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Magnetorheological fluids particles simulation through integration of Monte Carlo method and GPU accelerated technology

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Abstract: In order to study the rheological characteristics of magnetorheological fluids, a simulation approach through integration of Monte Carlo method and GPU accelerated technology was proposed and the three-dimensional micro-structure of magnetic particles in different strength magnetic fields were simulated. The Monte Carlo method to magnetic particles of magnetorheological fluids and its key steps such as particle modeling, magnetic energy equations calculating and system state updating were elaborated. Moreover, GPU accelerated technology was applied to the simulation of magnetorheological fluids to reduce computational time and a flowchart for the proposed approach was designed. Finally, a physics experiment was carried out and the three-dimensional simulation examples were provided. The comparison results indicated that proposed approach was feasible, efficient and outperforming others.

Keywords: Magnetorheological fluids; Magnetic particles; Monte Carlo method; GPU accelerated technology

1 Introduction

As a type of solid-liquid two phase functional material, the structure and performance of magnetorheological fluids (MRF) are controlled and constrained in an additional magnetic field. MRF can be treated as a kind of Newtonian fluids in no applied magnetic field, but a kind of non-Newtonian fluids in an applied magnetic field, and the fluids would be solidified and lose liquidity rapidly in an applied magnetic field. The transformation of rheological characteristics can be controlled and reversed easily so that magnetorheological fluids have been applied to several

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engineering fields such as aviation and aerospace, automotive industry, hydraulic transmission, biotechnology, medical care and other fields [**Hong** (2009)].

On one hand, the chain-like structure of magnetic particles in an applied magnetic field has an important effect on the yield stress of MRF. On the other hand, the time of forming chain-like structure and dynamic evolution process reflect the response characteristics of MRF. Thus, as an important factor for the study of rheological characteristics, the micro-structure of magnetorheological fluids has been an active research area since the last two decades [**Li and Peng** (2010)]. Many researchers have worked on the problem and proposed different solutions through experiment method, theory analysis and numerical simulation. However, the dynamic evolution of magnetorheological fluids micro-structure would take vast time and can not be observed easily through the experiment method. The theoretical analysis mainly depends on several simplified models, but can not get accurate results compared with the real physics experiment. Due to above reasons, the numerical simulation that variables and complex models can be imported has been applied to more and more science problems such as the simulation of magnetorheological fluids. Compared with conventional numerical simulation methods, the Monte Carlo simulation has many advantages such as high amenability to parallel computing, good adaptability to complex boundary conditions, easy physical representation of microscopic interactions and system implementation etc. In order to realize the accurate simulation and reduce the simulation time, GPU accelerated technology is applied to simulate the rheological characteristics of magnetorheological fluids.

The paper is organized as follows: some related works were outlined based on literature in section 2. A simulation approach through integration of Monte Carlo method and GPU accelerated technology was proposed in section 3. The simulation examples were put forward to validate the proposed Monte Carlo algorithm based on GPU in section 4. Our conclusions and future work were summarized in Section5.

2 Literature review

Recent publications relevant to this paper are mainly concerned with two research streams: The simulation of magnetorheological fluids and the Monte Carlo method. In this section, we try to summarize the relevant literature.

2.1 The simulation methods of magnetorheological fluids

Currently, there are a lot of numerical simulation methods and theories for the simulation of MRF micro-structure. The shape and structure of chain were analyzed by using molecular dynamics in the rotating magnetic field [**Sonia, Oscar,**

Miguel, and Gerald (2002)]. The dynamics of aggregated chains in magnetorheological suspensions subject to rotating magnetic fields were experimentally studied combining scattering dichroism and video microscopy experiments [**Wang Ruijing** (2005); **Sonia, Oscar, Miguel, and Gerald** (2005)]. The cluster chain was analyzed using the maximum entropy technique [**Coverdale, Chantrell, Martin, Bradbury, Hart, and Parker** (1998)]. The ferrofluid structure was studied by the Lattice Boltzmann method [**Xuan, Ye, and Li** (2005)]. A direct numerical simulation method based on the Maxwell stress tensor and a fictitious domain method had been developed to solve the flows with suspended paramagnetic particles [**Tae, Martien, Jaap, Patrick, and Han** (2008)]. A newly developed particle tracking scheme for fluids flow simulations on 3D unstructured grids was presented [**Stuart, Kleijn, and Kenjereš** (2011)]. The paramagnetic particles were simulated using one-stage smoothed profile method [**Kang and Suh** (2011)]. The magnetic particles were simulated using Monte Carlo method [**Peng, Min, Ma, and Yan** (2009); **Masayuki and Akira** (2004); **Akira** (2008); **Akira, Chantrell, Shin, and Coverdale** (1996); **Peng, Min, Ma, Luo, and Yan** (2009)].

2.2 The applications of Monte Carlo method

In recent years, with the computer science and technology development, computer could replace the conventional artificial methods to do a great deal of randomized trials based on mathematical models, so that Monte Carlo method has become an important approach for the random problems [**Xu** (1985); **Ji** (2004); **Lucre** (2003)]. As a kind of new numerical approach which rose with the development of computer technology, Monte Carlo method was not only used in physics and mathematics such as Monte Carlo particle transport simulation [**Zhao, Zhen, and Chen** (2005); **Xu, Huang, and Cai** (2010); **Kevin, Lin, and Thomas** (2004); **Rui, Rodrigo, Pedro , Filomena, and Fernando** (2006)] and the time saving algorithm for the Monte Carlo method of Metropolis [**Hsu and chang** (2007)], but also it was widely applied in medicine, material, machinery, management finance, insurance, biology, medicine, economic and other fields. For example, a method that relied exclusively on Monte Carlo simulation in order to compute numerically optimal portfolio values for utility maximization problems was proposed [**Jak'sa, Levon, and Fernando** (2003)].

2.3 Discussion

Although many approaches for the simulation of magnetorheological fluids have been developed in above literature, they have some common disadvantages summarized as follows. Firstly, most of researchers have not considered the simulation efficiency, especially for thousands of magnetic particles or much more. Secondly,

the accuracy of simulation has been analyzed rarely. Finally, few researches have focused on the three-dimensional simulation for micro-structure of magnetic particles. Based on our past research on the computer simulation of magnetorheological fluids and Monte Carlo method, this paper tries to tackle the above problems.

In this research, a simulation algorithm based on Monte Carlo method is proposed to simulate the rheological characteristics of magnetorheological fluids, and the power of GPU is applied to reduce the simulation time and realize accurate simulation.

3 The Monte Carlo method based on GPU

In order to formulate the problem in mathematical expression, the following notations are introduced first:

d	Average diameter of magnetic particles
δ	Thickness of steric layer
H	Strength of magnetic field
e_i^t	Total energy of magnetic particle $i$at state t
e_H	Energy due to the presence of an applied magnetic field
e_M	Energy due to the interaction of neighboring particles
e_R	Energy due to the overlapping of surfactant coating layers
E^t	Total energy of magnetic particles at state t
ΔE	Change of total energy between two states
n	Number of magnetic particles
m_i	Magnetic moment of magnetic particle i
μ_0	Permeability of free space
r_{ij}	Center distance of particles$i$and j
ε	Surfactant molecules per unit area of particle surface
k	Boltzmann's constant
T	Absolute temperature of magnetorheological fluids
a_{ij}	Surface distance of particles$i$and j
λ	Multiplier
θ	Increment
M	Modulus
Δ	Maximum displacement value of the magnetic particle
s_i^t	Position of magnetic particle $i$at state t
S^t	System state of magnetic particles at state t
$P(t,t+1)$	Probability from an old state $t$to a new state $t+1$

R	Random number
β_0	Constant
N	Number of cycles
t	Index of the current cycle
α	Acceleration factor

3.1 Particle model

There are two classic particle models for magnetorheological fluids: spherical particle model and spherocylinder particle model. In order to reduce the computation time, spherical particle model is adopted in this paper and the spherical particle model is shown in Fig.1.

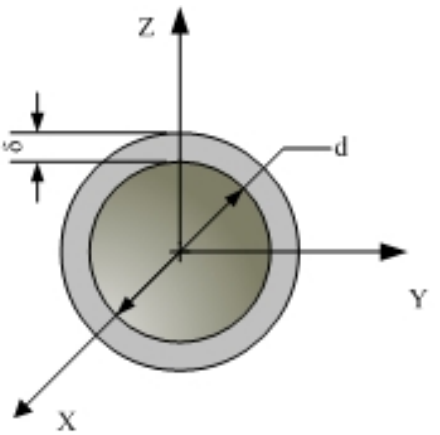

Figure 1: Spherical particle model

3.2 Magnetic energy between magnetic particles

The motion of a magnetic particle is typically caused by three kinds of energies: The energy e_H due to the presence of an applied magnetic field H, the interaction energy of the neighboring particles (e_M) and the energye_R due to the overlapping of the surfactant coating layers. The above-mentioned energies can be calculated as follows [**Liu, Zhou, Wang, and Teng** (1997)]:

$$e_i = e_H + e_M + e_R \tag{1}$$

$$e_H = -\vec{m} \cdot \vec{H} \tag{2}$$

$$e_M = \frac{\mu_0}{4\pi r_{ij}^3}\left\{\vec{m}_i \cdot \vec{m}_j - \frac{3}{r_{ij}^2}(\vec{m}_i \cdot \vec{r}_{ij})(\vec{m}_j \cdot \vec{r}_{ij})\right\} \tag{3}$$

$$e_R = 2\pi d^2 \varepsilon kT\left\{2 - \frac{a+2}{\delta}\ln\frac{(1+2\delta)}{(d+a)} - \frac{a}{\delta}\right\} \tag{4}$$

Thus, the total energy of magnetic particles can be calculated as follows:

$$E = \sum_{i=1}^{n} e_i \tag{5}$$

3.3 System state updating

In this paper, the position of magnetic particle *i* at state *t* can be expressed as a three-tuple as follows:

$s_i^t = (x_i^t, y_i^t, z_i^t)$

Thus, according to the method based on random number, the position of magnetic particle *i* at state *t*+ 1 can be calculated as follows [**Frenkel and Smit** (1996)]:

$$\begin{aligned} x_i^{t+1} &= x_i^t + (R_1 - 0.5)\Delta \\ y_i^{t+1} &= y_i^t + (R_2 - 0.5)\Delta \\ z_i^{t+1} &= z_i^t + (R_3 - 0.5)\Delta \end{aligned} \tag{6}$$

Obviously, the values of random numbers R_1, R_2, and R_3 play an important role in Monte Carlo method. Thus, once a new state appears the values of random numbers R_1, R_2, and R_3 should be modified accordingly and the updated rule can be defined as follows:

$$\begin{cases} \beta_{t+1} = \lambda\beta_t + \theta(\bmod M) & t = 0, 1, \cdots, n \\ R = \beta_{t+1}/M \end{cases} \tag{7}$$

The system is composed of various magnetic particles and can be abstracted as a set at state t shown as follows:

$S^t = \{s_1^t, s_2^t, \ldots, s_n^t\}$

According to the theory of Monte Carlo method, magnetic particles prefer to move to a new position randomly with a probability which is determined by the change of total energy between two states. In this paper, the probability from an old state t to a new state $t + 1$ can be calculated as follows:

$$P(t, t+1) = \begin{cases} \exp(-\Delta E/kT) & for\ \Delta E > 0 \\ 1 & for\ \Delta E \le 0 \end{cases} \tag{8}$$

$$\Delta E = E^{t+1} - E^t \tag{9}$$

3.4 GPU accelerated technology

The simulation of magnetic particles consumes vast computational time. Generally, with the increase of magnetic particles, the computational complexity of searching for an optimal state in a large solution space will increase more quickly. The tests show that it usually takes about several hours to carry out a three-dimensional simulation for about 1000 magnetic particles. In other words, the three-dimensional simulation of magnetorheological fluids with a mass volume fraction would not be realized within an acceptable time. Due to being massively parallel in nature, GPU is designed to process a very high volume of data [**Kalling, Evans, Orlov, Schissel, Maingi, Menardd, and Sabbagh** (2011)]. In order to reduce the computational time, GPU accelerated technology is applied to Monte Carlo method and an improved algorithm through integration of Monte Carlo method and GPU accelerated technology is proposed.

The GPU can be considered as a computer device and its architecture is shown as in Fig.2. A GPU is composed of several kernels consists of grids and a grid can be divided into many blocks, and large number of threads can run parallelly with no conflicts in a block. They can take an effective way to share data and execute simultaneously through the "sharing memory" [**Benjamin, Peter, and Tobias** (2010); **Tobias, Peter, Wolfgang, and Johannes** (2009); **Christopher and John** (2011)].

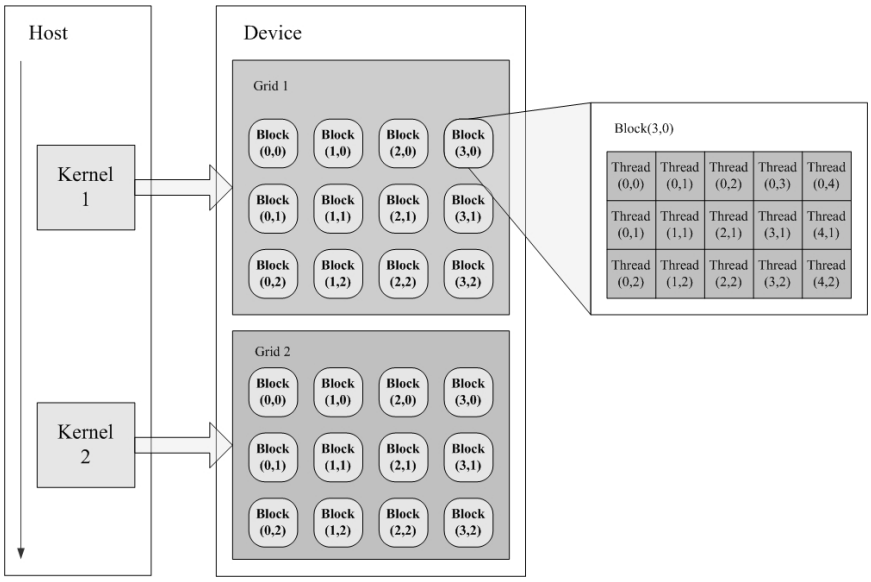

Figure 2: The GPU device architecturel

According to the GPU device architecture, simulation area can be divided into a series of grid units and each grid unit contains a particle or more particles shown as in Fig.3. Thus, a magnetic particle can be treated as a thread and the larger number of magnetic particles can be mapped into a grid. With the increase of magnetic particles, a single GPU maybe not meet the calculation speed and multi-GPU would be used.

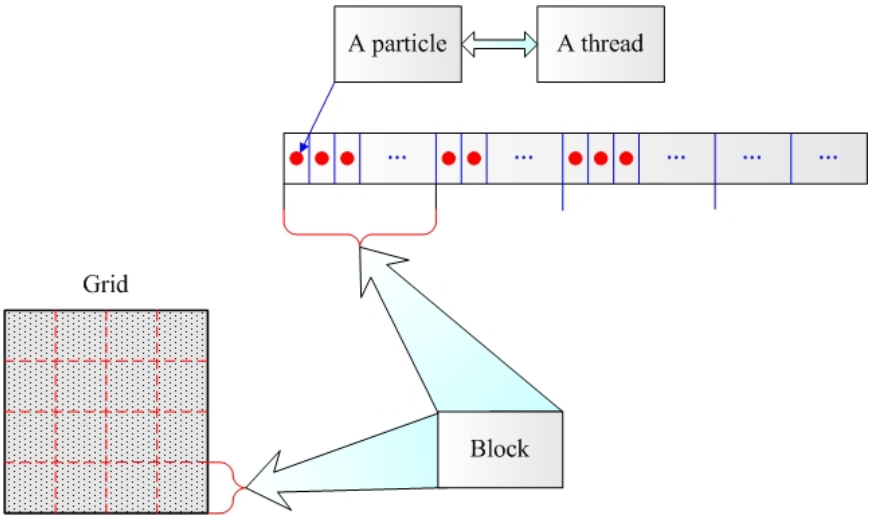

Figure 3: The divided schematic diagram for simulation area

3.5 Flowchart of the proposed algorithm

According to the above description about the Monte Carlo method and GPU accelerated technology, the proposed algorithm is an iterative algorithm and can be coded easily on the computer, and the flowchart of the proposed algorithm can be summarized as Fig.4.

4 The simulation example

In this section, the proposed approach through integration of Monte Carlo method and GPU accelerated technology is applied to simulate magnetorheological fluids in the different strength magnetic fields. In order to verify the validity of the proposed approach for the three-dimensional simulation of magnetorheological fluids, a physics experiment is carried out. The simulation results are contrasted with the physics experiment results and the computational efficiency of the proposed approach is compared with other methods.

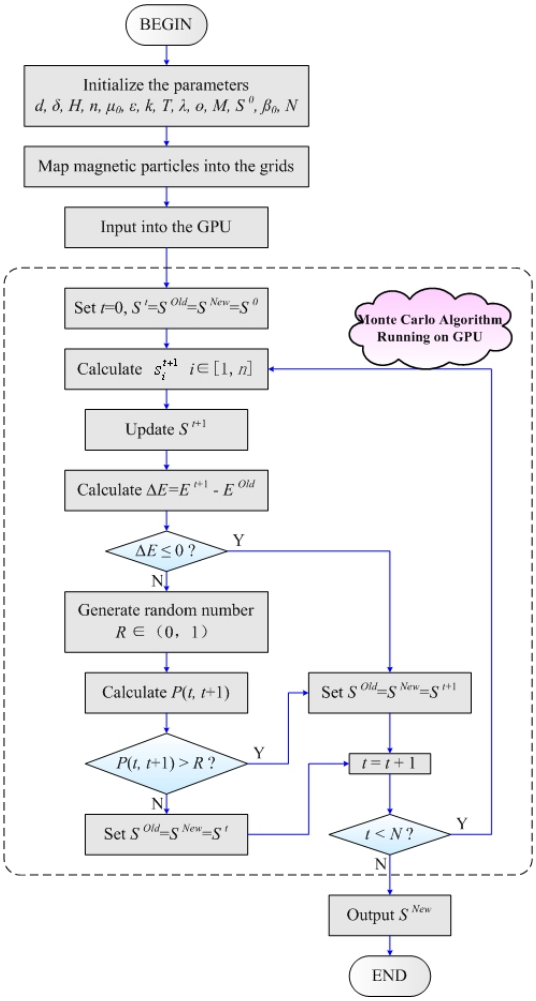

Figure 4: Flowchart of the proposed algorithm

4.1 Parameters for simulation example

In this paper, the number of magnetic particles can be taken as n=400. The thickness of the steric layer can be expressed as $\delta = 0.15d$. T =300$k$is the absolute temperature of the MRF. The dimension of particle d=1μm. The permeability of free space $\mu_0 = 4\pi\times10^{-7}(H/m)$. The multiplier λ=97, the increment ? =3, Modulus$M$=1000. The number of cycles N=30000. The strength of the magnetic field H= 0G, 5G, 15G, 25G, respectively.

4.2 The three-dimensional micro-structure of magnetic particles

In this sub-section, the effects of the magnetic field strength on micro-structure of magnetic particles are studied with H=0G, 5G, 15G and 25G, respectively. The three-dimensional simulation results are illustrated in Fig.5. Fig.5a shows that the magnetic particles are distributed randomly in the absence of the magnetic field (H=0G). Several magnetic particles are moving to form chain-like structures in a uniform magnetic field (H=5G) as shown in Fig.5b. Many chain-like structures are formed in a much stronger magnetic field (H=15G) as shown in Fig.5c. With the increase of magnetic field, some chain-like structures move towards longer and thicker as shown in Fig.5d. This is because the magnetic particles are magnetized so that the attraction of the magnetic field induces the magnetic particles form chain-like structures and the repulsive forces take the chain-like structures to be approximately parallel line in an applied magnetic field.

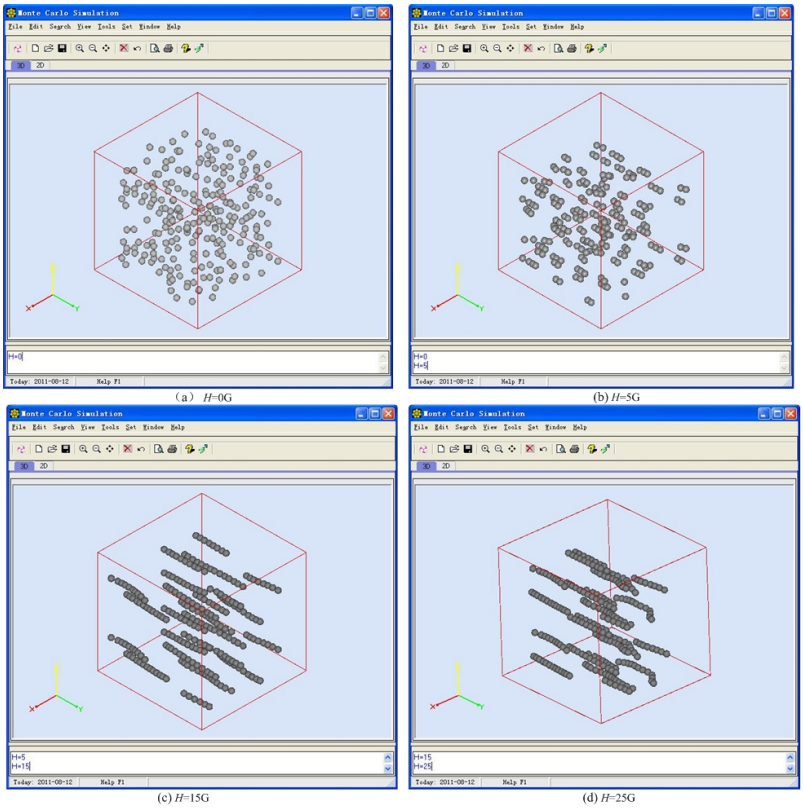

Figure 5: Influences of magnetic field strength on micro-structure in a three-dimensional simulation system

4.3 The physics experiment

Fig.6 shows the physics experiment results about distributions of magnetic particles on the same condition. In order to compare the simulation results with physics experiment results preferably, the two-dimensional simulation results based on the proposed algorithm are presented in Fig.7 and the simulation results are in a good accordance with these of experiment values. In other words, the proposed approach through integration of Monte Carlo method and GPU accelerated technology is feasible for the simulation of magnetorheological fluids.

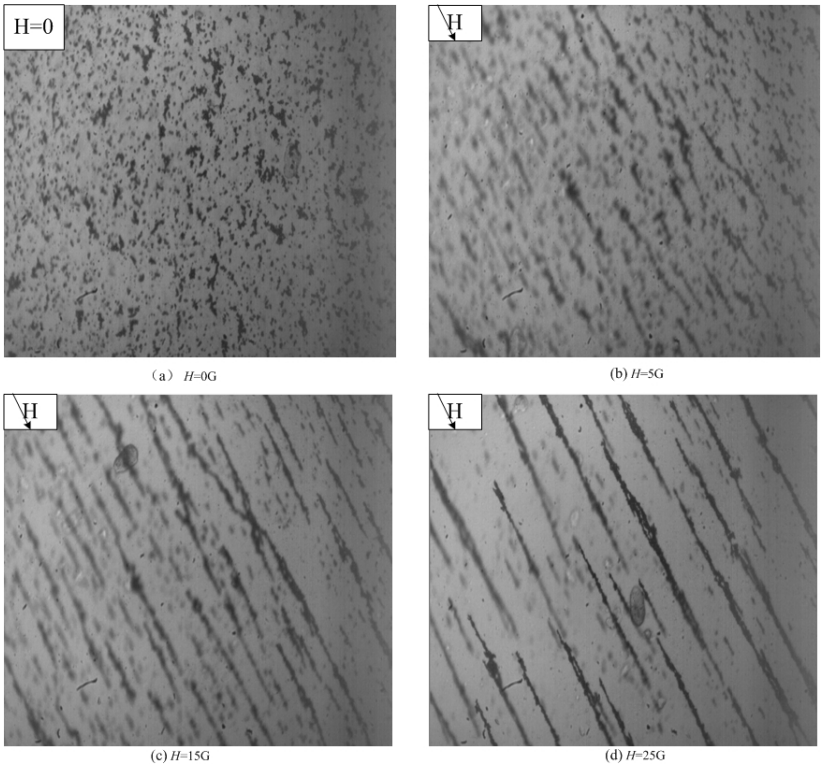

Figure 6: Video microscopy pictures of the micro-structure for different magnetic field strength

4.4 Efficiency analysis of the proposed algorithm

A high computational efficiency is important to a numerical method, so it is necessary to investigate the factors which may improve the computational efficiency. In

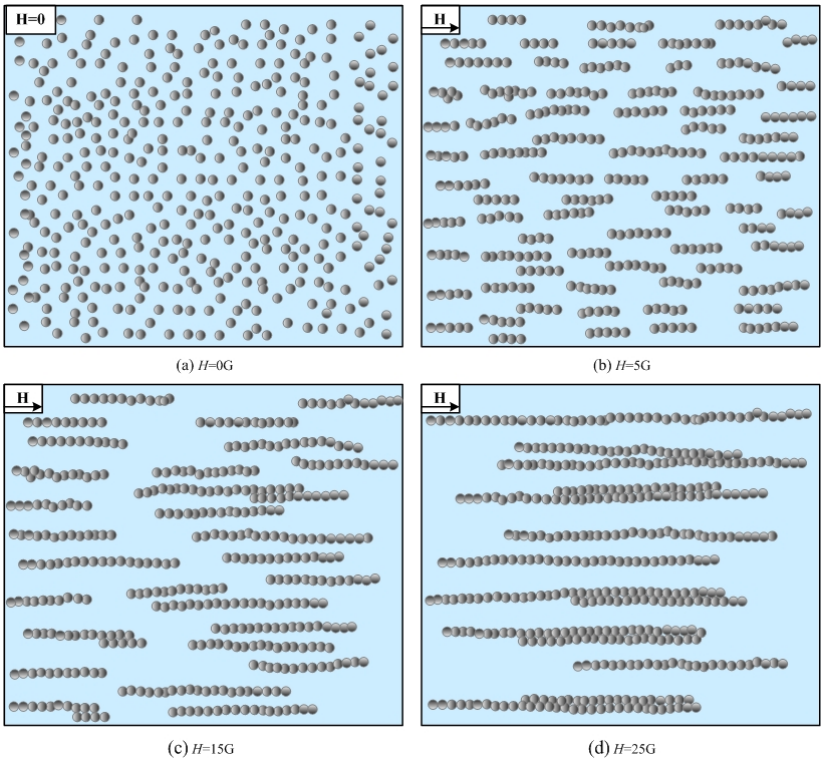

Figure 7: Influences of magnetic field strength on micro-structure in a two-dimensional area

this sub-section, we compare the simulation time of CPU with GPU in the simulations of magnetorheological fluids at the different number of magnetic particles. Here, CPU uses E5700 and GPU uses Quadro FX3400 in this paper. The efficiency of simulation for the magnetic particles system is shown in Fig.8. Compared with CPU, the simulation time is reduced obviously through the application of GPU accelerated technology. Fig.9 shows that the acceleration factor (α) becomes more and more large with the increase of magnetic particles. In other words, GPU accelerated technology has an advantage on the simulation of magnetic particles and the proposed algorithm can be used to simulate the magnetorheological fluids with a mass volume fraction.

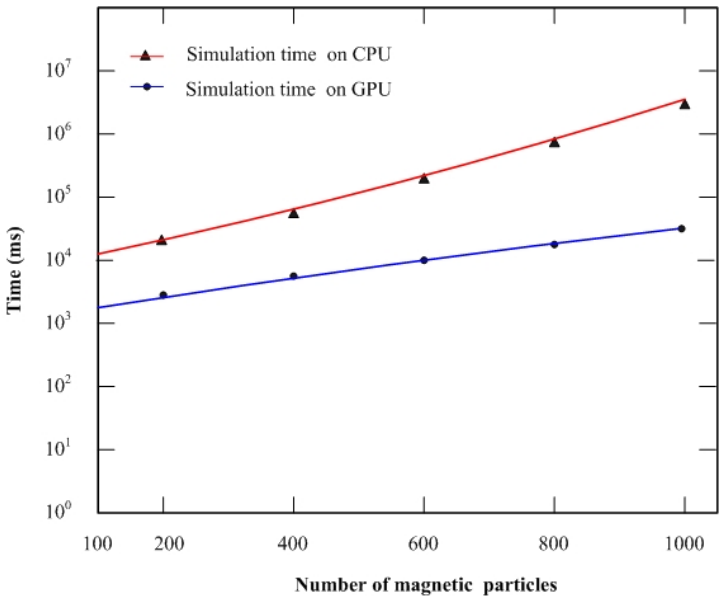

Figure 8: The simulation time of magnetic particles simulation system on GPU compared with on CPU

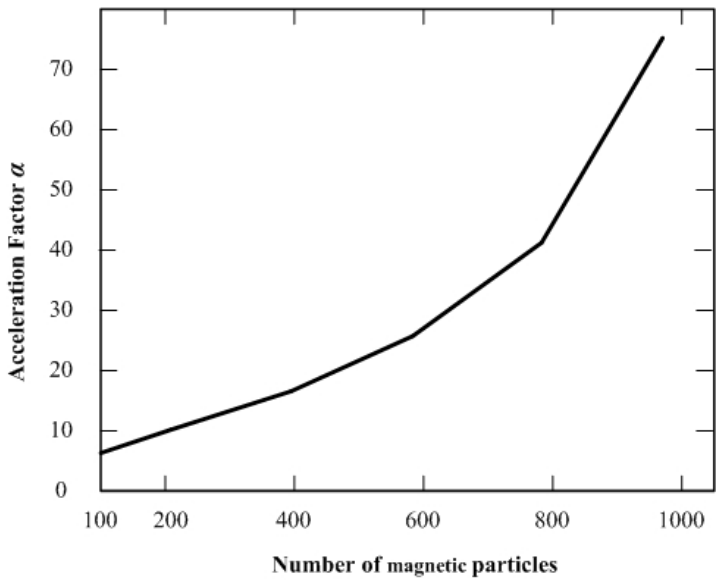

Figure 9: The acceleration factor of magnetic particles simulation system on GPU compared with on CPU

5 Conclusions and future work

In this paper, we had investigated the micro-structure of magnetic particles in a uniform magnetic field using a simulation approach through integration of Monte Carlo method and GPU accelerated technology. In order to verify the feasibility and efficiency of Monte Carlo algorithm running on GPU, a physics experiment was carried out and the simulation examples were provided. The simulation results were consistent with the physics experiment results and the simulation time was reduced greatly based on GPU accelerated technology.

In this paper, the physics experiment and the simulation were carried out in a uniform magnetic field. In future studies, the authors plan to investigate the microstructure of magnetic particles in a variational magnetic field and the application of different particle models would also be an important research field for authors.

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