Visualization of Energy Minimization in Ferromagnetic Systems

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Abstract

Many different studies of ferromagnetism and anti-ferromagnetism models have presented theories on energy minimization. These studies, however, do not give visual confirmation of what is occurring during minimization. We wish to study how the energy minimizes locally in a ferromagnetic system. Where does the energy dissipate once the magnetic field is applied? Are there regions that exhibit a chaotic nature before eventually aligning with an external magnetic field? It has been demonstrated that the energy of the system will minimize in the presence of an external magnetic field. However, regions within the lattice may not converge at the same rate. Our goal is to develop and apply a visual tool to the system, which would allow users to visualize the minimization process. In this paper, we describe a model and visualization system designed to illustrate the principles of energy minimization in ferromagnetic systems.

1 Introduction

While magnets and magnetic fields are ubiquitous and largely understood, the subtle properties of atomic magnetic dipoles include complicated interactions between individual atoms and electrons [2, 5, 9, 10, 11, 12]. A better understanding of these magnetic, molecular interactions could be applied to various applications such as creating faster, more efficient random access memory (RAM) in modern computers.

We constructed software that models and visualizes magnetic dipoles in a lattice and studied how the dipoles interacted with one another. Our software models the energy minimization that naturally occurs in ferromagnetic materials using a basic model for the Hamiltonian. Then, our software uses OpenGL to produce real-time three-dimensional renderings of the interactions between magnetic dipoles.

Additionally, the software models the interaction of the dipoles with an external magnetic field. This serves to demonstrate real life scenarios and to provide a litmus test as to whether or not the energy minimization is being modeled appropriately and accurately. Finally, our software models thermodynamic effects. By modeling the thermodynamic energy (heat) of the system, our software can show things like the threshold at which a material loses its ferromagnetic properties.

2 Background

2.1 Physics

The Heisenberg model is a simple n-vector model that allows us to represent magnetic dipoles in a lattice and gives the Hamiltonian of an individual dipole. *The Hamiltonian directly corresponds to the total energy of the system.* A minimization of the total Hamiltonian indicates that the system has been allowed to align internally in the absence of an external magnetic field or has aligned with the external magnetic field. The Heisenberg model uses the Nearest Neighbor Principle in the calculation of the Hamiltonian. The Nearest Neighbor Principle states that only the surrounding dipoles' orientation will be considered to be most significant in calculation of the Hamiltonian. The surrounding dipoles in our system will be located above, below, left, right, in front and behind. The Heisenberg model defines the Hamiltonian of the jth dipole to be:

$$H_j = -\sum_i \vec{m}_i \cdot \vec{a}_j - \vec{B} \cdot \vec{a}_j \tag{1}$$

The $\vec{a}_j$ is the vector that represents the jth dipole in the lattice. The $\sum_i \vec{m}_i \cdot \vec{a}_j$ is the nearest neighbor sum where $\vec{m}_i$ is the vector that represents the neighboring dipole. $\vec{B}$ is the magnetic field of the system. An assumption of the Heisenberg model is that the magnitude of the dipole moment is one.

Additionally, we wish to model the effect of temperature on the Hamiltonian in the system. The energy of the jth dipole due to temperature is given by:

$$E_j = \frac{F}{2} k_b T \tag{2}$$

T is the temperature of the entire system and k_b is the Boltzman constant. F represents the degrees of freedom. For our system, there are three rotational degrees of freedom. We will assume that this energy is due to the rotational kinetic energy of the jth dipole given by:

$$KE_j = \frac{1}{2} I \omega^2 \tag{3}$$

The I is the moment of inertia and ω is the angular velocity defined by:

$$\omega = \frac{\Delta\theta}{\Delta t} \tag{4}$$

If we substitute ω from $Eq.(4)$ into $Eq.(3)$ and set the kinetic energy equal to the thermal energy from $Eq.(2)$ and solve for T we get formula for the temperature as a function of $\Delta\theta$:

$$T = \frac{1}{3}\Big(\frac{I}{k_b \Delta t^2}\Big)\Delta\theta^2 \tag{5}$$

Using this relationship between the temperature and $\Delta\theta$, we can model the temperature of the system by altering the amount of random rotation ($\Delta\theta$). Another physical quantity that we will use is the magnetization. This is a measure of how the system has aligned with an external magnetic field. The magnetization is given by:

$$\vec{M} = \frac{1}{N} \sum_j \vec{a}_j \tag{6}$$

Typically we will take projections of the magnetization in the direction of the external magnetic field. This scalar quantity represents how much the dipoles have aligned with the external magnetic field.

Physically, we expect that applying these formulas will exhibit the following behaviors to system: If the temperature is zero ($T = 0$), the system will minimize its energy and all vectors will align. If the temperature is not zero ($T \neq 0$), then we expect that the energy will *stabilize* but may not become completely minimal. Lastly, if the temperature rises above the Curie temperature, the system will be unable to minimize and the dipole moments will not align. However, in the presence of a magnetic field, the system will exhibit paramagnetism, a form of magnetism that only exists in the presence of an external magnetic field. The algorithm we developed to model the system is presented in section 3.

2.2 Visualization

Many scientific visualization techniques have been developed for representing and understanding three-dimensional scalar and vector fields. Perhaps the most straightforward technique for visualizing a vector field is to use a series of lines or glyphs that

are tangent to the vector field. This technique is known as vector plots or hedgehogs [7].

In addition to the vector field, we also wish to visually represent the Hamiltonian that exists throughout the three-dimensional domain. Volume rendering is a classic visualization technique that uses color and opacity to represent a 3D scalar field. The process begins by assigning a scalar value to each point in the domain. A *transfer function* is defined to map each scalar value to a distinct color and level of transparency [8]. The image is rendered by taking a number of 2D slices through the 3D volume that is to be rendered. The slices are colored—or texture mapped—according to the transfer function at each point in the domain. The final image is constructed by compositing the transparency values within the slices to form a final 2D image that accurately depicts the 3D volume.

Field et al. have developed a technique that combines volume rendering with other vector field representations to visualize multiple quantities in the same three dimensional domain [3]. Our work is inspired by these techniques and we seek to expand these methods to better understand the minimization of the Hamiltonian.

3 Minimizing the Hamiltonian

We first randomly initialized the orientation of each dipole in a lattice consisting of 20^3 dipole vectors. Our initial implementation of a Monte Carlo method to minimize the Hamiltonian proved to be computationally expensive. Instead, we employed an iterative approach described in the next section.

3.1 An Iterative Algorithm for Minimizing the Hamiltonian

After the dipoles were randomly initialized, an iterative approach is applied to find the orientation of the system that yields the minimum Hamiltonian. The technique we developed for updating the lattice involves a simple manipulation of $Eq.(1)$. The Hamiltonian calculation involves a summation of its nearest neighbors added to the magnetic field. We take this to be one vector $\vec{K}_j$ defined for the jth dipole to be

$$\vec{K}_j = (\sum_i \vec{m}_i + \vec{B}) \tag{7}$$

To update the lattice we add $\eta(\vec{K}_j - \vec{a}_j)$ to $\vec{a}_j$ for each dipole, η is a small user-defined constant that is on the order of 10^{-2}. This constant relates to the type of material, the value of the time step, and the rotational inertia. It is defined by the user to attain the desired behavior of the system.

In figure 1, we show the results of our iteration method on the alignment of the dipoles for various magnetic field strengths. We apply the magnetic field in the direction of the x-axis. The alignment of the dipoles is represented by the magnetization projected

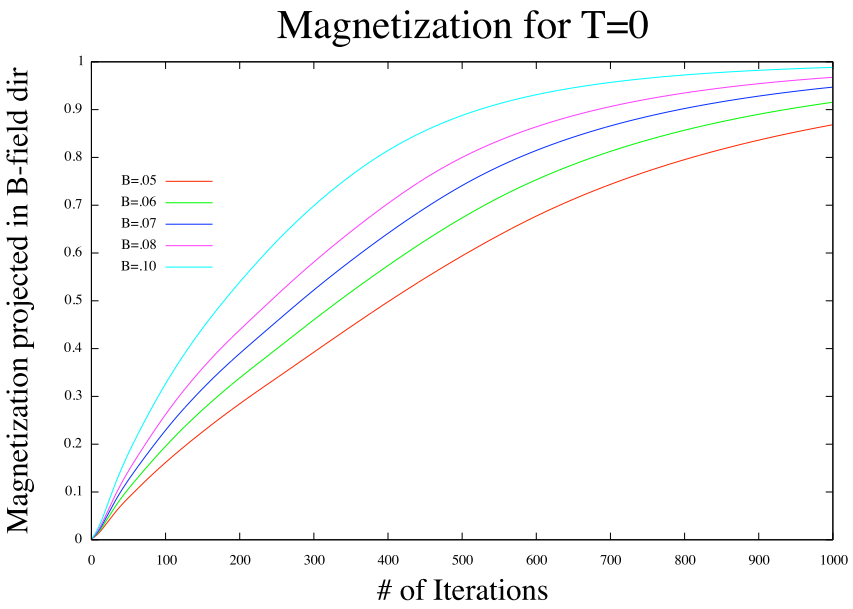


Figure 1: The magnetization approaches 1.0 for a system with no temperature and a magnetic field. If the magnetic field is stronger the graph approaches it more quickly. This figure demonstrates exactly how we expect the energy to minimize.

in the direction of the external magnetic field. Perfect alignment with the magnetic field would yield a magnetization of 1.0. As expected applying a stronger magnetic field causes the dipoles to align more rapidly than a weaker magnetic field.

3.2 Incorporation of Temperature

In order to incorporate temperature into our system, we evaluated *Eq.*(5) and assigned $\frac{1}{3}\left(\frac{I}{k_b \Delta t^2}\right) = 1$. This makes the relationship between temperature and the average change in the angle very manageable. However, we lose the physical interpretation of the temperature until further unit analysis is performed. The next step is to allow our system to have random rotations of the dipoles because we want our system to have a *freedom* in movement that non-zero temperature implies. We use the Central Limit Theorem (which was first explored by De Moivre[1]) to achieve a Gaussian-like distribution in which we could control the average angle and the variance independently. Figure 2 shows some plots of energy minimization at different temperatures. This figure demonstrates how temperature affects the minimization for a given magnetic field.

4 Visualization

In the next section, we describe visualization methods developed to better understand the orientation and alignment of the dipole vectors and the three dimensional convergence patterns of the Hamiltonian minimization.

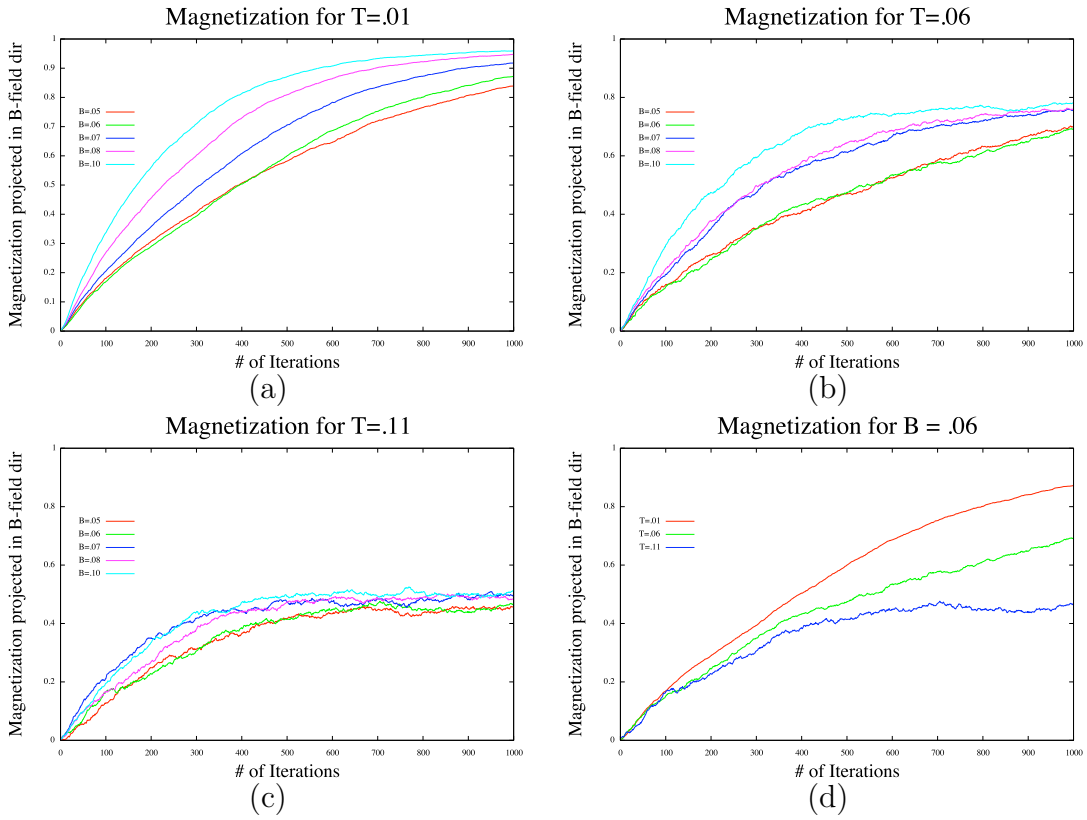


Figure 2: (a)-(c):These plots show the magnetization for three temperatures. These temperatures were experimentally determined to be *interesting*, because they showed how much temperature could affect the system. (d): This plot shows magnetization for a constant magnetic field with three different temperatures.

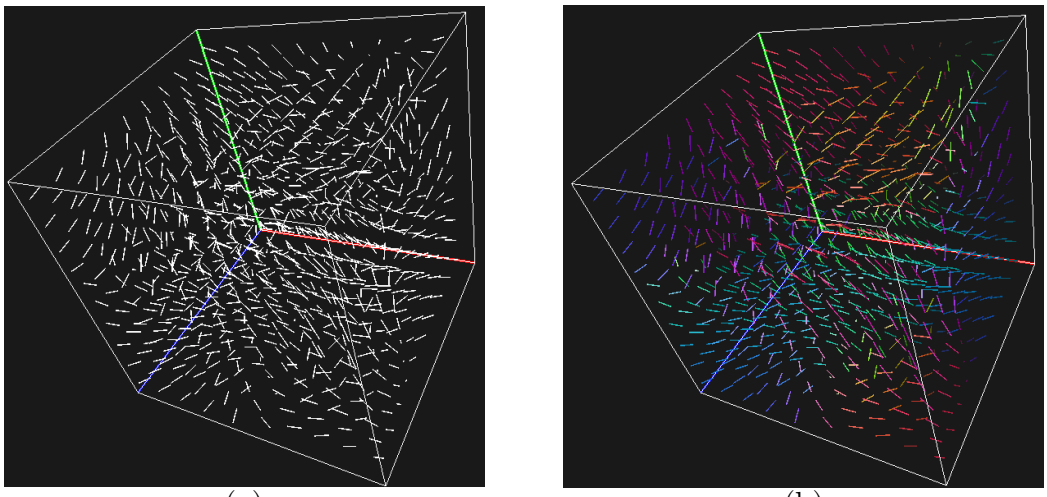
4.1 Dipoles

An initial visualization method for representing the dipole is to simply construct a line segment or glyph in the direction of each vector. This technique, known as vector plots or hedgehogs, is traditionally an effective method for representing vector fields. However, we are predominantly interested in the alignment of the dipoles and this simple technique is not entirely sufficient. Figure 3(a) illustrates how the orientation of the three dimensional vector glyphs within a lattice becomes difficult to interpret without additional information, as the orientation of the 3D glyphs become occluded by other glyphs.

In order to make the orientation of the vectors visually salient, we color the dipoles according to their orientation. We assign each of the coordinate axis a separate and orthogonal color in RGB color space (X⇒red, Y⇒blue, Z⇒green). Since each components range is -1 to 1, we developed a mapping function as follows:

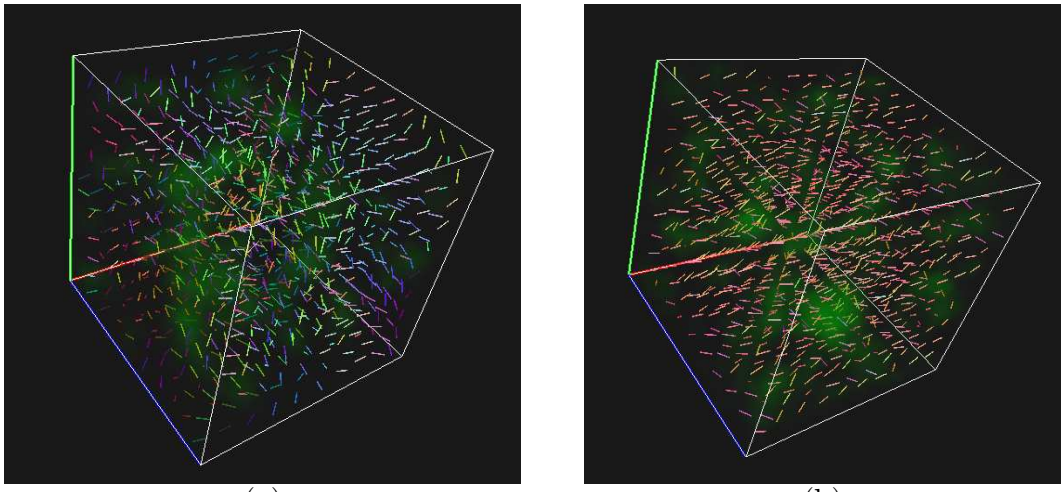
$$f(w) = \frac{w+1}{2} \tag{8}$$

where w is the X, Y, or Z component and $f(w)$ corresponds to R, G, and B, re-



(a) (b)

Figure 3: A visualization of the dipoles that have been allowed to partially align. (a): Shows no coloring (b): Shows a coloring of the dipole that indicates the direction of the dipole



(a) (b)

Figure 4: (a):This figure shows the lattice minimizing. We see there are definite regions of minimization. The volume-rendered regions of green indicate that the Hamiltonian has not completely minimized. (b): This figure is simmilar to (a) except that it has an applied external magnetic field. Here we can see that the Hamiltonian is minimizing in the dirrection of the magnetic field and volume render indicates regions where the system is *struggling* to minimize.

spectively. The result is that the vectors that are aligned are colored a similar color (Figure 3.b).

4.2 Volume Rendering the Hamiltonian

Volume rendering is a classic visualization technique that uses color and opacity to represent a 3D scalar field. We use volume rendering in order to represent the Hamiltonian of the system. This allows the user to directly identify regions where the Hamiltonian is minimizing and how the minimization occurs. Figure 4 shows two different volume renderings. It is clear that there exist regions where the Hamiltonian is not minimizing as quickly as other regions. It is also clear from these visualizations that the lattice does not uniformly minimize and that there are identifiable regions where initial dipole alignment greatly affects the convergence rate of the minimization of the Hamiltonian.

Figure 5 shows a plot of the magnetization similar to the plots in figure 2. Additionally, it shows the volume renderings that correspond to several time points throughout the minimization. Figure 5(a) show how the system is completely unaligned at the initial time step. It is clear from the volume rendering that there exists absolutely no minimization in the Hamiltonian. Examining figures 5(b) and (c), it is clear that as more iterations occur, the isolated regions of anti-alignment *shrink* in physical size. Eventually, the system becomes almost completely aligned with the magnetic field, which is clear from figure 5(d).

Figure 6 show that addition of temperature does not affect the existence of these anti-alignment regions. However it can be seen by comparison of figure 5(b) and figure 6(b) that a system with temperature *aids* the existence of these regions allowing them to be maintained longer. Additionally in figure 6(d), it is clear that there is a bit of variation in the dipole directions in neighboring dipoles. This variation is due to random rotations that are simulating the temperature.

4.3 User Interface

In order to allow the program be more useful and accessible a user interface was developed. We implement the Graphics Language User Interface (GLUI) extension for OpenGL. This is a open source extension that allowed for buttons, control of variables, movement of and through visualization, and display of current data. In Figure 7, the relevant data and controls are displayed for the user to manipulate, which allows the software to be more controllable.

5 Conclusions and Future Outlook

By visualizing magnetic dipoles, we are gaining insight into ferromagnetism and energy minimization. Our goal is to give scientists a better tool to look at ferromag-

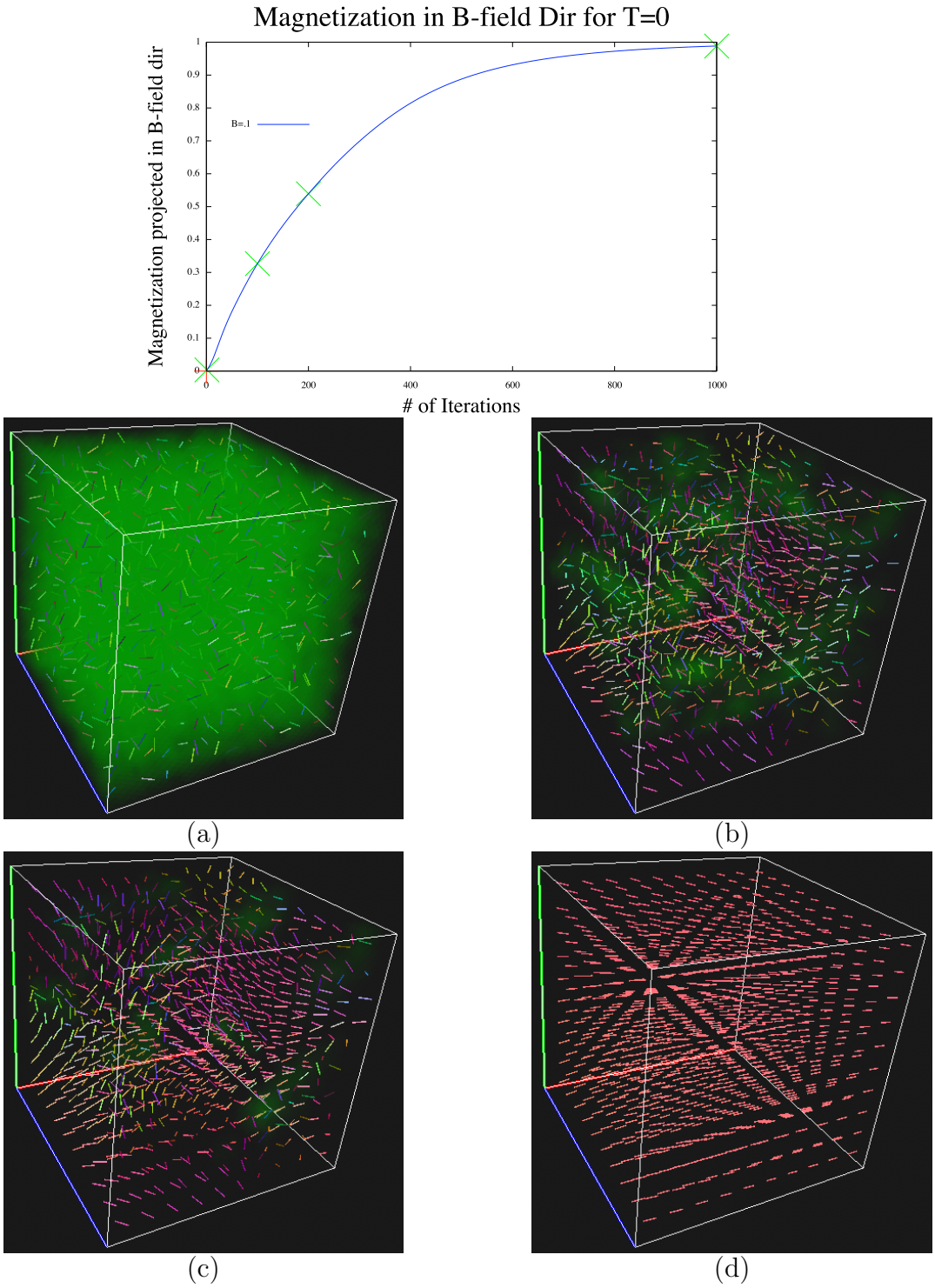


Figure 5: (top) A plot of magnetization projected in the direction of the magnetic field where temperature is not considered in the calculation. This plot and additional figures demonstrate the connection between minimization and volume rendering. The green X's on the plot of the magnetization indicate where we are taking snapshots of the volume rendering corresponding to (a)-(d), respectively. (b) and (c) clearly demonstrate that there exist regions where the initial dipole orientation lead to a slower alignment.

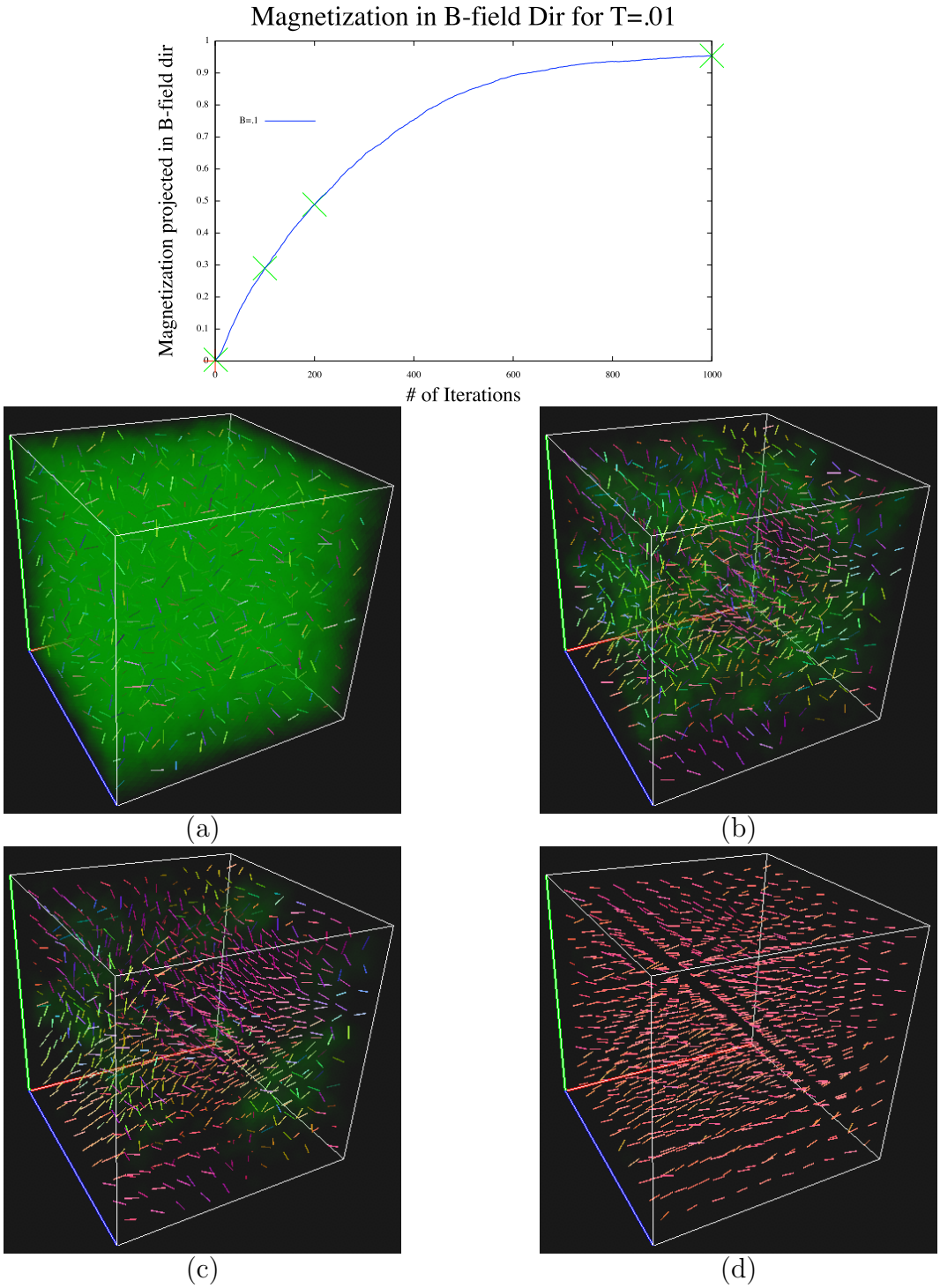


Figure 6: (top) A plot of magnetization projected in the direction of the magnetic field where temperature is considered in the calculation. This plot and additional figures demonstrate the connection between Hamiltonian minimization and volume rendering when temperature is considered. The green X's on the plot of the magnetization indicate where we are taking snapshots of the volume rendering corresponding to (a)-(d), respectively. Note: In comparison to Figure 5, these plots align more slowly because temperature is considered.

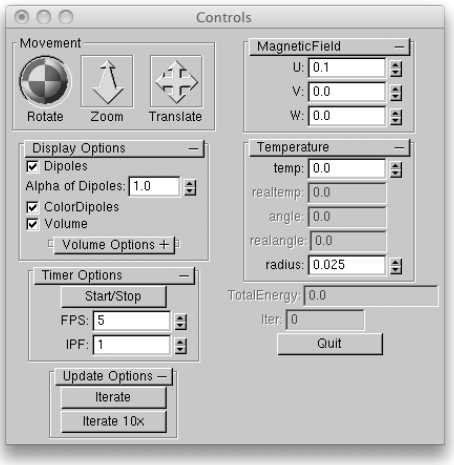


Figure 7: A user interface for our software that allow easy access to information and controls to operate the software.

netism. We hope that additionally we will be able to use our visualization to give individuals who have not previously studied ferromagnetism a better understanding of what underlying processes exist. Our visualization can demonstrate the Curie temperature—the temperature at which a system can no longer be minimized—to someone who has never had a single course in college level physics.

Our scheme for drawing dipoles and volume rendering is a starting point. We hope that our research is only the first of many visual tools to allow a better understanding of energy minimization in ferromagnetic systems. If our techniques were readapted to utilize the graphics processing unit (GPU), we might be able to see better real-time visualizations of large lattices. Additionally one could look at processing the lattice on a super-computer or multi-core system. This would allow us to have faster updating of large lattices. Lastly, this research could also benefit from visualization on a virtual reality system, as it would allow the user to have a better perception of the lattice.

6 Acknowledgments

We would like to thank Dr. Athan Petridis of Drake University for his expert advice on some of the physics. Additionally, Zack Kertzman provided several helpful insights at key times in our research. We would like to thank Drake Undergraduate Science Collaborative Institute for funding this research during the summer of 2007. Finally, we would like to thank the Drake University Student Travel and Research Fund.

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