Ewald summation for the rotlet singularity of Stokes flow

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Abstract

Ewald summation is an efficient method for computing the periodic sums that appear when considering the Green's functions of Stokes flow together with periodic boundary conditions. We show how Ewald summation, and accompanying truncation error estimates, can be easily derived for the rotlet, by considering it as a superposition of electrostatic force calculations.

1 Introduction

The fundamental free-space singularities of Stokes flow are (see e.g. [9]) the stokeslet S, the stresslet T and the rotlet Ω. They are defined (up to a constant) as

$$S_{jl}(\boldsymbol{r}) = \frac{\delta_{jl}}{r} + \frac{r_j r_l}{r^3}, \tag{1}$$

$$T_{jlm}(\boldsymbol{r}) = \frac{r_j r_l r_m}{r^5}, \tag{2}$$

$$\Omega_{jl}(\boldsymbol{r}) = \epsilon_{jlm}\frac{r_m}{r^3}. \tag{3}$$

These singularities are central when solving Stokes' equation using boundary integral methods [9]. In the context of flow simulations it is common to use periodic boundary conditions [1], in which case periodic sums of the above singularities must be considered. Due to the relatively slow decay of the singularities with respect to distance, some kind of special method is required for this. A well-established alternative is that of Ewald summation, which has its roots in electrostatic lattice calculations. It was derived by P.P. Ewald [3], and has as its central idea to split the kernel of the summation into one short-range component and one long-range component (for an introduction see e.g. [2]). To use Ewald summation for a given kernel function, one must first derive an Ewald decomposition of it. Such decompositions are available in the literature for the stokeslet [5, 10] and the stresslet [4]. For the rotlet, a decomposition can be found in [8].

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We will here show how a decomposition for the rotlet, which in the end is identical to that in [8], can be derived by drawing a parallel to Ewald summation for the electrostatic force potential. Not only does this parallel give us a shortcut for deriving the decomposition, it also allows us to derive truncation error estimates by using results which are well-known in the context of electrostatics.

2 Rotlet sum in free space

We consider the rotlet defined as

$$\Omega_{jl}(\boldsymbol{r}) = \epsilon_{jlm}\frac{r_m}{r^3}. \tag{4}$$

For a set of N point sources $\boldsymbol{f}^n$ at locations $\boldsymbol{x}^n \in \mathbb{R}^3$, the corresponding velocity field (which we will also refer to as the rotlet potential) at a target point $\boldsymbol{x}$ is

$$u_j(\boldsymbol{x}) = \sum_{n=1}^{N} \Omega_{jl}(\boldsymbol{x} - \boldsymbol{x}^n) f_l^n \tag{5}$$

$$= \sum_{n=1}^{N} \epsilon_{jlm}\frac{x_m - x_m^n}{|\boldsymbol{x} - \boldsymbol{x}^n|^3} f_l^n. \tag{6}$$

Recognizing that the kernel $\boldsymbol{r}/r^3$ is also used for electrostatic force calculations [6], we choose to write this is as

$$u_j(\boldsymbol{x}) = \epsilon_{jlm}\left(\sum_{n=1}^{N}\frac{\boldsymbol{x} - \boldsymbol{x}^n}{|\boldsymbol{x} - \boldsymbol{x}^n|^3} f_l^n\right)_m. \tag{7}$$

Defining

$$\boldsymbol{F}_l(\boldsymbol{x}) = \sum_{n=1}^{N}\frac{\boldsymbol{x} - \boldsymbol{x}^n}{|\boldsymbol{x} - \boldsymbol{x}^n|^3} f_l^n, \tag{8}$$

we can write the potential as

$$u_j(\boldsymbol{x}) = \epsilon_{jlm} F_{lm}(\boldsymbol{x}), \tag{9}$$

where $F_{lm} = (\boldsymbol{F}_l)_m$. This means that we can use any method available for electrostatic force computations to compute $\boldsymbol{F}_1$–$\boldsymbol{F}_3$ at all target points, and then combine them as in (9) to get $\boldsymbol{u}$.

3 Ewald summation for the rotlet

We now consider the case where we have N source points contained in the box $L_1 \times L_2 \times L_3$, which we will refer to as the primary cell. The periodic potential is then defined as the potential from all source points in all periodic replications of the primary cell,

$$u_j(\boldsymbol{x}) = \sum_{\boldsymbol{p}\in\mathbb{Z}} \sum_{n=1}^{N} \Omega_{jl}(\boldsymbol{x} + \boldsymbol{\tau}(\boldsymbol{p}) - \boldsymbol{x}^n) f_l^n, \tag{10}$$

where $\boldsymbol{\tau}(\boldsymbol{p}) = (L_1 p_1, L_2 p_2, L_3 p_3)$ represents a periodic shift. The slow decay of Ω makes this sum only conditionally convergent, which is why it is instead computed using Ewald summation. For the electrostatic potential, the Ewald summation for the periodic sum is [2]

$$\begin{aligned}\sum_{\boldsymbol{p}\in\mathbb{Z}} \sum_{n=1}^{N} \frac{\boldsymbol{x} + \boldsymbol{\tau}(\boldsymbol{p}) - \boldsymbol{x}^n}{|\boldsymbol{x} + \boldsymbol{\tau}(\boldsymbol{p}) - \boldsymbol{x}^n|^3} q^n = &\sum_{\boldsymbol{p}\in\mathbb{Z}} \sum_{n=1}^{N} G^R(\boldsymbol{x} + \boldsymbol{\tau}(\boldsymbol{p}) - \boldsymbol{x}^n) q^n \\ &+ \frac{4\pi i}{V} \sum_{\boldsymbol{k}\neq 0} \frac{k_m}{k^2} e^{-k^2/4\xi^2} \sum_{n=1}^{N} q^n e^{-i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}_n)},\end{aligned} \tag{11}$$

where

$$G^R(\boldsymbol{r}, \xi) = \frac{\boldsymbol{r}}{r^3} \left(\operatorname{erfc}(\xi r) + \frac{2\xi r}{\sqrt{\pi}} e^{-\xi^2 r^2} \right). \tag{12}$$

Here $V = L_1 L_2 L_3$ is the volume of the primary cell, and $k_i \in \{2\pi n/L_i : n \in \mathbb{Z}\}$ are the Fourier space vectors. The first sum is called the real space sum; it contains the short-range behavior of the kernel and converges rapidly in real space. The second sum is called the Fourier space sum; it contains the long-range behavior of the kernel and converges rapidly in Fourier space, due to its smoothness. The Ewald parameter ξ controls how short-range and smooth the two components are.

For the periodic rotlet potential (10), we can make a similar decomposition,

$$u_j(\boldsymbol{x}) = u_j^R(\boldsymbol{x}) + u_j^F(\boldsymbol{x}), \tag{13}$$

where u^R is the real space sum and u^F is the Fourier space sum,

$$u_j^R(\boldsymbol{x}) = \sum_{\boldsymbol{p}\in\mathbb{Z}} \sum_{n=1}^{N} \Omega_{jl}^R(\boldsymbol{x} + \boldsymbol{\tau}(\boldsymbol{p}) - \boldsymbol{x}^n, \xi) f_l^n, \tag{14}$$

$$u_j^F(\boldsymbol{x}) = \frac{1}{V} \sum_{\boldsymbol{k}\neq 0} \widehat{\Omega}_{jl}^F(\boldsymbol{k}, \xi) \sum_{n=1}^{N} f_l^n e^{-i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}_n)}. \tag{15}$$

Using (8) and (9), we can identify the real and Fourier space kernels from the Ewald decomposition of the electrostatic force (11)–(12), which gives us

$$\Omega_{jl}^R(\boldsymbol{r}, \xi) = \epsilon_{jlm} \frac{r_m}{r^3} \left(\operatorname{erfc}(\xi r) + \frac{2\xi r}{\sqrt{\pi}} e^{-\xi^2 r^2} \right), \tag{16}$$

$$\widehat{\Omega}_{jl}^F(\boldsymbol{k}, \xi) = \epsilon_{jlm} 4\pi i \frac{k_m}{k^2} e^{-k^2/4\xi^2}. \tag{17}$$

3.1 Zero wave number term

The term corresponding to $\boldsymbol{k} = 0$ is omitted from the Fourier space sum (15), as $\widehat{\Omega}^F$ is singular at the origin. The term corresponds to a constant "ground level" throughout the domain, and whether or not a correction for this is required depends on the physics of the problem. For the electrostatic potential no correction is required, which relates to the basic assumption of charge neutrality [2]. In Stokes flow, a reasonable requirement is that the periodic flow should have a zero mean. Denoting by D_j the face of the primary cell in the x_j-direction (lying in the plane $x_j = 0$), the zero mean flow requirement can be stated as

$$\langle u_j \rangle := \frac{1}{A_j} \int_{D_j} u_j(\boldsymbol{x}) \mathrm{d}S(\boldsymbol{x}) = 0, \tag{18}$$

where $A_j = \int_{D_j} \mathrm{d}S(\boldsymbol{x})$. For the stokeslet potential the $\boldsymbol{k} = 0$ term is zero, and it is shown in [10] that this is due to a balancing pressure gradient in the direction of the point forces. For the stresslet potential the periodic sum does generate a mean flow, and a correction term was derived in [1] for the case when the sum represents an integral over the surface of a rigid body.

To derive a result for the rotlet, we will now repeat the steps of the derivation in [1]. To that end, we will consider the periodic potential from a point source of strength $\boldsymbol{f}$ located at $\boldsymbol{x}_s$. The Fourier transform of the periodic sum (10) is then

$$u_j(\boldsymbol{x}) = \frac{4\pi i}{V} \sum_{\boldsymbol{k} \neq 0} \frac{k_m}{k^2} f_l e^{-i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}_s)} + \widehat{\Omega}^0_{jl} f_l, \tag{19}$$

(this can be by seen by considering the limit $\xi \to \infty$ of the Ewald sum). Here $\widehat{\Omega}^0$ is a correction for the $\boldsymbol{k} = 0$ term omitted in the sum. Inserting (19) into (18) and assuming no implicit summation over j in the following derivation, we get the requirement

$$\epsilon_{jlm} \frac{4\pi i}{V} \sum_{\boldsymbol{k} \neq 0} \frac{k_m}{k^2} f_l \int_{D_j} e^{-i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}_s)} \mathrm{d}S(\boldsymbol{x}) + A_j \widehat{\Omega}^0_{jl} f_l = 0. \tag{20}$$

The surface D_j covers exactly one period in the directions perpendicular to x_j. Hence, the integral is nonzero only if $k_i = 0$ for $i \neq j$, such that

$$\sum_{\boldsymbol{k} \neq 0} \frac{k_m}{k^2} \int_{D_j} e^{-i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}_s)} \mathrm{d}S(\boldsymbol{x}) = \delta_{mj} \sum_{k_j \neq 0} \frac{k_j}{k_j^2} A_j e^{-k_j (\boldsymbol{x}_s)_j}. \tag{21}$$

Inserting this into (20), we get that the correction term is zero,

$$\widehat{\Omega}^0_{jl} = -\epsilon_{jlj} \frac{4\pi i}{V} \sum_{k_j \neq 0} \frac{k_j}{k_j^2} A_j e^{-k_j (\boldsymbol{x}_s)_j} = 0, \tag{22}$$

since $\epsilon_{ijk} = 0$ if $i = k$. This means that the periodic rotlet sum produces zero mean flow, and no correction term is needed in the Ewald summation.

3.2 Self interaction

When the target point $\boldsymbol{x}$ in the periodic sum (10) is one of the source points, i.e. $\boldsymbol{x} = \boldsymbol{x}^i$ for some $i \in [0, N]$, then the term corresponding to $\boldsymbol{p} = 0$ and $n = i$ should be deleted from the summation, as it is singular. This is commonly referred to as removing the self interaction of the point.

When computing the periodic sum using Ewald summation, the part of the self interaction that ends up in the real space sum is easy to remove, by simply omitting the corresponding term in the summation. Part of the self interaction may however end up in the Fourier space sum, in which case a correction term must be added (this is the case for the electrostatic and stokeslet potentials [2, 7]).

In the case of the rotlet, the self interaction correction turns out to be zero. One way of seeing this is by considering the limit

$$\lim_{\boldsymbol{r}\to 0} \left(\Omega(\boldsymbol{r}) - \Omega^R(\boldsymbol{r})\right) = 0, \tag{23}$$

which can be shown by a series expansion of $\widehat{\Omega}^R$ around $\boldsymbol{r} = 0$. This means that all of the self interaction is contained in the real space component, such that no correction has to be added. Another way of seeing this is to consider the Fourier space sum for the case of $N = 1$,

$$u_j^F(\boldsymbol{x}^1) = \frac{1}{V} \sum_{\boldsymbol{k}\neq 0} \widehat{\Omega}_{jl}^F(\boldsymbol{k}, \xi) f_l = 0, \tag{24}$$

since $\widehat{\Omega}^F$ is odd in $\boldsymbol{k}$. This in turn implies (23).

3.3 Final form

Since no correction terms have to be added for self interaction or $\boldsymbol{k} = 0$, the final form for the rotlet Ewald sum is as already stated,

$$\begin{aligned}&\sum_{\boldsymbol{p}\in\mathbb{Z}} \sum_{n=1}^{N} \Omega_{jl}(\boldsymbol{x} + \boldsymbol{\tau}(\boldsymbol{p}) - \boldsymbol{x}^n) f_l^n = \\ &\sum_{\boldsymbol{p}\in\mathbb{Z}} \sum_{n=1}^{N} \Omega_{jl}^R(\boldsymbol{x} + \boldsymbol{\tau}(\boldsymbol{p}) - \boldsymbol{x}^n, \xi) f_l^n + \frac{1}{V} \sum_{\boldsymbol{k}\neq 0} \widehat{\Omega}_{jl}^F(\boldsymbol{k}, \xi) \sum_{n=1}^{N} f_l^n e^{-i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}_n)},\end{aligned} \tag{25}$$

where

$$\Omega_{jl}^R(\boldsymbol{r}, \xi) = \epsilon_{jlm} \frac{r_m}{r^3} \left(\operatorname{erfc}(\xi r) + \frac{2\xi r}{\sqrt{\pi}} e^{-\xi^2 r^2} \right), \tag{26}$$

$$\widehat{\Omega}_{jl}^F(\boldsymbol{k}, \xi) = \epsilon_{jlm} 4\pi i \frac{k_m}{k^2} e^{-k^2/4\xi^2}. \tag{27}$$

4 Truncation errors

When computing the Ewald sum (25) in practice, the real and Fourier space sums must be truncated at some truncation radius r_c and maximum wave number K, such that

$$|\boldsymbol{x} + \boldsymbol{\tau}(\boldsymbol{p}) - \boldsymbol{x}^n| \leq r_c \quad \text{and} \quad k \leq K. \tag{28}$$

Estimates for the error committed when truncating the rotlet Ewald sum can be derived from existing error estimates for the Ewald sum of the electrostatic force (11). Let $\Delta \boldsymbol{F}_l(\boldsymbol{x})$ be the error in a component $\boldsymbol{F}_l(\boldsymbol{x})$ (8) when computing it using some numerical method (e.g. truncated Ewald summation). The root mean square (RMS) error in $\boldsymbol{F}_l$ can then be defined as

$$\delta \boldsymbol{F}_l^2 = \frac{1}{N} \sum_{n=1}^{N} |\Delta \boldsymbol{F}_l(\boldsymbol{x}^n)|^2. \tag{29}$$

This error can be approximated as

$$\delta \boldsymbol{F}_l^2 \approx Q_l E, \tag{30}$$

where E depends on the method and

$$Q_l = \sum_{n=1}^{N} (f_l^n)^2. \tag{31}$$

Based on (9), we now define

$$\delta \boldsymbol{u}^2 = \frac{1}{N} \sum_{n=1}^{N} \sum_{j,l,m=1}^{3} (\epsilon_{jlm} \Delta F_{lm}(\boldsymbol{x}^n))^2. \tag{32}$$

Assuming the error to be equally distributed in all coordinate directions, we replace ϵ_{jlm}^2 by its average

$$\overline{\epsilon_{jlm}^2} = \frac{1}{27} \sum_{j=1}^{3} \sum_{l=1}^{3} \sum_{m=1}^{3} \epsilon_{jlm}^2 = \frac{2}{9}, \tag{33}$$

such that, combining (29), (32) and (33),

$$\delta \boldsymbol{u}^2 \approx \frac{2}{9} \sum_{j,l=1}^{3} \delta \boldsymbol{F}_l^2 \approx \frac{2}{3} \sum_{l=1}^{3} Q_l E = \frac{2}{3} Q E, \tag{34}$$

where

$$Q = \sum_{l=1}^{3} Q_l = \sum_{n=1}^{N} |\boldsymbol{f}^n|^2. \tag{35}$$

In the case of Ewald summation, a classic result by Kolafa & Perram [6] gives a very accurate RMS error estimate for the electrostatic force potential, under the assumption of randomly distributed sources and a Gaussian error distribution. The resulting estimates for the real and Fourier space truncation errors are

$$E^R = \frac{4}{V r_c} e^{-2\xi^2 r_c^2}, \tag{36}$$

$$E^F = \frac{4\xi^2}{\pi V K} e^{-K^2/2\xi^2}. \tag{37}$$

Together with (34), this gives us the error estimate for rotlet Ewald sum:

$$\delta \boldsymbol{u} = \delta \boldsymbol{u}^R + \delta \boldsymbol{u}^F, \tag{38}$$

where

$$\delta \boldsymbol{u}^R \approx \sqrt{\frac{8Q}{3V r_c}} e^{-\xi^2 r_c^2}, \tag{39}$$

$$\delta \boldsymbol{u}^F \approx \sqrt{\frac{8\xi^2 Q}{3\pi V K}} e^{-K^2/4\xi^2}. \tag{40}$$

These estimates are very accurate, just like their electrostatic counterparts. Figures 1 and 2 show an example with $\xi = 20$ and 1000 rotlet point sources randomly distributed in the unit cube, with errors in real and Fourier space computed by comparing to a converged reference solution. The estimates follow the measured RMS errors extremely well, until full numerical precision is obtained around $K/\xi \approx 12$ in Fourier space and $\xi r_c \approx 6$ in real space. These relations actually give full numerical accuracy for a wide range of parameters, as the error estimates are strongly dominated by their exponential terms.

The real space error estimate can be improved by explicitly evaluating the integral estimated in [6]. The resulting error estimate,

$$\delta \boldsymbol{u}^R \approx \sqrt{\frac{8\pi Q}{3V r_c}\left(\operatorname{erfc}(\xi r_c)^2 + \sqrt{\frac{2}{\pi}}\xi r_c \operatorname{erfc}(\sqrt{2}\xi r_c)\right)}, \tag{41}$$

follows the measured RMS error estimate more closely also for small ξr_c ("Better estimate" in Figure 2). In practice the difference might however not be significant enough to merit using the more cumbersome expression.

5 Concluding remarks

By making use of the correspondence between the rotlet and the kernel for the electrostatic force, we have derived an Ewald summation for the periodic rotlet potential (25)–(27), as well as accurate truncation error estimates (38)–(40) for the Ewald sum. Coupled with a fast Ewald summation method, such as the spectral Ewald method [7], these results allow the periodic rotlet potential to be computed rapidly and with controlled precision.

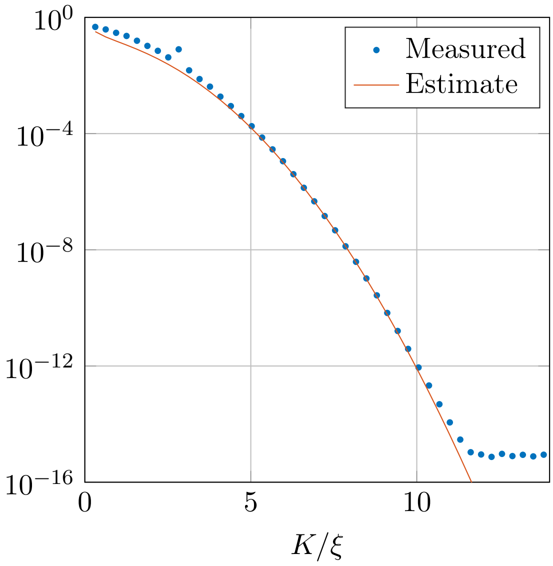

Figure 1: Fourier space RMS truncation error (relative) for $\xi = 20$ and 1000 random sources in the unit cube. Estimate computed using (40).

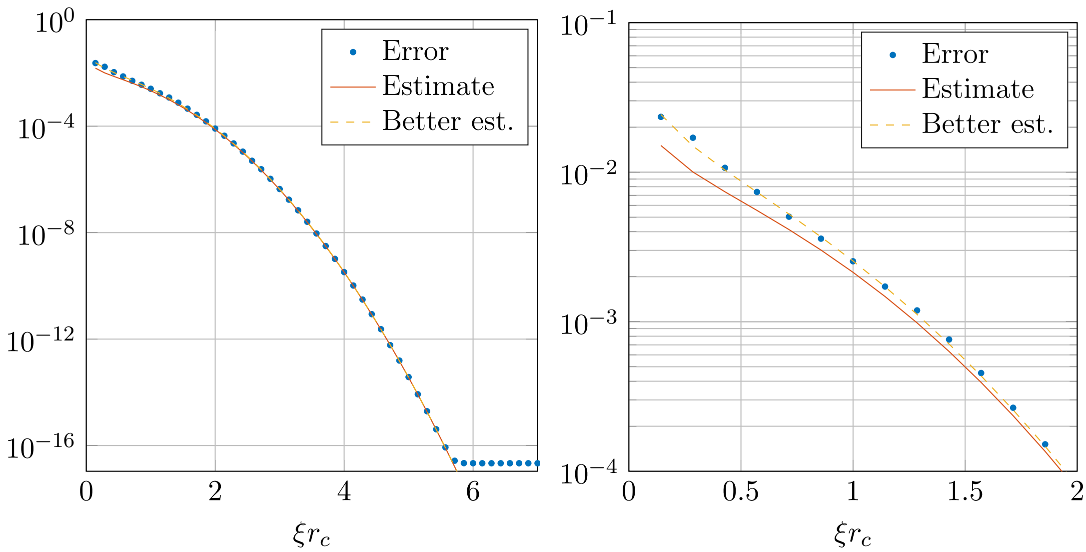

Figure 2: Real space RMS truncation error (relative) for $\xi = 20$ and 1000 random sources in the unit cube. Estimate computed using (39), better estimate computed using (41).

6 Supplementary material

The Ewald decomposition for the rotlet described in this text has been implemented in the Spectral Ewald package, which is available as open source software at `http://github.com/ludvigak/SE_unified` . The package includes a script (`SE_Rotlet/demo.m`) that generates the plots of Figures 1 and 2.

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