Finite Element Mesh Based Hybrid Monte Carlo Micromagnetics

Lei Xu

1 College of Engineering, Peking University, Beijing, China xulei_1988@pku.edu.cn

To deal with magnetic problem at finite temperature, hybrid Monte Carlo (HMC) micromagnetics method has been proposed in the past years. Previous study of HMC micromagnetics is based on finite difference mesh (FDM), FDM usually consists of identical micromagnetic cells, the fast Fourier transformation (FFT) algorithm can be applied to speed up the simulation, but FDM has difficulty in dealing with irregular shaped model. To overcome the geometry difficulty encountered in FDM, the finite element mesh (FEM) based HMC micromagnetics method is developed in this work. For the ellipsoidal shaped single domain magnetic particle, the decrease of coercive field versus temperature can be explained by FEM-HMC micromagnetics, and the numerical results agree well with analytical ones. The FEM-HMC micromagnetics method could be a useful tool in dealing with magnetic problem with irregular shape at finite temperature, it has promising application in the study of engineering device.

Index Terms—Finite element, finite temperature, hybrid Monte Carlo, micromagnetics

I. INTRODUCTION

THE GROWING application of magnetic material and the improving large-scale computational ability are the main impetus to the further development of the computational micromagnetics. For the study of real engineering problem, the thermal fluctuation and irregular shaped boundary are often inevitable and have significant effect on the micromagnetic simulation.

At finite temperature, not only the minimum energy state, but also other configurations of magnetization texture could contribute to the quasi-static equilibrium state according to their corresponding Boltzmann distribution. In order to obtain the correct Boltzmann distribution for the magnetization in thermal equilibrium, the hybrid Monte Carlo (HMC) micromagnetic has been developed [1], [2] in recent years. Previous application of the HMC is based on finite difference mesh (FDM) [1], [2], so it has difficulty in dealing with irregular shaped model. So the hybrid Monte Carlo micromagnetic method based on finite element mesh (FEM-HMC) has been developed in this work. To verify the correctness of FEM-HMC method, the magnetic properties of ellipsoidal Stoner-Wohlfarth model at finite temperature has been studied by the FEM-HMC micromagnetics. The results calculated by FEM-HMC micromagnetics is consistent with analytical results. The FEM-HMC micromagnetics enables magnetic model to be more geometrically accurate, so it has promising application in the study of real engineering device with complex structure at finite temperature.

II. HYBRID MONTE CARLO MICROMAGNETICS

The total free energy \( \mathcal{F} \) for a determined magnetization texture is the summation of Zeeman energy, exchange energy, demagnetization energy and anisotropy energy, etc. The demagnetization energy in each element is calculated by the hybrid FE-BE method proposed by Fredkin and Koehler [3].

The reduced HMC Hamiltonian for the magnetic model can be expressed as the summation of the free energy and a kinetic-like term

\[
h = \frac{1}{2} \sum_e V_e \mathbf{P}_e^2 + \frac{1}{k_B T} \mathcal{F} [M_e] \quad (1)
\]

The magnetization vector \( M_e \) and the quantity \( \mathbf{P}_e \) can form a pair of conjugate variables, which lead to the following equations of fictitious motion.

\[
\frac{1}{V_e} \frac{dM_e}{dt} = \mathbf{P}_e \\
\frac{1}{V_e} \frac{d\mathbf{P}_e}{dt} = -\frac{1}{k_B T} \frac{\delta \mathcal{F}}{\delta M_e}
\]

To ensure \( |M_e| = M_s \) at low temperature, a Lagrange multiplier \( \mathcal{F}_L \) is also added to the free energy, which can be written as

\[
\mathcal{F}_L [M_e] = \sum_e \frac{1}{4 M_s^4} (M_e^2 - M_s^2)^2 V_e \quad (2)
\]

where \( \lambda \) is the Lagrange parameter. The temperature dependence of saturation magnetization is dealt by solving the Brillouin function [1]. The temperature dependence for uniaxial anisotropy constant is scaled in the form as [1], [2]

\[
\frac{K_1 (T)}{K_1 (0)} = \left( \frac{M_s (T)}{M_s (0)} \right)^\eta \quad (3)
\]

The simulation in this work will focus on the correctness of FEM-HMC micromagnetics method, the scaling coefficient \( \eta \) and the quantum number in Brillouin function are fixed as 3 and 1/2 respectively. Values of saturation magnetization and uniaxial anisotropy constant calculated by the Brillouin function at certain temperatures are shown in Table 1 the decrease of saturation magnetization and uniaxial anisotropy constant near the curie temperature is obvious.

In the application of HMC simulation, the initial configuration of \( M_e \) in each element can be arbitrary, and configuration of the conjugate momenta \( \mathbf{P}_e \) can be generated by Gaussian distribution \( \exp \left( -\sum_e V_e \mathbf{P}_e^2 / 2 \right) \), then the initial Hamiltonian \( h (0) \) can be calculated from the initial conjugate variables of \( M_e \) and \( \mathbf{P}_e \). New configuration of \( M_e \) and \( \mathbf{P}_e \) are obtained by leapfrog integration algorithm. Calculate the Hamiltonian \( h (t) \) by the new configuration of \( M_e \) and \( \mathbf{P}_e \),
TABLE I

Temperature dependence of saturation magnetization and uniaxial anisotropy constant, the scaling coefficient and quantum number in Brillouin function are 3 and 1/2 respectively.

<table>
<thead>
<tr>
<th>$T/T_C$</th>
<th>$M_s(T)/M_s(0)$</th>
<th>$K_1(T)/K_1(0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>0.5</td>
<td>0.9575</td>
<td>0.8048</td>
</tr>
<tr>
<td>0.9</td>
<td>0.5254</td>
<td>0.1451</td>
</tr>
</tbody>
</table>

if $\Delta h = h(t) - h(0) < 0$, the new configuration is accepted, otherwise, the new configuration is accepted with a probability $\exp(-\Delta h)$. Magnetization configuration satisfy the Boltzmann distribution can then be generated by repeating above steps.

III. RESULTS AND DISCUSSION

The ellipsoidal magnetic particle can be easily discretized by the finite element mesh, the M-H loops and coercive fields under finite temperature can be obtained by applying the FEM-HMC micromagnetics simulation. The correctness of the numerical results is checked by comparing with the analytical results given by Stoner-Wohlfarth model.

Fig. 1. Ellipsoidal magnetic model discretized by tetrahedral mesh.

The $x$, $y$, $z$ semi-axis of the ellipsoidal model have lengths of 3nm, 3nm and 9nm respectively. Tetrahedron element is used to discretize the ellipsoidal model, shown in Fig. 1, the total element number is 829. The free energy of the Stoner-Wohlfarth single-domain model in external magnetic field can be expressed as

$$
\frac{F}{V} = -2\pi M_s^2 (N_x - N_z) \cos^2 (\phi - \theta) - M_s H_{ext} \cos \phi \quad (4)
$$

where $\theta$ is the angle between external field and the easy axis, $\phi$ is the angle between magnetization vector and the easy axis, $N_x$ and $N_z$ are the demagnetization factors along the easy axis and hard axis respectively. The demagnetization factors can be calculated analytically as $N_x = 0.4456$ and $N_z = 0.1087$ [4], numerical calculation by finite elements shown in Fig. 1 give the results as $N_x = 0.447$ and $N_z = 0.1061$, which agree well with analytical ones. At zero temperature, the saturation magnetization constant $M_s$ is 1000emu/cm$^3$, the exchange constant is $1.3 \times 10^{-6}$erg/cm. The external magnetic field is applied in three different direction along the easy axis, i.e. 0 degree, 45 degrees and 90 degrees, the corresponding M-H loops calculated by FEM-HMC are shown in Fig. 2(a), (b) and (c) respectively.

Fig. 2. M-H loops of ellipsoidal magnetic model under different temperature, the vertical axis is the normalized average magnetization with respect to $M_s(0)$ along the external field. The external field is applied along the easy axis with angle of 90 degree (a), 45 degrees (b) and 0 degrees (c).

TABLE II

Comparing results of coercive fields obtained by FEM-HMC micromagnetics and analytical study.

<table>
<thead>
<tr>
<th>$T/T_C$</th>
<th>0.1</th>
<th>0.5</th>
<th>0.9</th>
</tr>
</thead>
<tbody>
<tr>
<td>FEM-HMC (0 degree)</td>
<td>4425Oe</td>
<td>3975Oe</td>
<td>2188Oe</td>
</tr>
<tr>
<td>Analytical (0 degree)</td>
<td>4234Oe</td>
<td>4054Oe</td>
<td>2225Oe</td>
</tr>
<tr>
<td>FEM-HMC (45 degrees)</td>
<td>2125Oe</td>
<td>2025Oe</td>
<td>1125Oe</td>
</tr>
<tr>
<td>Analytical (45 degrees)</td>
<td>2117Oe</td>
<td>2027Oe</td>
<td>1120Oe</td>
</tr>
</tbody>
</table>

The decrease of coercive field with increasing temperature can be seen from Fig. 2, the comparing results of coercive field is shown in Table II, these numerical results agrees well with analytical results obtained by the analysis of the free energy shown in equation (4). So the correctness of FEM-HMC micromagnetics for arbitrary shaped model at finite temperature can be guaranteed.

REFERENCES