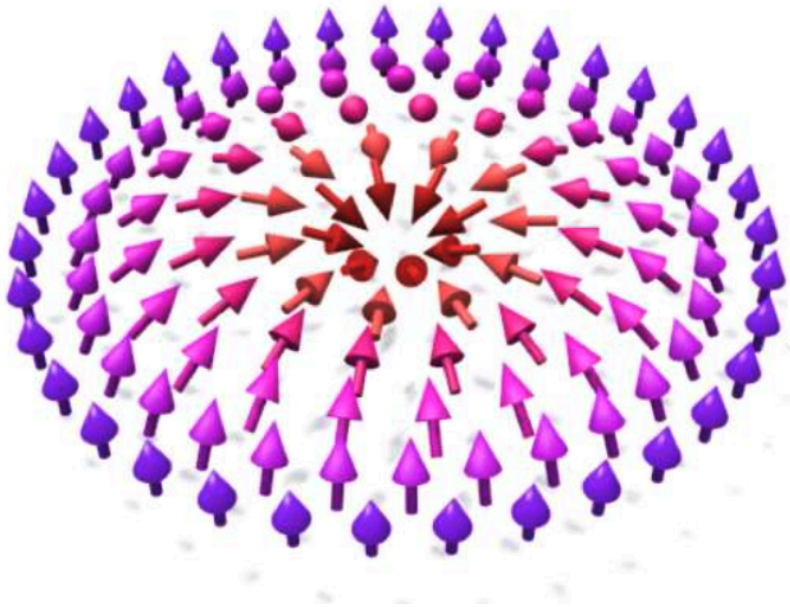
Imperial College London
Department of Earth Science and Engineering
MSc in Environmental Data Science and Machine Learning

Independent Research Project

Project Proposal



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Parallelisation and optimisation of Monte Carlo simulations in computational magnetism

Prepared by: M Gulam Nabi
CID: 02161232
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Supervisors:
Dr. Marijan Beg
Dr. Martin Lang

ABSTRACT:

Studying the phase space or conditions where the pseudo particles are stable can be intensive and expensive. Therefore, the simulation of spin-lattice systems using computational techniques is a catalyst for the development of this field. Techniques like Monte Carlo or Landau–Lifshitz–Gilbert can be used to investigate which interactions support anti-skyrmions, skyrmions of Bloch and Néel type[1], and Bloch point[6]. This is critical to study the feasibility of magnetic pseudo particles for data storage devices. The focus of this project is to create an open-source Python-based Monte Carlo simulator capable of running efficiently on both CPUs and GPUs. The second objective of this project involves using the developed simulator to replicate and validate findings from existing research. Furthermore, the simulator will be employed to investigate the stability of Skyrmions and Bloch points at room temperature, a novel inquiry that has not been previously explored. Moreover, the project aims to calculate the lifetime of Bloch points, an aspect crucial for assessing the feasibility of utilizing Bloch-point-based data storage.

INTRODUCTION:

Nanomagnetism

In 1962, Tony Skyrme developed a hypothetical object in which the vectors of a magnetic field are twisted and knotted in such a way that they result in a spin-effect, resulting in a 3D object that is a pseudo particle. An important feature is that the surrounding magnetic field is still uniform and that only this smallest possible area has been affected. It was named a skyrmion after him and for years they were just a useful tool in finding properties of subatomic particle interactions but no evidence for their actual existence was found at the time. Since then Magnetic skyrmions existence has been proven. They are meta-stable spin structures that naturally emerge due to interactions between atoms in a crystal lattice in magnetic materials.

Computational nanomagnetism

The creation and annihilation of skyrmions not only depends on different interactions arising due to crystal lattice but also on external factors like magnetic field and temperature. Studying the phase space or conditions where the skyrmions are stable can be intensive and expensive. Therefore, simulation of spin-lattice systems using computational techniques like Monte Carlo can be used to investigate which interactions support anti-skyrmions, skyrmions of Bloch and Néel type[1], and Bloch point[6]. These computational techniques can

shed light on the creation and annihilation processes of these pseudo particles and also explore other magnetic properties.

Importance:

1. Applications in data Storage with increased capacity, faster data access, and improved energy efficiency. Sensors and biomedical applications.
2. Applications in renewable energy technologies such as magnetic-based solar cells, magnetic fuel cells, and advanced batteries.

PROJECT OBJECTIVES:

1. Code the energy terms for both atomistic and continuous models.
2. Develop an open source Python based Monte Carlo simulation method from scratch that works on CPU and GPU.
3. Validate the simulator by reproducing the results from previous simulations and experimental research.
4. Study the stability of Skyrmions and Bloch points near room temperature.
5. Simulate conditions for annihilation and creation of Bloch point to collect telegraphic noise signal data.

BACKGROUND:

The magnetic interactions between the neighbouring atoms and external factors give rise to different energies:

1. Zeeman energy
2. Anisotropic energy
3. Dzyaloshinskii–Moriya (DM) interactions
4. Exchange energy

Models for energy computation

There are mainly two models to compute the energy terms, called atomistic and continuous models. The atomistic approach takes into account each atom's magnetic moment (**Si**) and its neighbour to calculate energy terms. Whereas, the continuous model takes into account a set of atoms and assigns a continuous vector field ($\boldsymbol{M}(\boldsymbol{ri},t)= |Ms|\cdot\mathbf{m}(\boldsymbol{ri},t)$). $\boldsymbol{M}$ is defined by

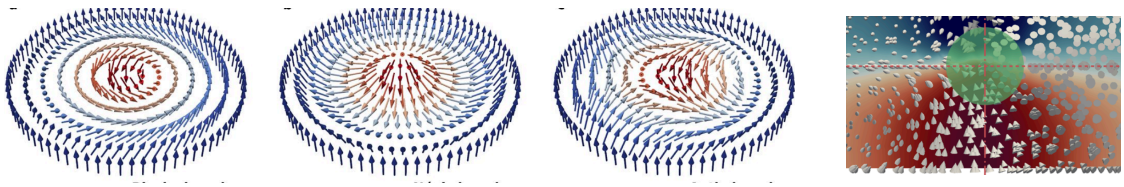
taking the average magnetic moment per unit volume. Hence, energy terms given for the continuous model are energy density.

Energy terms and their formulas based on model

Energy	Atomistic	Continuous(density)
Zeeman energy	$-\boldsymbol{B} \cdot \mathbf{S}i$	$-\boldsymbol{B}.\boldsymbol{M}$
Anisotropic energy	$-k \cdot (\mathbf{S}_i \cdot \boldsymbol{u})$	$-K\bullet(\boldsymbol{u}\bullet Sr)^2$
DMI energy	$\mathbf{d}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$	$-DM\cdot(\nabla\times M)$
Exchange energy	$-J \cdot \mathbf{S}i \cdot \mathbf{S}j$	$-A\bullet \mathbf{m}\bullet\nabla^2\mathbf{m}$

*details about the terms can be found in appendix 2.

The type of pseudo particle created depends on the strength and type of magnetic interaction[1,6].



Bloch skyrmion | Ńeel skyrmion | Anti-skyrmion | Bloch-point

Figure 1: Different pseudo particles

Now, that we have the required energy terms, we need a way to compute the relaxation of magnetization states.

Simulation techniques

1. Landau–Lifshitz–Gilbert equation or the stochastic Landau–Lifshitz–Gilbert equation (sLLG)[6, 7].
2. Energy minimization solvers, such as the steepest descent.
3. Markov chain Monte Carlo methods like Metropolis-Hastings.[1,2,5]

Choosing a model:

The choice of model depends on the system temperature and available compute power. LLG equations are computationally efficient and efficiently describe the system's time evolution and magnetization dynamics. But this method is applicable at zero temperature only. However, modifications to LLG such as stochastic LLG and sLLB capture some aspects of thermal effects and provide a more accurate description of magnetization dynamics at finite temperatures[7]. The energy minimisation solvers are the most computationally efficient, but share the same limitation as LLG. Monte Carlo simulations are not as efficient as the above two methods, however, they excel in broad temperature range applications. Hence, it can accurately capture thermal fluctuations. In particular, Monte Carlo (MC) simulations have been successfully used to study topological solitons in quantum field theories[1].

SCOPE AND DELIVERABLES:

Current progress:

1. Energy terms

Energy terms for different magnetic interactions have been prototyped in Python. A 3D lattice structure containing the magnetic moment vector of each atom is initialised using a NumPy array. Initialision is done using a class that creates the array and can initialise the vectors randomly or have the same direction to simulate the experimental initialisation at extremely high temperature or saturation magnetic field, respectively. Then the energy terms are calculated using the atomistic model.

2. Simulation

Monte Carlo is the method of choice since we will be studying relaxation near room temperature. In a study of skyrmions[1,2], the Monte Carlo approach was able to simulate at varying temperatures and the results accurately corresponded with the experimental results[2].

Since there are no open-source Monte Carlo simulation techniques available for nanomagnetism in Python. I have coded a rudimentary Monte Carlo approach that samples from the a Boltzmann distribution at a given temperature. However, the

simulation gets stuck sometimes and is time consuming. To overcome the latter, in the coming days, I plan to use the continuous model for energy terms and parallelise the process in Python using mpi4py.

Next steps:

1. Model Validation

After successfully developing the MC simulation, I will validate the model by reproducing experimental results related to the formation of magnetic skyrmion tubes8. Then, I will reproduce the results produced by Beg, M. Et al. to stabilise the Bloch point. Since the follow-up study is related to the Bloch points.

2. Improve Monte Carlo

CPU based parallelisation of Monte Carlo will be done by exploring packages like Dask/ Numba/mpi4py and for GPU based parallelisation, PyCUDA will be examined. The parallelisation and enhancement of Monte Carlo will be done in collaboration with fellow interns. If I have sufficient time I want to try a multimodal approach of using LLG/sLLG for a faster approach to the relaxation state and then using Monte Carlo to simulate the temperature fluctuations in the phase space near the equilibrium state.

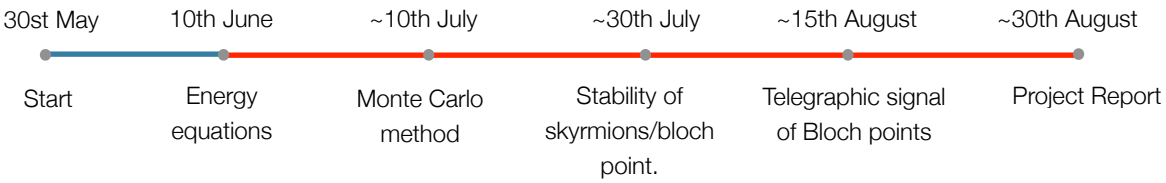
4. Bloch points and Telegraphic signals

One of the major applications is data storage for these pseudo particles. In the case of skyrmions, bit 1 is denoted by the existence of a skyrmion and 0 when there is no skyrmion. However, Bloch points are a better way to store the data because a Bloch point can store both 0 and 1 bit depending on the configuration, 'head-to-head' or 'tail-to-tail' Bloch point[6]. With the successful stabilisation of Bloch points as shown by Beg, M. Et al[6], Bloch points seem to be a feasible alternative for data storage applications.

To validate Bloch points as a viable option for data storage, it should be stable at room temperature and the lifetimes of bits should be reasonably high. The results produced by Beg, M. Et al[6,4] are at temperatures lower than the room temperature. So, the next step will be to study the stability/existence of Bloch points near room temperature. This study will be done utilizing an annealing schedule[1] at near-room temperatures. Also, the lifetimes of bloch points have not been addressed before. If time permits, I will use atomistic Monte Carlo simulations to study the field-dependent mean lifetimes of the Bloch points. This study will be based on the results produced by Hagemeister, J. Et al.[2] for skyrmions and telegraphic signal data as shown in Appendix Figure 1. The

telegraphic signal data will be generated by performing simulations at fields and temperatures near the phase boundary separating the annihilation and creation of Bloch points.

TIMELINE:



CONCLUSION:

This project endeavors to create an open-source Python-based Monte Carlo simulator capable of running efficiently on both CPUs and GPUs. The second objective of this project involves using the developed simulator to replicate and validate findings from existing research. Furthermore, the simulator will be employed to investigate the stability of Skyrmions and Bloch points at room temperature, a novel inquiry that has not been previously explored. Moreover, the project aims to calculate the lifetime of Bloch points, an aspect crucial for assessing the feasibility of utilizing Bloch-point-based data storage.

APPENDICES:

1. Telegraphic noise data

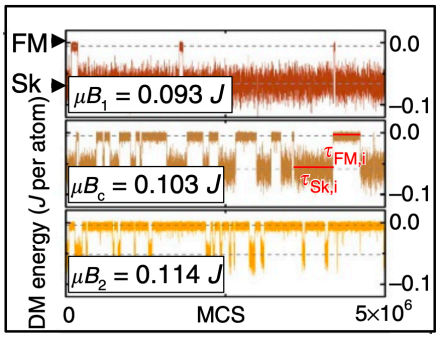


Figure 1: Telegraphic noise data for skyrmions from Haemeister, J. Et al.[2]

2. Energy terms

A) $\mathbf{S}_i = |S| \cdot \mathbf{s}_i$

Where I represents the indices. **Si** denotes a unit vector that represents the orientations of the magnetization of an arbitrary atom within a given volume.

B) Zeeman energy

$E_Z = -\boldsymbol{B} \cdot \mathbf{S}_i$

Where **B** is an external magnetic field.

C) Exchange energy

$Eex = -J \cdot \mathbf{S}i \cdot \mathbf{S}j$

Here we assume that the exchange integral value between all nearest neighbours' spins is constant and equals J.

$W_{ex} = -A \bullet \mathbf{m}(\boldsymbol{r},t) \cdot \nabla 2\mathbf{m}(\boldsymbol{r},t)$. **A** is the exchange constant.

D) DMI interaction

$E_{dmi} = \mathbf{d}ij \cdot (\mathbf{S}i \times \mathbf{S}j)$

Where $\mathbf{d}_{ij}$ is the Dzyaloshinskii vector, which is a positional vector with scale d pointing from vector $\mathbf{S}_i$ to $\mathbf{S}_j$.

$W_{dmi} = -D \bullet \mathbf{m}(\boldsymbol{r},t) \cdot (\nabla \times \mathbf{m}(\boldsymbol{r},t))$

Where **D** is the Dzyaloshinskii-Moriya energy constant.

E) Anisotropic energy

$E_a = -k \cdot (\mathbf{S}_i \cdot \boldsymbol{u})$

where k is the anisotropy constant, $\boldsymbol{u}$ is the unit vector along the preferential anisotropy axis, and the energy is set to minimum when these two vectors are parallel or anti-parallel.

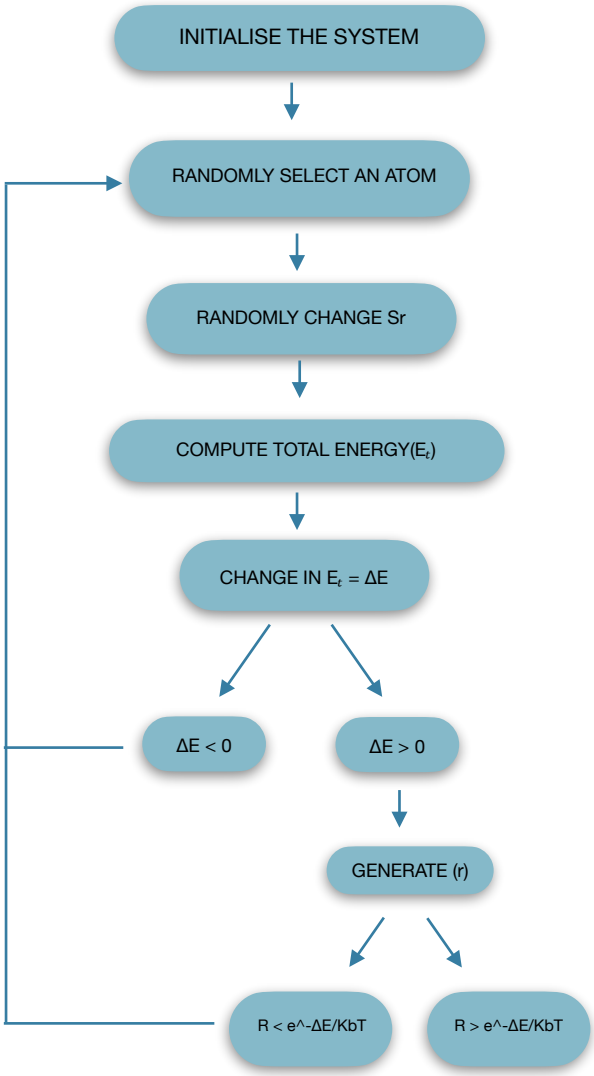
3. Monte Carlo Algorithm

1. Initialization: Initialise the system configuration. Initialision is done by spins oriented randomly or having the same direction to simulate the experimental initialisation at extreme higher temperatute or at saturation magnetic field respectively.
2. Site Selection: Randomly select a an atom within the lattice array. We'll refer to the spin at this site as **S**i. And change the spin based on the sampling method.
3. Compute total energy(Et): This can be done by summing up all the energy terms.
4. Change in energy (ΔE): Determine the change in energy that would occur if the spin **S**i at the selected site were changed.
5. Decision Making: Based on ΔE, we have to decide whether to accept the new spin or not:
    - If changing the spin would lead to a decrease in energy, then accept the new spin.
    - If changing the spin would result in an increase in energy, the accept only if a random number r sampled from normal(0,1), generated from a uniform distribution between 0 and 1, is less than r

      -ΔE/Kb.t

      $< e$

5. Iteration: Repeat steps 2 to 4 multiple times until an equilibrium state is reached.



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