Simple Simulation of Ferrofluid by Using Moldy

Xitian Deng
Guangzhou Middle School, Guangzhou 510665, China
Corresponding author’s email: angela@cas-harbour.org

Abstract. Ferrofluid is a new material created in recent hundred years, which has both flowability like liquids and magnetism that was only found in solid materials before. It is an amazing material but is not known well by people. Although there are some simulations of ferrofluid, the author of this paper thinks it is too complicated for the beginners of this field. In order to help beginners to understand ferrofluid, the author creates a very simple model of ferrofluid and simulates it. This model is very simple so that beginners can understand it easily. The molecular dynamic program used by the author is moldy, which is also simple and widely used. Considering moldy does not contain magnetic force, the author uses electric force to replace it, because these two forces share a lot of similarities. After simulation, the author uses VMD (Visual Molecular Dynamics) to see its structure and movement in microscope. The author thinks that it will really help the beginners to understand ferrofluid and enter this field easier and inspire researchers to create new materials.

1. Introduction
Ferrofluid is an amazing new material created in the recent century [1]. The most amazing property of ferrofluid is that when it attached to external magnetic field, it will show both flowability and magnetism. In macroscope, it is presented as soft spikes above its surface, which is unusual in the nature. In 2019, a group of researchers even created a permanently magnetic ferrofluid, which retains magnetism when the external magnetic field is removed. In addition, there are many mysteries in ferrofluid, waiting for people to study. A good way to get familiar with a new material is simulation. Though some simulations have been done, it is too complicated for beginners to get start. A molecular dynamic program called moldy is widely used for beginners, but it cannot simulate magnetic force. In this paper, the author suggests a way to use moldy to simulate ferrofluid and create a simple model. The paper will explain the feasibility of this model and the method to set parameters. The paper also suggests some reasons of the ferrofluid’s features formed. The author thinks it will inspire researchers to create new materials.

2. Simulation
Simulation is a good way for researchers to know new material. To do a simulation, the researchers need to analyze the interaction force and create an appropriate model [2]. In this simulation, the author uses the molecular dynamic program called moldy which has a lot of potential function [3]. There are two difficulties in doing this simulation. First, moldy does not contain the program to calculate magnetic potential. Second, components of ferrofluid are complicated for simulation.

To solve those problems, the author creates a simple model of ferrofluid. This simple model uses electric force to replace magnetic force. This method can work because electric force shows a lot of similarities with magnetic force. In addition, considering this model will not use in realistic application,
the author simplifies the molecular model of ferrofluid and ignores the carrier and active agent. Therefore, this model is easy to operate and it is friendly for the beginners to understand ferrofluid.

2.1. Input file
The input file used in this paper is shown below.

The simple model of ferrofluid molecule that set by author is made up by two atom that have same mass and opposite electric charges. Cause this is a simple model, the mass and electric charges can be set as any reasonable number. To get a better performance in VMD (visual molecular dynamic), the author used He and Ne as its atom name, because these two atoms have the same atomic radius.

The author chooses Lennard-Jones potential to do simulation [4]. There are two parameters in this potential function. They can be calculated or gained from experiment. As data for this a simple simulation had not been collected, the author set it approximately. This simulation mainly focuses on the electric potential, so the interaction potential can be set low.

2.2. Control file
There are many control parameters, the researchers can set them according to their needs. This paper only explains the important part of this simulation.

Moldy has an initial configuration to range molecules. Researchers do not want the result they get created by initial configuration. Thus, the first step is to set a high temperature to make the molecules move disorderly. In addition, the timestep and number of MD steps should be large enough for molecules to move disorderly. Meanwhile, in order to get a better result, the researchers need to put the molecules in a relative low density. Density is related to the number of the molecule, relative atomic mass and radius, which is set in input file. Researchers can get the density through simple calculation. Lastly, as later simulation needs to be restarted from the last one, it should be a command to save the configuration. The author’s suggestion is as follows.

After the first time of running, the researchers can get a disordered configuration. Now, researchers can make sure the following simulation is not created by initial configuration. So, in the following simulation, researchers will expect chain formation at low temperature like ferrofluids. Researchers can restart from the last simulation and set a low temperature to get the result. However, the
researchers will find the temperature grow much higher after temperature scaling. It is normal because moldy scaling does not calculate electric potential and the molecules do not form equilibria structure. The researchers should make the steps large enough till the temperature becomes relatively constant. Then, the researchers can do the steps above again till the temperature is low enough.

2.3. RDF

RDF (Radial Distribution Function) is a good way to check if the result is whether the researchers want or not [5]. The researchers expect chain formation at low temperature, which will show up as a strong signal in the correlation function between positive atoms and negative atoms. The researchers can set to print RDF in the control file, and read it in the output file. To get a clear version, the researchers can use Perl to run Plotrdf and plotting program to plot it. There is an example below.

![Figure 3. RDF function](image)

The green line in the picture is the RDF between positive and negative atoms. It shows that they have a strong connection. The purple line and blue line are the RDF of positive-positive and negative-negative, almost covering each other. This figure suggests that it may have chain formation. To have a better understanding of it, the researchers can divide the x coordinate with the radius of the atom that is set in input file. Then, the researchers can imagine the structure of it. If the RDF of the same pole molecules have a peak near 1.4, it will suggest each two molecules form a head to tail structure. If the peak is near 2, it will probably form some long chains.

2.4. VMD

If the researchers have seen the strong signal in RDF, they can use VMD (Visual Molecular Dynamics) to see the result [6]. The researchers can set to save dump file in the control file and use mdshak to convert it into pdb file that can read by VMD. There is another example and it clearly shows the chain formation that the researchers want to get.
3. Discussion about the External Field
The author introduced how to create ferrofluid molecules above, but an important character of ferrofluid is that when it attaches to external magnetic field, it will be magnetified. Although moldy cannot simulate this progress, it can simulate the structure in external field by using the simple model.

Moldy has “frameworks” function which can freeze atom in MD cells. By giving those atoms electric charges, the researchers can get any kind of external field as their want. In this part, the author will show some examples of the simple model of ferrofluid molecules interacting with external field.

3.1. With uniform electric field
By arranging frameworks atom regularly and giving them electric charges, the researchers can create a uniform electric field. The researchers can see the pole structure through using VMD. This pole structure is exactly like the realistic condition when ferrofluids are put into uniform magnetic field.

3.2. With inhomogeneous electric field

The author uses six layers of atoms with different electric charges to create an inhomogeneous electric field. By using lines drawing method, researchers can clearly see how the ferrofluid molecules arrange in the inhomogeneous electric field [6]. Those molecules are following induction lines, which is created by the electrified atom layers. Another exciting feature is the spiky shape at the top and bottom. This shape can also be seen when ferrofluid is attached to magnet. This may help researchers understand how those spikes form and why they are soft.

3.3. With monopole electric field

In the previous simulation, this model shows a lot of similarities with real ferrofluid. The author thinks researchers can use this model to simulate some conditions that do not happen in reality. In reality, monopole magnet does not exist, but the electrode can exist singly. Therefore, the author tries using this model to simulate the ferrofluid with monopole magnetic field.
The author creates a layer of atoms with electric charges and a layer of atoms that have no charges and low mass as a blocker to make it look better. In the simulation, the ferrofluid molecules form many spikes, which looks like touching a magnet to the bottom of ferrofluid’s container.

4. Conclusion
In this research, the author suggests a simple model to simulate ferrofluid with moldy and successfully gets the result that is close to reality. This research can really help people who are learning this subject at the beginning stage and give inspiration to other researchers.

However, it should be admitted that this research has many shortages. This is a very simple model that does not have many significant and realistic values to the leading edge. In addition, this model ignores the activator and carrier, which makes some features of ferrofluid disappeared, such as the low friction. To do a complex and realistic model, moldy is not competent. The researchers should use more advanced molecular dynamic program and create its own model. As the author mentions, this field has lots of mysteries and needs more studies. This research only can play a role as introduction of ferrofluid. The further study needs researchers to do it themselves.

Although this simulation has a lot of limitations, it also can give researchers some inspirations. This model used electric force to replace magnetic force and get a result which is close to ferrofluid. The researchers can try to create a new material like this model which probably has the same features of ferrofluid.

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References

[1] Huang L B, Torsten H, Dominik L M, Kaust 2019 On the Accurate Large-scale Simulation of Ferrofluids. ACM Trans. Graph., vol 38, No 4, Article 93

[2] Wu H A 2005 Introduction to Computational Mechanics Molecular Dynamics Simulation. Department of Mechanics and Mechanical Engineering University of Science and Technology of China

[3] Keith R 2001 Moldy User’s Manual. Department of Earth Sciences Parks Road Oxford OX1 3PR

[4] Barbosa D A, Piccoli F P 2018 Comparing the force due to the Lennard-Jones potential and the Coulomb force in the SPH Method, Journal of Ocean Engineering and Science 3, 310–315

[5] Fairushin I I, Khrapak S A, Mokshin A V 2020 Direct evaluation of the physical characteristics of Yukawa fluids based on a simple approximation for the radial distribution function, Results in Physics 19, 103359

[6] Theoretical and Computational Biophysics Group, November 27, 2016 VMD User's Guide Version 1.9.3, Online available, http://www.ks.uiuc.edu/Research/vmd/vmd-1.9.3/ug/ug.html, accessed on January 10th, 2021