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

Project Representative
Hide Sakaguchi — Institute for Research on Earth Evolution (IFREE), Japan Agency for Marine-Earth Science and Technology (JAMSTEC)

Authors
Hide Sakaguchi — Institute for Research on Earth Evolution (IFREE), JAMSTEC
Shigeo Wada — Department of Mechanical Science and Bioengineering, Osaka University
Kenichi Tsubota — Department of Biomechanics and Robotics, Tohoku University
Yoshitaka Kitagawa — Department of Biomechanics and Robotics, Tohoku University

Among four main topics in the research and development plan of DEM consortium studied in last three years, we focused to realize the large simulation of the collective behavior of multiple red blood cells, which is a typical example of the complex multi-phase systems with internal structures. Following the development of a two-dimensional blood flow model between parallel plates up to previous years, we made a great many successes in extending the blood flow model into a three dimensional model this year. Using our novel three-dimensional model, deformation of each individual blood cell, tank treading behavior and collective behavior were simulated.

Keywords: Read blood cell (RBC), Particle, Fluid, Multi-phase system, Internal structure, Discrete Element Method

1. Introduction

Materials, which are mixtures of solid and liquid, can be seen in many occasions such as ink for printing, fresh concrete and so on. Generally, those materials have significantly complex rheology and their flowing behavior is characterized by the percentage of solid fraction. However, the rheology becomes much more complex when the solid part forms an internal micro-structure composed of particles. In this case, even with the low percentage of solid fraction, the material shows more or less solid-like behavior. As a result, mathematical description of those material behaviors becomes extremely difficult.

Blood is kwon as a suspension in which solid blood cells, such as red blood cells (RBC), white blood cells (WBC) and platelets suspended in fluid plasma. Then, blood is also a good example of complex multi-phase systems with internal structure. However, the most distinguishable nature of blood is the fact that each individual RBC is highly deformable. Not only its deformability, but also the surface of a RBC, which is covered by thin membrane film, can independently react to the external force from the fluid inside a RBC. Consequently, the rheology of blood is one of the highest complex problems.

Actually, there is considerable indication that complex hemodynamics (blood fluid mechanics) play an important role in the development of artherosclerosis and other kinds of cardiovascular disease [1, 2], which is one of the most frequent causes of death in the industrialized world [3, 4].

It is therefore that the study of hemodynamics is to become a well representative for the urgent and practical part of the research on complex multi-phase system with internal structures. However, since the problem is highly complex, it is too difficult to construct a direct model and analytical solutions. Consequently, 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 elastic red blood cell model and its collective behavior.

2. Modeling of a three dimensional elastic red blood cell

In order to investigate the dynamical behavior of RBC in flowing blood, we built up a three dimensional model of an elastic RBC based on the minimum energy principle and carried out computer simulation of the RBC flow in a straight vessel.

Initially, RBC is modeled by a number of particles configuring RBC membrane. The number of particle depends on the number of RBC needed in the flow simulation. Particles are bonded together to form a triangular mesh by springs in three dimensional space. Each spring resists to either tension or compression. At the link of the springs, rotational resistance is considered. With these sets, the model can express the mechanical behavior of membrane. Elastic energy of the membrane is considered for changes in the length of the element and the angle between the neighboring elements. In addition, area constraint for each triangle is introduced to express internal pressure within RBC. The details can be seen in the work of Wada and Kobayashi [5].

In Figure 1, a series of snapshots of biconcave self-deformation from original spherical shape based on minimum energy principal is shown. The final configuration in Figure 1 is identical indeed to the real RBC observed in vitro.

With this highly deformable RBC model, we performed a simulation of a single RBC pushed into a thin blood vessel with assumed fluid pressure difference at the entrance and the exit (Figure 2). As is shown in the left top of Figure 2, the diameter of RBC is larger than that of blood vessel. Here, the red object is the side view of a biconcave RBC. As you can see in the following snapshots in Figure 2, the RBC adjusts itself by bending the body due to the small diameter of the blood vessel. In reality, a RBC which size is much lager

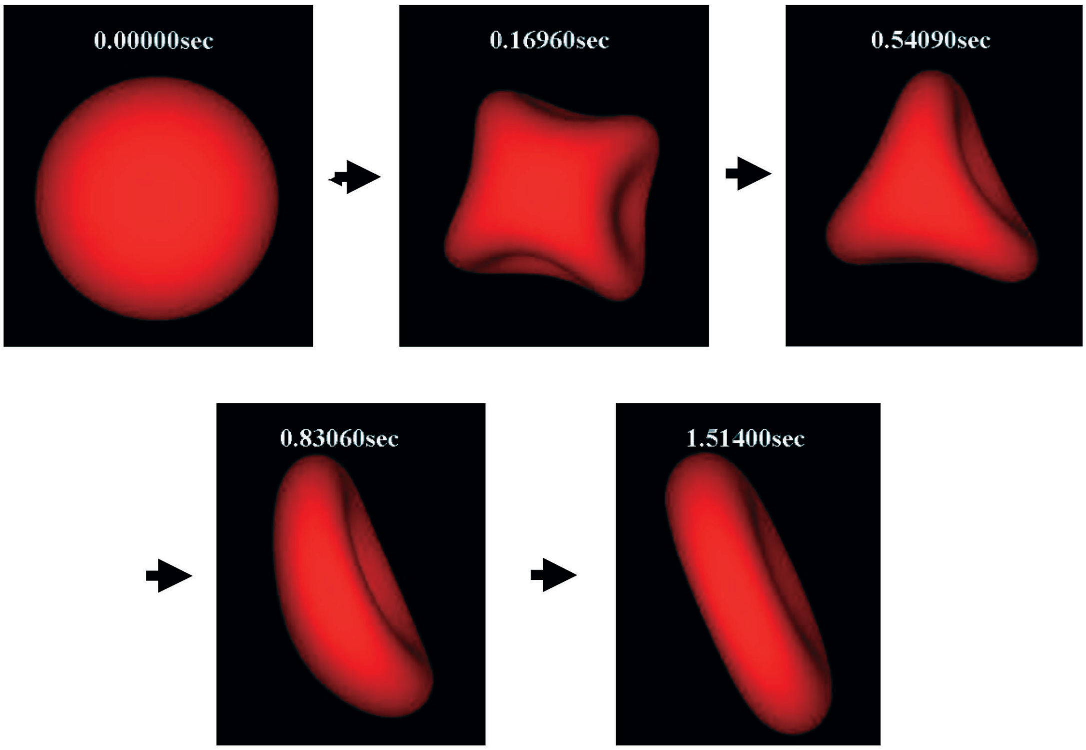

Fig. 1 Self-deformation of a single RBC.

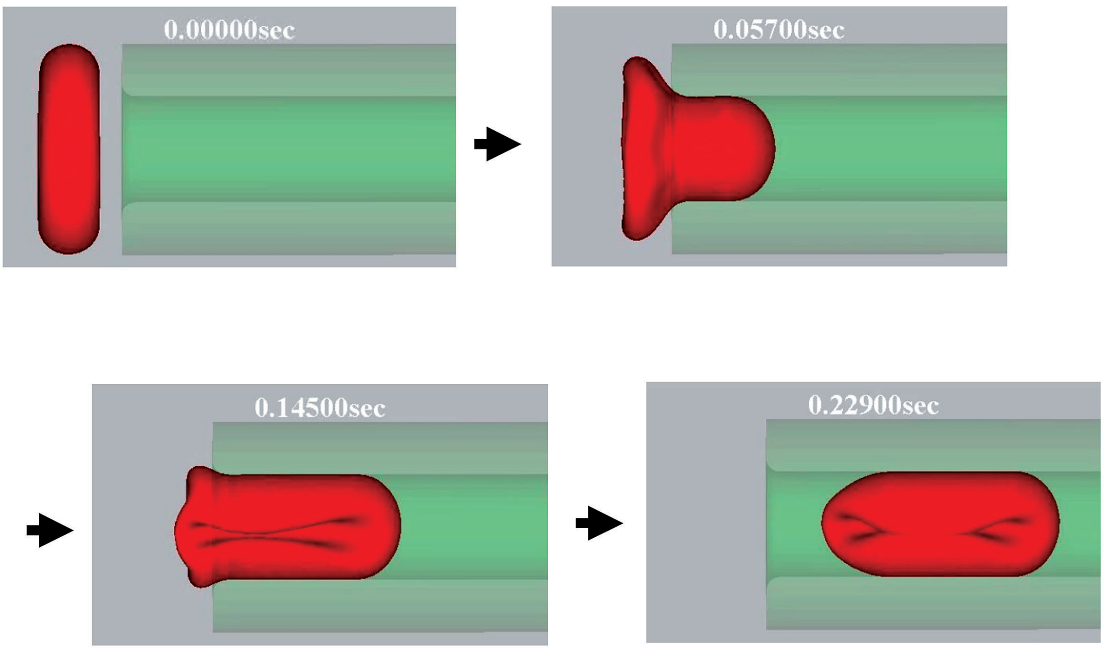

Fig. 2 A RBC in a thin blood vessel.

than the diameter of blood vessel can flow in the thin vessel freely. In this sense, modeling of this deformability is very important to understand the true mechanism of blood flow.

3. Collective Behavior of Multiple RBCs.

In contrast to the example simulation shown in the previous section, collective behavior under the influence of mechanical interaction between RBCs in the much larger vessels than RBC size is increasingly important to determine rheological properties of blood as a mass. In this section, some examples of our new three dimensional 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. In the following, the Poiseuille flow was assumed as the prescribed flow field.

Fig. 3 Small scale three dimensional RBC flow simulation.

In Figure 3, a snapshot of a small scale testing simulation result is shown. Depending on the deformability of each RBC and the shear force contrast, which is determined by the elastic properties and flow filed, the RBCs concentrate in the center of the vessel and tank treading behavior is observed in the simulation.

After verifying the model by the small scale simulations, we extended the model for large scale simulations (128 nodes on ES). Figure 4 and Figure 5 are the typical snapshots of the results. We will make detailed analyses for the result soon.

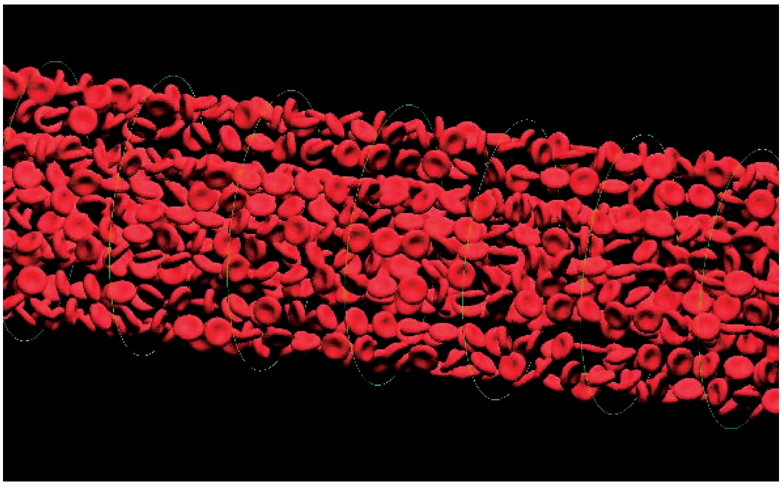

Fig. 4 Large scale three dimensional RBC flow simulation - Low RBC fraction.

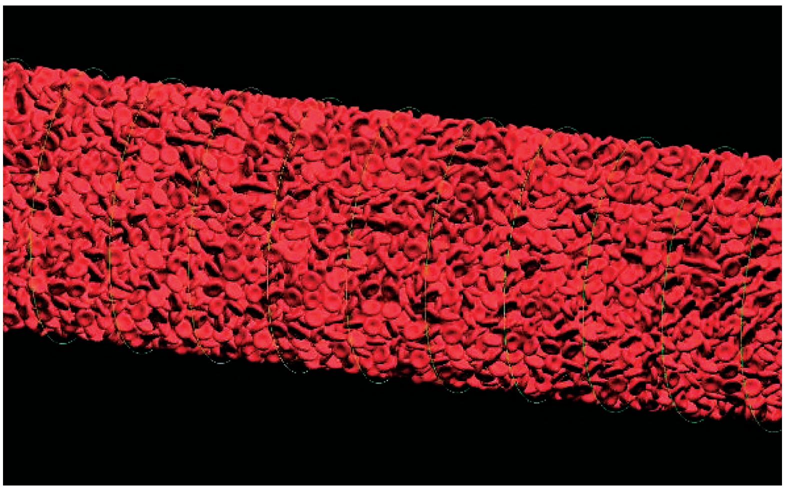

Fig. 5 Large scale three dimensional RBC flow simulation - High RBC fraction.

4. Conclusion

Implementation for the three dimensional realistic multiple RBC flow model on the Earth Simulator and the preliminary simulation results were all done. Toward the year 2006 and 2007, we will further continue to develop more and more realistic models, such as branching and deformable blood vessels.

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DEMによる内部構造を持つ複雑多相系の粒子モデル

プロジェクト責任者
阪口　　秀　　独立行政法人海洋研究開発機構　地球内部変動研究センター

著者
阪口　　秀　　独立行政法人海洋研究開発機構　地球内部変動研究センター
和田　成生　　大阪大学基礎工学部
坪田　健一　　東北大学大学院工学研究科　バイオロボティクス専攻
北川　義隆　　東北大学大学院工学研究科　バイオロボティクス専攻

昨年度までにDEMコンソーシアムでは、地球シミュレーターの共同プロジェクトの枠組みの中で、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てきた。幾つかのサブトピックスの中で、17年度は、計算資源を血流問題に重点的に割り当て、当初の予定通り、前年度までに開発された変形性赤血球の集団流れモデルを3次元モデルに拡張した。この3次元モデルの完成によって、今後、よりリアルなシミュレーションを行う基盤を作り上げた。

キーワード：赤血球, 粒子, 流体, 多相体, 内部構造, 個別要素法