Implementation of the "Hyperdynamics of Infrequent Events" Method for Acceleration of Thermal Switching Dynamics of Magnetic Moments

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***Abstract*—For acceleration of the calculations of thermal magnetic switching, we report the use of the Voter method, recently proposed in chemical physics (also called "hyperdynamics of the infrequent events"). The method consists of modification of the magnetic potential so that the transition state remains unchanged. We have found that the method correctly describes the mean first passage time even in the case of small damping (precessional case) and for an oblique angle between the anisotropy and the field directions. Due to the costly evaluation of the lowest energy eigenvalue, the actual acceleration depends on its fast computation. In the current implementation, it is limited to intermediate time scale and to small system size.**

***Index Terms*—Computational magnetics, numerical methods, spin dynamics and relaxation.**

THE major problem of current magnetic recording media is the superparamagnetic effect, which limits the stability of stored information. The use of numerical techniques is one of the tools which are applied to predict the thermal stability of recorded information. The main problem in such calculations is related to the timescale of interest ranging from picoseconds to years. It is difficult to envisage a single numerical techniques covering the whole timescale of the decay process. The integration of the stochastic Landau–Lifshitz–Gilbert (LLG) equation is normally plausible up to time of the order of nanoseconds [1]. At a large time scale, the kinetic Monte Carlo-based method with computationally costly energy barrier calculations is used [2], [3]. For an intermediate time scale, we have been working on the possibility to accelerate calculations, using the Monte Carlo technique with quantified time step (TQMC) [4]. Although the acceleration of the calculations was significant, we have found that the TQMC technique only correctly describes the switching in the so-called thermal regime when the influence of the magnetization precession is small. Additionally, there exist also methods which use the temperature acceleration dynamics [5], [6]. For example, Xue and Victora [6] employed the equivalence principle of time and temperature over long time range. The method is based on the supposition of the Arrhenius–Neel law with one unique temperature-independent attempt frequency for all reversal events and, therefore, is limited to the cases when this idea is true.

Here, we implement the Voter method (also called "hyperdynamics of the infrequent events"), [7], [8] which was recently proposed and used to calculate the diffusional processes of atoms on the surface, achieving an acceleration of the calculation up to 8000 times. Voter has tested the method using the molecular dynamics approach for particle diffusion. However, the magnetization diffusion has some peculiarities. Due to the presence of the precessional term, the dynamical equation of motion (the LLG equation) does not have a simple Newtonian form and the diffusional properties does not correspond to that of a simple Brownian particle [4]. This was the reason why the TQMC did not produce the same dynamics as the direct integration of the stochastic LLG equation, when the precessional effects were strong. Because of that, we also have to check the use of the Voter method with respect to correct description of the precessional effects.

The method consists in modification of the external potential, based on the Hessian energy matrix (the matrix of second derivatives $\partial^2 E/\partial x_i \partial x_j$, where x_i are the system coordinates), so that the transition state remains unchanged. An additional external boost potential, ΔV_b is slowly switched on at the minimum, rising its value, and is switched off near the transition surface, i.e., where the first eigenvalue of the Hessian matrix ε_1 becomes negative. The Langevin dynamics (LD) is then performed in this modified potential. The total time for the escape of the particle from the minimum can be evaluated as the sum of modified times at each timestep Δt_b, which could be computed from the LD timestep in the modified potential, Δt_{LD}, as the following:

$$\Delta t_b = \Delta t_{\mathrm{LD}} \exp(\Delta V_b(t)/k_B T).$$

Here, T is the temperature and k_B is the Boltzman constant.

We have implemented the method for collection of noninteracting magnetic particles with external field applied at some angle to their anisotropy axis. According to the Voter's suggestion, we have tried two forms of the boost potentials to accelerate the stochastic dynamical calculations

$$\Delta V_{b1} = a\theta(\varepsilon 1)\varepsilon_1^2 \quad \Delta V_{b2} = b\frac{a\theta(\varepsilon 1)\varepsilon_1^2}{1 + 2a\theta(\varepsilon 1)\varepsilon_1^2}. \qquad (1)$$

Here, θ is the standard Heaviside function and a and b are arbitrary parameters which could be tuned. On one hand, these parameters must be as large as possible to achieve the acceleration.

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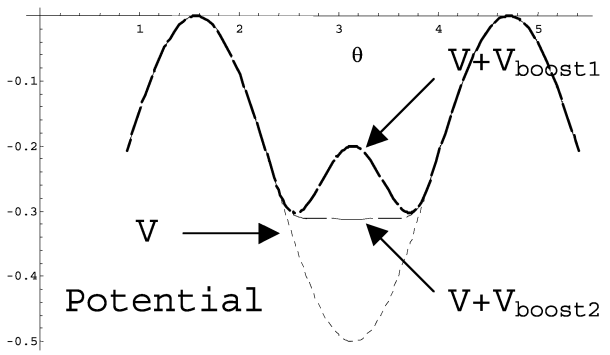

Fig. 1. Initial potential for a magnetic moment, (3), and two possible boosting potentials (1), as function of magnetic moment angle θ and in the absence of external applied field.

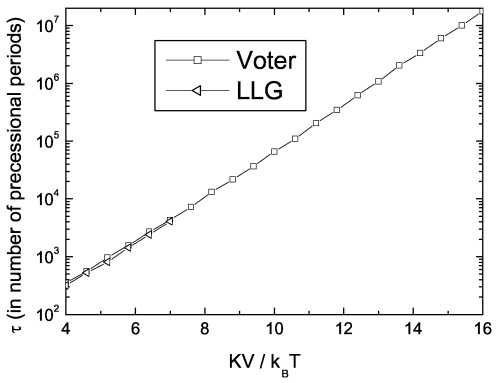

Fig. 2. Switching time obtained with direct LLG calculations and with the Voter's method for a magnetic particle at zero applied field.

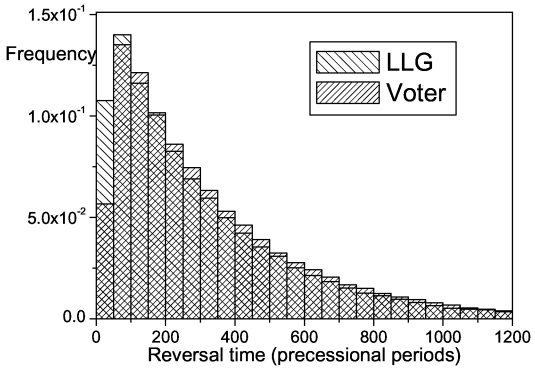

Fig. 3. Histogram showing the distribution of reversal times for both LLG calculations and Voter's method with energy barrier value $KV/k_BT = 4$.

On the other hand, the tuning of these parameters could be performed based on the fact that the equilibrium statistics should be achieved in the minimum, i.e., the number of LD time steps performed in the modified potential before the particle is escaped from the minimum must be large enough. The difference between the two potentials is that the second one, although more difficult to evaluate, produces much smoother modification and does not introduce a "crest" in the minimum, from which the particle could be scattered (see Fig. 1).

The implementation of the method requires the constant evaluation of the lowest eigenvalue of the correspondent Hessian matrix. The direct normal mode analysis is a time consuming procedure which depends strongly on the system size and would limit the acceleration achieved by the method. The iterative methods, such as the Gauss–Siegel, which could use the previous value as initial guess, could be very helpful. A. Voter [8] also suggested replacing the direct evaluation of ε_1 by its approximate evaluation by means of the numerical minimization (with respect to the parameter s) of the following expression:

$$\varepsilon^{num}(s) = \frac{[E(x+\eta s) + E(x-\eta s) - 2E(x)]}{\eta^2} \qquad (2)$$

where η is a small parameter.

At the first stage, we have implemented the method to calculate the escape time for an ensemble of noninteracting magnetic particles with uniaxial anisotropy and external applied field with the total energy

$$E_{\text{int}} = -KV(\vec{m}\cdot\vec{e})^2 - VM_s(\vec{m}\cdot\vec{H}app) \qquad (3)$$

where K is the anisotropy value, V is the particle volume, e is the direction of the anisotropy, H_{app} is the applied field and m is the magnetic moment, normalized to the saturation value M_s.

The averaged time for the particle to escape from the minimum is calculated using the Voter method and compared to that obtained from the direct integration of the LLG equation with a random term representing temperature fluctuations. Fig. 2 presents results of the calculations for switching time for an ensemble of uniaxial particles averaged over many realizations. The computation is stopped when the standard deviation from the average value is below 1%. It is clear that Voter's method for reasonable computational time is much faster than the direct LLG integration. Remarkably, the method reproduces correctly all the features of the dynamics, including the precession. Fig. 3 presents the histogram for switching time of a particle for energy barrier value $KV/k_BT = 4$. It shows that the accelerated dynamics correctly reproduces the form of the log-normal distribution although the general tendency of the Voter distribution is the displacement to larger values.

We have checked the results for different values of the damping parameters and different angles between the applied field and the anisotropy directions. Fig. 4 presents the results for an angle between the anisotropy direction and applied field of 45 degrees and for different values of the tuning parameter a. Therefore, unlike the TQMC method, the hyperdynamics method correctly reproduces the influence of the ellipticity of the precessional cone on the thermal switching statistics.

The real acceleration of the method depends on the efficiency to calculate the lowest eigenvalue of a complex large system. Therefore, for the small barriers case, the direct integration of the LLG equation is faster. To compare, we present in Fig. 5 the ratio between the average CPU time used in the Voter method [using direct lowest eigenvalue evaluation in system described by (3)] and the average CPU time used in the LD dynamics. The acceleration in calculation appears for barrier values larger than $KV/k_BT = 7$. For this "straightforward" implementation, the acceleration up to 24 times in CPU time has been reached. More sophisticated methods will improve this ratio. The method was also checked for the linear chain of exchange coupled magnetic moments and gave a satisfactory result.

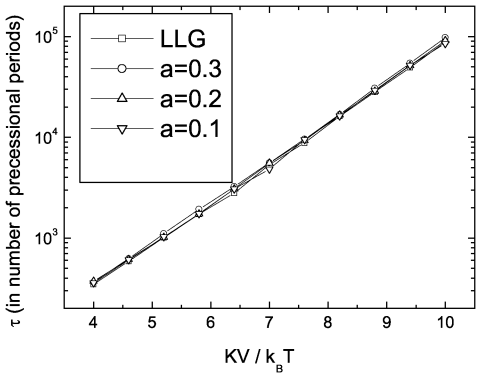

Fig. 4. Average switching time for a magnetic moment with an applied field (0.2 K/Ms, 0.2 K/Ms, 0) and the easy axis parallel to z direction. Results for different values of parameter a are represented, as well as LLG direct calculations.

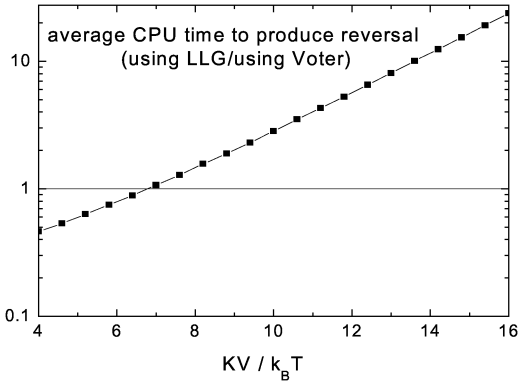

Fig. 5. Comparison of real time performance: Average total CPU time to produce reversal in LLG calculations divided by the same quantity using Voter's method. The line $y = 1$ represents equal performance and greater number reflects better efficiency of the tested method.

However, the real acceleration has an important limitation. Indeed, the acceleration involves the modification of the external potential and is stopped when its curvature is changed. This is independent of the system temperature and is going to be inefficient when its value is small. This effect is different from the TQMC method in which the acceleration involves the ratio KV/k_BT, rather then KV only.

In conclusion, we have implemented the method of "Hyperdynamics of infrequent events" to accelerate the molecular dynamics simulations in the case of magnetization dynamics achieving an acceleration up to 24 times. Higher acceleration seems also possible if one uses more sophisticated modern methods to evaluate rapidly the lowest eigenvalue of the Hessian matrix. In comparison to the time-quantified Monte Carlo [4], the main advantage of the method is the correct description of the influence of the precession on the thermal switching process. In contrast to the temperature accelerated method by Xue and Victora [6], this method does not suppose apriori the Arrhenius–Neel law with one unique temperature-independent attempt frequency. It may successfully be used when various reversal modes, with different attempt frequencies, coexist during the thermal magnetization process. The limitations of the method make it useful for intermediate timescale, up to hundreds of nanoseconds, for example, for the dynamic coercivity calculations. Higher time scale seems not reachable.

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