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A Full Eulerian Method For Fluid-Structure Interaction Problems

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Abstract

An efficient and scalable numerical method for massively parallel computing of fluid-structure interaction systems has been developed for biomedical applications. To facilitate the treatment of complex geometry, a full Eulerian method is employed to couple the incompressible motions of fluid and hyperelastic materials. Instead of implicitly solving the pressure Poisson equation, a novel artificial compressibility method with adaptive parameters, which are determined to guarantee the computed field to be nearly incompressible, is proposed. In both weak and strong scaling tests, the developed solver attains excellent scalability on the K computer. A sustained performance of 4.54 Pflops (42.7% of peak) has been achieved for a microchannel flow involving more than 5 million deformable bodies using 6.96×10^{11} grid points with 663,552 compute cores. We study arteriole blood flows in a brain to gain insight into dynamic interactions among motions of plasma and blood cells, which are relevant to initial thrombus formations.

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1. Introduction

Fluid-Structure Interaction (FSI) phenomena appear in a number of biological systems. Thereamong, blood flow plays important roles in life-sustaining and exhibits phenomenologically rich behavior owing to its multi-physics nature, the complicated geometry, and the suspension of blood cells. Recent advances in high-performance computing and numerical methods have promoted interest in hemodynamic simulations [1,2,3], and encouraged large-scale computations [4,5,6,7,8,9] as grand challenges. In this paper, we shall focus on deformable body motions, of which the improved understandings would gain insight into an initial thrombus formation and an exaggerated platelet aggregation to cause myocardial and cerebral infarctions [10,11]. In a microcirculation system, a Red Blood Cell (RBC) subjected to a shearing or squeezing fluid motion undergoes large deformation. Such a distinctive deformability and a dense particulate flow nature dictate rheological properties relevant to transport phenomena and hemostasis processes [12]. Especially, a platelet dispersion is strongly affected by the RBC-induced fluid fluctuation rather than the thermal one [13]. The significance of the hydrodynamic effect on the thrombus formation has become commonly recognized [14,15,16,17]. Recently, numerical simulations have been performed to predict e.g. three-dimensional motions of two platelets in a

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shear flow[18], and two-dimensional[19] and three-dimensional[20] blood flows (in vessels of 50μm height and 20μm diameter, respectively) including a number of platelets and RBCs. In order to obtain practically important knowledge of the integrated dynamics in e.g. a brain arteriole of 100μm or larger diameter, it is essential to perform large-scale computation at the realistic scale since the system is hydrodynamically and geometrically nonlinear in size. For this purpose, our strategy in formulation and algorithm will be outlined below.

When addressing moving interface problems, one has preferably employed a Lagrangian method using a moving finite element mesh[21,22,23] because it is suited for describing an elastic constitutive law. For relatively simple systems, these approaches are satisfactory and have been applied to a wide variety of biological problems. However, for a system involving complicated geometry of solid and/or a large number of bodies, it additionally requires a great effort to reconstruct the mesh at each time step. Moreover, in massively parallel computing, one encounters a nontrivial issue how the respective quantities on the Eulerian and Lagrangian meshes are adequately communicated without loss of parallel efficiency. 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[24,25,26,27]. The authors have formulated the basic equations for general FSI problems suited to the finite difference method using regular Cartesian grids to be consistent with conventional computational algorithms for incompressible flows[28,29,30?,31,32]. The developed method has revealed practical advantages of geometrical flexibility[20,31] since it can directly access voxel data and avoid a breakdown caused by the mesh distortion problem in a large deformation. Further, in view of computational efficiency, it readily gets great performance out of SIMD processing and reduces a computational-load imbalance in a domain decomposition for parallel programs. The full Eulerian method allows us to utilize efficient computational techniques cultivated in the field of stencil computations, that would be an advantage in the realization of massively parallel computing.

So far, several scalar-type supercomputer systems have achieved over 1 Pflops sustained performance on LINPACK, corresponding to a dense matrix solver[33]. However, among stencil computations, in which the discretized form of the basic equations often reduces to a sparse matrix, no application for popular fliud and/or solid problems has reached over 1 Pflops sustained performance. In particular, an iterative procedure for implicitly solving the pressure Poisson equation included in the standard algorithm for incompressible flows occupies a considerable amount of the computational time (as well as repetitive communications in parallel computing) and therefore makes it difficult to exploit the system performance. To drastically improve the situation, a novel algorithm, which includes no iterative procedure for solving the Poisson equation, will be proposed. We follow a revived Artificial Compressibility Method (ACM)[34], which is unlike the original ACM[35] for the steady flow problem or the implicit ACM[36] but explicitly solves a pressure evolution equation in a time-stepping manner. We introduce a projection step and an optimization procedure, where the adaptive parameters are dynamically determined to *mathematically* guarantee the computed field to be nearly incompressible.

This paper is organized as follows. In §2, the basic equation set for the full Eulerian FSI simulation is briefly presented and the novel ACM with the adaptive parameters is introduced. In §3, the performance in the weak and strong scaling analyses are reported. In §4, the results of the blood flow simulations are discussed. In §5, some perspectives are provided to conclude the paper.

2. Simulation methods

The fluid and solid are assumed to be incompressible and to possess the same density and viscosity, as in many analyses for biological systems. The governing equations are the mass and momentum conservations:

$$\nabla \cdot \boldsymbol{v} = 0, \tag{1}$$

$$\rho\left(\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v}\cdot\nabla\boldsymbol{v}\right) = \nabla\cdot\boldsymbol{\sigma} + \left(-\frac{\Delta P}{L_x}\right)\boldsymbol{e}_x, \tag{2}$$

where $\boldsymbol{v}$ denotes the velocity vector, ρ the density, t the time, $\boldsymbol{e}_x$ the unit vector in x direction, and $\boldsymbol{\sigma}$ the Cauchy stress. To pump the fluid and solid, the uniform pressure gradient $-\Delta P/L_x$ (here, L_x is the inlet-outlet length in x direction of the computational domain, and $-\Delta P$ is the inlet-outlet pressure drop) is applied to the system. The Cauchy stress is written in a mixture form of the Newtonian fluid and the neo-Hookean material, namely,

$$\boldsymbol{\sigma}(\boldsymbol{x}) = -p(\boldsymbol{x})\boldsymbol{I} + 2\mu\left(\boldsymbol{D}(\boldsymbol{x}) - \tfrac{1}{3}\mathrm{tr}(\boldsymbol{D}(\boldsymbol{x}))\boldsymbol{I}\right) + G\phi_s(\boldsymbol{x})\left(\tilde{\boldsymbol{B}}(\boldsymbol{x}) - \tfrac{1}{3}\mathrm{tr}(\tilde{\boldsymbol{B}}(\boldsymbol{x}))\boldsymbol{I}\right), \tag{3}$$