

Utilization of COMSOL Multiphysics' JAVA API for the Implementation of a Micromagnetic Modeling and Simulation Package with a Customized User Interface

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Abstract: One of the big advantages of COMSOL Multiphysics is the possibility to implement user-defined partial differential equations (PDE) which can be coupled to COMSOL's predefined application modes. However, using the tool's standard user interface requires manual implementation of the PDEs and a multitude of problem-specific parameters. This process is not just error-prone but also very time consuming. As an alternative to this manual implementation one can use COMSOL's Java Application Programming Interface which provides an easy and efficient way to create a user-defined simulation package. Here, we demonstrate the usage of COMSOL's Java Application Programming Interface by our implementation of a micromagnetic modeling and simulation package. Therein, the Landau-Lifshitz-Gilbert equation is coupled to Maxwell's equation for the magnetic field. With this implementation the magnetic properties of structures with dimensions in the order of several nanometers can be analyzed.

Keywords: Micromagnetics, Java API, magnetic nanostructures, magnetic nanoparticles, Landau-Lifshitz-Gilbert equation.

1. Introduction

Nanostructured magnetic materials have recently been focused by many research groups because of their particular properties and potential application in many interesting fields, e.g. data storage, biomedicine and smart materials. In order to calculate the magnetic properties of nano-sized structures hosting only a small number of magnetic moments like magnetic molecules, spin-discrete simulation techniques like quantum and classical Monte Carlo and spin dynamics simulations [1] are well established. Moving on to larger magnetic structures like magnetic nanoparticles or multi-

layer systems, the number of atomic moments is growing dramatically. If the density of moments becomes large enough the spin-discrete equations of motion can be replaced by partial differential equations which describe the magnetic moment as a continuous function of space and time. These continuous modeling and simulation techniques are known under the name of *Micromagnetics*.

2. Micromagnetic Modeling

The orientation of the continuous magnetic moment within a micromagnetic description is determined by minimizing the systems total energy with respect to competing energy contributions, such as the exchange energy, the Zeeman energy, the anisotropy energy, and the demagnetization energy. These energy contributions are explained in the following section.

2.1 Energy contributions

The exchange energy causes that neighboring magnetic moments align in a preferred way relative to each other. In ferromagnetic materials, adjacent magnetic moments align parallel to one another, whereas in antiferromagnetic materials an antiparallel orientation is preferred. Second, the Zeeman energy accounts for the interaction between magnetic moments and external magnetic fields. Minimal Zeeman energy is obtained, when magnetic moments lie parallel to the external magnetic field. The third contribution, the anisotropy energy, causes magnetic moments to align with certain preferred directions in case of an easy-axis anisotropy or to orient perpendicular to that direction in case of an easy-plane anisotropy. In contrast to the above described energy contributions, the demagnetization energy or stray-field energy is determined by long-range interactions. This

means that the demagnetization energy at a certain point of the micromagnetic system depends on the entire configuration whereas the other energy contributions explained above only depend on their local environment. The demagnetization energy causes the formation of magnetic domains.

2.2 Micromagnetic equations

All energy contributions mentioned in Sec. 2.1 add up to the total energy of the micromagnetic system. Minimizing this total energy leads to the well-known static Brown equation or to the time-dependent Landau-Lifshitz-Gilbert equation (LLG) Eq. (1) [2]. The LLG describes the precessional motion of magnetic moments according to

$$\frac{\partial \mathbf{m}}{\partial t} = -\mu_0 \gamma \mathbf{m} \times \mathbf{H}_{eff} + \mu_0 \alpha \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial t} \quad (1)$$

$$\mathbf{H}_{eff} = -\frac{2A_{ex}}{\mu_0 M_S} \Delta \mathbf{m} + \frac{2K_1}{\mu_0 M_S} \langle \mathbf{m}, \mathbf{e} \rangle \mathbf{e} + \mathbf{H}_{dem} + \mathbf{H}_{ext} \quad (2)$$

The effective field \mathbf{H}_{eff} given by Eq. (2) contains the contributions from the exchange interaction, the anisotropy, the demagnetization field, and the Zeeman energy. The coupling of the LLG Eq. (1) to Maxwell's equations is realized via the demagnetization field \mathbf{H}_{dem} . This set of equations can be transformed into a weak formulation which allows one to implement them directly in COMSOL Multiphysics.

3. Micromagnetic Modeling with COMSOL Multiphysics

In COMSOL Multiphysics, two application modes are needed to accomplish micromagnetic simulations. In the first place, the application mode "PDE, weak form" is used to implement the micromagnetic equations, namely the LLG and a corresponding norm condition in their weak formulation. Second, the "Magnetic fields" application mode is used to calculate the demagnetizing or stray field.

3.1 Weak Form Modeling

In order to obtain the weak formulation of the micromagnetic equations, the equations have to be multiplied by a set of test functions $\boldsymbol{\psi}$. Then they have to be integrated over the entire problem domain. Subsequently, Green's formula is used to integrate by parts. After implying the

Neumann boundary condition, a variational formulation of the original problem is achieved. This formulation, together with the Dirichlet boundary condition and a norm condition, yields the weak formulation of the micromagnetic PDE problem [3]. This formulation can be implemented in COMSOL Multiphysics. Therefore, the so-called test operator has to be used. The test operator may not be mistaken with the test functions used above. It rather generates the test functions for the variable it operates on.

$$\int_{\Omega} \langle \boldsymbol{\psi}, \frac{\partial \mathbf{m}}{\partial t} - \alpha \times \frac{\partial \mathbf{m}}{\partial t} \rangle d\Omega = \frac{2A_{ex}}{\mu_0 M_S} \sum_{x,y,z} \int_{\Omega} \langle \left(\mathbf{m} \times \frac{\partial \mathbf{m}}{\partial x_i} \right), \frac{\partial \boldsymbol{\psi}}{\partial x_i} \rangle d\Omega + \frac{2K}{\mu_0 M_S} \int_{\Omega} \langle \boldsymbol{\psi}, \mathbf{m} \times \mathbf{e} \rangle \langle \mathbf{m}, \mathbf{e} \rangle d\Omega + \int_{\Omega} \langle \boldsymbol{\psi}, \mathbf{H}_{dem} + \mathbf{H}_{ext} \rangle d\Omega \quad (3)$$

$$\frac{\partial \mathbf{m}}{\partial n} = \mathbf{0} \quad (4)$$

$$|\mathbf{m}| = 1 \quad (5)$$

3.2 Stray Field Computation

As mentioned in Sec. 2.2, the LLG is coupled to the magnetic stray field via the effective magnetic field \mathbf{H}_{eff} Eq. (2). The computation of the stray field is very elaborate and different approaches can be used. In our case, the predefined application mode "Magnetic fields" is used and for that reason the stray field is computed using the magnetic vector potential in the context of Maxwell's equations. The stray field has to be computed for every iteration step because of the bidirectional coupling of the magnetic moment and the stray field. Due to its long-range nature, the computation of the stray field is very time consuming compared to the calculation of the other energy contributions of the LLG Eqs. (1) and (2). Hence, alternative methods for a more efficient calculation of the stray field are commonly used. [4]. In this work, we use the magnetic vector potential approach. In Fig. 1 the stray field of a homogeneously magnetized cube as a result of a simulation with COMSOL Multiphysics is shown.

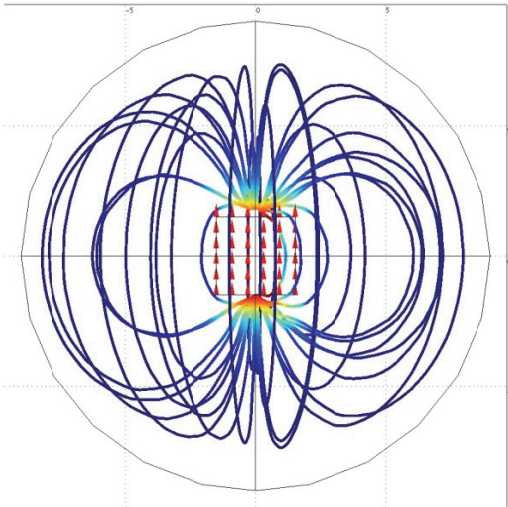


Figure 1: Stray field of a homogeneously magnetized cube computed with COMSOL

3.3 Coupling of Maxwell's equations to the stray field and the micromagnetic equations

The stray field \mathbf{H}_{dem} in Eq. (2) corresponds to the magnetic field \mathbf{H} in the equations of COMSOL's application mode "Magnetic fields", Eqs. (6) and (7).

$$\sigma \frac{\partial \mathbf{A}}{\partial t} + \nabla \times \mathbf{H} = \mathbf{J}_e \quad (6)$$

$$\mathbf{B} = \nabla \times \mathbf{A} \quad (7)$$

For a bidirectional coupling, the expressions used by COMSOL for the components of the magnetic field, have to be built into the weak form of the micromagnetic equations as well. This way, the stray field for a given configuration of the magnetic moment is computed which in turn changes the actual configuration and results in a new magnetic moment.

3.4 Simulation Process

The simulation of the micromagnetic system has to be performed in a certain way, in order to achieve convergence. First, a proper initial configuration has to be generated. If the initial configuration is too far away from a realistic configuration, the problem cannot be solved. As time-dependent simulations are much easier to handle, every simulation starts with a few time-dependent steps, even if one is only interested in the stationary state of the system. The time-dependent steps serve as pre-conditioning to get reasonable initial values. After this pre-conditioning, stationary as well as time-dependent simulations can be done.

4. Validation of the Simulation Model

In order to check the implementation of the micromagnetic equations in COMSOL, it is necessary to compare results achieved in COMSOL to some kind of reference results, i.e. analytical results or results from other software packages. The Micromagnetic Modeling Group of NIST offers a set of standardized example problems. For these problems, detailed simulation results can be referenced online [5]. In our case, μMag Standard problem #3 is chosen as a reference.

4.1 μMag Standard Problem #3

In μMag Standard Problem #3, a cuboid magnetic nanoelement with arbitrary material parameters is considered. Two different magnetic states are expected for this kind of structure:

1. *Flower state*: a homogeneous magnetization structure,
2. *Vortex state*: a curl- or vortex-like structure of the magnetic moment.

Depending on the edge length of the nano cube, one of these states forms the stationary state.

Magnetic domains are areas of homogeneous magnetization within magnetic materials. Usually, a magnetic sample consists of multiple magnetic domains. By splitting up the magnetic material in domains, the stray field energy can be reduced. At the same time exchange- and anisotropy energy have to be considered. In most cases, splitting up the magnetic material into domains results in a lower total energy of the magnetic system. In relatively small systems, the additional stray field and anisotropy energy contributions cannot be compensated by the stray field energy. Consequently, single-domain particles are formed.

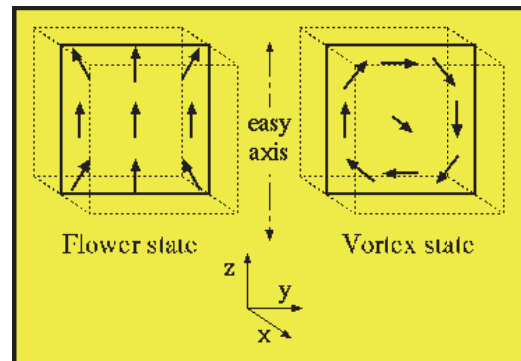


Figure 2: Possible magnetic states of a cubic nanoelement, μMag Standard Problem #3 [5]

4.2 Validation Model

To validate the implementation of the micromagnetic equations in COMSOL, the following material parameters have been chosen according to [6]:

- $K = 6.2831583 \text{ J/m}^3$,
- $A_{ex} = 1.773528 \cdot 10^{-12} \text{ J/m}$,
- $M_S = 10^6 \text{ A/m}$,
- $K_m = 6.2831583 \cdot 10^5 \text{ J/m}$,
- $l_{ex} = 5.3128 \cdot 10^{-9} \text{ m}$,
- $a = b = c = 30 \cdot 10^{-9} \dots 60 \cdot 10^{-9} \text{ m}$.

The edge length of the cube is varied in the range of 30 to 60 nanometers, because the transition between the two magnetic states is expected at $8 \cdot l_{ex} \approx 43 \cdot 10^{-9} \text{ m}$. Below this critical edge length, the flower state should be observed, whereas above the critical edge length, the vortex state should be obtained.

For the simulation it is not only necessary to model the micromagnetic system itself. In addition to that one needs to specify a surrounding volume which is essential for the calculation of the stray field. Alternatively, one could use infinite elements..

4.3 Results - Flower State

Below the critical edge length of $8 \cdot l_{ex}$ a homogeneous configuration of the magnetic moment, the so-called flower state can be observed, as shown in Fig. 3 for an edge length of 30 nm. After a few time-dependent steps for pre-conditioning, a stationary simulation has been performed. Fig. (3) depicts the stationary result. The surface plot shows the x-component of the magnetization \mathbf{M} , which is proportional to the magnetic moment \mathbf{m} . The arrow plot shows the direction of the magnetic moment \mathbf{m} in selected positions. By integrating the components of the magnetization over the whole magnetic volume, the following values have been determined in units of the saturation magnetization.

- $M_{x,avg} = -0.001$
- $M_{y,avg} = 0.001$
- $M_{z,avg} = 0.985$

When compared to the official μMag results, the following discrepancies and similarities can be found. The average magnetization in x- and y-direction is very small as compared to the total magnetization. Most of the μMag results do not

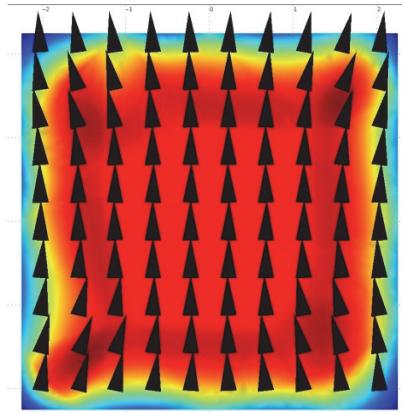


Figure 3: Result of the simulation of μMag Standard Problem #3 with an edge length of 30 nm in COMSOL. The magnetic moment has an orientation parallel to the z-axis of the cube, which is called a flower state.

include these values. However, this is what one would expect for a homogeneous configuration of the magnetization and the magnetic moment. When comparing the average magnetization in the z-direction a difference of +1.34% to the average value of all μMag results is noticed. This difference lies within the statistical error over all submitted μMag results. Together with the obtained orientation of the magnetization, the results for an edge length below the critical edge length can be considered reasonable and conclusive.

4.4 Results – Vortex State

For an edge length above the critical edge length, a vortex-like structure of the magnetic moment is expected. Fig. 4 shows the result for a simulation with an edge length of 60 nm. Each, the x- and z-components of the magnetization cancel out due to the vortex structure. In the y-direction, differences between 1.56% and 3.59% are noticed between our results and the μMag results. Again, this lies within the statistical error of all results submitted to Mag. So, the validation shows that the implementation of the micromagnetic equations is correct and can now be used for simulating arbitrary micromagnetic problems.

4. JMicomag

For the efficient usage of our newly implemented micromagnetic modeling features in COMSOL Multiphysics, the customized user interface “JMicomag” has been developed,

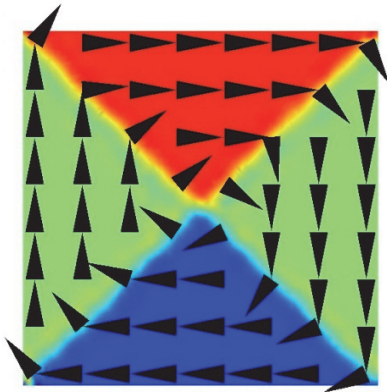


Figure 4: Simulation result for a cube with an edge length of 60 nm, which is above the critical edge length. As expected, a vortex-like structure can be observed.

taking advantage of COMSOL's Java Application Programming Interface (API). In this way, the manual implementation of the PDEs and problem-specific parameters is avoided which saves time and simplifies the modeling process.

4.1 COMSOL's Java API

On the basis of COMSOL's Java API, standalone applications can be developed. Every simulation file can be exported to a corresponding *Model Java-file* and vice versa, every Model Java-file, generated by COMSOL or externally, can directly be implemented in COMSOL. Consequently several steps in the modeling process can be simplified or automatized.

4.2 JMicomrag User Interface

In our micromagnetic modeling interface "JMicomrag" all manual parameter inputs as well as the corresponding PDEs are packaged and hidden from the user. To perform a simulation the user has to go through the following steps. First, the user defines the project name and the storage location. After this, the geometry has to be defined. In doing so, the user simply chooses one of the predefined geometry types, e.g. a sphere or a cube, and then fills in the main dimensions of the chosen structure (see Fig. 5). All necessary input fields are highlighted automatically. Afterwards, the material parameters have to be provided. Every user input is checked formally by "JMicomrag". Moreover, the user can specify simulation details on the "COMSOL Settings" page. In addition to that, at every step the user can check the input in the summary window on the "Project Properties"

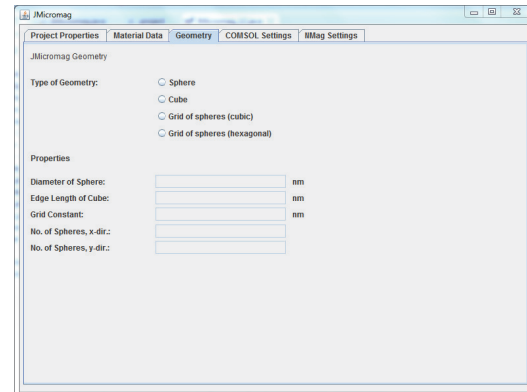


Figure 5: Geometry settings page of JMicomrag user interface, geometry type and main dimensions can be defined.

page. All settings and values are collected in there. After providing all necessary data, the simulation files are generated. The Model Java-file can easily be imported into COMSOL by the user. The Model Java-file contains the equations, the geometry, parameters and additional settings. The simulation can then be started with just one mouse-click. Furthermore, we have implemented the possibility to generate the simulation files for the micromagnetic modeling and simulation software package Nmag [7], with the same input data that is used to generate the COMSOL simulation files.

5. Conclusions and Outlook

We have created a micromagnetic simulation package by implementing the weak formulation of the Landau-Lifshitz-Gilbert equation and its coupling to Maxwell's equations within COMSOL Multiphysics. Using our implementation, we obtained a good agreement with other simulation results based on a standard micromagnetic problem. Furthermore, we developed the specialized user interface "JMicomrag" which allows the user to perform micromagnetic simulations in a very efficient and user friendly way. With these enhancements, COMSOL Multiphysics can be used to simulate and evaluate micromagnetic problems for arbitrary geometries and materials. Based on the existing implementation different extensions to this basic formalism can be implemented, e.g. the implementation of different types of the magnetic anisotropy. At the moment, only uniaxial anisotropies are implemented, but higher order anisotropies can easily be inserted within the existing framework. On the other hand, the user interface "JMicomrag" can be

enhanced. For example changes of the PDEs can be transferred to the user interface. Moreover, it is possible to raise the level of automation. Currently “JMicomag” generates the simulation files that have to be imported manually into COMSOL Multiphysics. It is imaginable that the functionality of “JMicomag” can be extended, so that import and simulation can be started within “JMicomag” and not within COMSOL Multiphysics.

7. Acknowledgement

This work was supported by the DFG (FOR945 “Nanomagnets”).

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