

CSC/WCPM joint seminar

Coupling atomistic and continuum modelling of magnetism

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P5.23 Seminar room, Department of Physics, 5th Floor

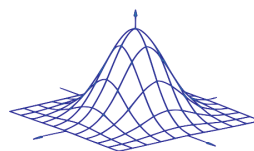
Abstract: Physical properties of materials are often highly dependent on the underlying microstructure and affected by presence of defects and/or heterogeneities at the atomistic length scale. Multiscale atomistic-continuum models allow investigating the influence of the small-scale phenomena on macroscopic quantities without using the fine-scale resolution over the entire computational domain.

The dynamic behaviour of ferromagnetic materials can be simulated either at the atomistic scale, where spin magnetic moments of individual atoms are considered while atomic positions are fixed, or at the continuum scale, where the evolution of volume-averaged coarse-grained quantities, such as magnetisation, is described by the specific PDEs. Interfacing these descriptions by domain partitioning, which implies the existence of an explicit interface between atomistic and continuum regions, leads to some computational difficulties, such as the mismatch between nonlocal atomistic interactions and local continuum description and, in the case of dynamics, high frequency wave reflections at the interface due to change in discretisation.

In this talk, the technique of introduction of numerically-damped quasi-nonlocal atoms at the proximity of the interface, which interact differently with the atomistic and the continuum regions and which absorb high frequency waves, is discussed. To illustrate the applicability of the developed method, examples of a propagation of spin waves and a motion of domain walls in ferromagnetic materials with crystallographic defects are shown.

A buffet lunch is available from 12:45 pm.

More info: <http://warwick.ac.uk/wcpm/seminars>



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