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Temporal upscaling in micromagnetism via heterogeneous multiscale methods

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ABSTRACT

We consider a multiscale strategy addressing the disparate scales in the Landau–Lifschitz equations in micromagnetism. At the microscopic scale, the dynamics of magnetic moments are driven by a high frequency field. On the macroscopic scale we are interested in simulating the dynamics of the magnetisation without fully resolving the microscopic scales.

The method follows the framework of heterogeneous multiscale methods and it has two main ingredients: a micro- and a macroscale model. The microscopic model is assumed to be known exactly whereas the macromodel is incomplete as it lacks effective quantities. The two models use different temporal and spatial scales and effective parameter values for the macromodel are computed on the fly, allowing for improved efficiency over traditional one-scale schemes.

For the analysis, we consider a single spin under a high frequency field and show that effective quantities can be obtained accurately with step-sizes much larger than the size of the microscopic scales required to resolve the microscopic features. Numerical results both for a single magnetic particle as well as a chain of interacting magnetic particles are given to validate the theory.

1. Introduction

Suppose that we are given an ensemble of particles $\{i\}_{i=1}^{N}$, each of them possessing a magnetic moment represented by $\mathbf{m}_i(t) \in \mathbb{R}^3$, for all $t \in [0, T]$. At a microscopic level, the dynamics of the particle i is modelled by the Landau–Lifschitz (LL) equation, [1]:

$$\frac{d}{dt}\mathbf{m}_i = -\beta \mathbf{m}_i \times \mathbf{H}_i - \gamma \mathbf{m}_i \times (\mathbf{m}_i \times \mathbf{H}_i), \quad i = 1, \ldots, N. \tag{1}$$

The first term on the right hand side accounts for the precessional motion of the magnetisation $\mathbf{m}_i$ around a field $\mathbf{H}_i$, while the nonlinear term is responsible for damping the magnetisation towards the field $\mathbf{H}_i$. In general, the effective field $\mathbf{H}_i$ includes the effects of different short and long range interactions. The short range terms are due to exchange interactions, material anisotropy, and applied external field. The exchange interaction makes the neighbouring particles be aligned with each other. The name material anisotropy comes from the fact that when no external field is applied, the direction of the magnetic moments would be aligned in certain directions in the crystal lattice. The long range terms include magnetostatic, and the magnostrictive energies. The former accounts for the interaction of the magnetic moments over long distances, and the

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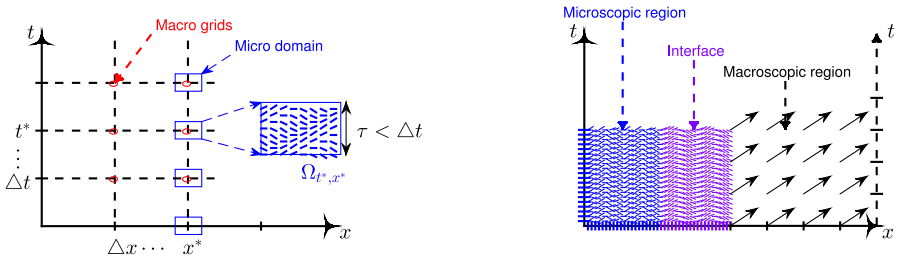

Fig. 1. (Left) A multiscale strategy based on upscaling: The macroscopic model lacks some information in the centre of the micro boxes, e.g., at (t^*, x^*). The missing effective parameter values are then computed by carrying out local, in time and space, microscopic simulations in small boxes, e.g., Ω_{t^*,x^*}. The micro problems should be synchronised with the corresponding coarse scale data and the effective quantities are computed and upscaled from the micro to the macro level. (Right) A multiscale strategy based on domain partitioning: Different mathematical laws are valid at different regions. The macroscopic region does not see the small scale variations in the microscopic domain. These two regions are connected by an interface. The interface acts as a transition region and conditions are often imposed to ensure the consistency between the microscopic and the macroscopic quantities.

latter is related to the relation between the applied stress and change in the magnetisation, see [2,3] for more details. In the presence of short range interactions, $\mathbf{H}_i$ is given by

$$\mathbf{H}_i = \sum_j J_{ij}\mathbf{m}_j + K_{ani}\langle \mathbf{p} \cdot \mathbf{m}_i \rangle \mathbf{p} + \tilde{\mathbf{H}},$$

where J_{ij} is the exchange coefficient between the particles i and j, $\mathbf{p}$ is the material anisotropy which is the energetically favourable direction of magnetisation, and $\tilde{\mathbf{H}}$ is an external field interacting with the particles. The long range interactions are ignored in the present study. The theoretical results in this paper will cover the contribution of the external field $\tilde{\mathbf{H}}$ only, but the method itself will be extended and tested when short range interactions are also present.

We are often interested in the dynamics of the magnetisation at scales much larger than the size of the spatial and temporal variations at a particle level. It is, however, computationally unaffordable to solve the microscopic model over the entire domain to simulate *macroscopic dynamics* of the magnetisation. The macroscopic quantities can be defined as e.g., local averages, in time and space, of the magnetisations of the particles. In general, it is not possible to write explicit equations for these local averages unless certain restrictive assumptions/approximations are made. Such an approach, however, lacks generality as the approximation may not be valid e.g., in the vicinity of microscopic irregularities, such as defects. To treat microscopic irregularities, it is therefore necessary to develop multiscale strategies that can iterate back and forth between an accurate microscopic and a computationally efficient macroscopic model. The microscopic model is expensive and, therefore, should be used only when necessary.

Analytical approaches have been used to derive macroscopic rules from a given microscopic model, see e.g., [4,5] for macroscopic rules describing the expected values of spin magnetic moments at nonzero temperatures, and [2,6] for examples of macroscopic rules at zero temperature starting from models at atomistic and electronic levels respectively. From a numerical point of view, there are two common types of multiscale strategies to couple the disparate scales in multiscale problems. *The first approach* is the domain partitioning strategy which implies an explicit interface between mathematical laws valid at different scales. Such methods have been developed e.g., in [7–10]. An important issue that arises in a domain partitioning strategy is the error at the interface, where two different descriptions are coupled. This issue has been addressed in [10] by introducing a damping band near the interface so that high frequency variations of the fine scale solution are damped out. *The second approach* is to use methods based on upscaling, where a macroscopic model is assumed everywhere and the microscopic information is upscaled to the macromodel only in a small part of the domain. The upscaling may be due to a one way information passing from the micro- to the macromodel, see e.g., [11], where macroscopic parameters are derived from atomistic simulations. In the present paper, however, the aim is to design and analyse an upscaling algorithm, which uses a two way coupling between the macro- and the micromodels. Such an approach is useful in situations where the magnetic behaviour is non-uniform, so that a typical one way upscaling strategy would break down. Schematics of the domain partitioning and upscaling approaches are given in Fig. 1.

In this article, as a first step towards designing general multiscale methods such as the upscaling strategy illustrated in Fig. 1 (the left schematic), we propose and analyse an upscaling strategy based on heterogeneous multiscale methods (HMM) [12], to couple disparate scales in the LL equations. The algorithm assumes a macromodel where some data in the model are missing. These data are then computed and upscaled by carrying out simulations in localised, in time and space, microscopic domains. The analysis part of this paper is limited to temporal upscaling only, and therefore the theoretical setting consists of a case where the effective field $\mathbf{H}$ includes only the influence of a time-dependent external field $\tilde{\mathbf{H}}$ and no particle interactions are involved. Since we do not have any interaction, such as exchange, among the particles, we regard all particles as being identical and rewrite the LL equation (1) as

$$\frac{d}{dt}\mathbf{m}^\varepsilon(t) = -\beta \mathbf{m}^\varepsilon \times \mathbf{H}^\varepsilon - \gamma \mathbf{m}^\varepsilon \times (\mathbf{m}^\varepsilon \times \mathbf{H}^\varepsilon)\,. \tag{2}$$