \quad R^-(t, \cdot) := r_h^j.
\]

The following theorem shows that the scheme (5) approximates weak solutions of (1) in the sense of [1].

**Theorem 2.3** Suppose \(|m_h^0(z)| = 1\) for all \(z \in \mathcal{N}\) and let \((m_h^j)_{j=0,1,...,J}, (r_h^j)_{j=0,1,...,J}\) solve (5). Assume that \(m_h^0 \rightarrow m_0\) in \(W^{1,2}(\Omega; \mathbb{R}^3)\) for \(h \rightarrow 0\). For \(k, h, \varepsilon \rightarrow 0\) satisfying \(\varepsilon = o(h^{-2}||m_h^0||)\) there exists a weak solution \(m \in W^{1,2}(\Omega; \mathbb{R}^3)\) of (1) such that \(m\) sub-converges to \(m\) in \(W^{1,2}(\Omega; \mathbb{R}^3)\). In particular, \(|m| = 1 \text{ a.e. in } \Omega_T, \ m(0) = m_0\) in the sense of traces, and \(m\) satisfies an energy law and (2) in the sense of distributions, i.e., for all \(w \in C^\infty(\Omega_T; \mathbb{R}^3)\) and all \(0 < T' < T\) there holds

\[
\int_{\mathcal{L}_T} m \cdot w \ dx dt + \alpha \int_{\mathcal{L}_T} (m \times m_t) \cdot w \ dx dt = -(1 + \alpha^2) \int_{\mathcal{L}_T} (m \times \nabla m) : \nabla w \ dx dt,
\]

\[
\frac{1}{2} ||\nabla m(T')||_2^2 + \frac{\alpha}{1+\alpha^2} \int_{\mathcal{L}_T} ||m_t||_2^2 dt \leq \frac{1}{2} ||\nabla m(0)||_2^2 + o(1).
\]

**Proof.** We sketch the proof of the theorem and refer the reader to [4] for details. Given any \(T'\) such that \(Jk > T' > 0\), summation of the estimate in Lemma 2.1 over \(j = 0, 1, ..., J'\) shows

\[
\frac{1}{2} ||\nabla M^+(T')||_2^2 + \frac{\alpha}{1+\alpha^2} \int_{0}^{T'} ||M_t||_2^2 dt \leq \frac{1}{2} ||\nabla M(0)||_2^2 + o(1).
\]

(6)

This bound yields the existence of \(m \in W^{1,2}(\Omega_T; \mathbb{R}^3)\) such that, as \(k, h, \varepsilon \rightarrow 0\) (for appropriate subsequences),

\[
M \rightarrow m \text{ in } W^{1,2}(\Omega_T; \mathbb{R}^3), \quad \nabla M^+, \nabla M^- \rightarrow \nabla m \text{ in } L^2(\Omega_T; \mathbb{R}^3), \quad M^+, M^- \rightarrow m \text{ in } L^2(\Omega_T; \mathbb{R}^3)
\]

and \(M^+ \rightarrow m\) in \(L^\infty(0, T; W^{1,2}(\Omega; \mathbb{R}^3))\). Since \(|M^+(t, z)| = 1\) for every \(z \in \mathcal{N}\) and almost all \(t \in (0, T)\), there holds for every \(K \subset T_h\),

\[
|||M^+|^2 - 1|||_{L^2(K)} \leq Ch ||\nabla ((|M^+|^2 - 1)|||_{L^2(K)} = 2Ch ((|\nabla M^+|||_{L^2(K)} \leq 2Ch ||\nabla M^+|||_{L^2(K)},
\]

which implies \(|M^+| \rightarrow 1\) in \(L^2(\Omega_T; \mathbb{R}^3)\), and hence \(|m| = 1\) almost everywhere in \(\Omega_T\). Equation (5) may be written as follows: letting \(w_h(t) := I_h w(t, \cdot) \in \mathcal{M}_h\) be the nodal interpolant of \(w \in C^\infty(\Omega_T; \mathbb{R}^3)\), we have

\[
\int_0^T (M_t, \mathcal{M}, w_h)_h dt + \alpha \int_0^T (\mathcal{M} \times M_t, \mathcal{M}, w_h)_h dt = (1 + \alpha^2) \int_0^T (\mathcal{M} \times \Delta_h \mathcal{M}, \mathcal{M}, w_h)_h dt + \int_0^T (R^- \times \mathcal{M}, w_h)_h dt. \quad (7)
\]
Properties of nodal interpolation and (6) allow to prove that

\[
\int_0^T (M_t, w_h) dt = \int_0^T (m_t, w) & \quad \text{and} \quad \int_0^T (\bar{M} \times M_t, w_h) dt = \int_0^T (m \times m_t, w) dt.
\]

The first term on the right-hand side of (7) requires a more careful treatment. There holds

\[
(\bar{M} \times \bar{\Delta}_h \bar{M}, w_h)_h = (\text{Id} - I_h)(\bar{M} \times w_h), \bar{\Delta}_h \bar{M})_h + (\nabla (I_h - \text{Id})(\bar{M} \times w_h), \nabla \bar{M} + (\nabla (\bar{M} \times w_h), \nabla \bar{M}.
\]

Estimates for nodal interpolation and (6) imply that the first two terms on the right-hand side converge to 0 when integrated over \((0, T)\). Owing to properties of the vector product we have \((\nabla (\bar{M} \times w_h), \nabla \bar{M}) = (\bar{M} \times \nabla w_h, \nabla \bar{M})\) and this identity allows to pass to the limit, i.e.,

\[
\int_0^T (\bar{M} \times \bar{\Delta}_h \bar{M}, w_h) dt = \int_0^T (m \times \nabla w, \nabla m) dt = \int_0^T (\nabla (m \times w), \nabla m) dt.
\]

Finally, noting that the last term in the right-hand side of (7) converges to 0 and that the trace operator is weakly continuous proves the theorem. \(\Box\)

### 3 Improved Fixed-Point Iteration

Our iterative method for the approximate solution of (3) is based on the observation that \(n_h = \bar{m}_j^{l+1/2}\) in (3) solves

\[
\frac{2}{k} (n_h, w_h)_h - \frac{2\alpha}{k} (n_h \times \bar{m}_j^l, w_h)_h - (1 + \alpha^2) (n_h \times \bar{\Delta}_h n_h, w_h)_h = \frac{2}{k} (\bar{m}_j^l, w_h)_h,
\]

where we used that \(d_L \bar{m}_j^{l+1} = \frac{2}{k} (n_h - \bar{m}_j^l)\). This motivates the following iteration that provides solutions of (5).

**Algorithm A.** Set \(n_0^l := m_0^l\) and \(\ell := 0\). (i) Compute \(n_{h+1}^l \in V_h\) such that for all \(w_h \in V_h\) there holds

\[
\frac{2}{k} (n_{h+1}^l, w_h)_h - \frac{2\alpha}{k} (n_{h+1}^l \times m_j^l, w_h)_h - (1 + \alpha^2) (n_{h+1}^l \times \bar{\Delta}_h n_{h+1}^l, w_h)_h = \frac{2}{k} (m_j^l, w_h)_h. 
\]  

(8)

(ii) If \(\|\bar{\Delta}_h (n_{h+1}^l - n_{h}^l)\|_h \leq \varepsilon/(1 + \alpha^2)\) then set \(m_{h+1}^l := 2n_{h+1}^l - m_j^l\) and stop; otherwise set \(\ell := \ell + 1\) and go to (i).

**Theorem 3.1** Suppose that \(m_j^l \in V_h\) satisfies \(|m_j^l(z)| = 1\) for all \(z \in N\). For all \(\ell \geq 0\) there exists a unique solution \(n_h^{l+1}\) to (8) such that for all \(\ell \geq 1\) holds

\[
\|n_{h+1}^l - n_h^l\|_h \leq \Theta \|n_{h+1}^l - n_{h}^{l-1}\|_h \quad \text{with} \quad \Theta := c_1^2 k h^{-2}(1 + \alpha^2),
\]

i.e., Algorithm A converges if \(\Theta < 1\). If \(m_{h+1}^l := 2n_{h+1}^l - m_j^l\) is the output of Algorithm A then there holds (5) with \(r_h^l = (1 + \alpha^2) \bar{\Delta}_h(n_{h+1}^l - n_h^l)\).

**Proof.** Unique solvability follows from the Lax-Milgram lemma by observing that the left-hand side of (8) defines a non-symmetric, elliptic bilinear form \(a(n_h, w_h)\) on \(V_h \times V_h\). Next, choosing \(w_h = n_h^{l+1}(z) \varphi_h\) in (8), properties of the discrete inner product \((\cdot, \cdot)_h\) and properties of the vector product yield \(|n_h^{l+1}(z)| \leq |m_j^l(z)| = 1\) for all \(z \in N\). We subtract two subsequent equations in (i) to verify for \(e_{h+1}^l := n_{h+1}^l - n_h^l\)

\[
\frac{2}{k} (e_{h+1}^l, w_h)_h - \frac{2\alpha}{k} (e_{h+1}^l \times m_j^l, w_h)_h - (1 + \alpha^2)(e_{h+1}^l \times \bar{\Delta}_h n_{h+1}^l, w_h)_h - (1 + \alpha^2)(n_{h+1}^l \times \bar{\Delta}_h e_{h+1}^l, w_h)_h = 0
\]

for all \(w_h \in V_h\). For \(w_h = e_{h+1}^l\) this implies

\[
\frac{2}{k} ||e_{h+1}^l||_h^2 \leq (1 + \alpha^2)||n_{h+1}^l||_{L^\infty} \|\bar{\Delta}_h e_{h+1}^l\|_h \leq (1 + \alpha^2)c_2^2 h^{-2}\|e_{h+1}^l\|_h,\]

where we used \(||n_{h}^l||_{L^\infty} \leq 1\) and (4). This proves (9). If \(m_{h+1}^l := 2n_{h+1}^l - m_j^l\) then there holds with \(\mu = (1 + \alpha^2)\)

\[
(d_t m_h^{l+1}, w_h)_h + \alpha (m_h^{l+1/2} \times d_t m_h^{l+1}, w_h)_h - \mu (m_h^{l+1/2} \times \bar{\Delta}_h m_h^{l+1/2}, w_h)_h = \mu (m_h^{l+1/2} \times \bar{\Delta}_h [m_h^l - m_h^{l+1}], w_h)_h.
\]

This finishes the proof of the theorem. \(\Box\)
4 Numerical Experiments

For our numerical experiments we choose \( \Omega := (-1/2, 1/2)^2 \), \( T := 1/20 \), \( \alpha := 1 \), and

\[
m_0(x) := \begin{cases} 
(0, 0, -1) & \text{for } |x| \geq 1/2, \\
(2xA, A^2 - |x|^2)/(A^2 + |x|^2) & \text{for } |x| \leq 1/2,
\end{cases}
\]

where \( A = A(x) := (1 - 2|x|)^4/4 \). For uniform triangulations \( T_j \) of \( \Omega \) into right-angled triangles of diameter \( h_j = \sqrt{2} \times 2^{-j} \) for \( j = 4, 5, 6 \) and with \( h_j = h_j^2/10 \) and \( \epsilon_j = h_j^{5/2} \) we used Algorithm A to compute solutions of (5). The initial \( m_0 \in V_h \) was chosen as the nodal interpolant of \( m_0 \). We remark that in all of our simulations, Algorithm A converged within at most 25 iterations. The left plot in Figure 1 displays the energy \( E(M(t)) = \frac{1}{2}||\nabla M^+(t)||_W^2 \) and the \( W^{1,\infty} \) semi-norm \( ||\nabla M^+(t)||_{W^{1,\infty}} \) as functions of \( t \in (0, T) \) for the numerical approximations obtained on the triangulations \( T_j \) for \( j = 4, 5, 6 \). We observe that the energies are uniformly bounded, indicating robustness of our method, and that the \( W^{1,\infty} \) semi-norm attains the maximum value among functions in \( V_h \) that have unit length at all nodes, indicating that this choice of initial data leads to singular solutions of (1). The two snapshots of the numerical solution shown in Figure 1 explain how the (discrete) finite-time blow-up occurs: At \( t = 0.0352 \) the solution vector at the origin and the surrounding ones point into opposite directions. Then, the vector at the origin changes its direction and all vectors point in the same direction at \( t = 0.0391 \).

![Fig. 1 Energy \( E(M(t)) \) and \( W^{1,\infty} \) semi-norm \( |M(t)|_{1,\infty} = ||\nabla M^+(t)||_{W^{1,\infty}} \) in an example leading to maximal gradients (left). Snapshots of the numerical solution on triangulation \( T_6 \) in a neighborhood of the origin for \( t = 0.0352 \) and \( t = 0.0391 \) (right).](image)

References