Influence of space discretization size in 3D micromagnetic modelling

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I. Introduction

To improve the magnetic properties of ferromagnetic materials, one needs to qualify relations between the microscopic material properties and the macroscopic magnetic behavior. Large computer resources nowadays allow to do this using micromagnetic ab initio simulations for larger, bulk like samples. Here, the size of the sample is limited by computer resource restrictions on the number of spatial discretizations in the sample.

II. Spatial discretization

In the three dimensional numerical scheme, the sample is discretized in N cubic finite difference (FD) cells with edges of length Δ. The evolution of the magnetization in every FD cell is computed through time stepping the Landau-Lifshitz equation using time steps δt [1]. In each time step the effective field incorporating the exchange, anisotropy, magnetostatic, magneto-elastic and applied field has to be evaluated twice in every FD cell.

In classical micromagnetic simulations, the exchange length is seen as a maximum discretization size since on a larger scale, magnetization nonuniformities are possible. However, in order to simulate larger bulk like samples, one could aim at a larger discretization size Δ resulting in a local averaging of the variations in magnetization. To test this, numerical experiments are performed on an iron sample with dimensions of $0.32\,\mu m \times 1.28\,\mu m \times 0.32\,\mu m$. The discretization length Δ is $2.5\,nm$, which is slightly smaller then the exchange length in pure iron ($2.8\,nm$), $5.0\,nm$ and $10.0\,nm$ which leads to respectively 8 388 608, 1 048 576 and 131 072 FD cells. The hysteresis loops are shown in Fig. 1. They are simulated when applying a magnetic field along the longest edge of the sample.

The loops are almost identical: they have the same slope and enclose a similar surface. Table I shows the used time step δt, the number of microscopic time steps and the total CPU time. A smaller time step δt is needed when a smaller discretization Δ is used[1],

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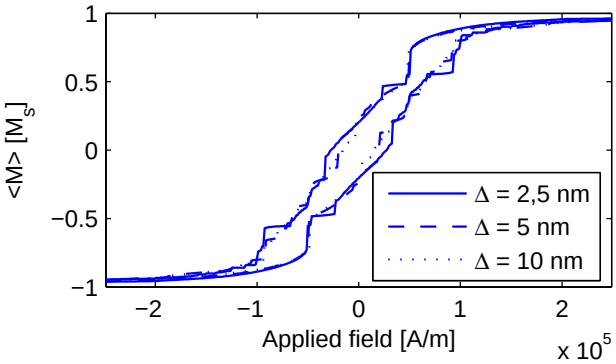

Fig. 1. Hysteresis loops for an identical iron sample using different discretization lengths

resulting in a massive increase in number of microscopic time steps needed to simulate the loops (cfr. column 3). Furthermore, the huge number of FD cells when a small Δ is used, results in a slow evaluation of the effective field in each FD cell every time step. Combined with the large number of time steps, it explains the massive differences in CPU time.

TABLE I
Simulation data for different discretization lengths

$\Delta\ [nm]$	$\delta t\ [ps]$	$\#\ \delta t$	CPU time
2.5	0.5	27 036	$103.25\,h$
5.0	1.0	14 627	$8.55\,h$
10	5.0	1 463	$7.46\,min$

III. Conclusions

The small differences in Fig. 1 justify the use of discretization lengths larger then the exchange length in the model. However, the discretization size should be sufficiently small with respect to the thickness of domain walls ($70\,nm$ in Fe) and the dimensions of vortex states (about 35 nm in Fe). Considering this together with the massive differences in CPU time and memory needs justifies the use of a discretization length up to $10\,nm$.

References

[1] B. Van de Wiele, F. Olyslager and L. Dupré, "Fast numerical 3D-scheme for the simulation of hysteresis in ferromagnetic grains", accepted for publication in *Journal of Applied Physics*.

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