Particle Modeling for Complex Multi-Phase System with Internal Structures using DEM

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Complex multi-phase systems with internal structures are generally categorized as highly non-linear materials. Especially when they are in non-equilibrium state, it is extremely difficult to describe and understand the behavior. Simulations that rely on tracing the motion of millions of particles are likely to remain central to such studies. For this purpose we have been developing various types of particle based code including the cubic lattice Ising model, Discrete Element Method (DEM) in broad sense coupled with fluid flow code. This year we focused on the contribution of particle modeling to 1) the study of the deformability of a red blood cell for the analysis of blood flow and blood vessel, 2) the computational statistical mechanics, and 3) particle-fluid mixed phase scenario. The common problems in those three topics are 1) difficulties in observation and measurement, 2) the existence of inter-phase interaction with complex structure, 3) strong non-linearity due to non-continuity, non-homogeneity, and large deformation. Therefore, direct simulations with large numbers of particles will be the best for understanding and prediction for those phenomena.

Keywords: Discrete Element Method, Complex system, Multi-phase system, Particle modeling

1. Introduction

In the studies of complex multi-phase system with internal structure, the ability to follow the motion of many particles has long been crucial both theoretically and experimentally. Despite the difficulties in data size and computational time, simulations that rely on tracing the motion of millions of particles are likely to remain central to such studies. In addition to particle models, hybrid models (particle and continuum media) are increasingly becoming attractive, especially in solid and fluid mixture and its phase transition.

Since we are dealing with "Complex multi-phase system with internal structures", it is natural to select particle models and hybrid models from the background above. Discrete Element Method (DEM) is a numerical method based on the particle model. This year we focused on the contribution of particle modeling to 1) the study of the deformability of a red blood cell for the analysis of blood flow and blood vessel, 2) the computational statistical mechanics, and 3) particle-fluid mixed phase scenario using DEM.

In the following section, we report the topics above respectively.

2. Deformability of a red blood cell and blood flow simulation

2.1. Simulation of the shape change of a red blood cell

It is well known that a red blood cell (RBC) has an ability to pass through a capillary with a diameter smaller than that of the RBC itself by changing its shape super flexibly. The flexibility of an RBC arises from the mechanical properties of the cell membrane consisting of a liquid bi-layer and an underlying skeletal network. However, it also depends on the shape as a shell structure. Therefore, in order to perform a realistic simulation to understand the mechanism of blood flow through a capillary, it is necessary

to describe the high deformability of a RBC based on the properties of the membrane.

For this purpose we developed the three dimensional elastic network-model to simulate the whole membrane of an RBC [1]. In this model, the shape of an RBC is determined by finding nodal positions to minimize the sum of the elastic energies. Since the derivative of the total energy with respect to the position vector at a node provides an internal force acting on the nodal point, nodal positions are determined by solving the equation of motion of mass points assigned to the nodes moved by the internal force and an external force applied.

It was assumed that the shape of an RBC in a natural state (stress free state) was a biconcave disc with a diameter of 8.30 μm, a minimum thickness of 1.01 μm, a maximum thickness of 2.18 μm, a surface area of 138 μm^2, and a volume of 122 μm^3. Simulation was carried out from a state where the RBC was approaching the entrance of a capillary with a diameter of 6 μm by aligning its axis with the axis of the capillary.

Figure 1 shows the shape change of an RBC as the cell was drawn in the capillary by a suction pressure of 50dyn/cm^2. The total elastic energy generated in the RBC increased until the cell was completely drawn in the capillary. The internal force acting on the membrane which increased with increasing the elastic energy resisted to the shape change of the RBC. However, in going deeper in the capillary, the shape of the RBC gradually changed in such a manner that it decreased the total elastic energy and pass through the capillary easily.

2.2. A particle method computer simulation of blood flow

For the first step toward a realistic blood flow simulation including the effect of the deformability of RBC, a two dimensional simulation was performed. In the model, Navior-Stokes equations were solved for blood plasma flow using a particle method in which continuum body was discretized by moving particles. In this study, moving particle semi-implicit (MPS) method [2] was used as a particle method, where the particle number density was kept to be its reference value in order to express the incompressibility condition. For RBC, a two-dimensional circular membrane model was constructed.

A simulation result revealed change in RBC shape and position in flowing plasma, as is shown in Figure 2. At the initial state, the plasma flow with the fixed RBC was steady seen on top. Poiseuille flow of the blood plasma was obtained in the upstream side of the RBC. The fluid force due to pressure seems higher at the upstream side than the downstream. The RBC was subjected to the pressure force near the wall, leading to compression of the RBC in the direction perpendicular to the vessel walls. These forces drove the RBC to move toward the downstream side, and caused deformation of the RBC in parachute-like shape.

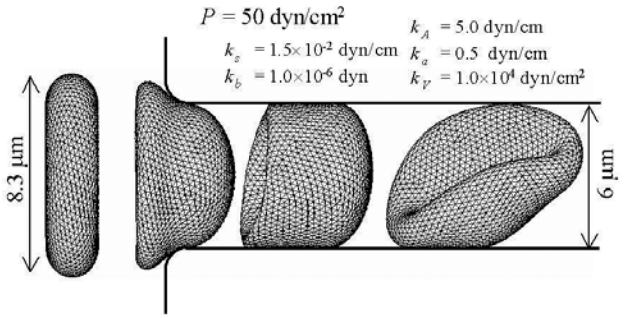

Fig. 1 Shape change of an RBC at the entrance of a capillary.

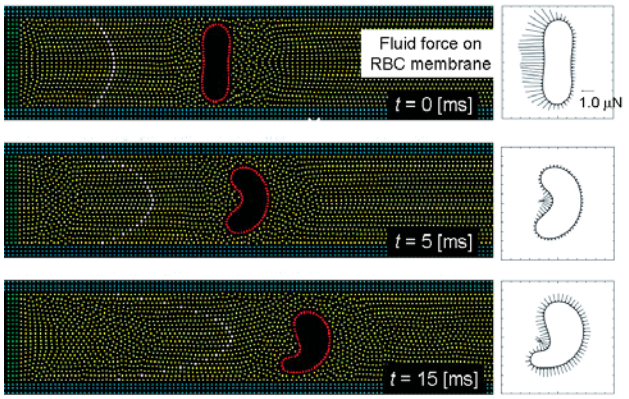

Fig. 2 Motion and deformation of RBC due to fluid pressure under blood plasma flow.

3. The computational statistical mechanics

3.1. Cubic Ising model

We performed highly accurate Monte Carlo simulations for simple cubic Ising model. The largest lattice simulated is $6648 \times 6648 \times 6656$ using 512 nodes and 4096 processors of the Earth Simulator. Each simulation contains multi-spin coded 64 systems, and therefore total DOFs in one simulation reaches to 19 trillion (19×10^12), which is the world record of number of bodies of a simulation. These extremely large scale computations were accomplished by means of the Earth Simulator. We found that the spontaneous magnetization m(t), as is shown in Figure 3, where , in a temperature range $0.0 < 1/t < 0.0004$. An analysis of the magnetization distribution near criticality yields a new determination of the critical point: $K_c = J/k_B T_c = 0.2216547$, which is three times accurate than the previously most accurate data.

For the case of full nodes (512 nodes, 4096 processors) computation, the model consists of $6648 \times 6648 \times 6656$ lattices and 64 parallel processing updated 19 trillion DOFs simultaneously. This is the world record in this field.

3.2. A new method of investigating equilibrium properties from non-equilibrium work

A new method of investigating thermal equilibrium natures from non-equilibrium work is proposed. This method enables us to calculate thermal equilibrium values of physical quantities, even the free energy, with help of the

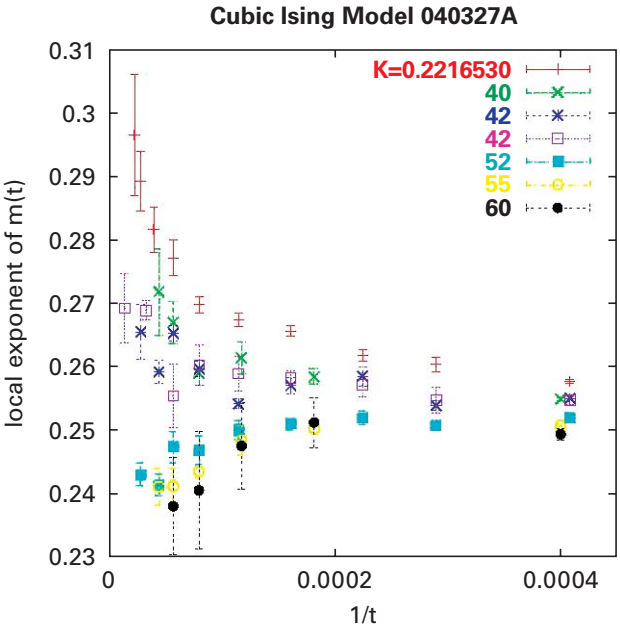

Fig. 3 Phase transition diagram of spontaneous magnetization from the simulation using 512 nodes of the Earth Simulator.

information of non-equilibrium work. The ides is based on non-equilibrium thermodynamics, that is, Jarzynski equality. The Jarzynski equality connects with non-equilibrium work and a difference of thermal equilibrium free energy in theoretically. We checked the usability of the equality and clarified some problems through an application for Lennard-Jones (spline) particle system as an application of DEM.

Figure 4 is the results of the simulation: Pressure, for instance of physical observational, and Helmholtz free energy are shown. Global behavior of pressure is plotted in a temperature-density plane. A horizontal axis represents the temperature of heat bath and vertical axis does the cubic root of fractional density. The pressure is computed from the Virial theorem and re-weighted with the exponential work. Here, we used a N = 8000 system and an operation interval was taken to be t_{op} = 100. We took 10 samples for 30 different temperatures. Some isobars are shown in this figure.

4. Particle-fluid mixed phase scenario - Simulation of solid particle sedimentation in a viscous, Newtonian fluid

In most works of particle sedimentation simulations, it is assumed that particles do not collide under relatively a low particle concentration. In this study the simulation was carried out to measure the detailed data of fluid flow around particles interacting with other particles, which directly relates to a formula of settling velocity. These measurements can never be performed in physical experiments. In the numerical simulation, it was confirmed that the velocity of particles decreased as the particle concentration increased, which corresponds to the experimental results. The simulation conditions are summarized in Table 1 and the snapshots and fluid velocity profile are plotted in Figure 5.

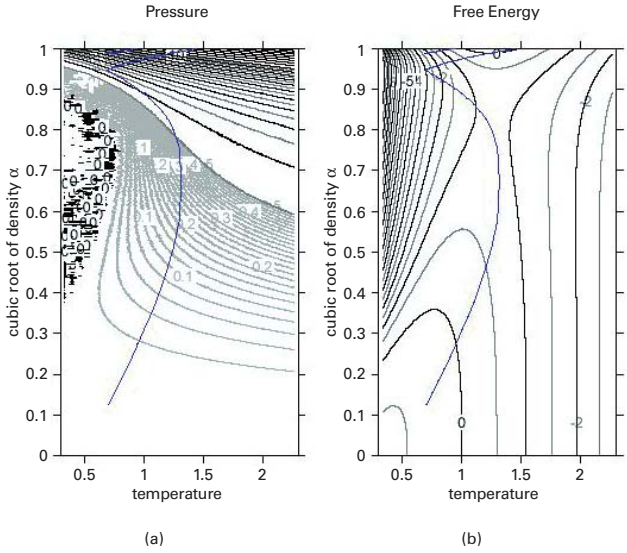

Fig. 4 (a) Global behavior of pressure and (b) Helmholtz free energy landscape.

Table 1 Simulation conditions.

System size	24m × 24m × 72m
The number of particles	1000, 5000, 10000, 15000, 20000
The number of fluid lattice	96 × 96 × 288 = 2,654,208
Density of solid particles	2450 kg/m^3
Density of fluid	1000 kg/m^3
Viscosity of fluid	100 Pa・s
Reynolds number	30

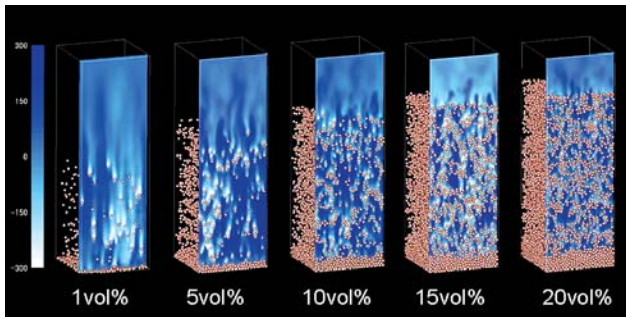

Fig. 5 Snapshots of DEM particles and DNS fluid flow velocity profiles.

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