Imperial College London

Department of Earth Science and Engineering

MSc in Applied Computational Science and Engineering

Independent Research Project
Final Report

Search for a Bloch point using the Mean-field model

by

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Abstract

Recent research on skyrmions suggests that magnetic skyrmions may revolutionize the way to store and process data. As interest in materials with Dzyaloshinskii-Moriya interaction gradually increases, researchers are actively searching for other topologically stable quasi-particles, such as the Bloch point. Although the finite element micromagnetic simulations and the finite difference based Monte Carlo simulations have been used to investigate the Bloch point, an efficient model that can represent the structure of the Bloch point correctly and introduce the influence of temperature still needs to be studied, as the finite element model is unable to represent Bloch points' structures well and the Monte Carlo model is inefficient. In this project, the Mean-field model is designed and applied in the combination of materials with different chiralities. Using the Mean-field model, it is found that two types of stable Bloch points emerge at the interface between two layers. Additionally, it's also found that the system undergoes hysteretic behavior and the two types of Bloch points can be switched to each other when varying the external magnetic field. This paper demonstrates that the Bloch point is a promising topologically stable quasi-particle and is expected to become a novel spintronic device. Simultaneously this paper provides an efficient and powerful model for computational micromagnetics.

1 Introduction

1.1 Background

Stepping into the 21^{st} century, the demand for data has increased rapidly as data science and artificial intelligence have flourished. Simultaneously, memory devices have reduced in size, with the widespread use of embedded devices such as smartphones. Traditional hard disk drives(HDDs) have disadvantages such as low storage density and slow read/write speeds, which gradually fail to meet the needs of modern data storage and processing. Therefore, tremendous efforts should be focused on the investigation of new memories with non-volatility, high data density, mutability(allowing information to be overwritten), and long life expectancy. [1, 2, 3]

With the discovery of magnetic skyrmions[4, 5], materials with the Dzyaloshinskii-Moriya interaction (DMI)[6, 7] have become the focus of research. A Bloch point is a singularity in a ferromagnet at which the vector of the spontaneous magnetization does not exist. [8, 9] So far, studies have demonstrated the existence of the Bloch point in the combination of materials with different chiralities. [10] Due to the interaction between contrary chiralities materials in the system, the local magnetization at the center of the interface between the two materials vanishes and the Bloch point appears. The topologically stable Bloch points may not lose information after a power-off, which means it offers a prospect as a nanometer-scale nonvolatile memory.[11] The diameters of Bloch points range from 1 to $100\,\mathrm{nm}$(as small as a few atom spacings), which means that the storage density could be high.

Simultaneously, it has also been demonstrated that there are two types of stable Bloch points and these two states have been proven to be interconvertible by changing the external magnetic field. [10] That means Bloch points promise to be a mutable memory. Existing research has shown that it is possible to store a 10-character word in ASCII code using 80 Bloch points. [12] Therefore, in a search for potential future spintronic devices, research on the stability, manipulability and temperature sensitivity of Bloch points may represent an important new avenue for research.

1.2 Problem Statement

To investigate whether the Bloch point can be used as a novel spintronic device, especially the computer memory, we need to study:

- the stability of the two types of Bloch points
- whether the two types of Bloch points can be switched between and how to manipulate it
- the effect of temperature on the properties of Bloch points

The system studied in this project can be modelled as Fig 1:

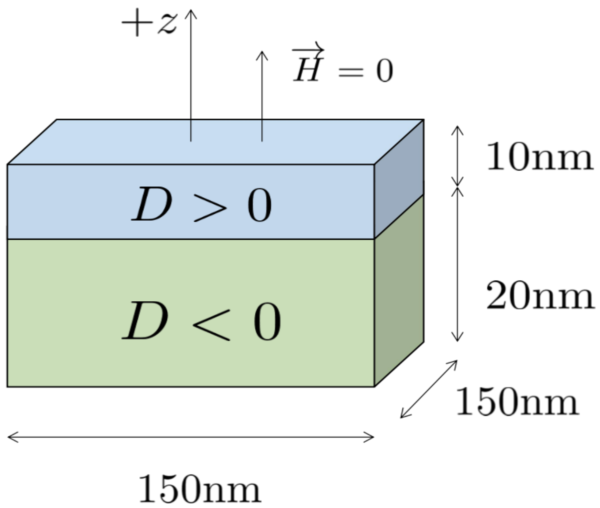


Figure 1: The geometry of the complex system. The system is made up of cubic B20 FeGe materials with the upper and lower layers having opposite chiralities. Specifically, the upper material has a positive DMI constant($D > 0$) while the lower material has a negative DMI constant($D < 0$). Further material parameters can be found in the Code metadata section. The length and width of the two layers are $150\mathrm{nm}$ respectively. The thicknesses of the upper and lower layers are $10\mathrm{nm}$ and $20\mathrm{nm}$ respectively. More details on the choice of thicknesses can be found in Marijan's paper[10]. For the convenience of the subsequent description, the direction from the lower layer to the upper layer is defined as the positive out-of-plane $+z$ direction. The vector $\mathbf{H}$ indicates the external magnetic field.

From the model, it is found that the upper and lower layers of material have opposite chiralities, which is the key point in generating the Bloch point. The materials studied in the project are cubic B20 FeGe with the opposite chiralities, more details about the materials can be found in the Code metadata section.

Using the Mean-field model for simulation, we have the following results:

- Two types of stable Bloch points emerge at the interface between two layers.
- The system undergoes hysteretic behavior which means that the two Bloch points can switch between with the vary of the external magnetic field.
- When the temperature rises to infinity, the magnetization of the whole system disappear. Furthermore, the Mean-field model is temperature sensitive, which means that the results of the simulation change by varying the temperature.

1.3 Literature Review

Ferromagnetic materials are an important class of materials, especially for storing and processing data. The study of micromagnetism has a long history. With the development of modern computing techniques, micromagnetic simulations could be performed before an expensive and time-consuming experiment in order to navigate the parameter space that would otherwise be impossible to study in detail. [13] The most common method used to explore the properties of Bloch points is the finite element micromagnetic simulations[10]. This simulation method, however, sets the length of the magnetization to a constant $\mathrm{M_s}$, which means that at the point where Bloch point appears, the length of the magnetization is still set to the non-zero constant $\mathrm{M_s}$. In reality, however, the length of the magnetization at this singularity should be 0. [8] Furthermore, this simulation method does not introduce the effect of temperature on this magnetic system. In detail, this model cannot simulate the case where the temperature is greater than 0 which is the real situation where the Bloch-point-based memory is actually applied. In summary, a model that could vary the magnetization in length and that could introduce the effects of temperature on the simulations is needed urgently.

The recently proposed Micromagnetic Monte Carlo model [14] is able to change not only the directions of magnetization for different atoms but also the magnetization's length atom by atom. This novel model is also applicable both below and above the Curie temperature. This model remedies some shortcomings of the finite element micromagnetic simulations model. However, due to the features of the Monte Carlo algorithm, the changes in both direction and length of magnetization are random, thus, there is an uncertainty in the direction of changes. In Lepadat's report[14], we can find that the probability of acceptance of each change for each atom is only about 0.5, which means that about half of the simulations are not valid. From the above description, it is obvious that the Monte Carlo model is not highly efficient, especially in the simulation of large-scale systems. Although the speed of simulation could be increased by using parallel techniques or by using more efficient hardware devices such as GPUs, it cannot address the fundamental issue of efficiency. The key point is that the Monte Carlo model is based on an evolutionary search for the equilibrium ground state. The core point of the Monte Carlo method is to do an estimation based on random sampling at the cost of a statistical error. An ideal model of relaxing the system to the equilibrium state should be a model in which each change can be made in a specific direction depending on reality instead of each change being an attempt with no defined direction.

To summarise, we should design a new model that possesses the following characteristics:

- The model should change the length of magnetization atom by atom to simulate the real situation of the Bloch point and then it is possible to represent the correct structure of the Bloch point.
- The model should be able to introduce the directions of change dynamically to make the algorithm more efficient.
- The model should be able to introduce the effect of temperature to study the temperature sensitivity of Bloch points.

This report will first introduce the concept of the effective field which gives the changes a dynamic direction and then will introduce a new model called the Mean-field model based on Hovorka's work [15] in the Methodology section. The simulations' results on stability and hysteresis using the Mean-field model are reported in the Results and Analysis section. Some interesting results are also reported in the Results section. Finally, the conclusion and discussion about the project are reported.

2 Methodology

2.1 Micromagnetics

Micromagnetics is the study of magnetic behaviour at nanometer scales. Micromagnetism as a continuum theory bridges the gap between quantum theory, dealing with atomic scales, and Maxwell's theory, dealing with macroscopic dimensions. After that, it can be explained well about the micromagnetics, the magnetization processes, and the hysteresis of ordered spin structures such as skyrmions and Bloch points. This project will therefore use computational micromagnetics techniques to study the Bloch point. In the continuum theory, the quantum spins $(\mathbf{S})$ are replaced by a continuous vector field $\mathbf{M}(\mathbf{r}, t)$ which describes the magnetization at a certain point in time (t) and at a certain position in space $(\mathbf{r})$.

In order to use computers to assist with experiments, we first discretize the continuous materials. The finite difference method(FDM) is the most popular discretization technique for the simulation of micromagnetics. Due to the simple geometry of the study object in this project, FDM, with the restriction of regular meshes but the application in high-performance algorithms, is an ideal method. Therefore, the finite difference discretization and then the continuous Mean-field model is used to find the equilibrium of a magnetic system in this project.

2.2 Static Micromagnetics

Static micromagnetics study the stable magnetization configurations and hence is an important model to study the stability of Bloch points. Simultaneously, it's also a valuable model for the investigation of material properties such as hysteresis. The prerequisite for a stable magnetization configuration is to find the minimum of the total free energy(E) for the system. The algorithms mentioned in Literature review section and the Mean-field algorithm are all used to minimize system energy.

The configuration with the energetic minimum is found when the derivative $\delta E(\mathbf{m})/\delta\mathbf{m}$ equals 0 ideally. The iteration, thus, should be along the direction of the derivative to minimize the total free energy. Therefore, from the defining equation of $\mathbf{H}_{\text{eff}}$ (Eq.1), the effective field indicates the ideal direction of iteration and then can be used to update the status of the system at each iteration. In the Mean-field model, the effective field is introduced to avoid the error from random sampling and to make sure all changes will be accepted.

$$\mathbf{H}_{\text{eff}} = -\frac{1}{\mu_0 \mathrm{M_s}} \frac{\delta E(\mathbf{m})}{\delta \mathbf{m}} \tag{1}$$

where μ_0 is a constant describing the vacuum permeability, $\mathbf{m}$ is the unit vector of $\mathbf{M}$ and M_{s} is the saturation magnetization. In the initial system, therefore, we have $\mathbf{M} = M_{\text{s}} \cdot \mathbf{m}$. The magnetization magnitude is initialized as M_{s}, due to the strong exchange interaction in the system. The value of M_{s} is determined by the material, the value used in this project is given in the Code metadata section.

Several typical contributions to free energy in FeGe are discussed below. The Zeeman energy term introduces the effect of the external magnetic field. The interaction of Exchange energy term and Dzyaloshinskii-Moriya energy term is the key to the formation of skrmions and Bloch points.

2.2.1 Zeeman energy

Zeeman energy is the potential energy of the ferromagnet in an external magnetic field. The Zeeman energy of a magnetic body can be expressed as:

$$E_z = -\mu_0 \mathrm{M_s} \int_V \mathbf{m} \cdot \mathbf{H} \mathrm{dV} \tag{2}$$

where V is the volume of the target material and $\mathbf{H}$ is the external magnetic field. From the Eq.1, we can calculate the effective field of Zeeman energy term:

$$\mathbf{H}_{\text{eff}}^{\text{z}} = \mathbf{H} \tag{3}$$

2.2.2 Exchange energy

Exchange interaction is a quantum mechanical effect, however, in the continuum theory, the general form of it can be expressed as

$$E_{\text{ex}} = -\mathrm{A} \int_V \mathbf{m} \cdot \nabla^2 \mathbf{m} dV \tag{4}$$

$$\mathbf{H}_{\text{eff}}^{\text{ex}} = \frac{2A}{\mu_0 \mathrm{M_s}} \nabla^2 \mathbf{m} \tag{5}$$

where $A = \frac{\mathrm{JM_s^2} n}{a}$ is the exchange energy constant, and the ∇^2 is the Laplacian operator. Note that the neighboring two spins are parallel if J > 0 while they are anti-parallel if J < 0.

2.2.3 Dzyaloshinskii-Moriya energ

Dzyaloshinskii-Moriya interaction is the source for chiral spin textures such as skyrmions and Bloch points. As a result of the lack of inversion symmetry in the crystal structure, the bulk DMI appears. The bulk DMI is used in the project, therefore, all subsequent DMIs indicate the bulk DMI. The general form of the bulk DMI can be expressed to be:

$$E_{\text{dmi}} = \mathrm{D} \int_V \mathbf{m} \cdot (\nabla \times \mathbf{m}) \mathrm{dV} \tag{6}$$

$$\mathbf{H}_{\text{eff}}^{\text{dmi}} = -\frac{2\mathrm{D}}{\mu_0 \mathrm{M_s}} \nabla \times \mathbf{m} \tag{7}$$

where D $= -dM_s^2 n/a^2$ is the coupling constant depending on the atomistic coupling constants d and the lattice spacing a. and the $\nabla\times$ is the Curl operator. Note that the positive and negative signs of D indicate different chirality repectively.

2.3 Energy minimization and stopping criteria

In order to find the configuration with the Bloch point, the system needs to be relaxed to the equilibrium state. Based on the definition of the equilibrium state, the system should satisfy Brown's condition(Eq.8) when the configuration with the energetic minimum is found, at which point the iteration stops. In the Mean-field model, the stopping criteria can be expressed as Eq.9

$$\mathbf{M} \times \frac{\delta E}{\delta \mathbf{M}} = 0 \tag{8}$$

$$\mathbf{M} \times \mathbf{H}_{\text{eff}} = 0 \tag{9}$$

where $\mathbf{M}$ indicates the magnetizations, E indicates the total energy of the system and $\mathbf{H}_{\text{eff}}$ indicates the effective fields of the system.

When simulating the Bloch point, it is found that the stopping criteria is invalid when a Bloch point appears in the system. Analyzing its invalidation, the magnetization is not continuous at the point where the Bloch point emerges since the Bloch point is the singularity of the system.

In order to make the iterations stop and the Mean-field algorithm convergent when a Bloch point emerges, thus avoiding inefficient iterations, an extra condition is added to the stopping criteria based on the physical nature of the Bloch point. Through a large number of simulations, we believe that a Bloch point appears when the angle of magnetization at the interface between the two materials is $107°$ or even greater(but smaller than $180°$), at which point the iteration should be stopped. In details, the iteration stops when:

$$(iter > max_{\text{iters}}) \vee (\mathbf{M} \times \mathbf{H}_{\text{eff}} = 0) \vee (107° \leq \theta_{\text{interface}} \leq 180°) = \text{True} \tag{10}$$

where the $iter$ indicates the current number of iterations, max_{iters} indicates the max iterations used in simulations and the $\theta_{\text{interface}}$ indicates the angles' array of magnetizations at the interface. Note that one of the stopping condition term $\mathbf{M} \times \mathbf{H}_{\text{eff}} = 0$ should be replaced by the similar term $\mathbf{m} \times \mathbf{h}_{\text{eff}} = 0$, where $\mathbf{m}$ indicates the unit vector of the magnetizations and $\mathbf{h}_{\text{eff}}$ indicates the unit vector of the effective field $\mathbf{H}_{\text{eff}}$. The reason for this is that the directions of magnetizations in the system cannot be exactly the same as the directions of the effective field during the simulation. The lengths of these two items therefore inflate the error of the experiment.

2.4 Mean-field model

Based on Hovorka's work [15], we have the continuous Mean-field model to relax the system to the equilibrium state. Due to the introduction of the effective field and NumPy's powerful matrix calculation, the Mean-field model is highly efficient as it updates all the lattices at once in each iteration, and the iteration proceeds in the direction of the system's energy reduction. The pseudo code of the continuous Mean-field model is given by:

Algorithm 1 Relax the system using the Mean-field model

Require : temperature T, max iterations max_{iters}, changing rate λ
Require : Initialize the system with a uniform magnetisation configuration in $+z$ or $-z$ direction.

$iter \leftarrow 0$
$\mathbf{M}_{\text{old}} \leftarrow \mathbf{M}_{\text{ini}}$
do
 Calculate effective field: $\mathbf{H}_{\text{eff}} = \frac{2\text{A}}{\mu_0 \text{M}_\text{s}} \nabla^2 \mathbf{m} - \frac{2\text{D}}{\mu_0 \text{M}_\text{s}} \nabla \times \mathbf{m} + \mathbf{H}$
 Update the length: $\mathbf{M}_{\text{len}} = M_\text{s} \cdot \mathcal{L}\left(\beta \mu_0 \left|\mathbf{H}_{\text{eff}}\right|\right) \cdot \frac{\mathbf{H}_{\text{eff}}}{\left|\mathbf{H}_{\text{eff}}\right|}$
 where $\mathcal{L}(x) = \coth x - \frac{1}{x}$ is the Langevin function and the parameter $\beta = \frac{1}{\text{K}_\text{b} T}$ introduces temperature to the algorithm.
 Update the direction: $\mathbf{M}_{\text{dir}} = \mathbf{M}_{\text{old}} + \lambda \cdot (\mathbf{M}_{\text{len}} - \mathbf{M}_{\text{old}})$
 Compute update: $\mathbf{M}_{\text{new}} = |\mathbf{M}_{\text{len}}| \cdot \frac{\mathbf{M}_{\text{dir}}}{|\mathbf{M}_{\text{dir}}|}$
 Apply update: $\mathbf{M}_{\text{old}} = \mathbf{M}_{\text{new}}$
 Update the counter of iterations: $iter \leftarrow iter + 1$
 Calculate new effective field: $\mathbf{H}_{\text{eff}_{\text{new}}} = \frac{2\text{A}}{\mu_0 \text{M}_\text{s}} \nabla^2 \mathbf{m}_{\text{new}} - \frac{2\text{D}}{\mu_0 \text{M}_\text{s}} \nabla \times \mathbf{m}_{\text{new}} + \mathbf{H}$
while $iter \geq max_{\text{iters}}$ or $\mathbf{m}_{\text{new}} \times \mathbf{H}_{\text{eff}_{\text{new}}} = 0$

The iteration of the Mean-field model can be expressed in Fig.2:

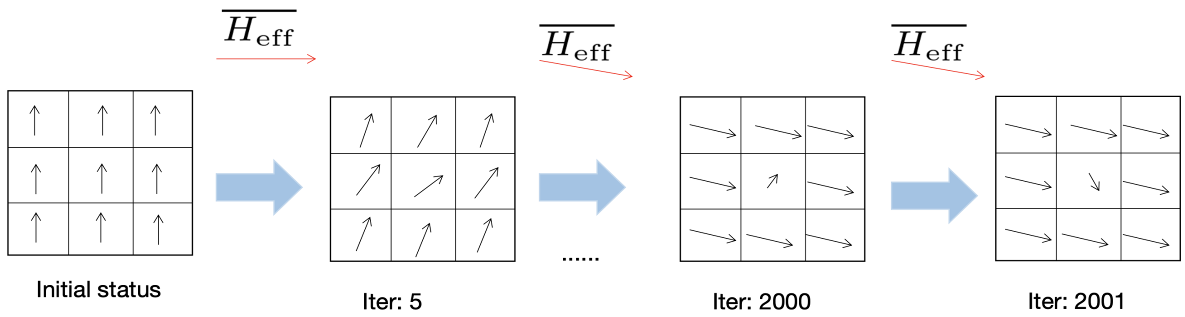


Figure 2: The schematic representation of the magnetization update during the iterations of the Mean-field algorithm. The directions of magnetization are initialized upwards. At this point, the directions of the effective fields of the system are assumed to the right. When the number of iterations is 5, the state of the system is shown in the second sub-figure and the system's effective fields change accordingly. Repeat the process until the system reaches the 2000^{th} iteration, for example, surrounded magnetization and the system's effective fields are in the same direction. In subsequent iterations, only the centre's magnetization changes dramatically. Note that this is only a schematic representation and does not represent the real process. In the real case, the system's $\mathbf{H}_{\text{eff}}$ is usually different lattice by lattice.

2.4.1 Initialization

The system is initialized with a uniform magnetisation configuration in the $+z$ or $-z$ direction to avoid the experimental impact of the initial state. The length of the magnetization is initialized to be the saturation magnetisation $M_{\text{s}} = 384\text{kAm}^{-1}$.

2.4.2 Compute the effective field

The effective field is the ideal state of magnetization at this iteration and its calculation formula is given below(Eq.11). Therefore, the magnetization is expected to move closer to the effective field spacially. Although, the exchange and Dzyaloshinskii-Moriya interaction are quantum mechanical effects, there is no need to focus on the interactions between neighbouring lattices as a result of the effective field. Based on NumPy's powerful matrix's computation, the whole system can be updated at once to substantially improve efficiency.

$$\mathbf{H}_{\text{eff}} = \frac{2\text{A}}{\mu_0 \text{M}_\text{s}} \nabla^2 \mathbf{m} - \frac{2\text{D}}{\mu_0 \text{M}_\text{s}} \nabla \times \mathbf{m} + \mathbf{H} \tag{11}$$

2.4.3 Update the magnetization

The update for the magnetization can be done by two steps:

1) The update for the length
2) The update for the direction

Geometrically, the process can be expressed as:

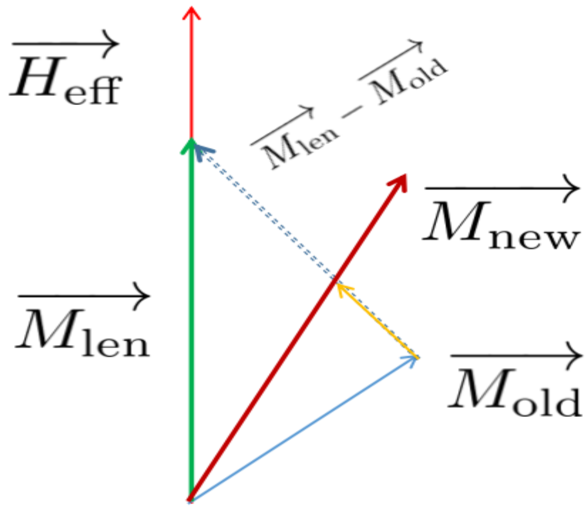


Figure 3: The Geometric schematic of updating magnetization. In this schematic, the light blue arrow indicates the magnetic state of the last iteration, the red arrow indicates the effective field, the green arrow indicates the result of updating length, the blue dashed arrow indicates the vary from $\mathbf{M}_{\text{old}}$ to $\mathbf{M}_{\text{len}}$, , the yellow arrow indicates the decayed vary which makes sure the real vary direction of this iteration and finally the dark red arrow indicates the updated state of magnetization at this iteration.

From the illustration shown above, after two steps' of updating(the vector in green and that in yellow), the new magnetization(the vector in dark red) is progressively closer to the effective field(the vector in red). The expressions used to update in two steps are given in the pseudo code.

3 Code Metadata

3.1 Code structure

As the implementation of this project is based on Object-Oriented Python, the organization of the code is given by the Unified Modeling Language(Fig.4) diagram: More details could be found from my open source repository `https://github.com/ese-msc-2021/irp-zl1021`.

3.2 Environment and dependencies

- Operating System: macOS Monterey 12.1
- Compiler: Python 3.8
- Dependencies:
  - NumPy[16]
  - discretisedfield[17]
  - micromagneticmodel[18]
  - oommfc[19]
  - Matplotlib[20]

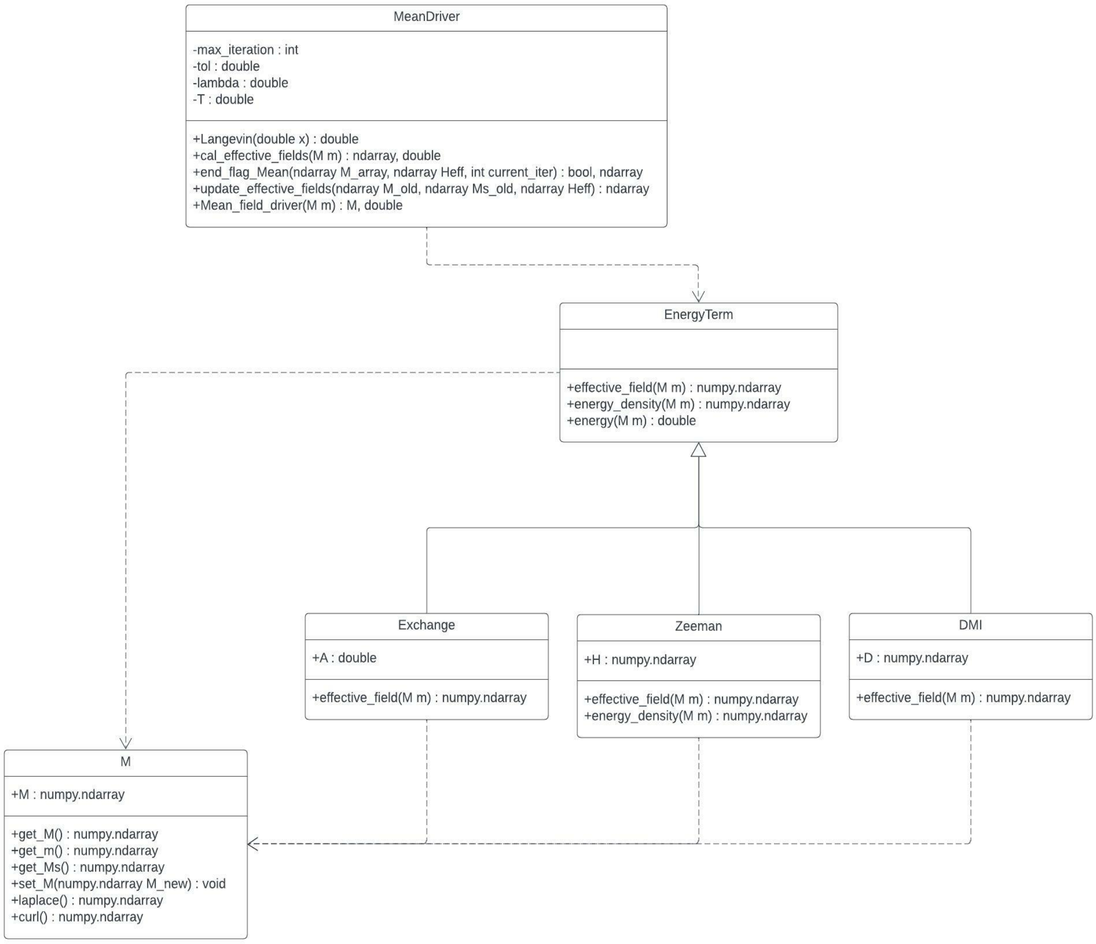


Figure 4: Code organisation diagram in UML.

3.3 Parameters used in the project

The cubic B20 FeGe material parameters [21] used in simulations are: saturation magnetisation $M_{\mathrm{s}} = 384\mathrm{kAm}^{-1}$, exchange energy constant $A = 8.78\mathrm{pJm}^{1}$, and Dzyaloshinskii-Moriya energy constant $|D| = 1.58\mathrm{mJm}^{-2}$.

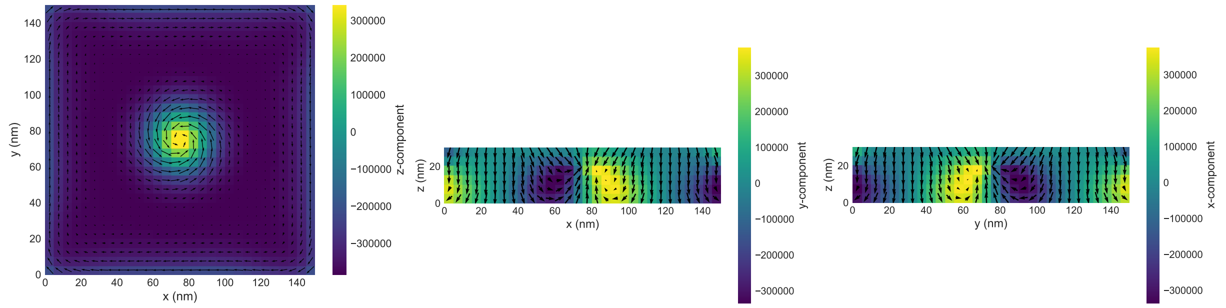
Some parameters of the two types of Bloch points is given by:

Table 1: Parameters for the two types of Bloch points.

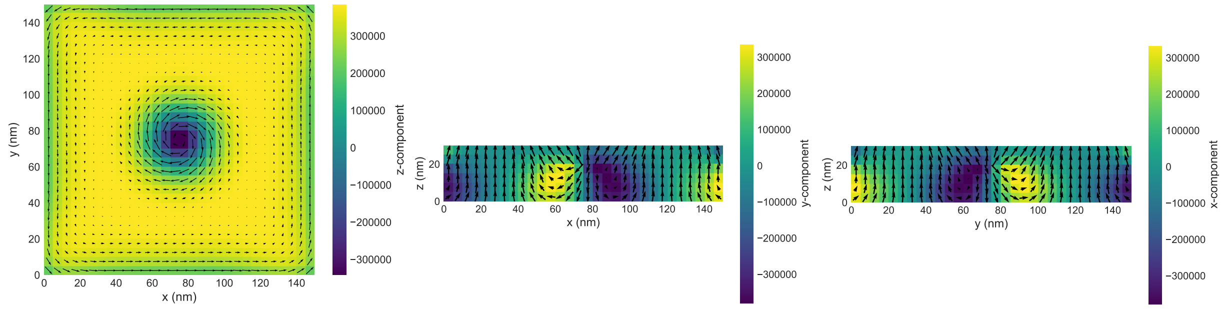
Type of BP	No.Cells	Size of cell(nm)	$\mu_0 H(\mathrm{T})$	Temperature(K)	Iter rate λ
Head-to-Head	(30, 30, 6)	(5, 5, 5)	-0.1	0	0.005
Tail-to-Tail	(30, 30, 6)	(5, 5, 5)	0.1	0	0.005

4 Results and Analysis

4.1 Stability



(a) The profile in z-direction of H-H BP (b) The profile in y-direction of H-H BP (c) The profile in x-direction of H-H BP



(d) The profile in z-direction of T-T BP (e) The profile in y-direction of T-T BP (f) The profile in x-direction of T-T BP

Figure 5: The structures of the two types of Bloch points. The three sub-figures on the first row show the structure of the Head-to-Head Bloch point. The interface's $\mathbf{M}$ point at each other. The three sub-figures on the second row show the structure of the Tail-to-Tail Bloch point. The interface's $\mathbf{M}$ point in the opposite direction of each other.

The Bloch point based spintronic device is a promising candidate of low-power and high-density memory. The first challenge in developing Bloch-points-based spintronic devices is the magnetic stability. The Mean-field model mentioned above is used to explore whether a Bloch point appears at the interface in the system mentioned in the Introduction section(Fig.1). For comparison with physics experiments, the cubic B20 FeGe is used in the project, and the realistic material parameters are given in the Code metadata section.

Using the experimental parameters given in Table1, the two types of Bloch points, which are Head-to-Head Bloch point and Tail-to-Tail Bloch point, emerge at the interface when the equilibrium state is obtained. The structures of the two types of Bloch points is shown in the Fig.5. The structure of Head-to-Head Bloch point can be observed from three orthogonal directions in the Fig.5(a), (b) and (c) respectively. As can be observed in the Fig.5(b) and (c) sub-figures, at the centre of the interface between the upper and lower layers, the magnetization are in opposite directions and have roughly the same length. This means that the magnetization at this point offset each other and end up in a state where the magnetization is zero. That means a noncontinuous singularity emerges, the singularity is in accordance with the definition of the Bloch point. The magnetization at the interface point towards each other, hence this type of Bloch point is known as the Head-to-Head Bloch point. Similarly, the Fig.5(d), (e) and (f) sub-figures shows the structure of the Tail-to-Tail Bloch point. The magnetization offset each other at the centre of the interface and they point in opposite directions to each other.

Additionally, special attention needs to be paid to the center of the interface where a Bloch point appears. In previous work[10], the precise magnetization configuration at this point cannot be obtained because the micromagnetic models assume the magnitude is constant. The encouraging thing is that the Mean-field algorithm can change both the length and the direction of the magnetization. We can therefore observe the change in the length and direction of the centre point.

4.2 Hysteretic behaviour

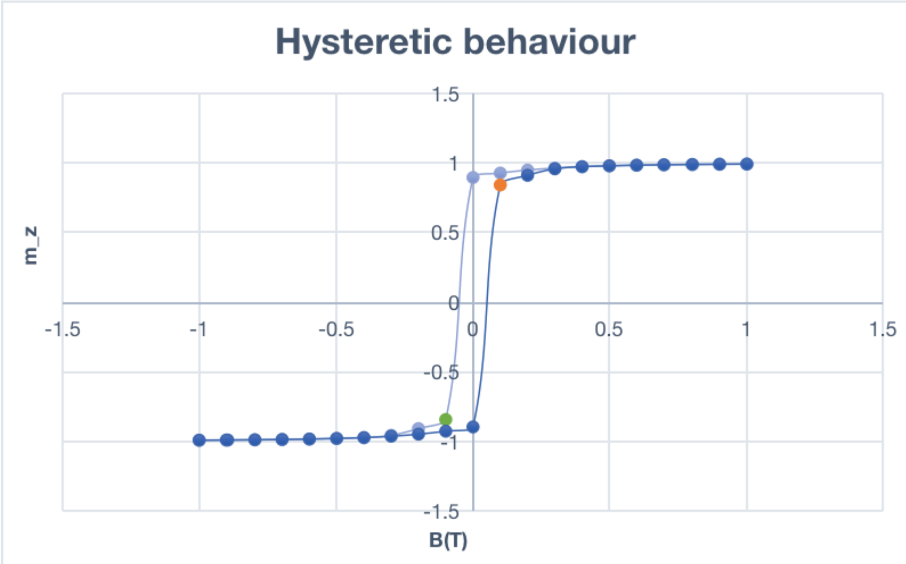


Figure 6: The hysteretic behaviour of the system. The hysteresis loops are represented as the dependence of the average out-of-plane magnetisation component m_z on the external magnetic field $\mathbf{B} = \mu_0\mathbf{H}$. The orange dot indicates the Head-to-Head Bloch point emerges, and the green one indicates the Tail-to-Tail Bloch point emerges. From the hysteresis loops, we can conclude that the two types of Bloch points can be switched into each other by varying the external magnetic field.

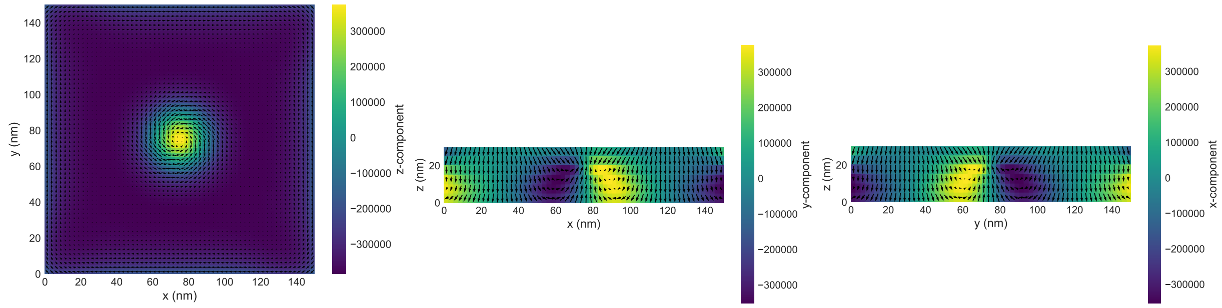
The second challenge of developing Bloch-points-based spintronic devices is the magnetic mutability. Using our Mean-field model, it is proven that the two types of Bloch points can be switched between by changing the external magnetic field. The simulations' parameters is same to that used in the study of stability. The external magnetic field used in the simulations is in the out-of-plane $+z$ direction and it varies between $1\mathrm{T}$ and $-1\mathrm{T}$ in steps of $0.1\mathrm{T}$. After changing the external magnetic field, the Mean-field is used to relax the system to the configuration with energetic minimum. And then the initial status of next simulation is set using the resulting magnetization. The mapping relationship between the average out-of-plane magnetization component m_z and the external magnetic field $B = \mu_0\mathbf{H}$ is represented in the Fig.6.

The diagram indicates the hysteretic behaviour of the system and two types of Bloch points exist in the system. The two types of Bloch points are represented in the Fig.6 by orange and green dots respectively. Moreover, it is note that the system cannot be relaxed to any other equilibrium state at any point in the hysteresis loop, which demonstrates that our system exist the bistability. In addition, one can manipulate the two Bloch points to switch between the Head-to-Head and the Tail-to-Tail configurations. In summary, the Bloch point is a promising memory since these two types of Bloch points is able to be used to store 0 and 1 respectively and the read/write operation is able to be completed by changing the external magnetic field.

Compared to Marijan's simulation results[10], the hysteretic loop changes particularly rapidly when $\mathbf{B} = \mu_0\mathbf{H}$ varies between $-0.1\mathrm{T}$ and $0.1\mathrm{T}$, which could be due to instability caused by the absence of the Demagnetization and the anisotropy energy term. The simulated material is isotropic, and accordingly, the anisotropy and demagnetization energy terms are neglected in this project. However, ignoring the effects of anisotropy and demagnetization may lead to a reduction in system stability and then lead to the extremely rapid changes in the figure.

4.3 Other study cases

4.3.1 Effect of lattice size



(a) The profile in z-direction (b) The profile in y-direction (c) The profile in x-direction

Figure 7: The structure of the Head-to-Head Bloch point when the lattice size is set as (2.5nm, 2.5nm, 5nm). Each lattice is 2.5nm long, 2.5nm wide and 5nm high. The shape of the lattice changes from a cube to a rectangle.

The material size and shape are fixed and only the number of lattices in the $x-$ and y-direction is changed from 30 to 60. Using the parameters mentioned in table 1, the final configuration of magnetization is shown above in Fig.7. Compared with the Fig.5(a), (b) and (c), the Head-to-Head Bloch point still appears at the interface of the disk, which means that the size of lattice cannot affect the results of the simulations.

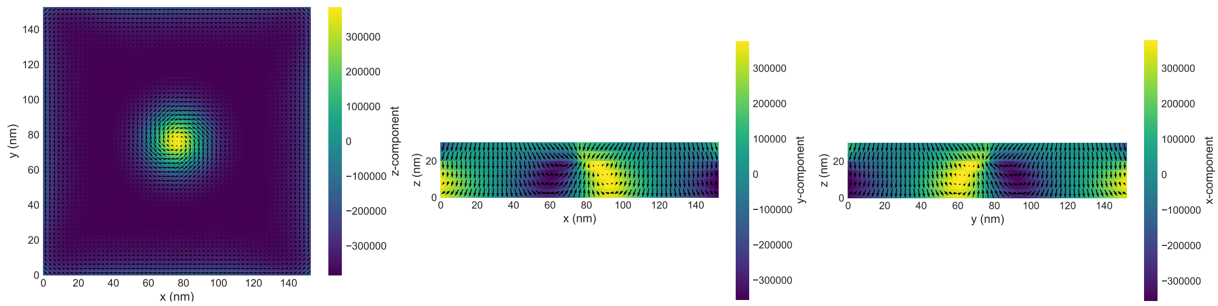
Simultaneously, when the size of lattice decreases, simulations will be more accurate, since more details is included into the model. Accordingly, the running time becomes longer, the running time spent for the Fig.5(a),(b) and (c) is about $200\mathrm{s}$ while that for the Fig.7 is about $400\mathrm{s}$. Analysing the reasons for this phenomenon, the running time spent at each iteration is extended. However, the number of iterations used in the two cases are similar, because with each update, within the machine, NumPy is updating the entire lattice at once.

4.3.2 Effect of lattice geometry

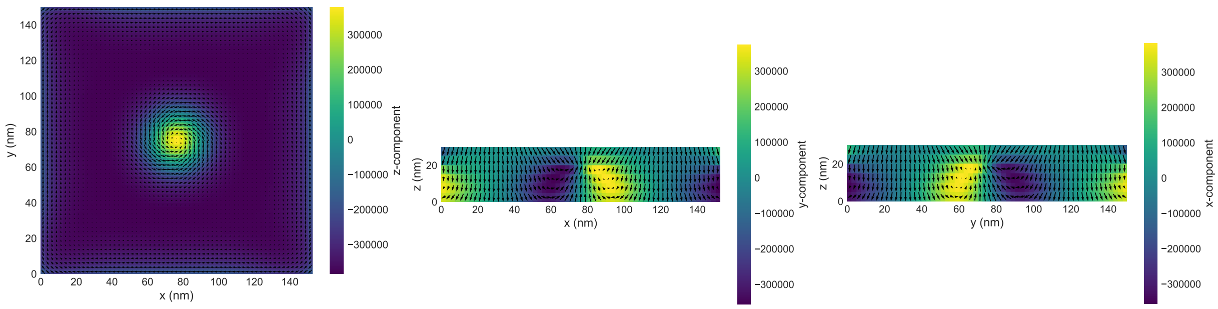
As the finite difference method used in the Mean-field model has more severe requirements for the geometry of the lattice, the effect of lattice geometry is study here. The geometry used in Fig.5 is a cube, while Fig.7 uses a rectangular cube for discretization. From the comparison figures, it can be concluded that the geometry of the lattice has little effect on the simulations, which means that the simulations could be applied for more complex systems.

4.3.3 Effect of lattice number

The three sub-figures in the first row in Fig.8 represent the case where the numbers of lattices in both the x and y directions are odd numbers. The three sub-figures in the second row in Fig.8 represent the case where the number of lattices in x direction is an odd number while that in y direction is an even number.



(a) The profile in z-direction of case 1 (b) The profile in y-direction of case 1 (c) The profile in x-direction of case 1



(d) The profile in z-direction of case 2 (e) The profile in y-direction of case 2 (f) The profile in x-direction of case 2

Figure 8: The structures of Head-to-Head Bloch point when using an odd number and an even number or using two odd numbers as the numbers of lattice in x or/and y directions. The three sub-figures in the first row indicate study case 1: the number of lattice is (61, 61, 6) and the three sub-figures in the second row indicates study case 2: (61, 60, 6). From the two set of results, we can conclude that the number of lattice cannot effect the result of simulation.

4.3.4 Effect of temperature

When the temperature rises to infinity, the magnetization will disappear. The effect of temperature is introduced by the β and then the Langevin's function to change the length of the magnetization. However, the connection between the temperature and the β is uncertain.

4.3.5 Boundary conditions

Ubermag[18] is an open source package to study the particles such as skyrmions and Bloch points using the computational micromagnetics. To ensure the accuracy of the calculation of the energy terms, the results of effective field in the Mean-field model are validated against those of Ubermag.

For the boundary condition of exchange energy term, the experimental results demonstrate that the boundary condition for exchange energy term is the standard Neumann boundary condition of second order accuracy. The boundary condition is given by:

$$\frac{\delta \mathbf{M}}{\delta \mathbf{n}} = 0 \tag{12}$$

For the boundary condition for DMI energy term, there is no existing literature on the boundary condition of bulk DMI. After much experimentation and verification with Ubermag, we found that the boundary condition for the bulk DMI energy term is the Dirichlet BC of second order accuracy. The Dirichlet BC is given by:

$$\mathbf{M} = 0 \tag{13}$$

However, due to time constraints, it is unable to give a clear mathematical proof or provide additional verification at this time. Next, based on Abert's work[22], I have the following guesses: energy terms have different effects on the interior and surface of the material, therefore, the system reaches its equilibrium state when Brown's condition(Eq.8 and Eq.9) and the Boundary condition(Eq.14) are satisfied at the same time.

$$\mathbf{m} \times \mathbf{B} = 0 \tag{14}$$

Similar to the effective field in the Brown's condition, the boundary term $\mathbf{B}$ is the ideal status of the next iteration's magnetization at the boundary. The boundary term $\mathbf{B}$ for the three energy terms are given by:

$$\begin{aligned} \mathbf{B} &= \mathbf{B}_{\mathsf{z}} + \mathbf{B}_{\mathsf{ex}} + \mathbf{B}_{\mathsf{dmi}} \\ &= \mathbf{0} + 2A\frac{\delta\mathbf{m}}{\delta\mathbf{n}} - D\mathbf{n} \times \mathbf{m} \\ &= 2A\frac{\delta\mathbf{m}}{\delta\mathbf{n}} - D\mathbf{n} \times \mathbf{m} \end{aligned} \tag{15}$$

Since the spatial derivatives of the magnetization $\mathbf{m}$ are always perpendicular to the magnetization due to the micromagnetic unit-sphere constraint, the boundary condition could be transformed to Eq16.

$$\mathbf{B} = 2A\frac{\delta\mathbf{m}}{\delta\mathbf{n}} - D\mathbf{n} \times \mathbf{m} = 0 \tag{16}$$

where $\mathbf{n}$ is the normal vector to the boundary serface. Based on the boundary condition for the exchange energy term, we have:

$$\begin{aligned} D\mathbf{n} \times \mathbf{m} &= 0 \\ \Longrightarrow |\mathbf{n}| \cdot |\mathbf{m}| \cdot \sin\theta &= 0 \\ \Longrightarrow \mathbf{m} = 0 \text{ or } \theta = 0 \text{ or } \theta &= \pi \end{aligned} \tag{17}$$

where θ indicates the angle between $\mathbf{m}$ and $\mathbf{n}$. When $\theta = 0$ or $\theta = \pi$, $\frac{\delta\mathbf{m}}{\delta\mathbf{n}} \neq 0$, which contradicts the conclusions drawn from exchange's boundary condition mentioned above. In summary, $\mathbf{m} = 0$ (Dirichlet BC) is the boundary condition for the DMI term.

5 Discussion and Conclusions

5.1 Discussion

Overall, the IRP is an enjoyable and fulfilling process. In the process, the most difficult tasks are:

- Finding and verifying the correct boundary conditions for the DMI and exchange energy term.
- Finding and verifying the correct stopping criteria in order to make the Mean-field algorithm convergent before arrive at the max iterations.
- Finding a set of valid and efficient parameters in order to make a Bloch point emerges at the interface of the system.

From the results and analysis section, it is obvious that the Mean-field model is a valid and high-efficient simulation algorithm to relax the magnetic system to the equilibrium state. The strengths are given by:

- The Mean-field model is valid. Using our Mean-field model, we can find that two types of Bloch points exist in the system stably, which fits the reality.
- Since the Mean-field model allows the change of the length, the structure of the Bloch point can be obtained in details, which bridges the gap of the obvious work.

- The Mean-field model introduces the effect of temperature, which also makes up for the micromagnetic model. Meanwhile, introducing temperature to the model is also helpful for study the possibility of using Bloch points as memory at the room temperature.
- The Mean-field model is high efficient compared to the Monte Carlo model, since the updates in Mean-field model are all accepted. For a magnetic system with $30 * 30 * 6$ lattices, the Mean-field algorithm only needs about 2000 iterations to converge. The whole process takes only $200\mathrm{s}$ to complete.

There are still some limitations due to time constraints. The four listed below are worthy of more in-depth study in the future.

- The demagnetization and anisotropy energy terms are not included in the model. However, it's easy to add them to the model because there is no need to change the framework of the Mean-field model.
- Verified with Ubermag[18], it's been found that the boundary condition for DMI term is the Dirichlet condition by experiments. The rigorous mathematical proof, however, due to time constraints, cannot be given now.
- The stopping criteria used to make the Mean-field algorithm convergent needs more study in the future. The key point is that it is essential to find a valid stop condition for the singularity.
- The connection between the temperature and the parameter β should also be study in the future.

5.2 Conclusions

The study object of this thesis is the Bloch point which is a promising spintronic memory. In order to investigate whether the Bloch point can be used as memory, the stability and hysteretic behaviour are studied. In order to find the equilibrium state of the system and then study the Bloch point's static features, the Mean-field model is designed and applied in this project. In Fig. 5, the Mean-field model shows the detailed structure of Bloch points and also introduces the effect of temperature to the simulations. Simultineously, the Mean-field model is high efficient due to its certain updating direction along the direction of the effective field. In the Fig.5, the simulations' results indicates that two types of Bloch points exist in the system stably and simulations' results also indicate that the two types of Bloch points are able to switch between each other by applying different external magnetic field in Fig.6. The conclusions of this thesis could indicate that the Bloch-points-based memory could be one of the future orientations of research in the field of computer storage.

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