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A geometrically consistent incremental variational formulation for phase field models in micromagnetics

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ABSTRACT

Magnetic materials have been finding increasingly wider areas of application in industry ranging from magnetic cores of transformers, motors, generators to recording devices and components in magnetostrictive actuators and sensors. We focus here on the continuum modeling of such materials, which have an inherent coupling between the magnetic and mechanical characteristics. This coupling results from the existence and rearrangement of microstructural domains with uniform magnetization. The understanding and efficient simulation of these highly nonlinear and dissipative mechanisms, which occur on the microscale, is an important challenge of the current research. We present a rate-type *incremental variational principle* for a dissipative micro-magneto-elastic model. It describes the quasi-static evolution of both *magnetic as well as mechanically driven* magnetic domains, which also *incorporates the surrounding free space*. The model incorporates characteristic size-effects that are observed and reported in the literature. The associated Euler equations arising from the variational principle for the coupled problem are shown to be consistent with the Landau–Lifschitz equation, containing the damping term of the Landau–Lifschitz–Gilbert equation that describes the time evolution of the magnetization. A particular challenge is the algorithmic preservation of the geometric constraint on the magnetization director field, that remains constant in magnitude. We propose a novel finite element formulation for the monolithic treatment of the variational-based *symmetric three-field problem*, considering the mechanical displacement, the magnetization director, and the magnetic potential induced by the magnetization as the primary fields. Here, the geometric property of the magnetization director is exactly preserved pointwise by nonlinear *rotational updates at the nodes*. Numerical simulations treat domain wall motions for magnetic field- and stress-driven loading processes, including the extension of the magnetic potential into the free space.

1. Introduction

The phenomenon of ferromagnetism in solids is characterized on the macroscopic level by a local magnetization that remains even after a complete withdrawal of the applied magnetic field and the stresses. At the microscale level, ferromagnetic materials are composed of several homogeneously magnetized regions, called *magnetic domains*, whose evolution in time is driven by external magnetic fields and stresses applied to a sample of the material. This causes the characteristic 'butterfly' field-induced strain and ferromagnetic hysteresis curves on the macroscale. It is this property of *dissipative magnetostriction*, that ferromagnetic materials exhibit a magneto-mechanical coupled response and hence find use as the active components in sensors and actuators. Some examples of this class of materials are Terfenol-D ($Tb_{1-x}Dy_xFe_2$), Cobalt–Iron-Oxide ($CoFe_2O_4$) and Nickel–Iron-Oxide ($NiFe_2O_4$) which show mechanical deformations induced by the application of magnetic fields. Elementary effects and the modeling ideas for ferromagnetic materials are described in Kittel [1], Cullity [2] and Spaldin [3]. Recent interest focuses on the construction of new, so-called *multiferroic composites* with strong magnetic–electric (ME) coupling, see for example Fiebig [4], Eerenstein et al. [5] or Nan et al. [6]. The macroscopic properties of ferromagnetic materials are determined through the evolution of the domain walls and the rotation of the magnetic moment between the *easy axes* under the application of external magnetic field and stresses. These time dependent changes are dissipative in nature and therefore result in magnetic hysteresis that is typically observed at the macroscale. The description of these effects through numerical models of continuum physics is a subject of present research and may broadly be classified into two categories namely, phenomenological macro-modeling approaches that do not resolve the magnetic domains and micromagnetics that involves the explicit characterization of the domain walls. For

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macroscopic models that describe the dissipative effects in ferromagnetic materials based on the concept of internal variables, the reader is directed to magnetostrictive models that are described in the works Smith et al. [7], Linnemann et al. [8] and Miehe et al. [9]. The work Miehe et al. [10] considers a dissipative model for multiferroic composites.

In order to improve the predictive quality of such macroscale models and to have a better understanding of the underlying micromechanical driving forces, a greater emphasis on the construction of micro-mechanically motivated experiments as well as microscale models is called for. The development of such models started with the seminal work of Landau and Lifschitz [11], where the fundamentals of the so-called *domain theory* of magnetization in rigid bodies as a consequence of energy minimization have been laid. In the 1960s, Brown [12] laid the basis of the theory of *micromagnetics*, which is based on variational principles. The essential difference between domain theory and micromagnetics is that the former assumes a certain structure of the domains a priori and proceeds by optimizing this assumed structure with respect to the energy, while the latter delivers an optimum microstructure directly by solving the micromagnetic equations. Here, traditional approaches are restricted to the description of ferromagnetic effects in rigid bodies and neglect magneto-mechanical coupling. The magnetization vector

$$\boldsymbol{M} = m_s \boldsymbol{m} \quad \text{with} \quad \boldsymbol{m} \in \mathcal{S}^{d-1} \tag{1}$$

is introduced as a continuum field variable, which describes the continuous evolution of the magnetization on a microscale. The saturation magnetization m_s is taken as a constant, or more precisely, only temperature dependent. The underlying geometric structure of the magnetization director $\boldsymbol{m}$ in (1), where $\mathcal{S}^{d-1}$ denotes the hypersphere in the $\mathcal{R}^d$, constitutes the essential difference with respect to the microelectric problems (e.g. phase-field models for ferroelectric domains in Zhang and Bhattacharya [13], Schrade et al. [14]) that employ a polarization vector as the order parameter which has no constraint on its magnitude. This so-called Heisenberg–Weiss relation create a special demand on the theoretical formulations and in particular, their numerical implementation. The foundations of the ferromagnetic domains in literature is well developed. We refer to the classic overview provided by Kittel [1] and a more recent outlook in Hubert and Schäfer [15]. When ignoring for a moment the magneto-mechanical coupling effects, the domain theory for *rigid bodies* is based on the Landau–Lifschitz energy functional

$$E(\boldsymbol{m}) = \int_{\mathcal{B}} \left[\frac{\alpha}{2}|\nabla \boldsymbol{m}|^2 + \varphi(\boldsymbol{m}) - m_s \boldsymbol{m}\cdot\boldsymbol{h}\right] dV + \frac{\kappa}{2}\int_{\mathcal{R}^3} |\nabla\phi|^2\, dV, \tag{2}$$

the minimization of which, for a given external magnetic field $\boldsymbol{h}$, gives the shape of the magnetic domain. Here, the functional is valid along with the additional constraint $\text{div}[\boldsymbol{m} - \nabla\phi] = 0$, i.e. the third Maxwell equation, where for a given magnetization $\boldsymbol{m}$, ϕ is the corresponding magnetic potential. The contributions to the free energy comprise the gradient term, the non-convex term $\varphi(\boldsymbol{m})$, whose energy landscape characterizes the easy axes of magnetization, and finally, the magnetostatic part. The central problem in the solution of such *equilibrium theories* is the presence of the non-convex energy term φ. This applies equally to micro-magneto-elastic theories, where we additionally have elastic and magnetostrictive terms in the free energy, see Kittel [1] and Hubert and Schäfer [15]. This is the motivation behind considering *relaxation methods* for the solution of non-convex variational problems which are dealt with, in the works of James and Kinderlehrer [16], DeSimone [17] and DeSimone and James [18]. Here, laminate-type structures are adopted to characterize the magnetic microstructure. Further, in a 'large body limit,' the gradient term in (2) and thus the boundary of the microstructure is neglected ($\alpha = 0$). Relaxation methods for rigid ferromagnetic materials are described in DeSimone et al. [19]. Formulations that include elastic couplings are outlined in the work DeSimone and James [18]. Numerical algorithms for implementation in non-convex variational problems are found in Prohl [20] as well as Kruzik and Prohl [21]. In contrast, classical approaches to *dynamic theories* (or more correctly, quasi-static viscous theories) of domain evolution consider the celebrated Landau–Lifschitz–Gilbert Equation (LLG, see Gilbert [22]), which describes the temporal evolution of the magnetization. This equation characterizes a phase-field that is consistent with the geometric constraint $(1)_2$. Micro-magneto-elastic theories with domain evolution based on the LLG are found in Zhang and Chen [23,24], as well as the recent descriptions on the magneto-electric effects in multiferroic materials are in Li et al. [25].

However, the literature seems to be lacking a fundamental variational principles of an incremental dissipative nature, where the LLG arises as an Euler equation. This motivates the extension of the incremental variational principles for macro-magneto-mechanical problems with *locally* evolving internal variables proposed in Miehe et al. [9], towards *gradient-extended* dissipative structures with *balance-type* evolution equations for order parameters which describe the magnetization. Furthermore, the algorithmic implementation of the LLG equation involving the space- and time-discretization that is consistent with the geometric structure of the magnetization director field is particularly challenging. This has led to the implementation of projection techniques or different norm preserving numerical methods, in order to have the discretized problem capture the aforementioned geometric structure. Weinan and Wang [26], Prohl [20] and Kruzik and Prohl [21] present some solutions. In Lewis and Nigam [27] aspects of the geometrical integration on spherical manifolds is considered with a particular emphasis on micromagnetic problems. A consistent and descriptive numerical treatment within the framework of finite elements is however, not given. The problem of satisfying the constraint $(1)_2$ bears a striking resemblance to the geometrically exact descriptions of finite deformation of shell structures with inextensible directors as described in Simó et al. [28].

With these aspects in mind, the *construction of geometrically exact, variational-based numerical models for the dynamic (or quasi-static) temporal evolution of magnetic domains in ferromagnetic and magnetostrictive materials is the key focus of this work.* The challenge on the theoretical side is the formulation of a *variational principle* in terms of the rates of the primary variables of the multi-field problem of micro-magneto-elasticity which, among other things, returns a Landau–Lifschitz–Gilbert-type evolution equation for the magnetization as an Euler equation. On the computational side, the key challenge is the construction of a new space- and time-discrete *algorithmic procedure* for micromagnetic problems that preserves the geometric properties of the magnetization director.

We propose a geometrically exact finite element method for micro-magneto-elasticity that accounts for the rotational nature of the magnetization director. Our work is inspired by Lewis and Nigam [27] on geometric integration on spheres with application to micromagnetics, and also by the sequence of works by Simó and coworkers [29,28] on geometrically exact shell models that account for an exact rotational treatment of the shell directors. These ideas on the parameterization of rotations and their consistent implementation into time-space-discrete finite element methods serve as guideline for the construction of geometrically exact numerical methods in micromagnetics. In our proposed formulation, we consider the magnetization director as a geometric object, that is treated appropriately. With that guideline at hand, we outline a computational scenario for the evolution of magnetic domains that is characterized by the following three ingredients: