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A fast integral equation method for solid particles in viscous flow using quadrature by expansion

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ABSTRACT

Boundary integral methods are advantageous when simulating viscous flow around rigid particles, due to the reduction in number of unknowns and straightforward handling of the geometry. In this work we present a fast and accurate framework for simulating spheroids in periodic Stokes flow, which is based on the completed double layer boundary integral formulation. The framework implements a new method known as quadrature by expansion (QBX), which uses surrogate local expansions of the layer potential to evaluate it to very high accuracy both on and off the particle surfaces. This quadrature method is accelerated through a newly developed precomputation scheme. The long range interactions are computed using the spectral Ewald (SE) fast summation method, which after integration with QBX allows the resulting system to be solved in *M* log *M* time, where *M* is the number of particles. This framework is suitable for simulations of large particle systems, and can be used for studying e.g. porous media models.

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1. Introduction

Fluid flows involving microscopic, rigid particles are common both in nature and in industrial processes. The macroscopic properties of such systems are often determined by the particle interactions happening on the smallest scale of the flow. Examples of such systems can be found in sedimenting suspensions [17] and porous media modeling [13]. To fully understand the interactions between particles, and the effect those interactions have on the fluid flow, numerical simulation is a valuable tool. Stokes equations are often valid in this context, due to the small particle size and low fluid velocity. For problems governed by Stokes equations it is possible to use boundary integral methods, where the solution is represented as a layer potential from the boundaries of the domain (in this case the particle surfaces). Since the problem then is formulated as a boundary integral equation (BIE) on the union of the particle surfaces, the dimension of the domain which has to be discretized is reduced from \mathbb{R}^3 to \mathbb{R}^2 , significantly reducing the number of unknowns. This also removes the problem of combining a volume grid with moving boundaries, which can be challenging. However, boundary integral methods come with a set of challenges of their own, two of which can be considered major.

The first major challenge of boundary integral methods is that the resulting linear system after e.g. a Nyström discretization is dense, such that the cost of one left hand side evaluation is $O(N^2)$, where N is the number of unknowns. This

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puts a severe limit on the size of the systems that can be considered, even if a rapidly converging interative method is used. This can be overcome by evaluating the layer potential using a fast method, such as the fast multipole method (FMM) [16] or a fast Ewald summation method [14,24] (for periodic problems). These methods reduce the cost of one left hand side evaluation to $\mathcal{O}(N)$ and $\mathcal{O}(N \log N)$, respectively, thereby making boundary integral methods suitable for large-scale computations.

The second major challenge of boundary integral methods is that one needs accurate quadrature of singular and nearly singular integrals when evaluating the layer potential. Developing such methods which are accurate, fast and work for arbitrary geometries is a topic of current research, particularly for the problem of nearly singular quadrature in three dimensions. In two dimensions there are efficient methods for nearly singular quadrature which gain a lot of their power from the complex variable formulation [18,6]. In three dimensions the situation appears less resolved, though several different methods have been successfully used in practical applications [9,10,37,29,34,38]. A common feature of many of these methods is however that they are highly target specific, meaning that the cost grows rapidly if there are many nearly singular integrals to be evaluated.

Quadrature by expansion (QBX) [20,7] is a fairly new method for numerical integration of singular and nearly singular integrals. The method is built around evaluating layer potentials through local expansions, and comes equipped with a solid convergence theory [15]. It was originally presented for the Helmholtz kernel in two dimensions, but the principles of the method generalize directly both to three dimensions and other kernels. A promising feature of QBX is that it is possible to combine it with an FMM, thereby creating a fully O(N) method that is able to accurately evaluate the potential everywhere.

In this paper we extend the QBX framework to deal with the Stokes double layer potential in three dimensions, and combine it with the fast Ewald summation method presented in [2]. The result is a robust and scalable framework for computing Stokes flow around periodic systems of rigid, spheroidal particles. To limit the scope of the present paper, we restrict our attention to stationary particles. The method could easily be extended to dynamic problems – such as sedimentation – by coupling it to an ODE solver, as was done in [2].

The structure of this paper is as follows: In section 2 we state the necessary boundary integral formulation for Stokes flow around rigid particles. In section 3 we introduce QBX and discuss errors and parameter selection. In section 4 we show how QBX can be accelerated for our problem, leading to a computationally feasible method. In section 5 we briefly touch on the subject of Ewald summation, and how to combine it with QBX. Finally, in section 6 we present selected numerical results, which we draw both from validation tests and from an example application. We also include an appendix (Appendix A), which covers the computational details of the acceleration scheme presented in section 4.

2. Formulation

Our application of interest is that of rigid particles in a Newtonian fluid. The particles are assumed small enough that the Reynolds number is close to zero, such that we can model the flow as being Stokes flow, governed by the Stokes equations,

$$-\nabla P + \mu \Delta \boldsymbol{u} + \boldsymbol{f} = \boldsymbol{0},$$

$$\nabla \cdot \boldsymbol{u} = \boldsymbol{0}$$
(1)

We here limit ourselves to spheroidal particles with semi-axes *a* and *c*, and assume $\mu = 1$. The surface of such a particle, oriented along the *z* coordinate axis, can in Cartesian coordinates be described as

$$\frac{x^2 + y^2}{a^2} + \frac{z^2}{c^2} = 1.$$
(2)

If parametrized in the spherical coordinates $\theta \in [0, \pi]$ and $\varphi \in [0, 2\pi)$, the same surface is given by

$$x = a \sin(\theta) \cos(\varphi),$$

$$y = a \sin(\theta) \sin(\varphi),$$

$$z = c \cos(\theta).$$

(3)

The particles can be classified into three distinct subgroups: prolate (a < c), spherical (a = c), and oblate (a > c).

2.1. Boundary integral formulation

We are considering Stokes flow as described by the Stokes equations (1), which by virtue of being a set of linear partial differential equations with constant coefficients have solutions that can be represented using boundary integrals. For these representations, the essential Green's functions are the stokeslet *S*, the stresslet *T* and the rotlet R.¹

¹ Throughout this paper we use the Einstein convention that an index appearing twice in an expression implies a summation over the set {1, 2, 3}, except for when there is a \sum explicitly defining the index.

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