SP 11 Micromagnetic modelling

SP11 - Parallel Session 1

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SP11.1.02

Analogue simulation of three dimensional magnetic self assembly processes

P. Löthman, T. Hageman, L. Abelmann

Text We constructed a system in which we can study the dynamics of self-assembly processes on the macroscale. We insert 3D printed polymer objects of centimeter size with embedded permanent magnets inside a transparent cylinder with upward water flow. The turbulence in the water shakes the objects so that the system can probe the energy landscape and find the minimum energy state. We show that this experimental setup obeys fundamental thermodynamic properties: individual objects show Brownian motion with a well defined diffusion coefficient, the velocity of the objects is Maxwell-Boltzmann distributed, the Einstein relation is obeyed and object interaction follows Boltzmann statistics. By adjusting the water inflow, we can adjust the energy in the turbulence ("the temperature") by a factor of ten, so that we can simulate cooling. We used this system to investigate interaction between spheres, and show that rings are the minimum energy state if they consist of more than four spheres. as is predicted by theoretical studies. We discoverd that the object aspect ratio determines whether 1D (lines), 2D (plates) or 3D (crystals) structures are formed. Cylindrical objects form more regular crystals than spheroids or cubes. The setup can be regarded "analogue computer" for molecular dynamics studies. The simulation time is independent on the number of objects and entropy is inherently included. As such it offers an interesting complement to numerical simulations.

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SP11.1.03

Solving large-scale magnetostatic problems in finite-element micromagnetics with H2 matrices

S. Christophersen, S. Börm, R. Hertel

Text Simulating large-scale micromagnetic problems based on the Landau-Lifshitz-Gilbert equation requires highly efficient numerical methods to calculate the effective field at every time step. In finite-element micromagnetics, the long-range magnetostatic interaction is the computationally most critical contribution to the effective field. Established methods to calculate the magnetostatic field via a boundary integral [1] suffer from the occurrence of a densely populated matrix and thus an $O(N^2)$ scaling that precludes large-scale computations. Previous studies [2,3] have employed hierarchical matrix methods [4] which reduce the size of the boundary matrix to an $O(N \cdot \log N)$ type scaling. Here we show that the additional hierarchical structure provided by H2 matrices [5] can further improve dramatically the matrix compression, yielding almost linear complexity. We obtain matrix size reductions beyond 99% in test cases with more than 10^6 degrees of freedom, and we demonstrate the high accuracy of the computed field by means of comparison with analytic values.

1. D.R. Fredkin & T.R. Koehler, IEEE Trans. Magn. 26, 415 (1990).
2. A. Knittel et al., J. Appl. Phys. 105, 07D542 (2009).
3. A. Kakay, E. Westphal & R. Hertel, IEEE Trans. Magn. 46, 2303 (2010).
4. W. Hackbusch, Hierarchical Matrices: Algorithms and Analysis (Springer, 2015).
5. S. Börm, Efficient Numerical Methods for Non-local Operators: H2-matrix Compression, Algorithms and Analysis. 14, (European Mathematical Society, 2010).

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SP11.1.04

Massively parallel micromagnetic simulations of small-size nanoelements with applications to STT-MRAM devices

D. Berkov, E. Semenova

Text We present a new micromagnetic methodology for simulation of a large number of small-sized nanoelements by fully exploiting the high acceleration provided by modern GPUs only for large systems. The major target of the method is magnetization dynamics in nanoelements with sizes of 10 to 100 nm, which are of the primary interest for designing MRAM cells.

We apply our method to the spin-torque-induced magnetization switching of elliptical elements. Switching has been studied for two cases: the constant total current and the constant current density through the MRAM cell. By computing simultaneously the reversal of up to 1000 nanoparticles, we obtain the switching time dependence on the element size with a high statistical accuracy.

Comparison to the macrospin approach has shown that full-scale simulations are essential for nanoelement sizes > 40 x 50 nm. Switching times obtained by full-scale simulations exceed that of the macrospin model; this difference rapidly growths with the element size. Analysis of the switching process has shown that for moderate sizes (short ellipse axis b = 40 nm, long axis a < 90 nm) magnetization switches via the nucleation and growth of small reversed regions; for a > 90 nm reversal occurs via the domain wall propagation. We also demonstrate the relation between switching time and excitation of higher eigenmodes with increasing nanoelement size.

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SP11.1.05

A 2.5D micromagnetic solver for randomly distributed magnetic thin objects

A. Manzin, R. Ferrero

Text The micromagnetic simulation of large numbers of interacting magnetic nano-objects is a complex task, needing long computation time for the spatial discretization of the Landau-Lifshitz equation. This happens when modelling dot-arrays for magnetic storage and magneto-logic devices, spin-ice structures or magnetic nanosystems for biomedical applications. In the last example, the nano-objects can be randomly distributed in a 3D space (a biological fluid or a tissue), with variable orientation. In this case, 3D FFT techniques, typically used for the magnetostatic field calculation, cannot be applied, since they require structured meshes that are not suitable for objects non-aligned with the mesh grid.
Here, we present a novel 2.5D GPU-parallelized micromagnetic solver able to simulate high concentrations of thin nano-objects, randomly distributed in a 3D space. Each nano-object is discretized with a non-structured mesh, to well-reproduce complex shapes and very different mutual orientations. The exchange field is calculated with a finite difference approach able to handle non-structured meshes, while the magnetostatic field is separated into a local and a long-range contribution. The first term includes the interactions between mesh elements belonging to the same object, while the second term describes the interactions between different objects, via a dipole approximation. The numerical model is validated in test cases by comparison to standard 2D and 3D micromagnetic solvers.

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SP11 - Parallel Session 1

SP11.1.06

Numerical integration of generalized Landau-Lifshitz-Gilbert equation based on the mid-point rule

C. Serpico, M. d'Aquino, V. Scalera, M. Hudl, S. Bonetti

Text Magnetization dynamics described by the Landau-Lifshitz-Gilbert (LLG) equation has the property of preserving magnetization magnitude. This is expected to be correct for ferromagnets with a temperature well below Curie's temperature subject to fields up to the microwave frequency range. In magnetization dynamics excited in all-optical magnetic switching and under THz applied fields, magnetization magnitude is not preserved and this requires the use of generalized LLG equations[1]. In these equations, magnetization magnitude is not preserved due to the presence of longitudinal (along magnetization) relaxation terms. In this paper, we consider the numerical time integration of the generalized LLG equation by using time-stepping techniques based on the mid-point rule [2], for the problem of magnetization dynamics in thin films induced by THz-fields[3]. When relaxation is set to zero, the mid-point integration preserves the property of the exact conservation of magnetization amplitude. When relaxation is present, generalized LLG equations have a Lyapunov structure: the free energy of the system is a decreasing function of time for constant applied fields. In this respect, we analyze the accuracy in the preservation of the Lyapunov structure and the stability of the time-stepping as function of the time step.

[1] U. Atxitia et al., J. Phys. D: Appl. Phys. 50, 033003 (2017)
[2] M. d’Aquino et al., J. Comp. Phys. 209, 730 (2005)
[3] D. Polley et al., J. Phys. D 51, 084001 (2018)

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SP11 - Parallel Session 1

SP11.1.07

Coupled lattice and spin dynamics from second principle

X. He, A. Martin, E. Bousquet, M. Verstraete, P. Ghosez

Text We present second principle methods of coupled lattice and spin dynamics implemented in multibinit, which is a component of the Abinit project. While density functional theory (DFT) can predict structural, electronic, and magnetic properties of materials with high accuracy, the high computational cost hinders its usage in large systems, which is usually needed in dynamics simulations. We develop second principle methods to build coupled molecular and spin dynamics models, where the parameters of the lattice and spin effective Hamiltonians and their couplings are extracted from DFT results automatically. The strategies for building and solving the models will be discussed. With this method, it is possible to simulate large systems with both lattice and spin degrees of freedom while keeping the DFT accuracy.

SP11 - Parallel Session 2

SP11 - Parallel Session 2

SP11.2.02

Experimental and computational study of magnetization reversal in Dy-Co diffused Nd-Fe-B sintered magnets

J. Fliegans, G. Delette, C. Rado, D. Givord, N. Dempsey

Text Developing permanent magnets containing less or no heavy rare-earth elements requires a better understanding of the link between microstructure and coercivity.

In this study, core-shell microstructures have been obtained for Nd-Fe-B sintered magnets by the grain boundary diffusion process from a Dy-Co coating. This method allows a localization of Dy mainly near the grain boundary. Examination by SEM confirms that Dy is not homogeneously distributed.

Coercivity of Nd-Fe-B magnets has been measured with and without Dy diffusion at two different fabrication steps: after sintering and after optimal annealing. It has been found that Dy diffusion alone leads to an increase in Hcj of 30% while Dy diffusion combined with annealing raises the Hcj by 78%.

Micromagnetic simulations have been performed with the FEMME code to simulate the core-shell structure. A model consisting of 8 cubic grains was used. Each grain comprises a $Nd_2Fe_{14}B$ core surrounded by a $(Nd,Dy)_2Fe_{14}B$ shell. Moreover, the grains are separated by a non-magnetic grain boundary phase. A defect is localized in one of the grains, acting as the nucleation zone for magnetization reversal.

Simulations clearly show that the $(Nd,Dy)_2Fe_{14}B$ shell hinders the propagation of the reversed domains from the defect to neighboring grains. The coercivity is enhanced by 30-36%, in good agreement with the experimental results. A parametric study has been performed to analyze some microstructural features *i.e.* shell thickness and repartition.

SP 11 Micromagnetic modelling

SP11 - Parallel Session 2

SP11.2.03

Frequency engineering of spin-torque diode

P. Skirdkov, A. Khudorozhkov, K. Zvezdin, P. Vetoshko, A. Popkov, A. Zvezdin

Text One of the emerging novel spintronic technologies is a spin-torque diode. Based on the radio-frequency rectification phenomenon (so called spin-torque diode effect), it could be used for detecting radio-frequency signals and microwave energy harvesting, as its sensitivity significantly overcomes sensitivity of commonly used Schottky diodes. For implementing this technology into a working prototype, we present several configurations of spin-torque diode, considered by micromagnetic modeling, aiming at achieving high sensitivity, comparable to the one of Schottky diode, in a wide range of frequencies.
The first concept includes a spin-torque diode with both magnetic layers softly pinned at some tilt to each other using antiferromagnets with different Neel temperature. The resonance operating frequency of such dual exchange-pinned spin-torque diode can be significantly higher (up to 9.5 GHz) than that of a traditional free layer spin-torque diode. At the same time, it is possible to tune the frequency of such diode during the manufacturing by choosing the angle between the pinning fields. The second concept is a vortex spin-torque diode, represented by MTJ with tilted polarizer and vortex magnetization distribution in the free layer. In this case the resonant frequency can be moved down to 300-400 MHz. For both cases the impact of the bias current is also considered.
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