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A 3-D indirect boundary element method for bounded creeping flow of drops

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Abstract

The simulation of the flow of emulsions in porous media presents formidable challenges, due to the extremely complex evolving geometry. Methods based on boundary integral equations, suitable for creeping flows, reduce the effort dedicated to geometry representation, but can become computationally expensive. An efficient indirect boundary integral formulation representing deformable drops in a bounded Stokes flow, resulting in a set of Fredholm integral equations of the second kind, is presented. The boundary element method (BEM) based on the formulation employs an accurate numerical integration scheme for the singular kernels involved, an effective and accurate curvature and normal calculation method, and an adaptive remeshing method to simulate interfacial deformation of drops. Two benchmark problems are used to assess the accuracy of the method, and to investigate its behavior for large problems. The method is found to provide accurate results combined with well-posedness, making it suitable for use in accelerated fast multipole method algorithms.

Keywords: Multiphase flow; Porous media; Indirect BIE; Iterative solution

1. Introduction

The low Reynolds number flow of drops in complex geometries is of interest in many emerging applications, for example the geological sequestration of CO_2, and multiphase flows found in various components of fuel cells. In these cases, the size of the drops may be comparable to the size of the confining geometry, so that flow of a homogenized effective fluids is not an appropriate modeling avenue. Conversely, phenomena of particular interest include drop coalescence and breakup, and the interaction of drops with the confining geometry. While flows of drops in an unbounded fluid in various conditions have been studied extensively [1–11,14–24,46–49], confined flows are less common [12,13,25–33].

In the case of creeping flows with well-defined interfaces, the governing equations can be cast in the form of integral equations with boundary-only terms. In such cases, boundary integral techniques offer important advantages, principally resulting from the reduced meshing requirements. The major disadvantage of the boundary integral approach, namely the large dense systems that arise from the discretization of the boundary integral equation (BIE), has recently been overcome by the application of acceleration methods which reduce the storage and computation requirements by orders of magnitude [34,35]. One of the main requirements to ensure the success of such methods is that the problem is well posed, generally meaning that the BIE is a regular Fredholm equation of the second kind, i.e. for which the homogeneous form only admits the trivial solution. The integral equation presented here is constructed to fit this requirement.

The main idea of the indirect formulation is to define an integral representation formula that produces a well-posed second kind integral equation, i.e. it is uniquely solvable and possesses a bounded inverse operator and its analytical solution is given in terms of a Neumann series (regular or modified), which is a Picard iteration. Besides, it is well known that the number of iterations of an iterative

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numerical solution of a well-posed Fredholm equation of the second kind to fixed precision is bounded and it is independent of the number of degrees of freedom (for more details see Greengard et al. [34]).

A major difficulty encountered with the indirect formulation is the necessity of defining a different formulation for each type of boundary value problem, in order to obtain a uniquely solvable integral equation of the second kind, which can be used as the basis of a robust numerical scheme. Generally this is not straightforward, and to prove the well-posedness of the resulting integral equation it is necessary to carry out a formal analysis of the corresponding integral operators.

In what follows, first the construction of the BIE is discussed in detail, especially in relation to the well-posedness requirement. The numerical implementation requires three components, namely accurate numerical integration, evaluation of surface normals and curvatures, and adaptive remeshing. The algorithms used to satisfy each component are discussed in the second part of the paper, in which novel techniques and adaptations of existing ones are presented. In the third part, the method is benchmarked using the bounded flow of a drop in a container of varying size, and by comparing the flow of a drop under the action of buoyancy forces with the corresponding analytical solution. In addition, the performance of the various components of the dynamic simulation is studied. Finally, strengths and weaknesses of the method are discussed and conclusions are drawn.

2. Indirect boundary integral formulation

The schematic of a typical contained flow involving a carrier fluid and n droplets of immiscible fluid is shown in Fig. 1. Let Γ_0 denote the surface of the container and Ω_0 the volume of the carrying fluid, Γ_p the surface of droplet p, $p = 1, \ldots, n$, Ω_p the volume enclosed by Γ_p, and Ω the entire volume bounded by Γ_0. Suppose that a velocity field

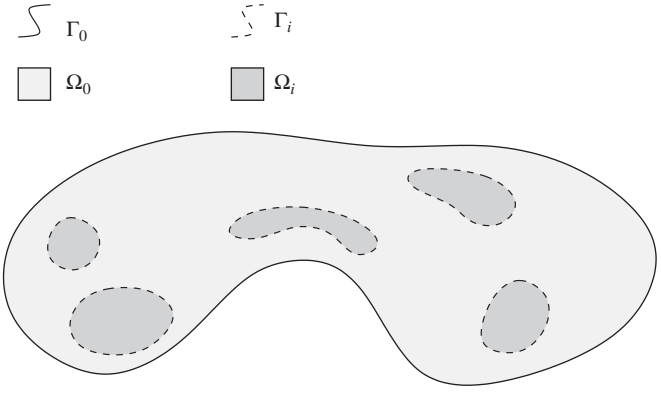

Fig. 1. Typical geometry of drops in a Stokes flow within a container. Velocities are specified on Γ_0, while each drop is characterized by a viscosity and a surface tension.

$\mathbf{U}(\mathbf{x}), \mathbf{x} \in \Gamma_0$ is specified as the boundary condition on the container surface.

The governing equations for the problem described in Fig. 1 are the Stokes equations:

$$\frac{\partial u_i}{\partial x_i} = 0, \quad \frac{\partial \sigma_{ij}}{\partial x_j} = 0, \tag{1}$$

where

$$\sigma_{ij} = \begin{cases} -P\delta_{ij} + \mu(\partial u_i/\partial x_j + \partial u_j/\partial x_i), & x \in \Omega_0, \\ -P\delta_{ij} + \lambda_p\mu(\partial u_i/\partial x_j + \partial u_j/\partial x_i), & x \in \Omega_p, \end{cases} \tag{2}$$

in which $\lambda_p = \mu_p/\mu$ is the ratio of the viscosity of drop p and the viscosity of the carrier fluid. The boundary conditions are

$$u_i(x) = U_i(x), \quad x \in \Gamma_0, \tag{3}$$

$$[\sigma_{ij}(x)n_j(x)]_S = \gamma_p n_i \frac{\partial n_k}{\partial x_k}, \quad x \in \Gamma_p. \tag{4}$$

Here, $[\,]_S$ denotes the jump across the surface of drop p from the outside Ω_0 to the inside Ω_p, while γ_p is the interface tension between the carrier fluid and fluid p. Surface velocity across each drop surface is continuous, i.e. $[u_i]_S = 0$.

Following standard practice in indirect boundary integral formulations [36], the velocity field is represented in terms of a distribution of double-layer densities ϕ on the container surface and distributions of single-layer densities ψ on each of the droplets' surfaces, resulting in

$$u_i(x) = \int_{\Gamma_0} K_{ij}(x,y)\phi_j(y)\,\mathrm{d}\Gamma_y + \sum_{p=1}^{n}\int_{\Gamma_p} Q_{ij}(x,y)\psi_j(y)\,\mathrm{d}\Gamma_y, \tag{5}$$

where the kernels $\mathbf{K}$ and $\mathbf{Q}$ are defined as

$$K_{ij}(x,y) = -\frac{3}{4\pi}\frac{(x_i - y_i)(x_j - y_j)(x_k - y_k)}{r^5}n_k(y), \tag{6}$$

$$Q_{ij}(x,y) = \frac{1}{8\pi}\left(\frac{\delta_{ij}}{r} + \frac{(x_i - y_i)(x_j - y_j)}{r^3}\right). \tag{7}$$

The immediate consequence of this choice of representation is the continuity of the velocity field across the droplet—carrier fluid interface. The Stokes equations are satisfied by setting the pressure field as

$$P(x) = B\int_{\Gamma_0}\frac{1}{2\pi}\frac{\partial}{\partial x_j}\left(\frac{x_k - y_k}{r^3}\right)n_j(y)\phi_k(y)\,\mathrm{d}\Gamma_y + B\sum_{p=1}^{n}\int_{\Gamma_p} -\frac{1}{4\pi}\frac{\partial}{\partial x_k}\left(\frac{1}{r}\right)\psi_k(y)\,\mathrm{d}\Gamma_y, \tag{8}$$

where

$$B = \begin{cases} \mu & \text{for } x \in \Omega_0, \\ \lambda_p\mu & \text{for } x \in \Omega_p,\ p = 1, 2, \ldots, n. \end{cases}$$

It is also noted that each drop may be characterized by an individual viscosity, although for simplicity a common