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Toward the multi-scale simulation for a human body using the next-generation supercomputer

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Abstract

We have developed novel numerical methods for fluid-structure and fluid-membrane interaction problems. The basic equation set is formulated in a full Eulerian framework. The method is based on the finite difference volume-of-fluid scheme with fractional step algorithm. It is validated through a numerical solution to a deformable vesicle problem, and applied to blood flows including red blood cells (RBCs) and platelets. Further, to gain insight into the mechanism of thrombus formation, a stochastic Monte Carlo model to describe the platelet-vessel wall interaction is incorporated into the Eulerian method. The effect of the RBCs on the platelet motion is discussed.

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1. Introduction

A 10-Peta-flops class supercomputer (the K computer) has been developed in the Next-Generation Supercomputer Project in Japan, and it will go into full-scale operation at the end of September 2012 [1]. The software development as well as the hardware development have been highly expected. Especially, the development of human body simulator has been assigned as a grand challenge program for the effective use of the K computer, in which the multi-scale and multi-physics natures of the living matter are emphasized. Under this concept, we have been developing the multi-scale simulator for a living human body. Basic strategy of the simulator is to utilize the medical image data taken by MRI, CT, or ultrasound for the prediction of disease and planning of therapy. For this purpose, we have developed full Eulerian Fluid-Structure Interaction (FSI) solver [2–8] without mesh generation procedure, which enables us to conduct the simulations directly from medical images. In this paper, we shall focus on the application to microcirculation systems including deformable blood cells.

Blood flow plays important roles in several functions to sustain life, and exhibits phenomenologically rich behavior owing to its multi-physics nature, the complex geometry, and the suspension of blood cells.

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In a microcirculation system with a sub-millimetric scale vessel, a red blood cell (RBC) subjected to a shearing fluid motion undergoes large deformation. Such a distinctive deformability and a dense particulate flow nature characterize rheological properties, which are relevant to transport phenomena and hemostatic processes [9]. Recent advances in high-performance computing and numerical methods have promoted interest in hemodynamic simulations [10–12]. In order to obtain practically important knowledge of the integrated dynamics, it is important to perform a large-scale computation close to the realistic scale since the system is hydrodynamically and geometrically nonlinear in size. An efficient and scalable numerical method is desirable for the large-scale computation.

Conventionally, the computational fluid dynamics is commonly described in an Eulerian way, while the computational structure dynamics is more straightforward to be described in an Lagrangian way. The coupling of the fluid and structure dynamics is a nontrivial task due to such a difference in the numerical framework. There are currently several approaches classified with respect to the computational treatment how the kinematic and dynamic interactions are coupled on the moving interface. When addressing moving interface problems, one has preferably employed the Lagrangian method using a moving finite element mesh. The numerical methods include Arbitrary Lagrangian Eulerian [13], Deforming-Spatial-Domain/Stabilized Space-Time [14] and Immersed Boundary [15] approaches. Once the body-fitted mesh is provided, the state-of-the-art Lagrangian approaches are satisfactory for achieving accurate predictions. However, for a system involving complex geometry of solid and/or a large number of bodies, it requires not only a high computational cost but also great efforts to generate the high quality mesh and to reconstruct the mesh topology when the mesh element is added/deleted. Moreover, in a large parallel computation, one encounters a nontrivial issue how the respective quantities on the Eulerian and Lagrangian meshes are adequately communicated to keep the load balance of each compute node.

To release the FSI simulation from the mesh generation/reconstruction procedure, and to extend the applicability to certain additional classes of problems, full Eulerian (fixed-mesh) methods have been developed [16–19]. Following an idea of a one-fluid formulation [20], in which one set of governing equations is written over the whole field, as frequently used in multiphase flow simulations, the authors have formulated the basic equations for general FSI problems suited to the finite difference method [4, 7]. The developed method has revealed practical advantages of geometrical flexibility [2, 3, 8] since it can directly access voxel data and avoid a breakdown in a large deformation owing to the absence of the mesh distortion problem. The monolithic formulation discretized on regular grids systematically offers numerical stability conditions [5]. Further, in view of computational efficiency, it readily exploits vector processing and reduces a computational-load imbalance in parallel computing. The full Eulerian method allows us to utilize efficient computational techniques cultivated in the field of computational fluid dynamics, that is an advantage in the realization of massively parallel computing [21].

In this paper, firstly, the basic equations of the system consisting of Newtonian fluid and hyperelastic structure/membrane will be outlined. Secondly, the validity of the advocated numerical method will be demonstrated. Thirdly, the method will be applied to three-dimensional blood flows including blood cells in a capillary vessel and in a microchannel, and the relevance of the RBC to the thrombus formation will be discussed.

2. Basic equations

We consider a system comprised of Newtonian fluid and visco-hyperelastic material regions, and also membrane surfaces, which enclose portions of fluid. The fluid and solid phases are incompressible (namely, $\nabla \cdot \boldsymbol{v} = 0$, here, $\boldsymbol{v}$ is the velocity vector) with the identical density ρ as in many analyses for biological systems. We assume that the membrane has no thickness, but the elastic tension thereon causes the traction jump and thus the discontinuity of the fluid stress. Here, we shall briefly explain the Eulerian formulation [4, 7]. The momentum equation for the whole field is written monolithically as

$$\rho(\partial_t + \boldsymbol{v} \cdot \nabla)\boldsymbol{v} = \nabla \cdot \boldsymbol{\sigma} + |\nabla \phi| \boldsymbol{f}, \tag{1}$$

where $\boldsymbol{\sigma}$ denotes the Cauchy stress tensor, ϕ the volume fraction of a dispersed phase (namely, the VOF function [22]), and $\boldsymbol{f}$ the local force density vector to describe the traction jump.