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Scale Transitions in Magnetisation Dynamics

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Abstract. Multiscale modelling is a powerful technique, which allows for computational efficiency while retaining small-scale details when they are essential for understanding a finer behaviour of the studied system. In the case of materials modelling, one of the effective multiscaling concepts is domain partitioning, which implies the existence of an explicit interface between various material descriptions, for instance atomistic and continuum regions. When dynamic material behaviour is considered, the major problem for this technique is dealing with reflections of high frequency waves from the interface separating two scales. In this article, a new method is suggested, which overcomes this problem for the case of magnetisation dynamics. The introduction of a damping band at the interface between scales, which absorbs high frequency waves, is suggested. The idea is verified using a number of one-dimensional examples with fine/coarse scale discretisation of a continuum problem of spin wave propagation. This work is the first step towards establishing a reliable atomistic/continuum multiscale transition for the description of the evolution of magnetic properties of ferromagnets.

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1 Introduction

Experimental investigations of the magnetisation dynamics is currently a most active and challenging research field [1–6]. The scientific questions which are addressed in these studies focus e.g. on advanced magnetic materials for data storage and magnetic memories, with the aim of understanding the fundamental limit of magnetisation switching and reversal. Technical avenues to reach this fundamental limit are pursued experimentally, e.g. using optical control, current induced phenomena and all-thermal switching,

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and several breakthroughs have been reported. In these experimental works it has been found that a Laser pulse can be used to demagnetise a ferromagnetic sample on time scales of picoseconds down to femtoseconds [1–6]. These studies are still on a very fundamental level and for practical aspects it can be argued that in device design a setup involving a Laser might be a hinder.

On the theory side methodologies have been developed that are based on the concept of micromagnetism [7,8], which provides a framework for understanding magnetisation dynamics on length scales of micrometers and in which the magnetisation is considered as a continuum variable. In this approach, the magnetism is treated as a continuum vector field on a relatively large length scale. The power of being able to couple such continuum based theories to the recently emerging atomistic theory of magnetisation dynamics [9] is obvious. One could then treat larger sections of the simulation box that have less structure or detail using the continuum model, while smaller regions with more detail could be treated on an atomistic scale. However, it is not straightforward to take the necessary step in this multiscale approach to magnetisation dynamics. Nevertheless, a reliable theoretical tool which could serve as a complement to modern experimental works on magnetisation dynamics and ultrafast switching phenomena is highly desirable, both when it comes to understanding the mechanisms which play role, but also for predicting phenomena and novel materials/concepts.

There are multiple ways of performing multiscale simulations, one of which is domain partitioning, where there is an explicit interface between various material descriptions. Models of coupling atomistic and continuum descriptions were initially developed to describe the mechanical behaviour of solids [10]. There is a wide variety of methods, which are applicable in the case of quasistatic behaviour [11], however, modelling the dynamic behaviour is more problematic, in particular, wave reflections from the interface between two descriptions present a challenge for multiscale techniques. Recently a significant progress has been made in this area [12,13]; a modification of the equation of motion of atoms in the proximity of the atomistic/continuum interface was suggested, such that high frequency waves are damped in this region.

There are also multiscale techniques, which are developed for the simulation of the magnetic material properties. In [14], some aspects of constructing continuum micromagnetic description and estimating its parameters based on atomistic spin dynamics were discussed. In [15], a way of coarse-graining from the atomistic to micromagnetic description, with a gradual transition of discretisation between descriptions, was presented. However, the proposed method was limited to the static problem of finding equilibrium states in the domain partitioned into atomistic and micromagnetic regions. Recently a way of constructing a transition between two descriptions for dynamic problems was published [16]. This approach suggested an overlapping of the atomistic and the continuum regions where the exchange energies of the two models are mixed. The model was used to describe the dynamics of Bloch points, which were surrounded by the atomistic description, while the rest of the material was modelled as a continuum. However, the continuum model still had to be discretised down to the atomistic scale,