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FFT BASED SPECTRAL EWALD METHODS AS AN ALTERNATIVE TO FAST MULTIPOLE METHODS

Anna-Karin Tornberg

Abstract

In this paper, we review a set of fast and spectrally accurate methods for rapid evaluation of three dimensional electrostatic and Stokes potentials. The algorithms use the so-called Ewald decomposition and are FFT-based, which makes them naturally most efficient for the triply periodic case. Two key ideas have allowed efficient extension of these Spectral Ewald (SE) methods to problems with periodicity in only one or two dimensions: an adaptive 3D FFT that apply different upsampling rates locally combined with a new method for FFT based solutions of free space harmonic and biharmonic problems. The latter approach is also used to extend to the free space case, with no periodicity. For the non-radial kernels of Stokes flow, the structure of their Fourier transform is exploited to extend the applicability from the radial harmonic and biharmonic kernels.

A window function is convolved with the point charges to assign values on the FTT grid. Spectral accuracy is attained with a variable number of points in the support of the window function, tuning a shape parameter according to this choice. A new window function, recently introduced in the context of a non-uniform FFT algorithm, allows for further reduction in the computational time as compared to the truncated Gaussians previously used in the SE method.

1 Introduction

The direct evaluation of so called N-body problems yields a computational cost proportional to N^2. One example of such a problem is the evaluation of an electrostatic potential

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owing to N particles at locations $\mathbf{x}_n$, $n = 1, \ldots, N$ with charges q_n, at each of the particle locations,

$$\phi^{0P}(\mathbf{x}_m) = \sum_{n=1}^{N'} q_n \frac{1}{|\mathbf{x}_m - \mathbf{x}_n|}, \tag{1}$$

where N' indicates that the term $m = n$ is excluded from the sum.

Such sums also arise when solving boundary integral equations numerically. Discretizing the following integral over the boundary $\partial\Omega$ of $\Omega \subset \mathbb{R}^3$

$$\int_{\partial\Omega} \frac{f(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|}\, dS_{\mathbf{y}},$$

q_n is for each n the product of the function f evaluated at the quadrature point $\mathbf{x}_n$ and the quadrature weight at that point. Since the integrand is singular at $\mathbf{x} = \mathbf{y}$, the point $\mathbf{x}_m$ can naturally not be included in the sum.

As we use integral equations to solve the Stokes equations, we need instead to evaluate integrals that contain fundamental solutions of Stokes flow, like the Stokeslet

$$S(\mathbf{r}) = \frac{1}{r}\mathbf{I} + \frac{1}{r^3}\mathbf{r}\mathbf{r}, \quad \text{or} \quad S_{j\ell} = \frac{\delta_{j\ell}}{r} + \frac{r_j r_\ell}{r^3} \quad j, l = 1, 2, 3, \tag{2}$$

with $r = |\mathbf{r}|$ and where $\delta_{j\ell}$ is the Kronecker delta. Another fundamental solution of Stokes flow, the Stresslet, will be introduced later. The discrete sum containing the Stokeslet corresponding to Equation (1) becomes

$$\mathbf{u}^{0P}(\mathbf{x}_m) = \sum_{n=1}^{N'} S(\mathbf{x}_m - \mathbf{x}_n)\mathbf{f}_n, \quad m = 1, \ldots, N. \tag{3}$$

In electrostatic calculations, periodic boundary conditions are typically applied to accurately capture properties of a larger aggregate. Periodicity in only one or two directions can be applied for systems with different structures, such as membranes or nanopores. Similarly, it is common to apply periodic boundary conditions in some directions for fluid flows.

Assume that we have N particles with charge q_n located at $\mathbf{x}_n$, $n = 1, \ldots, N$, in a domain $\Omega = [0, L_1] \times [0, L_2] \times [0, L_3]$, where the system is charge neutral, i.e. $\sum_{n=1}^{N} q_n \equiv 0$. The electrostatic potential due to these charges, evaluated at these same locations, is given by the sum

$$\phi^{DP}(\mathbf{x}_m) = \sum_{\mathbf{p} \in P_D} \sum_{n=1}^{N,'} \frac{q_n}{|\mathbf{x}_m - \mathbf{x}_n + \mathbf{p}|}, \quad m = 1, \ldots, N. \tag{4}$$

The sum over $\mathbf{p}$ is a periodic replication of the charges, and $D = 0, 1, 2, 3$ indicates the number of periodic directions. The $N,'$ indicates that the term ($n = m$, $\mathbf{p} = \mathbf{0}$) is excluded from the sum. We define

$$
\begin{aligned}
&P_3 = \{(jL_1, lL_2, pL_3\} : (j, l, p) \in \mathbb{Z}^3\}, \quad && P_2 = \{(jL_1, lL_2, 0)\} : (j, l) \in \mathbb{Z}^2\},\\
&P_1 = \{(0, 0, pL_3\} : p \in \mathbb{Z}\}, && P_0 = \{(0, 0, 0\}\}.
\end{aligned} \tag{5}
$$

Here, we have chosen x and y as the periodic directions and z as the free direction in the doubly periodic case (2P), and x and y as the free and z as the periodic direction in the singly periodic case (1P).

In the triply periodic case, the sum given above is only conditionally convergent also for charge neutral systems, and the result will depend on the summation order, as is shown e.g. in the much cited paper by de Leeuw, Perram, and E. R. Smith [1980]. This is further discussed more recently by E. Smith [2008]. The Ewald summation formula for the triply periodic case was derived by Ewald [1921] in 1921. The resulting formula imposes two choices: a spherical summation order and an assumption that the dielectric constant of the surrounding medium is infinite, i.e. that it is a conductor. This is often referred to as "tin foil" boundary conditions. As shown in E. Smith [2008], charge neutrality is necessary also in the singly and doubly periodic cases for the sums to be convergent, but the results are independent on the summation order.

In the Ewald summation formula Ewald [1921], the potential is computed by splitting the contribution from each charge into a rapidly decaying part and a smooth part which is summed in Fourier space. The Ewald sum for evaluating the potential at a source location $\mathbf{x}_m$, $m = 1, \ldots, N$ under triply periodic boundary conditions is

$$
\begin{aligned}
\phi^{3P}(\mathbf{x}_m) = &\sum_{\mathbf{p}\in P_3} \sum_{n=1}^{N,'} q_n \frac{\operatorname{erfc}(\xi\,|\mathbf{x}_m - \mathbf{x}_n + \mathbf{p}|)}{|\mathbf{x}_m - \mathbf{x}_n + \mathbf{p}|} + \\
&+ \frac{4\pi}{V} \sum_{\mathbf{k}\neq\mathbf{0}} \sum_{n=1}^{N} q_n \frac{e^{-k^2/4\xi^2}}{k^2} e^{-i\mathbf{k}\cdot(\mathbf{x}_m - \mathbf{x}_n)} - \frac{2\xi}{\sqrt{\pi}} q_m.
\end{aligned} \tag{6}
$$

Here, the $N,'$ indicates that the term ($n = m$, $\mathbf{p} = \mathbf{0}$) is excluded from the real space sum and P_3 is given in Equation (5). The $\mathbf{k}$-vectors form the discrete set $\{2\pi(\frac{n_1}{L_1}, \frac{n_2}{L_2}, \frac{n_3}{L_3}) : (n_1, n_2, n_3) \in Z^3\}$, $k^2 = |\mathbf{k}|^2$ and $V = L_1 L_2 L_3$. Here, $\xi > 0$ is the decomposition parameter. The result is independent of this parameter, but it controls the relative decay of the real and reciprocal space sums. The last term is the so called self correction term. When evaluating the potential at a charge location, no contribution from this charge itself should be included, and this term is added for this purpose. The Ewald sums for the energy and electrostatic force are easily obtained from the expression for the potential, see e.g. Deserno and Holm [1998].

Ewald sums have also been derived for the doubly and singly periodic cases, see Grzybowski, Gwóźdź, and Bródka [2000] and Porto [2000] and references therein. The derivation of the singly periodic sum in Porto [ibid.], however left an integral expression for which no closed form was given, that could later be obtained following Fripiat, Delhalle, Flamant, and Harris [2010]. In Tornberg [2016], derivations of the Ewald $3P$, $2P$ and $1P$ sums are presented in a unified framework that gives a natural starting point for the design of a fast method.

The Stokeslet sum (Equation (3)) can be extended similarly to Equation (4). Hasimoto derived an Ewald type decomposition for the triply periodic case in 1959 Hasimoto [1959]. Instead of charge neutrality, here we have an assumption that there is a mean pressure gradient that balances the net force. Pozrikidis [1996] derived an alternative sum for the Stokes 3P case, using a different decomposition due to Beenakker [1986]. He further discussed also the 2P and 1P Stokeslet sums, however not stating all formulas explicitly. Explicit formulas for the 2P Stokeslet sum with the Hasimoto decomposition can be found in Lindbo and Tornberg [2011a].

1.1 Fast methods and the development of the Spectral Ewald method. As was noted above, the direct evaluation of the sum in Equation (1) has a computational complexity of $O(N^2)$ and so does the Ewald sum for the triply periodic case as given in Equation (6), but in addition with a much larger cost for the same value of N.

For free space problems such as Equation (1), the Fast Multipole Method (FMM) can reduce the $O(N^2)$ cost to $O(N)$ work, where the constant multiplying N will depend on the required accuracy. FMM was first introduced by Greengard and Rokhlin for the harmonic kernel in 2D and later in 3D Greengard and Rokhlin [1987] and Cheng, Greengard, and Rokhlin [1999] and has since been extended to other kernels, including the fundamental solutions of Stokes flow Tornberg and Greengard [2008] and Wang, Lei, Li, Huang, and Yao [2007]. The FMM has not been as popular for periodic problems, even if it can be extended to this case at an additional cost, see e.g. Gumerov and Duraiswami [2014] and the references therein.

For triply periodic problems in electrostatics, FFT-based methods have been the most popular and successfully used since the early 1990s. Here, the Ewald decomposition is used, with ξ in Equation (6) chosen such that the real space terms decay rapidly, and more work is put into the Fourier sum, which is accelerated with an FFT based method. With a proper scaling of ξ as N grows, the full algorithm yields a cost of $O(N \log N)$. One early method for evaluation of the electrostatic potential and force was the Particle Mesh Ewald (PME) method by Darden, York, and Pedersen [1993], later refined to the Smooth Particle Mesh Ewald (SPME) method by Essmann, Perera, Berkowitz, Darden, Lee, and Pedersen [1995]. See also the survey by Deserno and Holm [1998]. The SPME method

was extended to the fast evaluation of the triply periodic stokeslet sum by Saintillan, Darve, and Shaqfeh [2005].

The Spectral Ewald method. The Spectral Ewald (SE) method was first introduced for the triply periodic stokeslet sum in Lindbo and Tornberg [2010], and soon thereafter for the electrostatic problem Lindbo and Tornberg [2011b]. The PME methods mentioned above have a polynomial order of accuracy, and require a refinement of the FFT grid to reduce approximation errors. Specifically, in the SPME method, the point sources are convolved with B-splines of a fixed regularity and support to assign values on the FTT grid. In contrast, the SE method as it was introduced in Lindbo and Tornberg [2010, 2011b], is spectrally accurate. By using suitably scaled and truncated Gaussians, the approximation error is reduced spectrally fast as the number of points in the support of the truncated Gaussians is increased, and is not tied to the grid size. The idea of using Gaussians as window functions was of course not new, not in PME like methods, nor in the closely related non-uniform FFT methods, as discussed in Lindbo and Tornberg [2010, 2011b]. The key in the performance of the SE method was to tie a shape parameter of the Gaussian to the number of points in its support in order to minimize approximation errors.

Recently, we compared the use of Gaussians to a window function that was recently introduced by Barnett and Magland in connection to a non-uniform FFT algorithm Barnett and Magland [2017]. This window function is an approximation to the Kaiser-Bessel function that retains the desirable properties while reducing the cost of evaluation. Similarly to the Gaussians, we adjust a shape parameter for this window function with the number of points in the support. In Saffar Shamshirgar and Tornberg [2017a], we showed that this new Barnett-Magland window function is superior to the Gaussian and that the computational cost is further reduced for the same target accuracy.

FFT based methods are most efficient for the triply periodic case. In this case, FFTs can be used in all directions without any oversampling. As soon as there is a non-periodic direction, the grid has to be extended in that direction. In the doubly periodic case, De Joannis, Arnold, and Holm [2002] devised a method where the problem is extended to full periodicity, with a larger length in the non-periodic direction, and where a correction term is applied to improve on the result. Here, the increased length in the non-periodic direction simply means a zero-padding of the FFT, increasing in the number of grid points in that direction. The SE2P method by Lindbo and Tornberg [2012] takes a different approach, which needs a "mixed" transform; a discrete Fourier transform in the periodic variables and an approximation to the continuous Fourier integral transform in the free dimension. Also in this case the grid in the free dimension must be oversampled for an accurate approximation.

In the doubly periodic Ewald sum, there is a term that includes the contribution from the zero wave number in the periodic directions, i.e., that depends only on the variable in the free direction. An expansion based on Chebyshev polynomials offered an efficient evaluation if this $1D$ sum Lindbo and Tornberg [2012].

Recent developments. There were two main challenges to overcome when extending the Spectral Ewald method to the singly periodic (1P) case. With two free dimensions, an oversampling factor of four to six in each would increase the cost of FFTs by a factor of 16 to 64, which is clearly not desirable. Furthermore, the zero wave number in the periodic direction here yields a 2D sum as opposed to a 1D sum in the doubly periodic case, and it is not feasible to extend the approach in Lindbo and Tornberg [ibid.].

In Saffar Shamshirgar and Tornberg [2017b] we showed that it is sufficient to upsample only for small discrete wave numbers, and introduced an adaptive FFT and IFFT (denoted by AFT and AIFT) that only upsample for a select number of discrete modes in the periodic direction. As for the second challenge, the 2D sum is the free space solution to a 2D Poisson problem, and a recent idea for how to solve free space problems by the means of FFTs Vico, Greengard, and Ferrando [2016] can therefore be used. The treatment of the zero periodic wave number can now be treated in the same framework as the other modes, and will be included in the AFT mentioned above. This is done at a negligible extra cost. A typical increase in cost of the FFTs performed in the 1P case as compared to 3P is a factor of $2-3$. The gridding cost when applying the window function is essentially the same in both cases. The ratio of the total runtime cost for the SE1P method and the SE3P method is therefore even smaller.

In af Klinteberg, Saffar Shamshirgar, and Tornberg [2017], the approach to solve free space problems with FFTs was used to extend the SE method to problems without periodicity. The original idea in Vico, Greengard, and Ferrando [2016] is applicable for the harmonic and biharmonic kernels, here an extension was introduced such that sum of free space potentials could be evaluated for stokeslets, stresslets and rotlets.

We have very recently unified the treatment from free space up to triply periodic for the electrostatic problem Saffar Shamshirgar and Tornberg [2017a]. The 2P algorithm from Lindbo and Tornberg [2012] was here modified to make use of the advances made when developing the $1P$ method Saffar Shamshirgar and Tornberg [2017b]. The software is available Lindbo, af Klinteberg, and Saffar Shamshirgar [2016], including also the implementation of the new window function Barnett and Magland [2017].

Recently, Nestler, Pippig, and Potts [2015] developed an FFT based fast algorithm based on Ewald decomposition for triply, double and singly periodic problems. To the best of our knowledge, this is the only Ewald method with $O(N\log(N))$ complexity for singly periodic problems except our own. Their approach is however quite different as

compared to ours, as instead of discretizing the continuous Fourier transforms, they work with the analytical formulas containing special functions that are obtained from them.

Any method based on Ewald summation and acceleration by FFTs will be most efficient in the triply periodic case. As soon as there is one or more non-periodic directions, there will be a need for some oversampling of FFTs, which will increase the computational cost. For the fast multipole method (FMM), the opposite is true. The free space problem is the fastest to compute, and any periodicity will invoke an additional cost, which will become substantial or even overwhelming if the base periodic box has a large aspect ratio. Hence, implementing the FFT-based Spectral Ewald method for a free-space problem and comparing it to an FMM method will be the worst possible case for the SE method. Still, we did so for the free space summation of Stokes potentials in af Klinteberg, Saffar Shamshirgar, and Tornberg [2017], using an open source implementation of the FMM Greengard [2012]. It turned out that our SE method was competitive and often performed clearly better than the FMM (one can, however, expect this adaptive FMM to perform better for highly non-uniform point distributions).

Outline. The structure of this review is as follows: in Section 2 we discuss the derivation of the Ewald sums, and highlight the differences that occur due to different periodicities. We also introduce modifications based on the ideas in Vico, Greengard, and Ferrando [2016] to get formulas on a form amenable to numerical treatment for all Fourier modes. In Section 2, we introduce the triply periodic SE method, and discuss all the steps of the algorithm. This is the simplest case, and the extension of the Spectral Ewald method to different periodicities is discussed in the following section. These sections are all concerned with the evaluation of the electrostatic potential, and in Section 5 we discuss the extension to potentials of Stokes flow, before we summarize and conclude.

2 Ewald formulas for electrostatics

There is more than one way to derive the Ewald summation formula. One can e.g. utilize the fact that the electrostatic potential can be found as the solution to the Poisson equation

$$-\Delta\phi = 4\pi f^{DP}(\mathbf{x}), \quad f^{DP}(\mathbf{x}) = \sum_{\mathbf{p}\in P_D}\sum_{n} q_n \delta(\mathbf{x}-\mathbf{x}_n+\mathbf{p}), \quad \mathbf{x}\in\mathbb{R}^3. \tag{7}$$

The sum over $\mathbf{p}$ is a replication of the charges in the periodic directions, and $D = 0, 1, 2, 3$ indicates the number of periodic directions with P_D defined in Equation (5). We introduce a charge screening function, $\gamma(\xi, \mathbf{x})$ to decompose f^{DP} into two parts:

$$f^{DP}(\mathbf{x}) = \underbrace{f^{DP}(\mathbf{x}) - (f^{DP} * \gamma)(\mathbf{x})}_{:=f^{DP,R}(\xi,\mathbf{x})} + \underbrace{(f^{DP} * \gamma)(\mathbf{x})}_{:=f^{DP,F}(\xi,\mathbf{x})}.$$

The Poisson equation can be solved for each of the two parts of the right hand side to find $\phi^{PD,R}$ and $\phi^{PD,F}$, that can then be added. The screening function for which the classical Ewald decomposition is obtained is a Gaussian $\gamma(\xi, \mathbf{x})$, with the Fourier transform $\widehat{\gamma}(\xi, \mathbf{k})$, $\xi > 0$,

$$\gamma(\xi, \mathbf{x}) = \xi^3 \pi^{-3/2} e^{-\xi^2 |\mathbf{x}|^2}, \quad \widehat{\gamma}(\xi, \mathbf{k}) = e^{-|\mathbf{k}|^2/4\xi^2}. \tag{8}$$

The function $f^{DP,F}(\xi, \mathbf{x})$ is smooth, and a Fourier representation of the solution $\phi^{PD,F}$ will hence converge rapidly.

The Ewald sum for evaluating the potential at a source location $\mathbf{x}_m$, $m = 1, \ldots, N$ under different periodicity conditions becomes

$$\phi^{DP}(\mathbf{x}_m) = \phi^{DP,R}(\mathbf{x}_m, \xi) + \phi^{DP,F}(\mathbf{x}_m, \xi) - \frac{2\xi}{\sqrt{\pi}} q_m, \tag{9}$$

where

$$\phi^{DP,R}(\mathbf{x}_m, \xi) = \sum_{\mathbf{p} \in P_D} \sum_{n=1}^{N,'} q_n \frac{\operatorname{erfc}(\xi\, |\mathbf{x}_m - \mathbf{x}_n + \mathbf{p}|)}{|\mathbf{x}_m - \mathbf{x}_n + \mathbf{p}|}, \quad D = 0, 1, 2, 3. \tag{10}$$

This term can be derived by evaluating a convolution integral of $\gamma(\xi, \mathbf{x} - \mathbf{x}_n)$ with the harmonic Green's function (see e.g. Appendix A of Tornberg [2016]), then summing over all sources including periodic copies. Here, the $N,'$ indicates that the term ($n = m$, $\mathbf{p} = \mathbf{0}$) is excluded from the real space sum and P_D is given in Equation (5). The last term in Equation (9) is the so called self correction term. When evaluating the potential at a charge location, no contribution from this charge itself should be included, and this term is added for this purpose.

For the Fourier space contribution, it remains to solve

$$-\Delta \phi^{DP,F} = 4\pi f^{DP,F}(\mathbf{x}, \xi), \quad f^{DP,F}(\mathbf{x}, \xi) = \sum_{\mathbf{p} \in P_D} \sum_{n} q_n \gamma(\xi, \mathbf{x} - \mathbf{x}_n + \mathbf{p}), \quad \mathbf{x} \in \mathbb{R}^3. \tag{11}$$

with $\gamma(\xi, \mathbf{x})$ as defined in Equation (8), under appropriate boundary conditions.

Expanding $\phi^{3P,F}(\mathbf{x}, \xi)$ in a triply periodic Fourier sum, and using the expression for $\widehat{\gamma}(\xi, \mathbf{k})$ from Equation (8) to do the same for $f^{3P,F}(\mathbf{x}, \xi)$, we can solve Equation (11) and obtain

$$\phi^{3P,F}(\mathbf{x}_m, \xi) = \frac{4\pi}{V} \sum_{\mathbf{k} \neq \mathbf{0}} \sum_{n=1}^{N} q_n \frac{e^{-k^2/4\xi^2}}{k^2} e^{-i\mathbf{k}\cdot(\mathbf{x}_m - \mathbf{x}_n)}. \tag{12}$$

which is the summation over $\mathbf{k}$ in the second line of Equation (6).

For the doubly periodic case, we can expand $\phi^{2P,F}(\mathbf{x},\xi)$ and $f^{2P,F}(\mathbf{x},\xi)$ in Fourier series in the periodic x and y directions. The Fourier coefficients $\hat{\phi}_{\bar{\mathbf{k}}}(z)$ and $\hat{f}_{\bar{\mathbf{k}}}(z)$ will be indexed by $\bar{\mathbf{k}} = (k_1, k_2)$. These coefficients can be represented in terms of a Fourier transform in the non-periodic z-direction. Alternatively, we can insert these doubly periodic Fourier series into Equation (11), use orthogonality and for each wave vector $\bar{\mathbf{k}}$ obtain

$$(-\partial_z^2 + |\bar{\mathbf{k}}|^2)\hat{\phi}_{\bar{\mathbf{k}}}(z) = 4\pi \hat{f}_{\bar{\mathbf{k}}}(z).$$

In light of how we will later proceed with constructing a fast method to evaluate $\phi^{2P,F}(\mathbf{x},\xi)$, we take the first view point for $\bar{\mathbf{k}} \neq 0$, and the second for $\bar{\mathbf{k}} = 0$. We write

$$\phi^{2P,F}(\mathbf{x},\xi) = \bar{\phi}^{2P,F}(\mathbf{x},\xi) + \phi_0^{2P,F}(z,\xi), \tag{13}$$

with

$$\bar{\phi}^{2P,F}(\mathbf{x},\xi) = \frac{2}{L_1 L_2} \sum_{\bar{\mathbf{k}}\neq 0} \sum_{n=1}^{N} q_n \int_{\mathbf{R}} \frac{1}{k^2} e^{-k^2/4\xi^2} e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}_n)}\, d\kappa_3. \tag{14}$$

Here, we use $\mathbf{k} = (k_1, k_2, \kappa_3)$ to emphasize that κ_3 is a continuous variable. The term for $\bar{\mathbf{k}} = 0$, i.e. $k_1 = k_2 = 0$ is given by the free space solution of the $1D$ Poisson equation

$$-\frac{d^2}{dz^2}\phi_0^{2P,F}(z,\xi) = 4\pi \frac{\xi\pi^{-1/2}}{L_1 L_2} \sum_{n=1}^{N} q_n e^{-\xi^2|z-z_n|^2}. \tag{15}$$

The integral in Equation (14) can be evaluated analytically, and the Equation (15) has an explicit solution. The result is stated e.g. in section 9 of Tornberg [ibid.]. Those formulas are however only used for validation of the fast method. To develop the fast method, we will continue along a different path.

In the singly periodic case, we can similarly to the double periodic case expand in a Fourier series in the periodic direction z, and index coefficients by k_3. Also, in this case, we use the continuous Fourier transform to express the coefficients as long as $k_3 \neq 0$, and formulate the PDE for the $k_3 = 0$ coefficient. The explicit formulas can be found in Saffar Shamshirgar and Tornberg [2017b].

In the doubly periodic case, we need to solve a one-dimensional free space problem (Equation (15)), and in the singly periodic case a two-dimensional free space problem. For the free space case, the full problem is a three dimensional free space problem, i.e. Equation (11) for $D = 0$ under the boundary conditions $\phi^{0P,F}(\mathbf{x},\xi) \to 0$ as $|\mathbf{x}| \to 0$.

This solution can be expressed as a 3D Fourier integral in k-space, with a $1/k^2$ factor. It is integrable, and a change to spherical coordinates will for example remove the singularity.

The integral can however not be accurately approximated with values on a regular grid, which is needed for a fast treatment with FFTs.

2.1 Free space formulas with truncated Green's functions. Assume that we want to solve

$$-\Delta\phi = 4\pi f(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^{\dim}. \tag{16}$$

with free space boundary conditions ($\phi \to 0$ as $|\mathbf{x}| \to 0$), and dim $= 1, 2$ or 3.

Assume now that $f(\mathbf{x})$ is compactly supported within a domain $\tilde{\mathfrak{D}}$, a box with sides $\tilde{\mathbf{L}}$, $\tilde{\mathfrak{D}} = \{\mathbf{x} \,|\, x_i \in [0, \tilde{L}_i]\}$, and that we seek the solution for $\mathbf{x} \in \tilde{\mathfrak{D}}$. The largest point-to-point distance in the domain is $|\tilde{\mathbf{L}}|$. Let $\mathcal{R} \geq |\tilde{\mathbf{L}}|$. Without changing the solution, we can then replace the Green's function with a truncated version

$$G^{\mathcal{R}}(r) = G(r)\,\mathrm{rect}\left(\frac{r}{2\mathcal{R}}\right), \qquad \mathrm{rect}(\mathbf{x}) = \begin{cases} 1 & \text{for } |\mathbf{x}| \leq 1/2, \\ 0 & \text{for } |\mathbf{x}| > 1/2. \end{cases}$$

The Fourier transform of the truncated Green's function in 3D, where $G(r) = 1/r$ is Vico, Greengard, and Ferrando [2016]

$$\hat{G}^{\mathcal{R}}(k) = 8\pi \left(\frac{\sin(\mathcal{R}k/2)}{k}\right)^2,$$

with the well defined limit

$$\hat{G}^{\mathcal{R}}(0) = \lim_{k\to 0} \hat{G}^{\mathcal{R}}(k) = 2\pi\mathcal{R}^2.$$

We then have

$$\begin{aligned} \phi(\mathbf{x}) = \int_{\mathbb{R}^3} G(|\mathbf{x}-\mathbf{y}|) f(\mathbf{y})\, d\mathbf{y} &= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \hat{G}(k)\hat{f}(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x}}\, d\mathbf{k} \\ &= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \hat{G}^{\mathcal{R}}(k)\hat{f}(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x}}\, d\mathbf{k}, \end{aligned} \tag{17}$$

as long as the assumption introduced above is fulfilled s.t. supp$(f) \in \tilde{\mathfrak{D}}$, $\mathbf{x} \in \tilde{\mathfrak{D}}$ and $\mathcal{R}$ is chosen appropriately. Similar formulas can be derived in one and two dimensions.

2.2 Formulas for the k-space contributions. The decomposition of ϕ^{DP} into a real space part $\phi^{DP,R}$ and a Fourier space part $\phi^{DP,F}$ was introduced in Equation (10). The terms in the real space part have the same form independent of the periodicity of the problem, only the summation over periodic images changes, as given in Equation (10). For the

k-space contribution, we need to work with Fourier series in any periodic direction, and Fourier integrals elsewhere. The simplest case is hence the triply periodic case, where a discrete sum is obtained directly, and the result was given in Equation (12).

For the cases with mixed periodicity, there will be a sum over the discrete Fourier modes in the periodic direction(s). For the Fourier mode where the discrete wave number/wave vector is zero, the integral has a singularity. For this zero mode, we instead define the contribution as the solution to a free space problem. In the previous section, we discussed how to work with truncated Green's functions to obtain an expression in Fourier space for a mollified Green's function that has no singularity. Similarly, for the $0P$ case, we solve a 3D free space problem, with the right hand side given in Equation (11).

This treatment introduces no approximation under the assumption of a compactly supported right hand side. Our right hand sides are however sums of Gaussians and are not compactly supported. The Gaussians do however decay exponentially fast, and as we construct a numerical algorithm based on these formulas, this error source can controlled and made vanishingly small by the choice of $\mathcal{R}$.

With $\mathbf{k} = (k_1, k_2, \kappa_3)$, $k = |\mathbf{k}|$, we write for the $2P$ case,

$$\phi^{2P,F}(\mathbf{x},\xi) \approx \frac{2}{L_1 L_2} \sum_{k_1,k_2} \sum_{n=1}^{N} q_n \int_{\mathbf{R}} \hat{G}^{2P}_{\mathcal{R}}(\mathbf{k}) e^{-k^2/4\xi^2} e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}_n)}\, d\kappa_3. \tag{18}$$

where

$$\hat{G}^{2P}_{\mathcal{R}}(\mathbf{k}) = \begin{cases} 1/k^2 & k_1^2 + k_2^2 \neq 0 \\ (\mathcal{R}k \sin(\mathcal{R}k) + \cos(\mathcal{R}k) - 1)/k, & k_1 = 0, k_2 = 0, \kappa_3 \neq 0 \\ \mathcal{R}^2/2 & \mathbf{k} = 0. \end{cases} \tag{19}$$

With $\mathbf{k} = (\kappa_1, \kappa_2, k_3)$, $k = |\mathbf{k}|$, for the 1P case we write

$$\phi^{1P,F}(\mathbf{x},\xi) \approx \frac{1}{\pi L_3} \sum_{k_3} \sum_{n=1}^{N} q_n \int_{\mathbb{R}^2} \hat{G}^{1P}_{\mathcal{R}}(\mathbf{k}) e^{-k^2/4\xi^2} e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}_n)}\, d\kappa_1 d\kappa_2, \tag{20}$$

where

$$\hat{G}^{1P}_{\mathcal{R}}(\mathbf{k}) = \begin{cases} 1/k^2 & k_3 \neq 0 \\ (1 - J_0(\mathcal{R}k))/k^2 - \mathcal{R}\log(\mathcal{R}) J_1(\mathcal{R}k)/k & k_3 = 0, \kappa_1^2 + \kappa_2^2 \neq 0 \\ \mathcal{R}^2(1 - 2\log(\mathcal{R})/4. & \mathbf{k} = 0. \end{cases} \tag{21}$$

In the above, $k_i \in \{2\pi n/L_i, n \in \mathbb{Z}\}$. For the free space case, we have no discrete modes, and use $\mathbf{k} = (\kappa_1, \kappa_2, \kappa_3)$, $k = |\mathbf{k}|$, as we write

$$\phi^{0P,F}(\mathbf{x},\xi) \approx \frac{1}{2\pi^2} \sum_{n=1}^{N} q_n \int_{\mathbb{R}^3} \hat{G}^{0P}_{\mathcal{R}}(k) e^{-k^2/4\xi^2} e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}_n)}\, d\kappa_1 d\kappa_2 d\kappa_3, \tag{22}$$

where

$$\hat{G}^{0P}_{\mathcal{R}}(k) = \begin{cases} 2\sin^2(\mathcal{R}k/2)/k^2, & k \neq 0 \\ \mathcal{R}^2/2 & k = 0. \end{cases} \tag{23}$$

Here, $\hat{G}^{0P}_{\mathcal{R}}$ is scaled with a factor of $1/(4\pi)$ as compared to $\hat{G}^{\mathcal{R}}$ introduced in the previous section. Again, we want to emphasize that the $\approx$ sign in these equations arise due to the fact that we formally do not have compactly supported right hand sides for the free space problems. In practice, if the domain of support is set such that the Gaussians are sufficiently decayed, and the parameter $\mathcal{R}$ is chosen according to this, there will be no noticeable errors from this source in the FFT based algorithm that we will develop based on these formulas.

2.3 Truncation errors. Both the real space and k-space sums need to be truncated. They decay exponentially fast, and can for the triply periodic case be truncated such as to only include terms for which $|\mathbf{x}_m - \mathbf{x}_n + \mathbf{p}| < r_c$ in Equation (10) and $k = |\mathbf{k}| < 2\pi k_\infty / L$ (assuming $L_i = L$, $i = 1, 2, 3$ for a simpler expression. Excellent error estimates were derived by Kolafa and Perram [1992], and given ξ and an error tolerance, r_c and k_∞ can be appropriately chosen. See also Lindbo and Tornberg [2011b]. Even though the error estimates were derived for the triply periodic case, they work remarkably well also for the singly and doubly periodic cases Lindbo and Tornberg [2012] and Saffar Shamshirgar and Tornberg [2017b] and even for the free space case af Klinteberg, Saffar Shamshirgar, and Tornberg [2017] (see the discussion on the rotlet). For the Fourier space contribution this means that the discretized integrals are truncated at the corresponding k_∞.

3 The spectral Ewald method with full periodicity

As was just discussed, contributions to the real space sum will be ignored if the distance between the source location and the target evaluation point is larger than a cut-off radius r_c. Typically, a linked cell list or a Verlet list algorithm can be used to efficiently obtain a list of nearest neighbors Lindbo and Tornberg [2011b]. The real space sum in Equation (10) includes a summation over the periodic dimensions, which means that contribution from periodic images of the sources are also included if they are within this distance. We will now proceed to discuss the evaluation of the Fourier space sum (Equation (12)) in the triply periodic case.

3.1 Formulas and algorithmic steps. The triply periodic case is the most straight forward, and also computationally most efficient since periodicity is naturally handled by FFTs. The fast method that we propose follows the structure of methods within the PME

family: point charges are distributed on a uniform grid using an interpolation (window) function, an FFT is applied, a multiplication is made in k-space with an appropriately modified Green's function (depending on the choice of window function), an inverse FFT is applied, and the window function is used once more to evaluate the result at irregular evaluation (target) points.

Let us denote the window function by $\mathcal{W}(\mathbf{x})$, and assume $\mathcal{W}(-\mathbf{x}) = \mathcal{W}(\mathbf{x})$. Note the trivial identity $\hat{\mathcal{W}}_{\mathbf{k}}\hat{\mathcal{W}}_{\mathbf{k}}\hat{\mathcal{W}}_{\mathbf{k}}^{-2} \equiv 1$ and introduce

$$\widehat{\widetilde{H}}_{\mathbf{k}} = \frac{e^{-k^2/4\xi^2}}{k^2}\hat{\mathcal{W}}_{\mathbf{k}}^{-2}\hat{H}_{\mathbf{k}} \tag{24}$$

where

$$\hat{H}_{\mathbf{k}} = \sum_{n=1}^{N} q_n \hat{\mathcal{W}}_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{x}_n}. \tag{25}$$

With this, the expression for $\phi^{3P,F}(\mathbf{x}_m, \xi)$ in Equation (12) becomes

$$\phi^{3P,F}(\mathbf{x}_m, \xi) = \frac{4\pi}{V}\sum_{\mathbf{k}\neq\mathbf{0}} \hat{\mathcal{W}}_{\mathbf{k}}\widehat{\widetilde{H}}_{-\mathbf{k}} e^{-i\mathbf{k}\mathbf{x}_m}. \tag{26}$$

The fact that a product in Fourier space is equal to a convolution in real space implies that $H(\mathbf{x})$ is given by

$$H(\mathbf{x}) = \sum_{n=1}^{N} q_n \int_{\Omega} \delta(\mathbf{x}-\mathbf{x}_n)\mathcal{W}(\mathbf{y}-\mathbf{x})_* \, d\mathbf{y} = \sum_{n=1}^{N} q_n \mathcal{W}(\mathbf{x}-\mathbf{x}_n)_*, \tag{27}$$

where $\mathcal{W}(\mathbf{x})_* = \sum_{\mathbf{p}\in P_D} \mathcal{W}(\mathbf{x}+\mathbf{p})$.

Furthermore, Parseval's formula yields

$$\begin{aligned}\phi^{3P,F}(\mathbf{x}_m, \xi) &= 4\pi \int_{\Omega} \widetilde{H}(\mathbf{x}) \left[\int_{\Omega} \delta(\mathbf{y}-\mathbf{x}_m)\mathcal{W}(\mathbf{y}-\mathbf{x})_* \, d\mathbf{y}\right] d\mathbf{x} \\ &= 4\pi \int_{\Omega} \widetilde{H}(\mathbf{x})\mathcal{W}(\mathbf{x}-\mathbf{x}_m)_* \, d\mathbf{x},\end{aligned} \tag{28}$$

where we have suppressed the dependence on ξ in the notation for $\widetilde{H}(\mathbf{x})$.

For simplicity, we will in the following assume that $L_1 = L_2 = L_3 = L$ such that the periodic domain as defined above (Equation (4)) is $\Omega = [0, L]^3$.

1. Introduce a uniform grid over Ω of size M^3 and evaluate $H(\mathbf{x})$ on this grid using Equation (27).

2. Apply an FFT to evaluate $\hat{H}$.
3. Evaluate $\widehat{\widetilde{H}}_{\mathbf{k}}$ according to Equation (24).
4. Apply an IFFT to evaluate $\widetilde{H}(\mathbf{x})$ on the uniform grid.
5. Evaluate the integral (Equation (28)) with the trapezoidal rule to arrive at the final result, $\phi^{3P,F}(\mathbf{x}_m, \xi)$.

There are two sources of errors. Truncation errors arise as only a finite number of Fourier modes are included. Given an error tolerance, the grid size M is chosen from the truncation error estimate as $M = 2k_\infty$. Approximation errors enter due to the approximation of the integral in Equation (28). We will discuss window functions that do not have compact support, and hence, truncation of the window function will also contribute to the approximation error.

3.2 Window functions and approximation errors. In the Spectral Ewald method as presented in e.g. Lindbo and Tornberg [2011b], truncated Gaussians have been used as window functions. Here, we use $\mathfrak{W}(\mathbf{x}) = g(\mathbf{x}, \xi, \eta)$, where

$$g(\mathbf{x}, \xi, \eta) = \left(\frac{2\xi^2}{\pi\eta}\right) e^{-2\xi^2|\mathbf{x}|^2/\eta} \tag{29}$$

The function has been normalized to 1. The Fourier transform is known, $\hat{g}(\mathbf{k}, \xi, \eta) = e^{-\eta|\mathbf{k}|^2/8\xi^2}$. With this choice of window function, the scaling step in Equation (24) becomes

$$\widehat{\widetilde{H}}_{\mathbf{k}} = \frac{e^{-(1-\eta)k^2/4\xi^2}}{k^2}\hat{H}_{\mathbf{k}}.$$

This relation to the Gaussian factor in the Ewald formula is the reason for defining g as in Equation (29) with both ξ and the new shape parameter η.

Another class of window functions that has been commonly used is cardinal B-splines Essmann, Perera, Berkowitz, Darden, Lee, and Pedersen [1995] and Deserno and Holm [1998]. The degree of the B-spline is chosen, which gives a fixed (small) support size, and a certain regularity. If the FFT gris has a grid size $h = L/M$, an approximation error of $O(h^p)$ will be introduced, where p depends on the regularity. Hence, to decrease the approximation error, the grid size M must be increased.

For the Gaussian window function, we truncate at $|x| = |y| = |z| = w$, where $2w = Ph$ such that we have P^3 points in the support. With $\eta = (2w\xi/m)^2$, we can show Lindbo and Tornberg [2011b] that the error committed in approximating Equation (28) by the trapezoidal rule can be bounded by

$$C\left(e^{-\pi^2P^2/(2m)^2} + \operatorname{erfc}(m/\sqrt{2})\right). \tag{30}$$

The first term is the quadrature error, and the second term is due to the truncation of the Gaussians. With $m = c\sqrt{\pi P}$ (where $c = 1$ found close to optimal for electrostatics), we obtain an exponential decay of the error with P.

Hence, for any given P, we scale the window function to achieve the optimal balance between resolution and truncation. We do not need to increase the grid size to reduce the approximation errors - we instead increase P and scale the window function properly. This allows for the grid size to be selected solely according to the Kolafa-Perram estimate for the truncation of the Fourier Ewald sum.

Recently, Barnett and Magland introduced a new window function in their work in the non-uniform FFT method Barnett and Magland [2017]. This new window function is an approximation of the so called Kaiser-Bessel function, which can be shown to yield low error levels but is expensive to compute. To use this window function, we set $\mathfrak{W}(\mathbf{x}) = B(x,\beta)B(y,\beta)B(z,\beta)$, where

$$B(x,\beta) = \begin{cases} e^{\beta\sqrt{1-(x/w)^2}}/e^{\beta} & -w \le x \le w \\ 0 & \text{otherwise.} \end{cases}$$

This defintion effectively yields a truncation, and again with $2w = Ph$, there are P^3 points in the support. The Fourier transform of this window function is not analytically known. By the structure of the function, it is sufficient to compute a 1D FFT (or at most three 1D FFTs if all dimensions are different), to obtain the transform numerically. This can then be used in the scaling step (Equation (24)).

Although not proven yet, from numerical evidence Saffar Shamshirgar and Tornberg [2017a] we can predict that the approximation error comparable to Equation (30) is

$$C\left(\beta^2 e^{-2\pi P^2/\beta} + \operatorname{erfc}(\sqrt{\beta})\right). \tag{31}$$

Hence, also here we can choose a parameter (β) to balance the resolution and truncation. In Saffar Shamshirgar and Tornberg [ibid.] we find $\beta = 2.5P$ close to optimal, and with this an approximation error that decays like $Ce^{-2.5P}$.

Hence, this window function shares many properties with the Gaussian, and the approximation errors decay faster with P ($Ce^{-2.5P}$ as compared to $Ce^{-\pi P/2}$). In Saffar Shamshirgar and Tornberg [ibid.] it is shown that the evaluation costs for the two window functions are comparable for the same P, and hence that the new BM window function is computationally more efficient.

4 The spectral Ewald method for different periodicities

In the previous section, we introduced the Spectral Ewald method for the triply periodic electrostatic problem. In the case of one or more non-periodic direction(s), we have to

make some modifications. Our formulas now involve integrals defining inverse Fourier transforms in Equations (18), (20) and (22), respectively. In addition, the evaluation of $H(\mathbf{x})$ in Equation (27) will be slightly different, and we start at this end.

In the triply periodic case, we introduced a uniform grid of grid size M^3 on $[0, L)^3$ with $h = L/M$. Now, we need to extend the grid in the non-periodic direction to accomodate the support of the window functions. We set $\tilde{L} = L + Ph$, and $\tilde{M} = M + P$ s.t. $h = L/M = \tilde{L}/\tilde{M}$. Approximating the Fourier integrals with the trapezoidal rule, we obtain discrete sums that can be evaluated with FFTs. The errors that we introduce are similar to the errors introduced by discretization of the integral in Equation (28), as was discussed in Section 3.2.

In analogy with the triply periodic case, we define a $\widehat{\widetilde{H}}(\mathbf{k})$ as $\widehat{\widetilde{H}}_{\mathbf{k}}$ in Equation (24) with the factor $1/k^2$ replaced by $\hat{G}^{DP}(\mathbf{k})$ (i.e. $\hat{G}^{3P}(\mathbf{k}) = 1/|\mathbf{k}|^2 = 1/k^2$). Consider e.g. the singly periodic case, then we have

$$\tilde{H}(\mathbf{x}) = \frac{1}{(2\pi)^2} \sum_{k_3} \int_{\mathbb{R}^2} \widehat{\widetilde{H}}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} \, d\kappa_1 \, d\kappa_2$$

where $\mathbf{k} = (\kappa_1, \kappa_2, k_3)$. For $k_3 \neq 0$ we have $\hat{G}^{1P}(\mathbf{k}) = 1/|\mathbf{k}|^2 = 1/(\kappa_1^2 + \kappa_2^2 + k_3^2)$ (Equation (21)). To evaluate this integral accurately for all discrete k_3 we need to discretize it on a finer grid in k-space than a regular FFT of $H(x)$ above would yield. Hence, for the $1P/2P$ cases, there are $2/1$ non-periodic directions that need this refinement.

The simplest way to achieve this is to define a global upsampling factor s_g and extend the domain to $s_g \tilde{L}$ in any non-periodic direction. This is a so-called zero padding in real space, which leads to a denser sampling of modes in Fourier space. Applying an FFT on a grid of size $s_g \tilde{M}$ in a non-periodic direction, yields a sampling in κ for $\kappa = 2\pi n/(s_g \tilde{L})$, $n = -s_g \tilde{M}/2, \ldots, s_g \tilde{M}/2 - 1$. An upsampling such that $s_g \tilde{M}$ is 4 up to 6 times larger than M can be needed depending on the accuracy requirement. This yields a large extra cost especially in the 1P case, with FFTs that are 16 or even 36 times larger than in the triply periodic case.

In Saffar Shamshirgar and Tornberg [2017b], we show that it is sufficient to apply upsampling to a band of discrete k_3 modes with small magnitude, and introduce an adaptive FFT and IFFT. With the AFFT, a typical increase in computational cost relative to the FFT without oversampling is a factor of $2-3$, with global upsampling it is $16-36$. For the doubly periodic case, upsampling is only needed in one dimension. Hence, the cost of global upsampling is not so overwhelming and was used in the first 2P implementation in Lindbo and Tornberg [2012].

In this implementation Lindbo and Tornberg [ibid.], the treatment of the zero mode $k_1 = k_2 = 0$, was done separately. In the final Ewald formula, there is an explicit 1D

sum for this term (see e.g. section 9 of Tornberg [2016]), and an expansion with Chebyshev polynomials was used for efficient evaluation. Again, moving to the singly periodic (1P) case, the corresponding term is a 2D sum, and cannot be evaluated as efficiently. This is where the idea of solving free space problems with FFTs as introduced by Vico, Greengard, and Ferrando [2016] enters. Now we consider the 2D free space Poisson problem corresponding to $k_3 = 0$ instead of the solution written as a sum in the Ewald formula. By introducing the truncated Green's function for the free space problem and then it's Fourier transform, we arrived at the definition in Equation (21) of $\hat{G}^{1P}(\mathbf{k})$ for $k_3 = 0$. It has a finite limit as $|\mathbf{k}| \to 0$, also given in the definition. Hence, this can be treated as all the other discrete k_3 modes. An oversampling factor of $s_0 = 1 + \sqrt{2}$ is sufficient for this mode. With this approach, the $k_3 = 0$ mode can be included almost for free.

This approach to solve free space problems is used for the free space case with no periodicity. With $\hat{G}^{0P}(\mathbf{k})$ defined in Equation (23), an upsampling factor of $1 + \sqrt{3}$ in each dimension is sufficient for full accuracy. A precomputation can however be made, to reduce the needed upsampling to a factor of 2, which is the minimum upsampling for computing an aperiodic convolution. This was first introduced for potentials of Stokes flow in af Klinteberg, Saffar Shamshirgar, and Tornberg [2017].

An extension of the domain length from L to $\tilde{L}$ to fit the support of the window function does not guarantee that the Gaussians in the right hand side of Equation (11) will be sufficiently decayed in this domain. As was discussed in af Klinteberg, Saffar Shamshirgar, and Tornberg [ibid.], an additional extension is however needed only if $\tilde{M}$ is picked larger than necessary for a given error tolerance (for a fixed P this reduces the support width Ph of the window function and hence $\tilde{L}$).

Very recently, we have treated all cases of periodicity in a unified framework Saffar Shamshirgar and Tornberg [2017a], also introducing the new window function as suggested by Barnett and Magland [2017]. Hence, this includes an implementation of the 2P method with both adaptive FFT and free space FFT treatment of the $k_3 = 0$ term, features that differ from the original 2P method Lindbo and Tornberg [2012].

5 Extension to fundamental solutions for Stokes flow

One fundamental solution for Stokes flow, the stokeslet, was introduced in Equation (2). The triply periodic SE method for the stokeslet is very similar in structure to that for electrostatics. We however work with vector point sources (forces) and the Fourier representation of the stokeslet is a matrix for each $\mathbf{k}$. Another important fundamental solution, needed e.g. when formulating second kind integral equations for Stokes flow, is the stresslet, as given by

$$T_{j\ell m}(\mathbf{r}) = -6\frac{r_j r_\ell r_m}{r^5} \quad j,\ell,m = 1,2,3. \tag{32}$$

The stresslet has three indicies and the triply periodic SE method will involve 6 FFTs for the source components, and three inverse FFTs for the components of the solution. Unlike the stokeslet, the stresslet does not by construction generate a divergence free velocity field. The correction term needed to impose a zero mean flow through a periodic cell was derived in af Klinteberg and Tornberg [2014]. Available truncation error estimates for the Ewald sums from Lindbo and Tornberg [2010] and af Klinteberg and Tornberg [2014] are summarized in af Klinteberg, Saffar Shamshirgar, and Tornberg [2017], as additional estimates needed for the free space case are derived.

For the free space case in af Klinteberg, Saffar Shamshirgar, and Tornberg [ibid.], we write the stokeslet and the stresslet as a differential operator acting on r, which is the Green's function for the biharmonic equation. For the stokeslet, this becomes

$$S_{j\ell} = \left(\delta_{j\ell}\nabla^2 - \nabla_j\nabla_\ell\right) r \quad j,l = 1,2,3.$$

Using the approach from Vico, Greengard, and Ferrando [2016] for the biharmonic kernel, which is a radial kernel, we can use this structure to extend the treatment to the stokeslet and the stresslet. Similarly, the rotlet is based on the harmonic kernel.

The doubly periodic case for the stokeslet was treated in Lindbo and Tornberg [2011a], in line with the 2P treatment of electrostatics in Lindbo and Tornberg [2012]. The extension to the 2P and 1P cases for both the stokeslet and stresslet in line with the new unified treatment of electrostatics as discussed in the previous section has not yet been done.

6 Summary and future work

We have in this paper reviewed the development of the Spectral Ewald methods. We have mainly considered their application to electrostatic problems, but also discussed the extension to Stokes flow. With the recent developments in Saffar Shamshirgar and Tornberg [2017b] and Saffar Shamshirgar and Tornberg [2017a], we now have a method for electrostatics that offers a unified treatment for problems with different periodicities, from triply periodic down to free space.

Compared to the triply periodic case, which is the most efficient, each non-periodic dimension increases the computational cost, but with the adaptive FFTs only to a limited amount. The cost of the algorithm associated with the window functions is essentially independent of the FFT grid size. Since that cost is reduced with the new Barnett-Magland window function, the increase in the FFT cost will have a larger impact when measuring computational cost relative to the triply periodic case. In this setting, and for typical parameter choices, we noted in Saffar Shamshirgar and Tornberg [2017b] that the doubly periodic case is only marginally more expensive than the triply periodic, and the singly periodic and free space cases are up to two and four times as expensive, respectively.

These FFT based methods are alternatives to fast multipole methods for evaluating electrostatic and Stokes potentials, and we have shown that the SE method is competitive with FMM Greengard [2012] for the free space summation of Stokes potentials, where it is at its largest disadvantage af Klinteberg, Saffar Shamshirgar, and Tornberg [2017]. We expect the SE method to do better the more periodic directions we have, and the FMM to do better relative to the SE method the more non-uniform the distribution of points get. Hence, this is not to conclude that one method is always better than the other, but only to remark that an FFT based SE method can be a competitive alternative to the FMM method. There is an additional value in having a method that can be used for different periodicities, thereby keeping the structure intact and easing the integration with the rest of the simulation code, concerning, e.g., modifications of quadrature methods in a boundary integral method to handle near interactions.

Future work involves extending the unified treatment for the harmonic kernel of electrostatics also to stokeslets and stresslets. In order for this to be possible it remains first to derive the appropriate Ewald summation formulas for the singly periodic stokeslet and for the singly and doubly periodic stresslet sums, as we are not aware of any suitable decompositions.

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Anna-Karin Tornberg
Department of Mathematics
Royal Institute of Technology (KTH)
Sweden
akto@kth.se