Fast Multipole Method for the Biharmonic Equation

Nail A. Gumerov and Ramani Duraiswami
Perceptual Interfaces and Reality Laboratory,
Department of Computer Science and UMIACS,
University of Maryland, College Park, MD 20742

May 17, 2005

Abstract

The evaluation of sums (matrix-vector products) of the solutions of the three-dimensional biharmonic equation can be accelerated using the fast multipole method, while memory requirements can also be significantly reduced. We develop a complete translation theory for these equations. It is shown that translations of elementary solutions of the biharmonic equation can be achieved by considering the translation of a pair of elementary solutions of the Laplace equations. The extension of the theory to the case of polyharmonic equations in $\mathbb{R}^3$ is also discussed. An efficient way of performing the FMM for biharmonic equations using the solution of a complex valued FMM for the Laplace equation is presented. Compared to previous methods presented for the biharmonic equation our method appears more efficient. The theory is implemented and numerical tests presented that demonstrate the performance of the method for varying problem sizes and accuracy requirements. In our implementation, the FMM for the biharmonic equation is faster than direct matrix vector product for a matrix size of 550 for a relative L_2 accuracy $\epsilon_2 = 10^{-4}$, and $N = 3550$ for $\epsilon_2 = 10^{-12}$.

1 Introduction

Many problems in fluid mechanics, elasticity, and in function fitting via radial-basis functions, at their core, require repeated evaluation of the sum

$$v(\mathbf{y}_j) = \sum_{i=1}^{N} u_i \Phi(\mathbf{y}_j - \mathbf{x}_i), \quad j = 1, ..., M \tag{1}$$

where $\Phi(\mathbf{y} - \mathbf{x}_i) : \mathbb{R}^3 \to \mathbb{R}$ is a solution of the three-dimensional biharmonic equation (e.g., the Green's function or a multipole solution) centered at $\mathbf{x}_i$.This sum must be evaluated at locations $\mathbf{y}_j$, and u_i are some coefficients. Straightforward computation of these sums, which also can be considered to be multiplication of a $M \times N$ matrix with elements $\Phi_{ji} = \Phi(\mathbf{y}_j - \mathbf{x}_i)$ by a N vector with components u_i to obtain a M vector with components $v_j = v(\mathbf{y}_j)$, obviously requires $O(MN)$ operations and $O(MN)$ memory locations to store the matrix. The point sets $\mathbf{y}_j$ (the target set) and $\mathbf{x}_i$ (the source set) in these problems may be different, or the same. If the points $\mathbf{y}_j$ and $\mathbf{x}_i$ coincide, the evaluation of Φ may have to be appropriately regularized in case Φ is singular (e.g., in a boundary element application, quadrature over the element will regularize the function). In the sequel we assume that this issue, if it arises, is dealt with, and not concern ourselves with it.

In its original form, the Fast Multipole Method, introduced by Greengard and Rokhlin [1], is an algorithm for speeding up such sums, for the case that the function Φ is a multipole of the Laplace equation. FMM inspired algorithms have since appeared for the solution of various problems of both matrices associated with the Laplace potential, and with those of other equations (the biharmonic, Helmholtz, Maxwell) and in unrelated areas (for general radial basis functions).

Previous work related to the FMM for the biharmonic equations has usually appeared in the context of Stokes flow or linear elastostatics. A description of this work may be found in the comprehensive review paper of Nishimura [2]. One approach to the FMM for sums of the biharmonic Green's function and its derivatives, avoids the problem of building a translation theory for this equation. These Green's functions are represented as sums of Laplace solutions [3]. Another approach is based on expanding the biharmonic functions in Taylor series [4, 5]. Other related FMMs are those that treat the problem of Stokes flow or linear elastostatics, but not directly applicable to the biharmonic translation, have appeared in the context of Stokes flow or elasticity. These may not have the efficiency of an FMM derived from a consideration of the elementary solutions of the biharmonic equation. Also we can mention publication [6], where kernel independent FMM is developed and applied to solution of Stokes and other equations. We elaborate on these comments in the section below.

1.1 Comparison with other FMMs for the biharmonic and related equations

Perhaps the first to apply the FMM to problems related to the three dimensional biharmonic equation was the paper by Sangani and Mo [7], who considered Stokes flow around particles. The method relied on expansions suggested by Lamb [8], and translation formulae, that are $O\left(p^4\right)$ when there are $O\left(p^2\right)$ terms in the Lamb expansion. A version of the FMM for 2D elasticity/Stokes flow that employs complex analysis was presented in Greengard et al. [9], and is thus difficult to extend to $\mathbb{R}^3$. Popov and Power [5] used Taylor series representations to develop a multipole translation theory for linear elasticity problems. Their results show a cross-over (when the FMM algorithm is faster than the direct approach) for 1.1×10^4 unknowns, though the error that is incurred is hard to establish, as they used an iteration error criterion, which does not have a corresponding value here. They mention that the largest order of Taylor series considered is 5 in their paper. Fu et al. [3], made the observation that the biharmonic Green's function, and its other derivatives could, via elementary manipulations, be written as sums of Laplace multipoles multiplied by source or target dependent coefficients. For example the biharmonic Green's function, can be written as

$$\begin{aligned} |\mathbf{x}-\mathbf{y}| &= \sqrt{(x_1-y_1)^2+(x_2-y_2)^2+(x_3-y_3)^2} \\ &= \frac{|\mathbf{x}|^2+|\mathbf{y}|^2}{|\mathbf{x}-\mathbf{y}|} - 2x_1\frac{1}{|\mathbf{x}-\mathbf{y}|}y_1 - 2x_2\frac{1}{|\mathbf{x}-\mathbf{y}|}y_2 - 2x_3\frac{1}{|\mathbf{x}-\mathbf{y}|}y_3. \end{aligned}$$

This allowed them to use an existing Laplace multipole method software and achieve an FMM for the elastostatics problem. This approach requires more Laplace solutions to represent higher order derivatives. The use of this technique for the solution of Stokes problems was presented in [10]. In these papers no explicit "break-even" data was presented.

Nishimura presents a review of the FMM work in this area (and several others) in the comprehensive review paper [2]. Yoshida et al. improved on the economy with which elasticity problem solutions were represented via Laplace solutions. They built a solution of the problem based on the Neuber-Papkovich representation of the displacement field, which can be expressed in terms of four harmonic functions. The formulation includes functions of the type $\phi(\mathbf{r})$ and $\mathbf{r}\phi(\mathbf{r})$, where ϕ is harmonic. The translation method presented in this case by Yoshida [11, 12] shows that the complexity of solution of the elastostatic problem using the FMM in these papers is equivalent to solution of four independent 3D Laplace equations. Fast translation methods for the Laplace equation presented in [13, 14] where also employed by these authors.

Another field that has seen the use of the FMM for sums of biharmonic and polyharmonic Green's functions is radial-basis interpolation. The biharmonic function is an optimal radial basis function in a certain sense [15], and scattered data interpolation using these in $\mathbb{R}^3$ has been pursued by many authors. Chen and Suter [4] used a Taylor series based FMM to speed the evaluation of spline interpolated 3D data. From their results a cross-over point of 13000 for $p = 3$ and of 18000 for $p = 4$ can be inferred. Carr et al. [16] report on the application of the FMM to a problem of interpolation with biharmonic splines. They do not present any details of how their FMM is developed and refer to some unpublished work. Published work of these authors for the case of the multiquadric function, which arises from regularizing the biharmonic Green's function, is given in [17]. Here, the authors employ special polynomial expansions for translation and polynomial convolution for fast translation. It reports a cross-over point for the $\mathbb{R}^3$ multiquadric of between 2000 and 4000 for an accuracy of 10^{-6}.

1.2 Contributions of this paper

The work presented in this paper thus appears to differ substantially from those in the literature. It presents a complete multipole translation theory for the biharmonic and polyharmonic equations in $\mathbb{R}^3$, which is of utility in its own right. Further, we present an efficient way of dealing with translations and the FMM and present cross-over results which appear to be significantly faster.

Translation Theory for the Biharmonic Equation: We develop a translation theory for the solutions of the biharmonic (and polyharmonic) equation from first principles. As is well known, solutions to the biharmonic equation Φ can be expressed as a pair of solutions to the Laplace equation (ϕ, ψ) so that

$$\Phi(\mathbf{r}) = \phi(\mathbf{r}) + (\mathbf{r}\cdot\mathbf{r})\,\psi(\mathbf{r}).$$

Our translation theory *maintains this form of the solution* so that, the translated representation of a solution $\Phi(\mathbf{r})$ in a new coordinate system, $\hat{\Phi}(\hat{\mathbf{r}})$ can be represented as

$$\hat{\Phi}(\hat{\mathbf{r}}) = \hat{\phi}(\hat{\mathbf{r}}) + (\hat{\mathbf{r}}\cdot\hat{\mathbf{r}})\,\psi(\hat{\mathbf{r}}).$$

We note that the representation in terms of the solutions of the Laplace equations applies for any biharmonic functions (e.g., the Green's function, its derivatives), and the number of Laplace equation solutions in the representation is always two. A complete error analysis of the translation is provided, and efficient methods for translation using a rotation, coaxial-translation, rotation scheme similar to that presented in [18] for the Laplace equation, and elaborated in [19] is described. Explicit expressions for the translation operator are derived, as these are useful in their own right, such as for the solution of boundary value problems (see e.g., [20, 21]). We also discuss the extension of this method to the solutions of the polyharmonic equation.

Efficient Implementation and Testing in a Complex Laplace FMM Code: We present a method to implement the FMM for the real biharmonic equation as a single complex FMM for the Laplace equation. This observation allows us to use a very efficient Laplace FMM software we have developed [19]. We present a complete testing of the algorithm for various problem sizes and imposed accuracy requirements. We first show that our algorithm obeys the derived error bounds well. The FMM for the biharmonic equation is found to require about 50 percent more time than the corresponding case for the Laplace equation. We observe a crossover (i.e., when the FMM is faster than direct multiplication that is given in the table below.

Relative L_2 error imposed	p	Cross over N biharmonic	Cross over N Laplace for same p
10^{-4}	4	550	320
10^{-7}	9	1350	900
10^{-12}	19	3400	2500

2 Factored solutions of the biharmonic equation

2.1 Spherical basis functions

We consider the biharmonic equation in 3-D satisfied by a function $\psi(\mathbf{r})$, and given by

$$\nabla^4 \psi = 0, \tag{2}$$

where ∇^2 is the Laplace operator $\nabla \cdot (\nabla)$. The transformation between spherical coordinates and Cartesian coordinates with a common origin $(x, y, z) \to (r, \theta, \varphi)$ is given by

$$x = r \sin\theta \cos\varphi, \quad y = r \sin\theta \sin\varphi, \quad z = r \cos\theta. \tag{3}$$

The gradient and Laplacian of a function ψ in spherical coordinates are

$$\nabla \psi = \mathbf{i}_r \frac{\partial \psi}{\partial r} + \mathbf{i}_\theta \frac{1}{r} \frac{\partial \psi}{\partial \theta} + \mathbf{i}_\varphi \frac{1}{r \sin\theta} \frac{\partial \psi}{\partial \varphi}, \tag{4}$$
$$\nabla \cdot (\nabla \psi) = \nabla^2 \psi = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2 \psi}{\partial \varphi^2}.$$

where $(\mathbf{i}_r, \mathbf{i}_\theta, \mathbf{i}_\varphi)$ is a right-handed orthonormal basis in spherical coordinates.

Solutions of the biharmonic equation in spherical coordinates can be expressed in the factored form ("separation of variables")

$$\psi_n^m(r, \theta, \varphi) = \Pi_n(r) \Theta_n^m(\theta) \Phi^m(\varphi), \tag{5}$$

where the function Θ_n^m is periodic with period π and Φ^m is periodic with period 2π. The spherical harmonics provide such a periodic basis

$$Y_n^m(\theta, \varphi) = \Theta_n^m(\theta) \Phi^m(\varphi) = N_n^m P_n^{|m|}(\mu) e^{im\varphi}, \quad \mu = \cos\theta, \tag{6}$$
$$N_n^m = (-1)^m \sqrt{\frac{2n+1}{4\pi} \frac{(n-|m|)!}{(n+|m|)!}}, \quad n = 0, 1, 2, ...; \quad m = -n, ..., n,$$

where $P_n^{|m|}(\mu)$ are the associated Legendre functions [22]. The spherical harmonics are also sometimes called surface harmonics of the first kind, tesseral for $m < n$ and sectorial for $m = n$. We will use the definition of the associated Legendre function $P_n^m(\mu)$ that is consistent with the value on the cut $(-1, 1)$ of the hypergeometric function $P_n^m(z)$ (see Abramowitz and Stegun, [22]). These functions can be obtained from the Legendre polynomials $P_n(\mu)$ via the Rodrigues' formula

$$P_n^m(\mu) = (-1)^m \left(1 - \mu^2\right)^{m/2} \frac{d^m}{d\mu^m} P_n(\mu), \quad P_n(\mu) = \frac{1}{2^n n!} \frac{d^n}{d\mu^n} \left(\mu^2 - 1\right)^n. \tag{7}$$

Our definition of spherical harmonics coincides with that of Epton and Dembart [23], except for a factor $\sqrt{(2n+1)/4\pi}$, which we include to make them an orthonormal basis over the sphere.

The dependence of the function Π_n on the radial coordinate, in Eq. (5), is described by

$$\left[\frac{d}{dr}\left(r^2\frac{d}{dr}\right)-n(n+1)\right]^2\Pi_n=0. \tag{8}$$

This equation has four linearly independent solutions of type $\Pi_n = r^\alpha$ for $\alpha = n+2, n, -n+1$, and $-n-1$. So we the biharmonic equation has the following elementary solutions:

$$\begin{aligned} R_n^m(\mathbf{r}) &= \alpha_n^m r^n Y_n^m(\theta,\varphi), \quad R_{(2)n}^m(\mathbf{r}) = r^2 R_n^m(\mathbf{r}), \\ S_n^m(\mathbf{r}) &= \beta_n^m r^{-n-1} Y_n^m(\theta,\varphi), \quad S_{(2)n}^m(\mathbf{r}) = r^2 S_n^m(\mathbf{r}), \\ n &= 0,1,2,...; \quad m=-n,...,n. \end{aligned} \tag{9}$$

where $\alpha_n^m$and β_n^m are some normalization constants, which can be set to the unity or selected by special way to simplify recursion and other functional relations between the elementary solutions. We note that the R-solutions are regular inside any finite domain, while the S-solutions have a singularity at $r=0$. Function $S_{(2)0}^0(\mathbf{r}) \sim r$ is finite at $r=0$, while its derivatives are singular at this point. This function is proportional to the whole-space Green's function for the biharmonic operator, $G(\mathbf{r},\mathbf{r}_0) = |\mathbf{r}-\mathbf{r}_0|$, which satisfies

$$\nabla^4 G(\mathbf{r},\mathbf{r}_0) = \nabla^4|\mathbf{r}-\mathbf{r}_0| = -8\pi\delta(\mathbf{r}-\mathbf{r}_0), \tag{10}$$

where δ is the Dirac delta-function. We also note that solutions $R_n^m(\mathbf{r})$ and $S_n^m(\mathbf{r})$ are solutions of the Laplace equation, $\nabla^2\psi = 0$, in finite and infinite domains (in the later case the origin is excluded) and function $S_{(1)0}^0(\mathbf{r}) \sim r^{-1}$ is proportional to the whole-space Green's function for the Laplace operator, $|\mathbf{r}-\mathbf{r}_0|^{-1}$.

2.2 Factorization of the Green's function

Let us start by considering factorization of the biharmonic Green's function $G(\mathbf{r},\mathbf{r}_0) = |\mathbf{r}-\mathbf{r}_0|$, where $\mathbf{r}_0$ can be thought as the location of source, and $\mathbf{r}$ as the field point. Due to the symmetry the role of these points can be exchanged. Assuming $r_0 = |\mathbf{r}_0| > 0$ consider the field of the source in the vicinity of the origin for $r = |\mathbf{r}| < r_0$. The Green's function can be written as

$$\begin{aligned} G(\mathbf{r},\mathbf{r}_0) &= [(\mathbf{r}-\mathbf{r}_0,\mathbf{r}-\mathbf{r}_0)]^{1/2} = \left(r^2-2rr_0\cos\gamma+r_0^2\right)^{1/2} = \frac{r^2-2rr_0\cos\gamma+r_0^2}{\left(r^2-2rr_0\cos\gamma+r_0^2\right)^{1/2}} \\ &= \left(r^2-2rr_0\cos\gamma+r_0^2\right)\frac{1}{r_0}\sum_{n=0}^{\infty}\left(\frac{r}{r_0}\right)^n P_n(\cos\gamma), \quad r<r_0, \end{aligned} \tag{11}$$

where γ is the angle between vectors $\mathbf{r}$ and $\mathbf{r}_0$ and we used the generating function for the Legendre polynomials. Using the recurrence relation for the Legendre polynomials $(2n+1)\mu P_n(\mu) = nP_{n-1}(\mu) + (n+1)P_{n+1}(\mu)$ this can be rewritten in the form

$$G(\mathbf{r},\mathbf{r}_0) = \sum_{n=0}^{\infty}\left(\frac{r_0^{-n-1}r^{n+2}}{2n+3} - \frac{r_0^{-n+1}r^n}{2n-1}\right)P_n(\cos\gamma), \quad r<r_0, \tag{12}$$

Further we will use the addition theorem for spherical harmonics in the form

$$P_n(\cos\gamma) = \frac{4\pi}{2n+1}\sum_{m=-n}^{n} Y_n^{-m}(\theta_0,\varphi_0)Y_n^m(\theta,\varphi), \tag{13}$$

where (θ_0, φ_0) and (θ, φ) are spherical polar angles of $\mathbf{r}_0$ and $\mathbf{r}$, respectively. Substituting this into Eq. (12) and using definitions (9), we obtain the following factorization of the Green's function for the biharmonic equation

$$G(\mathbf{r}, \mathbf{r}_0) = 4\pi \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{1}{\alpha_n^m \beta_n^{-m}(2n+1)} \left[\frac{S_n^{-m}(\mathbf{r}_0) R_{(2)n}^m(\mathbf{r})}{2n+3} - \frac{S_{(2)n}^{-m}(\mathbf{r}_0) R_n^m(\mathbf{r})}{2n-1} \right], \quad r < r_0. \quad (14)$$

Note that factorization of the Green's function for the Laplace equation can be written in the form

$$|\mathbf{r} - \mathbf{r}_0|^{-1} = \frac{1}{r_0} \sum_{n=0}^{\infty} \left(\frac{r}{r_0} \right)^n P_n(\cos\gamma) = 4\pi \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{S_n^{-m}(\mathbf{r}_0) R_n^m(\mathbf{r})}{\alpha_n^m \beta_n^{-m}(2n+1)}, \quad r < r_0. \quad (15)$$

2.3 Reduction of the solution of biharmonic equation to solution of two harmonic equations

There are several ways how to deal with factored solutions of the harmonic and biharmonic equations. The first way is to develop a translation theory for the biharmonic equation, similarly to the available theories for the Laplace equation (e.g., [1, 24, 14, 23]). We developed all necessary formulae to proceed in this way. However, in our study we found a second way, which simply reduces solution of the biharmonic equation to two harmonic equations with some modification of the translation operators. Computationally both methods have about the same complexity, and since the latter method seems simpler in terms of presentation and background theory, we will proceed in this paper with it.

The method is based on the observation that any solution of the biharmonic equation $\psi(\mathbf{r})$ can be expressed via two independent solutions of the Laplace equation, $\phi(\mathbf{r})$ and $\omega(\mathbf{r})$:

$$\psi(\mathbf{r}) = \phi(\mathbf{r}) + r^2\omega(\mathbf{r}), \quad \nabla^2\phi(\mathbf{r}) = 0, \quad \nabla^2\omega(\mathbf{r}) = 0, \quad \nabla^4\psi(\mathbf{r}) = 0, \quad r^2 = \mathbf{r}\cdot\mathbf{r}. \quad (16)$$

Therefore if we be able to perform operations required for the FMM for the harmonic functions and then modify them for compositions of type (16) we can solve the biharmonic equation with the same method.

2.4 Function representations and translations

One of the key parts of the FMM is the translation theory. Let $\psi(\mathbf{r})$ be an arbitrary scalar function, $\psi : \Omega(\mathbf{r}) \to \mathbb{C}$, where $\Omega(\mathbf{r}) \subset \mathbb{R}^3$. For a given vector $\mathbf{t} \in \mathbb{R}^3$ We define a new function $\widehat{\psi} : \widehat{\Omega}(\mathbf{r}) \to \mathbb{C}$, $\widehat{\Omega}(\mathbf{r}) \subset \mathbb{R}^3$ such that in $\widehat{\Omega}(\mathbf{r}) = \Omega(\mathbf{r}+\mathbf{t})$ the values of $\widehat{\psi}(\mathbf{r})$ coincide with the values of $\psi(\mathbf{r}+\mathbf{t})$ and treat $\widehat{\psi}(\mathbf{r})$ as a result of action of translation operator $\mathcal{T}(\mathbf{t})$ on $\psi(\mathbf{r})$:

$$\widehat{\psi} = \mathcal{T}(\mathbf{t})[\psi], \quad \widehat{\psi}(\mathbf{r}) = \psi(\mathbf{r}+\mathbf{t}), \quad \mathbf{r} \in \widehat{\Omega}(\mathbf{r}) \subset \mathbb{R}^3. \quad (17)$$

A function can be represented by an infinite set of coefficients derived by taking its scalar product with basis functions. For example, let $\phi(\mathbf{r})$ be a regular solution of the Laplace equation inside a sphere Ω_a of radius a, that includes the origin of the reference frame. Then it can be represented in the form

$$\phi(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \phi_n^m R_n^m(\mathbf{r}), \quad (18)$$

where ϕ_n^m are the expansion coefficients over the basis $\{R_n^m(\mathbf{r})\}$. Similarly we can consider a solution of the Laplace equation $\phi(\mathbf{r})$ which is regular outside the sphere Ω_a in which case it can be expanded over the basis functions $\{S_n^m(\mathbf{r})\}$. The translated function $\widehat{\phi}(\mathbf{r})$ can also be expanded over bases $\{R_n^m(\mathbf{r})\}$ or $\{S_n^m(\mathbf{r})\}$ with expansion coefficients $\widehat{\phi}_n^m$. Due to linearity of the translation operator the sets $\left\{\widehat{\phi}_n^m\right\}$ and $\{\phi_n^m\}$ are related by a linear operator, which can be represented as a translation matrix, which is a representation of the translation operator in the respective bases. The entries of the translation matrix can be found by reexpansion of the elementary solutions, which can be written in the form of addition theorems

$$
\begin{aligned}
R_n^m(\mathbf{r}+\mathbf{t}) &= \sum_{n'=0}^{\infty}\sum_{m'=-n'}^{n'} (R|R)_{n'n}^{m'm}(\mathbf{t}) R_{n'}^{m'}(\mathbf{r}), \qquad (19)\\
S_n^m(\mathbf{r}+\mathbf{t}) &= \sum_{n'=0}^{\infty}\sum_{m'=-n'}^{n'} (S|R)_{n'n}^{m'm}(\mathbf{t}) R_{n'}^{m'}(\mathbf{r}), \quad |\mathbf{r}|<|\mathbf{t}|,\\
S_n^m(\mathbf{r}+\mathbf{t}) &= \sum_{n'=0}^{\infty}\sum_{m'=-n'}^{n'} (S|S)_{n'n}^{m'm}(\mathbf{t}) S_{n'}^{m'}(\mathbf{r}), \quad |\mathbf{r}|>|\mathbf{t}|,
\end{aligned}
$$

where $\mathbf{t}$ is the translation vector, and $(R|R)_{n'n}^{m'm}$, $(S|R)_{n'n}^{m'm}$, and $(S|S)_{n'n}^{m'm}$ are the four index regular-to-regular, singular-to-regular, and singular-to-singular reexpansion coefficients (sometimes called also local-to-local, multipole-to-local, and multipole-to-multipole translation coefficients). Explicit expressions for these coefficients for the Laplace equation can be found elsewhere (see e.g., [23, 19]). For example, if we have two expansions, one as in (18), and the other as

$$
\widehat{\phi}(\mathbf{r}) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \widehat{\phi}_n^m R_n^m(\mathbf{r}), \qquad (20)
$$

over the same basis, then we also can write

$$
\begin{aligned}
\sum_{n=0}^{\infty}\sum_{m=-n}^{n} \widehat{\phi}_n^m R_n^m(\mathbf{r}) &= \widehat{\phi}(\mathbf{r}) = \phi(\mathbf{r}+\mathbf{t}) = \sum_{n'=0}^{\infty}\sum_{m'=-n'}^{n'} \phi_{n'}^{m'} R_{n'}^{m'}(\mathbf{r}+\mathbf{t}) \qquad (21)\\
&= \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left[\sum_{n'=0}^{\infty}\sum_{m'=-n'}^{n'} (R|R)_{nn'}^{mm'}(\mathbf{t})\phi_{n'}^{m'}\right] R_n^m(\mathbf{r}),
\end{aligned}
$$

which shows that

$$
\widehat{\phi}_n^m = \sum_{n'=0}^{\infty}\sum_{m'=-n'}^{n'} (R|R)_{nn'}^{mm'}(\mathbf{t})\phi_{n'}^{m'}, \qquad (22)
$$

assuming that all the series converge absolutely and uniformly.

Consider now translation of solution of the biharmonic equation represented in form (16). We have

$$
\begin{aligned}
\widehat{\psi}(\mathbf{r}) &= \mathcal{T}(\mathbf{t})[\psi(\mathbf{r})] = \mathcal{T}(\mathbf{t})[\phi(\mathbf{r}) + (\mathbf{r}\cdot\mathbf{r})\,\omega(\mathbf{r})] = \phi(\mathbf{r}+\mathbf{t}) + [(\mathbf{r}+\mathbf{t})\cdot(\mathbf{r}+\mathbf{t})]\,\omega(\mathbf{r}+\mathbf{t}) \qquad (23)\\
&= \widehat{\phi}(\mathbf{r}) + \left[r^2 + 2(\mathbf{r}\cdot\mathbf{t}) + t^2\right]\widehat{\omega}(\mathbf{r}).
\end{aligned}
$$

If we want now to represent the translated solution in the form (16), i.e.

$$
\widehat{\psi}(\mathbf{r}) = \widetilde{\phi}(\mathbf{r}) + r^2\widetilde{\omega}(\mathbf{r}), \qquad (24)
$$

then we need to relate the expansion coefficients of functions $\widetilde{\phi}(\mathbf{r})$ and $\widetilde{\omega}(\mathbf{r})$ and $\widehat{\phi}(\mathbf{r})$ and $\widehat{\omega}(\mathbf{r})$. Assuming that all these harmonic functions are represented in the same basis, e.g. $\{R_n^m(\mathbf{r})\}$ and noting that $\widetilde{\omega}(\mathbf{r})$ depends on $\widehat{\omega}(\mathbf{r})$ only ($\widehat{\phi}(\mathbf{r})$ does not contribute to the non-harmonic function $r^2\widetilde{\omega}(\mathbf{r})$), we can write taking into account the linearity of all operations considered:

$$\widetilde{\phi}_n^m = \sum_{n'=0}^{\infty}\sum_{m'=-n'}^{n'} \widehat{\phi}_{n'}^{m'} + \sum_{n'=0}^{\infty}\sum_{m'=-n'}^{n'} C_{(1)nn'}^{mm'}(\mathbf{t})\,\widehat{\omega}_{n'}^{m'}, \quad \widetilde{\omega}_n^m = \sum_{n'=0}^{\infty}\sum_{m'=-n'}^{n'} C_{(2)nn'}^{mm'}(\mathbf{t})\,\widehat{\omega}_{n'}^{m'}, \tag{25}$$

where $C_{(1)nn'}^{mm'}$ and $C_{(2)nn'}^{mm'}$ are the entries of the matrices, which we can call "conversion" matrices, once they convert solution from the form (23) to a standard form (24). These matrices depend in which basis $\{R_n^m(\mathbf{r})\}$ or $\{S_n^m(\mathbf{r})\}$ the conversion is performed. As follows from the consideration below these matrices are sparse and the conversion operation is computationally cheap compared to the translation operation.

Finally we note that in the FMM we do not translate the function, but rather change the center of expansion. For example, by local-to-local translation from center $\mathbf{r}_{*1}$ to center $\mathbf{r}_{*2}$ we mean representation of the *same* function in the regular bases centered at these point respectively. Since for representations of the same function we have

$$\sum_{n=0}^{\infty}\sum_{m=-n}^{n} \phi_n^m R_n^m(\mathbf{r}-\mathbf{r}_{*1}) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \widehat{\phi}_n^m R_n^m(\mathbf{r}-\mathbf{r}_{*2}), \tag{26}$$

it is not difficult to see that the expansion coefficients are related by Eq. (22), where the translation vector is $\mathbf{t} = \mathbf{r}_{*2}-\mathbf{r}_{*1}$.The same relates to the multipole-to-local and multipole-to-multipole translations, where we use the $S|R$ and $S|S$ matrices instead of the $R|R$ translation matrix. Normalized elementary solutions of the Laplace equation

Normalization factors α_n^m and β_n^m in Eq. (9) can be selected arbitrarily. For example, all of these coefficients can be set to be equal 1. However, we can choose these coefficients in a way that differential and translation relations take some simple, or convenient for operation form, as will be done below. This follows Epton and Dembart [23] who used the following normalization for the spherical basis functions for the Laplace equation:

$$\begin{aligned} \alpha_n^m &= (-1)^n\, i^{-|m|}\sqrt{\frac{4\pi}{(2n+1)\,(n-m)!(n+m)!}}, \quad \beta_n^m = i^{|m|}\sqrt{\frac{4\pi\,(n-m)!(n+m)!}{2n+1}}, \\ n &= 0,1,...., \quad m=-n,...,n. \end{aligned} \tag{27}$$

2.4.1 Differential relations

Let us introduce new independent variables ξ and η instead of Cartesian coordinates x and y according to

$$\xi = \frac{x+iy}{2}, \quad \eta = \frac{x-iy}{2}; \quad x=\xi+\eta, \quad y=-i(\xi-\eta). \tag{28}$$

We can then consider the following differential operators

$$\partial_z = \frac{\partial}{\partial z}, \quad \partial_\eta = \frac{\partial}{\partial x} + i\frac{\partial}{\partial y}, \quad \partial_\xi \equiv \frac{\partial}{\partial x} - i\frac{\partial}{\partial y}. \tag{29}$$

It is shown in Ref. [23] that the differentiation relations for normalized elementary solutions of the Laplace equation can be written as

$$
\begin{aligned}
\partial_z R_n^m(\mathbf{r}) &= -R_{n-1}^m(\mathbf{r}), \quad \partial_z S_n^m(\mathbf{r}) = -S_{n+1}^m(\mathbf{r}), \\
\partial_\eta R_n^m(\mathbf{r}) &= iR_{n-1}^{m+1}(\mathbf{r}), \quad \partial_\eta S_n^m(\mathbf{r}) = iS_{n+1}^{m+1}(\mathbf{r}), \\
\partial_\xi R_n^m(\mathbf{r}) &= iR_{n-1}^{m-1}(\mathbf{r}), \quad \partial_\xi S_n^m(\mathbf{r}) = iS_{n+1}^{m-1}(\mathbf{r}).
\end{aligned}
\tag{30}
$$

2.4.2 Polynomial representations

It is noticeable, that functions $R_n^m(\mathbf{r})$ are polynomials of variables (ξ, η, z). This fact is well-known as the regular solutions of the Laplace equation can be expressed via the polynomial basis. For particular normalization (27) the explicit expressions are the following

$$
\begin{aligned}
R_n^m(\mathbf{r}) &= \sum_{l=0}^{n-|m|} (-1)^l\, i^{n-l} \sigma_{n-l}^m \frac{\xi^{(n+m-l)/2} \eta^{(n-m-l)/2} z^l}{\left(\frac{n+m-l}{2}\right)! \left(\frac{n-m-l}{2}\right)! l!}, \\
\sigma_n^m &= \begin{cases} 1, & n+m = 2k \\ 0, & n+m = 2k+1 \end{cases}, \quad k = 0, \pm 1, \ldots,
\end{aligned}
\tag{31}
$$

where we introduced symbol σ_n^m which is 1 for even $n+m$ and zero otherwise. This expression can be derived by considering differential relations (30) recursively, and taking into account that $R_0^0(\mathbf{r}) = 1$, or can be proved using induction and the same differential relations. Note that according Eqs. (9) and (27) we have

$$
S_n^m(\mathbf{r}) = \frac{\beta_n^m}{\alpha_n^m} r^{-2n-1} R_n^m(\mathbf{r}) = (-1)^{n+m} (n-m)!(n+m)! r^{-2n-1} R_n^m(\mathbf{r}). \tag{32}
$$

So Eqs. (28) and (31) yield the following expression for these functions

$$
S_n^m(\mathbf{r}) = \frac{(-1)^{n+m}(n-m)!(n+m)!}{r^{2n+1}} \sum_{l=0}^{n-|m|} \frac{(-1)^l\, i^{n-l} \sigma_{n-l}^m \xi^{(n+m-l)/2} \eta^{(n-m-l)/2} z^l}{\left(\frac{n+m-l}{2}\right)! \left(\frac{n-m-l}{2}\right)! l!}, \quad r^2 = 4\xi\eta + z^2. \tag{33}
$$

2.4.3 Reexpansion coefficients

The use of the normalized basis functions yields extremely simple expressions for the reexpansion coefficients entering Eq. (19) [23]:

$$
\begin{aligned}
(R|R)_{n'n}^{m'm}(\mathbf{t}) &= R_{n-n'}^{m-m'}(\mathbf{t}), \quad |m'| \leqslant n', \\
(S|R)_{n'n}^{m'm}(\mathbf{t}) &= S_{n+n'}^{m-m'}(\mathbf{t}), \quad |m'| \leqslant n', \quad |m| \leqslant n, \\
(S|S)_{n'n}^{m'm}(\mathbf{t}) &= R_{n'-n}^{m-m'}(\mathbf{t}), \quad |m| \leqslant n.
\end{aligned}
\tag{34}
$$

2.4.4 Factorization of the Green's function

For the Green's function for the Laplace equation we can rewrite Eq. (15) using the normalized basis functions

$$
|\mathbf{r} - \mathbf{r}_0|^{-1} = 4\pi \sum_{n=0}^{\infty} \sum_{m=-n}^{n} (-1)^n S_n^{-m}(\mathbf{r}_0) R_n^m(\mathbf{r}), \quad r < r_0. \tag{35}
$$

Factorization of the Green's function for the biharmonic equation (14) can be written as

$$G(\mathbf{r},\mathbf{r}_0) = r^2 \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \frac{(-1)^n S_n^{-m}(\mathbf{r}_0) R_n^m(\mathbf{r})}{2n+3} - r_0^2 \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \frac{(-1)^n S_n^{-m}(\mathbf{r}_0) R_n^m(\mathbf{r})}{2n-1}, \quad r < r_0. \tag{36}$$

This is consistent with decomposition of an arbitrary solution in form (16).

2.5 Rotational-coaxial translation decomposition

If the infinite series over the basis functions of type (18) are truncated with p terms with respect to degree n ($n = 0, ..., p-1$) the total number of expansion coefficients for basis functions of the first kind will be p^2. Translations using the dense truncated reexpansion matrices of size $p^2 \times p^2$ performed by straightforward way will require then $O(p^4)$ operations. This cost can be reduced to $O(p^3)$ using the rotational-coaxial translational decomposition (or "point-and-shoot" method in Rokhlin's terminology) (e.g. see [18, 19]), since the rotations and coaxial translations can be performed at a cost of $O(p^3)$ operations. We also note that at the rotation transforms solution of the biharmonic equation given in form (16) remains in the same form, since the rotation transform preserves r^2. This method was described first in Ref. [18].

2.5.1 Coaxial translations

A coaxial translation is translation along the polar axis or the z-coordinate axis, i.e. this is the case when the translation vector $\mathbf{t} = t\mathbf{i}_z$, where $\mathbf{i}_z$ is the basis unit vector for the z-axis. The peculiarity of the coaxial translation is that it does not change the order m of the translated coefficients, and so translation can be performed for each order independently. For example, Eq. (22) for the coaxial local-to-local translation will be reduced to

$$\widehat{\phi}_n^m = \sum_{n'=|m|}^{\infty} (R|R)_{nn'}^m(t)\phi_{n'}^m, \quad m = 0, \pm 1, ..., \quad n = |m|, |m|+1, ... \tag{37}$$

The three index coaxial reexpansion coefficients $(F|E)_{nn'}^m$ ($F, E = S, R$; $m = 0, \pm 1, \pm 2, ...,\quad n, n' = |m|, |m|+1, ...$) are functions of the translation distance t only and can be expressed via the general reexpansion coefficients as

$$(F|E)_{nn'}^m(t) = (F|E)_{nn'}^{mm}(t\mathbf{i}_z), \quad F, E = S, R; \quad t \geqslant 0. \tag{38}$$

Using Eq. (34) we have for normalized basis functions with α_n^m and β_n^m from (27):

$$\begin{aligned} (R|R)_{nn'}^m(t) &= r_{n'-n}(t), \quad n' \geqslant |m|, \\ (S|R)_{nn'}^m(t) &= s_{n+n'}(t), \quad n, n' \geqslant |m|, \\ (S|S)_{nn'}^m(t) &= r_{n-n'}(t), \quad n \geqslant |m|, \end{aligned} \tag{39}$$

where the functions $r_n(t)$ and $s_n(t)$ are

$$r_n(t) = \frac{(-t)^n}{n!}, \quad s_n(t) = \frac{n!}{t^{n+1}} \quad n = 0, 1, ..., \quad t \geqslant 0, \tag{40}$$

and zero for $n < 0$. This show that for given m matrices $\{(R|R)_{nn'}^m(t)\}$ are upper triangular, $\{(S|S)_{nn'}^m(t)\}$ are lower triangular, and $\{(S|R)_{nn'}^m(t)\}$ is a fully populated matrix. The latter matrix is symmetric, while $\{(S|S)_{nn'}^m(t)\} = \{(R|R)_{n'n}^m(t)\}$, i.e. these matrices are transposes of each other. It is also important to note that the coaxial translation matrices are real.

2.5.2 Rotations

To perform translation with an arbitrary vector **t** using the computationally cheap coaxial translation operators, we first must rotate the original reference frame to align the z-axis of the rotated reference frame with **t**, translate and then perform an inverse rotation.

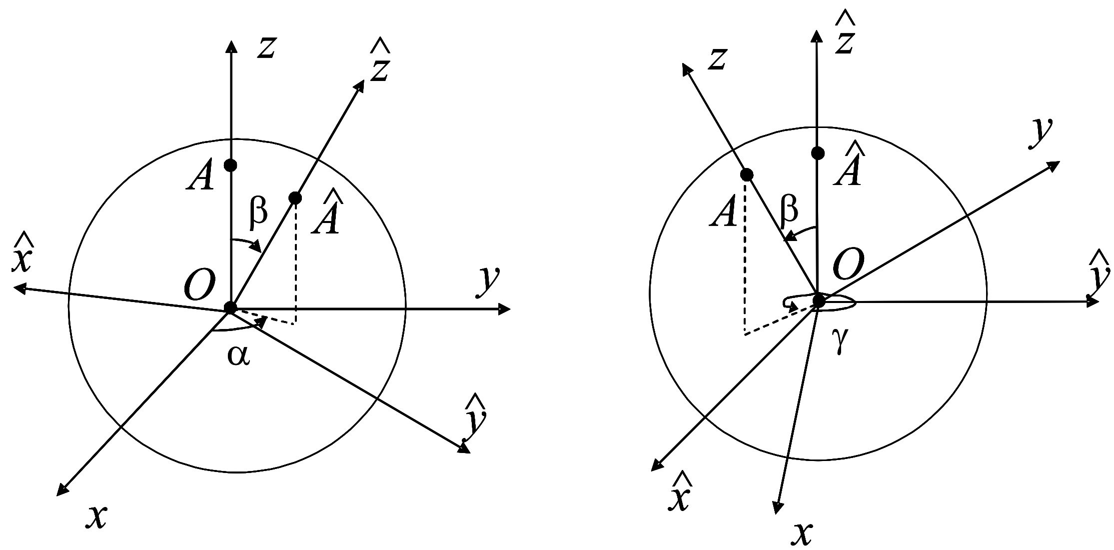

Figure 1: The figure on the left shows the transformed axes $(\hat{x}, \hat{y}, \hat{z})$ in the original reference frame (x, y, z). The spherical polar coordinates of the point $\hat{A}$ lying on the $\hat{z}$ axis on the unit sphere are (β, α). The figure on the right shows the original axes (x, y, z) in the transformed reference frame $(\hat{x}, \hat{y}, \hat{z})$. The coordinates of the point A lying on the z axis on the unit sphere are (β, γ). The points O, A, and $\hat{A}$ are the same in both figures. All rotation matrices can be derived in terms of these three angles α, β, γ.

An arbitrary rotation in three dimensions can be characterized by three Euler angles, or angles α, β, and γ that are simply related to them. For the forward rotation, when (θ, φ) are the spherical polar angles of the rotated z-axis in the original reference frame, then $\beta = \theta$, $\alpha = \varphi$; for the inverse rotation with $\left(\widehat{\theta}, \widehat{\varphi}\right)$ the spherical polar angles of the original z-axis in the rotated reference frame, $\beta = \widehat{\theta}$, $\gamma = \widehat{\varphi}$ (see Fig. 1). An important property of the spherical harmonics is that their degree n does not change on rotation, i.e.

$$Y_n^m(\theta, \varphi) = \sum_{m'=-n}^{n} T_n^{m'm}(\alpha, \beta, \gamma) Y_n^{m'}\left(\widehat{\theta}, \widehat{\varphi}\right), \quad n = 0, 1, 2, ..., \quad m = -n, ..., n, \tag{41}$$

where (θ, φ) and $\left(\widehat{\theta}, \widehat{\varphi}\right)$ are spherical polar angles of the same point on the unit sphere in the original and the rotated reference frames, and $T_n^{m'm}(\alpha, \beta, \gamma)$ are the rotation coefficients.

Rotation transform for solution of the Laplace equation factorized over the regular spherical basis functions (9) can be performed as

$$\begin{aligned}\phi(\mathbf{r}) &= \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\phi_n^m R_n^m(\mathbf{r}) = \sum_{n=0}^{\infty} r^n \sum_{m=-n}^{n}\phi_n^m \alpha_n^m Y_n^m(\theta,\varphi) \\ &= \sum_{n=0}^{\infty}\sum_{m'=-n}^{n}\left[\sum_{m=-n}^{n} T_n^{m'm}(\alpha,\beta,\gamma)\,\alpha_n^m \phi_n^m\right] r^n Y_n^{m'}\left(\widehat{\theta},\widehat{\varphi}\right) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\widehat{\phi}_n^m R_n^m(\widehat{\mathbf{r}}),\end{aligned} \tag{42}$$

where $\mathbf{r}$ and $\widehat{\mathbf{r}}$ are coordinates of the same field point in the original and rotated frames, while ϕ_n^m and $\widehat{\phi}_n^m$ are the respective expansion coefficients related as

$$\widehat{\phi}_n^m = \sum_{m'=-n}^{n}\frac{T_n^{mm'}(\alpha,\beta,\gamma)\,\alpha_n^{m'}}{\alpha_n^m}\phi_n^{m'}. \tag{43}$$

The same holds for the multipole expansions where in Eq. (43) we replace the normalization constants α_n^m and $\alpha_n^{m'}$ with β_n^m and $\beta_n^{m'}$, respectively. In case $\alpha_n^m = \beta_n^m$ the rotation coefficients for the regular and singular basis functions are the same.

The rotation coefficients $T_n^{m'm}(\alpha,\beta,\gamma)$ can be decomposed as

$$T_n^{m'm}(\alpha,\beta,\gamma) = e^{im\alpha}e^{-im'\gamma}H_n^{m'm}(\beta), \tag{44}$$

where $\left\{H_n^{m'm}(\beta)\right\}$ is a dense real symmetric matrix. Its entries can be computed using an analytical expression, or by a fast recursive procedure (see [19]), which starts with the initial value

$$H_n^{m'0}(\beta) = (-1)^{m'}\sqrt{\frac{(n-|m'|)!}{(n+|m'|)!}}P_n^{|m'|}(\cos\beta), \quad n=0,1,..., \quad m'=-n,...,n, \tag{45}$$

and further propagates for positive m:

$$H_{n-1}^{m',m+1} = \frac{1}{b_n^m}\left\{\frac{1}{2}\left[b_n^{-m'-1}(1-\cos\beta)H_n^{m'+1,m} - b_n^{m'-1}(1+\cos\beta)H_n^{m'-1,m}\right] - a_{n-1}^{m'}\sin\beta H_n^{m'm}\right\}, \tag{46}$$

where $n=2,3,...,\quad m'=-n+1,...,n-1,\quad m=0,...,n-2$, and $a_n^m = b_n^m = 0$ for $n<|m|$, and

$$\begin{aligned} a_n^m &= a_n^{-m} = \sqrt{\frac{(n+1+m)(n+1-m)}{(2n+1)(2n+3)}}, \quad \text{for } n \geqslant |m|, \\ b_n^m &= \begin{cases} \sqrt{\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}}, & 0\leqslant m\leqslant n, \\ -\sqrt{\frac{(n-m-1)(n-m)}{(2n-1)(2n+1)}}, & -n\leqslant m<0. \end{cases}\end{aligned} \tag{47}$$

For negative m coefficients $H_n^{m'm}(\beta)$ can be found using symmetry $H_n^{-m',-m}(\beta) = H_n^{m'm}(\beta)$.

We note that inverse rotation can be performed using the matrix $\left\{\left(T^{-1}\right)_n^{m'm}(\alpha,\beta,\gamma)\right\}$, which is the complex conjugate transposed of $\left\{T_n^{m'm}(\alpha,\beta,\gamma)\right\}$ and can be simplified using Eq. (44):

$$\begin{aligned}\left(T^{-1}\right)_n^{m'm}(\alpha,\beta,\gamma) &= \overline{T_n^{mm'}(\alpha,\beta,\gamma)} = e^{-im'\alpha}e^{im\gamma}H_n^{mm'}(\beta) \\ &= e^{-im'\alpha}e^{im\gamma}H_n^{m'm}(\beta) = T_n^{m'm}(\gamma,\beta,\alpha).\end{aligned} \tag{48}$$

In the "point-and-shoot" method the angle γ can be selected arbitrarily, since the direction of the translation vector $\mathbf{t}$ is characterized only by the two angles, α and β. For example, one could simply set $\gamma = 0$. We found however, that setting $\gamma = \alpha$ can be computationally cheaper for small truncation numbers p ($p < 7$), since in this case the forward and inverse translation operators coincide, $\left\{ \left(T^{-1}\right)_n^{m'm} (\alpha, \beta, \alpha) \right\} = \left\{ T_n^{m'm} (\alpha, \beta, \alpha) \right\}$ (for the normalization $\alpha_n^m = \beta_n^m = 1$).

3 Matrices for conversion to harmonic form

In this section we derive explicit expressions for the conversion matrices (25) in the regular and singular bases of normalized solutions of the Laplace equation. For this purpose let us consider expansion of functions $(\mathbf{r} \cdot \mathbf{t}) R_n^m (\mathbf{r})$ and $(\mathbf{r} \cdot \mathbf{t}) S_n^m (\mathbf{r})$ over the bases of functions $\{R_n^m (\mathbf{r})\}$ and $\{r^2 R_n^m (\mathbf{r})\}$ and $\{S_n^m (\mathbf{r})\}$ and $\{r^2 S_n^m (\mathbf{r})\}$, respectively. We present the result in the form of a few lemmas.

Lemma 1 (1) *Let $R_n^m (\mathbf{r})$ be a normalized regular elementary solution of the Laplace equation (31). Then*

$$\xi R_n^m (\mathbf{r}) = -i \frac{n+m+2}{2} R_{n+1}^{m+1} (\mathbf{r}) - \frac{i}{2} z R_n^{m+1} (\mathbf{r}), \quad n = 0, 1, ..., \quad m = -n, ..., n. \tag{49}$$

Proof. Using the polynomial representations (31) we have

$$\begin{aligned}
\xi R_n^m (\mathbf{r}) &= \sum_{l=0}^{n-|m|} \frac{(-1)^l i^{n-l} \sigma_{n-l}^m \xi^{(n+m-l+2)/2} \eta^{(n-m-l)/2} z^l}{\left(\frac{n+m-l}{2}\right)! \left(\frac{n-m-l}{2}\right)! l!} \\
&= \sum_{l=0}^{n-|m|} \frac{(-1)^l i^{n-l} \sigma_{n-l}^m \xi^{((n+1)+(m+1)-l)/2} \eta^{((n+1)-(m+1)-l)/2} z^l}{\left(\frac{(n+1)+(m+1)-l}{2} - 1\right)! \left(\frac{(n+1)-(m+1)-l}{2}\right)! l!} \\
&= -i \sum_{l=0}^{n+1-|m+1|} \frac{(-1)^l i^{n+1-l} \sigma_{n+1-l}^{m+1} \xi^{((n+1)+(m+1)-l)/2} \eta^{((n+1)-(m+1)-l)/2} z^l}{\left(\frac{(n+1)+(m+1)-l}{2} - 1\right)! \left(\frac{(n+1)-(m+1)-l}{2}\right)! l!} \\
&\quad + \sum_{l=n+1-|m+1|+1}^{n-|m|} \frac{(-1)^l i^{n-l} \sigma_{n-l}^m \xi^{((n+1)+(m+1)-l)/2} \eta^{((n+1)-(m+1)-l)/2} z^l}{\left(\frac{(n+1)+(m+1)-l}{2} - 1\right)! \left(\frac{(n+1)-(m+1)-l}{2}\right)! l!} \\
&= -i \sum_{l=0}^{n+1-|m+1|} \frac{(n+1)+(m+1)-l}{2} \frac{(-1)^l i^{n+1-l} \sigma_{n+1-l}^{m+1} \xi^{((n+1)+(m+1)-l)/2} \eta^{((n+1)-(m+1)-l)/2} z^l}{\left(\frac{(n+1)+(m+1)-l}{2}\right)! \left(\frac{(n+1)-(m+1)-l}{2}\right)! l!} \\
&= -i \frac{n+m+2}{2} R_{n+1}^{m+1} (\mathbf{r}) + \frac{i}{2} \sum_{l=0}^{n+1-|m+1|} \frac{(-1)^l i^{n+1-l} \sigma_{n+1-l}^{m+1} \xi^{((n+1)+(m+1)-l)/2} \eta^{((n+1)-(m+1)-l)/2} z^l}{\left(\frac{(n+1)+(m+1)-l}{2}\right)! \left(\frac{(n+1)-(m+1)-l}{2}\right)! (l-1)!} \\
&= -i \frac{n+m+2}{2} R_{n+1}^{m+1} (\mathbf{r}) - \frac{i}{2} \sum_{l=0}^{n-|m+1|} \frac{(-1)^l i^{n-l} \sigma_{n-l}^{m+1} \xi^{(n+(m+1)-l)/2} \eta^{(n-(m+1)-l)/2} z^{l+1}}{\left(\frac{n+(m+1)-l}{2}\right)! \left(\frac{n-(m+1)-l}{2}\right)! l!} \\
&= -i \frac{n+m+2}{2} R_{n+1}^{m+1} (\mathbf{r}) - \frac{i}{2} z R_n^{m+1} (\mathbf{r}).
\end{aligned}$$

■

Corollary 2 *Let $R_n^m(\mathbf{r})$ be a normalized regular elementary solution of the Laplace equation (31). Then*

$$\eta R_n^m(\mathbf{r}) = -i\frac{n-m+2}{2}R_{n+1}^{m-1}(\mathbf{r}) - \frac{i}{2}zR_n^{m-1}(\mathbf{r}), \quad n=0,1,..., \quad m=-n,...,n. \tag{50}$$

Proof. According Eqs. (9) and (27) we have for complex conjugate

$$\overline{R_n^m(\mathbf{r})} = (-1)^m R_n^{-m}(\mathbf{r}). \tag{51}$$

Since $\overline{\eta} = \xi$ (see Eq. (28)) we obtain using Lemma 1:

$$\begin{aligned}
\eta R_n^m(\mathbf{r}) &= \overline{\overline{\eta R_n^m(\mathbf{r})}} = (-1)^m \overline{\xi R_n^{-m}(\mathbf{r})} = (-1)^m \overline{\left[-i\frac{n-m+2}{2}R_{n+1}^{-m+1}(\mathbf{r}) - \frac{i}{2}zR_n^{-m+1}(\mathbf{r})\right]} \\
&= (-1)^m \left[i\frac{n-m+2}{2}(-1)^{m-1}R_{n+1}^{m-1}(\mathbf{r}) + \frac{i}{2}z(-1)^{m-1}R_n^{m-1}(\mathbf{r})\right] \\
&= -i\frac{n-m+2}{2}R_{n+1}^{m-1}(\mathbf{r}) - \frac{i}{2}zR_n^{m-1}(\mathbf{r}).
\end{aligned}$$

■

Lemma 3 (2) *Let $R_n^m(\mathbf{r})$ be a normalized regular elementary solution of the Laplace equation (31). Then*

$$zR_n^m(\mathbf{r}) = -\frac{1}{2n+1}\left[(n+m+1)(n-m+1)R_{n+1}^m(\mathbf{r}) + r^2R_{n-1}^m(\mathbf{r})\right], \quad n=0,1,..., \quad m=-n,...,n. \tag{52}$$

Proof. Using the following identity for the associated Legendre functions

$$\mu P_n^m(\mu) = \frac{n+m}{2n+1}P_{n-1}^m(\mu) + \frac{n-m+1}{2n+1}P_{n+1}^m(\mu), \tag{53}$$

and definition of the basis functions (9) we can find

$$\begin{aligned}
zR_n^m(\mathbf{r}) &= \alpha_n^m N_n^m e^{im\varphi} r^{n+1} \mu P_n^{|m|}(\mu) \qquad (54)\\
&= \alpha_n^m N_n^m e^{im\varphi} r^{n+1}\left[\frac{n+|m|}{2n+1}P_{n-1}^{|m|}(\mu) + \frac{n-|m|+1}{2n+1}P_{n+1}^{|m|}(\mu)\right] \\
&= \frac{1}{2n+1}\left[(n+|m|)\frac{\alpha_n^m N_n^m}{\alpha_{n-1}^m N_{n-1}^m}r^2R_{n-1}^m(\mathbf{r}) + (n-|m|+1)\frac{\alpha_{(1)n}^m N_n^m}{\alpha_{n+1}^m N_{n+1}^m}R_{n+1}^m(\mathbf{r})\right].
\end{aligned}$$

Since

$$\alpha_n^m N_n^m = \frac{(-1)^{n+m} i^{-|m|}}{(n+|m|)!}, \tag{55}$$

we obtain the statement of the lemma. ■

Lemma 4 (3) *Let $R_n^m(\mathbf{r})$ be a normalized regular elementary solution of the Laplace equation (31). Then*

$$\begin{aligned}
(\mathbf{r}\cdot\mathbf{t})R_n^m(\mathbf{r}) &= -\frac{(it_x+t_y)(n+m+2)(n+m+1)R_{n+1}^{m+1}(\mathbf{r})}{2(2n+1)} \qquad (56)\\
&\quad -\frac{(it_x-t_y)(n-m+2)(n-m+1)R_{n+1}^{m-1}(\mathbf{r}) + 2t_z(n+m+1)(n-m+1)R_{n+1}^m(\mathbf{r})}{2(2n+1)} \\
&\quad +\frac{r^2\left[(it_x+t_y)R_{n-1}^{m+1}(\mathbf{r}) + (it_x-t_y)R_{n-1}^{m-1}(\mathbf{r}) - 2t_zR_{n-1}^m(\mathbf{r})\right]}{2(2n+1)}.
\end{aligned}$$

Proof. Follows from Eqs. (49)-(52) and

$$(\mathbf{r}\cdot\mathbf{t})R_n^m(\mathbf{r}) = (xt_x + yt_y + zt_z)\,R_n^m(\mathbf{r}) = \left[(t_x - it_y)\,\xi + (t_x + it_y)\,\eta + t_z z\right]R_n^m(\mathbf{r}). \tag{57}$$

■

Lemma 5 (4) *Let $S_n^m(\mathbf{r})$ be a normalized singular elementary solution of the Laplace equation (31). Then*

$$\begin{aligned}(\mathbf{r}\cdot\mathbf{t})S_n^m(\mathbf{r}) &= \frac{(it_x+t_y)\,(n-m-1)\,(n-m)S_{n-1}^{m+1}(\mathbf{r})}{2\,(2n+1)} \\ &+\frac{(it_x-t_y)\,(n+m-1)\,(n+m)S_{n-1}^{m-1}(\mathbf{r}) + 2t_z\,(n-m)\,(n+m)S_{n-1}^{m}(\mathbf{r})}{2\,(2n+1)} \\ &-\frac{r^2\left[(it_x+t_y)\,S_{n+1}^{m+1}(\mathbf{r}) + (it_x-t_y)\,S_{n+1}^{m-1}(\mathbf{r}) - 2t_z S_{n+1}^{m}(\mathbf{r})\right]}{2\,(2n+1)}.\end{aligned} \tag{58}$$

Proof. Follows from Eqs. (32) and (56). ■

Lemma 6 (5) *Let $\widehat{\phi}_n^m$, $\widehat{\omega}_n^m$, $\widetilde{\phi}_n^m$, and $\widetilde{\omega}_n^m$ be coefficients of expansions of harmonic functions $\widehat{\phi}(\mathbf{r})$, $\widehat{\omega}(\mathbf{r})$, $\widetilde{\phi}(\mathbf{r})$, and $\widetilde{\omega}(\mathbf{r})$ over the normalized regular basis $\{R_n^m(\mathbf{r})\}$ that satisfy relation*

$$\widetilde{\phi}(\mathbf{r}) + r^2\widetilde{\omega}(\mathbf{r}) = \widehat{\phi}(\mathbf{r}) + \left[r^2 + 2\,(\mathbf{r}\cdot\mathbf{t}) + t^2\right]\widehat{\omega}(\mathbf{r}). \tag{59}$$

Then

$$\begin{aligned}\widetilde{\phi}_n^m &= \widehat{\phi}_n^m + t^2\widehat{\omega}_n^m - \frac{(it_x+t_y)\,(n+m)\,(n+m-1)\widehat{\omega}_{n-1}^{m-1}}{2n-1} \\ &\quad-\frac{(it_x-t_y)\,(n-m)\,(n-m-1)\widehat{\omega}_{n-1}^{m+1} + 2t_z(n+m)\,(n-m)\,\widehat{\omega}_{n-1}^{m}}{2n-1} \\ \widetilde{\omega}_n^m &= \widehat{\omega}_n^m + \frac{1}{2n+3}\left[(it_x+t_y)\,\widehat{\omega}_{n+1}^{m-1} + (it_x-t_y)\,\widehat{\omega}_{n+1}^{m+1} - 2t_z\widehat{\omega}_{n+1}^{m}\right].\end{aligned} \tag{60}$$

Proof. Follows from Eqs. (56) and (59) by grouping the terms multiplying functions $R_n^m(\mathbf{r})$ and $r^2R_n^m(\mathbf{r})$ and comparing coefficients. ■

Lemma 7 (6) *Let $\widehat{\phi}_n^m$, $\widehat{\omega}_n^m$, $\widetilde{\phi}_n^m$, and $\widetilde{\omega}_n^m$ be coefficients of expansions of harmonic functions $\widehat{\phi}(\mathbf{r})$, $\widehat{\omega}(\mathbf{r})$, $\widetilde{\phi}(\mathbf{r})$, and $\widetilde{\omega}(\mathbf{r})$ over the normalized singular basis $\{S_n^m(\mathbf{r})\}$ that satisfy relation (59). Then*

$$\begin{aligned}\widetilde{\phi}_n^m &= \widehat{\phi}_n^m + t^2\widehat{\omega}_n^m + \frac{(it_x+t_y)\,(n-m+1)\,(n-m+2)\widehat{\omega}_{n+1}^{m-1}}{2n+3} \\ &\quad+\frac{(it_x-t_y)\,(n+m+1)\,(n+m+2)\widehat{\omega}_{n+1}^{m+1} + 2t_z(n-m+1)\,(n+m+1)\,\widehat{\omega}_{n+1}^{m}}{2n+3} \\ \widetilde{\omega}_n^m &= \widehat{\omega}_n^m - \frac{1}{2n-1}\left[(it_x+t_y)\,\widehat{\omega}_{n-1}^{m-1} + (it_x-t_y)\,\widehat{\omega}_{n-1}^{m+1} - 2t_z\widehat{\omega}_{n-1}^{m}\right].\end{aligned} \tag{61}$$

Proof. Follows from Eqs. (58) and (59) by grouping the coefficients of the functions $S_n^m(\mathbf{r})$ and $r^2S_n^m(\mathbf{r})$ and comparison of the coefficients. ■

Relations (60) and (61) in fact determine the entries of the conversion matrices (25). These matrices are sparse, since only 4 elements $\widehat{\omega}_n^m$ are needed to determine $\widetilde{\omega}_n^m$ and $\widetilde{\phi}_n^m$. Note that in the FMM where the translation is decomposed into rotation and coaxial translation operations, the conversion operation can be performed for a lower cost after the coaxial translation. Conversion formulae for coaxial translation can be obtained easily from Eqs. (60) and (61) by setting $t_x = t_y = 0$, $t_z = t$. So we have for expansions over the regular basis $\{R_n^m(\mathbf{r})\}$:

$$\begin{aligned} \widetilde{\phi}_n^m &= \widehat{\phi}_n^m + t^2\widehat{\omega}_n^m - 2t\frac{(n+m)(n-m)}{2n-1}\widehat{\omega}_{n-1}^m, \\ \widetilde{\omega}_n^m &= \widehat{\omega}_n^m - \frac{2t}{2n+3}\widehat{\omega}_{n+1}^m. \end{aligned} \tag{62}$$

For expansion over the singular basis $\{S_n^m(\mathbf{r})\}$ we have:

$$\begin{aligned} \widetilde{\phi}_n^m &= \widehat{\phi}_n^m + t^2\widehat{\omega}_n^m + 2t\frac{(n+m+1)(n-m+1)}{2n+3}\widehat{\omega}_{n+1}^m, \\ \widetilde{\omega}_n^m &= \widehat{\omega}_n^m + \frac{2t}{2n-1}\widehat{\omega}_{n-1}^m. \end{aligned} \tag{63}$$

4 Polyharmonic equations

While we will not pursue this here, the method presented above can be easily extended to solution of polyharmonic equations of type

$$\nabla^{2k}\psi = 0, \quad k = 3, 4, ... \tag{64}$$

The Green's functions of these functions are often used in radial basis function interpolation. In this case solution in spherical coordinates can be represented in the form

$$\psi(\mathbf{r}) = \phi_1(\mathbf{r}) + r^2\phi_2(\mathbf{r}) + r^4\phi_3(\mathbf{r}) + ... + r^{2k-2}\phi_k(\mathbf{r}) = \sum_{j=1}^{k} r^{2j-2}\phi_j(\mathbf{r}), \tag{65}$$

where $\phi_j(\mathbf{r})$, $j = 1, ..., k$. The translation operator acts on this solution as follows

$$\begin{aligned} \widehat{\psi}(\mathbf{r}) &= \mathcal{T}(\mathbf{t})[\psi(\mathbf{r})] = \mathcal{T}(\mathbf{t})\left[\sum_{j=1}^{k}(\mathbf{r}\cdot\mathbf{r})^{2j-2}\phi_j(\mathbf{r})\right] = \sum_{j=1}^{k}[(\mathbf{r}+\mathbf{t})\cdot(\mathbf{r}+\mathbf{t})]^{2j-2}\widehat{\phi}_j(\mathbf{r}) \\ &= \sum_{j=1}^{k}\left[r^2 + 2(\mathbf{r}\cdot\mathbf{t}) + t^2\right]^{j-1}\widehat{\phi}_j(\mathbf{r}), \end{aligned} \tag{66}$$

where we used the binomial expansion. As shown above the conversion operator provides a transform, which can be written as

$$\begin{aligned} \left[r^2 + 2(\mathbf{r}\cdot\mathbf{t}) + t^2\right]\widehat{\phi}_j(\mathbf{r}) &= \Phi_j^{(1,1)}(\mathbf{r}) + r^2\Phi_j^{(1,2)}(\mathbf{r}), \\ \left[r^2 + 2(\mathbf{r}\cdot\mathbf{t}) + t^2\right]^2\widehat{\phi}_j(\mathbf{r}) &= \left[r^2 + 2(\mathbf{r}\cdot\mathbf{t}) + t^2\right]\Phi_j^{(1,1)}(\mathbf{r}) + r^2\left[r^2 + 2(\mathbf{r}\cdot\mathbf{t}) + t^2\right]\Phi_j^{(1,2)}(\mathbf{r}) \\ &= \Phi_j^{(2,1)}(\mathbf{r}) + r^2\Phi_j^{(2,2)}(\mathbf{r}) + r^4\Phi_j^{(2,2)}(\mathbf{r}), ... \\ \left[r^2 + 2(\mathbf{r}\cdot\mathbf{t}) + t^2\right]^{j-1}\widehat{\phi}_j(\mathbf{r}) &= \sum_{l=1}^{j} r^{2l-2}\Phi_j^{(j-1,l)}(\mathbf{r}). \end{aligned} \tag{67}$$

where $\Phi_j^{(j-1,l)}(\mathbf{r})$ are harmonic functions. So we can rewrite Eq. (66) as

$$\widehat{\psi}(\mathbf{r}) = \sum_{j=1}^{k} \sum_{l=1}^{j} r^{2l-2} \Phi_j^{(j-1,l)}(\mathbf{r}) = \sum_{l=1}^{k} r^{2l-2} \sum_{j=l}^{k} \Phi_j^{(j-1,l)}(\mathbf{r}) = \sum_{l=1}^{k} r^{2l-2} \widetilde{\phi}_l(\mathbf{r}), \tag{68}$$

where

$$\widetilde{\phi}_l(\mathbf{r}) = \sum_{j=l}^{k} \Phi_j^{(j-1,l)}(\mathbf{r}). \tag{69}$$

Eq. (68) represents the translated solution in the same form as the original solution (compare with Eq. (65)). Therefore, solution of k-harmonic equation can be reduced to solution of k Laplace equations (e.g. the triharmonic equation solution can be expressed in terms of three harmonic functions), with modification of the translation operators, which include multiplications by sparse conversion matrices. Such multiplications can be greatly simplified using the rotational-coaxial translation decompositions.

5 Fast multipole method

5.1 Mapping a real biharmonic function to a complex harmonic function

A nice property of the harmonic and biharmonic equations is that they can be solved for both real and complex-valued functions. If the function is complex valued one can simply solve the problem for real and imaginary parts. In this case one can rewrite the equations in terms of real spherical harmonics and translation operators, which, however, makes the formulae more involved. So it is preferable to operate with complex functions. In terms of the use of the FMM we found that it only needs to be slightly modified, so an FMM matrix vector product routine for the complex Laplace equation can be used for the biharmonic equation for real valued functions, which is the practical case typically encountered.

To show how this works, let us first consider solution of the Laplace equation for real valued function $\phi(\mathbf{r})$. Assume that this function is expanded over the regular basis according Eq. (18). Then due to the property (51) of normalized spherical basis functions we have

$$\overline{\phi(\mathbf{r})} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \overline{\phi_n^m R_n^m(\mathbf{r})} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} (-1)^m \overline{\phi_n^m} R_n^{-m}(\mathbf{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} (-1)^m \overline{\phi_n^{-m}} R_n^m(\mathbf{r}). \tag{70}$$

Since $\phi(\mathbf{r}) = \overline{\phi(\mathbf{r})}$, comparing this with Eq. (18) and taking into account uniqueness of the expansion over the basis, we can find that expansion coefficients of real functions satisfy relation

$$\phi_n^m = (-1)^m \overline{\phi_n^{-m}}, \quad n = 0, 1, ..., \quad m = -n, ..., n. \tag{71}$$

Now, let us consider a complex valued harmonic function

$$\Psi(\mathbf{r}) = \phi(\mathbf{r}) + i\omega(\mathbf{r}), \quad \Psi_n^m = \phi_n^m + i\omega_n^m, \tag{72}$$

where ϕ and ω are real, and functions Ψ, ϕ, and ω can be expanded over basis $\{R_n^m(\mathbf{r})\}$ with coefficients Ψ_n^m, ϕ_n^m, and ω_n^m. We have then relation (71), which is valid for coefficients of real functions ϕ_n^m and ω_n^m :

$$\Psi_n^m - i\omega_n^m = \phi_n^m = (-1)^m \overline{\phi_n^{-m}} = (-1)^m \left(\overline{\Psi_n^{-m}} + i\overline{\omega_n^{-m}}\right) = (-1)^m \overline{\Psi_n^{-m}} + i\omega_n^m, \tag{73}$$
$$\Psi_n^m - \phi_n^m = i\omega_n^m = -(-1)^m \overline{\left(i\omega_n^{-m}\right)} = -(-1)^m \left(\overline{\Psi_n^{-m}} - \overline{\phi_n^{-m}}\right) = -(-1)^m \overline{\Psi_n^{-m}} + \phi_n^m.$$

This yields

$$\phi_n^m = \frac{1}{2}\left[\Psi_n^m + (-1)^m \overline{\Psi_n^{-m}}\right], \quad \omega_n^m = \frac{1}{2i}\left[\Psi_n^m - (-1)^m \overline{\Psi_n^{-m}}\right]. \tag{74}$$

It is not difficult to check that this relation holds also if Ψ_n^m, ϕ_n^m, and ω_n^m are expansion coefficients of Ψ, ϕ, and ω over basis $\{S_n^m(\mathbf{r})\}$. Thus, if harmonic function $\Psi(\mathbf{r})$ is known via its expansion coefficients, then expansion coefficients of its real and imaginary parts can be easily retrieved. This maps harmonic function $\Psi(\mathbf{r})$ to biharmonic function $\psi(\mathbf{r})$ represented as Eq. (16).

As the translation process of biharmonic function is concerned, we, first, perform translation of coefficients Ψ_n^m to $\widehat{\Psi}_n^m$ using translation operators for the Laplace equation, second, we determine $\widehat{\phi}_n^m$ and $\widehat{\omega}_n^m$ from $\widehat{\Psi}_n^m$ according to Eq. (74), third, we convert $\widehat{\phi}_n^m$ and $\widehat{\omega}_n^m$ to $\widetilde{\phi}_n^m$ and $\widetilde{\omega}_n^m$ according Eqs. (60) and (61), and, finally, we form $\widetilde{\Psi}_n^m = \widetilde{\phi}_n^m + i\widetilde{\omega}_n^m$, which is a representation of the translated biharmonic function. This is shown on a flow chart in Fig. 2.

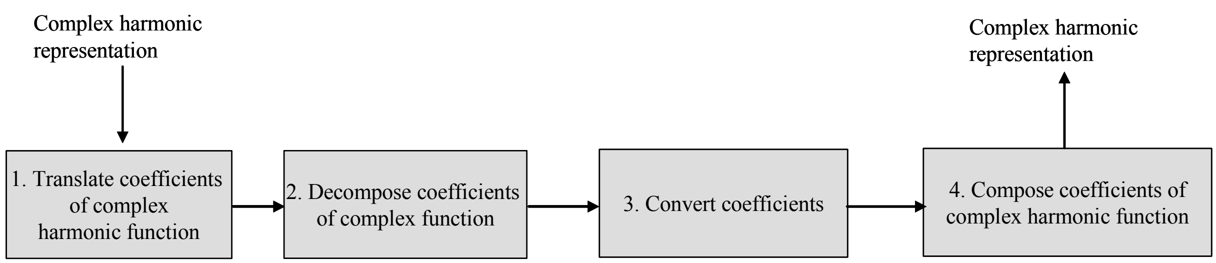

Figure 2: A flow chart for translation of solutions of the biharmonic equation using complex harmonic representation.

As we mentioned above the conversion operator can be simplified in the case of coaxial translation. The flow chart corresponding to this case is shown in Fig. 3.

5.2 Basic FMM algorithm

In the Introduction we mentioned several different approaches for fast solution of the Laplace equation, including various modifications of the FMM. Generally speaking any solver for Laplace equation can be adjusted to solve the biharmonic equation, as soon as translation operators are modified according the scheme on Fig. 2. We will not present details of the basic FMM algorithm, which are well described in the original papers of Greengard, Rokhlin, and others [1, 24]. Our implementation of the Laplace solvers is described in a recent publication [19], where we also provided operational and memory complexity, error analysis, and comparison of two fastest versions of the FMM currently available.

The algorithm is designed to provide fast summation (or matrix-vector multiplication)

$$\psi(\boldsymbol{\rho}_j) = \sum_{i=1}^{N} \Phi(\boldsymbol{\rho}_j, \mathbf{r}_i) q_i, \quad j = 1, ..., M, \tag{75}$$

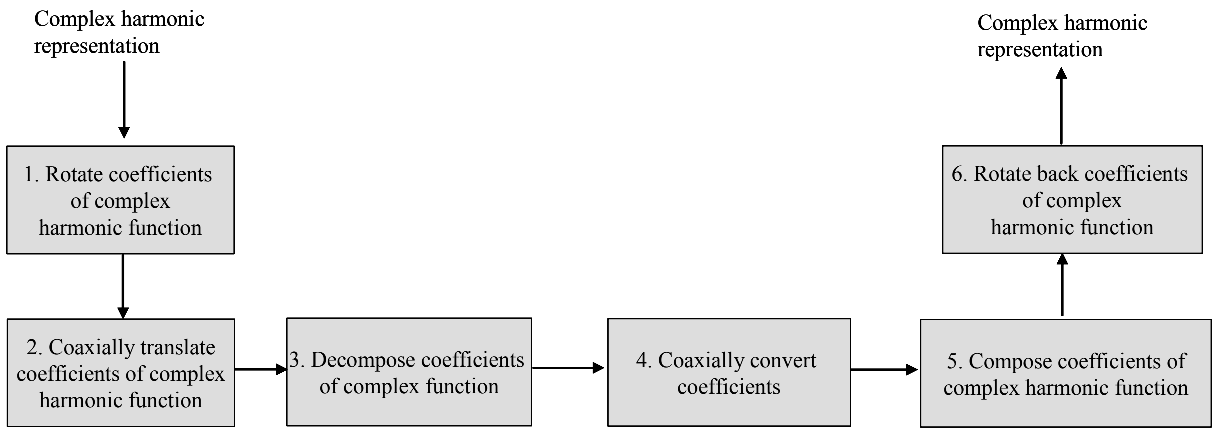

Figure 3: A flow chart for translation of solutions of the biharmonic equation using complex harmonic representation and rotation-coaxial translation decomposition.

where q_i are intensities of the sources located at $\mathbf{r}_i$, $\Phi(\boldsymbol{\rho}_j, \mathbf{r}_i)$ source function (in the present paper we use the Green's function for the biharmonic equation (14), $\Phi(\boldsymbol{\rho}_j, \mathbf{r}_i) = G\left(\boldsymbol{\rho}_j, \mathbf{r}_i\right)$), and $\psi(\boldsymbol{\rho}_j)$ is the solution evaluated at $\boldsymbol{\rho}_j$. This problem appears, e.g. in 3D interpolation, or in solution of equations using the boundary element method, where the boundary of the domain is discretized, so $\mathbf{r}_i$ and q_i are the nodes and weights of the respective quadratures. Solution of the problems involving derivatives (e.g. normal to the surface) can be easily reduced to summations of type (75), where one can use differential properties of the basis function (30). A methodology for differentiation of functions represented by their expansions (differential operators in the space of coefficients) can be found in Ref. [25].

The algorithm consists of two main parts: the preset step, which includes setting the data structure (building and storage of the neighbor lists, etc.) and precomputation and storage of all translation data. The data structure is generated using the bit interleaving technique described in [25], which enables spatial ordering, sorting, and bookmarking. While the algorithm is designed for two independent data sets (N arbitrary located sources and M arbitrary evaluation points), for the current tests we used the same source and evaluation sets of length N, which is also called the problem size. For a problem size N, the cost of building the data structure based on spatial ordering is $O(N \log N)$, where the asymptotic constant is much smaller than the constants in the $O(N)$ asymptotics of the main algorithm. The number of levels could be arbitrarily set by the user or found automatically based on the clustering parameter (the maximum number of sources in the smallest box) for optimization of computations of problems of different size.

Figure 4 shows the main steps of the standard FMM, assuming that the preset part is performed initially. Here Steps 1 and 2 constitute the upward pass in the box hierarchy, Steps 3,4, and 5 form the downward pass and Steps 6 and 7 relate to final summation. The upward pass is performed for boxes in the source hierarchy, while the downward pass and final summation are performed for the evaluation hierarchy. By "near neighborhood" we mean the box itself and its immediate neighbors, which consists of 27 boxes for a box not adjacent to the boundary, and the "far neighbors", are boxes from the parent near neighborhood (of the size of the given box), which do not belong to the close neighborhood. The number of such boxes is 189 in case the box is sufficiently separated from the boundary of the domain.

For solution of the biharmonic equation translation operators shown in Fig. 4 should be ex-

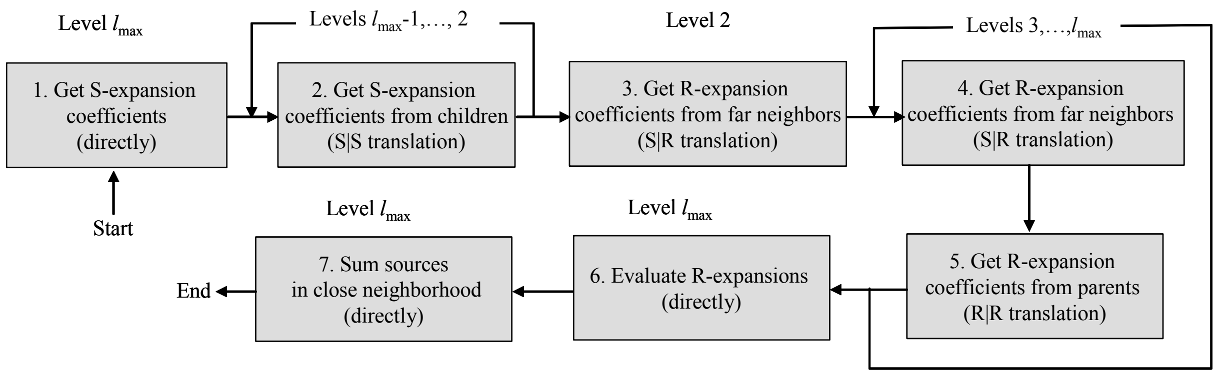

Figure 4: A flow chart of the standard FMM.

panded according to Fig. 2 in general case, and according to Fig. 2 if translations are decomposed to rotations and coaxial translations. In the numerical examples shown below we used such decomposition.

5.3 Numerical tests

To validate the theory and conduct some performance tests we developed software for the FMM for solutions of the biharmonic equation. The code was realized in Fortran 95 and compiled using the Compaq 6.5 Fortran compiler. All computations were performed in double precision. The CPU time measurements were conducted on a 3.2 GHz dual Intel Xeon processor with 3.5 GB RAM. In the tests we studied a benchmark case where N sources are uniformly randomly distributed inside a unit cube. The intensities of the sources generally were assigned randomly, while for consistency of error measurements we often used sources of the same intensity.

5.3.1 Computation of errors

To validate accuracy of the FMM we measured the relative error in the L_2 norm evaluated over M random points in the domain:

$$\epsilon_2 = \left[\frac{\sum_{j=1}^{M} \left| \psi_{exact}\left(\mathbf{r}_j\right) - \psi_{approx}\left(\mathbf{r}_j\right) \right|^2}{\sum_{j=1}^{M} \left| \psi_{exact}\left(\mathbf{r}_j\right) \right|^2} \right]^{1/2}, \tag{76}$$

where $\psi_{exact}(\mathbf{r})$ and $\psi_{approx}(\mathbf{r})$ are the exact and approximate solutions of the problem.

The exact solution was computed by straightforward summation of the source potentials (27). This method is acceptable for relatively low M, while for larger M the computations become unacceptably slow, and the error can be measured by evaluation of the errors at smaller number of the evaluation points. We found experimentally that the relative L_2-norm error evaluated over 100 points is quite close to the error evaluated over the full set for $N < 100000$. So we used this partial error measure to evaluate the computation error.

The error of the FMM depends on several factors. It is mainly influenced by the truncation number, p, which is the number of terms in the outer summation ($n = 0, ..., p-1$). We note that the total number of expansion coefficients for a single harmonic function for a truncation number p is p^2, since the order changes as $m = -n, ..., n$, in the truncated series representation of a harmonic

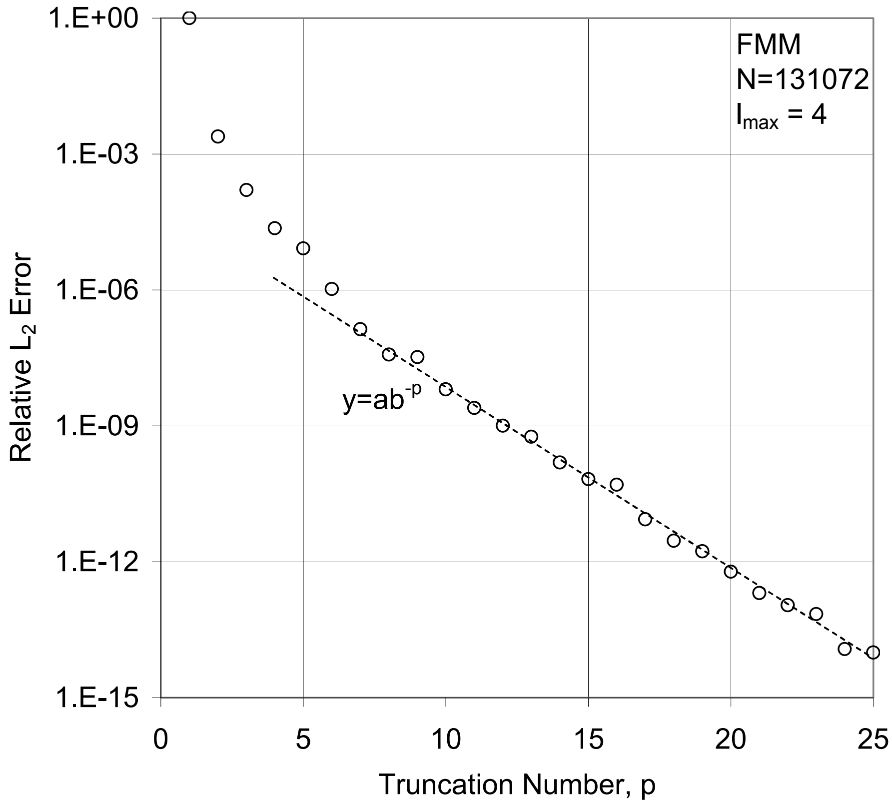

Figure 5: A dependence of the relative FMM error in the L_2 norm (ϵ_2) computed over 100 random points on the truncation number p for $N = 2^{17} = 131072$ sources of equal intencity distributed uniformly randomly inside a unit cube. The maximum level of space subdivision $l_{\max} = 4$. For $p > 6$ the error can be approximated by dependence $\epsilon_2 = ab^{-p}$.

function. We used this truncation for representation of harmonic functions $\phi(\mathbf{r})$ and $\omega(\mathbf{r})$ in decomposition of the biharmonic function $\psi(\mathbf{r})$ (see Eq. (16)), and accordingly we truncated all translation operators to matrices, where the maximum order m and degree n are $p-1$.

Figure 5 shows the dependence of the relative L_2 error evaluated over $M = 100$ points on p for fixed N. It is seen that for larger p this error decays exponentially. However even $p \sim 4$ provide a reasonably small error, which might be sufficient for computation of some practical problems. It is noticeable that ϵ_2 almost does not depend on N. This is shown in Figure 5. This is due to the growth of the norm of function $\psi(\mathbf{r})$ (see Eq. 75) with N. If one is interested with absolute error in L_∞ norm, then to keep it constant for increasing N we should increase $p \sim \log N$. We conducted corresponding numerical experiments for harmonic functions, which are reported in [19].

5.3.2 Performance

Once some truncation number providing sufficient accuracy is selected, the FMM should be optimized in terms of selection of optimum maximum level of space subdivision, $l_{\max}$. As is discussed in [19], for the Laplace equation $l_{\max}$ is proportional to $\log N$ and, in fact, for fixed p theoretically should depend only on the clustering parameter s, which is the maximum number of sources in the

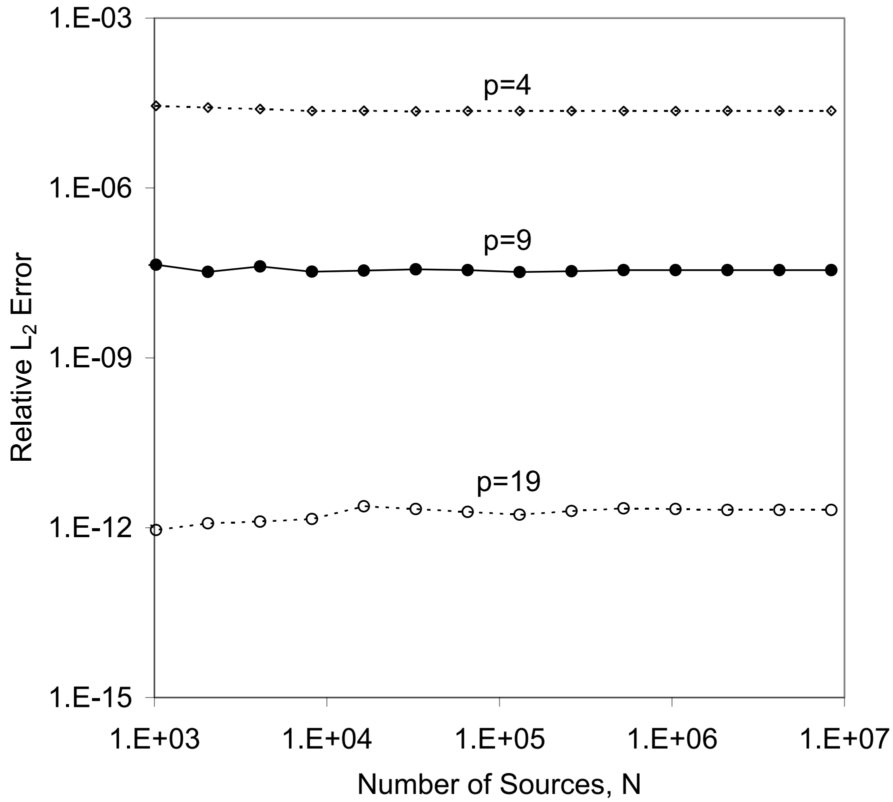

Figure 6: Dependences of the relative error ϵ_2 on the size of the problem for different truncation numbers. Computations made for settings described in Fig. 5 and 7. $l_{\max}$ was selected for the optimum CPU time of the algorithm.

smallest box of space subdivision. This is also true for the biharmonic equation. Accordingly, we varied this parameter to achieve the minimum CPU time for each case reported.

Figure 7 shows the dependences of the CPU time required for the "run" part of the FMM algorithm. It is seen that independently on p the complexity of the FMM is linear with respect to N, which is consistent with the theory. The direct summation method scaled as $O(N^2)$. We note that the break-even points, $N = N_*$, (the points at which the CPU time of the direct method coincides with the CPU time of the FMM) depend on the truncation number (or on the accuracy of computations) and on the implementation of the algorithm. In our implementation of the 3D biharmonic solver we obtained $N_* = 550$ for $p = 4$, $N_* = 1350$ for $p = 9$, and $N_* = 3550$ for $p = 19$. Note that we obtained the break-even numbers $N_* = 320, 900$, and 2500 for $p = 4, 9$, and 19 using the same "point-and-shoot" method for the Laplace equation for real functions [19].

Figure 8 shows the CPU times required for the "run" parts of the FMM algorithm for the Laplace and biharmonic equations (both for real functions). It is seen that, in fact solution of the biharmonic equation is faster than just sum of two Laplace equations. There are a couple of reasons for that. First, in both cases we use the same data structure and the translation operators for a single Laplace equation can be used for the biharmonic equation. Second, even though the translation for the biharmonic equation more costly than for the Laplace equation, the direct

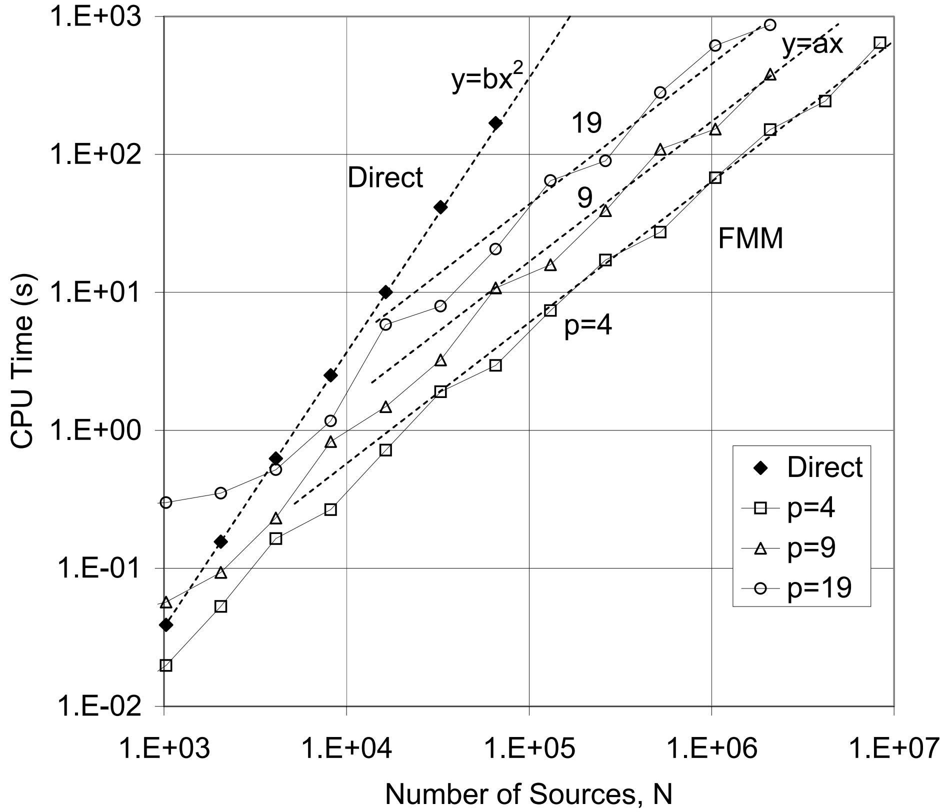

Figure 7: Dependences of the CPU (run) time, measured on Intel Xeon 3.2 GHz processor (3.5 GB RAM) on the size of the problem. Computations performed using the direct summation and the FMM with different truncation numbers shown near the curves. Sources (Green's function for biharmonic equation) of equal intencities are distributed uniformly randomly inside a cube. The series of the FMM data are connected with the solid lines. The dashed lines show asymptotic complexities of the algorithms at large N.

summation in the neighborhoods of the evaluation points for the both equations have the same cost. Therefore translations take not 100% of the CPU time, but just a part . Moreover, the optimization of the algorithm leads to balancing of the costs of translations and direct summations. So, theoretically, one can expect only 50% (not 100%) CPU time increase for solution of the biharmonic equation compared to the Laplace equation. These numbers are close to that we observed in actual computations for the maximum difference in the CPU times, e.g. for $N = 2^{19}$ the increase of the CPU time was 59% , and for $N = 2^{20}$ we had 36% increase (note that the ratio of the CPU times varies, due to the discrete change of the maximum level of space subdivision, which means that the translations may constitute not exactly 50% of the run time of the algorithm).

Figure 8 also shows the time needed to preset the FMM. As we mentioned above this step should be performed only once for a given set of source and evaluation points and includes setting of the data structure and precomputation of the translation operators. Even if it performed every time when the FMM run routine is called, it does not substantially affect the execution time, since it may contribute only 10% or so to the total computation time (so the FMM can be used for computation of dynamic system with moving sources). The graph of the preset time shows jumps,

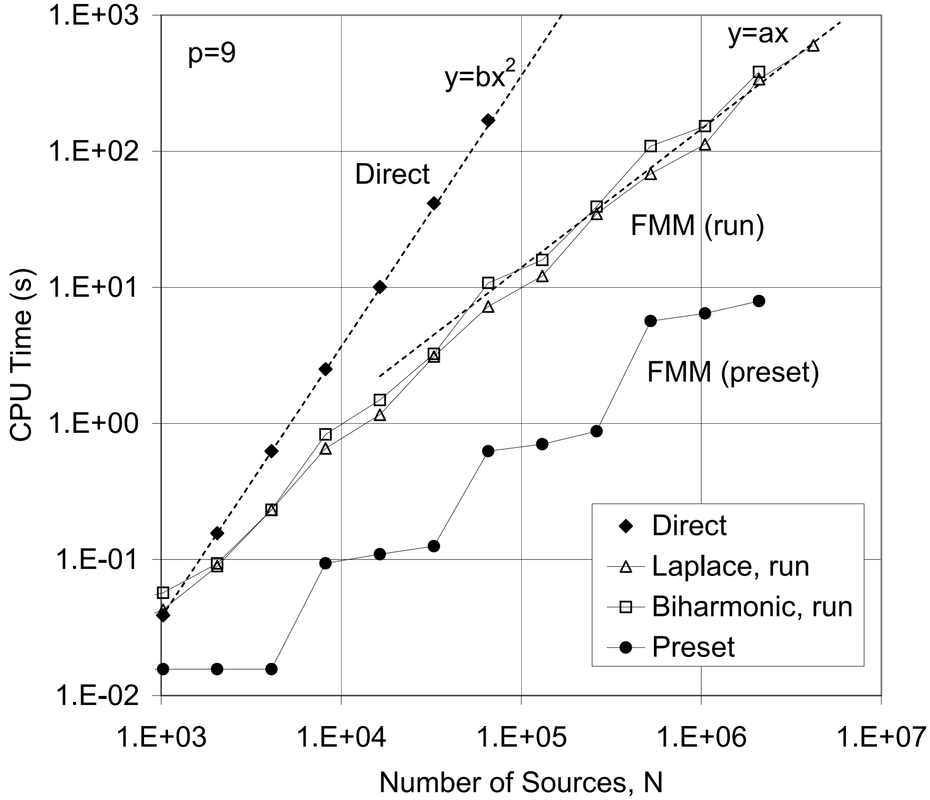

Figure 8: A comparison of the CPU times for the direct summation (the dark rhombs), the "run" parts of the FMM algorithms for the Laplace (the triangles) and the biharmonic (the squares) equations, and the "preset" step of the FMM algorithm (the dark discs). The FMM for the Laplace and biharmonic equation was employed with $p = 9$ and the same data structure. Other settings are the same as in Fig. 7.

which are related to the change of the maximum level of space subdivision. Almost the same CPU time is required to preset the FMM for different number of data points and the same $l_{\max}$.

6 Conclusions

We developed a fast method to solve a biharmonic equation in three dimensions based on the FMM for the Laplace equation. The method modifies translation operators and such modifications can be used with any solver of the Laplace equation employing translations or reexpansions including tree codes and various version of the FMM. Numerical tests show good performance in terms of accuracy and speed.

7 Acknowledgments

We would like to gratefully acknowledge the partial support of NSF awards 0086075 and 0219681.

References

[1] L. Greengard and V. Rokhlin, A fast algorithm for particle simulations, J. Comput. Phys. 73 (1987) 325-348.

[2] N. Nishimura, Fast multipole accelerated boundary integral equation methods, Appl Mech .55 (2002) 299-324.

[3] Y. Fu, K. J. Klimkowski, G.J.Rodin, E. Berger, J.C. Browne, J.K. Singer, R. Van de Geijn, and K. S.Vemaganti, A fast solution method for three-dimensional many-particle problems of linear elasticity, Int. J. Numer. Meth. Engng. 42 (1998) 1215-1229.

[4] F. Chen and D. Suter, Fast evaluation of vector splines in three dimensions, J. Computing 61(3) (1998) 189-213.

[5] V. Popov and H. Power, An O(N) Taylor series multipole boundary element method for three-dimensional elasticity problems, Eng. Anal. Boundary Elem. 25 (2001) 7–18.

[6] L. Ying, G. Biros, D. Zorin, and H. Langston, A new parallel kernel-independent fast multipole method, ACM SC'03, Phoenix, AZ, 2003.

[7] A S. Sangani and G. Mo, An O(N) algorithm for Stokes and Laplace interactions of particles, Phys. Fluids 8 (1996) 1990-2010.

[8] J. Happel and H. Brenner, Low Reynolds Number Hydrodynamics, Prentice- Hall, 1965 (reprinted by Martinus Nijhoff, Kluwer Academic Publishers, 1983).

[9] L. Greengard, M.C. Kropinski, A. Mayo, Integral methods for Stokes flow and isotropic elasticity in the plane, J. Comput. Phys. 125 (1996) 403-414.

[10] Y. Fu and G.J. Rodin, Fast solution method for three-dimensional Stokesian many-particle problems, Commun. Numer. Meth. Eng. 16 (2000) 145-149.

[11] K. Yoshida, Applications of Fast Multipole Method to Boundary Integral Equation Method, Ph.D. thesis, Dept. of Global Environment Eng., Kyoto Univ., Japan, 2001.

[12] K. Yoshida, N. Nishimura, and S. Kobayashi, Application of new fast multipole boundary integral equation method to elastostatic crack problems in three dimensions, J. Struct. Eng. JSCE 47A (2001) 169–179.

[13] L. Greengard and V. Rokhlin, A new version of the fast multipole method for the Laplace equation in three dimensions, Acta Numerica 6 (1997) 229-269.

[14] H. Cheng, L. Greengard, and V. Rokhlin, A fast adaptive multipole algorithm in three dimensions, J. Comput. Phys. 155 (1999) 468-498.

[15] J. Duchon, Splines minimizing rotation-invariant semi-norms in Sobolev spaces. In W. Schempp and K. Zeller (eds.), Constructive Theory of Functions of Several Variables, 571 in Lecture Notes in Mathematics, Springer-Verlag, Berlin (1977) 85-100.

[16] J. C. Carr, R. K. Beatson, J. B. Cherrie, T. J. Mitchell, W. R. Fright, B. C. McCallum, and T. R. Evans, Reconstruction and representation of 3D objects with radial basis functions, ACM SIGGRAPH 2001, Los Angeles, CA (2001) 67-75.

[17] J. B. Cherrie , R. K. Beatson , and G. N. Newsam, Fast evaluation of radial basis functions: methods for generalised multiquadrics in $\mathbb{R}^n$, SIAM J.Sci. Comput. 23(5) (2002) 1549-1571.

[18] C.A. White and M. Head-Gordon, Rotation around the quartic angular momentum barrier in fast multipole method calculations, J. Chem. Phys. 105(12) (1996) 5061-5067.

[19] N.A. Gumerov and R. Duraiswami, Comparison of the Efficiency of Translation Operators Used in the Fast Multipole Method for the 3D Laplace Equation, Univ. of Maryland Dept. Computer Science, Technical Report CS TR#-4701, UMIACS TR# - 2005-09, 2005.

[20] S. Kim, Stokes flow past three spheres: An analytic solution, Phys. Fluids 30 (1987) 2309-2314.

[21] A. V. Filippov, Phoretic motion of arbitrary clusters of N spheres, J. Colloid and Interface Sci. 241 (2001) 479–491.

[22] M. Abramowitz and I.A. Stegun, Handbook of Mathematical Functions, National Bureau of Standards, Wash., D.C.,1964.

[23] M.A. Epton and B. Dembart, Multipole translation theory for the three-dimensional Laplace and Helmholtz equations, SIAM J. Sci. Comput. 4(16) (1995) 865-897.

[24] L. Greengard, The Rapid Evaluation of Potential Fields in Particle Systems, MIT Press, Cambridge, MA, 1988.

[25] N.A. Gumerov and R. Duraiswami, Fast Multipole Methods for the Helmholtz Equation in Three Dimensions, Elsevier, 2005.