Behavior of μMAG Standard Problem No. 2 in the Small Particle Limit

M. J. Donahue, D. G. Porter, R. D. McMichael
National Institute of Standards and Technology,
Gaithersburg, MD 20899

J. Eicke
Institute for Magnetics Research, George Washington University,
Washington, DC 20052

Abstract— **For a uniformly magnetized rectangular particle with dimensions in the ratio 5 : 1 : 0.1, the coercive and switching fields in the $(1,1,1)$ direction are determined to be $H_c/M_s = 0.057069478$ and $H_s/M_s = 0.057142805$. Previous micromagnetic computations of coercive and switching fields that did not approach these values for small particles are analyzed. It is shown that the disagreement was primarily due to a disparity in the method of calculating demagnetization energy. Corrected simulations are shown to agree with analytically determined values.**

I. Introduction

When solutions to the first μMAG standard problem failed to show good agreement, [1] a simpler standard problem was designed to examine the details of how different numerical techniques yield different solutions. The second μMAG standard problem considers a rectangular particle with dimensions $L : d : t$ in the ratio $5:1:0.1$. Only exchange and magnetostatic energy terms are considered. The coercive field along the $(1,1,1)$ direction is to be calculated as a function of the ratio of particle size to exchange length $l_{\rm ex} = (2A/\mu_0 M_s^2)^{1/2}$. Here A is the exchange stiffness coefficient in J/m and M_s is the saturation magnetization in A/m. Published solutions [2], [3], [4] show much better agreement than the results from the first problem. It was expected that for a small enough particle size, exchange energy would dominate, and the coercive field predicted by all calculations would converge to the coercive field of a uniformly magnetized particle. As seen in Fig. 1 however, significant differences were observed for small simulated particles. In this paper we provide analytic values of the coercive and switching fields in the small particle limit. Our previous calculations [3] (labeled "OOMMF 1.0" in Fig. 1) are examined in detail to determine and correct the sources of error when simulating small particles. New solutions are computed by a corrected solver. [5]

II. Small Particle Theory

In this section we analyze the equations of our micromagnetic model in the small particle limit. The intent is to examine whether the numerical methods used in our micromagnetic simulations behave properly in this limit, not to predict the physical behavior of small magnetic particles. Many important influences on the physical behavior

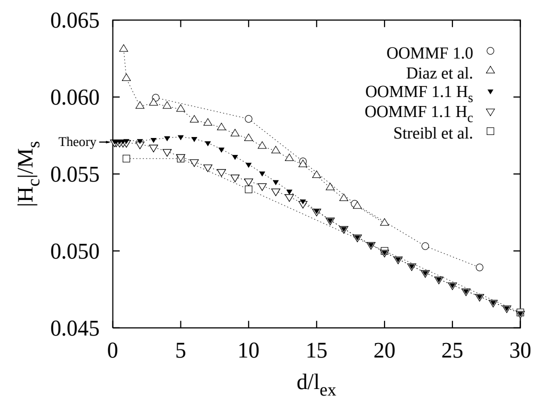

Fig. 1. Coercive (H_c) and switching (H_s) fields of standard problem 2 as a function of particle size as computed by several micromagnetic simulations. New results are labeled OOMMF 1.1.

of small magnetic particles are neglected by our model.

In our model, as the particle size decreases, the exchange energy becomes dominant to the point that magnetization is uniform throughout the particle. In this limit, exchange may be treated as a constraint that the magnetization is uniform, and analysis of magnetic reversal need consider only energy terms due to demagnetizing and external fields. Analysis is simplified by normalizing all field and magnetization quantities to the saturation magnetization of the particle M_s, and all energy densities to the quantity $\mu_0 M_s^2$.

A uniformly magnetized ellipsoid has a uniform demagnetizing field, $\mathbf{h}_{\rm d} = -\mathbf{D}\mathbf{m}$, where $\mathbf{m}$ is a column vector of the components of normalized magnetization along the principal axes of the ellipsoid, and $\mathbf{D}$ is a diagonal matrix of demagnetizing factors.

The demagnetizing energy density of the ellipsoid is

$$e_{\rm d} = \frac{1}{2}\mathbf{m}^T\mathbf{D}\mathbf{m}. \tag{1}$$

For rectangular particles, uniform magnetization does not result in a uniform demagnetizing field. However, the demagnetizing energy density has the same form as (1). For the standard problem, the demagnetizing factors are $D_{(1,0,0)} = 0.021829576$, $D_{(0,1,0)} = 0.11522396$, and

$D_{(0,0,1)} = 0.86294646$. [6] The quantity $\mathbf{Dm}$ is the average demagnetizing field over the volume of the particle. Because the magnetization is uniform, the average field value is sufficient to compute the total demagnetization energy.

Analysis of magnetization reversal considers the total energy density under the influence of an applied field $\mathbf{h}_\mathrm{a}$,

$$e = \frac{1}{2}\mathbf{m}^T\mathbf{D}\mathbf{m} - \mathbf{h}_\mathrm{a}^T\mathbf{m}. \quad (2)$$

The coercive field, H_c, is defined relative to a unit vector in the direction of the applied field, $\hat{\mathbf{u}}$. After saturation by a large field in the direction of $\hat{\mathbf{u}}$, H_c is the largest value of H for which an applied field of $-H\hat{\mathbf{u}}$ yields a magnetization with $\hat{\mathbf{u}}^T\mathbf{m} > 0$. The switching field, H_s, is the magnitude of applied field at which a local minimum of (2) disappears. In many circumstances, H_c and H_s are equal, because $\hat{\mathbf{u}}^T\mathbf{m} = 0$ only during a switching event. When solving standard problem 2 for uniformly magnetized particles, however, H_c and H_s are not equal. The magnetization of the particle rotates past the plane perpendicular to the applied field direction before the switching event. Lagrange multiplier analysis yields expressions for $\mathbf{m}$ and $\mathbf{h}_\mathrm{a}$ in terms of Lagrange multiplier λ. The stationary points of (2) correspond to the roots of a rational function which is sixth order in λ. At coercivity, the constraint that $\mathbf{h}_\mathrm{a}^T\mathbf{m} = 0$ corresponds to a rational function that is third order in λ. Solving the system of equations yields a value for H_c. At the switching field H_s, one of the stationary points of (2) disappears. Solving for the applied field magnitude at which one of the roots of the sixth order rational function disappears yields a value for H_s. The values of H_c and H_s in the small particle limit are $H_c/M_s = 0.057069478$ and $H_s/M_s = 0.057142805$.

III. Simulation Analysis

Our previous solutions [3] were computed using a discretization of the particle into a two-dimensional grid of square cells. The magnetization was assumed to be uniform within each cell, represented by a single spin. A sequence of external fields was applied to the spin assembly. For each applied field value, the evolution of the system of spins was computed by the Landau-Lifshitz equation until the maximum torque on all spins fell below a threshold value, indicating an equilibrium magnetization for the applied field had been reached. In the following sections, we examine several details of these computations for small particles, seeking the reasons they do not approach the values predicted by Section II.

A. Demagnetization Energy

In reference [3] (open circles in Fig. 1), the normalized demagnetization energy density of the simulated particle is computed as

$$e_\mathrm{d} = \frac{1}{2N}\sum_i \mathbf{m}_i^T\mathbf{h}_{\mathrm{d},i}, \quad (3)$$

where the sum is over the N cells in the grid, and the values $\mathbf{h}_{\mathrm{d},i}$ are the demagnetizing field sampled at the center point of each cell.

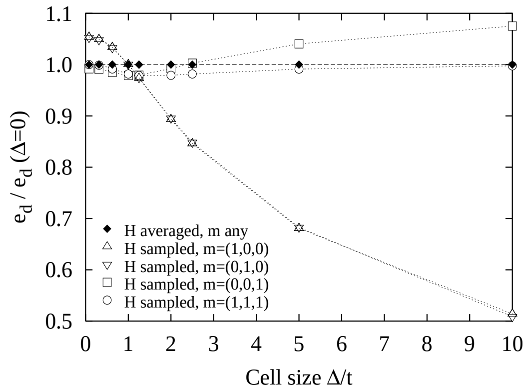

Fig. 2. Computed demagnetization energy as a function of cell size for a uniformly magnetized $5:1:0.1$ rectangular particle. Cell size is expressed relative to particle thickness t. The energy is calculated using either sampled demagnetizing fields (open symbols) or averaged demagnetizing fields (solid diamonds).

Fig. 2 displays the computed demagnetization energy as a function of cell size for several directions of uniform magnetization. For each direction, the demagnetization energy is plotted normalized to the analytical value computed from (1). It is clear that the formulation in (3) suffers from errors that are not eliminated by refinement of the two-dimensional grid.

When the magnetization is in the plane of the film (the nearly overlapping $m = (1,0,0)$ and $m = (0,1,0)$ curves), the field at distance a from a charged edge drops off roughly proportional to $\tan^{-1}(t/(2a))$. Because this is concave up, a field sample taken at the center of a cell will underestimate the average in-plane field strength, resulting in the low values for the energy at coarse discretization seen in Fig. 2. This error can be reduced by refining the discretization. However, because the sample grid is two dimensional, the field samples always come from the center of the film, where the field is stronger than near the top or bottom surfaces. Therefore, for very small cell size Δ, the energy is overestimated. Analogous considerations explain the discrepancies in the $m = (0,0,1)$ plot.

Fortunately, these errors can be removed without requiring three-dimensional discretization. Each sampled value of the demagnetizing field in (3) may be replaced with the average value of the demagnetizing field over the entire cell. The expressions necessary for calculation of the demagnetizing fields averaged over each cell are known. [6] They are considerably more complex than the expressions for the sampled field values, but they may still be expressed as convolution integrals, so fast Fourier methods are available, and the additional complexity only contributes to the initialization phase of a simulation. (Due to the large number of terms, rounding error can be significant, so the demagnetization tensor should be computed using a technique such as doubly compensated summation. [7]) As seen in Fig. 2, the demagnetization energy computed using cell-averaged demagnetizing fields does not depend on discretization and agrees with the analytic result.

B. Rounding Errors in Exchange Energy Calculation

In reference [3], the normalized exchange energy density is computed using an eight-neighbor cosine scheme: [8]

$$e_{\mathrm{ex},i} = \frac{A}{3\mu_0 M_s^2 \Delta^2} \sum_{k\in \mathrm{nn_i}} (1 - \mathbf{m}_i^T \mathbf{m}_k), \qquad (4)$$

where A is the exchange stiffness constant, Δ is the cell size, and k sums over the nearest and next-nearest neighbors on the square 2D grid. When the angle θ between neighboring spins is small, $1 - \mathbf{m}_i^T\mathbf{m}_k \approx 1 - (1 - \theta^2/2)$ and the $\theta^2/2$ term is lost in rounding, i.e., in floating point arithmetic $1 - \theta^2/2 = 1$. In this case the outer subtraction from 1 does not contribute to the error, but only exposes what has already been lost.

If one could regroup the expression $1 - (1 - \theta^2/2)$ as $(1 - 1) + \theta^2/2$, then rounding errors would be significantly reduced. This is accomplished by the alternative expression

$$e_{\mathrm{ex},i} = \frac{A}{3\mu_0 M_s^2 \Delta^2}\, \mathbf{m}_i^T \sum_{k\in \mathrm{nn_i}} (\mathbf{m}_i - \mathbf{m}_k). \qquad (5)$$

Here the subtraction is done before other floating point operations, and the dot product is computed between vectors which are nearly perpendicular, which is numerically better behaved.

If the exchange coupling A/Δ^2 is large, due to either large A or small Δ, then the spins will be nearly aligned and roundoff errors can become a significant fraction of the total energy. This can cause a misalignment between the calculated effective field direction and the gradient of the energy surface; if we require each simulation step to lower the total energy, then such misalignment forces the simulation step size to be reduced. This unnecessary stiffening of the problem is evidenced by some simulations performed for this paper, where using (5) in place of (4) reduced the computation time by several orders of magnitude.

C. Uncertainty in Critical Fields

Our simulations compute the sequence of equilibrium states corresponding to a sequence of applied fields. Although extrapolation methods have been proposed to determine critical switching fields from such data [9], we simply report the mid-point of the field step at which we observe a discontinuity as H_s. Thus, we do not determine H_s to finer resolution than the size of the field step which leads to the discontinuity. In this paper, the (reduced) field step size $|\Delta \mathbf{h}_\mathrm{a}|$ near the switching field was 0.0000276.

There are additional uncertainties, however. When the applied field is stepped, the location of the local energy minimum shifts, and it can happen that when the simulation is subsequently allowed to relax, it falls to a minimum different from the one being tracked, giving the mistaken impression that the first minimum has disappeared. This is an important effect in dynamic studies, [10] but is an error in the quasi-static situation being studied here and results in an underreporting of the switching field. For this to occur, the starting point for the relaxation procedure (i.e., the equilibrium position from the previous field step) must have an energy higher than the energy barrier surrounding the minimum of interest. The total energy of the system increases as the switching field is approached, so the difference in energy between the relaxation starting point and the desired equilibrium point is not more than $\Delta\mathbf{h}_\mathrm{a}^T\mathbf{m} < |\Delta\mathbf{h}_\mathrm{a}|$. This means that if an energy minimum is prematurely lost, it must be shallower than $|\Delta\mathbf{h}_\mathrm{a}| = 0.0000276$. If we compare to a particle of equal volume at finite temperature, obeying $t = t_0 \exp(\Delta E/kT)$ with attempt period $t_0 = 10^{-9}$ s, observation time $t = 60$ s, and NiFe material parameters, then an energy well of this depth would be unstable at temperature $T > 0.006(d/l_\mathrm{ex})^3$ K. For the largest particle considered here, $d/l_\mathrm{ex} = 30$, corresponding to $T = 160$ K.

On the other hand, the simulation will report an equilibrium exists when the torque $|\mathbf{m}\times\mathbf{h}|$ at all spins is less than a specified threshold value. This test is insufficient if the energy surface is very flat, resulting in an overestimate of the switching field. This problem can be controlled by making the threshold small, which in the present study was set to 10^{-6} (normalized units). If we assume $|d\mathbf{m}/dt| \approx \gamma|\mathbf{m}\times\mathbf{h}|M_s$, with gyromagnetic ratio $\gamma = 2.21\times10^5$ m/As and (say) $M_s = 8\times10^5$ A/m, then at $|\mathbf{m}\times\mathbf{h}| = 10^{-6}$, a 1% change in $\mathbf{m}$ requires about 56 ns.

IV. Results

After making the corrections to our micromagnetic solver indicated above, new solutions for μMAG standard problem 2 were computed. Both the coercive and switching fields were determined for particles with width from 0.125 to 30 times the exchange length. The results are plotted in Fig. 1 along with the previously published results [2], [3], [4]. For a particle with width 0.25 times the exchange length, we compute $H_c/M_s = 0.05707$ and $H_s/M_s = 0.05713$ using a field step of $|\Delta\mathbf{h}_\mathrm{a}| = 0.0000276$. We compute the same results for a particle of width 0.125 times the exchange length, indicating these values are a good estimate for the limit as $\Delta \to 0$. The theoretical values for both coercive and switching field for a uniformly magnetized particle from Section II are also marked on the graph. (The two values are indistinguishable at the scale of the graph.) The new simulation results agree with the theoretical solution in the small particle limit while the previously published solutions did not.

In the improved micromagnetic solver, the demagnetizing energy is completely accurate up to the assumption that the magnetization is uniform in each cell. It is still important that discretization of the problem be fine enough to resolve spatial variations of magnetization, but there is no need for finer discretization beyond that to resolve spatial variations in the demagnetizing field. The averaging of demagnetizing fields over uniformly magnetized cells accounts for those variations. This means that as the magnetization of the particle becomes more uniform, coarse discretizations can compute accurate results.

References

[1] R. D. McMichael and M. J. Donahue, <URL: http://www.ctcms.nist.gov/%7Erdm/std1/prob1report.html> (unpublished).

[2] L. Lopez-Diaz, O. Alejos, L. Torres, and J. I. Iniguez, J. Appl. Phys. **85**, 5813 (1999).

[3] R. D. McMichael, M. J. Donahue, D. G. Porter, and J. Eicke, J. Appl. Phys. **85**, 5816 (1999).

[4] B. Streibl, T. Schrefl, and J. Fidler, J. Appl. Phys. **85**, 5819 (1999).

[5] M. J. Donahue and D. G. Porter, <URL: http://math.nist.gov/oommf/> (unpublished).

[6] A. J. Newell, W. Williams, and D. J. Dunlop, Journal of Geophysical Research **98**, 9551 (1993).

[7] N. J. Higham, in *Accuracy and Stability of Numerical Algorithms* (SIAM, Philadelphia, 1996), pp. 96–97.

[8] M. J. Donahue and R. D. McMichael, Physica B **233**, 272 (1997).

[9] A. Hubert and W. Rave, Phys. Stat. Sol. (B) **211**, 815 (1999).

[10] D. G. Porter, IEEE Trans. Magn. **34**, 1663 (1998).