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

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Following the research and development up to previous years, we made further developments of the study of the complex multi-phase systems with internal structures. This year we focused on 1) Large scale simulation of the collective behavior of multiple red blood cells, 2) DNS/DEM coupling simulation for hindered settling behavior, 3) Development of a new scheme of Discrete Element Method for solid/fluid multi-material simulations using four particles interaction.

Keywords: Particle, Fluid, Multi-phase system, Internal structure, Discrete Element Method

1. Introduction

Mixtures of particles and fluid or that of solids and fluid can be seen in many occasions. However, they show significantly complex behavior depending on the density of particle or solid part. This is because internal micro-structures composed of particles or solids induce highly heterogeneous, unisotropic and non-linear responses. As a result, mathematical description of those material behaviors becomes extremely difficult.

Numerical simulations, rely on tracing the motion of many particles, are likely to remain central to such studies. In this report, we will focus on the following three topics related to the problem of mixtures of particles and fluid: 1) Collective behavior of multiple red blood cells, 2) Hindered settling behavior, 3) A new scheme of Discrete Element Method for solid/fluid multi-material simulations using four particles interaction

2. Collective Behavior of Multiple RBCs

2.1. Flow model for multiple RBCs [1]

In the much larger vessels than RBC size, collective behavior under the influence of mechanical interaction between RBCs is increasingly important to determine rheological properties of blood as a mass. In this section, a simulation method for multiple RBCs is proposed toward understanding of rheological properties of blood from a viewpoint of multi-scale mechanics. Assuming macroscopic flow field is not affected by each RBC motion, macroscopic flow field was prescribed by theoretical/numerical analysis. The difference in the velocities between the RBC and the prescribed flow field determined momentum and viscous forces acting on RBC. In addition, reaction force is introduced in the case of contact of RBCs.

2.2. Simulation model and parallel computing technique

A two-dimensional blood flow model between parallel plates was constructed using $10 \times 20 = 1200$ RBCs, as shown in Fig. 1(a). Each RBC was modeled by 100 particles. The size of the model was 200 μm in axial flow length and 75 μm in distance between the plates. The Poiseuille flow was assumed as the prescribed flow field. The ES system

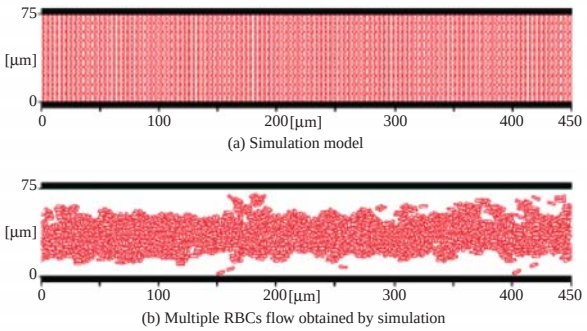

Fig. 1 Large-scale simulation of flow of multiple RBCs using parallel computing technique

[2], a vector/parallel super computer system, was used to simulate the problem, in which we used 80 processors and 12 hours in real time (960 hours in CPU time). The parallel computation with standard MPI library was employed, and the simulation region was divided into 80 regions as the same number of the processors. Preliminary numerical experiments showed that the data communication time greatly affected computing time in the simulation. Therefore, the communication was performed per 1000 calculation steps, which did not change the essential result from that obtained in the case of full communication.

2.3. Results

As for the simulation codes developed for 80 processors on the ES system, vector operation ratio, average vector length and parallel efficiency were 99.30%, 203.19 and 98.69%, respectively. These specs were acceptable to use 1024 processors in the ES system. The code enabled us to calculate blood flow in 98.9 [s] in the simulation time, in which RBCs were able to travel from the inlet to the outlet.

The simulation result demonstrated that RBCs flew downstream due to fluid force and concentrated to the flow axis, as shown in Fig. 1(b). This axial concentration, corresponding to experimental observation, would play an important role in distributing the RBCs into the daughter vessels at bifurcation [1]. In order to understand this kind of collective behavior in RBCs flow, however, further studies are necessary to clarify the characteristics the model parameters introduced into RBC model [1,3], and to investigate effects of the assumption on the prescribed flow field on the simulation results.

3. DNS/DEM coupling simulation for hindered settling behavior

In order to propose a formula of hindered settling velocity, the effect of concentration and size distribution of particles on the settling velocity of a particle in suspension was investigated by the experiment and computer simulation.

In the experiment, the sedimentation behavior of particles which distributed uniformly in a rectangle container was observed using a high-speed camera at low particle concentration, and the settling velocity of a particle in suspension was obtained by analyzing the pictures. At high concentration, settling velocity of each particle cannot be observed visually with the high-speed camera. Then, particles were distributed uniformly in a cylindrical container and sedimentation velocity of interface between particles layer and fluid was observed. In the result, it was confirmed that as the particle concentration increased, the velocity of a particle decreased, the variation of each particle velocity became large, and the effect of the particle size distribution increased.

The simulation was carried out to obtain the detailed data which cannot be obtained experimentally and is useful to propose an equation of settling velocity. On such a purpose, a direct numerical simulation (DNS) was used to calculate the fluid flow of the surface of a particle closely so that the effect of fluid flow on a particle behavior can be investigated, and a particle behavior was calculated by the discrete element method (DEM). Furthermore, we tried to develop the large-scale simulation in order to represent more realistic simulation system because very many particles are needed to reproduce the particles with particle size distribution.

Figure 2 shows the relation of the sedimentation velocity and concentration obtained by simulation and experiment at high concentration. The vertical axis expresses a velocity ratio, that is, expresses the hindered settling velocity to the settling velocity of a single particle. The experimental data was measured by an apparatus as shown in Figure 3 and so there are no wall effect. Therefore, the experiment data agrees with Steinour's well. The simulation result also corresponds with Steinour's in a tendency. However, the value of simulation is lower than Steinour's and Experimental result. It seems that the precision of simulation depends on the ratio of cell size of DNS to particle size. Used cell size is one-

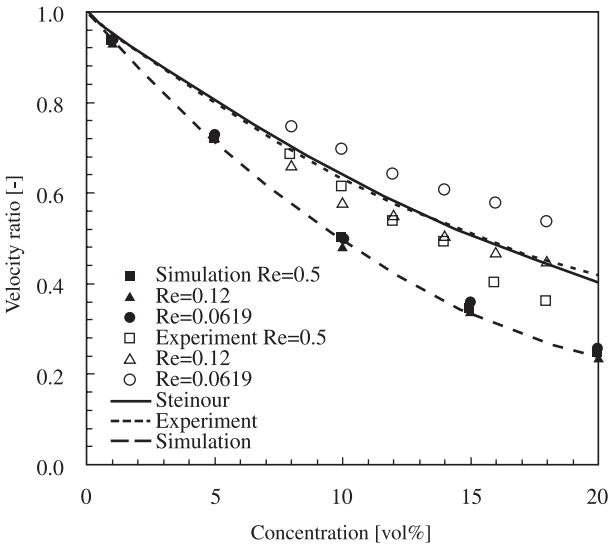

Fig. 2 Effect of concentration on settling velocity of particle

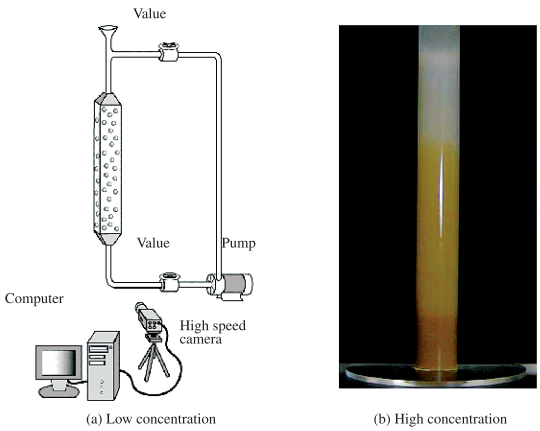

Fig. 3 Experimental apparatus

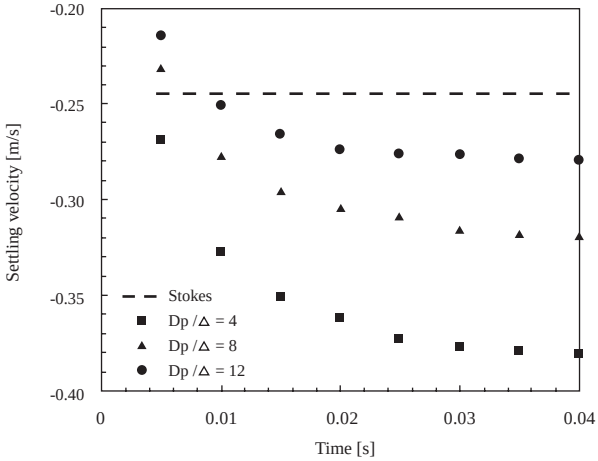

Fig. 4 Effect of grid size of DNS on settling velocity of one particle

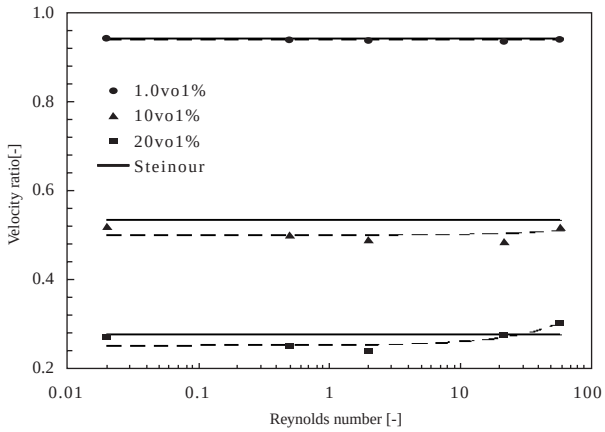

Fig. 5 Effect of Reynolds number on settling velocity particle

eighth of particle diameter for the simulation. However it is not enough cell size. Figure 4 shows the settling velocity of single particle at different cell size. The settling velocity is close to the theoretical value of Stokes as cell size becomes small. Therefore, it is suggested that the simulation result in Figure 2 is insufficiency of precision and if cell size is smaller the simulation value may be close to values of Steinour and experiment.

Next, the effect of Reynolds number on settling velocity is shown in Figure 5. The effect of Reynolds number was investigated by changing a fluid viscosity and fixing other parameters. It turned out that the reduction rate of settling velocity as particle concentration increases becomes small when Reynolds number is higher, and it was remarkable at high concentration. It is thought that if the Reynolds number becomes high a fluid flow exfoliates from the particle surface and so drag force decreases. As a result, settling velocity at high Reynolds number was higher than that at low Reynolds number.

4. A new scheme of Discrete Element Method for solid/fluid multi-material simulations using three-dimensional four particle interaction

4.1. Introduction of QDEM

From the view point of the mechanics of materials, all tectonic processes of the solid Earth involve movement of solid, molten material, and fluid. Another point is the interior of the Earth is not made of the same material nor has homogeneous nature all the way through. Depending on the depth from the surface, temperature, pressure, and chemical environment to a large extent define the nature of materials and various resultant aspects of deformation and flow. For example, convection in the mantle, driven by the thermal gradient between the core and lithosphere, occurs by solid-state deformation and flow of the rocks and minerals. Deformation in the shallow crust, on the other hand, is dominated by brittle processes, predominantly sliding on pre-existing plate boundary or fault systems.

However, the scenario mentioned above is still a hypothesis based on the indirect observations near the surface of the Earth. The reality is that the dynamics of the interior of the Earth is basically unobservable physics both in terms of time and space. Under such uncertain circumstances, numerical simulations play a key role to virtually observe the complex behavior of the solid Earth system and to understand the entire self-consistent dynamics of multi-materials phenomena as well as its long-term behavior.

Realistic simulations of the tectonic processes including mantle convection, plate subduction, and magma flow require the consideration of a wide variety of complex rheologies. One of the difficulties within self-consistent multi-materials/multi-phenomena models, capturing various rheologies, such as elasticity, plasticity, failure, friction, fluid flow properties and their temperature and pressure dependency, is that the individual behavior cannot be considered in isolation [4]. In other words, one set of field equations can contain one kind of rheology, although it can be applied to multi-components mixed materials. For very simple example, if a material which behaves like solid at low temperature and behaves like fluid at high temperature is subject to a large temperature contrast, one must choose either of the models: 1) a fluid model with high viscosity contrast, 2) a solid model with high creep effect. In either case, numerical instabilities may be unavoidable due to the enormous material parameter contrasts in addition to the complexity in the formulation if one follows the traditional continuum mechanics approach. Hence, it is worth developing a new specific computational scheme to deal with multi-materials and multi-rheologies for the numerical simulations of the solid Earth.

Motivated by the discussion above, a new method for numerical simulations which inherits the advantages of particle-based methods, with which micro-continuum mechanics is implemented to express the three dimensional multi-materials and multi-rheologies without solving complex field equations. The new method proposed here, namely, QDEM (Quadraple Discrete Element Method) is a kind of DEM but

the interaction of particles is defined not by two particles but by four particles. The four particles are not necessary to touch each other but are located in neighbor each other to form a tetrahedron by connecting the center of their mass which contains no other mass center of a particle. Assuming a micro-continuum for each tetrahedron where rheological models in continuum mechanics can be considered, we formulate the relationship between the motion of four particles and the stress developed in the tetrahedron. Once stress-force conversion for a tetrahedron is established, the rest of procedures are equal to those of DEM.

4.2. Isotropic elastic solid

One of the general forms of an elastic solid for the solid Earth simulation, including the fundamental physics, such as pressure, temperature and other potential energy is described by the functions

$$\begin{aligned} \boldsymbol{t}(\mathrm{t}) &= \mathrm{func\_}\boldsymbol{t}(\boldsymbol{F}, \theta, \mathrm{Grad}\theta, \boldsymbol{X}), \\ \boldsymbol{q}(\mathrm{t}) &= \mathrm{func\_}\boldsymbol{q}(\boldsymbol{F}, \theta, \mathrm{Grad}\theta, \boldsymbol{X}), \\ \varepsilon(\mathrm{t}) &= \mathrm{func\_}\varepsilon(\boldsymbol{F}, \theta, \mathrm{Grad}\theta, \boldsymbol{X}) \end{aligned} \tag{1}$$

where $\boldsymbol{t}$ is the Cauchy stress tensor, t is the time, $\boldsymbol{q}$ is the heat flux vector, ε is the internal energy, func_ represents a function, $\boldsymbol{F}$ is the deformation gradient tensor, θ is the temperature and $\boldsymbol{X}$ is the position at the reference [5]. Here, for simplicity, let us assume that the material properties are independent of the temperature, which means there is no heat and energy flow. Then, the material is called *purely elastic*. Further simplification may be made by introducing the symmetry conditions. As a result, equations (1) are simply reduced into

$$\boldsymbol{t}(\mathrm{t}) = \mathrm{func\_}\boldsymbol{t}(\boldsymbol{F}). \tag{2}$$

As you can seen in (2), the Cauchy stress tensor t only depends on the deformation gradient tensor $\boldsymbol{F}$. Actually this is a broad definition of *isotropic elastic solid* - Elastic stress is determined only from the information of reference configuration and current configuration. Inversely speaking, if we can well define the deformation gradient tensor $\boldsymbol{F}$ in a particle system, we can give three dimensional isotropic elastic properties in that system. This concept is important and it was the first step to develop QDEM.

Since the deformation gradient tensor $\boldsymbol{F}$ maps vectors from the reference configuration d$\boldsymbol{X}$ onto vectors in the current configuration d$\boldsymbol{x}$,

$$\mathrm{d}\boldsymbol{x} = \boldsymbol{F}\mathrm{d}\boldsymbol{X} \tag{3}$$

and is therefore also known as a *two-point-tensor*. Thus, to determine the nine components of the deformation gradient tensor $\boldsymbol{F}$, a set of mapping of minimum three linear independent vectors in a body is required. If four points not arranged in a same plane are given, then three linear independent vectors in a space can be defined. Those four points are the vertexes of a tetrahedron. Therefore, finding a tetrahedral local arrangement of four particles in neighbor and tracing it from the reference configuration to the current configuration, we can define the deformation gradient tensor for those four particles explained in Figure 6.

However, the deformation of the tetrahedron described by $\boldsymbol{F}$ in Figure 6 contains both pure stretch and rigid rotation as is interpreted by two polar decompositions of $\boldsymbol{F}$,

$$\boldsymbol{F} = \boldsymbol{RU} = \boldsymbol{VR}. \tag{4}$$

Then, we need to remove the effect of rigid rotation in $\boldsymbol{F}$, since the stress tensor of an isotropic elastic solid in (2) actually depends only on the left stretch tensor $\boldsymbol{V}$ or on the right stretch tensor $\boldsymbol{U}$ in (4). Choosing the left Cauchy-Green deformation tensor, one obtains

$$\boldsymbol{B} = \boldsymbol{F}\boldsymbol{F}^{\mathrm{T}} = \boldsymbol{V}\boldsymbol{R}\boldsymbol{R}^{\mathrm{T}}\boldsymbol{V} = \boldsymbol{V}^2 \tag{5}$$

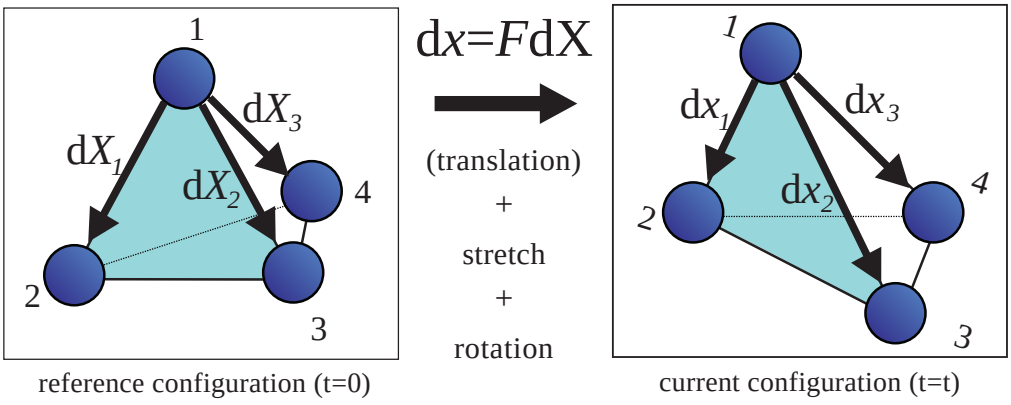

Fig. 6 The deformation gradient tensor $\boldsymbol{F}$: Three linear independent vectors defined in a system of four neighboring particles arranged in a tetrahedron and the mapping of vectors from the reference configuration d$\boldsymbol{X}$ onto vectors in the current configuration d$\boldsymbol{x}$

and (5) shows that the tensor $\boldsymbol{B}$ is not affected by rigid rotation any more.

Now, (2) is rewritten as

$$\boldsymbol{t}(\mathrm{t}) = \mathrm{func}\_\boldsymbol{t}'(\boldsymbol{B}). \tag{6}$$

From the theory in material equations for isotropic bodies, the representative form of the functional of the stress tensor for isotropic elastic solid is thus given by an isotropic tensor function of the tensor $\boldsymbol{B}$ (see the details of the derivation in the literature, such as [5]) : it implies

$$\boldsymbol{t}(\mathrm{t}) = a_0\boldsymbol{I} + a_1\boldsymbol{B} + a_2\boldsymbol{B}^2 \tag{7}$$

where a_0, a_1, and a_2 are the scalar functions of the tensor invariants of I_B, II_B, and III_B.

Choosing the proper scalar functions of a_0, a_1, and a_2 to match with the real material property, we here obtained the formulation of the stress tensor for isotropic elastic solid in QDEM The stress tensor in (7) defines the stress developed among four neighboring particles due to their relative motion that are described by $\boldsymbol{B}$.

4.3. Isotropic viscous fluid

For viscous fluid, the dependency of the deformation gradient tensor $\boldsymbol{F}$ for elastic solid is replaced to a dependency on the velocity gradient tensor $\boldsymbol{L}$ and the density ρ. Likewise $\boldsymbol{F}$, $\boldsymbol{L}$ consists of stretching part and rotating part. From the point of objectivity, the stress tensor may depend on the symmetric part of $\boldsymbol{L}$, if we assume isotropic viscous fluid. $\boldsymbol{L}$ can be uniquely decomposed into symmetric and anti-symmetric parts,

$$\boldsymbol{L} = 1/2\,(\boldsymbol{L} + \boldsymbol{L}^{\mathrm{T}}) + 1/2\,(\boldsymbol{L}\text{-}\boldsymbol{L}^{\mathrm{T}}) = \boldsymbol{D} + \boldsymbol{W}. \tag{8}$$

In the same manner of (7), the representative form of the functional of the stress tensor for isotropic viscous fluid is

$$\begin{aligned}\boldsymbol{t}(\mathrm{t}) &= b_0\boldsymbol{I} + c_1\boldsymbol{D} + c_2\boldsymbol{D}^2\\ b_0 &= -p + c_0\end{aligned} \tag{9}$$

where p is the pressure term, which is a function of the density ρ and c_0, c_1, and c_2 are the scalar functions of the tensor invariants of I_D, II_D, and III_D. If we wish to model Newtonian fluid, then the quadratic term drops out from (9). However, incompressibility is not explicitly introduced in QDEM, but expressed by a higher bulk modulus value which is the parameters of the pressure increment term versus volume change since each particle moves independently.

In QDEM, the velocity gradient tensor $\boldsymbol{L}$ can be defined also on the four neighboring particles arranged in a tetrahedron. In this case, $\boldsymbol{L}$ maps the relative position vectors d$\boldsymbol{x}$ on the relative velocity vectors d$\boldsymbol{v}$

$$\mathrm{d}\boldsymbol{v} = \boldsymbol{L}\mathrm{d}\boldsymbol{x} \tag{10}$$

Hence, we understand how the two different rheologies of an elastic solid and a viscous fluid can be introduced in the same particle system using the four particle relationship in QDEM. It is, clearly, possible that those two rheologies can be mixed.

4.4. From stress to force

Up to the previous arguments, the way how to relate the motion of four particles in neighbor to the stress stored among them for isotropic elastic solid and viscous fluid was explained. However, the closed formulation for QDEM has not been completed yet. Because (7) or (9) does not give forces on particles but gives stress among four particles. It is, therefore, in need to convert the stress tensor for a tetrahedron to the force vector acting on the particles.

In QDEM, the stress developed in the volume of each tetrahedron is homogeneously constant. Therefore, the way to subdivide this volume to define the interfacing planes is the key issue to estimate the contributing force acting on the four particles. There are many ways to divide a tetrahedron into four blocks. Considering the stress homogeneously distributed in the tetrahedron, we have developed a new method which uniquely divides an arbitrary tetrahedron into four equi-volume blocks. Although the details of the method are not explained here, one tetrahedron can be subdivided into four equi-volume blocks by twelve triangular surfaces. Figure 7 shows the interfacing surfaces of each domain of four blocks. Once these surfaces are defined, the stress vector for each triangular surface will be given from the stress tensor, and it will then be converted into the force acting on the surface of each block. Finally, all the surface forces on each block are

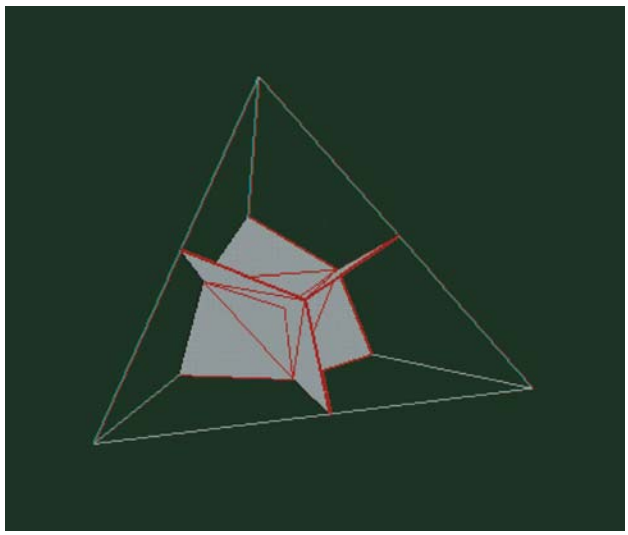

Fig. 7 Skelton of interfacing planes

summed up and transposed into the force acting on the vertex of the tetrahedron as a part of the force on a particle.

The motion of each particle is determined individually by solving the motion of equation from the resultant force and the body force. This procedure is exactly identical to the way of DEM.

4.5. Discussion

Introducing a micro-continuum mechanics into the particle based modeling, we showed a new computational scheme, named QDEM, to implement three dimensional multi-materials and muti-rheologies into particle based models. In this sense, QDEM can be categorized as a DEM interpretation of FEM-β [6]. Although the example rheologies considered in this paper may be too simple for the simulation of the solid Earth discussed in the section of introduction, the scheme is far less complicated and solvable for practical purposes. One of the main advantages of QDEM is to be easy to combine with the ordinary DEM since the main framework is similar except the part of the particle interaction.

In Figure 8, snapshots of uni-axial compression simulation of viscous-elastic material with large strain (10%), as an example of QDEM simulation, are shown.

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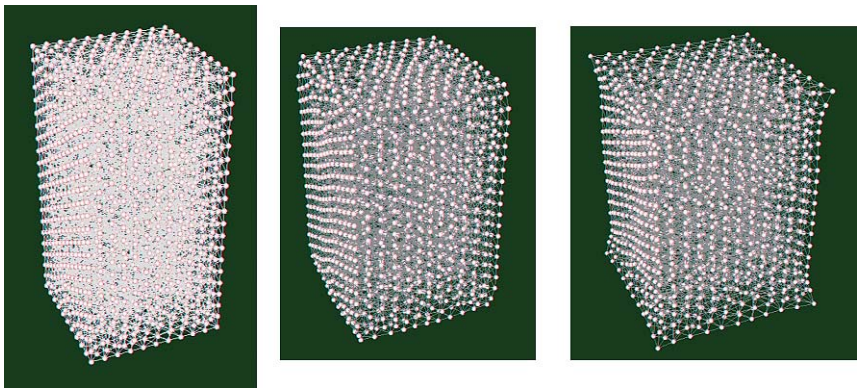

Fig. 8 Example simulation using QDEM

DEMによる内部構造を持つ複雑多相系の粒子モデル

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前年度までの本プロジェクトを継続し、気相、液相、固相が混在している場で、とくに内部構造を作りながら複雑な振る舞いを示す系に対して、粒子に基づく離散モデル(DEM-Discrete Element Method)と粒子－連続体カップリングモデルを構築し、大規模シミュレーションのための計算手法と技術を開発した。そして、幾つかの重要な応用問題に適用し、複雑多相系現象の解明と解析、予測に応用し、本報告では、1)血流シミュレーション：流体と柔らかい固体の相互作用問題として、赤血球の変形性が毛細血管における流れ抵抗と分岐流に与える影響の解明、2)流体内粒子沈降シミュレーション：気流のある場における微粒子運動の解析、3)地盤・岩盤・プレート運動シミュレーション：固体－粒状体－流体からなる地球内部及び表面物質の運動・破壊・流動解析のための4体粒子モデルの新たな開発について報告する。

キーワード：粒子，流体，多相体，内部構造，個別要素法