ASC Report No. 02/2012

An Effective Integrator for the Landau-Lifshitz-Gilbert Equation

P. Goldenits, G. Hrkac, D. Praetorius, D. Suess

Institute for Analysis and Scientific Computing
Vienna University of Technology — TU Wien
www.asc.tuwien.ac.at ISBN 978-3-902627-05-6

Most recent ASC Reports

01/2012	*A. Arnold, L. Neumann, W. Hochhauser* Stability of glued and embedded Glass Panes: Dunkerley straight Line as a conservative Estimate of superimposed buckling Coefficients
43/2011	*G. Hastermann, P. Lima, L. Morgado, E. Weinmüller* Numerical Solution of the Density Profile Equation with p-Laplacians
42/2011	*M. Aurada, J.M. Melenk, D. Praetorius* Mixed Conforming elements for the large-body limit in micromagnetics: a finite element approach
41/2011	*P. Amodio, T. Levitina, G. Settanni, E.B. Weinmüller* On the Calculation of the Finite Hankel Transform Eigenfunctions
40/2011	*D.P. Hewett, S. Langdon, J.M. Melenk* A high frequency hp boundary element method for scattering by convex polygons
39/2011	*A. Jüngel* Semiconductor Device Problems
38/2011	*L. Neumann, A. Arnold, W. Hochhauser* Zur Stabilität von geklebten und geklotzten Glasscheiben: Beurteilung der Dunkerley'schen Geraden zur Beulwertbestimmung
37/2011	*A. Dick, O. Koch, R. März, E. Weinmüller* Collocation Schemes for Nonlinear Index 1 DAEs with a Singular Point
36/2011	*J.A. Carrillo, S. Hittmeir, A. Jüngel* Cross diffusion and nonlinear diffusion preventing blow up in the Keller-Segel model
35/2011	*P. Fuchs, A. Jüngel, M. von Renesse* On the Lagrangian structure of quantum fluid models

Institute for Analysis and Scientific Computing
Vienna University of Technology
Wiedner Hauptstraße 8–10
1040 Wien, Austria

E-Mail: admin@asc.tuwien.ac.at
WWW: http://www.asc.tuwien.ac.at
FAX: +43-1-58801-10196

ISBN 978-3-902627-05-6

An Effective Integrator for the Landau-Lifshitz-Gilbert Equation

P. Goldenits * **G. Hrkac** ** **D. Praetorius** *** **D. Suess** ****

* *Institute for Analysis and Scientific Computing, Vienna University of Technology, 1040 Wien, Wiedner Hauptstraße 8-10, Austria, (e-mail: petra.goldenits@tuwien.ac.at).*
** *Institute for Analysis and Scientific Computing, Vienna University of Technology, 1040 Wien, Wiedner Hauptstraße 8-10, Austria and Department of Materials Science and Engineering, University of Sheffield, S1 3JD Sheffield, Mappin Street, UK, (e-mail: g.hrkac@sheffield.ac.uk).*
*** *Institute for Analysis and Scientific Computing, Vienna University of Technology, 1040 Wien, Wiedner Hauptstraße 8-10, Austria, (e-mail: dirk.praetorius@tuwien.ac.at).*
**** *Institute of Solid State Physics, Vienna University of Technology, 1040 Wien, Wiedner Hauptstraße 8-10, Austria, (e-mail: dieter.suess@tuwien.ac.at).*

Abstract: 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 from the mathematics literature, we examine LLG including the total magnetic field induced by physical phenomena described in terms of exchange energy, anisotropy energy, magnetostatic energy, as well as Zeeman energy. Besides a strong non-linearity and a non-convex side constraint, the non-local dependence of the demagnetization field from the magnetization represents a challenging task for the numerical integrator. In our numerical scheme, only the highest order term, namely the exchange contribution, is treated implicitly, whereas the remaining contributions are computed explicitly. This is, in particular, advantageous for the computation of the demagnetization field by means of the popular approach of Fredkin et al. (1990). Furthermore, our scheme requires to solve only one linear system per time-step and allows a simplified computation of the arising system matrices by mass-lumping. Finally, the proposed integrator is mathematically reliable in the sense that we prove unconditional convergence for the approximation of a weak solution.

Keywords: finite elements, micromagnetism, Landau-Lifshitz-Gilbert equation, time-integration, non-convex, non-local, non-linear, demagnetization field

1. INTRODUCTION

The understanding of the dynamic behaviour of a micromagnetic body under the influence of certain micromagnetic phenomena is essential and of utter relevance for the development of magnetic materials. In the literature, the Landau-Lifshitz-Gilbert equation (LLG) is well-accepted to model the dynamics of micromagnetism. A variety of applications such as for example the development of magneto-resistive storage devices as well as the amount of numerical issues makes LLG of interest for both, physicists and mathematicians.

In our contribution we consider a polyhedral bounded Lipschitz domain $\Omega \subset \mathbb{R}^3$ and a fixed time interval $(0, \tau)$. Let $\mathbf{m}_0 : \Omega \to \mathbb{S}^2 = \{\mathbf{x} \in \mathbb{R}^3 | \, |\mathbf{x}| = 1\}$ be some given initial state. Then, the non-dimensional formulation of LLG reads

$$\begin{aligned}\mathbf{m}_t = &-\frac{\alpha}{1+\alpha^2}\mathbf{m} \times (\mathbf{m} \times \mathbf{h}_{\rm eff}(\mathbf{m}, \mathbf{f})) \\ &- \frac{1}{1+\alpha^2}\mathbf{m} \times \mathbf{h}_{\rm eff}(\mathbf{m}, \mathbf{f}),\end{aligned} \quad (1)$$

$$\mathbf{m}(0) = \mathbf{m}_0 \quad \text{in } \Omega, \quad (2)$$

$$\partial_{\boldsymbol{\nu}}\mathbf{m} = 0 \qquad \text{on } (0, \tau) \times \partial\Omega, \quad (3)$$

where the (unknown) magnetization is denoted by a vector-valued function $\mathbf{m} : (0, \tau) \times \Omega \to \mathbb{S}^2$ which satisfies the non-convex side constraint $|\mathbf{m}| = 1$ a.e. in $(0, \tau) \times \Omega$. Here, $\alpha > 0$ refers to the Gilbert damping parameter which depends only on the material. Moreover, $\mathbf{m}_t$ is the time derivative of $\mathbf{m}$, and $\mathbf{h}_{\rm eff}(\mathbf{m}, \mathbf{f})$ denotes the total magnetic field and is given by the negative variation of the Gibbs Free energy

$$\mathbf{h}_{\rm eff}(\mathbf{m}, \mathbf{f}) = -\frac{\delta e(\mathbf{m})}{\delta \mathbf{m}}. \quad (4)$$

In this work, the bulk energy $e(\cdot)$ consists of exchange energy, anisotropy energy, magnetostatic energy, as well as Zeeman energy and thus reads

$$e(\mathbf{m}) = \frac{C_{\rm ex}}{2}\int_\Omega |\nabla \mathbf{m}|^2 + C_{\rm ani}\int_\Omega \Phi(\mathbf{m}) + \frac{1}{2}\int_\Omega \mathbf{m}\cdot\nabla u - \int_\Omega \mathbf{f}\cdot\mathbf{m}. \tag{5}$$

Here, Φ refers to the anisotropy density, $\mathbf{f}$ denotes an applied external field, and ∇u is the demagnetization field. The latter is obtained from the magnetostatic Maxwell's equations with u being the solution $u = (u^{\rm int}, u^{\rm ext})$ of the full space transmission problem

$$\begin{aligned} \Delta u^{\rm int} &= \operatorname{div}\mathbf{m} && \text{in } \Omega,\\ \Delta u^{\rm ext} &= 0 && \text{in } \mathbb{R}^3\backslash\overline{\Omega},\\ [u] &= 0 && \text{on } \Gamma,\\ [\partial_{\boldsymbol\nu} u] &= -\mathbf{m}\cdot\boldsymbol{\nu} && \text{on } \Gamma,\\ u^{\rm ext}(\mathbf{x}) &= \mathcal{O}\big(1/|\mathbf{x}|\big) && \text{as } |\mathbf{x}|\to\infty. \end{aligned} \tag{6}$$

Here, $[u]$ and $[\partial_{\boldsymbol\nu} u]$ denote the jumps of u and its normal derivative across the boundary Γ of Ω. The contribution of the magnetostatic potential, thus involves certain 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.

In Goldenits et al. (2012), we discuss several approaches from the literature to solve (6) numerically. In the present work, we restrict ourselves to the hybrid FEM-BEM approach proposed in Fredkin et al. (1990), which is mostly used in the physics literature: Let u_1 be the (up to an additive constant) unique solution of the Neumann problem

$$\begin{aligned} \Delta u_1 &= \operatorname{div}\mathbf{m} && \text{in } \Omega,\\ \partial_{\boldsymbol\nu} u_1 &= \mathbf{m}\cdot\boldsymbol{\nu} && \text{on } \Gamma, \end{aligned} \tag{7}$$

and extend u_1 by zero to the entire space $\mathbb{R}^3$. With u the magnetostatic potential determined by (6), the remainder $u_2 = u - u_1$ satisfies

$$\begin{aligned} \Delta u_2 &= 0 && \text{in } \mathbb{R}^3\backslash\Gamma,\\ [u_2] &= u_1|_\Gamma && \text{on } \Gamma,\\ [\partial_{\boldsymbol\nu} u_2] &= 0 && \text{on } \Gamma,\\ u_2(\mathbf{x}) &= \mathcal{O}(1/|\mathbf{x}|) && \text{as } |\mathbf{x}|\to\infty. \end{aligned} \tag{8}$$

Here and in the following, $u_1|_\Gamma$ denotes the interior trace $u_1|_\Gamma$ of u_1. As is known from potential theory, the unique solution of (8) is the double-layer potential $u_2 = Ku_1|_\Gamma$ where

$$(Ku_1|_\Gamma)(\mathbf{x}) := \frac{1}{4\pi}\int_\Gamma \frac{(\mathbf{y}-\mathbf{x})\cdot\boldsymbol{\nu}(\mathbf{y})}{|\mathbf{y}-\mathbf{x}|^3}\, u_1(\mathbf{y}) \tag{9}$$

for all $\mathbf{x} \in \mathbb{R}^3\backslash\Gamma$ and with $\boldsymbol{\nu}$ the exterior unit normal vector on Γ. According to the jump of K across Γ, one can show that u_2 on Ω is characterized by the inhomogeneous Dirichlet problem

$$\begin{aligned} \Delta u_2 &= 0 && \text{in } \Omega,\\ u_2 &= (K - 1/2)u_1|_\Gamma && \text{on } \Gamma, \end{aligned} \tag{10}$$

and we have $\nabla u = \nabla u_1 + \nabla u_2$ in Ω.

Remark. We stress that the factor $c = 1/2$ for the trace jump $(K - c)u_1|_\Gamma$ of the double-layer potential $Ku_1|_\Gamma$ in Ω holds only almost everywhere on Γ, where Γ is flat. At corners or on edges of Γ, the factor c depends on the interior angle of Ω.

In order to provide a numerical scheme, we obtain that supplemented by the same initial and boundary conditions (2) and (3), the classical formulation of LLG, cf. (1), can equivalently be stated as

$$\alpha\,\mathbf{m}_t + \mathbf{m}\times\mathbf{m}_t = \mathbf{h}_{\rm eff}(\mathbf{m},\mathbf{f}) - (\mathbf{m}\cdot\mathbf{h}_{\rm eff}(\mathbf{m},\mathbf{f}))\mathbf{m}, \tag{11}$$

cf. e.g. Goldenits (2012) for a detailed proof. We emphasis, that this alternative formulation still is non-linear in consideration of the magnetization $\mathbf{m}$ but is linear in consideration of its time derivative $\mathbf{m}_t$. Formulation (11) will serve as the basis for our finite element (FE) scheme to solve LLG numerically, where we approximate $\mathbf{m}_h(t,\cdot) \approx \mathbf{m}(t,\cdot)$ and $\mathbf{v}_h(t,\cdot) \approx \mathbf{m}_t(t,\cdot)$ for all times $t \in (0,\tau)$. Note that, due to the non-convex constraint $|\mathbf{m}| = 1$ 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 $\mathcal{T}_h$ denote a quasi-uniform and regular triangulation of the domain Ω into tetrahedra and $\mathcal{N}_h$ 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. To discretize the time interval, we consider a uniform partition $0 = \tau_0 < \tau_1 < \cdots < \tau_J = \tau$ with time-step size $k = k_j := \tau_{j+1} - \tau_j$ for $j = 0,\dots,J-1$. For each (discrete) function $\boldsymbol{\varphi}$, $\boldsymbol{\varphi}^j$ denotes the evaluation $\boldsymbol{\varphi}(\tau_j)$ at time τ_j. Now, let

$$\mathcal{M}_h = \big\{\boldsymbol{\phi}_h \in \mathcal{V}_h \big| |\boldsymbol{\phi}_h(\mathbf{z})| = 1 \text{ for all } \mathbf{z}\in\mathcal{N}_h\big\} \tag{12}$$

be the restricted finite element set, where our solution $\mathbf{m}_h^j \approx \mathbf{m}(\tau_j)$ is sought due to the non-convex constraint $|\mathbf{m}| = 1$. Furthermore, for $\boldsymbol{\phi}_h \in \mathcal{M}_h$, let

$$\mathcal{K}_{\boldsymbol{\phi}_h} = \big\{\boldsymbol{\psi}_h \in \mathcal{V}_h \big| \boldsymbol{\psi}_h(\mathbf{z})\cdot\boldsymbol{\phi}_h(\mathbf{z}) = 0 \text{ for all } \mathbf{z}\in\mathcal{N}_h\big\} \tag{13}$$

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

To obtain a numerical integrator for LLG, we follow the idea of Alouges (2008), where the small particle limit $\mathbf{h}_{\rm eff}(\mathbf{m}) = \Delta\mathbf{m}$ is considered: We proceed by setting $\mathbf{v} = \mathbf{m}_t$ in (11) and by discretizing the weak form of it according to our framework. We treat the term of highest order implicitly, namely the exchange contribution, whereas the remaining three terms of the effective magnetic field $\mathbf{h}_{\rm eff}(\mathbf{m},\mathbf{f}) = C_{\rm ex}\Delta\mathbf{m} + \mathbf{h}_{\rm low}(\mathbf{m},\mathbf{f})$ with

$$\mathbf{h}_{\rm low}(\mathbf{m},\mathbf{f}) := -C_{\rm ani}D\Phi(\mathbf{m}) - \nabla u + \mathbf{f} \tag{14}$$

are computed explicitly. For the numerical integrator, we set

$$\mathbf{h}_{\rm low}(\mathbf{m}_h^j,\mathbf{f}_h^j) := -C_{\rm ani}D\Phi(\mathbf{m}_h^j) - \nabla u_h^j + \mathbf{f}_h^j. \tag{15}$$

Here, $u_h^j := u_{1h}^j + u_{2h}^j \in \mathcal{S}^1(\mathcal{T}_h)$ denotes an FE solution of the superposition ansatz of Fredkin et al. (1990), where we proceed as follows: First, let $u_{1h} \in \mathcal{S}^1(\mathcal{T}_h)$ with e.g. $\int_\Omega u_{1h} = 0$ be the unique FE solution of

$$\int_\Omega \nabla u_{1h}\cdot\nabla v_h = \int_\Omega \mathbf{m}\cdot\nabla v_h \tag{16}$$

for all $v_h \in \mathcal{S}^1(\mathcal{T}_h)$ with $\int_\Omega v_h = 0$. Second, let $u_{2h} \in \mathcal{S}^1(\mathcal{T}_h)$ be the unique solution of the Dirichlet problem

$$\int_\Omega \nabla u_{2h}\cdot\nabla v_h = 0 \tag{17}$$

for all $v_h \in \mathcal{S}^1(\mathcal{T}_h)$ with $v_h|_\Gamma = 0$, which additionally satisfies the inhomogeneous discrete Dirichlet condition $u_{2h}|_\Gamma = S_h(K-1/2)u_{1h}|_\Gamma$. Here, S_h maps the continuous boundary data $(K-1/2)u_{1h}|_\Gamma$ onto some discrete boundary data in $\mathcal{S}^1(\mathcal{T}_h|_\Gamma)$, where $\mathcal{T}_h|_\Gamma$ denotes the induced triangulation of the boundary Γ into flat surface triangles. A possible choice for the approximation operator S_h is given by the Clément-Operator

$$J_h v := \sum_{\mathbf{z}\in\mathcal{N}_h\cap\Gamma} v_\mathbf{z}\beta_\mathbf{z} \quad \text{with} \quad v_\mathbf{z} := \frac{1}{|\gamma_\mathbf{z}|}\int_{\gamma_\mathbf{z}} v.$$

Here, $\gamma_\mathbf{z}$ denotes the surface node-patch

$$\gamma_\mathbf{z} := \bigcup\{T|_\Gamma : T \in \mathcal{T}_h \text{ with } \mathbf{z} \in T\} \subseteq \Gamma$$

of a boundary node $\mathbf{z} \in \mathcal{N}_h \cap \Gamma$. Moreover, $\beta_\mathbf{z} \in \mathcal{S}^1(\mathcal{T}_h)$ is the corresponding hat function.
Finally, the discrete demagnetization field is defined by $\nabla u_h = \nabla u_{1h} + \nabla u_{2h}$.

Considering the last term in (15), we stress that $\mathbf{f}_h^j \approx \mathbf{f}(\tau_j)$ approximates the given applied field $\mathbf{f}$. If $\mathbf{f}$ is continuous in time, a valid choice is the evaluation $\mathbf{f}_h^j := \mathbf{f}(\tau_j)$ of $\mathbf{f}$ at time τ_j. If $\mathbf{f}$ is continuous in space and time, $\mathbf{f}_h^j \in \mathcal{V}_h$ can be chosen to be the nodal interpolant of $\mathbf{f}(\tau_j)$ which further simplifies the implementation.

Finally, with the nodal interpolation operator $\mathcal{I}_h : C(\overline{\Omega}) \to \mathcal{S}^1(\mathcal{T}_h)$, we include the so-called mass-lumping of the L^2-scalar-product to compute the arising mass-matrices only approximately. This results in corresponding matrix blocks which are diagonal instead of sparse only. The proposed time-splitting scheme now reads as follows:

Algorithm. Input: Discretized initial data $\mathbf{m}_h^0 \in \mathcal{M}_h$, damping parameter $\alpha > 0$, parameter $0 < \theta \leq 1$, counter $j = 0$.

(i) Compute $\mathbf{v}_h^j \in \mathcal{K}_{\mathbf{m}_h^j}$ by solving the (regular) linear system

$$\begin{aligned} \alpha \int_\Omega \mathcal{I}_h(\mathbf{v}_h^j \cdot \boldsymbol{\psi}_h) + \int_\Omega \mathcal{I}_h((\mathbf{m}_h^j \times \mathbf{v}_h^j)\cdot\boldsymbol{\psi}_h) \\ = -C_{\text{ex}} \int_\Omega \nabla(\mathbf{m}_h^j + \theta k \mathbf{v}_h^j)\cdot\nabla\boldsymbol{\psi}_h \\ + \int_\Omega \mathbf{h}_{\text{low}}(\mathbf{m}_h^j, \mathbf{f}_h^j)\cdot\boldsymbol{\psi}_h \end{aligned} \tag{18}$$

for all test functions $\boldsymbol{\psi}_h \in \mathcal{K}_{\mathbf{m}_h^j}$ from the discrete tangential space.

(ii) Define $\mathbf{m}_h^{j+1} \in \mathcal{M}_h$ by setting

$$\mathbf{m}_h^{j+1}(\mathbf{z}) = \frac{\mathbf{m}_h^j(\mathbf{z}) + k\mathbf{v}_h^j(\mathbf{z})}{|\mathbf{m}_h^j(\mathbf{z}) + k\mathbf{v}_h^j(\mathbf{z})|} \tag{19}$$

for all nodes $\mathbf{z} \in \mathcal{N}_h$ and go to (i).

Output: Sequence of functions $\mathbf{v}_h^j \in \mathcal{K}_{\mathbf{m}_h^j}$ as well as $\mathbf{m}_h^{j+1} \in \mathcal{M}_h$ for $j \geq 0$. ■

Some remarks are in order to comment on the well-posedness and the advantages of the proposed algorithm:

- According to the Lemma of Lax-Milgram, (18) admits a unique solution $\mathbf{v}_h^j \in \mathcal{K}_{\mathbf{m}_h^j}$.
- As a consequence of the orthogonality relation $\mathbf{m}_h^j(\mathbf{z})\cdot\mathbf{v}_h^j(\mathbf{z}) = 0$, one has $|\mathbf{m}_h^j(\mathbf{z}) + k\mathbf{v}_h^j(\mathbf{z})|^2 = |\mathbf{m}_h^j(\mathbf{z})|^2 + k^2|\mathbf{v}_h^j(\mathbf{z})|^2 \geq 1$. Therefore, the discretized magnetization $\mathbf{m}_h^{j+1} \in \mathcal{M}_h$ defined in step (ii) of our Algorithm is well-defined.
- We stress that only one (sparse) linear system (18) has to be solved per time-step and the non-convex side constraint $|\mathbf{m}| = 1$ is fulfilled node-wise. The assembly of this system is the topic of the subsequent Section 3.
- Although, one may also drop the nodal interpolation $\mathcal{I}_h$ in the linear system (18), we put emphasis on the fact that the use of mass-lumping for the cross product contribution of (18) is implementationally very attractive.
- An explicit treatment of the non-local contribution stemming from the magnetostatic potential ∇u is included, i.e. the computation of $\mathbf{m}_h^{j+1}$ only requires the approximate field ∇u_h^j from the previous time-step. Put differently, the approach by Fredkin et al. (1990) is only used once per time-step. This results in the solution of two additional (sparse) linear systems per time-step.
- Formally, the Crank-Nicholson type scheme $\theta = 1/2$ is of second order in time, whereas $\theta = 1$ corresponds to an implicit Euler scheme.
- Instead of the approach of Fredkin et al. (1990) to approximate the demagnetization field ∇u, also other approaches can be used. The same applies for the assumptions on and the discretization of the exterior field $\mathbf{f}$. We refer to the remarks in Section 4 and Goldenits et al. (2012) for further details.

3. IMPLEMENTATION

In this section, we focus on the computation of $\mathbf{v}_h^j \in \mathcal{K}_{\mathbf{m}_h^j}$ in step (i) of our algorithm. Emphasis is put on the assembly and structure of the matrices of the linear system (18), which is posed on the subspace $\mathcal{K}_{\mathbf{m}_h^j}$ of the FE space $\mathcal{V}_h = \mathcal{S}^1(\mathcal{T}_h)^3$. Let $\beta_i \in \mathcal{S}^1(\mathcal{T}_h)$ denote the canonical hat function associated with the node $\mathbf{z}_i \in \mathcal{N}_h$. We define $\boldsymbol{\beta}_{i+(\ell-1)n} := \beta_i\mathbf{e}_\ell$ with the ℓ-th unit vector $\mathbf{e}_\ell \in \mathbb{R}^3$ and note that $\boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_{3N}$ is the canonical basis of $\mathcal{V}_h$.

In a first step, we rewrite the variational form (18) as follows: Find $\mathbf{v}_h^j \in \mathcal{K}_{\mathbf{m}_h^j}$ such that

$$a(\mathbf{v}_h^j, \boldsymbol{\psi}_h) + b^j(\mathbf{v}_h^j, \boldsymbol{\psi}_h) = L^j(\boldsymbol{\psi}_h) \tag{20}$$

for all $\boldsymbol{\psi}_h \in \mathcal{K}_{\mathbf{m}_h^j}$, where we use the abbreviate notation

$$a(\boldsymbol{\phi}_h, \boldsymbol{\psi}_h) = \alpha \int_\Omega \mathcal{I}_h(\boldsymbol{\phi}_h \cdot \boldsymbol{\psi}_h) + \theta k C_{\rm ex} \int_\Omega \nabla \boldsymbol{\phi}_h \cdot \nabla \boldsymbol{\psi}_h, \tag{21}$$

$$b^j(\boldsymbol{\phi}_h, \boldsymbol{\psi}_h) = \int_\Omega \mathcal{I}_h((\mathbf{m}_h^j \times \boldsymbol{\phi}_h) \cdot \boldsymbol{\psi}_h), \tag{22}$$

$$\begin{aligned} L^j(\boldsymbol{\psi}_h) = -C_{\rm ex} \int_\Omega \nabla \mathbf{m}_h^j \cdot \nabla \boldsymbol{\psi}_h \\ - C_{\rm ani} \int_\Omega D\Phi(\mathbf{m}_h^j) \cdot \boldsymbol{\psi}_h \\ - \int_\Omega \nabla u_h^j \cdot \boldsymbol{\psi}_h + \int_\Omega \mathbf{f}_h^j \cdot \boldsymbol{\psi}_h. \end{aligned} \tag{23}$$

Due to the choice of the basis functions $\boldsymbol{\beta}_{i+(\ell-1)n} = \beta_i \mathbf{e}_\ell$, the bilinear form $a(\cdot,\cdot)$ from (21) corresponds to a symmetric block diagonal matrix

$$\mathbf{A} = \begin{pmatrix} \mathbf{A}^0 & & \\ & \mathbf{A}^0 & \\ & & \mathbf{A}^0 \end{pmatrix} \in \mathbb{R}^{3N \times 3N}_{\rm sym} \tag{24}$$

with symmetric blocks $\mathbf{A}^0 \in \mathbb{R}^{N\times N}_{\rm sym}$, where

$$\begin{aligned} \mathbf{A}^0_{ii'} &= \alpha \int_\Omega \mathcal{I}_h(\beta_i \beta_{i'}) + \theta k C_{\rm ex} \int_\Omega \nabla \beta_i \cdot \nabla \beta_{i'} \\ &= \alpha |\omega_i| \, \delta_{ii'} + \theta k C_{\rm ex} \int_\Omega \nabla \beta_i \cdot \nabla \beta_{i'}, \end{aligned} \tag{25}$$

with $\omega_i = \bigcup \{ T \in \mathcal{T}_h \, : \, \mathbf{z}_i \in T\}$ the volume patch associated with the node $\mathbf{z}_i \in \mathcal{N}_h$. Here, $\delta_{ii'}$ denotes Kronecker's delta with $\delta_{ii'} = 1$ for $i = i'$ and $\delta_{ii'} = 0$ otherwise. The occurring integrals can be computed by closed formulae. Note that $\mathbf{A}^0$ is the (positively weighted) sum of the standard stiffness and an approximated diagonal mass matrix. Consequently, $\mathbf{A}^0$ and hence $\mathbf{A}$ are positive definite sparse matrices and do not depend on the time step τ_j.

For the bilinear form $b^j(\cdot,\cdot)$ from (22), we use the identity $\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = (\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c}$ to see

$$\begin{aligned} b^j(\boldsymbol{\phi}_h, \boldsymbol{\psi}_h) &= \int_\Omega \mathcal{I}_h((\mathbf{m}_h^j \times \boldsymbol{\phi}_h) \cdot \boldsymbol{\psi}_h) \\ &= \int_\Omega \mathcal{I}_h((\boldsymbol{\phi}_h \times \boldsymbol{\psi}_h) \cdot \mathbf{m}_h^j). \end{aligned}$$

To derive the corresponding matrix $\mathbf{B} \in \mathbb{R}^{3N\times 3N}$, note that $\beta_i \mathbf{e}_\ell \times \beta_{i'} \mathbf{e}_{\ell'} = \beta_i \beta_{i'} \, \mathbf{e}_\ell \times \mathbf{e}_{\ell'}$ and

$$\mathbf{e}_1 \times \mathbf{e}_2 = \mathbf{e}_3, \quad \mathbf{e}_2 \times \mathbf{e}_3 = \mathbf{e}_1, \quad \mathbf{e}_3 \times \mathbf{e}_1 = \mathbf{e}_2,$$

and

$$\mathbf{e}_\ell \times \mathbf{e}_\ell = 0.$$

By choice of the basis functions $\boldsymbol{\beta}_{i+(\ell-1)n} = \beta_i \mathbf{e}_\ell$, $\mathbf{B}$ therefore has some block structure of the type

$$\mathbf{B} = \begin{pmatrix} \mathbf{0} & +\mathbf{B}^3 & -\mathbf{B}^2 \\ -\mathbf{B}^3 & \mathbf{0} & +\mathbf{B}^1 \\ +\mathbf{B}^2 & -\mathbf{B}^1 & \mathbf{0} \end{pmatrix} \in \mathbb{R}^{3N\times 3N} \tag{26}$$

with diagonal blocks $\mathbf{B}^\ell \in \mathbb{R}^{N\times N}$, where

$$\mathbf{B}^\ell_{ii'} = \int_\Omega \mathcal{I}_h(\beta_i \beta_{i'} \mathbf{m}_h^j \cdot \mathbf{e}_\ell) = |\omega_i| \, \mathbf{m}_h^j(\mathbf{z}_i) \cdot \mathbf{e}_\ell \, \delta_{ii'}.$$

Clearly, $\mathbf{B}$ is a sparse matrix which is skew-symmetric and positive semidefinite, since $b^j(\boldsymbol{\phi}_h, \boldsymbol{\psi}_h) = -b^j(\boldsymbol{\psi}_h, \boldsymbol{\phi}_h)$ and $b^j(\boldsymbol{\phi}_h, \boldsymbol{\phi}_h) = 0$.

Altogether, the system matrix $\mathbf{M} = \mathbf{A} + \mathbf{B} \in \mathbb{R}^{3N\times 3N}$ is positive definite and hence regular. Therefore the variational formulation (20) has even a unique solution if posed on the entire space $\mathcal{V}_h = \mathcal{S}^1(\mathcal{T}_h)^3$. However, $\mathbf{v}_h^j$ is determined by solving (20) in the subspace $\mathcal{K}_{\mathbf{m}_h^j}$. We realize the linear constraints

$$\mathbf{m}_h^j(\mathbf{z}) \cdot \mathbf{v}_h^j(\mathbf{z}) = 0 \quad \text{for all } \mathbf{z} \in \mathcal{N}_h \tag{27}$$

by a Lagrange multiplier ansatz, i.e. we obtain the unknown coefficients $\boldsymbol{\nu} \in \mathbb{R}^{3N}$ of

$$\mathbf{v}_h^j = \sum_{m=1}^{3N} \boldsymbol{\nu}_m \boldsymbol{\beta}_m \quad \text{by solution of} \quad \begin{pmatrix} \mathbf{M} & \boldsymbol{\Lambda}^T \\ \boldsymbol{\Lambda} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\nu} \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{0} \end{pmatrix}.$$

Here, $\boldsymbol{\lambda} \in \mathbb{R}^N$ is the Lagrange multiplier and $\boldsymbol{\Lambda}\boldsymbol{\nu} = \mathbf{0}$ realizes the constraints (27). Consequently, the Lagrange matrix reads

$$\boldsymbol{\Lambda} = \begin{pmatrix} \boldsymbol{\Lambda}^1 & \boldsymbol{\Lambda}^2 & \boldsymbol{\Lambda}^3 \end{pmatrix} \in \mathbb{R}^{N\times 3N}$$

with

$$\boldsymbol{\Lambda}^\ell \in \mathbb{R}^{N\times N}, \quad \boldsymbol{\Lambda}^\ell_{ii'} = kh^2 \mathbf{m}_h^j(\mathbf{z}_i) \cdot \mathbf{e}_\ell \, \delta_{ii'},$$

i.e. the matrices $\boldsymbol{\Lambda}^\ell$ are diagonal and scaled by kh^2 in order to stabilize the scheme.

4. CONVERGENCE RESULT

The definition of a weak solution to LLG is based on the idea of Alouges et al. (1992) and reads as follows:

Definition. Let $\mathbf{m}_0 \in H^1(\Omega; \mathbb{S}^2)$ be a given initial magnetization. Then, $\mathbf{m}$ is called a *weak solution* to LLG, if there holds for all times $\tau > 0$:

(i) $\mathbf{m} \in H^1(\Omega_\tau; \mathbb{S}^2)$ with $\mathbf{m}(\mathbf{x}, 0) = \mathbf{m}_0(\mathbf{x})$ in the sense of traces;

(ii) for all $\boldsymbol{\phi} \in C_0^\infty(\Omega_\tau; \mathbb{R}^3)$, there holds

$$\begin{aligned} \int_{\Omega_\tau} \mathbf{m}_t \cdot \boldsymbol{\phi} - \alpha \int_{\Omega_\tau} (\mathbf{m} \times \mathbf{m}_t) \cdot \boldsymbol{\phi} \\ = \int_{\Omega_\tau} (\mathbf{h}_{\rm eff}(\mathbf{m}, \mathbf{f}) \times \mathbf{m}) \cdot \boldsymbol{\phi}; \end{aligned} \tag{28}$$

(iii) for almost all $t \in (0, \tau)$, there holds

$$\begin{aligned} \frac{1}{2} \int_\Omega |\nabla \mathbf{m}(t)|^2 + C_1 \int_{\Omega_\tau} |\partial \mathbf{m}_t|^2 \\ \le \frac{1}{2} \int_\Omega |\nabla \mathbf{m}_0|^2 + C_2, \end{aligned} \tag{29}$$

with positive constants $C_1, C_2 > 0$ which depends only on $\mathbf{f}$, Ω and $\alpha > 0$.

We interpolate the discrete solution $\mathbf{m}_h^j$ for $j = 1, \ldots, J$ of the numerical integrator from Section 2 as a continuous, piecewise affine function in time: For all $\mathbf{x} \in \Omega$ and all times $t \in (0, \tau)$ with $j = \{0, \ldots, J-1\}$ such that $t \in [jk, (j+1)k)$, we define

$$\mathbf{m}_{hk}(t, \mathbf{x}) := \frac{t - jk}{k} \mathbf{m}_h^{j+1}(\mathbf{x}) + \frac{(j+1)k - t}{k} \mathbf{m}_h^j(\mathbf{x}). \tag{30}$$

The following convergence theorem generalizes the result of Alouges (2008), yields reliability of the proposed algorithm, and even proves existence of global weak solutions. We stress that no coupling of the time-step size k and the space-mesh size h is imposed.

Convergence Theorem. Let $\theta \in (1/2, 1]$ be a fixed parameter and let $\mathcal{T}_h$ be a family of shape-regular triangulations of the magnetic domain Ω with mesh-size $h \to 0$. Let the hat functions $\{\beta_i\}$ associated with $\mathcal{T}_h$ fulfill

$$\int_\Omega \nabla\beta_i \cdot \nabla\beta_{i'} \leq 0 \quad \text{for all } i \neq i'. \tag{31}$$

For the discrete initial magnetization $\mathbf{m}_h^0 \in \mathcal{M}_h$, we assume $\mathbf{m}_h^0 \to \mathbf{m}_0$ in $H^1(\Omega)$ as $h \to 0$. Then, there holds weak convergence in $H^1(\Omega_\tau)$ of a subsequence of the in time interpolated discrete magnetization $\mathbf{m}_{hk}$ from (30) to a weak solution $\mathbf{m}$ of LLG as $(h,k) \to 0$.

Remark. Due to Bartels (2005), condition (31) implies the following energy estimate for the exchange energy in step (ii) of the algorithm:

$$\int_\Omega |\nabla\mathcal{I}_h(\frac{\boldsymbol{\phi}_h}{|\boldsymbol{\phi}_h|})|^2 \leq \int_\Omega |\nabla\boldsymbol{\phi}_h|^2 \tag{32}$$

for all $\boldsymbol{\phi}_h \in \mathcal{V}_h$ with $|\boldsymbol{\phi}_h(\mathbf{z})| \geq 1$ and for all nodes $\mathbf{z} \in \mathcal{N}_h$.

Remark. Under certain assumptions one may approximate the demagnetization field ∇u as well as the applied external field $\mathbf{f}$ differently without changing the result of the convergence theorem:

- We assume that the approximation $\mathcal{P}_h\mathbf{m}_h^j$ related to the demagnetization field $\mathcal{P}\mathbf{m} = \nabla u$ as its discrete counterpart, fulfills the following properties
$$\|\mathcal{P}_h\mathbf{m}_h^j\|_{L^2(\Omega)} \leq C_\mathcal{P}\,\|\mathbf{m}_h^j\|_{L^2(\Omega)} \tag{33}$$
as well as
$$\|\mathcal{P}\mathbf{m} - \mathcal{P}_h\mathbf{m}\|_{L^2(\Omega_\tau)} \to 0 \quad \text{as } h \to 0 \tag{34}$$
with a positive constant $C_\mathcal{P} > 0$.

- We note that the approximate stray-field operator $\mathcal{P}_h\mathbf{m}_h^j = \nabla u_h$, which is given by the approach of Fredkin et al. (1990) and discussed above, fulfills property (33) as well as (34). A detailed proof is given in Goldenits et al. (2012).

- We consider the approximation $\mathbf{f}_{hk}$ in space and time of an applied external field $\mathbf{f}$, which is given by
$$\mathbf{f}_{hk}(t,\mathbf{x}) = \mathbf{f}_h^j(\mathbf{x}) \quad \text{for all} \quad t_j \leq t \leq t_{j+1}, \mathbf{x} \in \Omega.$$
We note that any discretization $\mathbf{f}_{hk}$ of $\mathbf{f}$ which satisfies
$$\|\mathbf{f} - \mathbf{f}_{hk}\|_{L^2(\Omega_\tau)} \to 0 \quad \text{as } (h,k) \to 0 \tag{35}$$
will provide an admissible choice in the sense that the convergence theorem holds. In particular, it is also possible to deal with discontinuous applied fields.

- The discretization of continuous $\mathbf{f}$ by nodal interpolation in time or in space-time, as proposed in Section 2, guarantees (35).

5. SKETCH OF PROOF

In this section we briefly comment on the essential arguments to prove the convergence theorem. A rigorously elaborated proof is given in Goldenits (2012).

In a first step, we aim for convergence properties of the output $\mathbf{v}_h^j$ and $\mathbf{m}_h^j$ for $j > 0$ of our algorithm. To this end, we also interpret the output function $\mathbf{v}_h^j$ as a piecewise constant function in time: For all $\mathbf{x} \in \Omega$ and all times $t \in (0,\tau)$ with $j = \{0, \ldots, J\}$ such that $t \in [jk, (j+1)k)$, we define

$$\mathbf{v}_{hk}(t,\mathbf{x}) := \mathbf{v}_h^j(\mathbf{x}).$$

On the one hand, the definition of $\mathbf{m}_{hk}$ in (30) as well as the non-convex property $|\mathbf{m}_h^j(\mathbf{x})| \leq 1$ for $j \geq 0$ and all $\mathbf{x} \in \Omega$, which holds due to step (ii) of our time-splitting scheme, implies $|\mathbf{m}_{hk}(t,\mathbf{x})| \leq 1$. On the other hand and by use of the test function $\boldsymbol{\psi}_h = \mathbf{v}_h^j$ in (18), one may deduce some stability estimate

$$\begin{aligned}\frac{1}{2}\int_\Omega |\nabla\mathbf{m}_h^J|^2 + kC\sum_{j=0}^{J-1}\int_\Omega |\mathbf{v}_h^j|^2 \\ \leq \frac{1}{2}\int_\Omega |\mathbf{m}_h^0|^2 \\ + \frac{k}{C_{\text{ex}}}\sum_{j=0}^{J-1}\int_\Omega \mathbf{h}_{\text{low}}(\mathbf{m}_h^j, \mathbf{f}_h^j)\cdot\mathbf{v}_h^j.\end{aligned} \tag{36}$$

This yields uniform boundedness of $\mathbf{m}_{hk}$ in $H^1(\Omega_\tau)$ as well as of $\mathbf{v}_{hk}$ in $L^2(\Omega_\tau)$. Therefore, we may extract a subsequence of $\mathbf{v}_{hk}$ and $\mathbf{m}_{hk}$, respectively, such that

$$\mathbf{m}_{hk} \rightharpoonup \mathbf{m} \quad \text{weakly in } H^1(\Omega_\tau) \text{ as } (h,k) \to 0, \tag{37}$$

$$\mathbf{m}_{hk} \to \mathbf{m} \quad \text{strongly in } L^2(\Omega_\tau) \text{ as } (h,k) \to 0, \tag{38}$$

$$\mathbf{v}_{hk} \rightharpoonup \mathbf{v} \quad \text{weakly in } L^2(\Omega_\tau) \text{ as } (h,k) \to 0, \tag{39}$$

with certain $\mathbf{v} \in L^2(\Omega_\tau;\mathbb{R}^3)$ and $\mathbf{m} \in H^1(\Omega_\tau;\mathbb{R}^3)$. The remaining part of the proof is dedicated to the stepwise verification that the limit $\mathbf{m}$ is a weak solution to LLG, see Definition 4. We remark that this also involves the proof of $\mathbf{v} = \mathbf{m}_t$ to link the limits (37)–(39).

ACKNOWLEDGEMENTS

The authors acknowledge support of the Viennese Science and Technology Fund (WWTF) through the research project MA09–029 *Micromagnetic Simulation and Computational Design of Future Devices.*

REFERENCES

F. Alouges. A new finite element scheme for Landau-Lifchitz equations. Discrete and Continuous Dynamical Systems Series S, Vol. 1, 2008, 187-196.

F. Alouges, and A. Soyeur. On global weak solutions for Landau-Lifshitz equations: existence and nonuniqueness. *Nonlinear Analysis*, 18:1071–1084, 1992.

S. Bartels. Stability and convergence of finite-element approximation schemes for harmonic maps. *SIAM J. Numer. Anal.*, 43:220–238, 2005.

D. Fredkin, and T. Koehler. Hybrid method for computing demagnetizing fields. *IEEE Transactions on Magnetics*, 26:415–417, 1990.

P. Goldenits, G. Hrkac, M. Page, D. Praetorius, T. Schrefl, and D. Süss. Effective Simulation of the Dynamics of Ferromagnetism. Work in progress, 2012.

P. Goldenits. Phd-Thesis. Institute for Analysis and Scientific Computing, Vienna University of Technology.