



Optimal control for a coupled spin-polarized current and magnetization system

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Abstract

This paper is devoted to an optimal control problem of a coupled spin drift-diffusion Landau–Lifshitz–Gilbert system describing the interplay of magnetization and spin accumulation in magnetic-nonmagnetic multilayer structures, where the control is given by the electric current density. A variational approach is used to prove the existence of an optimal control. The first-order necessary optimality system for the optimal solution is derived in one space-dimension via Lagrange multiplier method. Numerical examples are reported to validate the theoretical findings.

Keywords Micromagnetism · Landau–Lifshitz–Gilbert equation · Optimal control · Faedo–Galerkin approximation

Mathematics Subject Classification (2010) 45K05 · 46S50 · 49L20 · 49L25 · 91A23 · 93E20

1 Introduction

The classical theory of micromagnetism describes the dynamics of ferromagnetic materials occupying a domain in the absence of electric currents and for constant temperature (below the Curie temperature). The process of magnetization is described by so called Landau–Lifshitz–Gilbert (LLG) equation, see [13, 17]. A more general approach is to consider the interactions between spin accumulation and the magnetization on magnetic and nonmagnetic multilayer structures [12, 24, 25, 29, 30, 34]—

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which has wide applications in various magnetic devices, e.g., in magnetic tunnel junctions and magnetic domain walls [26, 31]. Moreover, a number of technological applications of these phenomena have been seen, e.g., in racetrack memories, magnetic vortex oscillators [21, 23]. In this paper, we study the optimal control problem for a coupled spin drift-diffusion Landau–Lifshitz–Gilbert system on a magnetic multilayer. A formal description of our problem is as follows.

Let $D, \tilde{D} \subset \mathbb{R}^d$ ($d = 1, 2, 3$) be two bounded Lipschitz domains such that $D \subset \tilde{D}$, and let ∂D and $\partial \tilde{D}$ be their boundaries, respectively. For any $T > 0$, we denote $D_T := (0, T) \times D$, $\tilde{D}_T := (0, T) \times \tilde{D}$, $\partial D_T := (0, T) \times \partial D$, and $\partial \tilde{D}_T := (0, T) \times \partial \tilde{D}$. In the whole paper, we denote by ∂_t the time derivative and ∂_ν the normal derivative.

Let $\mathbf{m} : D_T \rightarrow \mathbb{R}^3$ and $\mathbf{s} : \tilde{D}_T \rightarrow \mathbb{R}^3$ be, respectively, magnetization and spin accumulation. We extend \mathbf{m} by zero outside D . In this work, we want to control the dynamics of \mathbf{m} governed by the boundary value problem with the Landau–Lifshitz–Gilbert (LLG) equation

$$\begin{cases} \partial_t \mathbf{m} = -\gamma_0 \mathbf{m} \times (\mathbf{H}_{\text{eff}}(\mathbf{m}) + c\mathbf{s}) + \alpha \mathbf{m} \times \partial_t \mathbf{m} & \text{in } D_T, \\ \partial_\nu \mathbf{m} = 0 & \text{on } \partial D_T, \\ \mathbf{m}(0, \cdot) = \mathbf{m}_0(\cdot) & \text{in } D, \end{cases} \quad (1.1)$$

and the problem with the diffusion equation

$$\begin{cases} \partial_t \mathbf{s} = -\nabla \cdot \mathbf{J} - \frac{2D_0}{\lambda_1} \mathbf{s} - \frac{2D_0}{\lambda_2} \mathbf{s} \times \mathbf{m} & \text{in } \tilde{D}_T, \\ \partial_\nu \mathbf{s} = 0 & \text{on } \partial \tilde{D}_T, \\ \mathbf{s}(0, \cdot) = \mathbf{s}_0(\cdot) & \text{in } \tilde{D}, \end{cases} \quad (1.2)$$

where the spin current \mathbf{J} is a 3×3 matrix defined by

$$\mathbf{J} = \frac{\beta' \mu_\beta}{e} \mathbf{m} \otimes \mathbf{j} - D_0 (\nabla \mathbf{s} - \beta \beta' \mathbf{m} \otimes (\nabla \mathbf{s} \cdot \mathbf{m})) \quad \text{in } \tilde{D}_T \quad (1.3)$$

with the given electric current density $\mathbf{j} : \tilde{D}_T \rightarrow \mathbb{R}^3$, which is the control variable of the problem.

The physical meanings of the variables in (1.1)–(1.3) are given below.

- \mathbf{m} denotes the magnetization.
- \mathbf{s} denotes the spin accumulation.
- The effective field \mathbf{H}_{eff} reads

$$\mathbf{H}_{\text{eff}}(\mathbf{m}) = -D\mathcal{E}(\mathbf{m}), \quad (1.4)$$

which is deduced from the Landau–Lifshitz energy $\mathcal{E}(\mathbf{m})$. For simplicity, in this work $\mathcal{E}(\mathbf{m})$ is the exchange energy

$$\mathcal{E}(\mathbf{m}) = \frac{1}{2} \int_D |\nabla \mathbf{m}|^2 dx.$$

In this case, $\mathbf{H}_{\text{eff}}(\mathbf{m}) = \Delta \mathbf{m}$.

- \mathbf{J} denotes the spin current.
- \mathbf{j} is the applied current density field.

- γ_0 and α are the gyromagnetic ratio and the nondimensional empiric Gilbert damping parameter, respectively.
- D_0 is the diffusion coefficient. The parameters λ_1 and λ_2 are the characteristic length of the spin-flip relaxation and the mean free path of an electron, respectively.
- The parameters β and β' are the nondimensional spin polarization parameters of the magnetic layers.

For notational simplicity we assume that the constants $\gamma_0, c, e, \mu\beta$ are equal to 1, while λ_1, λ_2 are equal to 2 so that (1.1), (1.2), and (1.3) have simpler forms to write. Moreover we choose $\beta' = 1$ and $0 < \beta < 1$ so that $\beta\beta' \in (0, 1)$ in order that (1.2) is parabolic; see [3, Lemma 5].

In case of $\mathbf{j} = \mathbf{0}$, and $\mathbf{s} = \mathbf{0}$, (1.1)–(1.3) reduces to the standard LLG equation, the well-posedness of which is studied, e.g., in [6, 8, 16, 20, 33] and references therein. In [12], the authors have employed a Galerkin approximation to prove the existence of global weak solution of (1.1)–(1.3) in three space-dimensions. By using energy methods, the authors in [14] established the existence of a global smooth solution of spin-polarized transport equation in two space-dimensions; see also [25] for the existence of a smooth solution in one dimensional case. Recently a decoupled time-marching scheme was analyzed and its unconditional convergence of the integrator towards a weak solution of the underlying problem was established in [3].

An optimal control problem subject to LLG equation has been studied by Dunst et al. in [9]. The authors in [9] have shown the existence of an optimal solution and derived its necessary first-order optimality system in the one space-dimension. Moreover, they have shown convergence of the time semi-discrete optimality system towards the optimality system of the original problem. We also refer to see [4, 5] for optimal control type problems subject to LLG equation.

Our goal is to study an associated optimal control problem to (1.1)–(1.3). Let $\bar{\mathbf{m}} : [0, T] \times D \rightarrow \mathbb{S}^2$ be a given function and let

$$\begin{aligned}
 F(\pi) = & \frac{\kappa}{2} \int_0^T \|\mathbf{m} - \bar{\mathbf{m}}\|_{\mathbb{L}^2}^2 \, dt + \frac{1}{2} \int_0^T \left(\delta_1 \|\mathbf{j}\|_{\mathbb{L}^2(\bar{D})}^2 + \delta_2 \|\nabla \mathbf{j}\|_{\mathbb{L}^2(\bar{D})}^2 + \delta_3 \|\Delta \mathbf{j}\|_{\mathbb{L}^2(\bar{D})}^2 \right) dt \\
 & + \frac{1 - \kappa}{2} \Psi(\mathbf{m}(T))
 \end{aligned}
 \tag{1.5}$$

for $\pi = (\mathbf{m}, \mathbf{s}, \mathbf{j})$ with some nonnegative constants $\kappa, \delta_1, \delta_2$ and δ_3 . The term $\Psi(\mathbf{m}(T))$ represents the terminal payoff. In Definition 2.2 it is given as a Lipschitz continuous function defined on \mathbb{L}^2 . In Section 5 for numerical simulations we choose $\Psi(\mathbf{u}) = \|\mathbf{u} - \bar{\mathbf{m}}(T)\|_{\mathbb{L}^2}^2$.

We find an admissible weak solution $\pi^* = (\mathbf{m}^*, \mathbf{s}^*, \mathbf{j}^*)$ which minimizes the cost functional, i.e.,

$$F(\pi^*) = \min_{\pi} F(\pi) \quad \text{subject to (1.1)–(1.3)}.
 \tag{1.6}$$

A minimizer π^* of (1.6) is constructed via the variational method. For a minimizing sequence of admissible weak solutions $\pi_n = (\mathbf{m}_n, \mathbf{s}_n, \mathbf{j}_n)$, we employ uniform bounds along with Fatou’s lemma to prove existence of a minimizer of (1.6). Once a minimizer π^* of (1.6) is obtained, we ask for its necessary optimality system — which may be used for a gradient descent method to numerically approximate π^* . To deduce necessary first-order optimality system of π^* , we need higher regularity of

the solutions—which is why, we consider more regular control \mathbf{j} in (1.6) and restrict our study to one space-dimension, see, e.g., proof of Lemma 4.2. Due to the presence of nonlinear non-Lipschitz drift in (1.1), the classical Pontryagin’s maximum principle is not immediate. We use the Lagrange multiplier method to deduce the necessary first-order optimality system corresponding to minimizer π^* in one space-dimension. Due to the coupled system of state equations, it is more challenging to show that π^* is a regular point of some appropriate function (cf. Lemma 4.4) — a crucial step for applying the Lagrange multiplier theorem.

The remaining part of this paper is organized as follows. We detail the technical framework, and state the main result in Section 2. Section 3 is devoted to show the existence of an optimal solution of (1.6). In Section 4, we first deduce improved stability properties of the weak solution in one space dimension and then use these estimates to obtain a necessary first-order optimality system for the optimal solution π^* via the Lagrange multiplier method. Moreover, improved regularity properties of the adjoint variables and the optimal control are obtained. Computational studies for the switching dynamics are reported in the final section.

2 Technical framework and statement of the main results

Throughout this paper, we use the letter C to denote a generic positive constant, which may take different values at different occurrences. In the sequel, we denote by \mathbb{L}^p the space $L^p(D; \mathbb{R}^3)$, by $\mathbb{L}^p(\tilde{D})$ the space $L^p(\tilde{D}; \mathbb{R}^3)$, by \mathbb{H}^ℓ the Sobolev space $W^{\ell,2}(D; \mathbb{R}^3)$, and by $\mathbb{H}^\ell(\tilde{D})$ the Sobolev space $W^{\ell,2}(\tilde{D}; \mathbb{R}^3)$ for any integer $\ell \geq 1$ and real number $p \geq 1$. We write $\mathbb{H}^{-1}(\tilde{D})$ for the dual of $\mathbb{H}_0^1(\tilde{D})$. Moreover, for any $T > 0$, let $L^m(\mathbb{H}^\ell) := L^m(0, T; \mathbb{H}^\ell)$ and $L^m(\mathbb{H}^\ell(\tilde{D})) := L^m(0, T; \mathbb{H}^\ell(\tilde{D}))$ denote the standard Bochner spaces for any $m, \ell \geq 1$. The inner products in $\mathbb{L}^2(D)$ and $\mathbb{L}^2(\tilde{D})$ are denoted by $(\cdot, \cdot)_D$ and $(\cdot, \cdot)_{\tilde{D}}$.

We now define notion of weak solution for the problem (1.1)–(1.3).

Definition 2.1 (Weak Solution) Let $\mathbf{s}_0 \in \mathbb{H}^1(\tilde{D})$ and $\mathbf{m}_0 \in \mathbb{H}^1$ with $|\mathbf{m}_0| = 1$ a.e. in D . We say that (\mathbf{m}, \mathbf{s}) is a weak solution to the problem (1.1)–(1.3) if the following hold:

- i) $\mathbf{m} \in L^\infty(\mathbb{H}^1)$, $\partial_t \mathbf{m} \in \mathbb{L}^2(D_T)$, and $|\mathbf{m}| = 1$ a.e.;
- ii) $\mathbf{s} \in L^\infty(\mathbb{L}^2(\tilde{D})) \cap L^2(\mathbb{H}^1(\tilde{D}))$, $\partial_t \mathbf{s} \in L^2(\mathbb{H}^{-1}(\tilde{D}))$;
- iii) For almost all $t \in (0, T)$

$$\begin{aligned}
 (\partial_t \mathbf{m}, \boldsymbol{\phi})_D - \alpha (\mathbf{m} \times \partial_t \mathbf{m}, \boldsymbol{\phi})_D &= (\mathbf{m} \times \nabla \mathbf{m}, \nabla \boldsymbol{\phi})_D - (\mathbf{m} \times \mathbf{s}, \boldsymbol{\phi})_D, \quad \forall \boldsymbol{\phi} \in \mathbb{H}^1, \\
 (\partial_t \mathbf{s}, \boldsymbol{\psi})_{\tilde{D}} &= (\mathbf{J}, \nabla \boldsymbol{\psi})_{\tilde{D}} - (D_0 \mathbf{s}, \boldsymbol{\psi})_{\tilde{D}} - (D_0 \mathbf{s} \times \mathbf{m}, \boldsymbol{\psi})_{\tilde{D}}, \quad \forall \boldsymbol{\psi} \in \mathbb{H}^1(\tilde{D});
 \end{aligned}$$

- iv) $\mathbf{m}(0, \cdot) = \mathbf{m}_0$ and $\mathbf{s}(0, \cdot) = \mathbf{s}_0$ in the trace sense.

Note that it follows from the formulation of (1.1) that $|\mathbf{m}|$ is constant. (This is a well-known property of magnetization which states that below the Curie temperature, the magnitude of the magnetization is constant.) Hence we assume $|\mathbf{m}| = |\mathbf{m}_0| = 1$. The existence of global weak solutions for (1.1)–(1.3) is detailed in [3, 12]. We

assume in this paper that the given data are smooth enough, so that uniqueness holds; see [7, Theorem 1.3]. The following theorem holds:

Theorem 2.1 *Let $s_0 \in \mathbb{H}^1(\tilde{D})$ and $\mathbf{m}_0 \in \mathbb{H}^1$ with $|\mathbf{m}_0| = 1$ a.e. in D , and $D_0 : \tilde{D} \rightarrow \mathbb{R}^+$ be a measurable function such that*

$$0 < D_* \leq D_0(x) \leq D^*, \quad \text{for almost all } x \in \tilde{D} \tag{2.1}$$

for some positive constants D_* and D^* . Then for any $\mathbf{j} \in L^2(\mathbb{H}^1(\tilde{D}))$, there exists a weak solution (\mathbf{m}, \mathbf{s}) of (1.1)–(1.3) in the sense of Definition 2.1. Moreover, the following estimates hold:

$$\begin{cases} \|\mathbf{s}\|_{L^\infty(\mathbb{L}^2(\tilde{D}))}^2 + \|\nabla \mathbf{s}\|_{L^2(\mathbb{L}^2(\tilde{D}))}^2 \leq C \|\mathbf{j}\|_{L^2(\mathbb{L}^2(\tilde{D}))}^2, \\ \|\partial_t \mathbf{m}\|_{L^2(\mathbb{L}^2)}^2 + \|\nabla \mathbf{m}\|_{L^\infty(\mathbb{L}^2)}^2 \leq C(\alpha) \|\mathbf{s}\|_{L^2(\mathbb{L}^2(\tilde{D}))}^2 + \|\mathbf{m}_0\|_{\mathbb{H}^1}^2, \\ \|\partial_t \mathbf{s}\|_{L^2(\mathbb{H}^{-1}(\tilde{D}))} \leq C \left(\|\mathbf{j}\|_{L^2(\mathbb{H}^1(\tilde{D}))} + \|\mathbf{s}\|_{L^2(\mathbb{L}^2(\tilde{D}))} + \|\nabla \mathbf{s}\|_{L^2(\mathbb{L}^2(\tilde{D}))} \right). \end{cases} \tag{2.2}$$

Thanks to the above theorem, the set \mathcal{U}_{ad} of all triplets $\pi = (\mathbf{m}, \mathbf{s}, \mathbf{j})$, where \mathbf{j} belongs to $L^2(\mathbb{H}^2(\tilde{D}))$ and (\mathbf{m}, \mathbf{s}) is the weak solution to the corresponding problem (1.1)–(1.3), is non-empty. The reason to require more smoothness in \mathbf{j} is to obtain more smoothness in the solution (\mathbf{m}, \mathbf{s}) , as will be explained later. With this at hand, we rewrite the minimization problem (1.6) as follows.

Definition 2.2 Let the assumptions of Theorem 2.1 hold true. Let $\bar{\mathbf{m}} : [0, T] \times D \rightarrow \mathbb{S}^2$ be a given function, and Ψ be a given Lipschitz continuous function on \mathbb{L}^2 . A tuple $\pi^* = (\mathbf{m}^*, \mathbf{s}^*, \mathbf{j}^*) \in \mathcal{U}_{\text{ad}}$ is said to be a weak optimal solution of (1.6) if

$$F(\pi^*) = \inf_{\pi \in \mathcal{U}_{\text{ad}}} F(\pi).$$

We finish this section by stating the main results of this article, the proofs of which will be presented in Sections 3 and 4.3. The first theorem states the existence of a weak optimal solution π^* .

Theorem 2.2 *There exists at least one weak optimal solution $\pi^* \in \mathcal{U}_{\text{ad}}$ of (1.6) in the sense of Definition 2.2.*

In case of one spatial dimension, optimal solution π^* may satisfy first-order optimality conditions. For $d = 1$, we consider the following equation for spin accumulation $\mathbf{s} : \tilde{D}_T \rightarrow \mathbb{R}^3$, see [25],

$$\begin{cases} \partial_t \mathbf{s} = -\nabla \mathbf{J} - D_0 \mathbf{s} - D_0 \mathbf{s} \times \mathbf{m} & \text{in } \tilde{D}_T, \\ \partial_\nu \mathbf{s} = 0 & \text{on } \partial \tilde{D}_T, \\ \mathbf{s}(0, \cdot) = \mathbf{s}_0 & \text{in } \tilde{D}, \end{cases} \tag{2.3}$$

where the spin current \mathbf{J} is a vector defined by

$$\mathbf{J} = \mathbf{m} \mathbf{j} - D_0(\nabla \mathbf{s} - \beta \mathbf{m} \langle \nabla \mathbf{s}, \mathbf{m} \rangle) \quad \text{in } \tilde{D}_T \tag{2.4}$$

with the given electric current density $\mathbf{j} : \tilde{D}_T \rightarrow \mathbb{R}$. Here, $\langle \cdot, \cdot \rangle$ denotes the Euclidean inner product in \mathbb{R}^3 .

The next theorem derives the first-order optimality system to be solved to simulate the optimal solution $(\mathbf{m}^*, \mathbf{s}^*, \mathbf{j}^*)$ numerically. The second-order optimality system is not easy to derive due to lack of regularity of the solution of the control problem.

Theorem 2.3 *Let $d = 1$, $\mathbf{m}_0 \in \mathbb{H}^2$, $\mathbf{s}_0 \in \mathbb{H}^2(\tilde{D})$, and $D_0 \in H^2(\tilde{D})$ with $D_* > 2\beta D^*$. Let $\pi^* = (\mathbf{m}^*, \mathbf{s}^*, \mathbf{j}^*)$ be a weak optimal solution of (1.6) subject to (1.1), (2.3), and (2.4); see Theorem 2.2. Then there exists $(\mathbf{z}_1, \mathbf{z}_2) \in L^2(\mathbb{L}^2) \times L^2(\mathbb{L}^2(\tilde{D}))$ such that for a.e. $t \in [0, T]$, there hold*

$$0 = (\delta_1 \mathbf{j}^* - \delta_2 \Delta \mathbf{j}^*, \delta \mathbf{j})_{\tilde{D}} + \delta_3 (\Delta \mathbf{j}^*, \Delta \delta \mathbf{j})_{\tilde{D}} - (\nabla \mathbf{z}_2, \mathbf{m}^* \delta \mathbf{j})_{\tilde{D}} \quad \forall \delta \mathbf{j} \in L^2(H^2(\tilde{D})), \tag{2.5}$$

$$\begin{aligned} 0 = & -(\partial_t \mathbf{z}_1, \delta \mathbf{m})_D + \kappa (\mathbf{m}^* - \bar{\mathbf{m}}, \delta \mathbf{m})_D - \alpha_1 (\mathbf{z}_1, \Delta \delta \mathbf{m})_D - \alpha_1 (\mathbf{z}_1, 2 \langle \nabla \mathbf{m}^*, \nabla \delta \mathbf{m} \rangle \mathbf{m}^* + |\nabla \mathbf{m}^*|^2 \delta \mathbf{m})_D \\ & + \alpha_2 (\mathbf{z}_1, \mathbf{m}^* \times \Delta \delta \mathbf{m} + \delta \mathbf{m} \times \Delta \mathbf{m}^* + \delta \mathbf{m} \times \mathbf{s}^*)_D + \alpha_1 (\mathbf{z}_1, \delta \mathbf{m} \langle \mathbf{m}^*, \mathbf{s}^* \rangle + \mathbf{m}^* \langle \delta \mathbf{m}, \mathbf{s}^* \rangle)_D \\ & - (\nabla \mathbf{z}_2, \delta \mathbf{m} \mathbf{j}^*)_D - \beta (\nabla \mathbf{z}_2, D_0 \delta \mathbf{m} \langle \nabla \mathbf{s}^*, \mathbf{m}^* \rangle)_D + (\mathbf{z}_2, D_0 \mathbf{s}^* \times \delta \mathbf{m})_D \\ & - \beta (\nabla \mathbf{z}_2, D_0 \mathbf{m}^* \langle \nabla \mathbf{s}^*, \delta \mathbf{m} \rangle)_D \quad \forall \delta \mathbf{m} \in L^2(\mathbb{H}^2) \cap H^1(\mathbb{L}^2), \end{aligned} \tag{2.6}$$

$$\begin{aligned} 0 = & -(\partial_t \mathbf{z}_2, \delta \mathbf{s})_{\tilde{D}} + \alpha_2 (\mathbf{z}_1, \mathbf{m}^* \times \delta \mathbf{s})_{\tilde{D}} - \alpha_1 (\mathbf{z}_1, \delta \mathbf{s} - \mathbf{m}^* \langle \mathbf{m}^*, \delta \mathbf{s} \rangle)_{\tilde{D}} + (\mathbf{z}_2, D_0 \delta \mathbf{s} + D_0 \delta \mathbf{s} \times \mathbf{m}^*)_{\tilde{D}} \\ & - (\nabla \mathbf{z}_2, -D_0 \nabla \delta \mathbf{s} + \beta D_0 \mathbf{m}^* \langle \nabla \delta \mathbf{s}, \mathbf{m}^* \rangle)_{\tilde{D}} \quad \forall \delta \mathbf{s} \in L^2(\mathbb{H}^2(\tilde{D})) \cap H^1(\mathbb{L}^2(\tilde{D})), \end{aligned} \tag{2.7}$$

$$\mathbf{z}_1(T) = -\frac{1-\kappa}{2} \nabla \Psi(\mathbf{m}^*(T)), \quad \mathbf{z}_2(T) = 0, \tag{2.8}$$

where $\alpha_1 = \alpha/(1 + \alpha^2)$ and $\alpha_2 = 1/(1 + \alpha^2)$. The pair $(\mathbf{z}_1, \mathbf{z}_2)$ is called adjoint variables.

3 Existence of optimal control: proof of Theorem 2.2

In this section, we prove the existence of a weak optimal solution π^* of (1.6), i.e., we verify Theorem 2.2. Let $\Lambda = \inf_{\pi \in \mathcal{U}_{\text{ad}}} F(\pi)$. For $\mathbf{j} = \mathbf{0}$, the problem (1.1)–(1.3) has a weak solution (\mathbf{m}, \mathbf{s}) with $|\mathbf{m}| = 1$. Thus Λ is finite. Let $\pi_n = (\mathbf{m}_n, \mathbf{s}_n, \mathbf{j}_n)$, $n \in \mathbb{N}$ be a minimizing sequence of weak solutions, i.e.,

$$\lim_{n \rightarrow \infty} F(\pi_n) = \Lambda.$$

Since Λ is finite, there exists $R > 0$ such that

$$\|\mathbf{j}_n\|_{L^2(\mathbb{H}^2(\tilde{D}))}^2 \leq R. \tag{3.1}$$

Again, since π_n is a weak solution of (1.1)–(1.3), the following estimates hold, see [12],

$$\begin{aligned} \|\partial_t \mathbf{m}_n\|_{L^2(\mathbb{L}^2)}^2 + \|\nabla \mathbf{m}_n\|_{L^\infty(\mathbb{L}^2)}^2 & \leq C(\alpha) \|\mathbf{s}_n\|_{L^2(\mathbb{L}^2(\tilde{D}))}^2 + \|\mathbf{m}_0\|_{\mathbb{H}^1}^2, \\ \|\mathbf{s}_n\|_{L^2(\mathbb{L}^2(\tilde{D}))}^2 + \|\nabla \mathbf{s}_n\|_{L^2(\mathbb{L}^2(\tilde{D}))}^2 & \leq C \|\mathbf{j}_n\|_{L^2(\mathbb{L}^2(\tilde{D}))}^2, \\ \|\partial_t \mathbf{s}_n\|_{L^2(\mathbb{H}^{-1}(\tilde{D}))} & \leq \|\mathbf{J}_n\|_{L^2(\mathbb{L}^2(\tilde{D}))} + 2D^* \|\mathbf{s}_n\|_{L^2(\mathbb{L}^2(\tilde{D}))} \\ & \leq C \left(\|\mathbf{j}_n\|_{L^2(\mathbb{H}^1(\tilde{D}))} + \|\mathbf{s}_n\|_{L^2(\mathbb{L}^2(\tilde{D}))} + \|\nabla \mathbf{s}_n\|_{L^2(\mathbb{L}^2(\tilde{D}))} \right). \end{aligned} \tag{3.2}$$

Thus, thanks to (3.1) and (3.2), there exist subsequences of $\{\mathbf{s}_n\}$, $\{\mathbf{m}_n\}$ and $\{\mathbf{j}_n\}$ (not relabeled) such that

$$\begin{cases} \mathbf{m}_n \rightharpoonup \mathbf{m}^* & \text{in } L^2(\mathbb{L}^2) \text{ and a.e. } D_T \\ \mathbf{m}_n \rightharpoonup \mathbf{m}^* & \text{in } H^1(D_T) \\ \mathbf{s}_n \rightarrow \mathbf{s}^* & \text{in } L^2(\mathbb{L}^2(\tilde{D})) \text{ and a.e. } \tilde{D}_T \\ \nabla \mathbf{s}_n \rightharpoonup \nabla \mathbf{s}^* & \text{in } L^2(\mathbb{L}^2(\tilde{D})) \\ \partial_t \mathbf{s}_n \rightharpoonup \partial_t \mathbf{s}^* & \text{in } L^2(\mathbb{H}^{-1}(\tilde{D})) \\ \mathbf{j}_n \rightharpoonup \mathbf{j}^* & \text{in } L^2(\mathbb{H}^2(\tilde{D})) \\ \mathbf{j}_n \rightarrow \mathbf{j}^* & \text{in } L^2(\mathbb{L}^2(\tilde{D})) \text{ and a.e. } \tilde{D}_T \end{cases} \tag{3.3}$$

for some functions \mathbf{s}^* , \mathbf{m}^* and \mathbf{j}^* . In view of the convergence results as in (3.3), the uniform bounds in (3.1) and (3.2) together with Fatou’s lemma, one can easily pass to the limit in the weak formulations for $(\mathbf{m}_n, \mathbf{s}_n, \mathbf{j}_n)$ to verify that the limiting function $(\mathbf{m}^*, \mathbf{s}^*, \mathbf{j}^*)$ satisfies i-iv) of Definition 2.1, except $|\mathbf{m}^*(t, x)| = 1$ a.e. $(t, x) \in D_T$. We can achieve the unit length condition for \mathbf{m}^* in the following way. Let $\phi_0 \in C_0^\infty(D)$. Take the test function $\phi = \mathbf{m}^* \phi_0$ in iii) of Definition 2.1. Then one has

$$\frac{d}{dt} \int_D |\mathbf{m}^*|^2 \phi_0 \, dx = 0,$$

and therefore $|\mathbf{m}^*(t, x)| = |\mathbf{m}_0(x)| = 1$ a.e. D_T . Consequently, $\pi^* = (\mathbf{m}^*, \mathbf{s}^*, \mathbf{j}^*) \in \mathcal{U}_{\text{ad}}$. It remains to show that π^* is a minimum. Observe that F is measurable, non-negative and lower semi-continuous convex function. Thus, by using Fatou’s lemma, we have

$$0 \leq \Lambda = \inf_{\pi \in \mathcal{U}_{\text{ad}}} F(\pi) \leq F(\pi^*) \leq \lim_{n \rightarrow \infty} F(\pi_n) = \Lambda,$$

i.e., $F(\pi^*) = \inf_{\pi \in \mathcal{U}_{\text{ad}}} F(\pi)$. This completes the proof.

Remark 3.1 One may formulate the control problem for \mathbb{H}^1 -control and show the existence of an optimal solution and hence the optimal control. In Theorem 2.2, we have taken \mathbb{H}^2 -valued control, which play a crucial role to deduce optimality conditions for optimal solution π^* .

4 Optimality system for $d = 1$

Theorem 2.2 ensures the existence of an optimal solution $(\mathbf{m}^*, \mathbf{s}^*, \mathbf{j}^*)$ of (1.6) in any spatial dimension $d = 1, 2, 3$. In order to deduce the necessary optimality system associated with the tuple $(\mathbf{m}^*, \mathbf{s}^*, \mathbf{j}^*)$, one needs higher regularity for the solution, and therefore needs to restrict to one spatial dimension. From now onwards, we consider D and \tilde{D} to be bounded Lipschitz domains in \mathbb{R} and the spin accumulation $\mathbf{s} : \tilde{D}_T \rightarrow \mathbb{R}^3$ satisfies (2.3) and (2.4).

4.1 Regularity of weak solution

We wish to deduce improved stability properties for a weak solution of the problem (1.1), (2.3), and (2.4).

Lemma 4.1 *For $d = 1$, let the assumptions of Theorem 2.1 hold true and $D_0 \in H^2(\tilde{D})$ with $D_* > 2\beta D^*$. Let (\mathbf{m}, \mathbf{s}) be a weak solution of the problem (1.1), (2.3), and (2.4). Then*

i) $\mathbf{m} \in L^\infty(\mathbb{H}^1) \cap L^2(\mathbb{H}^2) \cap H^1(\mathbb{L}^2)$, i.e., there exists a constant $C > 0$ such that

$$\|\mathbf{m}\|_{L^\infty(\mathbb{H}^1)} + \|\mathbf{m}\|_{L^2(\mathbb{H}^2)} + \|\mathbf{m}\|_{H^1(\mathbb{L}^2)} \leq C.$$

ii) $\mathbf{s} \in L^\infty(\mathbb{H}^1(\tilde{D})) \cap L^2(\mathbb{H}^2(\tilde{D}))$, i.e., there exists a constant $C > 0$ such that

$$\|\mathbf{s}\|_{L^\infty(\mathbb{H}^1(\tilde{D}))} + \|\mathbf{s}\|_{L^2(\mathbb{H}^2(\tilde{D}))} \leq C.$$

Proof Proof of i): It is easy to establish $\mathbf{m} \in L^\infty(\mathbb{H}^1) \cap H^1(\mathbb{L}^2)$. It remains to show $\mathbf{m} \in L^2(\mathbb{H}^2)$. Recalling that $\mathbf{H}_{\text{eff}}(\mathbf{m}) = \Delta \mathbf{m}$ and that we have assumed $\gamma_0 = c = 1$ in (1.1), we rewrite the (1.1) in the following form:

$$\partial_t \mathbf{m} - \alpha_1 \Delta \mathbf{m} = \alpha_1 |\nabla \mathbf{m}|^2 \mathbf{m} - \alpha_2 \mathbf{m} \times \Delta \mathbf{m} - \alpha_2 \mathbf{m} \times \mathbf{s} + \alpha_1 (\mathbf{s} - \mathbf{m} \langle \mathbf{m}, \mathbf{s} \rangle), \tag{4.1}$$

where $\alpha_1 = \alpha/(1 + \alpha^2)$ and $\alpha_2 = 1/(1 + \alpha^2)$, noting that $|\nabla \mathbf{m}|^2 = -\mathbf{m} \cdot \Delta \mathbf{m}$ due to $|\mathbf{m}| = 1$. This equivalence can be shown by taking the cross product to the left of both sides of (1.1), using $|\mathbf{m}| = 1$ and the elementary identity $\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = \mathbf{b} \langle \mathbf{a}, \mathbf{c} \rangle - \mathbf{c} \langle \mathbf{a}, \mathbf{b} \rangle$, and rearranging the resulting equation.

Formally we multiply (4.1) with $-\Delta \mathbf{m}$, and use the Cauchy–Schwarz inequality, the boundedness of \mathbf{m} together with the Gagliardo–Nirenberg inequality

$$\|X\|_{L^4(\tilde{D})} \leq C \|X\|_{H^1(\tilde{D})}^{\frac{1}{4}} \|X\|_{L^2(\tilde{D})}^{\frac{3}{4}} \quad \text{for } \tilde{D} \subset \mathbb{R}$$

to have

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\nabla \mathbf{m}\|_{\mathbb{L}^2}^2 + \alpha_1 \|\Delta \mathbf{m}\|_{\mathbb{L}^2}^2 &\leq \sigma \|\Delta \mathbf{m}\|_{\mathbb{L}^2}^2 + C(\sigma, \alpha_1, \alpha_2) \left(\|\nabla \mathbf{m}\|_{\mathbb{L}^4}^4 + \|\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 \right) \\ &\leq \sigma \|\Delta \mathbf{m}\|_{\mathbb{L}^2}^2 + C(\sigma, \alpha_1, \alpha_2) \left((\|\nabla \mathbf{m}\|_{\mathbb{L}^2} + \|\Delta \mathbf{m}\|_{\mathbb{L}^2}) \|\nabla \mathbf{m}\|_{\mathbb{L}^2}^3 + \|\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 \right) \\ &\leq (\sigma + \tilde{\sigma}) \|\Delta \mathbf{m}\|_{\mathbb{L}^2}^2 + C(\sigma, \tilde{\sigma}, \alpha_1, \alpha_2) \left(\|\nabla \mathbf{m}\|_{\mathbb{L}^2}^6 + \|\nabla \mathbf{m}\|_{\mathbb{L}^2}^4 + \|\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 \right), \end{aligned}$$

for some $\sigma, \tilde{\sigma} > 0$ which can be chosen such that $\sigma + \tilde{\sigma} < \alpha_1$. Combining this with the estimate for \mathbf{s} in (2.2) we conclude that $\mathbf{m} \in L^2(\mathbb{H}^2)$. Hence assertion i) follows.

Proof of ii): First we note that (2.3) and (2.4) imply, after rearranging the equation,

$$\begin{aligned} \partial_t \mathbf{s} - D_0 \Delta \mathbf{s} &= -\nabla \langle \mathbf{j}, \mathbf{m} \rangle + \nabla D_0 (\nabla \mathbf{s} - \beta \mathbf{m} \langle \nabla \mathbf{s}, \mathbf{m} \rangle) - \beta D_0 \mathbf{m} \langle \Delta \mathbf{s}, \mathbf{m} \rangle \\ &\quad - \beta D_0 \nabla \mathbf{m} \langle \nabla \mathbf{s}, \mathbf{m} \rangle - \beta D_0 \mathbf{m} \langle \nabla \mathbf{s}, \nabla \mathbf{m} \rangle - D_0 \mathbf{s} - D_0 \mathbf{s} \times \mathbf{m}. \end{aligned} \tag{4.2}$$

Then we formally multiply (4.2) by $-\Delta \mathbf{s}$ and integrate w.r.t x to obtain

$$\frac{1}{2} \frac{d}{dt} \|\nabla \mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 + D_* \|\Delta \mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 \leq T_1 + T_2 + \dots + T_5, \tag{4.3}$$

where

$$\begin{aligned}
 T_1 &:= |(\nabla(\mathbf{m}j), \Delta\mathbf{s})_{\mathbb{L}^2(\tilde{D})}|, \\
 T_2 &:= \left|(\nabla D_0(\nabla\mathbf{s} - \beta\mathbf{m}\langle\nabla\mathbf{s}, \mathbf{m}\rangle), \Delta\mathbf{s})_{\mathbb{L}^2(\tilde{D})}\right|, \\
 T_3 &:= |\beta(D_0\mathbf{m}\langle\Delta\mathbf{s}, \mathbf{m}\rangle, \Delta\mathbf{s})_{\mathbb{L}^2(\tilde{D})}|, \\
 T_4 &:= \left|\beta(D_0\nabla\mathbf{m}\langle\nabla\mathbf{s}, \mathbf{m}\rangle, \Delta\mathbf{s})_{\mathbb{L}^2(\tilde{D})} + \beta(D_0\mathbf{m}\langle\nabla\mathbf{s}, \nabla\mathbf{m}\rangle, \Delta\mathbf{s})_{\mathbb{L}^2(\tilde{D})}\right|, \\
 T_5 &:= \left|(D_0\mathbf{s} + D_0\mathbf{s} \times \mathbf{m}, \Delta\mathbf{s})_{\mathbb{L}^2(\tilde{D})}\right|.
 \end{aligned}$$

By using the Cauchy–Schwarz inequality, the embedding $\mathbb{H}^1 \hookrightarrow \mathbb{L}^\infty$, and (2.1), we have

$$\begin{aligned}
 T_1 &\leq \|\Delta\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})} \left(\|\nabla\mathbf{m}\|_{\mathbb{L}^2} \|j\|_{\mathbb{H}^1(\tilde{D})} + \|\nabla j\|_{\mathbb{L}^2(\tilde{D})}\right) \\
 &\leq \epsilon \|\Delta\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 + \frac{1}{2\epsilon} \|\nabla\mathbf{m}\|_{\mathbb{L}^2}^2 \|j\|_{\mathbb{H}^1(\tilde{D})}^2 + \frac{1}{2\epsilon} \|\nabla j\|_{\mathbb{L}^2(\tilde{D})}^2, \\
 T_2 &\leq \epsilon \|\Delta\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 + C(\epsilon, \beta) \|\nabla\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2, \\
 T_3 &\leq \beta D^* \|\Delta\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2, \\
 T_4 &\leq 2\beta D^* \|\nabla\mathbf{m}\|_{\mathbb{L}^\infty} \|\nabla\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})} \|\Delta\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})} \\
 &\leq 2\beta D^* \|\nabla\mathbf{m}\|_{\mathbb{H}^1} \|\nabla\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})} \|\Delta\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})} \\
 &\leq 2\beta D^* (\|\nabla\mathbf{m}\|_{\mathbb{L}^2} + \|\Delta\mathbf{m}\|_{\mathbb{L}^2}) \|\nabla\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})} \|\Delta\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})} \\
 &\leq \epsilon \|\Delta\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 + C(\epsilon, \beta, D^*) (\|\nabla\mathbf{m}\|_{\mathbb{L}^2}^2 + \|\Delta\mathbf{m}\|_{\mathbb{L}^2}^2) \|\nabla\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2, \\
 T_5 &\leq 2D^* \|\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})} \|\Delta\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})} \\
 &\leq \epsilon \|\Delta\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 + C(\epsilon, D^*) \|\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2.
 \end{aligned}$$

Combining all the estimates we obtained from (4.3)

$$\begin{aligned}
 \frac{1}{2} \frac{d}{dt} \|\nabla\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 + (D_* - 4\epsilon - \beta D^*) \|\Delta\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 &\leq C(\epsilon, \beta, D^*) \left\{ \|\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 + \|\nabla j\|_{\mathbb{L}^2(\tilde{D})}^2 + \|\nabla\mathbf{m}\|_{\mathbb{L}^2}^2 \|j\|_{\mathbb{H}^1(\tilde{D})}^2 \right. \\
 &\quad \left. + \left(\|\nabla D_0\|_{L^\infty(\tilde{D})}^2 + \|\nabla\mathbf{m}\|_{\mathbb{L}^2}^2 + \|\Delta\mathbf{m}\|_{\mathbb{L}^2}^2\right) \|\nabla\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 \right\}.
 \end{aligned}$$

By choosing ϵ sufficiently small and using the given assumption $D_* > 2\beta D^*$, we obtain after integrating over $[0, t]$ and invoking Gronwall’s Lemma

$$\begin{aligned}
 \|\nabla\mathbf{s}(t)\|_{\mathbb{L}^2(\tilde{D})}^2 + \int_0^t \|\Delta\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 d\tau &\leq C \int_0^t \left(\|\mathbf{s}\|_{\mathbb{L}^2(\tilde{D})}^2 + \|\nabla j\|_{\mathbb{L}^2(\tilde{D})}^2 + \|\nabla\mathbf{m}\|_{\mathbb{L}^2}^2 \|j\|_{\mathbb{H}^1(\tilde{D})}^2 \right) d\tau \\
 &\quad \times \exp\left(C \int_0^t \left(\|\nabla D_0\|_{L^\infty(\tilde{D})}^2 + \|\nabla\mathbf{m}\|_{\mathbb{L}^2}^2 + \|\Delta\mathbf{m}\|_{\mathbb{L}^2}^2\right) d\tau\right).
 \end{aligned}$$

In view of the estimation of i) and the estimate for \mathbf{s} in (2.2), we complete the proof. □

As we mentioned, we need improved regularity for the solution (\mathbf{m}, \mathbf{s}) . To get improved regularity, we need to consider more regular control $j \in L^2(H^2(\tilde{D}))$.

Lemma 4.2 For $d = 1$, let the assumptions of Lemma 4.1 hold with $\mathbf{m}_0 \in \mathbb{H}^2$, $s_0 \in \mathbb{H}^2(\tilde{D})$, and $j \in L^2(H^2(\tilde{D}))$. Then the weak solution (\mathbf{m}, s) of (1.1), (2.3) and (2.4) satisfies the following improved regularity:

- i) $\mathbf{m} \in L^2(\mathbb{H}^3) \cap L^\infty(\mathbb{H}^2) \cap H^1(\mathbb{H}^1) \hookrightarrow C(\mathbb{H}^2)$.
- ii) $s \in L^2(\mathbb{H}^3(\tilde{D})) \cap L^\infty(\mathbb{H}^2(\tilde{D})) \cap H^1(\mathbb{H}^1(\tilde{D})) \hookrightarrow C(\mathbb{H}^2(\tilde{D}))$.

Proof Proof of i): Let $\mathbf{m}_0 \in \mathbb{H}^2$. Denote $\mathbf{M} = \nabla \mathbf{m}$. Differentiating (4.1) with respect to the spatial variable, we formally have

$$\begin{aligned} \partial_t \mathbf{M} - \alpha_1 \Delta \mathbf{M} &= 2\alpha_1 \langle \nabla \mathbf{M}, \nabla \mathbf{m} \rangle \mathbf{m} + \alpha_1 |\nabla \mathbf{m}|^2 \mathbf{M} - \alpha_2 [\mathbf{M} \times \Delta \mathbf{m} + \mathbf{m} \times \Delta \mathbf{M}] \\ &\quad - \alpha_2 [\mathbf{M} \times \mathbf{s} + \mathbf{m} \times \nabla \mathbf{s}] + \alpha_1 [\nabla \mathbf{s} - \mathbf{M} \langle \mathbf{m}, \mathbf{s} \rangle - \mathbf{m} \langle \langle \mathbf{m}, \nabla \mathbf{s} \rangle + \langle \mathbf{M}, \mathbf{s} \rangle \rangle]. \end{aligned} \tag{4.4}$$

Multiplying (4.4) by $-\Delta \mathbf{M}$ (formally), using integration by parts, the Cauchy–Schwarz inequality, and the boundedness of \mathbf{m} , we have after rearranging the equation

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\nabla \mathbf{M}\|_{\mathbb{L}^2}^2 + (\alpha_1 - \sigma_1) \|\Delta \mathbf{M}\|_{\mathbb{L}^2}^2 \\ \leq C \left\{ (1 + \|\mathbf{m}\|_{\mathbb{H}^2}^2) (\|\nabla \mathbf{m}\|_{\mathbb{L}^2}^2 + \|\nabla \mathbf{M}\|_{\mathbb{L}^2}^2) + \|\mathbf{s}\|_{\mathbb{H}^1(\tilde{D})}^2 (1 + \|\nabla \mathbf{m}\|_{\mathbb{L}^2}^2) \right\}, \end{aligned}$$

for some small $\sigma_1 > 0$ and $C \equiv C(\sigma_1, \alpha_1, \alpha_2) > 0$ being a generic constant, so that by choosing $\sigma_1 < \alpha_1$ and invoking Lemma 4.1, we deduce

$$\frac{d}{dt} \|\nabla \mathbf{M}\|_{\mathbb{L}^2}^2 + \|\Delta \mathbf{M}\|_{\mathbb{L}^2}^2 \leq C(1 + \|\mathbf{m}\|_{\mathbb{H}^2}^2) + C(1 + \|\mathbf{m}\|_{\mathbb{H}^2}^2) \|\nabla \mathbf{M}\|_{\mathbb{L}^2}^2.$$

By invoking Lemma 4.1 again and integrating over $(0, t)$ we infer

$$\begin{aligned} \|\nabla \mathbf{M}(t)\|_{\mathbb{L}^2}^2 + \int_0^t \|\Delta \mathbf{M}(\tau)\|_{\mathbb{L}^2}^2 d\tau &\leq C \int_0^t (1 + \|\mathbf{m}(\tau)\|_{\mathbb{H}^2}^2) d\tau + C \int_0^t (1 + \|\mathbf{m}(\tau)\|_{\mathbb{H}^2}^2) \|\nabla \mathbf{M}(\tau)\|_{\mathbb{L}^2}^2 d\tau \\ &\leq C + C \int_0^t (1 + \|\mathbf{m}(\tau)\|_{\mathbb{H}^2}^2) \|\nabla \mathbf{M}(\tau)\|_{\mathbb{L}^2}^2 d\tau. \end{aligned}$$

Gronwall’s Lemma and Lemma 4.1 yield

$$\|\nabla \mathbf{M}\|_{L^\infty(\mathbb{L}^2)}^2 + \|\Delta \mathbf{M}\|_{L^2(\mathbb{L}^2)}^2 \leq C(\alpha_1, \alpha_2, \|\mathbf{s}\|_{L^2(\mathbb{H}^1(\tilde{D}))}, \|\mathbf{m}_0\|_{\mathbb{H}^2}). \tag{4.5}$$

Again, we formally multiply (4.4) by $\partial_t \mathbf{M}$, and use a similar argument along with the estimate (4.5) to conclude that

$$\|\partial_t \mathbf{M}\|_{L^2(\mathbb{L}^2)}^2 \leq C(\alpha_1, \alpha_2, \|\mathbf{s}\|_{L^2(\mathbb{H}^1(\tilde{D}))}, \|\mathbf{m}_0\|_{\mathbb{H}^2}). \tag{4.6}$$

Hence from (4.5) and (4.6) together with Lemma 4.1, we get $\mathbf{m} \in L^2(\mathbb{H}^3) \cap L^\infty(\mathbb{H}^2) \cap H^1(\mathbb{H}^1) \hookrightarrow C(\mathbb{H}^2)$.

Proof of ii): Denote $\mathbf{S} = \nabla \mathbf{s}$. Upon differentiating (2.3) with respect to the spatial variable, we formally see that \mathbf{S} satisfies the following PDE:

$$\begin{aligned} \partial_t \mathbf{S} - D_0 \Delta \mathbf{S} &= -\mathbf{m} \Delta j - 2 \nabla \mathbf{m} \nabla j - j \Delta \mathbf{m} + \Delta D_0 [\mathbf{S} - \beta \mathbf{m} \langle \mathbf{S}, \mathbf{m} \rangle] \\ &\quad + 2 \nabla D_0 \left\{ \nabla \mathbf{S} - \beta \nabla \mathbf{m} \langle \mathbf{S}, \mathbf{m} \rangle - \beta \mathbf{m} \langle \nabla \mathbf{S}, \mathbf{m} \rangle - \beta \mathbf{m} \langle \mathbf{S}, \nabla \mathbf{m} \rangle \right\} \\ &\quad + D_0 \left\{ -\beta \Delta \mathbf{m} \langle \mathbf{S}, \mathbf{m} \rangle - 2\beta \nabla \mathbf{m} \langle \nabla \mathbf{S}, \mathbf{m} \rangle - 2\beta \nabla \mathbf{m} \langle \mathbf{S}, \nabla \mathbf{m} \rangle \right. \\ &\quad \left. - 2\beta \mathbf{m} \langle \nabla \mathbf{S}, \nabla \mathbf{m} \rangle - \beta \mathbf{m} \langle \Delta \mathbf{S}, \mathbf{m} \rangle - \beta \mathbf{m} \langle \mathbf{S}, \Delta \mathbf{m} \rangle \right\} - \nabla D_0 \mathbf{s} - D_0 \mathbf{S} \\ &\quad - \nabla D_0 \mathbf{s} \times \mathbf{m} - D_0 \mathbf{S} \times \mathbf{m} - D_0 \mathbf{s} \times \nabla \mathbf{m}. \end{aligned} \tag{4.7}$$

Multiplying (4.7) by $-\Delta \mathbf{S}$ (formally), and using the Cauchy–Schwarz inequality, the boundedness of \mathbf{m} , and (2.1), we obtain

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \|\nabla \mathbf{S}\|_{L^2(\tilde{D})}^2 + D_* \|\Delta \mathbf{S}\|_{L^2(\tilde{D})}^2 \\ & \leq (\epsilon + \beta D^*) \|\Delta \mathbf{S}\|_{L^2(\tilde{D})}^2 + C(\epsilon) \|\mathbf{m}\|_{\mathbb{H}^2}^2 \|\mathbf{j}\|_{H^2(\tilde{D})}^2 \\ & \quad + C(\epsilon, \beta) \|\Delta D_0\|_{L^2(\tilde{D})}^2 \|\mathbf{S}\|_{L^\infty(\tilde{D})}^2 + C(\epsilon, \beta) \|\nabla D_0\|_{L^\infty(\tilde{D})}^2 \{ \|\nabla \mathbf{S}\|_{L^2(\tilde{D})}^2 + \|\nabla \mathbf{m}\|_{L^\infty}^2 \|\mathbf{S}\|_{L^2(\tilde{D})}^2 \} \\ & \quad + C(\epsilon, \beta, D^*) \left\{ \|\Delta \mathbf{m}\|_{L^2}^2 \|\mathbf{S}\|_{L^\infty(\tilde{D})}^2 + \|\nabla \mathbf{m}\|_{L^\infty}^2 \|\nabla \mathbf{S}\|_{L^2(\tilde{D})}^2 + \|\nabla \mathbf{m}\|_{L^\infty}^4 \|\mathbf{S}\|_{L^2(\tilde{D})}^2 \right\} \\ & \quad + C(\epsilon) \left\{ D^* \|\mathbf{S}\|_{L^2(\tilde{D})}^2 + (\|\nabla D_0\|_{L^\infty(\tilde{D})}^2 + D^* \|\nabla \mathbf{m}\|_{L^\infty}^2) \|\mathbf{s}\|_{L^2(\tilde{D})}^2 \right\}. \end{aligned}$$

By using the result in part i), we deduce (noting the assumption on D_0)

$$\frac{1}{2} \frac{d}{dt} \|\nabla \mathbf{S}\|_{L^2(\tilde{D})}^2 + D_* \|\Delta \mathbf{S}\|_{L^2(\tilde{D})}^2 \leq (\epsilon + \beta D^*) \|\Delta \mathbf{S}\|_{L^2(\tilde{D})}^2 + C(\epsilon, \beta, D_0) \left\{ \|\mathbf{j}\|_{H^2(\tilde{D})}^2 + \|\mathbf{S}\|_{\mathbb{H}^1(\tilde{D})}^2 \right\}.$$

We take $\epsilon = D^*/2$ and use Gronwall’s lemma along with the assumptions on \mathbf{j} to conclude

$$\|\nabla \mathbf{S}\|_{L^\infty(L^2(\tilde{D}))}^2 + \|\Delta \mathbf{S}\|_{L^2(L^2(\tilde{D}))}^2 \leq C(\|\mathbf{s}_0\|_{(\mathbb{H}^2(\tilde{D}))}, \|\mathbf{m}_0\|_{\mathbb{H}^2}),$$

i.e.,

$$\|\mathbf{s}\|_{L^\infty(\mathbb{H}^2(\tilde{D}))}^2 + \|\mathbf{s}\|_{L^2(\mathbb{H}^3(\tilde{D}))}^2 \leq C(\|\mathbf{s}_0\|_{(\mathbb{H}^2(\tilde{D}))}, \|\mathbf{m}_0\|_{\mathbb{H}^2}). \tag{4.8}$$

Moreover, multiplying the equation (2.3) by $\partial_t \mathbf{s}$, and then using the Cauchy–Schwarz inequality, part i) as well as (4.8), we have for any $\epsilon > 0$

$$\begin{aligned} & \|\partial_t \mathbf{s}\|_{L^2(\tilde{D})}^2 + (1 - \beta) D_* \frac{d}{dt} \|\nabla \mathbf{s}\|_{L^2(\tilde{D})}^2 \\ & \leq \epsilon \|\partial_t \mathbf{s}\|_{L^2(\tilde{D})}^2 + C(\epsilon) \left(\|\mathbf{j}\|_{H^1(\tilde{D})}^2 \|\mathbf{m}\|_{\mathbb{H}^1}^2 + \|\nabla \mathbf{s}\|_{L^2(\tilde{D})}^2 \|\mathbf{m}\|_{\mathbb{H}^2}^2 + \|\mathbf{s}\|_{L^2(\tilde{D})}^2 \right) \\ & \leq \epsilon \|\partial_t \mathbf{s}\|_{L^2(\tilde{D})}^2 + C(\epsilon) \left(1 + \|\mathbf{j}\|_{H^1(\tilde{D})}^2 \right). \end{aligned}$$

Since $0 < \beta < 1$, we see that

$$\|\partial_t \mathbf{s}\|_{L^2(L^2(\tilde{D}))}^2 \leq C(\|\mathbf{s}_0\|_{(\mathbb{H}^2(\tilde{D}))}, \|\mathbf{m}_0\|_{\mathbb{H}^2}).$$

Lastly, by formally multiplying (4.7) with $\partial_t \mathbf{S}$, then applying the Cauchy–Schwarz inequality along with the estimate (4.8), one can arrive at the following estimate

$$\|\partial_t \mathbf{S}\|_{L^2(L^2(\tilde{D}))}^2 \leq C(\|\mathbf{s}_0\|_{(\mathbb{H}^2(\tilde{D}))}, \|\mathbf{m}_0\|_{\mathbb{H}^2}),$$

i.e.,

$$\|\mathbf{s}\|_{H^1(\mathbb{H}^1(\tilde{D}))}^2 \leq C(\|\mathbf{s}_0\|_{(\mathbb{H}^2(\tilde{D}))}, \|\mathbf{m}_0\|_{\mathbb{H}^2}).$$

This completes the proof. □

Remark 4.1 In the proof of Lemma 4.2, we have used integration by parts formula, which may be made rigorous by a standard argument using the Faedo–Galerkin method which uses the related eigenfunctions of the given operator.

4.2 Optimization problem and its analysis

With the help of the Lagrange multiplier theorem ([18, Chapter 9, Theorem 1]), we now deduce the optimality system for the optimal solution of (1.6) where the con-

straints (1.2) and (1.3) are replaced by (2.3) and (2.4). To this end, we define the spaces

$$\mathcal{M} := L^2(\mathbb{H}^2) \cap H^1(\mathbb{L}^2), \quad \mathcal{S} := L^2(\mathbb{H}^2(\tilde{D})) \cap H^1(\mathbb{L}^2(\tilde{D})), \quad \mathcal{J} := L^2(H^2(\tilde{D})). \quad (4.9)$$

Note that, in view of [10, Theorem 4, section 5.9.2, p. 306] we have

$$\mathcal{M} \hookrightarrow C(\mathbb{H}^1) \hookrightarrow L^\infty(\mathbb{L}^\infty) \quad \text{and} \quad \mathcal{S} \hookrightarrow C(\mathbb{H}^1(\tilde{D})) \hookrightarrow L^\infty(\mathbb{L}^\infty(\tilde{D})). \quad (4.10)$$

Moreover, we define four functions $e_1 : \mathcal{M} \times \mathcal{S} \times \mathcal{J} \rightarrow L^2(\mathbb{L}^2)$, $e_2 : \mathcal{M} \times \mathcal{S} \times \mathcal{J} \rightarrow L^2(\mathbb{L}^2(\tilde{D}))$, $e_3 : \mathcal{M} \times \mathcal{S} \times \mathcal{J} \rightarrow \mathbb{H}^1$ and $e_4 : \mathcal{M} \times \mathcal{S} \times \mathcal{J} \rightarrow \mathbb{H}^1(\tilde{D})$ by

$$e_1(\mathbf{m}, \mathbf{s}, \mathbf{j}) := \partial_t \mathbf{m} - \alpha_1 \Delta \mathbf{m} - \alpha_1 |\nabla \mathbf{m}|^2 \mathbf{m} + \alpha_2 \mathbf{m} \times \Delta \mathbf{m} + \alpha_2 \mathbf{m} \times \mathbf{s} - \alpha_1 (\mathbf{s} - \mathbf{m} \langle \mathbf{m}, \mathbf{s} \rangle),$$

$$e_2(\mathbf{m}, \mathbf{s}, \mathbf{j}) := \partial_t \mathbf{s} + \nabla \left\{ \mathbf{m} \mathbf{j} - D_0 (\nabla \mathbf{s} - \beta \mathbf{m} \langle \nabla \mathbf{s}, \mathbf{m} \rangle) \right\} + D_0 \mathbf{s} + D_0 \mathbf{s} \times \mathbf{m},$$

$$e_3(\mathbf{m}, \mathbf{s}, \mathbf{j}) := \mathbf{m}(0) - \mathbf{m}_0,$$

$$e_4(\mathbf{m}, \mathbf{s}, \mathbf{j}) := \mathbf{s}(0) - \mathbf{s}_0.$$

The cost functional F defined in (1.6) could be re-interpreted as a function from $\mathcal{M} \times \mathcal{S} \times \mathcal{J} \rightarrow \mathbb{R}$. With this set up, we now state the optimal control problem (1.6) in the following form.

Problem 4.1 Let $d = 1$, and $\bar{\mathbf{m}} : D_T \rightarrow \mathbb{S}^2$ be a given smooth function. Assume that $\mathbf{m}_0 \in \mathbb{H}^2$ with $|\mathbf{m}_0| = 1$ in D , $\mathbf{s}_0 \in \mathbb{H}^2(\tilde{D})$, and (2.1) holds. Minimize F subject to $\Gamma(\mathbf{m}, \mathbf{s}, \mathbf{j}) = 0$, where $\Gamma : \mathcal{M} \times \mathcal{S} \times \mathcal{J} \rightarrow L^2(\mathbb{L}^2) \times L^2(\mathbb{L}^2(\tilde{D})) \times \mathbb{H}^1 \times \mathbb{H}^1(\tilde{D})$ is defined by

$$\Gamma(\mathbf{m}, \mathbf{s}, \mathbf{j}) := \begin{pmatrix} e_1(\mathbf{m}, \mathbf{s}, \mathbf{j}) \\ e_2(\mathbf{m}, \mathbf{s}, \mathbf{j}) \\ e_3(\mathbf{m}, \mathbf{s}, \mathbf{j}) \\ e_4(\mathbf{m}, \mathbf{s}, \mathbf{j}) \end{pmatrix}. \quad (4.11)$$

Lemma 4.3 *The function $\Gamma : \mathcal{M} \times \mathcal{S} \times \mathcal{J} \rightarrow L^2(\mathbb{L}^2) \times L^2(\mathbb{L}^2(\tilde{D})) \times \mathbb{H}^1 \times \mathbb{H}^1(\tilde{D})$ is continuously Fréchet differentiable, with derivative*

$$\langle \Gamma'(\mathbf{m}, \mathbf{s}, \mathbf{j}), (\delta \mathbf{m}, \delta \mathbf{s}, \delta \mathbf{j}) \rangle = \begin{pmatrix} \langle e'_1(\mathbf{m}, \mathbf{s}, \mathbf{j}), (\delta \mathbf{m}, \delta \mathbf{s}, \delta \mathbf{j}) \rangle \\ \langle e'_2(\mathbf{m}, \mathbf{s}, \mathbf{j}), (\delta \mathbf{m}, \delta \mathbf{s}, \delta \mathbf{j}) \rangle \\ \langle e'_3(\mathbf{m}, \mathbf{s}, \mathbf{j}), (\delta \mathbf{m}, \delta \mathbf{s}, \delta \mathbf{j}) \rangle \\ \langle e'_4(\mathbf{m}, \mathbf{s}, \mathbf{j}), (\delta \mathbf{m}, \delta \mathbf{s}, \delta \mathbf{j}) \rangle \end{pmatrix},$$

where

$$\begin{aligned} & \langle e'_1(\mathbf{m}, \mathbf{s}, \mathbf{j}), (\delta \mathbf{m}, \delta \mathbf{s}, \delta \mathbf{j}) \rangle \\ &= \partial_t \delta \mathbf{m} - \alpha_1 \Delta \delta \mathbf{m} - \alpha_1 (2 \langle \nabla \mathbf{m}, \nabla \delta \mathbf{m} \rangle \mathbf{m} + |\nabla \mathbf{m}|^2 \delta \mathbf{m}) - \alpha_1 (\delta \mathbf{s} - \mathbf{m} \langle \mathbf{m}, \delta \mathbf{s} \rangle) \\ & \quad + \alpha_2 (\mathbf{m} \times \Delta \delta \mathbf{m} + \delta \mathbf{m} \times \Delta \mathbf{m} + \delta \mathbf{m} \times \mathbf{s} + \mathbf{m} \times \delta \mathbf{s}) + \alpha_1 (\delta \mathbf{m} \langle \mathbf{m}, \mathbf{s} \rangle + \mathbf{m} \langle \delta \mathbf{m}, \mathbf{s} \rangle), \\ & \langle e'_2(\mathbf{m}, \mathbf{s}, \mathbf{j}), (\delta \mathbf{m}, \delta \mathbf{s}, \delta \mathbf{j}) \rangle \\ &= \partial_t \delta \mathbf{s} + \nabla \left\{ \mathbf{m} \delta \mathbf{j} + \delta \mathbf{m} \mathbf{j} - D_0 \nabla \delta \mathbf{s} + D_0 \beta [\delta \mathbf{m} \langle \nabla \mathbf{s}, \mathbf{m} \rangle + \mathbf{m} \langle \nabla \mathbf{s}, \delta \mathbf{m} \rangle + \mathbf{m} \langle \nabla \delta \mathbf{s}, \mathbf{m} \rangle] \right\} \\ & \quad + D_0 (\delta \mathbf{s} + \delta \mathbf{s} \times \mathbf{m} + \mathbf{s} \times \delta \mathbf{m}), \\ & \langle e'_3(\mathbf{m}, \mathbf{s}, \mathbf{j}), (\delta \mathbf{m}, \delta \mathbf{s}, \delta \mathbf{j}) \rangle = \delta \mathbf{m}(0), \\ & \langle e'_4(\mathbf{m}, \mathbf{s}, \mathbf{j}), (\delta \mathbf{m}, \delta \mathbf{s}, \delta \mathbf{j}) \rangle = \delta \mathbf{s}(0). \end{aligned}$$

Proof We calculate the directional derivatives of e_1 in the directions $\delta \mathbf{m}$, $\delta \mathbf{s}$ and $\delta \mathbf{j}$ to obtain

$$\begin{aligned} \langle \partial_{\mathbf{m}} e_1(\mathbf{m}, \mathbf{s}, \mathbf{j}), \delta \mathbf{m} \rangle &= \partial_t \delta \mathbf{m} - \alpha_1 \Delta \delta \mathbf{m} - \alpha_1 \left(2 \langle \nabla \mathbf{m}, \nabla \delta \mathbf{m} \rangle \mathbf{m} + |\nabla \mathbf{m}|^2 \delta \mathbf{m} \right) \\ &\quad + \alpha_2 \left(\mathbf{m} \times \Delta \delta \mathbf{m} + \delta \mathbf{m} \times \Delta \mathbf{m} + \delta \mathbf{m} \times \mathbf{s} \right) + \alpha_1 \left(\delta \mathbf{m} \langle \mathbf{m}, \mathbf{s} \rangle + \mathbf{m} \langle \delta \mathbf{m}, \mathbf{s} \rangle \right), \\ \langle \partial_{\mathbf{s}} e_1(\mathbf{m}, \mathbf{s}, \mathbf{j}), \delta \mathbf{s} \rangle &= \alpha_2 \mathbf{m} \times \delta \mathbf{s} - \alpha_1 \left(\delta \mathbf{s} - \mathbf{m} \langle \mathbf{m}, \delta \mathbf{s} \rangle \right), \\ \langle \partial_{\mathbf{j}} e_1(\mathbf{m}, \mathbf{s}, \mathbf{j}), \delta \mathbf{j} \rangle &= 0. \end{aligned}$$

By using (4.10) we deduce

$$\begin{aligned} &\| \langle \partial_{\mathbf{m}} e_1(\mathbf{m}, \mathbf{s}, \mathbf{j}), \delta \mathbf{m} \rangle \|_{L^2(\mathbb{L}^2)} \\ &\leq \| \partial_t \delta \mathbf{m} \|_{L^2(\mathbb{L}^2)} + C(\alpha) \left(\| \Delta \delta \mathbf{m} \|_{L^2(\mathbb{L}^2)} + \| \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} \| \Delta \delta \mathbf{m} \|_{L^2(\mathbb{L}^2)} + \| \delta \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} \| \Delta \mathbf{m} \|_{L^2(\mathbb{L}^2)} \right. \\ &\quad \left. + \| \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} \| \nabla \delta \mathbf{m} \|_{L^2(\mathbb{L}^\infty)} \| \nabla \mathbf{m} \|_{L^\infty(\mathbb{L}^2)} + \| \delta \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} \| \nabla \mathbf{m} \|_{L^2(\mathbb{L}^\infty)} \| \nabla \mathbf{m} \|_{L^\infty(\mathbb{L}^2)} \right. \\ &\quad \left. + \| \delta \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} \| \mathbf{s} \|_{L^2(\mathbb{L}^2(\bar{D}))} + \| \mathbf{s} \|_{L^2(\mathbb{L}^2(\bar{D}))} \| \delta \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} \| \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} \right) \\ &\leq C(\mathbf{m}, \mathbf{s}, \mathbf{j}) \| \delta \mathbf{m} \|_{\mathcal{M}}, \end{aligned}$$

and

$$\| \langle \partial_{\mathbf{s}} e_1(\mathbf{m}, \mathbf{s}, \mathbf{j}), \delta \mathbf{s} \rangle \|_{L^2(\mathbb{L}^2)} \leq C(\alpha) \left(\| \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} + 1 + \| \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)}^2 \right) \| \delta \mathbf{s} \|_{L^2(\mathbb{L}^2(\bar{D}))} \leq C(\mathbf{m}, \mathbf{s}, \mathbf{j}) \| \delta \mathbf{s} \|_{\mathcal{S}}.$$

Define a linear operator $e'_1(\mathbf{m}, \mathbf{s}, \mathbf{j}) \in \mathcal{L}(\mathcal{M} \times \mathcal{S} \times \mathcal{J}; L^2(\mathbb{L}^2))$ by

$$\langle e'_1(\mathbf{m}, \mathbf{s}, \mathbf{j}), (\delta \mathbf{m}, \delta \mathbf{s}, \delta \mathbf{j}) \rangle = \langle \partial_{\mathbf{m}} e_1(\mathbf{m}, \mathbf{s}, \mathbf{j}), \delta \mathbf{m} \rangle + \langle \partial_{\mathbf{s}} e_1(\mathbf{m}, \mathbf{s}, \mathbf{j}), \delta \mathbf{s} \rangle + \langle \partial_{\mathbf{j}} e_1(\mathbf{m}, \mathbf{s}, \mathbf{j}), \delta \mathbf{j} \rangle. \tag{4.12}$$

Thus, e_1 is Gâteaux differentiable. Moreover, since e'_1 is continuous at $(\mathbf{m}, \mathbf{s}, \mathbf{j})$, the function e_1 is continuously Fréchet differentiable and the Fréchet derivative is given by (4.12).

For the function e_2 , we have

$$\begin{aligned} \langle \partial_{\mathbf{m}} e_2(\mathbf{m}, \mathbf{s}, \mathbf{j}), \delta \mathbf{m} \rangle &= \nabla \left(\delta \mathbf{m} \mathbf{j} + D_0 \beta [\delta \mathbf{m} \langle \nabla \mathbf{s}, \mathbf{m} \rangle + \mathbf{m} \langle \nabla \mathbf{s}, \delta \mathbf{m} \rangle] \right) + D_0 \mathbf{s} \times \delta \mathbf{m} \\ &= \mathbf{j} \nabla \delta \mathbf{m} + \delta \mathbf{m} \nabla \mathbf{j} + (\nabla D_0) \beta (\delta \mathbf{m} \langle \nabla \mathbf{s}, \mathbf{m} \rangle + \mathbf{m} \langle \nabla \mathbf{s}, \delta \mathbf{m} \rangle) \\ &\quad + D_0 \beta (\nabla \delta \mathbf{m} \langle \nabla \mathbf{s}, \mathbf{m} \rangle + \delta \mathbf{m} \langle \Delta \mathbf{s}, \mathbf{m} \rangle + \delta \mathbf{m} \langle \nabla \mathbf{s}, \nabla \mathbf{m} \rangle) \\ &\quad + \nabla \mathbf{m} \langle \nabla \mathbf{s}, \delta \mathbf{m} \rangle + \mathbf{m} \langle \Delta \mathbf{s}, \delta \mathbf{m} \rangle + \mathbf{m} \langle \nabla \mathbf{s}, \nabla \delta \mathbf{m} \rangle, \\ \langle \partial_{\mathbf{s}} e_2(\mathbf{m}, \mathbf{s}, \mathbf{j}), \delta \mathbf{s} \rangle &= \partial_t \delta \mathbf{s} + \nabla \left(-D_0 \nabla \delta \mathbf{s} + \beta D_0 \mathbf{m} \langle \nabla \delta \mathbf{s}, \mathbf{m} \rangle \right) + D_0 \delta \mathbf{s} + D_0 \delta \mathbf{s} \times \mathbf{m} \\ &= \partial_t \delta \mathbf{s} - (\nabla D_0 \nabla \delta \mathbf{s} + D_0 \Delta \delta \mathbf{s}) + \beta (\nabla D_0) \mathbf{m} \langle \nabla \delta \mathbf{s}, \mathbf{m} \rangle \\ &\quad + \beta D_0 \nabla \mathbf{m} \langle \nabla \delta \mathbf{s}, \mathbf{m} \rangle + \beta D_0 \mathbf{m} \langle \Delta \delta \mathbf{s}, \mathbf{m} \rangle + \beta D_0 \mathbf{m} \langle \nabla \delta \mathbf{s}, \nabla \mathbf{m} \rangle \\ &\quad + D_0 \delta \mathbf{s} + D_0 \delta \mathbf{s} \times \mathbf{m}, \\ \langle \partial_{\mathbf{j}} e_2(\mathbf{m}, \mathbf{s}, \mathbf{j}), \delta \mathbf{j} \rangle &= \nabla(\mathbf{m} \delta \mathbf{j}) = \nabla \mathbf{m} \delta \mathbf{j} + \mathbf{m} \nabla \delta \mathbf{j}. \end{aligned}$$

Moreover, we have the following bounds:

$$\begin{aligned}
 & \| \langle \partial_{\mathbf{m}} e_2(\mathbf{m}, \mathbf{s}, j), \delta \mathbf{m} \rangle \|_{L^2(\mathbb{L}^2(\tilde{D}))} \\
 & \leq \| \nabla \delta \mathbf{m} \|_{L^\infty(\mathbb{L}^2)} \| j \|_{L^2(\mathbb{L}^\infty(\tilde{D}))} + \| \delta \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} \| \nabla j \|_{L^2(\mathbb{L}^2(\tilde{D}))} \\
 & \quad + C(D^*, \beta) \left(\| \delta \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} \| \nabla \mathbf{s} \|_{L^2(\mathbb{L}^2(\tilde{D}))} \| \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} + \| \nabla \delta \mathbf{s} \|_{L^\infty(\mathbb{L}^2)} \| \nabla \mathbf{s} \|_{L^2(\mathbb{L}^\infty(\tilde{D}))} \| \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} \right. \\
 & \quad \left. + \| \delta \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} \| \Delta \mathbf{s} \|_{L^2(\mathbb{L}^2(\tilde{D}))} \| \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} + \| \delta \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} \| \nabla \mathbf{s} \|_{L^\infty(\mathbb{L}^2(\tilde{D}))} \| \mathbf{m} \|_{L^\infty(\mathbb{L}^2)} \right) \\
 & \leq C(\mathbf{m}, \mathbf{s}, j) \| \delta \mathbf{m} \|_{\mathcal{M}}, \\
 & \| \langle \partial_{\mathbf{s}} e_2(\mathbf{m}, \mathbf{s}, j), \delta \mathbf{s} \rangle \|_{L^2(\mathbb{L}^2(\tilde{D}))} \\
 & \leq \| \partial_t \delta \mathbf{s} \|_{L^2(\mathbb{L}^2(\tilde{D}))} + C(D^*, \beta) \left(\| \nabla \delta \mathbf{s} \|_{L^2(\mathbb{L}^2(\tilde{D}))} + \| \Delta \delta \mathbf{s} \|_{L^2(\mathbb{L}^2(\tilde{D}))} + \| \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)}^2 \| \nabla \delta \mathbf{s} \|_{L^2(\mathbb{L}^2(\tilde{D}))} \right. \\
 & \quad \left. + \| \nabla \mathbf{m} \|_{L^2(\mathbb{L}^\infty)} \| \nabla \delta \mathbf{s} \|_{L^\infty(\mathbb{L}^2(\tilde{D}))} \| \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} + \| \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)}^2 \| \Delta \delta \mathbf{s} \|_{L^2(\mathbb{L}^2(\tilde{D}))} \right. \\
 & \quad \left. + \| \delta \mathbf{s} \|_{L^2(\mathbb{L}^2(\tilde{D}))} + \| \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} \| \delta \mathbf{s} \|_{L^2(\mathbb{L}^2(\tilde{D}))} \right), \\
 & \| \langle \partial_j e_2(\mathbf{m}, \mathbf{s}, j), \delta j \rangle \|_{L^2(\mathbb{L}^2(\tilde{D}))} \\
 & \leq \| \mathbf{m} \|_{L^\infty(\mathbb{L}^\infty)} \| \nabla \delta j \|_{L^2(\mathbb{L}^2(\tilde{D}))} + \| \nabla \mathbf{m} \|_{L^\infty(\mathbb{L}^2)} \| \delta j \|_{L^2(\mathbb{L}^\infty(\tilde{D}))} \\
 & \leq C(\mathbf{m}, \mathbf{s}, j) \| \delta j \|_{\mathcal{J}}.
 \end{aligned}$$

Define the operator $e'_2(\mathbf{m}, \mathbf{s}, j) \in \mathcal{L}(\mathcal{M} \times \mathcal{S} \times \mathcal{J}; L^2(\mathbb{L}^2(\tilde{D})))$ by

$$\begin{aligned}
 \langle e'_2(\mathbf{m}, \mathbf{s}, j), (\delta \mathbf{m}, \delta \mathbf{s}, \delta j) \rangle &= \langle \partial_{\mathbf{m}} e_2(\mathbf{m}, \mathbf{s}, j), \delta \mathbf{m} \rangle + \langle \partial_{\mathbf{s}} e_2(\mathbf{m}, \mathbf{s}, j), \delta \mathbf{s} \rangle \\
 & \quad + \langle \partial_j e_2(\mathbf{m}, \mathbf{s}, j), \delta j \rangle. \tag{4.13}
 \end{aligned}$$

Thus, e_2 is Gâteaux differentiable. Moreover, since e'_2 is continuous at $(\mathbf{m}, \mathbf{s}, j)$, the function e_2 is continuously Fréchet differentiable and the Fréchet derivative is given by (4.13).

Similarly, we can show that e_3 and e_4 are continuously Fréchet differentiable, and their Fréchet derivatives are given by

$$\langle e'_3(\mathbf{m}, \mathbf{s}, j), (\delta \mathbf{m}, \delta \mathbf{s}, \delta j) \rangle = \delta \mathbf{m}(0) \quad \text{and} \quad \langle e'_4(\mathbf{m}, \mathbf{s}, j), (\delta \mathbf{m}, \delta \mathbf{s}, \delta j) \rangle = \delta \mathbf{s}(0).$$

Thus the function Γ is continuously Fréchet differentiable. This completes the proof. □

To apply the Lagrange multiplier theorem, one needs to check that a minimizer is a regular point of Γ defined in (4.11). We recall that a point $(\mathbf{m}^*, \mathbf{s}^*, j^*)$ is said to be a regular point of Γ if $e'_1(\mathbf{m}^*, \mathbf{s}^*, j^*), e'_2(\mathbf{m}^*, \mathbf{s}^*, j^*), e'_3(\mathbf{m}^*, \mathbf{s}^*, j^*), e'_4(\mathbf{m}^*, \mathbf{s}^*, j^*)$ are linearly independent. We have the following lemma.

Lemma 4.4 *Under the assumptions $D_0 \in H^2(\tilde{D})$ and $D_* > 2\beta D^*$, if $(\mathbf{m}^*, \mathbf{s}^*, j^*)$ is an optimal solution of Problem 4.1, then it is a regular point of Γ .*

Proof To show that $(\mathbf{m}^*, \mathbf{s}^*, j^*)$ is a regular point of Γ , it suffices to show that

$$(\mathbf{m}, \mathbf{s}, \mathbf{0}) \mapsto \langle \Gamma'(\mathbf{m}^*, \mathbf{s}^*, j^*), (\mathbf{m}, \mathbf{s}, \mathbf{0}) \rangle$$

is surjective. Let $(\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3, \mathbf{f}_4) \in L^2(\mathbb{L}^2) \times L^2(\mathbb{L}^2(\tilde{D})) \times \mathbb{H}^1 \times \mathbb{H}^1(\tilde{D})$ be given. Then we need to show the existence of $(\mathbf{m}, \mathbf{s}) \in \mathcal{M} \times \mathcal{S}$ such that

$$\begin{cases} \partial_t \mathbf{m} - \alpha_1 \Delta \mathbf{m} - \alpha_1 (2\langle \nabla \mathbf{m}^*, \nabla \mathbf{m} \rangle \mathbf{m}^* + |\nabla \mathbf{m}^*|^2 \mathbf{m}) - \alpha_1 (\mathbf{s} - \mathbf{m}^* \langle \mathbf{m}^*, \mathbf{s} \rangle) \\ \quad + \alpha_2 (\mathbf{m}^* \times \Delta \mathbf{m} + \mathbf{m} \times \Delta \mathbf{m}^* + \mathbf{m} \times \mathbf{s}^* + \mathbf{m}^* \times \mathbf{s}) + \alpha_1 (\mathbf{m} \langle \mathbf{m}^*, \mathbf{s}^* \rangle + \mathbf{m}^* \langle \mathbf{m}, \mathbf{s}^* \rangle) = \mathbf{f}_1, \\ \mathbf{m}(0) = \mathbf{f}_3, \end{cases} \tag{4.14}$$

and

$$\begin{cases} \partial_t \mathbf{s} + \nabla \left\{ \mathbf{m} \mathbf{j}^* - D_0 \nabla \mathbf{s} + D_0 \beta [\mathbf{m} \langle \nabla \mathbf{s}^*, \mathbf{m}^* \rangle + \mathbf{m}^* \langle \nabla \mathbf{s}^*, \mathbf{m} \rangle + \mathbf{m}^* \langle \nabla \mathbf{s}, \mathbf{m}^* \rangle] \right\} \\ \quad + D_0 (\mathbf{s} + \mathbf{s} \times \mathbf{m}^* + \mathbf{s}^* \times \mathbf{m}) = \mathbf{f}_2, \\ \mathbf{s}(0) = \mathbf{f}_4 \end{cases} \tag{4.15}$$

hold. We use several steps to solve the above coupled equations.

Step I (Discretization and projection in time): We use semi discretization in time with the semi-implicit Euler method. For some $N \in \mathbb{N}^* = \{1, 2, 3, \dots\}$, let

$$t_i = ik, \quad i = 0, \dots, N, \quad k = \frac{T}{N} \tag{4.16}$$

be a uniform partition of $[0, T]$. Since $\mathbf{m}^* \in C(\mathbb{H}^2)$ and $\mathbf{s}^* \in C(\mathbb{H}^2(\tilde{D}))$, see Lemma 4.2, the evaluation of these functions at t_i makes sense. Moreover,

$$\|\mathbf{m}_i^*\|_{\mathbb{W}^{1,\infty}} \leq \|\mathbf{m}_i^*\|_{\mathbb{H}^2} \leq C \quad \text{and} \quad \|\mathbf{s}_i^*\|_{\mathbb{W}^{1,\infty}(\tilde{D})} \leq \|\mathbf{s}_i^*\|_{\mathbb{H}^2(\tilde{D})} \leq C \quad \forall i = 0, \dots, N. \tag{4.17}$$

For \mathbf{f}_1 and \mathbf{f}_2 , this is not the case. Therefore, we define a projection operator in time. To this end, let X be a Hilbert space with inner product $(\cdot, \cdot)_X$. For each time step k , we define the set

$$\mathcal{P}_k := \left\{ \boldsymbol{\phi}_k : (0, T) \rightarrow X : \boldsymbol{\phi}_k|_{(t_j, t_{j+1})} \text{ is a constant in } X \right\}.$$

For any $f \in L^2(0, T; X)$, we define the projection $\Pi_k f \in \mathcal{P}_k$ via

$$\int_0^T (\Pi_k f - f, \boldsymbol{\phi}_k)_X dt = 0 \quad \forall \boldsymbol{\phi}_k \in \mathcal{P}_k. \tag{4.18}$$

Existence of such projection Π_k follows from the Lax–Milgram lemma. In view of the Cauchy–Schwarz inequality and (4.18) we see that

$$\|\Pi_k f\|_{L^2(0,T;X)}^2 = \int_0^T \|\Pi_k f\|_X^2 dt = \int_0^T (f, \Pi_k f)_X dt \leq \|f\|_{L^2(0,T;X)} \|\Pi_k f\|_{L^2(0,T;X)},$$

and therefore we obtain

$$\|\Pi_k f\|_{L^2(0,T;X)} \leq \|f\|_{L^2(0,T;X)}, \tag{4.19}$$

for all $f \in L^2(0, T; X)$.

For any $p_k \in \mathcal{P}_k$, we take $\boldsymbol{\phi}_k = \Pi_k f - f + f - p_k \in \mathcal{P}_k$ in (4.18) and use the Cauchy–Schwarz inequality to get

$$\|\Pi_k f - f\|_{L^2(0,T;X)} \leq \|f - p_k\|_{L^2(0,T;X)}.$$

Since $p_k \in \mathcal{P}_k$ is arbitrary and $\cup_{k>0} \mathcal{P}_k$ is dense in $L^2(0, T; X)$, we get from above that

$$\Pi_k f \rightarrow f \quad \text{in } L^2(0, T; X). \tag{4.20}$$

Let $\Pi_{1,k}$, $\Pi_{2,k}$, and $\Pi_{3,k}$ denote the projections associated with $X = \mathbb{L}^2$, $X = \mathbb{L}^2(\tilde{D})$, and $X = H^2(\tilde{D})$ respectively. In the following, we denote

$$\mathbf{m}_i^* = \mathbf{m}^*(t_i), \quad \mathbf{s}_i^* = \mathbf{s}^*(t_i), \quad \mathbf{f}_1^i = \Pi_{1,k}\mathbf{f}_1(t_i), \quad \mathbf{f}_2^i = \Pi_{2,k}\mathbf{f}_2(t_i), \quad \text{and} \quad \mathbf{j}_i^* = \Pi_{3,k}\mathbf{j}^*(t_i).$$

By using (4.19), we have

$$\begin{aligned} k \sum_{i=0}^{j-1} \|\mathbf{f}_1^{i+1}\|_{\mathbb{L}^2}^2 &\leq \|\Pi_{1,k}\mathbf{f}_1\|_{L^2(\mathbb{L}^2)}^2 \leq \|\mathbf{f}_1\|_{L^2(\mathbb{L}^2)}^2 \leq C, \\ k \sum_{i=0}^{j-1} \|\mathbf{f}_2^{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 &\leq \|\Pi_{2,k}\mathbf{f}_2\|_{L^2(\mathbb{L}^2(\tilde{D}))}^2 \leq \|\mathbf{f}_2\|_{L^2(\mathbb{L}^2(\tilde{D}))}^2 \leq C, \\ k \sum_{i=0}^{j-1} \|\mathbf{j}_{i+1}^*\|_{L^2(\tilde{D})}^2 &\leq \|\Pi_{3,k}\mathbf{j}^*\|_{L^2(L^2(\tilde{D}))}^2 \leq \|\mathbf{j}^*\|_{L^2(L^2(\tilde{D}))}^2 \leq C. \end{aligned} \tag{4.21}$$

Step II (Semi-discrete scheme and its solvability): We consider the following semi-discrete scheme for problems (4.14) and (4.15). Starting with $\mathbf{m}_0 = \mathbf{f}_3$ and $\mathbf{s}_0 = \mathbf{f}_4$, for $0 \leq i \leq N - 1$,

(i) compute $\mathbf{m}_{i+1} \in \mathbb{H}^1$ such that

$$\begin{aligned} &\left(\frac{1}{k}\mathbf{m}_{i+1}, \phi\right)_{\mathbb{L}^2} + \alpha_1(\nabla\mathbf{m}_{i+1}, \nabla\phi)_{\mathbb{L}^2} - \alpha_1(|\nabla\mathbf{m}_i^*|^2\mathbf{m}_{i+1}, \phi)_{\mathbb{L}^2} - \alpha_2(\nabla\mathbf{m}_{i+1}, \nabla\phi \times \mathbf{m}_{i+1}^*)_{\mathbb{L}^2} \\ &\quad - \alpha_2(\nabla\mathbf{m}_{i+1}, \phi \times \nabla\mathbf{m}_{i+1}^*)_{\mathbb{L}^2} + \alpha_2(\mathbf{m}_{i+1} \times (\Delta\mathbf{m}_{i+1}^* + \mathbf{s}_{i+1}^*), \phi)_{\mathbb{L}^2} \\ &= \left(\frac{1}{k}\mathbf{m}_i + \mathbf{f}_1^i + \alpha_1(\mathbf{s}_i - \mathbf{m}_{i+1}^*(\mathbf{m}_{i+1}^*, \mathbf{s}_i) - \mathbf{m}_i(\mathbf{m}_{i+1}^*, \mathbf{s}_{i+1}^*) - \mathbf{m}_{i+1}^*(\mathbf{m}_i, \mathbf{s}_{i+1}^*))\right. \\ &\quad \left. - \alpha_2\mathbf{m}_{i+1}^* \times \mathbf{s}_i + 2\alpha_1\langle \nabla\mathbf{m}_i^*, \nabla\mathbf{m}_i \rangle \mathbf{m}_{i+1}^*, \phi\right)_{\mathbb{L}^2} \quad \forall \phi \in \mathbb{H}^1, \end{aligned} \tag{4.22}$$

(ii) compute $\mathbf{s}_{i+1} \in \mathbb{H}^1(\tilde{D})$ such that

$$\begin{aligned} &\left(\frac{1}{k}\mathbf{s}_{i+1}, \psi\right)_{\mathbb{L}^2(\tilde{D})} + (D_0\nabla\mathbf{s}_{i+1}, \nabla\psi)_{\mathbb{L}^2(\tilde{D})} + (D_0\mathbf{s}_{i+1}, \psi)_{\mathbb{L}^2(\tilde{D})} + (D_0\mathbf{s}_{i+1} \times \mathbf{m}_{i+1}^*, \psi)_{\mathbb{L}^2} \\ &\quad - \beta(D_0\mathbf{m}_{i+1}^*\langle \nabla\mathbf{s}_{i+1}, \mathbf{m}_{i+1}^* \rangle, \nabla\psi)_{\mathbb{L}^2(\tilde{D})} \\ &= \left(\beta D_0[\mathbf{m}_{i+1}\langle \nabla\mathbf{s}_{i+1}^*, \mathbf{m}_{i+1}^* \rangle + \mathbf{m}_{i+1}^*\langle \nabla\mathbf{s}_{i+1}^*, \mathbf{m}_{i+1} \rangle] + \mathbf{m}_{i+1}\mathbf{j}_{i+1}^*, \nabla\psi\right)_{\mathbb{L}^2(\tilde{D})} \\ &\quad + \left(\frac{1}{k}\mathbf{s}_i - \mathbf{s}_{i+1}^* \times \mathbf{m}_{i+1}, \psi\right)_{\mathbb{L}^2(\tilde{D})} + (\mathbf{f}_2^{i+1}, \psi)_{\mathbb{L}^2(\tilde{D})} \quad \forall \psi \in \mathbb{H}^1(\tilde{D}). \end{aligned} \tag{4.23}$$

Existence of \mathbf{m}_{i+1} in step (i) given the existence of $\mathbf{m}_i \in \mathbb{H}^1$: Define a bilinear form

$\mathcal{A} : \mathbb{H}^1 \times \mathbb{H}^1 \rightarrow \mathbb{R}$ as

$$\begin{aligned} \mathcal{A}(\varphi, \phi) &= \left(\frac{1}{k}\varphi, \phi\right)_{\mathbb{L}^2} + \alpha_1(\nabla\varphi, \nabla\phi)_{\mathbb{L}^2} - \alpha_1(|\nabla\mathbf{m}_i^*|^2\varphi, \phi)_{\mathbb{L}^2} - \alpha_2(\nabla\varphi, \nabla\phi \times \mathbf{m}_{i+1}^*)_{\mathbb{L}^2} \\ &\quad - \alpha_2(\nabla\varphi, \phi \times \nabla\mathbf{m}_{i+1}^*)_{\mathbb{L}^2} + \alpha_2(\varphi \times (\Delta\mathbf{m}_{i+1}^* + \mathbf{s}_{i+1}^*), \phi)_{\mathbb{L}^2}. \end{aligned}$$

One can use (4.17) to show that $|\mathcal{A}(\phi, \phi)| \leq C(k, \alpha) \|\phi\|_{\mathbb{H}^1} \|\phi\|_{\mathbb{H}^1}$. Moreover, \mathcal{A} is \mathbb{H}^1 -coercive as

$$\begin{aligned} \mathcal{A}(\phi, \phi) &= \frac{1}{k} \|\phi\|_{\mathbb{L}^2}^2 + \alpha_1 \|\nabla \phi\|_{\mathbb{L}^2}^2 - \alpha_1 \left(|\nabla \mathbf{m}_i^*|^2 \phi, \phi \right)_{\mathbb{L}^2} - \alpha_2 \left(\nabla \phi, \phi \times \nabla \mathbf{m}_{i+1}^* \right)_{\mathbb{L}^2} \\ &\geq \left(\frac{1}{k} - \alpha_1 \|\nabla \mathbf{m}_i^*\|_{\mathbb{L}^\infty}^2 - C \|\nabla \mathbf{m}_{i+1}^*\|_{\mathbb{L}^\infty}^2 \right) \|\phi\|_{\mathbb{L}^2}^2 + \frac{\alpha_1}{2} \|\nabla \phi\|_{\mathbb{L}^2}^2 \\ &\geq \left(\frac{1}{k} - C \right) \|\phi\|_{\mathbb{L}^2}^2 + \frac{\alpha_1}{2} \|\nabla \phi\|_{\mathbb{L}^2}^2 \geq C \|\phi\|_{\mathbb{H}^1}^2, \end{aligned}$$

for k is sufficiently small which can be chosen to be independent of the iteration step. Here, in the last step we used again (4.17). Let

$$\begin{aligned} \ell(\phi) &:= \left(\frac{1}{k} \mathbf{m}_i + \mathbf{f}_1 + \alpha_1 (\mathbf{s}_i - \mathbf{m}_{i+1}^* \langle \mathbf{m}_{i+1}^*, \mathbf{s}_i \rangle) - \mathbf{m}_i \langle \mathbf{m}_{i+1}^*, \mathbf{s}_{i+1}^* \rangle - \mathbf{m}_{i+1}^* \langle \mathbf{m}_i, \mathbf{s}_{i+1}^* \rangle \right) \\ &\quad - \alpha_2 \mathbf{m}_{i+1}^* \times \mathbf{s}_i + 2\alpha_1 \langle \nabla \mathbf{m}_i^*, \nabla \mathbf{m}_i \rangle \mathbf{m}_{i+1}^*, \phi \Big)_{\mathbb{L}^2}. \end{aligned}$$

Then it is linear and bounded, since

$$\begin{aligned} |\ell(\phi)| &\leq \left(\frac{1}{k} \|\mathbf{m}_i\|_{\mathbb{L}^2} + \|\mathbf{f}_1\|_{\mathbb{L}^2} + C(\alpha) \left\{ \|\mathbf{s}_i\|_{\mathbb{L}^2(\tilde{D})} + \|\mathbf{s}_i\|_{\mathbb{L}^2(\tilde{D})} + \|\mathbf{m}_{i+1}^*\|_{\mathbb{L}^\infty} \|\mathbf{m}_i\|_{\mathbb{L}^2} \|\mathbf{s}_{i+1}^*\|_{\mathbb{L}^\infty(\tilde{D})} \right. \right. \\ &\quad \left. \left. + \|\mathbf{m}_{i+1}^*\|_{\mathbb{L}^\infty} \|\mathbf{s}_i\|_{\mathbb{L}^2(\tilde{D})} + \|\nabla \mathbf{m}_i\|_{\mathbb{L}^2} \|\nabla \mathbf{m}_i^*\|_{\mathbb{L}^\infty} \|\mathbf{m}_{i+1}^*\|_{\mathbb{L}^\infty} \right\} \|\phi\|_{\mathbb{L}^2} \leq C(k, \alpha) \|\phi\|_{\mathbb{H}^1}. \end{aligned}$$

Thus, by Lax–Milgram lemma, there exists a unique $\mathbf{m}_{i+1} \in \mathbb{H}^1$ such that (4.22) holds.

Existence of \mathbf{s}_{i+1} in step (ii) given the existence of $\mathbf{m}_{i+1} \in \mathbb{H}^1$ and $\mathbf{s}_i \in \mathbb{H}^1(\tilde{D})$: The same argument was done in step (i) can be used to obtain the existence of \mathbf{s}_{i+1} . The corresponding bilinear form to (4.23) is $\mathcal{B} : \mathbb{H}^1(\tilde{D}) \times \mathbb{H}^1(\tilde{D}) \rightarrow \mathbb{R}$ be the bilinear form defined by

$$\begin{aligned} \mathcal{B}(\varphi, \psi) &:= \left(\frac{1}{k} \varphi, \psi \right)_{\mathbb{L}^2(\tilde{D})} + \left(D_0 \nabla \varphi, \nabla \psi \right)_{\mathbb{L}^2(\tilde{D})} + \left(D_0 \varphi, \psi \right)_{\mathbb{L}^2(\tilde{D})} \\ &\quad - \beta \left(D_0 \mathbf{m}_{i+1}^* \langle \nabla \varphi, \mathbf{m}_{i+1}^* \rangle, \nabla \psi \right)_{\mathbb{L}^2(\tilde{D})} + \left(D_0 \varphi \times \mathbf{m}_{i+1}^*, \psi \right)_{\mathbb{L}^2(\tilde{D})}. \end{aligned}$$

We omit the details.

Step III (A priori estimates): Let $0 \leq i \leq N - 1$. We choose $\phi = \mathbf{m}_{i+1}$ and use the algebraic identity

$$\langle \mathbf{a}, \mathbf{a} - \mathbf{b} \rangle = \frac{1}{2} (|\mathbf{a}|^2 - |\mathbf{b}|^2 + |\mathbf{a} - \mathbf{b}|^2) \quad \forall \mathbf{a}, \mathbf{b} \in \mathbb{R}^3, \tag{4.24}$$

to get, after rearranging the terms,

$$\begin{aligned} &\frac{1}{2k} \left(\|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 - \|\mathbf{m}_i\|_{\mathbb{L}^2}^2 + \|\mathbf{m}_{i+1} - \mathbf{m}_i\|_{\mathbb{L}^2}^2 \right) + \alpha_1 \|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \\ &= \alpha_1 \left(|\nabla \mathbf{m}_i^*|^2 \mathbf{m}_{i+1}, \mathbf{m}_{i+1} \right)_{\mathbb{L}^2} + \alpha_2 \left(\nabla \mathbf{m}_{i+1}, \mathbf{m}_{i+1} \times \nabla \mathbf{m}_{i+1}^* \right)_{\mathbb{L}^2} \\ &\quad + \left(\mathbf{f}_1 + \alpha_1 (\mathbf{s}_i - \mathbf{m}_{i+1}^* \langle \mathbf{m}_{i+1}^*, \mathbf{s}_i \rangle) - \alpha_2 \mathbf{m}_{i+1}^* \times \mathbf{s}_i, \mathbf{m}_{i+1} \right)_{\mathbb{L}^2} \\ &\quad - \alpha_1 \left(\mathbf{m}_i \langle \mathbf{m}_{i+1}^*, \mathbf{s}_{i+1}^* \rangle + \mathbf{m}_{i+1}^* \langle \mathbf{m}_i, \mathbf{s}_{i+1}^* \rangle, \mathbf{m}_{i+1} \right)_{\mathbb{L}^2} + 2\alpha_1 \left(\langle \nabla \mathbf{m}_i^*, \nabla \mathbf{m}_i \rangle \mathbf{m}_{i+1}^*, \mathbf{m}_{i+1} \right)_{\mathbb{L}^2} \\ &= \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3 + \mathcal{I}_4 + \mathcal{I}_5. \end{aligned} \tag{4.25}$$

By using Young’s inequality and (4.17), we obtain, for any $\theta_1, \theta_2 > 0$,

$$\begin{aligned} |\mathcal{I}_1| &\leq \alpha_1 \|\nabla \mathbf{m}_i^*\|_{\mathbb{L}^\infty}^2 \|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \leq C \|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2, \\ |\mathcal{I}_2| &\leq \theta_1 \|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + C(\theta_1) \|\nabla \mathbf{m}_{i+1}^*\|_{\mathbb{L}^\infty}^2 \|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \leq \theta_1 \|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + C(\theta_1) \|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2, \\ |\mathcal{I}_3| &\leq C \left(\|\mathbf{f}_1^{i+1}\|_{\mathbb{L}^2}^2 + \|\mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2 + \|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \right), \\ |\mathcal{I}_4| &\leq C \left(\|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + \|\mathbf{m}_i\|_{\mathbb{L}^2}^2 \|\mathbf{s}_{i+1}^*\|_{\mathbb{L}^\infty(\bar{D})}^2 \right) \leq C \left(\|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + \|\mathbf{m}_i\|_{\mathbb{L}^2}^2 \right), \\ |\mathcal{I}_5| &\leq \theta_2 \|\nabla \mathbf{m}_i\|_{\mathbb{L}^2}^2 + C(\theta_2) \|\nabla \mathbf{m}_i^*\|_{\mathbb{L}^\infty}^2 \|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \\ &= \theta_2 \|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + \theta_2 \left(\|\nabla \mathbf{m}_i\|_{\mathbb{L}^2}^2 - \|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \right) + C(\theta_2) \|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2. \end{aligned}$$

Inserting these estimates into (4.25), multiplying the resulting equation by $2k$, and rearranging the terms, we deduce

$$\begin{aligned} \|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 - \|\mathbf{m}_i\|_{\mathbb{L}^2}^2 + \|\mathbf{m}_{i+1} - \mathbf{m}_i\|_{\mathbb{L}^2}^2 + 2k(\alpha_1 - \theta_1 - \theta_2) \|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \\ \leq Ck \left(\|\mathbf{f}_1^{i+1}\|_{\mathbb{L}^2}^2 + \|\mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2 \right) + Ck \left(\|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + \|\mathbf{m}_i\|_{\mathbb{L}^2}^2 \right) \\ + Ck \left(\|\nabla \mathbf{m}_i\|_{\mathbb{L}^2}^2 - \|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \right). \end{aligned}$$

The constant C may depend on $\alpha_1, \alpha_2, \theta_1, \theta_2, \|\mathbf{m}^*\|_{C(\mathbb{H}^2)}$, and $\|\mathbf{s}^*\|_{C(\mathbb{H}^2(\bar{D}))}$ (which in turn depend on $\|\mathbf{m}_0\|_{\mathbb{H}^2}$ and $\|\mathbf{s}_0\|_{\mathbb{H}^2(\bar{D})}$) but is independent of k . By choosing $\theta_1, \theta_2 > 0$ satisfying $\theta_1 + \theta_2 < \alpha_1$ and summing over $i = 0, \dots, j - 1$ for $j \in \{1, \dots, N\}$ we deduce

$$\begin{aligned} \|\mathbf{m}_j\|_{\mathbb{L}^2}^2 + \sum_{i=0}^{j-1} \|\mathbf{m}_{i+1} - \mathbf{m}_i\|_{\mathbb{L}^2}^2 + k \sum_{i=0}^{j-1} \|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \\ \leq C \|\mathbf{m}_0\|_{\mathbb{H}^1}^2 + Ck \sum_{i=0}^{j-1} \|\mathbf{f}_1^{i+1}\|_{\mathbb{L}^2}^2 + Ck \sum_{i=0}^{j-1} \|\mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2 + Ck \sum_{i=0}^j \|\mathbf{m}_i\|_{\mathbb{L}^2}^2, \\ \leq C \left(1 + k \sum_{i=0}^{j-1} \|\mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2 \right) + Ck \sum_{i=0}^j \|\mathbf{m}_i\|_{\mathbb{L}^2}^2, \end{aligned}$$

where in the last step we used (4.21). Applying the discrete Gronwall Lemma, we obtain

$$\|\mathbf{m}_j\|_{\mathbb{L}^2}^2 + \sum_{i=0}^{j-1} \|\mathbf{m}_{i+1} - \mathbf{m}_i\|_{\mathbb{L}^2}^2 + k \sum_{i=0}^{j-1} \|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \leq C \left(1 + k \sum_{i=0}^{j-1} \|\mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2 \right), \tag{4.26}$$

where $C > 0$ is a constant independent of the time step size k .

For higher order bound, formally we choose $\phi = -\Delta \mathbf{m}_{i+1}$ in (4.22), and use integration by parts along with (4.24) to obtain

$$\begin{aligned} \frac{1}{2k} \left(\|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 - \|\nabla \mathbf{m}_i\|_{\mathbb{L}^2}^2 + \|\nabla \mathbf{m}_{i+1} - \nabla \mathbf{m}_i\|_{\mathbb{L}^2}^2 \right) + \alpha_1 \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \\ = -\alpha_1 \left(|\nabla \mathbf{m}_i^*|^2 \mathbf{m}_{i+1}, \Delta \mathbf{m}_{i+1} \right)_{\mathbb{L}^2} + \alpha_2 \left(\mathbf{m}_{i+1} \times (\Delta \mathbf{m}_{i+1}^* + \mathbf{s}_{i+1}^*), \Delta \mathbf{m}_{i+1} \right)_{\mathbb{L}^2} \\ + \left(\alpha_2 \mathbf{m}_{i+1}^* \times \mathbf{s}_i - \alpha_1 (\mathbf{s}_i - \mathbf{m}_{i+1}^* (\mathbf{m}_{i+1}^*, \mathbf{s}_i)) - \mathbf{f}_1^{i+1}, \Delta \mathbf{m}_{i+1} \right)_{\mathbb{L}^2} \\ + \alpha_1 \left(\mathbf{m}_i (\mathbf{m}_{i+1}^*, \mathbf{s}_{i+1}^*) + \mathbf{m}_{i+1}^* (\mathbf{m}_i, \mathbf{s}_{i+1}^*), \Delta \mathbf{m}_{i+1} \right)_{\mathbb{L}^2} - 2\alpha_1 \left(\langle \nabla \mathbf{m}_i^*, \nabla \mathbf{m}_i \rangle \mathbf{m}_{i+1}^*, \Delta \mathbf{m}_{i+1} \right)_{\mathbb{L}^2} \\ = \mathcal{I}_6 + \mathcal{I}_7 + \mathcal{I}_8 + \mathcal{I}_9 + \mathcal{I}_{10}. \end{aligned} \tag{4.27}$$

Similarly to the above estimate, by using Young’s inequality and (4.17), we have, for any $\theta_1, \dots, \theta_5 > 0$,

$$\begin{aligned} |\mathcal{I}_6| &\leq \alpha_1 \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2} \|\nabla \mathbf{m}_i^*\|_{\mathbb{L}^\infty}^2 \|\mathbf{m}_{i+1}\|_{\mathbb{L}^2} \leq \theta_1 \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + C(\theta_1) \|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2, \\ |\mathcal{I}_7| &\leq \alpha_2 \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2} \|\mathbf{m}_{i+1}\|_{\mathbb{L}^\infty} (\|\Delta \mathbf{m}_{i+1}^*\|_{\mathbb{L}^2} + \|\mathbf{s}_{i+1}^*\|_{\mathbb{L}^2(\bar{D})}) \\ &\leq \theta_2 \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + C(\theta_2) \|\mathbf{m}_{i+1}\|_{\mathbb{H}^1}^2, \\ |\mathcal{I}_8| &\leq \theta_3 \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + C(\theta_3) (\|\mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2 + \|\mathbf{f}_1^{i+1}\|_{\mathbb{L}^2}^2) \leq \theta_3 \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + C(\theta_3) \left(1 + \|\mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2\right), \\ |\mathcal{I}_9| &\leq C \|\mathbf{s}_{i+1}^*\|_{\mathbb{L}^\infty(\bar{D})} \|\mathbf{m}_i\|_{\mathbb{L}^2} \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2} \leq \theta_4 \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + C(\theta_4) \|\mathbf{m}_i\|_{\mathbb{L}^2}^2, \\ |\mathcal{I}_{10}| &\leq \theta_5 \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + C(\theta_5) \|\nabla \mathbf{m}_i^*\|_{\mathbb{L}^\infty}^2 \|\nabla \mathbf{m}_i\|_{\mathbb{L}^2}^2 \leq \theta_5 \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + C(\theta_5) \|\nabla \mathbf{m}_i\|_{\mathbb{L}^2}^2, \end{aligned}$$

where all the constants may also depend on $\alpha_1, \alpha_2, \mathbf{m}^*, \mathbf{s}^*$, and \mathbf{f}_1 . Inserting all the above estimates into (4.27) and choosing $\theta_1, \dots, \theta_5 > 0$ such that $\sum_{i=1}^5 \theta_i < \alpha_1$, we have (after multiplying by $2k$)

$$\begin{aligned} \|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 - \|\nabla \mathbf{m}_i\|_{\mathbb{L}^2}^2 + \|\nabla \mathbf{m}_{i+1} - \nabla \mathbf{m}_i\|_{\mathbb{L}^2}^2 + k \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \\ \leq Ck(1 + \|\mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2) + Ck(\|\mathbf{m}_i\|_{\mathbb{L}^2}^2 + \|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2) + Ck(\|\nabla \mathbf{m}_i\|_{\mathbb{L}^2}^2 + \|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2) \\ \leq Ck(1 + \|\mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2) + Ck\left(1 + k \sum_{\ell=0}^i \|\mathbf{s}_\ell\|_{\mathbb{L}^2(\bar{D})}^2\right) + Ck(\|\nabla \mathbf{m}_i\|_{\mathbb{L}^2}^2 + \|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2) \end{aligned}$$

where in the last step we used (4.26). By summing over i from 0 to j for $j \in \{1, \dots, N\}$ and using (4.26) again, we deduce

$$\begin{aligned} \|\nabla \mathbf{m}_{j+1}\|_{\mathbb{L}^2}^2 - \|\nabla \mathbf{m}_0\|_{\mathbb{L}^2}^2 + \sum_{i=0}^j \|\nabla(\mathbf{m}_{i+1} - \mathbf{m}_i)\|_{\mathbb{L}^2}^2 + k \sum_{i=0}^j \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \\ \leq C\left(1 + k \sum_{i=0}^j \|\mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2\right) + C\left(1 + k^2 \sum_{i=0}^j \sum_{\ell=0}^i \|\mathbf{s}_\ell\|_{\mathbb{L}^2(\bar{D})}^2\right) + Ck \sum_{i=0}^{j+1} \|\nabla \mathbf{m}_i\|_{\mathbb{L}^2}^2 \\ \leq C\left(1 + k \sum_{i=0}^j \|\mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2\right), \end{aligned}$$

which implies

$$\begin{aligned} \|\nabla \mathbf{m}_{j+1}\|_{\mathbb{L}^2}^2 + \sum_{i=0}^j \|\nabla(\mathbf{m}_{i+1} - \mathbf{m}_i)\|_{\mathbb{L}^2}^2 + k \sum_{i=0}^j \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \tag{4.28} \\ \leq C\left(1 + k \sum_{i=1}^j \|\mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2\right), \end{aligned}$$

where the constant C depends on $\|\mathbf{m}_0\|_{\mathbb{H}^1}$, $\|\mathbf{m}^*\|_{C(\mathbb{H}^2)}$, $\|\mathbf{s}^*\|_{\mathbb{L}^2(\bar{D})}$, and T , but it is independent of k .

In order to derive the bound for \mathbf{m}_i from (4.26) and (4.28), we need to estimate $\sum_{i=1}^j \|\mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2$. Choosing $\psi = \mathbf{s}_{i+1}$ as test function in (4.23) and using the boundedness of \mathbf{m}^* , the Cauchy–Schwarz inequality, and Young’s inequality along with (2.1), we have for any $\theta > 0$

$$\begin{aligned} \frac{1}{2k} \left(\|\mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 - \|\mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2 + \|\mathbf{s}_{i+1} - \mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2 \right) + (D_* - \beta D^*) \|\nabla \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 + D_* \|\mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 \\ \leq \theta (\|\nabla \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 + \|\mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2) + C(\theta) \|\mathbf{m}_{i+1}\|_{\mathbb{L}^\infty}^2 \left\{ \|\nabla \mathbf{s}_{i+1}^*\|_{\mathbb{L}^2(\bar{D})}^2 + \|\mathbf{s}_{i+1}^*\|_{\mathbb{L}^2(\bar{D})}^2 + \|\mathbf{j}_{i+1}^*\|_{\mathbb{L}^2(\bar{D})}^2 \right\} \\ + C(\theta) \|\mathbf{f}_2^{i+1}\|_{\mathbb{L}^2(\bar{D})}^2. \end{aligned}$$

By using (4.17), we obtain after rearranging the equation

$$\begin{aligned} & \frac{1}{2k} \left(\|s_{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 - \|s_i\|_{\mathbb{L}^2(\tilde{D})}^2 + \|s_{i+1} - s_i\|_{\mathbb{L}^2(\tilde{D})}^2 \right) \\ & + (D_* - \beta D^* - \theta) \|\nabla s_{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 + (D_* - \theta) \|s_{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 \\ & \leq C(\theta) \|\mathbf{m}_{i+1}\|_{\mathbb{H}^1}^2 \left(1 + \|j_{i+1}^*\|_{L^2(\tilde{D})}^2 \right) + C(\theta) \|\mathbf{f}_2^{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2. \end{aligned}$$

By choosing θ such that $D_* - \beta D^* - \theta > 0$, using (4.26) and (4.28), and multiplying the resulting equation by $2k$, we deduce

$$\begin{aligned} & \|s_{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 - \|s_i\|_{\mathbb{L}^2(\tilde{D})}^2 + \|s_{i+1} - s_i\|_{\mathbb{L}^2(\tilde{D})}^2 + k \|s_{i+1}\|_{\mathbb{H}^1(\tilde{D})}^2 \\ & \leq Ck \left(1 + k \sum_{\ell=0}^i \|s_\ell\|_{\mathbb{L}^2(\tilde{D})}^2 \right) \left(1 + \|j_{i+1}^*\|_{L^2(\tilde{D})}^2 \right) + Ck \|\mathbf{f}_2^{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 \\ & \leq Ck \left(1 + \|j_{i+1}^*\|_{L^2(\tilde{D})}^2 \right) + Ck^2 \left(1 + \|j_{i+1}^*\|_{L^2(\tilde{D})}^2 \right) \sum_{\ell=0}^j \|s_\ell\|_{\mathbb{L}^2(\tilde{D})}^2 + Ck \|\mathbf{f}_2^{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 \end{aligned}$$

for any $j > i$. By summing over i from 0 to $j - 1$ for $j \in \{1, \dots, N\}$, we deduce

$$\begin{aligned} & \|s_j\|_{\mathbb{L}^2(\tilde{D})}^2 + \sum_{i=0}^{j-1} \|s_{i+1} - s_i\|_{\mathbb{L}^2(\tilde{D})}^2 + k \sum_{i=0}^{j-1} \|s_{i+1}\|_{\mathbb{H}^1(\tilde{D})}^2 \\ & \leq C \left(1 + k \sum_{i=0}^{j-1} \|j_{i+1}^*\|_{L^2(\tilde{D})}^2 \right) + Ck^2 \sum_{i=0}^{j-1} \left(1 + \|j_{i+1}^*\|_{L^2(\tilde{D})}^2 \right) \sum_{\ell=0}^j \|s_\ell\|_{\mathbb{L}^2(\tilde{D})}^2 \\ & + Ck \sum_{i=0}^{j-1} \|\mathbf{f}_2^{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2. \end{aligned}$$

By using (4.21), we have

$$\|s_j\|_{\mathbb{L}^2(\tilde{D})}^2 + \sum_{i=0}^{j-1} \|s_{i+1} - s_i\|_{\mathbb{L}^2(\tilde{D})}^2 + k \sum_{i=0}^{j-1} \|s_{i+1}\|_{\mathbb{H}^1(\tilde{D})}^2 \leq C + Ck \sum_{\ell=0}^j \|s_\ell\|_{\mathbb{L}^2(\tilde{D})}^2.$$

By using the discrete Gronwall lemma, we deduce

$$\|s_j\|_{\mathbb{L}^2(\tilde{D})}^2 + \sum_{i=0}^{j-1} \|s_{i+1} - s_i\|_{\mathbb{L}^2(\tilde{D})}^2 + k \sum_{i=0}^{j-1} \|s_{i+1}\|_{\mathbb{H}^1(\tilde{D})}^2 \leq C. \tag{4.29}$$

Using (4.29) in (4.26) and (4.28), we obtain

$$\max_{0 \leq i \leq N} \|\mathbf{m}_i\|_{\mathbb{H}^1}^2 + \sum_{i=0}^{N-1} \|\mathbf{m}_{i+1} - \mathbf{m}_i\|_{\mathbb{H}^1}^2 + k \sum_{i=0}^{N-1} \|\mathbf{m}_{i+1}\|_{\mathbb{H}^2}^2 \leq C, \tag{4.30}$$

where C is a constant independent of the time step size k .

Hence, by choosing $\psi = -\Delta s_{i+1}$ in (4.23) and using integration by parts along with (4.17), we have

$$\begin{aligned} & \frac{1}{2k} \left(\|\nabla s_{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 - \|\nabla s_i\|_{\mathbb{L}^2(\tilde{D})}^2 + \|\nabla(s_{i+1} - s_i)\|_{\mathbb{L}^2(\tilde{D})}^2 \right) + D_* \|\Delta s_{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 + D_* \|\nabla s_{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 \\ & \leq (\epsilon + \beta D^*) \|\Delta s_{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 + C(\epsilon, \beta, D_0) \|\mathbf{m}_{i+1}\|_{\mathbb{H}^1}^2 + C(\epsilon, \beta, D_0) \left(\|s_{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 + \|\nabla s_{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 \right) \\ & + C(\epsilon) \left(\|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \|j_{i+1}^*\|_{H^1(\tilde{D})}^2 + \|\mathbf{m}_{i+1}\|_{\mathbb{H}^1}^2 \|\nabla j_{i+1}^*\|_{L^2(\tilde{D})}^2 \right) + C(\epsilon) \|\mathbf{f}_2^{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2. \end{aligned}$$

Note, in the calculation above, we used the boundedness of D_0 ($D_0 \in H^2(\tilde{D})$) to have

$$\|\nabla D_0\|_{\mathbb{L}^\infty} \leq C. \tag{4.31}$$

By multiplying the above equation by $2k$, using (4.29) and (4.30), we deduce, after rearranging the equation and choosing ϵ such that $D_* - \epsilon - \beta D^* > 0$,

$$\begin{aligned} \|\nabla \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 - \|\nabla \mathbf{s}_i\|_{\mathbb{L}^2(\tilde{D})}^2 + \|\nabla(\mathbf{s}_{i+1} - \mathbf{s}_i)\|_{\mathbb{L}^2(\tilde{D})}^2 + k\|\Delta \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 \\ \leq Ck\left(1 + \|\mathbf{j}_{i+1}^*\|_{\mathbb{H}^1(\tilde{D})}^2 + \|\mathbf{f}_2^{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2\right) + Ck\|\nabla \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2. \end{aligned}$$

By summing over i from 0 to $j - 1$ for $j \in \{1, \dots, N\}$, using (4.21), and invoking the discrete Gronwall lemma, we deduce

$$\|\nabla \mathbf{s}_j\|_{\mathbb{L}^2(\tilde{D})}^2 + \sum_{i=0}^{j-1} \|\nabla(\mathbf{s}_{i+1} - \mathbf{s}_i)\|_{\mathbb{L}^2(\tilde{D})}^2 + k \sum_{i=0}^{j-1} \|\Delta \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\tilde{D})}^2 \leq C$$

for some constant $C > 0$ independent of k . Combining this equation with (4.29) gives

$$\max_{1 \leq j \leq N} \|\mathbf{s}_j\|_{\mathbb{H}^1(\tilde{D})}^2 + \sum_{i=0}^{N-1} \|\mathbf{s}_{i+1} - \mathbf{s}_i\|_{\mathbb{H}^1(\tilde{D})}^2 + k \sum_{i=0}^{N-1} \|\mathbf{s}_{i+1}\|_{\mathbb{H}^2(\tilde{D})}^2 \leq C. \tag{4.32}$$

Step IV (Continuation and its bound): Let $0 = t_0 < t_1 < t_2 \dots < t_N = T$ be a uniform partition of $[0, T]$ with time step size $k = T/N$ for some $N \in \mathbb{N}^*$. For any sequence $(\mathbf{x}_i)_{i=0}^N \subset \mathbb{X}$, where \mathbb{X} is a Banach space, we define the difference quotient $d_t \mathbf{x}_{i+1} = (\mathbf{x}_{i+1} - \mathbf{x}_i)/k$ for $0 \leq i \leq N - 1$. The global time interpolant $\mathbf{X}_k \in C(\mathbb{X})$ of $(\mathbf{x}_i)_{i=0}^N$ is defined via

$$\mathbf{X}_k(t) := \frac{t - t_i}{k} \mathbf{x}_{i+1} + \frac{t_{i+1} - t}{k} \mathbf{x}_i \quad \forall t \in (t_i, t_{i+1}].$$

Moreover, we define the piecewise constant interpolants (in time) \mathbf{X}_k^+ and \mathbf{X}_k^- as follows:

$$\mathbf{X}_k^+(t) := \mathbf{x}_{i+1}, \quad \mathbf{X}_k^-(t) := \mathbf{x}_i \quad \forall t \in (t_i, t_{i+1}] \tag{4.33}$$

with $\mathbf{x}_{-1} = \mathbf{x}_0$ and $\mathbf{x}_{N+1} = 0$.

We now show that the sequence $\{\partial_t \mathbf{M}_k\}$ is bounded in $L^2(\mathbb{L}^2)$. To do so, let $0 \leq i \leq N - 1$ and $t \in (t_i, t_{i+1}]$. Choosing the test function $\phi = d_t \mathbf{m}_{i+1}$ in (4.22) and using integration by parts, we obtain (recalling (4.17) again)

$$\begin{aligned} \|d_t \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + \frac{\alpha 1}{2k} \left(\|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 - \|\nabla \mathbf{m}_i\|_{\mathbb{L}^2}^2 + \|\nabla(\mathbf{m}_{i+1} - \mathbf{m}_i)\|_{\mathbb{L}^2}^2 \right) \\ \leq \frac{1}{2} \|d_t \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + C \|\mathbf{m}_{i+1}\|_{\mathbb{H}^2}^2 + C \left(\|\mathbf{f}_1^{i+1}\|_{\mathbb{L}^2}^2 + \|\mathbf{s}_i\|_{\mathbb{L}^2(\tilde{D})}^2 + \|\mathbf{m}_i\|_{\mathbb{H}^1}^2 \right). \end{aligned}$$

Hence, by using (4.28) and (4.32), as well as rearranging the equation, we have

$$\begin{aligned} \|d_t \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + \frac{1}{k} \left(\|\nabla \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 - \|\nabla \mathbf{m}_i\|_{\mathbb{L}^2}^2 + \|\nabla(\mathbf{m}_{i+1} - \mathbf{m}_i)\|_{\mathbb{L}^2}^2 \right) \leq C \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 \\ + C \left(1 + \|\mathbf{f}_1^{i+1}\|_{\mathbb{L}^2}^2 \right). \end{aligned}$$

Integrating over the time interval (t_i, t_{i+1}) and summing over i , we obtain

$$\begin{aligned} \|\partial_t \mathbf{M}_k\|_{L^2(\mathbb{L}^2)}^2 &= \sum_{i=0}^{N-1} \int_{t_i}^{t_{i+1}} \|d_t \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 dt \\ &\leq C \sum_{i=0}^{N-1} k \|\Delta \mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + C \left(1 + \sum_{i=0}^{N-1} k \|\mathbf{f}_1^{i+1}\|_{\mathbb{L}^2(\bar{D})}^2\right) \leq C, \end{aligned} \tag{4.34}$$

where we used (4.21) and (4.28) in the last step.

Next we show the boundedness of the sequence $\{\partial_t \mathbf{S}_k\}_{k>0}$ in $L^2(\mathbb{L}^2(\bar{D}))$. For $0 \leq i \leq N - 1$, let $t \in (t_i, t_{i+1}]$. Then using the test function $\psi = d_t \mathbf{s}_{i+1}$ in (4.23) and integration by parts, we get (recalling (4.17) and (4.31))

$$\begin{aligned} \|d_t \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 &+ \frac{1}{2k} \left(\|\sqrt{D_0} \nabla \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 - \|\sqrt{D_0} \nabla \mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2 + \|\sqrt{D_0} \nabla (\mathbf{s}_{i+1} - \mathbf{s}_i)\|_{\mathbb{L}^2(\bar{D})}^2 \right) \\ &+ \frac{1}{2k} \left(\|\sqrt{D_0} \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 - \|\sqrt{D_0} \mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2 + \|\sqrt{D_0} (\mathbf{s}_{i+1} - \mathbf{s}_i)\|_{\mathbb{L}^2(\bar{D})}^2 \right) \\ &\leq \frac{1}{2} \|d_t \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 + C \|\mathbf{s}_{i+1}\|_{\mathbb{H}^2(\bar{D})}^2 + C \|\mathbf{m}_{i+1}\|_{\mathbb{H}^1}^2 \left(1 + \|\mathbb{J}_{i+1}^*\|_{\mathbb{H}^1(\bar{D})}^2\right) \\ &+ C \left(\|\mathbf{m}_{i+1}\|_{\mathbb{L}^2}^2 + \|\mathbf{f}_2^{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 \right), \end{aligned}$$

or equivalently,

$$\begin{aligned} \|d_t \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 &+ \frac{1}{k} \left(\|\sqrt{D_0} \nabla \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 - \|\sqrt{D_0} \nabla \mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2 + \|\sqrt{D_0} \nabla (\mathbf{s}_{i+1} - \mathbf{s}_i)\|_{\mathbb{L}^2(\bar{D})}^2 \right) \\ &+ \frac{1}{k} \left(\|\sqrt{D_0} \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 - \|\sqrt{D_0} \mathbf{s}_i\|_{\mathbb{L}^2(\bar{D})}^2 + \|\sqrt{D_0} (\mathbf{s}_{i+1} - \mathbf{s}_i)\|_{\mathbb{L}^2(\bar{D})}^2 \right) \\ &\leq C \|\Delta \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 + C \left(1 + \|\mathbb{J}_{i+1}^*\|_{\mathbb{H}^1(\bar{D})}^2 + \|\mathbf{f}_2^{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 \right). \end{aligned}$$

Integrating over the time interval (t_i, t_{i+1}) and summing over i , we get

$$\begin{aligned} \|\partial_t \mathbf{S}_k\|_{L^2(\mathbb{L}^2(\bar{D}))}^2 &= \sum_{i=0}^{N-1} \int_{t_i}^{t_{i+1}} \|d_t \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 dt \\ &\leq C \sum_{i=0}^{N-1} k \|\Delta \mathbf{s}_{i+1}\|_{\mathbb{L}^2(\bar{D})}^2 + C \left(1 + \sum_{i=0}^{N-1} k \|\mathbb{J}_{i+1}^*\|_{\mathbb{H}^1(\bar{D})}^2 + \sum_{i=0}^{N-1} k \|\mathbf{f}_2^{i+1}\|_{\mathbb{L}^2(\bar{D})}^2\right) \leq C, \end{aligned} \tag{4.35}$$

where in the last step we used (4.21) and (4.32).

Step V (Solvability of (4.14) and (4.15)): In view of (4.30), (4.32), (4.34), and (4.35), there exists a constant $C > 0$, independent of the discretization parameter $k > 0$, such that

$$\begin{cases} \|\mathbf{M}_k^\pm\|_{L^2(\mathbb{H}^2)} + \|\mathbf{M}_k^\pm\|_{L^\infty(\mathbb{H}^1)} + \|\mathbf{M}_k\|_{L^2(\mathbb{H}^2)} + \|\mathbf{M}_k\|_{L^\infty(\mathbb{H}^1)} + \|\mathbf{M}_k\|_{H^1(\mathbb{L}^2)} \leq C, \\ \|\mathbf{S}_k^\pm\|_{L^2(\mathbb{H}^2(\bar{D}))} + \|\mathbf{S}_k^\pm\|_{L^\infty(\mathbb{H}^1(\bar{D}))} + \|\mathbf{S}_k\|_{L^2(\mathbb{H}^2(\bar{D}))} + \|\mathbf{S}_k\|_{L^\infty(\mathbb{H}^1(\bar{D}))} + \|\mathbf{S}_k\|_{H^1(\mathbb{L}^2(\bar{D}))} \leq C. \end{cases} \tag{4.36}$$

Inequality (4.30) and simple calculations reveal

$$\begin{aligned} \|\mathbf{M}_k^+ - \mathbf{M}_k\|_{L^2(\mathbb{L}^2)}^2 &= \sum_{j=0}^{N-1} \|\mathbf{m}_{j+1} - \mathbf{m}_j\|_{\mathbb{L}^2}^2 \int_{t_j}^{t_{j+1}} \left(\frac{t_{j+1} - t}{k}\right)^2 dt \\ &= \frac{k}{3} \sum_{j=0}^{N-1} \|\mathbf{m}_{j+1} - \mathbf{m}_j\|_{\mathbb{L}^2}^2 \rightarrow 0 \end{aligned}$$

as $k \rightarrow 0$. Similarly, it can be shown that $\mathbf{M}_k^- - \mathbf{M}_k \rightarrow \mathbf{0}$ in $L^2(\mathbb{L}^2)$ and $\mathbf{S}_k^\pm - \mathbf{S}_k \rightarrow \mathbf{0}$ in $L^2(\mathbb{L}^2(\tilde{D}))$. Therefore, it follows from (4.36) that there exists $(\mathbf{m}, \mathbf{s}) \in \mathcal{M} \times \mathcal{S}$ (defined by (4.9)) such that the following statements hold:

$$\left\{ \begin{array}{lll} \mathbf{M}_k \rightharpoonup \mathbf{m} \text{ in } L^2(\mathbb{H}^2) \text{ and } H^1(\mathbb{L}^2), & \mathbf{M}_k \overset{*}{\rightharpoonup} \mathbf{m} \text{ in } L^\infty(\mathbb{H}^1), & \mathbf{M}_k \rightarrow \mathbf{m} \text{ in } L^2(\mathbb{L}^2), \\ \mathbf{M}_k^\pm \rightharpoonup \mathbf{m} \text{ in } L^2(\mathbb{H}^2), & \mathbf{M}_k^\pm \overset{*}{\rightharpoonup} \mathbf{m} \text{ in } L^\infty(\mathbb{H}^1), & \mathbf{M}_k^\pm \rightarrow \mathbf{m} \text{ in } L^2(\mathbb{L}^2), \\ \mathbf{S}_k \rightharpoonup \mathbf{s} \text{ in } L^2(\mathbb{H}^2(\tilde{D})) \text{ and } H^1(\mathbb{L}^2(\tilde{D})), & \mathbf{S}_k \overset{*}{\rightharpoonup} \mathbf{s} \text{ in } L^\infty(\mathbb{H}^1(\tilde{D})), & \mathbf{S}_k \rightarrow \mathbf{s} \text{ in } L^2(\mathbb{L}^2(\tilde{D})), \\ \mathbf{S}_k^\pm \rightharpoonup \mathbf{s} \text{ in } L^2(\mathbb{H}^2(\tilde{D})), & \mathbf{S}_k^\pm \overset{*}{\rightharpoonup} \mathbf{s} \text{ in } L^\infty(\mathbb{H}^1(\tilde{D})), & \mathbf{S}_k^\pm \rightarrow \mathbf{s} \text{ in } L^2(\mathbb{L}^2(\tilde{D})). \end{array} \right. \tag{4.37}$$

Moreover, if $\mathbf{M}_k^{*\pm}$ are defined from $\mathbf{m}_i^* = \mathbf{m}^*(t_i)$ by (4.33) then, since $\mathbf{m}^* \in C([0, T], \mathbb{H}^2)$, it can be shown, using the uniform continuity of \mathbf{m}^* , that

$$\|\mathbf{M}_k^{*\pm} - \mathbf{m}^*\|_{L^2(\mathbb{H}^2)} \rightarrow 0 \text{ as } k \rightarrow 0. \tag{4.38}$$

We now prove that (\mathbf{m}, \mathbf{s}) given in (4.37) is a solution to (4.14) and (4.15). It follows from (4.22) and (4.23) that $\mathbf{M}_k, \mathbf{M}_k^\pm, \mathbf{M}_k^{*\pm}, \mathbf{S}_k,$ and \mathbf{S}_k^\pm satisfy the following equations

$$\begin{aligned} & \int_0^T (\partial_t \mathbf{M}_k, \boldsymbol{\phi})_{\mathbb{L}^2} dt + \alpha_1 \int_0^T (\nabla \mathbf{M}_k^+, \nabla \boldsymbol{\phi})_{\mathbb{L}^2} dt - \alpha_1 \int_0^T (|\nabla \mathbf{M}_k^{*-}|^2 \mathbf{M}_k^+, \boldsymbol{\phi})_{\mathbb{L}^2} dt \\ & \quad - \alpha_2 \int_0^T (\nabla \mathbf{M}_k^+, \nabla \boldsymbol{\phi} \times \mathbf{M}_k^{*+})_{\mathbb{L}^2} dt - \alpha_2 \int_0^T (\nabla \mathbf{M}_k^{*+} \times \nabla \mathbf{M}_k^+, \boldsymbol{\phi})_{\mathbb{L}^2} dt \\ & \quad - \alpha_2 \int_0^T (\nabla \mathbf{M}_k^{*+}, \nabla \boldsymbol{\phi} \times \mathbf{M}_k^+ + \boldsymbol{\phi} \times \nabla \mathbf{M}_k^+)_{\mathbb{L}^2} dt + \alpha_2 \int_0^T (\mathbf{M}_k^+ \times \mathbf{S}_k^{*+}, \boldsymbol{\phi}) dt \\ & = \int_0^T (\mathbf{F}_{1k}^- + \alpha_1 (\mathbf{S}_k^- - \mathbf{M}_k^{*+} \langle \mathbf{M}_k^+, \mathbf{S}_k^- \rangle - \mathbf{M}_k^- \langle \mathbf{M}_k^{*+}, \mathbf{S}_k^{*+} \rangle - \mathbf{M}_k^{*+} \langle \mathbf{M}_k^-, \mathbf{S}_k^{*+} \rangle) \\ & \quad - \alpha_2 \mathbf{M}_k^{*+} \times \mathbf{S}_k^- + 2\alpha_1 \langle \nabla \mathbf{M}_k^{*-}, \nabla \mathbf{M}_k^- \rangle \mathbf{M}_k^{*+}, \boldsymbol{\phi})_{\mathbb{L}^2} dt \quad \forall \boldsymbol{\phi} \in \mathbb{H}^1 \end{aligned} \tag{4.39}$$

and

$$\begin{aligned} & \int_0^T (\partial_t \mathbf{S}_k, \boldsymbol{\psi})_{\mathbb{L}^2(\tilde{D})} dt + \int_0^T (D_0 \nabla \mathbf{S}_k^+, \nabla \boldsymbol{\psi})_{\mathbb{L}^2(\tilde{D})} dt + \int_0^T (D_0 \mathbf{S}_k^+, \boldsymbol{\psi})_{\mathbb{L}^2(\tilde{D})} dt \\ & \quad + \int_0^T (D_0 \mathbf{S}_k^+ \times \mathbf{M}_k^{*+}, \boldsymbol{\psi})_{\mathbb{L}^2} dt - \beta \int_0^T (D_0 \mathbf{M}_k^{*+} \langle \nabla \mathbf{S}_k^+, \mathbf{M}_k^{*+} \rangle, \nabla \boldsymbol{\psi})_{\mathbb{L}^2(\tilde{D})} dt \\ & = \int_0^T (\beta D_0 [\mathbf{M}_k^+ \langle \nabla \mathbf{S}_k^{*+}, \mathbf{M}_k^+ \rangle + \mathbf{M}_k^{*+} \langle \nabla \mathbf{S}_k^{*+}, \mathbf{M}_k^+ \rangle] + \mathbf{M}_k^+ \mathbf{J}_k^{*+}, \nabla \boldsymbol{\psi})_{\mathbb{L}^2(\tilde{D})} dt \\ & \quad - \int_0^T (\mathbf{S}_k^{*+} \times \mathbf{M}_k^+, \boldsymbol{\psi})_{\mathbb{L}^2(\tilde{D})} dt + \int_0^T (\mathbf{F}_{2k}^+, \boldsymbol{\psi})_{\mathbb{L}^2(\tilde{D})} dt \quad \forall \boldsymbol{\psi} \in \mathbb{H}^1(\tilde{D}). \end{aligned} \tag{4.40}$$

We discuss the passing to the limit (when $k \rightarrow 0$) of (4.39) only. Similar arguments hold for (4.40). The convergence in (4.37) implies, for any $\boldsymbol{\phi} \in C^\infty(C^\infty(\tilde{D}))$,

$$\begin{aligned} \int_0^T (\partial_t \mathbf{M}_k, \boldsymbol{\phi})_{\mathbb{L}^2} dt & \rightarrow \int_0^T (\partial_t \mathbf{m}, \boldsymbol{\phi})_{\mathbb{L}^2} dt, \quad \int_0^T (\nabla \mathbf{M}_k^+, \nabla \boldsymbol{\phi})_{\mathbb{L}^2} dt \rightarrow (\nabla \mathbf{m}, \nabla \boldsymbol{\phi})_{\mathbb{L}^2} dt, \\ & \int_0^T (\mathbf{S}_k^-, \boldsymbol{\phi})_{\mathbb{L}^2} dt \rightarrow (\mathbf{s}, \boldsymbol{\phi})_{\mathbb{L}^2} dt. \end{aligned}$$

The convergence of the linear term

$$\int_0^T (\mathbf{F}_{1k}^-, \boldsymbol{\phi})_{\mathbb{L}^2} dt \rightarrow \int_0^T (\mathbf{f}_1, \boldsymbol{\phi})_{\mathbb{L}^2} dt$$

can be obtained by using (4.20) as follows:

$$\begin{aligned} \left| \int_0^T (\mathbf{F}_{1k}^- - \mathbf{f}_1, \boldsymbol{\phi})_{\mathbb{L}^2} dt \right| &= \left| \sum_{j=0}^{N-1} \int_{t_j}^{t_{j+1}} (\Pi_k \mathbf{f}(t_j) - \mathbf{f}_1(t), \boldsymbol{\phi})_{\mathbb{L}^2} dt \right| = \left| \sum_{j=0}^{N-1} \int_{t_j}^{t_{j+1}} (\Pi_k \mathbf{f}(t) - \mathbf{f}_1(t), \boldsymbol{\phi})_{\mathbb{L}^2} dt \right| \\ &\leq \|\boldsymbol{\phi}\|_{\mathbb{L}^2} \int_0^T \|\Pi_k \mathbf{f}_1(t) - \mathbf{f}_1(t)\|_{\mathbb{L}^2} dt \leq C \|\Pi_k \mathbf{f}_1 - \mathbf{f}_1\|_{L^2(\mathbb{L}^2)} \rightarrow 0, \quad k \rightarrow 0. \end{aligned}$$

The convergence of the nonlinear terms in (4.39) can be derived by using (4.36), (4.37), and (4.38). We present detailed estimates for one term, namely $\int_0^T (|\nabla \mathbf{M}_k^{*-}|^2 \mathbf{M}_k^+, \boldsymbol{\phi})_{\mathbb{L}^2} dt$. We have

$$\begin{aligned} &\left| \int_0^T (|\nabla \mathbf{M}_k^{*-}|^2 \mathbf{M}_k^+ - |\nabla \mathbf{m}^*|^2 \mathbf{m}, \boldsymbol{\phi})_{\mathbb{L}^2} dt \right| \\ &\leq \left| \int_0^T (|\nabla \mathbf{M}_k^{*-}|^2 (\mathbf{M}_k^+ - \mathbf{m}), \boldsymbol{\phi})_{\mathbb{L}^2} dt \right| + \left| \int_0^T ((|\nabla \mathbf{M}_k^{*-}|^2 - |\nabla \mathbf{m}^*|^2) \mathbf{m}, \boldsymbol{\phi})_{\mathbb{L}^2} dt \right| \\ &\leq \|\mathbf{m}^*\|_{C(\mathbb{H}^2)} \|\boldsymbol{\phi}\|_{\mathbb{H}^1} \|\mathbf{M}_k^+ - \mathbf{m}\|_{L^2(\mathbb{L}^2)} + \int_0^T \int_D (|\nabla \mathbf{M}_k^{*-}| + |\nabla \mathbf{m}^*|) |\boldsymbol{\phi}| |\nabla \mathbf{M}_k^{*-} - \nabla \mathbf{m}^*| |\mathbf{m}| dx dt \\ &\leq C \|\mathbf{M}_k^+ - \mathbf{m}\|_{L^2(\mathbb{L}^2)} + 2 \|\mathbf{m}^*\|_{C(\mathbb{H}^2)} \|\boldsymbol{\phi}\|_{\mathbb{H}^1} \|\mathbf{M}_k^{*-} - \mathbf{m}^*\|_{L^2(\mathbb{H}^1)} \|\mathbf{m}\|_{L^2(\mathbb{L}^2)} \\ &\leq C \|\mathbf{M}_k^+ - \mathbf{m}\|_{L^2(\mathbb{L}^2)} + C \|\mathbf{M}_k^{*-} - \mathbf{m}^*\|_{L^2(\mathbb{H}^1)} \rightarrow 0, \quad k \rightarrow 0. \end{aligned}$$

The convergence of other nonlinear terms in (4.39) can be shown in the same manner. Therefore, by letting $k \rightarrow 0$ in (4.39) we deduce

$$\begin{aligned} &\int_0^T (\partial_t \mathbf{m}, \boldsymbol{\phi})_{\mathbb{L}^2} dt + \alpha_1 \int_0^T (\nabla \mathbf{m}, \nabla \boldsymbol{\phi})_{\mathbb{L}^2} dt - \alpha_1 \int_0^T (|\nabla \mathbf{m}^*|^2 \mathbf{m}, \boldsymbol{\phi})_{\mathbb{L}^2} dt \\ &\quad - \alpha_2 \int_0^T (\nabla \mathbf{m}, \nabla \boldsymbol{\phi} \times \mathbf{m}^*)_{\mathbb{L}^2} dt - \alpha_2 \int_0^T (\nabla \mathbf{m}^* \times \nabla \mathbf{m}, \boldsymbol{\phi})_{\mathbb{L}^2} dt \\ &\quad - \alpha_2 \int_0^T (\nabla \mathbf{m}^*, \nabla \boldsymbol{\phi} \times \mathbf{m} + \boldsymbol{\phi} \times \nabla \mathbf{m})_{\mathbb{L}^2} dt + \alpha_2 \int_0^T (\mathbf{m} \times \mathbf{s}^*, \boldsymbol{\phi}) dt \\ &= \int_0^T (\mathbf{f}_1 + \alpha_1 (\mathbf{s} - \mathbf{m}^* \langle \mathbf{m}^*, \mathbf{s} \rangle - \mathbf{m} \langle \mathbf{m}^*, \mathbf{s}^* \rangle - \mathbf{m}^* \langle \mathbf{m}, \mathbf{s}^* \rangle) \\ &\quad - \alpha_2 \mathbf{m}^* \times \mathbf{s} + 2\alpha_1 \langle \nabla \mathbf{m}^*, \nabla \mathbf{m} \rangle \mathbf{m}^*, \boldsymbol{\phi})_{\mathbb{L}^2} dt \quad \forall \boldsymbol{\phi} \in \mathbb{H}^1, \end{aligned}$$

or equivalently (by using integration by parts),

$$\begin{aligned} &\int_0^T (\partial_t \mathbf{m}, \boldsymbol{\phi})_{\mathbb{L}^2} dt - \alpha_1 \int_0^T (\Delta \mathbf{m}, \boldsymbol{\phi})_{\mathbb{L}^2} dt - \alpha_1 \int_0^T (|\nabla \mathbf{m}^*|^2 \mathbf{m}, \boldsymbol{\phi})_{\mathbb{L}^2} dt \\ &\quad + \alpha_2 \int_0^T (\mathbf{m}^* \times \Delta \mathbf{m}, \boldsymbol{\phi})_{\mathbb{L}^2} dt + \alpha_2 \int_0^T (\mathbf{m} \times \Delta \mathbf{m}^*, \boldsymbol{\phi})_{\mathbb{L}^2} dt + \alpha_2 \int_0^T (\mathbf{m} \times \mathbf{s}^*, \boldsymbol{\phi}) dt \\ &= \int_0^T (\mathbf{f}_1 + \alpha_1 (\mathbf{s} - \mathbf{m}^* \langle \mathbf{m}^*, \mathbf{s} \rangle - \mathbf{m} \langle \mathbf{m}^*, \mathbf{s}^* \rangle - \mathbf{m}^* \langle \mathbf{m}, \mathbf{s}^* \rangle) \\ &\quad - \alpha_2 \mathbf{m}^* \times \mathbf{s} + 2\alpha_1 \langle \nabla \mathbf{m}^*, \nabla \mathbf{m} \rangle \mathbf{m}^*, \boldsymbol{\phi})_{\mathbb{L}^2} dt \quad \forall \boldsymbol{\phi} \in \mathbb{H}^1, \end{aligned}$$

which implies the first equation in (4.14).

To show the second equation in (4.14), namely $\mathbf{m}(0) = \mathbf{f}_3$, we choose the test function $\boldsymbol{\phi} \in C^\infty(C^\infty(D))$ such that $\boldsymbol{\phi}(T) = \mathbf{0}$. Then integration by parts gives

$$\int_0^T (\partial_t \mathbf{M}_k, \boldsymbol{\phi})_{\mathbb{L}^2} dt = - \int_0^T (\mathbf{M}_k, \partial_t \boldsymbol{\phi})_{\mathbb{L}^2} dt - (\mathbf{f}_3, \boldsymbol{\phi}(0))_{\mathbb{L}^2}.$$

Letting $k \rightarrow 0$ we obtain

$$\int_0^T (\partial_t \mathbf{m}, \phi)_{\mathbb{L}^2} dt = - \int_0^T (\mathbf{m}, \partial_t \phi)_{\mathbb{L}^2} dt - (\mathbf{f}_3, \phi(0))_{\mathbb{L}^2}.$$

Using integration by parts again gives the required result. Similarly, one can easily show that (\mathbf{m}, \mathbf{s}) satisfies (4.15), completing the proof of the lemma. \square

4.3 Proof of Theorem 2.3

Since $(\mathbf{m}^*, \mathbf{s}^*, j^*)$ is a regular point of Γ defined in (4.11) (cf. Lemma 4.4), one can use Lagrange multiplier theorem [18, Theorem 1, Chapter 9] to show that there exists $(\mathbf{z}_1, \mathbf{z}_2, \xi_1, \xi_2) \in L^2(\mathbb{L}^2) \times L^2(\mathbb{L}^2(\tilde{D})) \times (\mathbb{H}^2)^* \times \mathbb{H}^2(\tilde{D})^*$ such that the Lagrangian functional $L : \mathcal{M} \times \mathcal{S} \times \mathcal{J} \rightarrow \mathbb{R}$, given by

$$L(\mathbf{m}, \mathbf{s}, j) := F(\mathbf{m}, \mathbf{s}, j) + \sum_{i=1}^2 \langle \mathbf{z}_i, e_i(\mathbf{m}, \mathbf{s}, j) \rangle + \sum_{i=1}^2 \langle \xi_i, e_{i+2}(\mathbf{m}, \mathbf{s}, j) \rangle,$$

is stationary at the point $(\mathbf{m}^*, \mathbf{s}^*, j^*)$. In other words, $DL(\mathbf{m}^*, \mathbf{s}^*, j^*) = \mathbf{0}$, where

$$DL(\mathbf{m}^*, \mathbf{s}^*, j^*) := DF(\mathbf{m}^*, \mathbf{s}^*, j^*) + \sum_{i=1}^2 \langle \mathbf{z}_i, De_i(\mathbf{m}^*, \mathbf{s}^*, j^*) \rangle + \sum_{i=1}^2 \langle \xi_i, De_{i+2}(\mathbf{m}^*, \mathbf{s}^*, j^*) \rangle.$$

Thus, by computing the directional derivative of L with respect to j , \mathbf{m} and \mathbf{s} , respectively, we arrive at the optimality condition (2.5), the adjoint (2.6) with $\mathbf{z}_1(T) = -(1 - \kappa)\nabla\psi(\mathbf{m}^*(T))/2$, and the adjoint (2.7) with $\mathbf{z}_2(T) = \mathbf{0}$ respectively.

4.4 Regularity of the adjoint and optimal control

In view of the Lagrange multiplier theorem, the adjoint variables \mathbf{z}_1 and \mathbf{z}_2 satisfy $(\mathbf{z}_1, \mathbf{z}_2) \in L^2(\mathbb{L}^2) \times L^2(\mathbb{L}^2(\tilde{D}))$. But one can expect better regularity properties for these adjoint variables and the optimal control j^* . Regarding this, we have the following lemma.

Lemma 4.5 *Assume that $D_0 \in H^2(\tilde{D})$ with $D_* > 2\beta D^*$. Let $(\mathbf{m}^*, \mathbf{s}^*, j^*)$ be an optimal solution of Problem 4.1, and the adjoint variables $(\mathbf{z}_1, \mathbf{z}_2)$ satisfy the system (2.5), (2.6), and (2.7). Then*

- i) $\mathbf{z}_2 \in L^\infty(\mathbb{H}^1(\tilde{D})) \cap L^2(\mathbb{H}^2(\tilde{D})) \cap H^1(\mathbb{L}^2(\tilde{D}))$;
- ii) $j^* \in L^\infty(H^3(\tilde{D}))$;
- iii) $\mathbf{z}_1 \in L^\infty(\mathbb{H}^1) \cap L^2(\mathbb{H}^2) \cap H^1(\mathbb{L}^2)$.

Proof Proof of i): Testing (2.7) formally by \mathbf{z}_2 and using (2.1) along with the Cauchy–Schwarz inequality, we get

$$-\frac{1}{2} \frac{d}{dt} \|\mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 + (D_* - \beta D^*) \|\nabla \mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 \leq C \left(\|\mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 + \|\mathbf{z}_1\|_{\mathbb{L}^2}^2 \right).$$

Using the terminal condition $\mathbf{z}_2(T) = 0$ (see (2.8)) and the condition $(\mathbf{z}_1, \mathbf{z}_2) \in L^2(\mathbb{L}^2) \times L^2(\mathbb{L}^2(\tilde{D}))$, we deduce after integrating over $[t, T]$,

$$\mathbf{z}_2 \in L^\infty(\mathbb{L}^2(\tilde{D})) \cap L^2(\mathbb{H}^1(\tilde{D})). \tag{4.41}$$

Again, testing (2.7) formally by $-\Delta \mathbf{z}_2$ and using Young’s inequality with some $\epsilon > 0$:

$$\begin{aligned} -\frac{1}{2} \frac{d}{dt} \|\nabla \mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 + D_* \|\Delta \mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 &\leq (\epsilon + \beta D^*) \|\Delta \mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 \\ &+ C(\epsilon, \alpha, \beta) \left(\|\mathbf{z}_1\|_{\mathbb{L}^2}^2 + \|\nabla \mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 \left(\|\nabla \mathbf{m}^*\|_{\mathbb{L}^\infty}^2 + \|\nabla D_0\|_{\mathbb{L}^2(\tilde{D})}^2 \right) \right). \end{aligned}$$

Choosing $\epsilon < D_*/2$ and using (4.17) along with (4.41) we have, after integrating over $[t, T]$,

$$\mathbf{z}_2 \in L^\infty(\mathbb{H}^1(\tilde{D})) \cap L^2(\mathbb{H}^2(\tilde{D})). \tag{4.42}$$

Furthermore, testing (2.7) formally by $-\partial_t \mathbf{z}_2$, using integration by parts and Young’s inequality, after rearranging the equation, we have

$$\begin{aligned} \|\partial_t \mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 - \frac{1}{2} \frac{d}{dt} \|\sqrt{D_0} \nabla \mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 \\ \leq \epsilon \|\partial_t \mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 + C(\epsilon, \alpha, \beta) \left(\|\Delta \mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 + \|\nabla \mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 \left(\|\nabla D_0\|_{\mathbb{L}^\infty(\tilde{D})}^2 + \|\nabla \mathbf{m}^*\|_{\mathbb{L}^\infty}^2 \right) \right. \\ \left. + \|\mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 + \|\mathbf{z}_1\|_{\mathbb{L}^2}^2 \right). \end{aligned}$$

Choosing ϵ sufficiently small, using (4.42) and (4.17), and integrating over $[t, T]$ we infer

$$\mathbf{z}_2 \in H^1(\mathbb{L}^2(\tilde{D})).$$

Thus, we complete the proof of assertion i).

Proof of ii): Test (2.5) with j^* and $-\Delta j^*$ and then integrate with respect to x along with the Cauchy–Schwarz inequality. The resulting inequality becomes

$$\|j^*\|_{\mathbb{L}^2(\tilde{D})}^2 + \|\nabla j^*\|_{L^2(\tilde{D})}^2 + \|\Delta j^*\|_{L^2(\tilde{D})}^2 + \|\nabla \Delta j^*\|_{L^2(\tilde{D})}^2 \leq C \|\nabla \mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2.$$

Thanks to i), we see from the above estimate that $j^* \in L^\infty(H^3(\tilde{D}))$.

Proof of iii): Testing (2.6) with \mathbf{z}_1 , and $-\Delta \mathbf{z}_1$, we have, thanks to the Cauchy–Schwarz inequality, the boundedness of \mathbf{m}^* , and the embedding of \mathbb{L}^∞ between \mathbb{L}^2 and \mathbb{H}^1

$$\begin{aligned} -\frac{1}{2} \frac{d}{dt} \|\mathbf{z}_1\|_{\mathbb{L}^2}^2 + \alpha_1 \|\nabla \mathbf{z}_1\|_{\mathbb{L}^2}^2 &\leq \epsilon \|\nabla \mathbf{z}_1\|_{\mathbb{L}^2}^2 + C \|\bar{\mathbf{m}} - \mathbf{m}^*\|_{\mathbb{L}^2}^2 + C \left(\|\nabla \mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 + \|\mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 \|\mathbf{s}^*\|_{\mathbb{L}^\infty(\tilde{D})}^2 \right) \\ &+ C \left(1 + \|\mathbf{s}^*\|_{\mathbb{H}^1(\tilde{D})}^4 + \|\mathbf{m}^*\|_{\mathbb{H}^2}^4 + \|j^*\|_{H^1(\tilde{D})}^2 \right) \|\mathbf{z}_1\|_{\mathbb{L}^2}^2 \end{aligned}$$

and

$$\begin{aligned} -\frac{1}{2} \frac{d}{dt} \|\nabla \mathbf{z}_1\|_{\mathbb{L}^2}^2 + \alpha_1 \|\Delta \mathbf{z}_1\|_{\mathbb{L}^2}^2 &\leq \epsilon \|\Delta \mathbf{z}_1\|_{\mathbb{L}^2}^2 + C \left(\left(\|\mathbf{s}^*\|_{\mathbb{H}^1(\tilde{D})}^2 + \|\mathbf{m}^*\|_{\mathbb{H}^2}^4 + \|\mathbf{m}^*\|_{\mathbb{H}^2}^2 \right) \|\mathbf{z}_1\|_{\mathbb{H}^1}^2 \right. \\ &\left. + \|\bar{\mathbf{m}} - \mathbf{m}^*\|_{\mathbb{L}^2}^2 + \|\nabla \mathbf{z}_2\|_{\mathbb{L}^2(\tilde{D})}^2 \left(\|j^*\|_{H^1(\tilde{D})}^2 + \|\mathbf{s}^*\|_{\mathbb{H}^2(\tilde{D})}^2 \right) \right), \end{aligned}$$

for some $\epsilon > 0$. We now use part i) and part ii) above, Lemma 4.2, and the condition on $\mathbf{z}_1(T)$ given in (2.8) to conclude that $\mathbf{z}_1 \in L^\infty(\mathbb{H}^1) \cap L^2(\mathbb{H}^2)$. As in the proof of part i), by testing (2.6) with $\partial_t \mathbf{z}_1$, one can easily show that $\|\partial_t \mathbf{z}_1\|_{L^2(\mathbb{L}^2)}^2 \leq C$, which completes the proof of iii). \square

5 Numerical experiments

The following numerical experiments are carried out using the FEniCS automated code generation system (<https://fenicsproject.org>) version 2019 and the `tlm_adjoint` library (https://github.com/jrmaddison/tlm_adjoint). FEniCS enables a high-level syntax representation of the complex numerical equations, as well as an efficient implementation using automated tools. On the other hand, the `tlm_adjoint` library is used to derive the associated adjoint model, which computes the required derivatives of the cost functional [11, 15, 19, 27]. In general, the implementation only requires the users to define a suitable finite element function space, the computational domain and mesh, the weak formulation, and a few other specifics. The FEniCS system and the `tlm_adjoint` library enable automatic derivation of the finite element equation, the discrete tangent-linear and adjoint models. Nevertheless, we would like to lay out more details for pedagogical purpose. Generally, the PDE constrained optimization algorithm contains two main parts. The first part is to solve the forward problem, while the second part is to achieve optimization.

We elaborate the first part here. First we note that the weak equations in Definition 2.1 can be rewritten as

$$\begin{aligned} (\mathbf{m}_t, \boldsymbol{\phi})_D + \alpha_1 (\nabla \mathbf{m}, \nabla \boldsymbol{\phi})_D &= \alpha_1 (|\nabla \mathbf{m}|^2 \mathbf{m}, \boldsymbol{\phi})_D - \alpha_1 (\mathbf{m} \times (\mathbf{m} \times \mathbf{s}), \boldsymbol{\phi})_D \\ &\quad + \alpha_2 (\mathbf{m} \times \nabla \mathbf{m}, \nabla \boldsymbol{\phi})_D - \alpha_2 (\mathbf{m} \times \mathbf{s}, \boldsymbol{\phi})_D \end{aligned}$$

and

$$(\mathbf{s}_t, \boldsymbol{\psi})_{\tilde{D}} + a(\mathbf{s}, \boldsymbol{\psi}) = \frac{\beta' \mu_\beta}{e} (\mathbf{m} \otimes \mathbf{j}, \nabla \boldsymbol{\psi})_D,$$

with

$$\begin{aligned} a(\mathbf{s}, \boldsymbol{\psi}) := \frac{2}{\lambda_1} (D_0 \mathbf{s}, \boldsymbol{\psi})_{\tilde{D}} + (D_0 \nabla \mathbf{s}, \nabla \boldsymbol{\psi})_{\tilde{D}} - \beta \beta' (D_0 \mathbf{m} \otimes (\nabla \mathbf{s} \cdot \mathbf{m}), \nabla \boldsymbol{\psi})_D \\ + \frac{2}{\lambda_2} (D_0 \mathbf{s} \times \mathbf{m}, \boldsymbol{\psi})_D, \end{aligned}$$

where we recover the constants $\gamma_0, c, \beta', e, \mu_\beta, \lambda_1$, and λ_2 as in problem (1.1)–(1.3). The fully discrete schemes to solve these equations are (5.1) and (5.2) below. For the time discretization, we recall (4.16) and use the backward Euler scheme. The spatial discretization is determined by a shape-regular triangulation \mathcal{T}_h of D and $\tilde{\mathcal{T}}_h$ of \tilde{D} into tetrahedra such that the two triangulations agree on D .

The finite element spaces are defined by

$$\begin{aligned} \mathcal{S}^1(\mathcal{T}_h) &:= \{\boldsymbol{\phi}_h \in C(D; \mathbb{R}^3) : \boldsymbol{\phi}_h|_\tau \in (\mathcal{P}^1(\tau))^3 \text{ for all } \tau \in \mathcal{T}_h\}, \\ \mathcal{S}^1(\tilde{\mathcal{T}}_h) &:= \{\boldsymbol{\psi}_h \in C(\tilde{D}; \mathbb{R}^3) : \boldsymbol{\psi}_h|_\tau \in (\mathcal{P}^1(\tau))^3 \text{ for all } \tau \in \tilde{\mathcal{T}}_h\}, \end{aligned}$$

where $\mathcal{P}^1(\tau)$ is the space of polynomials of degree at most 1 on τ . Supposing that the normalized magnetization \mathbf{m}^j and spin accumulation \mathbf{s}^j at the j th time step are known, FEniCS uses Newton’s scheme to obtain $\tilde{\mathbf{m}}^{j+1}$ by solving the nonlinear system (5.1). Then, \mathbf{m}^{j+1} is obtained by normalizing $\tilde{\mathbf{m}}^{j+1}$. Afterwards, FEniCS calculates \mathbf{s}^{j+1} using the value of \mathbf{m}^{j+1} and \mathbf{s}^j by solving (5.2). The method here is the implicit Euler method due to the spin accumulation PDE (1.2) being linear. The complete algorithm reads as follows:

- (i) Find $\tilde{\mathbf{m}}_h^{j+1} \in \mathcal{S}^1(\mathcal{T}_h)$ such that

$$\begin{aligned} \left(\frac{\tilde{\mathbf{m}}_h^{j+1} - \mathbf{m}_h^j}{k}, \phi_h\right)_D + \alpha_1 \left(\nabla \tilde{\mathbf{m}}_h^{j+1}, \nabla \phi_h\right)_D \\ = \alpha_1 \left(|\nabla \mathbf{m}_h^j|^2 \tilde{\mathbf{m}}_h^{j+1}, \phi_h\right)_D - \alpha_1 \left(\tilde{\mathbf{m}}_h^{j+1} \times (\mathbf{m}_h^j \times \mathbf{s}_h^j), \phi_h\right)_D \\ + \alpha_2 \left(\tilde{\mathbf{m}}_h^{j+1} \times \nabla \tilde{\mathbf{m}}_h^{j+1}, \nabla \phi_h\right)_D - \alpha_2 \left(\tilde{\mathbf{m}}_h^{j+1} \times \mathbf{s}_h^j, \phi_h\right)_D. \end{aligned} \tag{5.1}$$

- (ii) Normalize $\tilde{\mathbf{m}}_h^{j+1}$ by

$$\mathbf{m}_h^{j+1} = \frac{\tilde{\mathbf{m}}_h^{j+1}}{|\tilde{\mathbf{m}}_h^{j+1}|} \text{ nodewise,}$$

i.e. \mathbf{m}_h^{j+1} is the normalized $\tilde{\mathbf{m}}_h^{j+1}$.

- (iii) Find $\mathbf{s}_h^{j+1} \in \mathcal{S}^1(\tilde{\mathcal{T}}_h)$ such that

$$\left(\frac{\mathbf{s}_h^{j+1} - \mathbf{s}_h^j}{k}, \psi_h\right)_{\tilde{D}} + a(\mathbf{s}_h^{j+1}, \psi_h) = \frac{\beta\mu\beta}{e} \left(\mathbf{m}_h^{j+1} \otimes \mathbf{j}, \nabla \psi_h\right)_D, \tag{5.2}$$

We note that (5.2) to find the spin accumulation has been used in [3].

The optimization part of the algorithm reads as follows: Given a target $\bar{\mathbf{m}}$, we introduce the standard procedures for achieving the minimizer π^* of the discretized cost functional $F(\pi_n)$ defined in (1.6). In general, the steps are:

1. Choose an initial guess for the current density $\mathcal{J}^{(0)} = \{\mathbf{j}_j^{(0)}\}_{j=1}^J$. The initial guess of control variables can be chosen based on physical laws or previous studies in order to save the computation time.
2. **For** $i = 0, 1, 2, \dots$ **do**:
 - (a) Determine $(\mathbf{M}^{(i)}, \mathbf{S}^{(i)}) = \{(\mathbf{m}_j^{(i)}, \mathbf{s}_j^{(i)})\}_{j=1}^J$ with $\mathcal{J}^{(i)}$ via the fully discretized coupled LLG-Spin accumulation system (5.1) and (5.2). The assembly code was generated by FEniCS using Gaussian quadrature for integration. We note that the upper index indicates the optimization step, whereas the lower index indicates the time step.
 - (b) Evaluate the cost functional $F(\Pi^{(i)})$ defined by (1.6) at $\Pi^{(i)} = (\mathbf{M}^{(i)}, \mathbf{S}^{(i)}, \mathcal{J}^{(i)})$.
 - (c) If the targeted value for the cost functional is fulfilled, terminate the iteration and set $\Pi^* = \Pi^{(i)}$. Otherwise, proceed to (d).
 - (d) Determine the next control variable $\mathcal{J}^{(i+1)} = \{\mathbf{j}_j^{(i+1)}\}_{j=1}^J$. Here, evaluations of the derivative $dF/d\mathcal{J}^{(i+1)}$ are used to determine a search direction

$d^{(i)}$ in which the functional F is decreasing. We used the L-BFGS-B algorithm [22], which is an iterative method for solving unconstrained nonlinear optimization problems from the Scipy library [32].

(e) Set $i = i + 1$ and return to (a).

Step (d) is crucial as the main task of the gradient based optimization is to determine an improved choice of control variable in order to achieve fast convergence to the optimal solution.

In Section 5.1 we show the numerical results for the case of one-dimensional domains D and \tilde{D} . Even though the analysis presented in previous sections does not apply for multi-dimensional domains, we still experiment with $D = \tilde{D} \subset \mathbb{R}^3$; the results are shown in Section 5.2. In all experiments in both sections, the cost functional $F(\pi)$, see (1.5), is defined with the terminal payoff

$$\Psi(\mathbf{m}(T)) = \|\mathbf{m}(T) - \bar{\mathbf{m}}\|_{\mathbb{R}^2}^2$$

and parameters

$$\delta_1 = \delta_2 = \delta_3 = 0.01.$$

We also choose $\kappa = 1$ in $F(\pi)$ for all simulations, except the ones in Section 5.1.4, where we experiment on different values of κ . The other parameters in (1.1), (1.2), and (1.3) are chosen to be

$$\gamma_0 = c = \beta' = e = \mu_\beta = D_0 = 1, \quad \lambda_1 = \lambda_2 = 2, \quad \beta = 0.5.$$

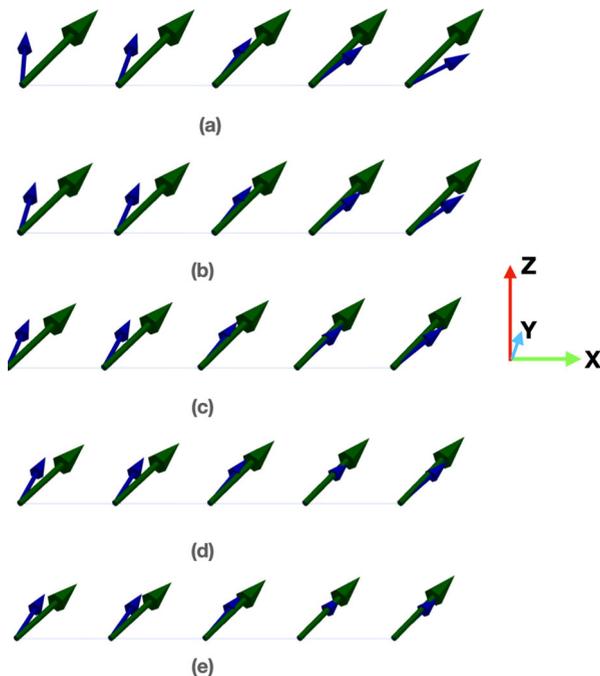


Fig. 1 Example 1: $j = 0$ and $\mathbf{m}_0 = (\sin(x), \cos(x)/\sqrt{2}, \cos(x)/\sqrt{2})$, no target. The blue arrows indicate the magnetization \mathbf{m} , while the green arrows indicate the spin accumulation \mathbf{s}

5.1 Experiments for 1D problem

In this section, we present numerical results for

$$D = \tilde{D} = [0, 1] \quad \text{and} \quad \mathcal{J}^{(0)} = 1.0.$$

The stopping criterion is

$$F(\Pi^i) < 0.005 \quad \text{or} \quad \left| \frac{F(\Pi^{(i)}) - F(\Pi^{(i-1)})}{F(\Pi^{(i-1)})} \right| \leq 10^{-10}. \quad (5.3)$$

We apply uniform partitions with space mesh size $h = 0.01$ and time step $k = 0.0005$. We observe that when a larger value of k is chosen, e.g., $k = 0.5$, the numerical simulation becomes unstable and Newton's method used to solve the nonlinear system (5.1) fails to converge.

5.1.1 No targets

Example 1: In this example, we show the evolutions of magnetization \mathbf{m} and the spin accumulation \mathbf{s} when the control variable $\mathbf{j} = 0$ and there are no targets (Fig. 1), with

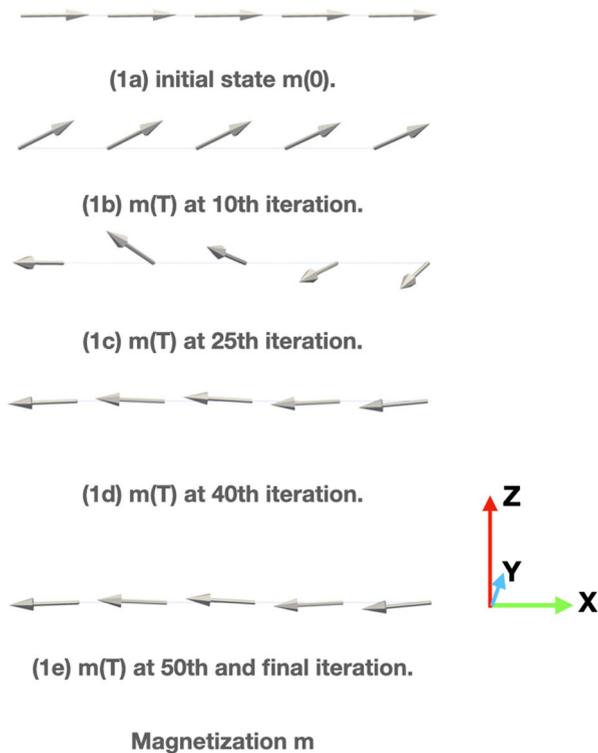


Fig. 2 Example 2: $\mathbf{m}_0 = (1, 0, 0)$ and $\bar{\mathbf{m}} = (-1, 0, 0)$

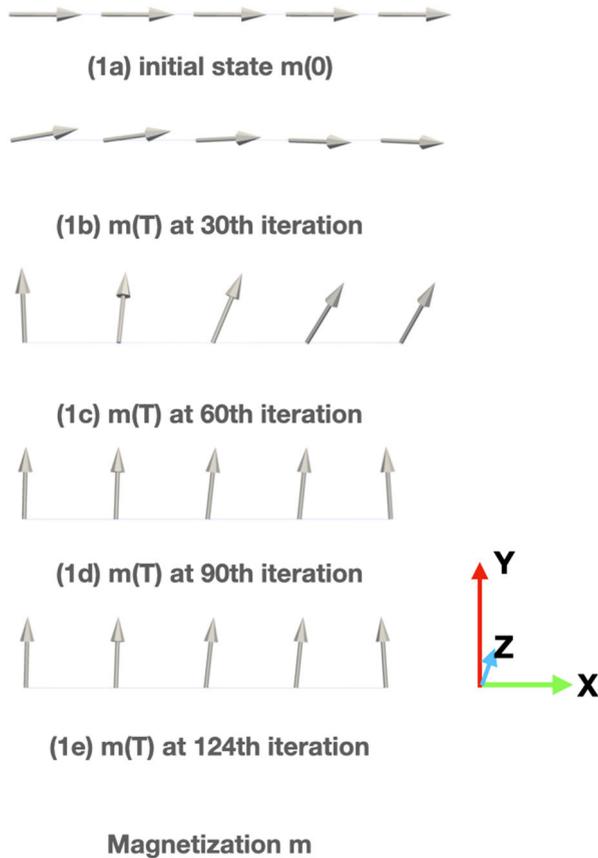


Fig. 3 Example 3: $\mathbf{m}_0 = (1, 0, 0)$ and $\bar{\mathbf{m}} = (0, 1, 0)$

the initial data \mathbf{m}_0 given by $\mathbf{m}_0 = (\sin(x), \cos(x)/\sqrt{2}, \cos(x)/\sqrt{2})$ and the terminal time $T = 0.3$.

5.1.2 Single targets

Example 2: In this example, the initial states, total running time, and the assimilation target are

$$\mathbf{m}_0(x) = (1, 0, 0), \quad \mathbf{s}_0(x) = (1, 1, 1), \quad T = 0.4, \quad \text{and} \quad \bar{\mathbf{m}} = (-1, 0, 0).$$

Figure 2 (1a)–(1e) show the progress of assimilation of \mathbf{m} . The final iteration shown in Fig. 2 (1e) gives a good approximation of the target magnetization $\bar{\mathbf{m}}$.

Example 3: In this example, the given data are

$$\mathbf{m}_0(x) = (1, 0, 0) \quad \mathbf{s}_0(x) = (1, 1, 1), \quad T = 0.4, \quad \text{and} \quad \bar{\mathbf{m}} = (0, 1, 0).$$

The simulation is presented in Fig. 3 (1a)–(1e).

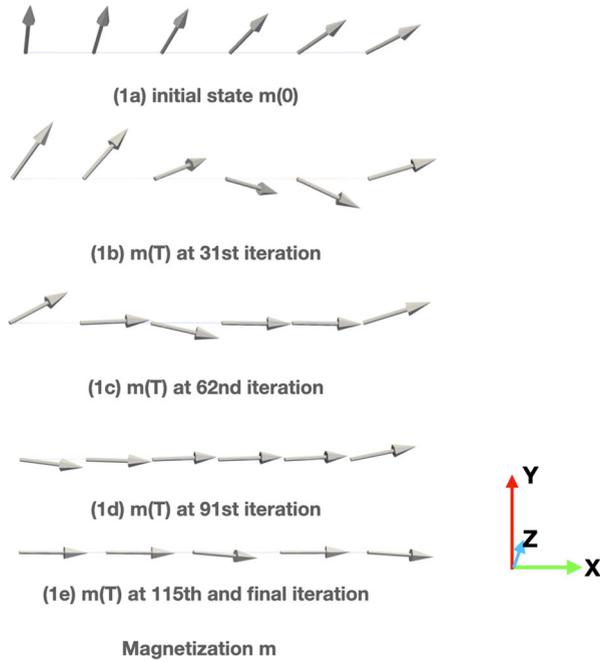


Fig. 4 Example 4: $\mathbf{m}_0 = (\sin(x), \cos(x)/\sqrt{2}, \cos(x)/\sqrt{2})$ and $\bar{\mathbf{m}} = (1, 0, 0)$

Example 4: In this example, the given data are

$$\mathbf{m}_0(x) = \left(\sin(x), \frac{\cos(x)}{\sqrt{2}}, \frac{\cos(x)}{\sqrt{2}} \right), \quad \mathbf{s}_0(x) = (1, 1, 1), \quad T = 0.3, \quad \text{and} \quad \bar{\mathbf{m}} = (1, 0, 0).$$

The simulation is presented in Fig. 4 (1a)–(1e).

For all three examples 2, 3, and 4, we show in Fig. 5 two comparisons. The left column (a) plots the cost functional F versus the optimization iteration. The right column (b) plots the relative change $\delta F/F$ versus the optimization iteration. A general decreasing trend can be seen which indicates the numerical method is valid.

5.1.3 Switching type initial and target profile

Example 5: In this example, we show the numerical simulations when the switching type initial conditions and the targets are given. The total time is chosen to be $T = 0.6$. The switching moment $T_s = 0.3$. The initial states are

$$\mathbf{m}_0(x) = \begin{cases} (1, 0, 0), & \text{when } x \in [0.0, 0.5) \\ \left(\sin(x), \frac{\cos(x)}{\sqrt{2}}, \frac{\cos(x)}{\sqrt{2}} \right), & \text{when } x \in [0.5, 1.0). \end{cases} \quad (5.4)$$

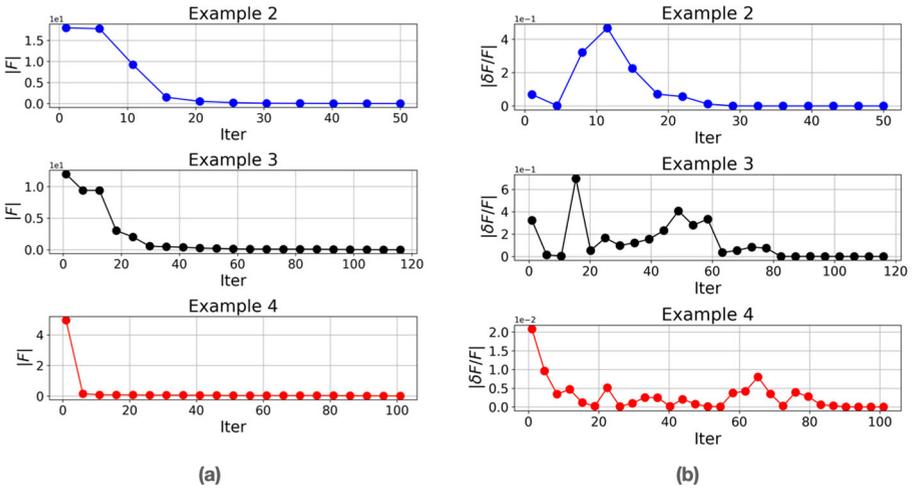


Fig. 5 Shown are the two comparisons. (a) shows cost functional F versus the optimization iteration in all three examples; (b) shows the relative change $\delta F/F$ versus the optimization iteration in all three examples

The switching targets are

$$\bar{\mathbf{m}}(x) = \begin{cases} (0, 1, 0) & \text{for } t \in [0, 0.3), \\ (0, -1, 0) & \text{for } t \in [0.3, 0.6). \end{cases} \tag{5.5}$$

Figure 6 shows the evolution of the optimal \mathbf{m}^* with respect to time t . Figure 6 (1d) is the simulation at the switching moment $t = 0.3$.

5.1.4 Multiple cost functional settings

In the following two examples, we choose different values of κ for the cost functional in (1.5).

Example 6: The given data are:

$$\mathbf{m}_0(x) = \left(\sin(x), \frac{\cos(x)}{\sqrt{2}}, \frac{\cos(x)}{\sqrt{2}} \right), \quad \mathbf{s}_0(x) = (1, 1, 1), \quad T = 0.3, \\ \bar{\mathbf{m}}(x) = (1, 0, 0), \quad \text{and } \kappa = 0.0.$$

Example 7: The given data are:

$$\mathbf{m}_0(x) = \left(\sin(x), \frac{\cos(x)}{\sqrt{2}}, \frac{\cos(x)}{\sqrt{2}} \right), \quad \mathbf{s}_0(x) = (1, 1, 1), \quad T = 0.3, \\ \bar{\mathbf{m}}(x) = (1, 0, 0), \quad \text{and } \kappa = 0.5.$$

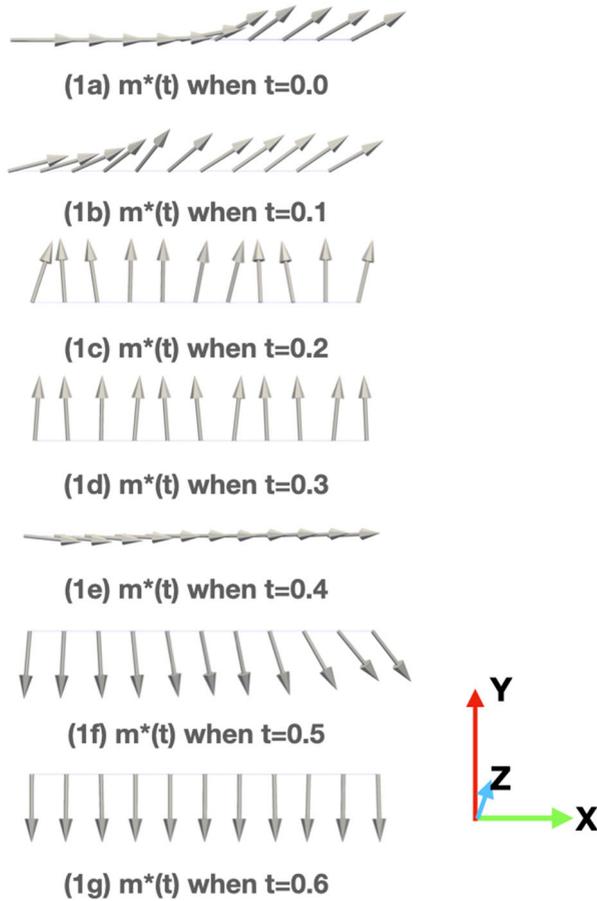


Fig. 6 Example 5: Optimal solutions \mathbf{m}^* with switching initial (5.4) and target profile (5.5)

The assimilation process for Example 6 is shown in Fig. 7 and for Example 7 in Fig. 8.

5.2 Experiments for 3D problem

In this section, we present numerical results for

$$D = \tilde{D} = [0, 1]^3 \quad \text{and} \quad \mathcal{J}^{(0)} = (1, 1, 1).$$

The same stopping criterion (5.3) is used. We apply uniform partition with space mesh size $h = 0.2$ and time step $k = 0.01$.

Example 8: In this example, the given data are

$$s_0(x, y, z) := (1, 1, 1), \quad \mathbf{m}_0(x, y, z) := (1, 0, 0), \quad \text{and} \quad \bar{\mathbf{m}} = (-1, 0, 0).$$

The progress of the assimilation is presented in Fig. 9 (a)–(d).

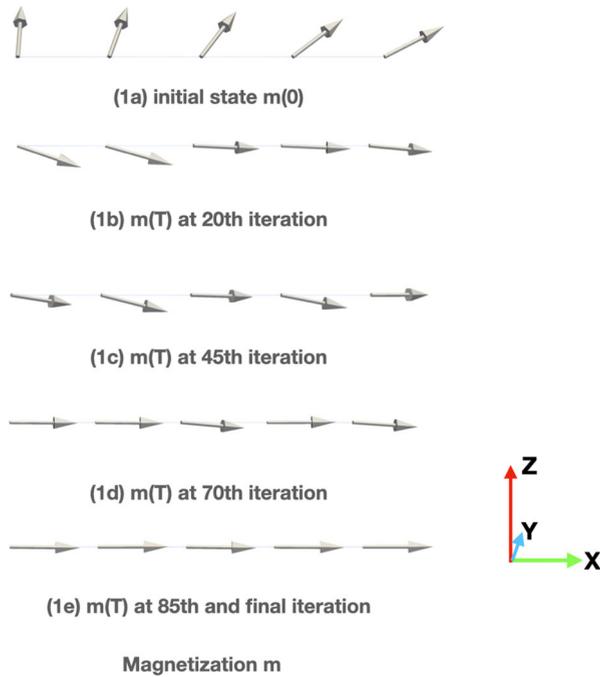


Fig. 7 Example 6: $\mathbf{m}_0(x) = (\sin(x), \cos(x)/\sqrt{2}, \cos(x)/\sqrt{2})$, $\bar{\mathbf{m}}(x) = (1, 0, 0)$, and $\kappa = 0.0$

Example 9: In this example, the given data are

$$\mathbf{s}_0(x, y, z) := (1, 1, 1), \quad \mathbf{m}_0(x, y, z) := (1, 0, 0), \quad \text{and} \quad \bar{\mathbf{m}} = (0, 1, 0).$$

It is noted that in order to achieve optimal control in this example, we need to add an extra external field, namely the Zeeman field, to the effective field in (1.4). Otherwise, the minimization of the cost functional cannot be obtained. The effective field in this example becomes

$$H_{\text{eff}} := \Delta \mathbf{m} - c \mathbf{e}_3,$$

where $\mathbf{e}_3 = (0, 0, 1)$ and c is some physical constant, chosen to be 1 in this example. The assimilation is shown in Fig. 10 (a)–(d).

Example 10: In this example, the given data are chosen to be

$$\mathbf{s}_0(x, y, z) := (1, 1, 1), \quad \mathbf{m}_0(x, y, z) := \left(\sin(x), \frac{\cos(x)}{\sqrt{2}}, \frac{\cos(x)}{\sqrt{2}} \right), \quad \text{and} \quad \bar{\mathbf{m}} = (1, 0, 0).$$

While the time step is chosen to be $k = 0.01$ as in the previous examples, here we have to choose a smaller spatial step, namely $h = 0.05$. This is due to the non-constant initial data \mathbf{m}_0 which results in larger interpolation errors at non-nodal points in D , even though at the nodal points normalization has been performed to ensure that $|\mathbf{m}| = 1$. These errors can be observed in Fig. 11 (c) (red color area). The progress of the assimilation is shown in Fig. 11 (a)–(d).

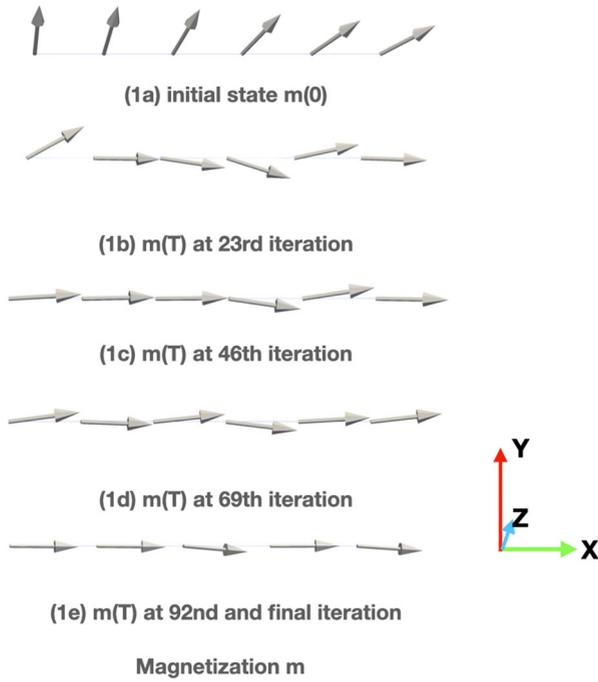


Fig. 8 Example 7: $m_0(x) = (\sin(x), \cos(x)/\sqrt{2}, \cos(x)/\sqrt{2})$, $\bar{m}(x) = (1, 0, 0)$, and $\kappa = 0.5$

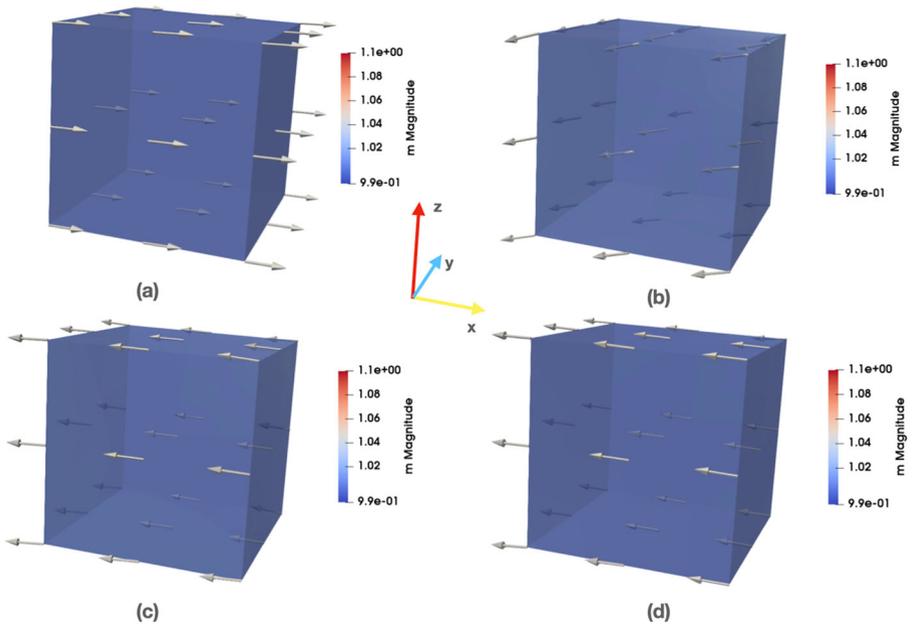


Fig. 9 Example 8: $m_0 = (1, 0, 0)$ and $\bar{m} = (-1, 0, 0)$. (a) shows the initial state; (b) shows the 10th iteration; (c) shows the 20th iteration; (d) shows the 36th and final iteration

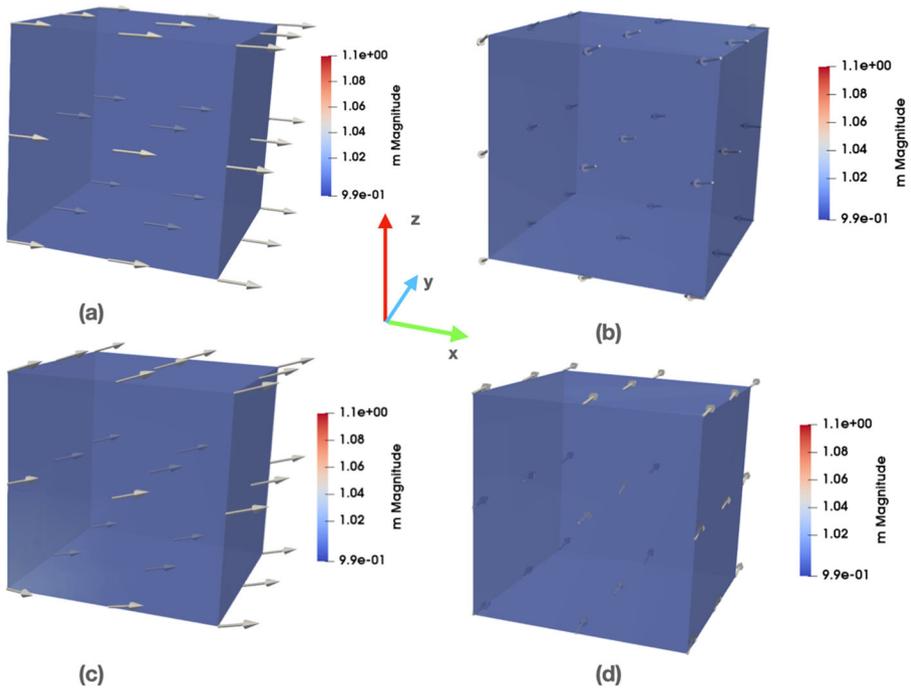


Fig. 10 Example 9: $\mathbf{m}_0 = (1, 0, 0)$ and $\bar{\mathbf{m}} = (0, 1, 0)$. (a) shows the initial state. (b) shows the 40th iteration. (c) shows the 80th iteration. (d) shows the 124th and final iteration

5.3 Discussion

The numerical simulations in Sections 5.1 and 5.2 showcase the availability of optimal control for a coupled spin-polarized current and magnetization system in a simple geometry. It is noted that, in order to provide a realistic physical interpretation and insight, a couple of issues need to be addressed. First, a more sophisticated geometry is needed. The typical case is a multilayer structure that consists of two ferromagnetic layers of given thickness that are separated by a nonmagnetic layer [1, 2, 28]. Second, more external fields should be included to the effective fields in the LLG equation. However, because this paper focuses on providing a mathematical framework for the optimal control problem, we only use the simple geometry to validate the mathematical analysis. We plan to investigate the optimal control of the coupled system in a more complicated setting in the near future.

6 Concluding remarks

In this paper, we proved the existence of the optimal solution of a coupled spin drift-diffusion Landau–Lifshitz–Gilbert system. We also showed the existence of the adjoint variables which define the first-order optimality system to be solved for the

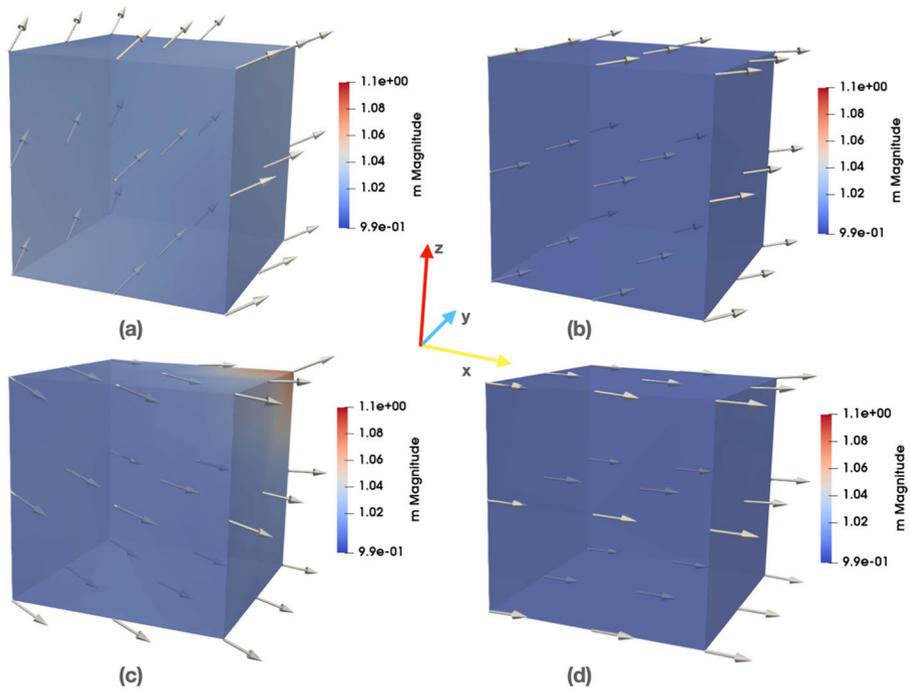


Fig. 11 Example 10: $\mathbf{m}_0 = \left(\sin(x), \frac{\cos(x)}{\sqrt{2}}, \frac{\cos(x)}{\sqrt{2}} \right)$ and $\bar{\mathbf{m}} = (1, 0, 0)$. (a) shows the initial state; (b) shows the 41th iteration; (c) shows the 92th iteration; (d) shows the 115th and final iteration

optimal solution. Theorem 2.3, Lemma 4.1, Lemma 4.2, Lemma 4.3, Lemma 4.4, and Lemma 4.5 hold only for one dimensional spatial variables, while Theorem 2.2 holds for more general dimensions.

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Declarations

Conflict of interest Authors declare no competing interests.

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