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A Treecode Algorithm for 3D Stokeslets and Stresslets

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Abstract. The Stokeslet and stresslet kernels are commonly used in boundary element simulations and singularity methods for slow viscous flow. Evaluating the velocity induced by a collection of Stokeslets and stresslets by direct summation requires $\mathcal{O}(N^2)$ operations, where N is the system size. The present work develops a treecode algorithm for 3D Stokeslets and stresslets that reduces the cost to $\mathcal{O}(N\log N)$. The particles are divided into a hierarchy of clusters and well-separated particle-cluster interactions are computed by a far-field Cartesian Taylor approximation. The terms in the approximation are contracted to promote efficient computation. Serial and parallel results display the performance of the treecode for several test cases. In particular the method has relatively simple structure and low memory usage and this enhances parallel efficiency for large systems.

AMS subject classifications: 65D99, 76D07

Key words: Stokeslet, stresslet, fast summation, treecode, Taylor approximation.

1 Introduction

The slow steady flow of an incompressible viscous fluid is governed by the Stokes equations,

$$\nabla^2\mathbf{u}-\nabla p=0, \tag{1.1a}$$

$$\nabla\cdot\mathbf{u}=0, \tag{1.1b}$$

where $\mathbf{u}$ is the fluid velocity, p is the pressure and the viscosity is taken to be unity. Many applications in fluid dynamics are modeled as particle interactions in Stokes flow,

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including for example particle-laden fluid jets [28], vibrations in microfluidic crystals [5], cilia- and flagella-driven flows [11,33], free-surface flows of liquid drops [27] and vesicle flows [36], among others. The Stokeslet and stresslet kernels are fundamental solutions of the Stokes equations given in 3D (up to a numerical prefactor) by

$$S_{ij}(\mathbf{x},\mathbf{y}) = \frac{\delta_{ij}}{|\mathbf{x}-\mathbf{y}|} + \frac{(x_i-y_i)(x_j-y_j)}{|\mathbf{x}-\mathbf{y}|^3}, \tag{1.2a}$$

$$T_{ijl}(\mathbf{x},\mathbf{y}) = \frac{(x_i-y_i)(x_j-y_j)(x_l-y_l)}{|\mathbf{x}-\mathbf{y}|^5}, \tag{1.2b}$$

where δ_{ij} is the Kronecker delta, $\mathbf{x}=(x_1,x_2,x_3)$, $\mathbf{y}=(y_1,y_2,y_3)$ and indices $i,j,l=1:3$ represent Cartesian coordinates. The Stokeslet and stresslet kernels are commonly used in boundary element simulations and singularity methods for slow viscous flow [29].

The ith component of the velocity induced by a set of Stokeslets and stresslets is

$$u_i(\mathbf{x}^m) = \sum_{\substack{n=1\\ n\neq m}}^{N} S_{ij}(\mathbf{x}^m,\mathbf{x}^n) f_j^n + \sum_{\substack{n=1\\ n\neq m}}^{N} T_{ijl}(\mathbf{x}^m,\mathbf{x}^n) h_j^n \nu_l^n, \quad i=1,2,3, \tag{1.3}$$

where $\mathbf{x}^m$ is a target particle, $\mathbf{x}^n$ is a source particle, f_j^n is a force weight, h_j^n is a dipole weight and ν_l^n are the components of a unit normal vector to a surface. Note that the Stokeslet term has an implicit sum over $j=1:3$ and the stresslet term has an implicit sum over $j,l=1:3$; for clarity in some places below these sums will be written out explicitly. Eq. (1.3) is written for the case in which the targets and sources coincide, but it is straightforward to handle problems where they are disjoint.

Evaluating the velocity (1.3) for $m=1:N$ by direct summation requires $\mathcal{O}(N^2)$ operations, which is prohibitively expensive when N is large. The same issue arises for interacting point masses, point charges and point vortices and many fast summation methods have been developed to reduce the cost, including particle-mesh methods [13, 20], the Fast Multipole Method (FMM) [19] and treecodes [4]. These methods reduce the operation count to $\mathcal{O}(N\log N)$ or $\mathcal{O}(N)$ in principle, while introducing approximations. The FMM and treecode use multipole expansions of particle clusters (near-field and far-field for the FMM, but only far-field for the treecode), while particle-mesh methods interpolate the particle strengths to a grid where often the fast Fourier transform (FFT) is used to compute the sum.

A number of these fast summation methods have been developed in the context of Stokes flow including a particle-mesh Ewald technique [31, 32] and a pre-corrected FFT method [38]. Several extensions of the FMM have also been developed for Stokes flow [7, 17, 24, 37, 39]. In one implementation [35], the Stokeslet and stresslet sums are decomposed into several terms which are computed by the FMM for Coulomb interactions [15]. The kernel-independent FMM [25, 26, 39] has been applied to simulate swimming microorganisms [30] using regularized Stokeslets [8,9]. Recently the Spectral Ewald (SE) method was developed for Stokes flow using Gaussian spreading functions [1, 2].