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Coupling of dynamical micromagnetism and a stationary spin drift-diffusion equation: A step towards a fully self-consistent spintronics framework

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ABSTRACT

We consider the coupling of the Landau–Lifshitz–Gilbert equation with a quasilinear diffusion equation to describe the interplay of magnetization and spin accumulation in magnetic-nonmagnetic multilayer structures. For this problem, we propose and analyze a convergent finite element integrator, where, in contrast to prior work, we consider the stationary limit for the spin diffusion. Numerical experiments underline that the new approach is more effective, since it leads to the same experimental results as for the model with time-dependent spin diffusion, but allows for larger time-steps of the numerical integrator.

1. Introduction and mathematical model

The classical theory of micromagnetism models the behavior of ferromagnetic materials for constant temperature far below the Curie point and in the absence of electric currents. To take the interactions between magnetization and spin-polarized currents into account, several extensions of the model based on the concept of spin-transfer have been proposed [1–7]. In this work, we consider the Landau–Lifshitz–Gilbert (LLG) equation

$$\partial_t \mathbf{m} = -\gamma_0 \mathbf{m} \times (\mathbf{H}_{\mathrm{eff}}(\mathbf{m}, \mathbf{f}) + c\mathbf{s}) + \alpha \mathbf{m} \times \partial_t \mathbf{m} \quad \text{in } \Omega_T, \tag{1a}$$

$$\partial_{\mathbf{n}} \mathbf{m} = \mathbf{0} \ \text{ on } (0, T) \times \partial\Omega, \quad \mathbf{m}(0) = \mathbf{m}^0 \ \text{ in } \Omega, \tag{1b}$$

where the sought vector field is the normalized magnetization $\mathbf{m}: \Omega_T \to \mathbb{R}^3$ with $|\mathbf{m}| = 1$. In (1a), $\Omega \subset \mathbb{R}^3$ is the volume occupied by some ferromagnetic body, $T > 0$ is some finite time, and $\Omega_T = (0, T) \times \Omega$ is the time-space domain. Moreover, $\gamma_0 > 0$ is the gyromagnetic ratio, $\alpha > 0$ is the Gilbert constant, and the effective field is given by

$$\mathbf{H}_{\mathrm{eff}}(\mathbf{m}, \mathbf{f}) = C_{\mathrm{exch}} \Delta \mathbf{m} + \boldsymbol{\pi}(\mathbf{m}) + \mathbf{f}. \tag{1c}$$

In (1c), the first term is the exchange contribution, with $C_{\mathrm{exch}} = 2A/(\mu_0 M_s) > 0$, $\boldsymbol{\pi}(\mathbf{m})$ collects the $\mathbf{m}$-dependent lower-order contributions (e.g., anisotropy field and stray field), and $\mathbf{f}$ comprises the $\mathbf{m}$-independent contributions (e.g., applied external field). In (1a), $\mathbf{s}: \Omega'_T \to \mathbb{R}^3$ denotes the spin accumulation, $\Omega' \subset \mathbb{R}^3$ is the volume of a conducting body such that $\Omega \subset \Omega'$, $\Omega'_T = (0, T) \times \Omega'$, and $c > 0$ is the corresponding coupling constant. The LLG equation is equipped with homogeneous Neumann boundary conditions and initial conditions (1b) for some initial state $\mathbf{m}^0: \Omega \to \mathbb{R}^3$ with $|\mathbf{m}^0| = 1$. The dynamics of the spin accumulation $\mathbf{s}$ is governed by the diffusion equation [3,8]

$$\partial_t \mathbf{s} = -\nabla \cdot \mathbf{J}_s - \frac{2D_0}{\lambda_{\mathrm{sf}}^2}\mathbf{s} - \frac{2D_0}{\lambda_{\mathrm{J}}^2}\mathbf{s} \times \mathbf{m} \quad \text{in } \Omega'_T, \tag{2a}$$

$$\partial_{\mathbf{n}} \mathbf{s} = \mathbf{0} \ \text{ on } (0, T) \times \partial\Omega', \quad \mathbf{s}(0) = \mathbf{s}^0 \ \text{ in } \Omega'. \tag{2b}$$

Here, D_0 denotes the diffusion coefficient, $\lambda_{\mathrm{sf}}, \lambda_{\mathrm{J}} > 0$ are characteristic lengths and $\mathbf{s}^0: \Omega' \to \mathbb{R}^3$ is some initial configuration. The spin current $\mathbf{J}_s$ reads

$$\mathbf{J}_s = \frac{\beta \mu_B}{e}\mathbf{m} \otimes \mathbf{J}_e - 2D_0(\nabla \mathbf{s} - \beta\beta' \mathbf{m} \otimes (\nabla \mathbf{s}^\top \mathbf{m})) \quad \text{in } \Omega'_T, \tag{2c}$$

where $\mathbf{J}_e: \Omega'_T \to \mathbb{R}^3$ is a given electric current density and the constants $\mu_B > 0$, $e > 0$, and $0 < \beta, \beta' < 1$ are the Bohr magneton, the electron electric charge, and polarization parameters, respectively. The above setting covers the case of multilayer structures, where Ω' denotes the volume of the entire multilayer sample,

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while Ω denotes its ferromagnetic part (see Section 4).

Existence of weak solutions of the nonlinear system (1)–(2) has been established in [8]. A first numerical scheme based on finite differences has been proposed and empirically validated in [9]. A convergent finite element integrator has been proposed, analyzed, and applied by the authors in [10,11]. The latter scheme extends the integrator of [12] and is unconditionally convergent towards a weak solution of the system, although each time-step decouples the integration of (1) and (2) and requires only to solve two linear systems (despite the overall nonlinearities).

The dynamics of the spin accumulation is much faster than the one of the magnetization [3]. If one is only interested in the magnetization dynamics, it is thus reasonable to treat the spin accumulation as in equilibrium, i.e., to consider the stationary case of the governing diffusion equation. With this approach, (2a) reduces to the boundary value problem

$$-\nabla\cdot(D_0(\nabla\mathbf{s} - \beta\beta'\mathbf{m}\otimes(\nabla\mathbf{s}^\top\mathbf{m}))) + \frac{D_0}{\lambda_{\mathrm{sf}}^2}\mathbf{s} + \frac{D_0}{\lambda_{\mathrm{J}}^2}(\mathbf{s}\times\mathbf{m}) = -\frac{\beta\mu_{\mathrm{B}}}{2e}\nabla\cdot(\mathbf{m}\otimes\mathbf{J}_{\mathrm{e}}) \quad \text{in } \Omega', \tag{3a}$$

$$\partial_{\mathbf{n}}\mathbf{s} = 0 \quad \text{on } \partial\Omega'. \tag{3b}$$

In the present work, as a novel contribution over [8–11], we analyze the numerical integration of (1a) coupled to (3a). We prove convergence of the algorithm towards a weak solution of the problem and compare the numerical results with those for (1)–(2). The latter is computationally more expensive, since it requires a smaller time-step size in order to resolve the dynamics of the spin accumulation.

2. Variational formulation and weak solution

We assume that $D_0 \in L^\infty(\Omega')$ satisfies $D_0 \ge D_*$ a.e. in Ω' for a positive constant D_*. For the moment, we omit the time-dependence of all quantities, assume $\mathbf{J}_{\mathrm{e}} \in \mathbf{H}(\mathrm{div}, \Omega')$, and consider the set $\mathcal{M} = \{\mathbf{m} \in \mathbf{L}^\infty(\Omega): |\mathbf{m}| \le 1 \text{ a.e. in } \Omega\}$. For $\mathbf{m} \in \mathcal{M}$, we define the bilinear form $a_{\mathbf{m}}: \mathbf{H}^1(\Omega') \times \mathbf{H}^1(\Omega') \to \mathbb{R}$ by

$$a_{\mathbf{m}}(\zeta_1, \zeta_2) = (D_0\nabla\zeta_1, \nabla\zeta_2)_{\Omega'} - \beta\beta'(D_0\mathbf{m}\otimes(\nabla\zeta_1^\top\mathbf{m}), \nabla\zeta_2)_{\Omega} + \lambda_{\mathrm{sf}}^{-2}(D_0\zeta_1, \zeta_2)_{\Omega'} + \lambda_{\mathrm{J}}^{-2}(D_0(\zeta_1\times\mathbf{m}), \zeta_2)_{\Omega} \tag{4}$$

for all $\zeta_1, \zeta_2 \in \mathbf{H}^1(\Omega')$. The variational formulation of (3) then reads as follows: find $\mathbf{s} \in \mathbf{H}^1(\Omega')$ such that, for all $\zeta \in \mathbf{H}^1(\Omega')$, it holds

$$a_{\mathbf{m}}(\mathbf{s}, \zeta) = \frac{\beta\mu_{\mathrm{B}}}{2e}(\mathbf{m}\otimes\mathbf{J}_{\mathrm{e}}, \nabla\zeta)_{\Omega} - \frac{\beta\mu_{\mathrm{B}}}{2e}(\mathbf{J}_{\mathrm{e}}\cdot\mathbf{n}, \mathbf{m}\cdot\zeta)_{\partial\Omega'\cap\partial\Omega}. \tag{5}$$

The following proposition characterizes the mapping $\mathbf{m}\mapsto\mathbf{s}$.

Proposition 1. *For all* $\mathbf{m} \in \mathcal{M}$, *there exists a unique solution* $\mathbf{s} \in \mathbf{H}^1(\Omega')$ *of* (5). *Moreover, it holds*

$$\|\mathbf{s}\|_{\mathbf{H}^1(\Omega')} \le \frac{\beta\mu_{\mathrm{B}}\|\mathbf{J}_{\mathrm{e}}\|_{\mathbf{H}(\mathrm{div},\Omega')}}{2D_*|e|\min\{1-\beta\beta', \lambda_{\mathrm{sf}}^{-2}\}}.$$

Proof. Recall $|\mathbf{m}| \le 1$ a.e. in Ω. It follows that the bilinear form $a_{\mathbf{m}}(\cdot,\cdot)$ is continuous and coercive, as $a_{\mathbf{m}}(\zeta,\zeta) \ge D_*\min\{1-\beta\beta', \lambda_{\mathrm{sf}}^{-2}\}\|\zeta\|_{\mathbf{H}^1(\Omega)}^2$ for all $\zeta \in \mathbf{H}^1(\Omega')$. Moreover, $F(\cdot)$ defined as the right-hand side of (5) is linear and continuous, as $|F(\zeta)| \le (\beta\mu_{\mathrm{B}}|e|^{-1}/2)\|\mathbf{J}_{\mathrm{e}}\|_{\mathbf{H}(\mathrm{div},\Omega')}\|\zeta\|_{\mathbf{H}^1(\Omega')}$ for all $\zeta \in \mathbf{H}^1(\Omega')$. Therefore, the result follows from the Lax–Milgram theorem.□

We suppose $\mathbf{f} \in C([0,T]; \mathbf{L}^2(\Omega))$ and $\mathbf{J}_{\mathrm{e}} \in C([0,T], \mathbf{H}(\mathrm{div}, \Omega'))$. In the spirit of [13–15], we introduce the notion of a weak solution of (1a) coupled to (3a):

Definition 2. Let $\mathbf{m}^0 \in \mathbf{H}^1(\Omega)$ with $|\mathbf{m}^0| = 1$ a.e. in Ω. Then, $\mathbf{m}: \Omega_T \to \mathbb{R}^3$ is called a weak solution of the coupling of (1) and (3) if the following properties (i)–(v) are satisfied:

(i) $\mathbf{m} \in \mathbf{H}^1(\Omega_T)$ and $|\mathbf{m}| = 1$ a.e. in Ω_T,
(ii) $\mathbf{m}(0) = \mathbf{m}^0$ in the sense of traces,
(iii) for a.e. $t \in (0,T)$ $\mathbf{s}(t) \in \mathbf{H}^1(\Omega')$satisfies (5)
(iv) for all $\boldsymbol{\varphi} \in \mathbf{H}^1(\Omega_T)$, it holds

$$(\partial_t\mathbf{m}, \boldsymbol{\varphi})_{\Omega_T} + \alpha(\partial_t\mathbf{m}\times\mathbf{m}, \boldsymbol{\varphi})_{\Omega_T} = -C_{\mathrm{exch}}\gamma_0(\nabla\mathbf{m}\times\mathbf{m}, \nabla\boldsymbol{\varphi})_{\Omega_T} + \gamma_0(\boldsymbol{\pi}(\mathbf{m})\times\mathbf{m}, \boldsymbol{\varphi})_{\Omega_T} + \gamma_0(\mathbf{f}\times\mathbf{m}, \boldsymbol{\varphi})_{\Omega_T} + c\gamma_0(\mathbf{s}\times\mathbf{m}, \boldsymbol{\varphi})_{\Omega_T},$$

(v) for a.e. time $T' \in (0,T)$, it holds

$$\|\nabla\mathbf{m}(T')\|_{\mathbf{L}^2(\Omega)}^2 + \alpha\int_0^{T'}\|\partial_t\mathbf{m}(t)\|_{\mathbf{L}^2(\Omega)}^2\,dt \le C, \tag{6}$$

where the constant $C > 0$ depends only on the data.

We point out that stronger (dissipative) bounds than (6) in terms of the Gibbs free energy require additional assumptions on $\boldsymbol{\pi}$ and $\mathbf{f}$; see [14,15].

3. Numerical algorithm

For the spatial discretization, let $\{\mathcal{T}_h^{\Omega'}\}_{h>0}$ be a quasi-uniform family of conforming tetrahedral triangulations of Ω' with mesh-size h. We assume that Ω is resolved, i.e., the restriction $\mathcal{T}_h^{\Omega} = \{K \in \mathcal{T}_h^{\Omega'}: K \subseteq \overline{\Omega}\}$ satisfies $\overline{\Omega} = \bigcup_{K\in\mathcal{T}_h^{\Omega}} K$. We denote by $\mathbf{V}_h(\Omega') = \mathcal{S}^1(\mathcal{T}_h^{\Omega'})^3$ the standard finite element space of globally continuous and piecewise affine functions from Ω' to $\mathbb{R}^3$ and define $\mathbf{V}_h(\Omega)$ analogously. The set of vertices of the triangulation $\mathcal{T}_h^{\Omega}$ is denoted by $\mathcal{N}_h^{\Omega}$. We define the set of admissible discrete magnetizations by

$$\mathcal{M}_h := \{\boldsymbol{\phi}_h \in \mathbf{V}_h(\Omega): |\boldsymbol{\phi}_h(\mathbf{z})| = 1 \text{ for all } \mathbf{z} \in \mathcal{N}_h^{\Omega}\} \subset \mathcal{M}$$

and consider, for $\boldsymbol{\phi}_h \in \mathcal{M}_h$, the discrete tangent space

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

We note that these definitions are inspired by mimicking the properties $|\mathbf{m}| = 1$ and $\mathbf{m}\cdot\partial_t\mathbf{m} = \frac{1}{2}\partial_t|\mathbf{m}|^2 = 0$ a.e. in Ω_T which are satisfied for each solution $\mathbf{m}$ of (1a).

For the time discretization, we consider a uniform partition of the time interval $[0,T]$ with time-step size $\Delta t = T/N$, i.e., $t_i = i\Delta t$ for $0 \le i \le N$. Algorithm 3 approximates $\mathbf{m}(t_i) \approx \mathbf{m}_h^i \in \mathcal{M}_h$ as well as $\partial_t\mathbf{m}(t_i) \approx \mathbf{v}_h^i \in \mathcal{K}_{\mathbf{m}_h^i}$. Instead of (5), we consider the following discrete problem: Given $\mathbf{J}_{\mathrm{e}}^i := \mathbf{J}_{\mathrm{e}}(t_i)$, find $\mathbf{s}_h^i \in \mathbf{V}_h(\Omega')$ such that, for all $\zeta_h \in \mathbf{V}_h(\Omega')$, it holds

$$a_{\mathbf{m}_h^i}(\mathbf{s}_h^i, \zeta_h) = \frac{\beta\mu_{\mathrm{B}}}{2e}(\mathbf{m}_h^i\otimes\mathbf{J}_{\mathrm{e}}^i, \nabla\zeta_h)_{\Omega} - \frac{\beta\mu_{\mathrm{B}}}{2e}(\mathbf{J}_{\mathrm{e}}^i\cdot\mathbf{n}, \mathbf{m}_h^i\cdot\zeta_h)_{\partial\Omega'\cap\partial\Omega}. \tag{7}$$

Proposition 1, shows that (7) is well-posed and that $\mathbf{s}_h^i \in \mathbf{V}_h(\Omega')$ satisfies

$$\|\mathbf{s}_h^i\|_{\mathbf{H}^1(\Omega')} \le \frac{\beta\mu_{\mathrm{B}}\|\mathbf{J}_{\mathrm{e}}\|_{C([0,T],\mathbf{H}(\mathrm{div},\Omega'))}}{2D_*|e|\min\{1-\beta\beta', \lambda_{\mathrm{sf}}^{-2}\}}. \tag{8}$$