Efficient Simulation of Ferromagnetic Spin Configuration

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1. Introduction to shape anisotropy

In ferromagnetic materials, spins of atoms prefer to align in a parallel way below the Curie temperature T_C, as a result of the ferromagnetic nearest-neighboring interaction. Classical Monte Carlo algorithm is a powerful and efficient tool to simulate the spin configuration of ferromagnets by using Heisenberg model. However, realistic ferromagnets usually involve many other interactions, like dipole-dipole interaction (DDI), crystalline anisotropy, Zeeman energy, etc.

Considering the boundary effect of ferromagnets, shape anisotropy will affect the spin configuration. This anisotropy comes from the long-ranged DDI. As a result in long thin ferromagnets, spins prefer to align parallel to the long side of ferromagnets. In addition, magnetic domains of flux-closure shape can be observed in ferromagnets, as the length and width of rectangle are approximately equivalent. These two kinds of spin configuration is related to not only the competition of the nearest-neighboring exchange interaction J and dipole-dipole interaction D, but also the shape of the ferromagnets. Shape anisotropy plays an important

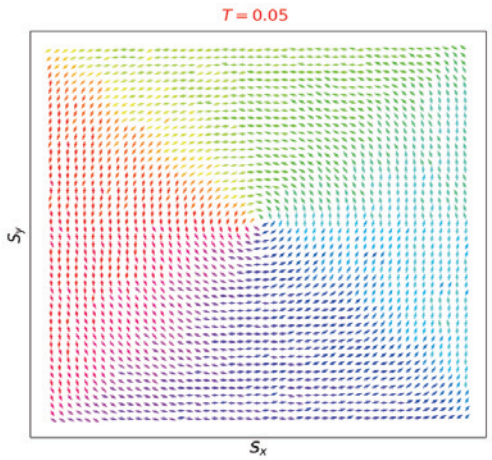

Fig. 1 Vortex spin configuration in 50×50 spins systems (J = 1, D = 0.1)

We simulate the spin configuration from a first-principle perspective and study the phase diagram of spin configuration with different system sizes and interaction constants.

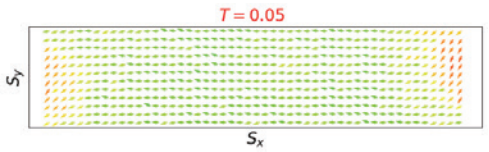

Fig. 2 Spin configuration parallel to long side in 50×12 spins systems (J = 1, D = 0.1)

All these interactions, except DDI, are short-ranged interactions, so the time complexity of simulating is in order of $O(N)$ per Monte Carlo steps (MCS). Here, N is the number of independent spins. Unfortunately, the long-ranged DDI exists between every two spins, so the time complexity is in order of $O(N^2)$ per Monte Carlo steps (MCS).

2. Efficient Simulation with Stochastic Cutoff (SCO) algorithm

In Monte Carlo simulation for magnetic systems, the great majority of the DDI terms is almost negligible, comparing to the exchange interaction, so they have hardly any influence on the accept-or-reject decision for new samplings. SCO algorithm utilizes this feature and switch most of the unimportant DDI terms to 0, and the others to a different $\overline{V}$ to satisfy the detailed balance condition.

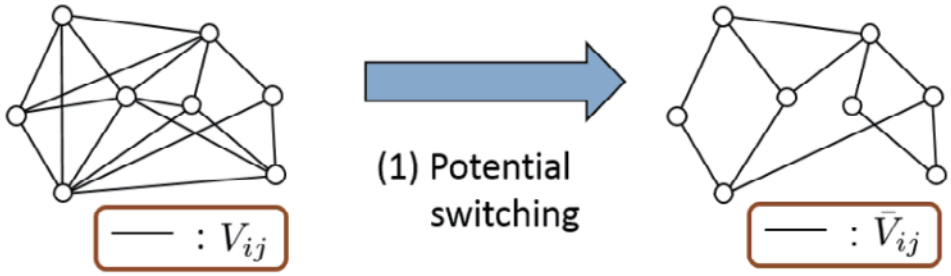

Fig. 3 SCO sets the majority of bonds to 0, whereas the values of remaining bonds are switched from V to $\overline{V}$. It is proven that the detailed balance condition is unchanged after the stochastic cutoff.

It has been tested and measured that SCO algorithm can speed-up the Monte Carlo simulation for large-scale ferromagnetic systems.

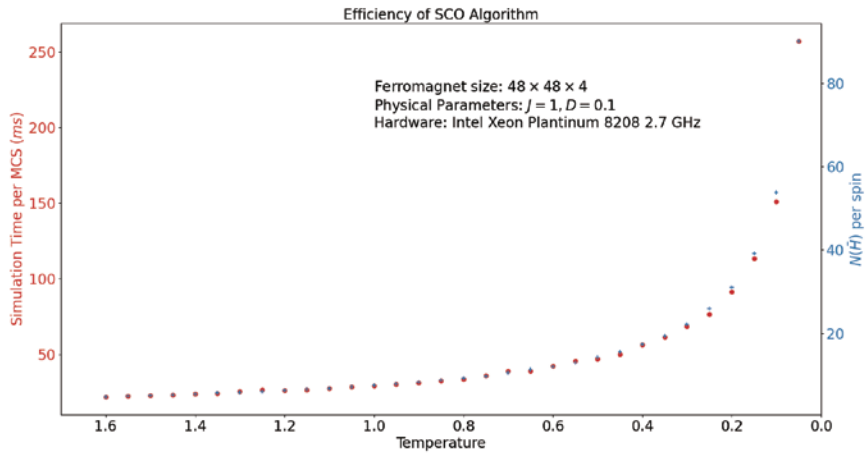

Fig. 4 Efficiency of SCO on Oakbridge-CX for $48 \times 48 \times 4$ ferromagnets. Following the decrease of temperature, more DDI terms are switched to non-zero $\overline{V}$, and the simulation time increases accordingly.

Reference

"Stochastic potential switching algorithm for Monte Carlo simulations of complex systems" *J. Chem. Phys.* **122,** 213110 (2005)

"Order-N cluster Monte Carlo method for spin systems with long-range interactions" *J. Comput. Phys.* **228,** 2629-2642 (2009)