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A distributed lagrange multiplier based computational method for the simulation of particulate-Stokes flow

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Abstract

In this paper we present a distributed lagrange multiplier (DLM) based Stokes flow algorithm for particulate flows. The entire fluid–particle domain is treated as a fluid. The "fluid" in the particle domain is ensured to move rigidly by adding a rigidity constraint. We modify the SIMPLER (Semi-Implicit Method for Pressure Linked Equations—Revised) algorithm for fluids (by Patankar [Numerical Heat Transfer and Fluid Flow, Taylor and Francis, London, 1980]), to account for the presence of the particle. The modification pertains to the presence of the rigidity constraint in the particle domain. We validate the algorithm with suitable test cases.

Keywords: Direct numerical simulation (DNS); Distributed lagrange multiplier (DLM) method; Control volume; SIMPLER; Particulate flows

1. Introduction

Advances in nano/micro-fabrication techniques over the past few years have enabled many new applications. The technology finds applications in chemical, biochemical and biomedical analysis. These devices comprise of electrical and mechanical components on small chips. Among various possible uses are the sorting and analysis of cells and particles that move in a fluid environment. Proper understanding of particle motion in a fluid medium, under conditions of varying fluid properties, particle size, concentration and body forces is essential for the design of these devices. Owing to small Reynolds numbers encountered in

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such flows the inertia term can be neglected. Hence, the problem reduces to solving the Stokes flow equations.

Particulate flow simulations under the Stokes flow assumption have been done by the Stokesian dynamics technique [1]. They adopted a quasi-Stokes approach where a creeping flow steady-state problem is solved for a given configuration of the particles. The particle velocities are obtained through the solution. The particles are then updated explicitly to a new configuration and a new Stokes problem is solved. This quasi-Stokes approach has been successfully applied to spherical particles in Newtonian fluids while also accounting for the Brownian motion. However, extension of the method to irregular shaped bodies in a fluid with varying properties (e.g. viscosity, temperature, etc.) is not straightforward.

The objective of the current work is to develop a general purpose direct numerical simulation (DNS) technique for particulate Stokes flows. DNS of particle motion in fluids is a tool that has been developed over the past several years [11,12,14,5–7,19,13,20,8,4,2,3]. In this approach the fluid equations are solved coupled with the equations of motion of the particles. DNS allows investigation of a wide variety of problems including particles in Newtonian or viscoelastic fluids [13,25] with constant or varying properties.

The DNS Stokes flow algorithm for particulate flows developed in this paper is based on the distributed lagrange multiplier (DLM) approach [5,19,20]. In the DLM approach the entire fluid–particle domain is considered to be a fluid. It is ensured that the 'fluid' occupying the particle domain moves rigidly by adding a rigidity constraint. We consider three-dimensional numerical simulations of flow around a sphere to validate the algorithm. However, our approach can very easily handle irregular shaped bodies [19,20,24] and can be used for the simulation of Brownian particles [23]. The application of earlier DLM formulations of Glowinski et al. [5,6] to non-spherical rigid bodies is given by Juarez et al. [15,16], Pan et al. [18], Glowinski et al. [9] and Glowinski [4].

The paper is organized as follows. In Section 2 we discuss the mathematical formulation of the problem. Section 3 contains a discussion of the proposed numerical scheme. Simulation results to validate the numerical algorithm are presented in Section 4. Section 5 contains summary.

2. The mathematical formulation

Let Ω be the computational domain which includes both the fluid and particle domain. Let P be the particle domain. Let the fluid boundary not shared with the particle be denoted by Γ. In this work we will assume a periodic boundary condition on Γ (except for the shear flow problem presented in Section 4.2). We will consider one particle in the computational domain. The particle can be of any shape but in this paper we will solve for a spherical particle. The entire fluid-particle domain is assumed to be a fluid. The governing equations (corresponding to Stokes flow) applicable in the fluid–particle domain are thus given by [19]

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{f} = \mathbf{0} \quad \text{in } \Omega, \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega, \tag{2}$$

$$\mathbf{u} = \text{periodic on } \Gamma, \tag{3}$$

$$\left.\begin{array}{ll} \nabla \cdot (\mathbf{D}[\mathbf{u}]) = \mathbf{0} & \text{in } P \\ \mathbf{D}[\mathbf{u}] \cdot \mathbf{n} = \mathbf{0} & \text{on } \partial P \end{array}\right\}, \tag{4}$$

where we assume neutrally buoyant particles (although the formulation is not restricted to this assumption), $\mathbf{u}$ is the fluid velocity, $\mathbf{n}$ is the outward normal on the particle surface and $\boldsymbol{\sigma}$ is the stress tensor.

Eq. (4) represents the rigidity constraint and Eq. (2) is the incompressibility constraint. The rigidity constraint, imposed only in the particle domain P, ensures that the deformation–rate tensor [19]