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Boundary integral equation analysis for suspension of spheres in Stokes flow

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ABSTRACT

We show that the standard boundary integral operators, defined on the unit sphere, for the Stokes equations diagonalize on a specific set of vector spherical harmonics and provide formulas for their spectra. We also derive analytical expressions for evaluating the operators away from the boundary. When two particle are located close to each other, we use a truncated series expansion to compute the hydrodynamic interaction. On the other hand, we use the standard spectrally accurate quadrature scheme to evaluate smooth integrals on the far-field, and accelerate the resulting discrete sums using the fast multipole method (FMM). We employ this discretization scheme to analyze several boundary integral formulations of interest including those arising in porous media flow, active matter and magneto-hydrodynamics of rigid particles. We provide numerical results verifying the accuracy and scaling of their evaluation.

1. Introduction

Suspension of spherical particles in Stokes flow acts as a mimetic model for several natural and engineering systems. Often, the physical phenomena of interest happen at scales much larger than the constituent particle sizes e.g., collective motion in bacterial suspensions [10], bulk rheology of polydisperse colloidal suspensions, pattern formations in electro- and magneto-rheological fluids [22] and self-assembly of particles [27]. Consequently, direct simulation methods that scale to large number of particles and that are numerically stable for long-time simulations are crucial to enable insights into these systems.

Several techniques have been developed in the past few decades for simulating the hydrodynamics of multiple spherical particles including the Stokesian dynamics approach (e.g., [4,11,47]), multipole methods (e.g., [8,37]), fictitious domain methods (e.g., [33]) and boundary integral methods (e.g., [1,9,34]). We refer the reader to [29] for a recent review on the broader topic of simulation methods for particulate flows. The present work combines features from both the multipole methods (spectral representations) and the boundary integral methods (second-kind formulations, fast algorithms) to arrive at a fast, spectrally accurate numerical method.

Our work is closely related to three recent efforts, that of Veerapaneni et al. [41], Vico et al. [43] and Singh et al. [38] (listed in chronological order). In [41], using the antenna theorems of [37], the spectrum of the "single-layer" Stokes boundary integral operator (BIO) was derived and applied to analyze certain integro-differential operators on the sphere; here, we extend this framework to all the other relevant BIOs. In [43], authors derived signatures of the BIOs that arise when solving

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Helmholtz or Maxwell equations in the frequency domain. The present work can be viewed as an extension of [43] to the Stokes equations. In [38], a Galerkin approach for evaluating Stokes BIOs on spheres was developed. The main difference from the present work is the choice of the basis functions: while *tensorial spherical harmonics* were used in [38], we chose a specific set of *vector spherical harmonics*. We show that this choice leads to much simpler formulas and diagonalization of most of the BIOs. Another important distinction is that the N-body hydrodynamic interactions of the particles were computing directly in [38], leading to a quadratic complexity in N whereas our method is linear in N via the use of Nyström's method for evaluating the smooth far-field integrals, accelerated by the fast multipole method (FMM) [16,18,39].

Synopsis. We consider several BIOs that arise when solving the Stokes equations and compute their signatures analytically on the unit sphere. This enables us to convert the classical task of *weakly-singular* integral evaluation to simple formula evaluation. We also present formulas for evaluating the operators at arbitrary target locations away from the sphere. Thereby, the issue of accurate evaluation of *nearly-singular* integrals also reduces to simple analytic expression evaluation. We then demonstrate the solution procedure for various physical problems using the standard integral equation formulations proposed in the literature.

The paper is organized as follows. In §2, we introduce the basis functions for representing scalar and vector fields on the sphere and the definitions of the boundary integral operators. In §3, we derive the signatures of these operators and the analytical formulas for evaluating the velocity and pressure away from a unit sphere given a certain form of the jump conditions. We use these formulas in §4 to develop a fast, spectrally accurate singular and nearly-singular integral evaluation scheme. Finally, in §5, we discuss the standard model problems in creeping flow of spherical particle suspensions, their reformulation as boundary integral equations and perform a series of numerical experiments to validate our solvers.

2. Mathematical preliminaries

In this section, we provide a summary of the spherical harmonic basis functions, which will be used to represent scalar and vector fields defined on the sphere, and also provide definitions for the classical boundary integral operators that arise when solving the Laplace and Stokes equations. The concepts discussed here are fairly standard e.g., see [21,32,35,42].

2.1. Spherical harmonic bases

Scalar spherical harmonics

Definition 2.1. Let θ and ϕ be the polar and azimuthal angles in the standard parametrization of the unit sphere. The scalar spherical harmonic Y_n^m of degree n and order m (for $|m| \le n$) is defined in terms of the associated Legendre functions P_n^m by

$$Y_n^m(\theta,\phi) = \sqrt{\frac{2n+1}{4\pi}}\sqrt{\frac{(n-|m|)!}{(n+|m|)!}}\, P_n^{|m|}(\cos\theta)\, e^{im\phi}. \tag{2.1}$$

Scalar spherical harmonics form an orthonormal basis of eigenfunctions of the Laplacian for square-integrable functions on the unit sphere. That is, any function $\sigma \in L^2(\mathbb{S}^2)$ has the expansion:

$$\sigma(\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \widehat{\sigma}_n^m\, Y_n^m(\theta,\phi), \quad \theta \in [0,\pi], \quad \phi \in [0,2\pi], \tag{2.2}$$

$$\text{where} \quad \widehat{\sigma}_n^m = \int_0^{2\pi}\int_0^{\pi} \sigma(\theta,\phi)\overline{Y_n^m(\theta,\phi)}\, \sin\theta\, d\theta d\phi. \tag{2.3}$$

For $\sigma \in C^\infty(\mathbb{S}^2)$, the finite-term approximation (truncating the outer sum to $n = 0 \ldots p$ in Eq. (2.2), which yields $(p+1)^2$ terms) is spectrally convergent with p [32]. One can use fast transforms for both the longitude (Fast Fourier Transform or FFT) and the latitude (Fast Legendre Transform or FLT) to implement a fast forward spherical harmonic transform that computes the coefficients for the approximation of order p in $\mathcal{O}(p^2 \log^2 p)$ operations. The inverse transform can be obtained in a similar fashion [30]. However, note that the break-even point for existing FLTs is large and typically, only the FFTs will be employed with a complexity of $\mathcal{O}(p^3 \log p)$ for forward and inverse transforms.

Vector spherical harmonics

Vector spherical harmonics are an extension of the scalar spherical harmonics to square-integrable vector fields on the sphere. They can in fact be defined in terms of scalar spherical harmonics and their derivatives.