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Optimal allocation of boundary singularities for stokes flows about pairs of particles

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ABSTRACT

Methods of allocation of singularities for the Method of Fundamental Solutions are proposed, implemented and applied to a Stokes flow about pairs of particles. New local normal and combined Stokeslets allocation methods are proposed to solve Stokes flows using a moderate number of singularities. In the proposed methods the singularities are located at surfaces inside the particles but dissimilar to the particles' shapes. Optimization of location of Stokeslets is performed for peanut-shaped and barrel-shaped particles. Convergence of numerical solution as a function of numbers of Stokeslets is evaluated and show substantial reduction in the needed number of Stokeslets compared to the prior methods in which Stokeslets are located at surfaces created similar to the particle shape. Using proposed methods of allocation of Stokeslets, patterns of pressure and velocity vector field near particles are obtained and discussed. The Stokes force exerted by a Stokes flow on the pair of particles is computed at different stages of their collective behavior including separate location of particles in proximity to each other, merging of particles, and re-orientation of cluster along the flow. These results help to determine the least stable location of particles' pair for the purpose of their separation off the flow.

1. Introduction

Present research is aimed at optimization of the Method of Fundamental Solutions (MFS) for a Stokes flow around pairs of particles of arbitrarily shape with variable local curvature radius. To obtain a Stokes flow solution using the minimum needed number of Stokeslets the singularities are located at surfaces inside the particles but dissimilar to the particles' shapes. The proposed approach substantially extends the recent studies of the optimal allocation of singularities (Stokeslets) for the Stokes flow about spherical particles [1–3], which used co-centered spherical surfaces for allocation of Stokeslets. The techniques described herein account for variable radius and convex-to-concave inflexion points of pairs of particles that have profound influence on the MFS convergence and sustainability.

A Stokes flow model describes fluid moving at low Reynolds numbers ($Re < 1$), so that convection terms in the governing Navier–Stokes equations are neglected. The condition $Re < 1$ corresponds to either slow motion, or small characteristic length, or large viscosity or combination of these factors. There are numerous practical applications of Stokes flows that require computing of flowfield such as micromechanical engineering (nano- and micro-filtration of multiphase mixtures, penetration of fluid drops in porous media and their hydrodynamic interactions), biomedical engineering (such as precise filtration of medicine, development of media capturing viruses, bacteria and cells, protein folding, and vascular and capillary blood flow) and aerospace engineering (for example, microchannel heat exchanger development), to name a few [4–10]. A distinct advantage of the MFS compared to the finite-element methods and finite-volume methods is that the MFS requires meshing only the boundary surface of computational domain as opposed to the entire 3-D domain. Therefore, the MFS is easily applicable to Stokes flows about particles and their pairs of an arbitrarily and changing shape.

Being one of the Boundary Element Methods (BEM) [4,11], the MFS (also known as the Boundary Singularity Method (BSM)) has demonstrated good accuracy using a moderate number of Stokeslets for the Stokes flows about spherical particles [1,2,6,12]. The authors of these cited papers obtained optimal allocations of singularities primarily for spherical particles. The problem with the MFS method is appearance of near-singular matrices with large condition numbers (the ratio of maximum-to-minimum eighenvalues) in cases when either the Stokeslets are located too close to observation points or the Stokeslets are located too close to each other [2]. Therefore Stokeslets can neither coincide with collocation points nor placed near the geometric center of spherical particle. The optimal radius of spherical surface at which

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Stokeslets are located has been determined in prior studies as a fraction of radius of spherical particle.

The prior MFS studies are focused on techniques to extend the MFS applicability, to reduce number of singularities required to achieve convergence and to avoid near-singular matrices. The developed approaches include the slender-body approach [7,8,13–16], the method of images [17–22], the method of regularized Stokeslets [23–26], and methods of allocation of Stokeslets outside of computational domain (also known as methods of submerged Stokeslets [1–3,5,12,27]). In the current study, the approach of submerged Stokeslets has been extended to particles with variable curvature radii associated with geometric properties of fused particles.

One of the techniques allocating the MFS singularities is based on the slender-body approach [8,13,14]. The necessary condition for validity of this approach is that one dimension (size of body) should be much larger than other dimensions ($\epsilon = l/b \le 0.005$), where l is a body length and b is the maximum characteristic length in other directions [15]. In frame of the slender body approach, Stokeslets are placed along the axis of the slender body. This method has been adopted for basic shapes including cylinders, helices, spheroids and other axisymmetric bodies (Clarke et al. [7], Cortez and Nicholas [16], Nitsche and Parthasarathi [25]), complex flagella swimming models, closed filaments and combined bodies (Johnson and Brokaw [15], Cortez and Nicholas [16]), flexible fibers and filaments (Tornberg and Shelley [8]), and various slender axisymmetric particles (Batchelor [13]), to name a few. The slender-body approach separates collocation points and singularities. However, this technique is limited to axisymmetric slender bodies and is not applicable to pairs of particles where the above slenderness condition is not satisfied.

To remove singularities associated with the close proximity of Stokeslets and collocation points, the Method of Regularized Stokeslets (MRS) is used for Stokes flow problems including flow about translating spheres (Cortez et al. [24]) and more complex shapes like cilia- and flagella-driven flows (Lobaton and Bayen [26] and Smith et al. [28]). The MRS has been introduced by Cortez et al. [24] and Cortez [29] and has been updated and improved by Lin [30] and Gonzalez [31]. The MRS is based on exact solution of Stokes equations for velocity in response to local force expressed by regularized delta functions. The MRS becomes another version of MFS specifically focused on elimination of singularities [11]. In frame of the MRS, the Green's function singularity has been removed [32] by distortion of the original Green's function (Stokeslet).

According to Zhao [3], the MRS with Stokeslets causes significant pressure oscillations in the obtained numerical solution, when the Stokeslets and collocation points are located at the same spherical surface. While the regularized Stokeslets remove oscillations of pressure near rigid surface, it still has significant error in pressure at the particle surface. This error is significant even for the value of regularization parameter corresponding to the minimum of error.

In the current study, the authors are focused on the method of submerged Stokeslets, which is anticipated to produce accurate Stokes flow solutions using a moderate number of Stokeslets. Besides, the approach does not create singular matrix even if two particles collide. Present paper proposes novel techniques of allocation of Stokeslets for particles of an arbitrarily shape forming as a result of merging of two or more particles. The goal is to achieve solution convergence using moderate number of Stokeslets for Stokes flows about generic shapes of pairs of particles. For liquid or gas droplets or solid particles, that are frozen liquid droplets, the spherical convex shape has the minimum surface for a given volume and nature always tries to minimize surface because of surface tension. While single particles typically have convex surface, the merged newly formed particles have combined convex and concave surfaces separated by inflexion points (see Figs. 5 and 7). The convex spherical part of surface is inherited from single spherical particles while the concave part of surface is formed where particles are merged. The proposed combined approach to allocation of Stokeslets accounts for intermittent convex and concave parts of surface of clusters or pair of particles.

In existing allocation methods, Stokeslets are placed at a submerged surface Γ_S similar in shape to the physical particle surface Γ but having smaller geometric scale (see Fig. 1). There are two Stokeslet allocation techniques widely used in frame of the method of submerged Stokeslets, namely, similar shape uniform (Fig. 1b) and non-uniform (Fig. 1a) methods (Zhao and Povitsky [1–3], Young, Tsai [27,33], and Aboelkassem and Staples [5]).

In frame of the uniform allocation scheme the surface Γ_S is divided to elementary surface cells of equal area and Stokeslets are placed at the centers of these cells. A non-uniform Stokeslet allocation scheme assumes equal number of Stokeslets at each lateral cross-section, which leads to more dense concentration of Stokeslets in the cross-sections with a smaller radius such as necks and poles (Figs. 1a and 5).

Young et al. [34,35 and 36] applied the MFS to 2-D and 3-D Stokes flows about spheres and inside cavities of various shapes. Their numerical experiments revealed a range of distances between Stokeslets and collocation points that produced acceptable convergence. Thus, for the Stokes flow about sphere they chose the normalized Stokeslets allocation depth of $D \approx 0.167$ under the spherical surface of the unity radius. The number of Stokeslets varied from 20 to 40 Stokeslets for the flow in circular cavity to more than 266 Stokeslets for the flow about complex shapes. Kolodziej and Klekiel [37] used the MFS to obtain parameters of Stokes flows through ducts of an arbitrarily cross-section. For the duct with square cross-section, they placed Stokeslets outside of flow domain at a distance of 10% of the square length.

Many studies adopt the uniform Stokeslet allocation method including Zhao and Povitsky [1–3] for Stokes flows about sets of spheres, Young et al. [33,38–41] for the lid driven cavity flow, Aboelkassem and Staples [8] for Stokes flow in curved duct and Young et al. [27] for Stokes flow inside the free-form cavities and about spherical particles. Zhao and Povitsky [1–3] applied uniform Stokeslet distribution scheme for the Stokes flow past a sphere and about ensembles of spherical particles for no-slip and partial-slip boundary conditions. They have determined that the optimal Stokeslet allocation is at spherical surface Γ_S with its normalized radius $\overline{a} = 0.7$ that corresponds to the Stokeslets' allocation depth $D = 0.3$ (Fig. 1). This submergence depth has been used for both uniform and non-uniform Stokeslet allocation schemes.

Apart of solutions of Stokes flow problems, allocations of boundary singularities are discussed by Goldberg and Cheng [42] and applied to heat transfer problem inside two merging spheres. They placed singularities over an imaginary sphere of a greater radius than the boundary surface. Tsai and Young [12] applied non-uniform Stokeslet allocation scheme to a peanut-shaped model solving 3-D Helmholtz problems.

Tsai et al. [43] used the non-uniform Stokeslet allocation scheme to place Stokeslets (referred to as source points) to solve an unsteady problem of motion of peanut-shaped particle in a viscous media. They used a combined temporal-spatial discretization scheme, i.e. they placed source points at the same spatial locations as collocation points but at different time levels that allows for the non-zero distance between Stokeslets and collocation points.

The MFS solution is formed by superposing the fundamental solutions to the Stokes equations. The strength of the singularities is then obtained by solving a system of linear equations formed by