Imperial College London

Department of Earth Science and Engineering

MSc in Applied Computational Science and Engineering

Independent Research Project
Project Plan

Monte Carlo simulator for the exploration of magnetic nanostructures

by

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1 Introduction

Scientist has been working for many years to develop computer simulations in the field of micromagnetics. Since analytical approaches address the limited micromagnetic problems, computer simulation can overcome this problem by varying parameters and measuring different observables, etc. Therefore, computational magnetism is now seen as an indispensable tool in the research process. In addition, computer simulations enable scientists to validate the theory, guide experiments, and justify design decisions. [1].

When studying the behaviour of phase transition in the classical spin model of magnetic materials, scientists have used several computational methods, such as the mean-field method. However, those methods either fail to model the critical temperature or cannot predict the critical temperature and critical exponents accurately [2]. Thus, high-quality simulations such as Monte-Carlo simulations are needed.

When the existing computational model is used to explore new magnetic phenomena of magnetic materials, scientists often need to modify computational models to align simulations with the experimental results. Instead of changing the source code of the model, a domain-specific language (DSL) is a viable alternative. DSL is a high-level programming language that can generate source code from DSL programs to make the simulation more efficient and simple. People have developed Devito [3], which can perform finite-difference discretisation. Finite difference discretisation is essential to many classical spin models of magnetic materials. However, Devito is not designed for computational micromagnetics purposes. Ubermag is another option [4]. Unfortunately, there is only a continuous model in Ubermag. Nevertheless, after an extensive literature review, there seem to be no studies that attempted to implement a domain-specific language for the atomistic computational magnetic model.

This project will focus on developing atomistic and continuous magnetic materials models using the Monte Carlo method. Following this, I will test the performance of these two models in determining a specific physical problem such as phase transition. The final goal is to create a domain-specific language package for the developed models.

2 Literature Review

2.1 Magnetic Moments

Magnetic moment is one of the most basic contents of magnetism. When modelling a piece of magnetic material, we consider it a collection of small magnets. Each magnet has its magnetic moment. As shown in Fig. 1 (a), a elementary magnetic moment $\mathrm{d}\boldsymbol{\mu}$ can be seen as a current loop I which around an elementary oriented loop area $\mathrm{d}\mathbf{S}$ [5]. The elementary magnetic moment has the form:

$$\mathrm{d}\boldsymbol{\mu} = I \, \mathrm{d}\mathbf{S} \tag{1}$$

After that, combining the magnetic moments $\boldsymbol{\mu}$ of many infinitesimal current loops produces a magnetic moment as shown in Fig. 1 (b). It is defined as

$$\boldsymbol{\mu} = I \int_S \mathrm{d}\mathbf{S} \tag{2}$$

where, the magnetic moment $\boldsymbol{\mu}$ points perpendicular to the plane of the loop of current, in addition, its direction is associated with the direction of current I [6].

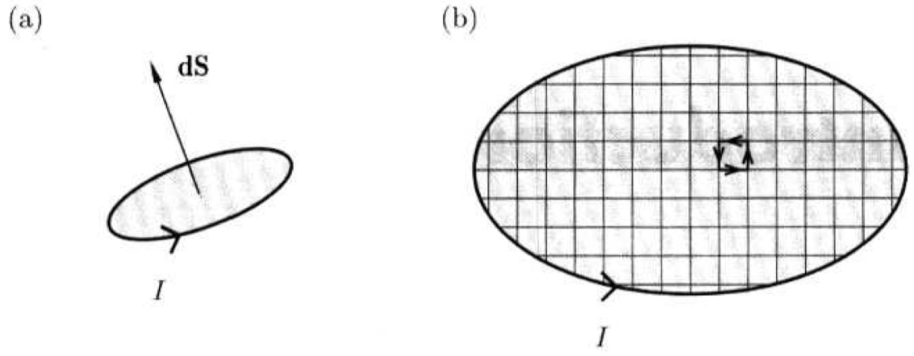


Figure 1: (a) an elementary magnetic moment. (b) a magnetic moment [5].

2.2 Computational model

Atomistic model In an atomistic model, we equal the magnetic material with a lattice of atomistic spins. Each spin $\boldsymbol{s_i}$ processes a local magnetic moment, which can be seen as a unit vector in $\mathbb{R}^3$ in most cases. There are currently several atomistic models for phase transitions in magnetic materials.

- **Ising model:** Ising was invented in 1925 as the first model to solve phase transitions in ferromagnets. It is a square lattice of atomic spins, where each atomic spin can be in one of two states. We called the two states -1 and $+1$. Since the Ising model only allows two states along an inflexible quantization axis, it is rarely used for modelling magnetic materials. [7].
- **Heisenberg model:** In contrast to the Ising model, where spins are allowed to be only -1 or 1, the spins are allowed to point in any direction in the Heisenberg model. Thus Heisenberg model can be seen as a natural extension of the Ising model. In addition, the Heisenberg model has already been extensively used to study the phase transitions of magnetic materials.
- **LLG model:** The Landau–Lifshitz–Gilbert atomistic spin model can be seen as the next-generation micromagnetic method for studying the time domain behavior of magnetic materials [7] .

The Heisenberg Hamiltonian At sufficiently low temperatures, magnetic moments of individual neighboring atoms order parallel or antiparallel to each other in ferromagnets and antiferromagnets, respectively. This interaction is well understood from the quantum perspective, but the accurate solution of this interaction in a solid material is very complex. Therefore, the simplified classical model such as Heisenberg model governed by Hamilton's equations is favored. The Hamiltonian of the Heisenberg model is [2]:

$$H_h = -\frac{1}{2}\sum_{ij} J_{ij}\mathbf{s}_i \cdot \mathbf{s}_j \tag{3}$$

where J_{ij} is a nearest-neighbour exchange parameter. $\mathbf{s}_i$ represents a normalized local magnetic moment of spin i. $\mathbf{s}_j$ is the nearest-neighbour normalized local magnetic moment of spin j. All spins are unit vectors in $\mathbb{R}^3$. $\mathbf{s}_i = \boldsymbol{\mu}_{\mathrm{i}}/\left|\mu\right|$, where $\boldsymbol{\mu}_{\mathrm{i}}$ is the magnetic moment of spin i, $|\mu|$ is its magnitude.

The full Hamiltonian The full Hailtonian consists of heisenberg term, zeeman term, DMI term, etc. When a single magnetic moment is placed into external magnetic fields $\mathbf{B}_i$, the zeeman Hamiltonian is:

$$H_z = -\mu\sum_i \mathbf{s}_i \cdot \mathbf{B}_i \tag{4}$$

Scientists discovered that chiral interactions might occur for some materials with an antisymmetric exchange. Moriya and Dzyaloshinski introduced this interaction. It is now called the Dzyaloshinski–Moriya Interaction (DMI). The Hamiltonian of DMI can is:

$$H_{dmi} = -\frac{1}{2}\sum_{ij} \mathbf{D}_{ij} \cdot (\mathbf{s}_i \times \mathbf{s}_j) \tag{5}$$

where D_{ij} is a nearest-neighbour DMI parameter. The full Hamiltonian with Heisenberg, DMI and Zeeman terms is:

$$H_{full} = -\frac{1}{2}\sum_{ij} J_{ij}\mathbf{s}_i \cdot \mathbf{s}_j - \frac{1}{2}\sum_{ij} \mathbf{D}_{ij} \cdot (\mathbf{s}_i \times \mathbf{s}_j) - \mu \sum_i \mathbf{s}_i \cdot \mathbf{B}_i \tag{6}$$

2.3 Monte-Carlo Algorithm

Metropolis Monte-Carlo (MMC) algorithm is an essential tool that enables us to study the phase transition of the classical spin model [8]. In the classical spin model, we equate a magnetic material with a lattice of particle spins, where the spins are uniformly distributed in the lattice. $\boldsymbol{r}\,(x_i, y_i, z_i)$ represents the position of each particle spin.

MMC algorithm is a Markov chain Monte Carlo method, which generates a sequence of random samples whose distributions converge to $P(x)$ [9]. The algorithm chooses whether to accept candidate spins produced by current states at each iteration. The acceptance ratio depends on transition probability. The transition probability w_{ij} is [8]:

$$w_{ij} = \begin{cases} \exp(-\Delta E/k_b T) & \text{when } \Delta E > 0 \\ 1 & \text{when } \Delta E \leq 0 \end{cases} \tag{7}$$

where the energy difference of the spin system $\Delta E = E_{\text{new}} - E_{\text{old}}$, k_b is the Boltmann constant and T is the Kelvin temperature. A simple example of the use of this method is shown in Algorithm 1.

Algorithm 1 Monte Carlo method.

Initialise the system.
Choose the simulation times N.
Choose S_m as an initial position.
for $i = 1$ to N **do**
    Produce a new position S_w using random method.
    if the energy difference$\Delta E <= 0$ **then**
        $S_{m+1} = S_w$
    else
        Generate a random number r with uniform(0,1).
        if $\exp(-\Delta E/k_b T) >= r$ **then**
            $S_{m+1} = S_w$
        else
            $S_{m+1} = S_m$
        end if
    end if
    $S_m = S_{m+1}$
end for

2.4 Domain-specific language

In this project, we will implement a domain-specific language(DSL) for computing the atomistic model of magnetic materials. The main guideline was the current available DSL package called Ubermag.

For example, when computing an integration on a discretised field such as the equation for winding number:

$$S = \frac{1}{4\pi} \iint \mathbf{m} \cdot \left(\frac{\partial \mathbf{m}}{\partial x} \times \frac{\partial \mathbf{m}}{\partial y} \right) \mathrm{d}x \, \mathrm{d}y \tag{8}$$

The Python code we implemented for computing S is [4]:

```
import discretisefield as df

J = 1
m = system.s.orientation.plane('z')
q = m @ (m.derivative('x') & m.derivative('y'))
S = 1 / (4*math.pi) * df.integral(q * df.dx*df.dy)
```

As shown in the script above, Ubermag encapsulates several DSL operations, such as derivative or integral on a discretised field m. In addition, DSL operations, including the laplacian, curl, and others, can be widely used to build models more efficiently. In addition, DSL operations include Laplacian operators and curl can be widely used to build magnetic models with higher efficiency.

3 Description of Problem and Objectives

As stated in the introduction, studies have shown that several computational methods, such as the mean-field method, perform poorly in predicting critical temperatures and critical exponents in the phase transition of the magnetic material. An important reason is that the collective effects of thermal fluctuation were neglected [10]. The Monte Carlo method is a better choice for solving phase transition problems. It describes the correlation between spins better. Moreover, some studies successfully applied that to the three-dimensional cubic Heisenberg model.

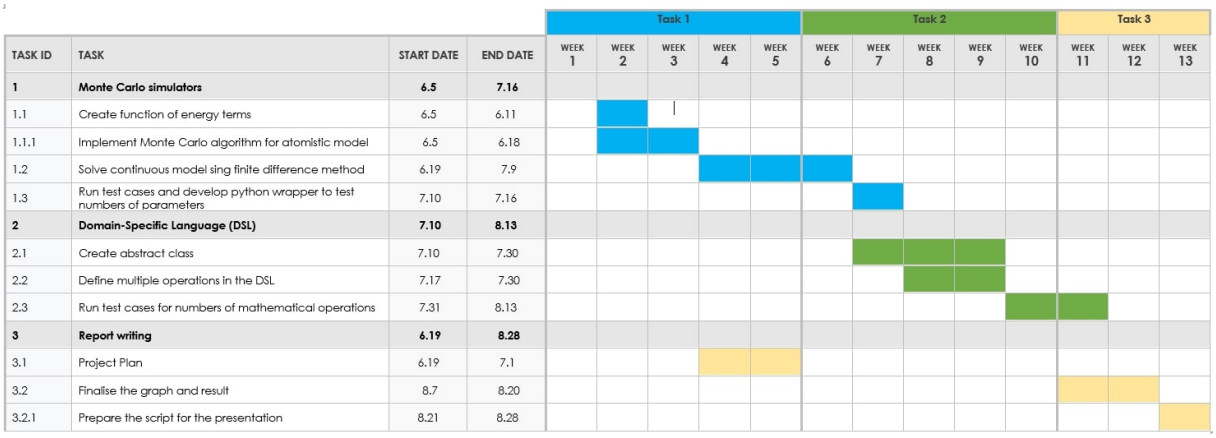
One of the challenges in computational science is that when studying the magnetic phenomena of new magnetic material, if the scientists use an open-source micromagnetic simulation package, sometimes, the simulations cannot reproduce what they saw in an experiment. That informs people that the system may have a new energy term. However, the new energy term itself is not explicit and cannot be created by varying geometry and material parameters. Scientists must try many combinations of energy terms, many different sums, dot product, cross product, nearest neighbours, etc. After that, they need to add that energy term to the package and recompile the source code. It is not feasible in most cases unless the scientists have solid experience in programming. Instead, they may be from diverse backgrounds such as experiments, pure theory, device design, etc. There are a few packages that perform domain-specific language to solve this problem. Although, no existing package can be directly applied to the atomistic model of magnetic materials.

There are 2 major objectives to achieve for this project,

- This project will develop atomistic and continuous computational models to simulate magnetic material. To do so, a Monte Carlo simulation will be used with the Metropolis Monte-Carlo algorithm. In addition to this, test the performance of these two models in determining phase transition problems.
- The project will create a domain-specific language that enables researchers to write neat, single-line, explicit equations or formulas for atomistic models.

4 Process to Data and Future Plan

As shown in Fig. 2, the gantt chart describes a timetable of the individual research project.



				Task 1					Task 2					Task 3		
TASK ID	TASK	START DATE	END DATE	WEEK 1	WEEK 2	WEEK 3	WEEK 4	WEEK 5	WEEK 6	WEEK 7	WEEK 8	WEEK 9	WEEK 10	WEEK 11	WEEK 12	WEEK 13
1	**Monte Carlo simulators**	**6.5**	**7.16**													
1.1	Create function of energy terms	6.5	6.11													
1.1.1	Implement Monte Carlo algorithm for atomistic model	6.5	6.18													
1.2	Solve continuous model sing finite difference method	6.19	7.9													
1.3	Run test cases and develop python wrapper to test numbers of parameters	7.10	7.16													
2	**Domain-Specific Language (DSL)**	**7.10**	**8.13**													
2.1	Create abstract class	7.10	7.30													
2.2	Define multiple operations in the DSL	7.17	7.30													
2.3	Run test cases for numbers of mathematical operations	7.31	8.13													
3	**Report writing**	**6.19**	**8.28**													
3.1	Project Plan	6.19	7.1													
3.2	Finalise the graph and result	8.7	8.20													
3.2.1	Prepare the script for the presentation	8.21	8.28													

Figure 2: Gantt chart of the individual research project.

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