SIMULATION OF MICROMAGNETIC PHENOMENA

Markus-A. B.W. Bolte
Prof. Dr.-Ing. Dietmar P.F. Möller
Fachbereich Informatik,
Arbeitsbereich Technische Informatiksysteme
Universität Hamburg,
Vogt-Kölln-Strasse 30, D-22527 Hamburg, Germany
E-Mail: mbolte@physik.uni-hamburg.de

Dr. Guido D. Meier
Alexander Thieme
Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung
Universität Hamburg,
Jungiusstrasse 11, D-20355 Hamburg, Germany
E-Mail: meier@physik.uni-hamburg.de

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ABSTRACT

The study of micromagnetism is a very active field of research with prospective applications in microelectronics, harddisk data storage as well as non-volatile random access memory. In recent years, the use of simulation tools has become one predominant factor in the rapid development of new devices as well as in the deepened understanding of underlying physical principles. To bridge the gap between theoretical predictions and experimental findings we extended an existing simulation package to allow directly comparison of experimental results with the theoretical background that is implemented in the simulation software. In general the comparison results in excellent fits. Moreover we increased the performance of the existing code which will enable further extensions and applications.

INTRODUCTION

A growing understanding of the ferromagnetic properties of micro- and nanometer sized structures have been the prerequisite for much of the technological advances that occurred in the last decades in the field of data storage. It is also likely a crucial factor in future developments of microelectronic and data storage devices such as the magnetic random access memory (MRAM) or the anticipated spin transistor (Datta and Das, 1990, Meier and Matsuyama 2000) which is one possible way to further decrease the size and increase the speed of computer componentware. The microscopic and thermodynamic theory of magnetism has been established well over 70 years ago with fundamental work from Landau, Lifshitz, Gilbert, and others (Landau and Lifshitz 1935; Gilbert 1955). The real challenge is to conclusively compare theory with experiments. Hence, the principles of micromagnetic simulation have become accepted as the main bridge over the last three decades. The importance of numerical and simulation techniques to micromagnetism has several reasons: First, due to the extremely large number of free variables (3N, with N being the number of electrons or cells in a specimen) there are only a limited number of special scenarios in which there exists an analytical solution, e.g., the rotational ellipsoid (Stoner Wohlfarth 1948; Aharoni 1998). Secondly, the existing theory offers solutions to a wide range of physical problems from magnetoresistance to domain wall motion and spin wave excitation. Thirdly, a few parameters suffice to provide a good approximation of real systems, and finally, its algorithms have become very fast and able to efficiently simulate large-scale samples while others, e.g., ab-initio approaches, are extremely time-consuming.

In the following paragraphs we give a brief introduction into the principles of micromagnetism, as well as the most important simulation aspects. Thereafter we discuss the structure and performance analysis of an implementation used in micromagnetism and our adaptations and extensions. Moreover we compare our simulation results with measurements done by several techniques, which show excellent fits.

Micromagnetic principles

The micromagnetic theory describes magnetic phenolmena such as hysteresis effects and domain walls and is based on the approximation to use a continuous magnetization vector instead of discrete magnetic moments located on the sites of the crystal lattice, i.e., on the atomic length scale. It also sets the scale in which this assumption is valid, i.e., the nanometer scale is the lower limit. In principle no upper limit exists apart from computational limitations. Initial works by (Landau and Lifshitz 1935; Gilbert 1955; Brown 1963) have given the theory a foundation that has become widely accepted and that holds true for a wide variety of applications. The foundation to micromagnetic theory is the equation of motion established from thermodynamic consideration (minimization of the Gibbs' free energy) by Landau, Lifshitz and Gilbert. It describes the change of a magnetization vector over time as a function of the effective magnetic field at the location of the vector and some parameters inherent in a magnetic system, i.e., the saturation magnetization M_s, which is the strength of the magnetization vector, the gyromagnetic constant γ and the damping constant α. Similar to the motion of a gyroscope where a gravitational field causes a precessional movement around the axis of the gravitational pull, the magnetization precedes around the direction of a local effective field H_{eff}. A sketch is shown in Figure 1.

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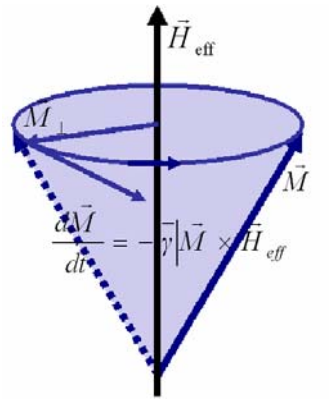

Figure 1: The Magnetization Vector Precedes around the Direction of the Effective Field. In a Real Sample the Damping Term of the LLG Equation Causes the Magnetization to Align with the Effective Field after a Characteristic Time.

To this precession the damping term is added that takes into account the fact that energy is exchanged with the surrounding system, thus the magnetization loses energy over time and tends to align with the field vector of the effective magnetic field at the location of the magnetization. Thus the equation of motion for the micromagnetic model is written in the form of the Landau-Lifshitz-Gilbert (LLG)-equation

$$\frac{d\vec{\mathrm{M}}}{d\mathrm{t}} = -\left|\bar{\gamma}\right|\vec{\mathrm{M}}\times\overrightarrow{\mathrm{H}_{\mathrm{eff}}} - \frac{\left|\bar{\gamma}\right|\alpha}{\mathrm{M_S}}\ \vec{\mathrm{M}}\times(\vec{\mathrm{M}}\times\overrightarrow{\mathrm{H}_{\mathrm{eff}}}). \qquad (1)$$

The effective field originates from the superposition of four different interactions between the spins of magnetic material (in the absence of mechanical forces we can neglect magnetostrictive effects). The sum of their energies is the total energy of the system which becomes minimal in stable spin configurations

$$E_{tot} = E_{exch} + E_{aniso} + E_{Zeeman} + E_{demag}. \qquad (2)$$

These four contributing terms are exchange energy, anisotropic energy, Zeeman energy, and de- or selfmagnetization energy. They have their origin in the quantum mechanical nature of magnetism and can not satisfactorily be understood without a comprehension of its principles. In quantum mechanics, electrons are described as wave functions, and the location of electrons can be seen as the square of the amplitude of such a function. The location cannot be determined with infinite accuracy, but rather has an uncertainty that depends on the electron's velocity (uncertainty principle). The integral of the wave function is normalized to one; the wave function can therefore be seen as the probability function of the location of the electron. From these basic considerations the electronic orbitals of atoms can be calculated; they determine the probability of electrons being at a certain location in relation to the atom's nucleus. The three space coordinates are transformed into integer quantum numbers that describe their energetic properties. Essential to magnetism is the electrons' fourth intrinsic attribute, its spin. It is directly proportional to the magnetic moment of the electron, the motion of which is described by the LLG equation. The electronic and magnetic properties of charged particles are inseparably connected by Maxwell's equations. More details can be taken from introductory physics books (Cohen-Tannoudji et al. 1996; and Jackson, 1998).

Energy terms

The energy of a solid state system can be calculated by taking into account all possible interactions of the electrons with each other and with outer electric and magnetic fields. As stated in the introduction, this is very costly concerning both time and computational resources. Within the theory of micromagnetism the electric and magnetic properties of many individual atoms are averaged to material constants such as the strength of the interaction of the spins of electrons in close proximity due to an overlap of their wave functions. This is an extremely strong but only close-range interaction known as the exchange coupling. The change in energy from this effect can be calculated as

$$E_{exch} = -J\sum_{i\neq j} S_i \cdot S_j, \qquad (3)$$

where J, also called exchange integral, is the shared volume of the wave functions of electrons i and j and S_i and S_j their spins. Here the indices can also stand for neighboring simulation cells. What the equation says is that when considering only the exchange coupling, the spins (magnetization vectors) of neighboring atoms (simulation cells) want to align parallel to make the exchange energy minimal. The exchange energy is normally determined by considering only nearest-neighbor atoms/ cells, but it does not take into account the spatially uneven (anisotropic) distribution of electrons according to their quantum numbers as mentioned above. This is done by introducing a term known as the anisotropy energy, which considers the shape of the electronic orbitals and the location of neighboring atoms in the lattice of a solid. For uniformly magnetized ferromagnets, the spins of the electrons tend to align to so-called easy axes as described by the Stoner-Wohlfarth-model for rotational ellipsoids (Stoner and Wohlfarth 1948). For example, for materials organized in hexagonal closed packed lattices, there is one principle easy axis, and its energy term is written as

$$E_{aniso} = K_{u1}\int_V \sin^2\phi dV + K_{u2}\int_V \sin^4\phi dV, \qquad (4)$$

where ϕ is the angle between magnetization and the easy axis, and K_{u1} and K_{u2} are uniaxial anisotropy constants, derived from Taylor series expansion. Typically the second order term is already much smaller than the first order anisotropy.

A third contribution is the Zeeman term that describes the influence of external magnetic fields on the spins. Basic electrodynamic calculations result in an added energy

$$E_{Zeeman} = -\int_V \vec{M}\vec{H}\, dV. \quad (5)$$

Here M is the magnetization of one simulation cell, which is the averaged unbalanced spin of all atoms represented by the cell, and H the external magnetic field. The scalar product of the two is then integrated over the cell volume V to derive the field energy. Again, the magnetization will seek to align itself to the direction of the outer field as described by the LLG-equation.
Exchange coupling and Zeeman interaction are competing against a fourth term that depends on the shape of the magnetic system. This demagnetization energy depends on the interaction of the magnetization with the stray field H_S generated by the magnetization itself, and is written as

$$E_{demag} = -\frac{1}{2}\int_V MH_S\, dV. \quad (6)$$

The magnetization can also be seen as magnetic polarization charges which are unbalanced at the surfaces of a structure. Just as with their electric equivalents, this creates a dipole field that is the stronger the more charges are unbalanced at the surface. This means, that under the influence of this interaction the magnetization vectors will try to be arranged parallel to a sample's surface, because then there would be no polarization charges. The stray field can be approximated as the field of a dipole that occurs between two charges with a relative displacement between them. The stray field is a long-range interaction between magnetizations and thus often becomes the dominating part of the effective field.

Domain walls

With the four competing energy terms described above the magnetization of ferromagnetic materials in zero-field environments generally tend to be arranged parallel to each other and preferably along easy axes in large volumes called Weiss areas (Weiss 1907) or domains, thus minimizing exchange and anisotropy energies, while on the boundaries the stray field (also called demagnetization field) is prevalent. This means that on the interfaces of these domains a change in the direction of the magnetization vectors occurs; this can be viewed as a wall between the different domains. Since their first discovery and investigations by (Bloch 1923, Néel 1955) and subsequent studies done by (Aharoni 1996) and others research on domain walls has become of major interest, because the electronic and magnetic properties of materials depend largely on the behavior of domain walls (Hertel and Kronmüller 1999). One has to differentiate between several types of walls: In the Bloch wall the magnetization vector rotates around an axis normal to the domain wall, leading to surface charges at the interface of the wall with other media. Another type, the Néel wall, is prevalent in thin films; here the vector rotates in plane of the structure. Other types, such as the cross-tie or the asymmetric Bloch wall are combinations of the fundamental types. Depending on parameters such as spatial extension and energy coefficients which configuration will appear (Ramstöck, Hartung and Hubert 1995).

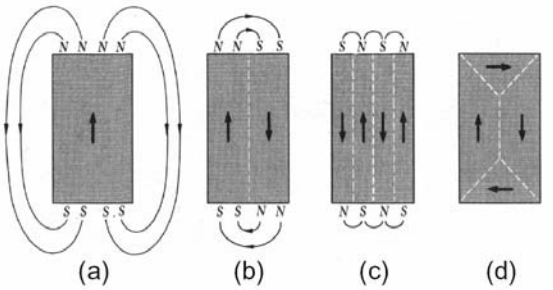

Figure 2: Formation of domains reduces the stray field. From left to right, the demagnetization energy is reduced by the formation of domains, especially by closure domains. Modified from (Hubert and Schäfer 1998)

Consider as a simple example the rectangular particle of Figure 2. Let us assume that the external field is zero, i.e., the Zeeman energy vanishes. We further assume that the particle possesses first order uniaxial anisotropy along the long axis. The remaining energy contributions are the demagnetization and the exchange energy, the latter of which tries to align all magnetic moments parallel. If exchange is the leading energy contribution, as it is true for small particles the configuration of Figure 2(a) is preferred. However, in this case the stray field of the particle is maximized which can be easily seen by the large number of free poles at the surface, equivalent with a high demagnetization energy being proportional to the stray field times the magnetization of the particle. The configuration of Figure 2(b) reduces the stray field energy at the cost of the generation of a domain wall in the middle of the rectangle. Within the wall magnetic moments are pointing in hard directions and cause anisotropy energy and also an exchange energy contribution. Depending on the material parameters and the size of the rectangle configuration (c) might further reduce the total energy. The arrangement of domains shown in Figure 2(d) is known as the Landau pattern and often occurs in nature, because it couples a major part of the magnetic flux inside the particle, thus minimizing the stray field, i.e., the demagnetization energy. Most of a multi-domain sample's magnetic energy is therefore contained in the domain walls.

COMPUTATION OF MICROMAGNETIC PROBLEMS

Science is concerned with understanding and controlling the materials and forces of nature for the benefit of humankind. Therefore it is necessary for scientists to analyze and improve the performance of systems, when the components of which originate from different domains. Examples include either adapting existing systems to new demands and/or conditions, or designing new applications such as those in mechatronics, automotive, avionics, aerospace, micromagnetics, etc. Such systems in-

clude components derived from many different science domains. In many cases, solutions to problems have been found by applying appropriate mathematical models and computer simulation to them. A recent White House report identifies computer modeling and simulation as one of the key enabling technologies of the 21st century. Its applications are virtually universal.

There are several excellent micromagnetic simulation packages available today, with different modeling schemes. We have decided on OOMMF – the object oriented micromagnetic framework, a project in the National Institute of Standard and Technology (NIST, http:\\math.nist.gov\oommf) for several reasons. First its code is freely available, making it possible to compare techniques and algorithms with established publications, a vital criterion for scientific research. With its modular architectural design it is also extensible and very flexible. It has also proven to be a very fast application for the dynamic 3D simulations of the rectangular magnetic samples that we mainly investigate.

OOMMF is implemented as a client/server-architecture in which the different components request and offer services via a service directory. These components include user interfaces for the input of the problem to be simulated, so-called solvers that progress the simulation time by stepwise integration of the above LLG ordinary differential equation (ODE), and display components for scalar and vector values. A script file gives a description of the problem; the exchange of data is performed via TCP ports. The code can be modified at three levels; first one can choose different display components and settings to vary the output format. Secondly, one can adjust material constants, the OOMMF components used and their input parameters to control sample and simulation attributes; and finally, a full and arbitrary access on the C++ code itself allows debugging, modification and extension of any component of the package. The main classes of the existing solver shall be explained in more detail in the following paragraphs, followed by a description of our extensions and adaptations as well as a comparison of our simulations with experiments done with various techniques.

Structure and Performance of the Program

A director component controls the loading of involved components and determines when a simulation run is complete. It insures that read/write access on individual simulation stages is not violated.

One can choose between two standard techniques to evolve the magnetization configuration towards a state of equilibrium: Either by minimizing the total energy by using a conjugate gradient technique to find the path to a local energy minimum, or by integrating the equation of motion mentioned above in small time steps. Only with the second method one can follow the dynamic changes in the magnetization configuration, which is why we will focus on this evolver. Each evolver has its own driver that controls stopping criteria and the progression from one time step to another as well as different simulation stages, i.e., when the strength of the external field is ramped up in the case of simulation of hysteresis curves.

The time evolver uses integration methods to further the simulation one step. For that, two disjoint simulation states are used so that the data is clearly separated. In the current state all information needed for the advance of the magnetization configuration is stored. The next configuration is then determined by either using a simple Euler or an adaptive Cash-Karp implementation of the Runge-Kutta method that was implemented to speed up computation. The magnetization vectors then are the foundation for the computation of the effective field; its value is stored as a foundation of the computation of the next time step. Last the time step itself is evaluated against some error restriction to determine whether the step has to be repeated with a smaller step size.

The analysis of the run time performance showed that most of the computing time (62 to 82%) is spent in computing the demagnetization energy (see Figure 3); the results are in good accordance with other findings (Berkov et al. 1993). The complexity is due to the long-range nature of the stray field and the current algorithm used to compute the same. Because the influence of the stray field converges only slowly, the interaction with the magnetization vectors of each cell of a sample has to be considered to derive the field strength at every simulation cell, so that for N cells one would have a $O(N^2)$ complex algorithm if one would use this crude method.

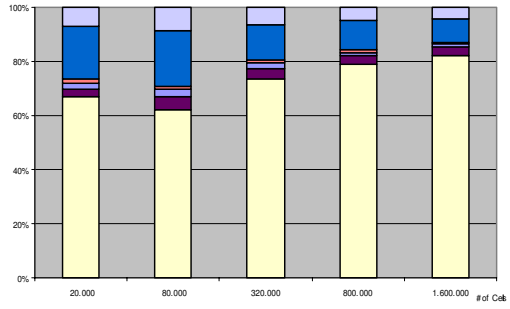

Figure 3: Break-up of the Runtime for Simulations with Different Input Sizes into the Main Routines. Colours represent (from bottom to top): Stray, Exchange, Anisotropy and Zeeman Field Computation, Integration and Computation of Derivative

In the existing simulation package a sophisticated algorithm as described in (Newell et al. 1993) is used which performs at O(N log N) due to Fast Fourier Transforms. This method uses a demagnetization tensor N to account for the shape of a magnetized body. The stray field

$$H_{Stray,i} = -\sum_j N(r_i - r_j) M_j \qquad (7)$$

can be seen as a convolution of two vectors in spatial coordinates. It can be substituted for a simple product in frequency space via FFT so that its complexity is O(NlogN), but the coefficient is large which is why it consumes most of the computation time.

Expansion and Results

From this introduction it can be seen that an effort to increase the computation speed should be focused on objectives: First, to decrease the number of steps necessary to derive a certain convergence criterion, and second, to reduce the time needed to compute one simulation step. The first objective can be obtained by applying well-known methods for integrating ODEs, such as Runge-Kutta integration or other methods. The second objective requires faster algorithms, especially for the demagnetization term. One possible way is to approximate the stray field by using a multipole expansion of the dipole field to a given order of accuracy as stated in (Yuan and Bertram 1992). The advantage for using this method, aside from having linear complexity, is that this algorithm would be parallelizable as suggested in (Singh et al. 1993). An excellent overview over the current state of the art is given in (Fidler and Schrefl 2000).
One important enhancement for the existing code due to speed up purposes is the implementation of a Cash-Karp Runge-Kutta algorithm as described in (Press et al. 2002). The commonly available code uses the Euler-method for integration with an adaptive time step derived from error estimation. The speedup achieved was significant; depending on the problem's stiffness as given by the damping constant α, up to a factor of 20 (for small damping and relatively small problems).
Another part of our work included adapting the output of the simulation package to our experimental setup to allow direct comparison between experiments and the established theory, as implemented in the OOMMF code. We are using the magnetic-force microscopy (MFM) and in collaboration with Dr. P. Fischer (Fischer 1998; Fischer 2001) from the Max-Planck-Institute for metal physics in Stuttgart magnetic transmission x-ray microscopy (MTXM) to investigate the magnetic properties of permalloy and iron-nickel samples. As shown by (Barthelmess et al. 2004) the MFM image can be effectively simulated using the second derivative of the magnetization's stray field in z-direction, while the MTXM-method shows the projection of the magnetization vectors on the axis of the transmitting x-ray beam as grey-scale values. The additional component to the OOMMF architecture takes the measuring height above the sample surface as a free parameter. Figure 4 shows examples of the good fits between experiment and simulation, others can be seen in (Meier et al. 2002; Barthelmess et al. 2003; Pels et al. 2004).
Another application of the additional feature is that it allows direct comparison between the two techniques, serving as a bridge between two standard measuring methods (Meier et al. 2004). Figure 5 shows one such example: The experimental data were taken from magnetic transmission x-ray microscopy (upper left), which basically takes an x-ray image of a ferromagnetic sample – the grey scale values corresponding to the scalar product of the sample's magnetization with the direction of the transmitting x-rays – as well as from magnetic-force microscopy (lower left). The right column shows the simulated magnetization image (upper right) yielding the same Landau structure as seen in the MTXM image, and the simulated MFM image (lower right) revealing the second derivative of the stray field akin to the one taken from magnetic-force microscopy. This example shows how the added module of the existing software package is a useful tool in both comparing and validating theoretical and experimental data, as well as bridging different measurement techniques.

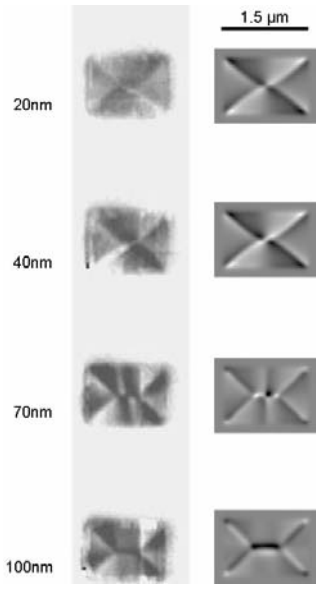

Figure 4: Magnetization patterns of 1x1.5µm² permalloy samples with different thicknesses as indicated in the figure, left measured by magnetic-force microscopy, right from micromagnetic simulations. From (Barthelmess et al. 2004).

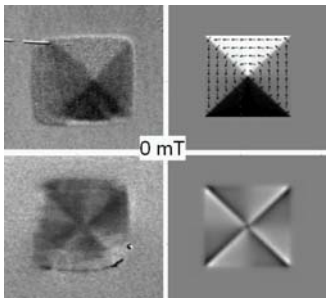

Figure 5: Isolated 2x2 m² sized Micro Contact. Modified from (Meier et al. 2004). See Text for Explanation.

CONCLUSIONS

We outlined the problem by giving a brief discourse on the fundamentals of micromagnetism. We described the structure of the simulation software and showed several ways to decrease computation time by using more effective integration schemes as well as faster, parallelizable algorithms for the stray field computation. We extended the existing code to enable direct comparison with and between experimental data observed with two measurement techniques, yielding good fits. Speedup and

extension provide a good foundation for fast simulations working hand-in-hand with micromagnetic experiments.

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AUTHOR BIOGRAPHIES

MARKUS-A. B. W. BOLTE is currently working on his master thesis in both Physics and Computer Science at the University of Hamburg, Hamburg, Germany, on the topic of simulation of micromagnetic structures.

DIETMAR P. F. MÖLLER is a professor of computer science and engineering and chair of computer science at the University of Hamburg, Hamburg, Germany. He is currently working on embedded computing systems, virtual and augmented reality, modeling and simulation, mobile autonomous systems, soft computing, medical informatics and nanostructures.

GUIDO D. MEIER is a division leader in the research group of Prof. U. Merkt at the Institute of Applied Physics of the University of Hamburg., Germany. His research activities include semiconductors, ferromagnets and hybrid devices of both materials on the micro- and nanometer scale.

ALEXANDER THIEME is a graduate student at the University of Hamburg working on his master of physics and his M.D. on the topic of simulation of biomolecular processes.