A 3D micromagnetic solver with time integration based on the Cayley transform

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The need of simulating phenomena at the exchange length scale as well as long-range interactions, such as the magnetostatic field, can make the spatial integration of the Landau-Lifshitz-Gilbert (LLG) equation very computationally demanding. Additionally, it's important to take great care in ensuring that the time integration preserves the magnetization amplitude with sufficiently large time-steps [1]. To overcome these challenges, we have developed a 3D micromagnetic solver that uses GPU-parallelization and an FFT-based approach for magnetostatic field evaluation [2]. To ensure that the magnetization constraint is maintained independently of the scheme order and time-step size, we utilize a geometric integration method based on the Cayley transform for time updates [3,4]. Specifically, we solve a generalized form of the LLG equation:

$$\dot{\mathbf{M}}(\mathbf{r},t) = \left[\mathbf{A}\big(\mathbf{M}(\mathbf{r},t)\big) + \sigma\mathbf{M}(\mathbf{r},t)\right] \times \mathbf{M}(\mathbf{r},t), \qquad (1)$$

where **A** is the generator that depends on the magnetization vector **M** and on the effective field [3]. Equation (1) is equivalent to the LLG equation for $\sigma = 0$; this form is particularly advantageous for the computation of static hysteresis loops, since the addition of term $\sigma\mathbf{M}$ can speed up the reaching of equilibrium, allowing the use of larger time-steps [5].

Here, we test the efficiency of the solver, focusing on the calculation of the equilibrium states of 3D nanostructures. The figure below shows the damping effect of parameter σ in the determination of the remanent state of a permalloy nanosphere, demonstrating that for values of σ in the order of the gyromagnetic ratio γ it is possible to reach equilibrium in less time with a reduced number N of time-steps ($\sigma = 0$: $N \approx 3\times10^6$; $\sigma = 9\gamma$: $N \approx 1\times10^5$). However, very high values of σ can lead to an overdamping. When $\sigma = 22.5\gamma$, the magnetization may remain stuck in a local energy minimum, if a not sufficiently strong equilibrium convergence condition is imposed, or may evolve very slowly towards the global minimum, reducing the computational advantage obtained with the numerical dampening ($N \approx 2\times10^5$)

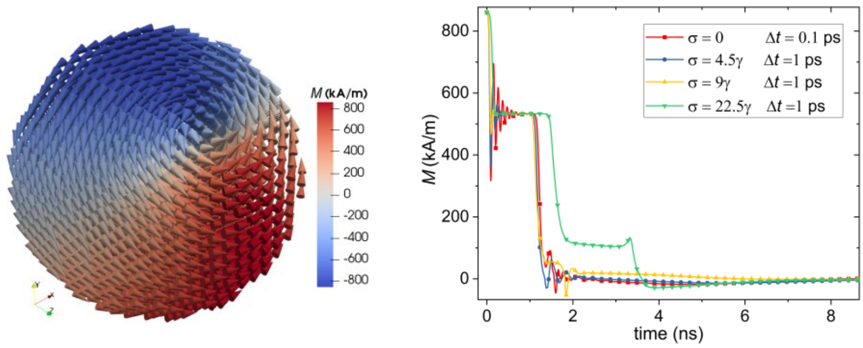

Figure 1: Left: Time evolution from saturation to remanence state of the radial component of the magnetization of a 100 nm permalloy nanosphere, showing the effect of σ. Right: Remanent state of the sphere; the cones represent the magnetization vector direction.

References

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