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Efficient Evaluation of the Rokhlin Translator in Multilevel Fast Multipole Algorithm

Ilari Hänninen and Jukka Sarvas

Abstract

In Multilevel Fast Multipole Algorithm (MLFMA) the direct evaluation of the Rokhlin translator is computationally expensive, and usually the cost is lowered by using local Lagrange interpolation in the evaluation, which requires oversampling of the translator. In this paper we improve the interpolation procedure by introducing a new, accurate, and fast oversampling technique based on the Fast Fourier Transform (FFT). In addition to speeding up the oversampling this also allows the use of lower number of points in the interpolation stencils improving the efficiency of the evaluation of the Rokhlin translator. We have optimized the interpolation parameters, i.e. the number of the stencil points and the oversampling factor, by using as the error criterion the accuracy in the translated (incoming) field rather than the usually used interpolation error. This choice leads to better optimized parameter pairs which further lowers the interpolation cost. We have computed and tabulated the optimized pairs for a wide range of target accuracies and the MLFMA division levels. These tables can be used for a good error control and maximal speed-up in practical computations.

Keywords: Lagrange interpolation, fast fourier transform, multilevel fast multipole algorithm, translator operator.

1 Introduction

Direct evaluation of the Rokhlin translator in the Multilevel Fast Multipole Algorithm (MLFMA) [1,2] is a computationally intensive operation. The number of directions for which the Rokhlin translator must be computed is large, and especially on the higher division levels the computing time for direct evaluation is significant. Similarly, on these levels the system memory needed to store the translation matrices is substantial. To overcome these problems interpolation methods for the Rokhlin transfer function based on the Lagrange interpolation have been suggested by several authors [3–5]. The accuracy of the interpolation depends on the oversampling factor and the number of points in the interpolation stencil. The higher the oversampling factor and the number of stencil points are, the more accurate the interpolation becomes.

As the number of needed interpolations is very large, it is important to optimize the interpolation procedure so that the number of stencil points is minimized. This can be achieved by using a high oversampling factor. However, the computational and storage costs of directly oversampling the Rokhlin transfer function are then high. It is thus essential to find such values for the oversampling factor and for the number of stencil points that are sufficient for the target accuracy and lead to a computationally efficient algorithm.

In this paper, we introduce an oversampling method based on the Fast Fourier Transform (FFT) that is much faster than directly computing the oversampled data points. This allows us, with low computational and storage costs, to use much larger oversampling factors and thus a smaller number of points in the interpolation stencil, which significantly improves the efficiency of the interpolation algorithm. We also study the interpolation error and the error in the translated field arising from the interpolation error in the Rokhlin translator. Although previously mainly the former error has been used to optimize the efficiency of the interpolation, this approach does not take into account the fact that the final error in the translated field may be much different.

We carry out the optimization for the interpolation procedure with respect to the field error, and use the FFT based oversampling to minimize the computational cost. We tabulate the optimized pairs of the stencil size and the oversampling factor for a large range of division levels and the relative field accuracies for $q = 1, \ldots, 8$ digits. The resulting table can be used to obtain optimal accuracy and maximal efficiency in practical computations.

2 Efficient Evaluation of the Rokhlin Translator

In the traditional MLFMA [6] the out-to-in translation with the Rokhlin translator T_L plays an important role. It translates an outgoing field, given by its far field pattern $F_\infty(\hat{\boldsymbol{k}})$, into an incoming field expanded in the plane waves as

$$F(\boldsymbol{D}+\boldsymbol{r}) \simeq \int_{|\hat{\boldsymbol{k}}|=1} F_\infty(\hat{\boldsymbol{k}}) T_L(\boldsymbol{D}, \hat{\boldsymbol{k}}) e^{ik\hat{\boldsymbol{k}}\cdot\boldsymbol{r}}\, d\hat{\boldsymbol{k}}, \tag{1}$$

where $\boldsymbol{D}$ is the translation vector from the center of the division cube containing the source to the center of a non-nearby target cube on the same division level. In (1) $\hat{\boldsymbol{k}}$ is the unit direction vector, the integration is over the surface of the unit sphere, and

$$T_L(\boldsymbol{D}, \hat{\boldsymbol{k}}) = \frac{ik}{4\pi} \sum_{n=0}^{L} i^n (2n+1) h_n^{(1)}(kD) P_n(\hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{D}}) \tag{2}$$

is the Rokhlin translator of order L with $D = |\boldsymbol{D}|$, $\hat{\boldsymbol{D}} = \boldsymbol{D}/D$, and the wave number k. The order L in (2) controls the approximation error (also called the truncation error) in the equation (1).

The integral in (1) is computed numerically, and therefore, $T_L(\boldsymbol{D}, \hat{\boldsymbol{k}})$ must be sampled in the sampling points $\hat{\boldsymbol{k}}_{mn}$, $m = 1, \ldots, L+1$, $n = -L, \ldots, L$ of the integration rule. For a large L this becomes costly if (2) is used directly, and so, the local interpolation of T_L by the Lagrange interpolation technique is used to speed-up the evaluation of $T_L(\boldsymbol{D}, \hat{\boldsymbol{k}}_{mn})$, [3–5]. The local interpolation is based on the fact that $T_L(\boldsymbol{D}, \hat{\boldsymbol{k}})$ is a trigonometric polynomial $T_L(\alpha)$ of order L, with $\alpha = \arccos(\hat{\boldsymbol{D}} \cdot \hat{\boldsymbol{k}})$, $-\pi \le \alpha \le \pi$,

$$T_L(\alpha) = \sum_{n=-L}^{L} b_n e^{in\alpha}, \tag{3}$$

as (2) shows, because P_n is the Legendre polynomial of degree n and $\hat{\boldsymbol{D}} \cdot \hat{\boldsymbol{k}} = \cos\alpha = \frac{1}{2}\left(e^{i\alpha} + e^{-i\alpha}\right)$. In [3] it it shown that if $T_L(\alpha)$ is interpolated with a uniform interpolation stencil of $2p$ points, $p \ge 1$, by using $2sL+1$ sampling points

$$\alpha_m = \frac{2\pi}{2sL+1} m, \quad m = -sL, \ldots, sL, \tag{4}$$

then the relative interpolation error

$$\frac{\max\limits_{-\pi\le\alpha\le\pi} \left|\tilde{T}_L(\alpha) - T_L(\alpha)\right|}{\max\limits_{-\pi\le\alpha\le\pi} |T_L(\alpha)|} \tag{5}$$

decreases rapidly as $\sim s^{-2p}$ with increasing s and fixed $p \geq 1$. Here $s \geq 1$ is the oversampling factor and $\tilde{T}_L$ is the interpolate of T_L given by the Lagrange interpolation,

$$\tilde{T}_L(\alpha) = \sum_{j=1}^{2p} T_L(\beta_j)\gamma_j(\alpha), \tag{6}$$

with the polynomials $\gamma_j(\alpha)$ defined as

$$\gamma_j(\alpha) = \prod_{\substack{k=1 \\ k \neq j}}^{2p} \frac{\alpha - \beta_k}{\beta_j - \beta_k}, \tag{7}$$

where the interpolation stencil points $\beta_j = \alpha_{m+j}$, $j = 1, \ldots, 2p$, and m is chosen so that $\beta_p \leq \alpha \leq \beta_{p+1}$, i.e. α is in the center interval of the stencil.

The numbers p and s must now be chosen so that the cost of the interpolation is reasonable for the target accuracy. By considering the interpolation error (5), Song and Chew [4] propose values $p = 3$ and $s = 5$ for $L \geq 50$ and the direct evaluation of $T_L(\boldsymbol{D}, \hat{\boldsymbol{k}})$ by (2) for $L < 50$.

Ergül and Gürel [5] examine the relation of the interpolation error (5) and the pairs (p, s) by numerical testing and tabulate the optimal pairs (p, s) for the relative interpolation accuracies 10^{-d_0}, $d_0 = 2, \ldots, 5$, and $L \geq 50$. For each d_0, the optimal pair (p, s) is taken to be that which leads to the least cost in oversampling by (2) and evaluating $T_L(\boldsymbol{D}, \hat{\boldsymbol{k}})$ by interpolation.

In MLFMA, however, it is essential to know what the resulting error is in the incoming field (1) due to the interpolation error in T_L. This aspect is not discussed in [4] or [5]. As expected, the error in the field is not the same as the interpolation error (5). This difference affects the accuracy criterion and the optimality in the choice of (p, s). Of course, the optimality also depends on the way the samples $T_L(\alpha_m)$ are computed and how low p can be used.

In this paper we greatly lower the cost of oversampling by using the FFT as follows. By (2) we directly only compute the samples $T_L(\alpha'_m)$ with $s = 1$, i.e. at the Nyquist sampling points

$$\alpha'_m = \frac{2\pi}{2L+1} m, \quad m = -L, \ldots, L. \tag{8}$$

Thereafter, we use FFT for computing the samples $T_L(\alpha_m)$ at the oversampling points α_m in (4) with $s > 1$. The cost of the oversampling in the fill-in of $T_L(\alpha_m)$ now becomes so low that only computing the samples $T_L(\alpha'_m)$ at the Nyquist rate counts. It turns out that the fill-in cost of $T_L(\alpha_m)$ with FFT method is about s times faster than by the direct computing with (2). With the low fill-in cost of $T_L(\alpha_m)$ the cost of evaluating T_L by interpolation from the samples $T_L(\alpha_m)$ becomes dominating and it is directly related to the length $2p$ of the stencil.

As an error criterion we have used the relative error in the field (1), and accordingly, we have determined the optimal pairs (p, s) so that $p \geq 2$ is the lowest integer by which the error criterion is satisfied with $s \leq 15$. In Section 5 we search and tabulate these pairs for the error levels 10^{-q}, $q = 1, \ldots, 8$, and the division levels $l = -1, \ldots, 10$. Here we number the division levels by $l = 0, \pm 1, \pm 2, \ldots$ so that on the level l the side of the division cube a_l equals to $2^{l-1}\lambda$. If some other choice and numbering of the levels is used, one can easily use our tables of (p, s) by interpolating the values between our levels.

Our (p, s)-tables show that the fixed choice $p = 3$, $s = 5$ in [4] yields the relative field accuracy of about 10^{-3}, in general. The (p, s) pairs recommended by [5] for levels $l \geq 3$ are not always optimal if FFT based faster oversampling is used, and with these pairs the expected relative accuracy 10^{-d_0}, $d_0 = 2, \ldots, 5$, is not always reached in the incoming field (1).

3 Lagrange Interpolation of Trigonometric Polynomials and Oversampling with FFT

Consider a trigonometric polynomial

$$T_L(\alpha) = \sum_{n=-L}^{L} b_n e^{in\alpha}, \quad -\pi \leq \alpha \leq \pi, \tag{9}$$

of order L, in general. We interpolate it at α by using samples $T_L(\beta_j)$ at equally spaced stencil points $\beta_1 < \ldots < \beta_{2p}$, $p \geq 1$, with spacing $h = 2\pi(2sL + 1)^{-1}$, and with $\beta_p \leq \alpha \leq \beta_{p+1}$. Due to the remainder of the Lagrange interpolation, e.g. see [7], and reasoning as in [3], we get for the interpolation error the estimate

$$\left|\tilde{T}_L(\alpha) - T_L(\alpha)\right| \leq \max_{\beta} \left|T_L^{(2p)}(\beta)\right| \frac{(2p)!}{(p!)^2} \left(\frac{h}{4}\right)^{2p}, \tag{10}$$

where $\tilde{T}_L(\alpha)$ is the interpolated value, $T_L^{(2p)}(\beta)$ is $(2p)$:th derivative of $T_L(\beta)$, and $s \geq 1$ is the oversampling factor. Due to Bernstein's lemma we have the estimate [3]

$$\max\left|T_L^{(2p)}(\alpha)\right| \le L^{2p}\max\left|T_L(\alpha)\right|, \tag{11}$$

which with (10) shows that the relative interpolation error defined by (5) for a fixed p decreases as $\sim s^{-2p}$ for increasing $s \ge 1$.

Accordingly, for an accurate interpolation we need to oversample T_L so that the spacing h of the stencil points is sufficiently dense. After having by (2) directly computed the samples

$$u(m) = T_L(\alpha'_m), \tag{12}$$

where α'_m are given by (8), we use the centered Fourier transform $\mathcal{F}_{2L+1}$,

$$\left(\mathcal{F}_{2L+1}u\right)(n) = \sum_{m=-L}^{L} u(m)e^{-i\frac{2\pi}{2L+1}nm}, \tag{13}$$

$n = -L, \ldots, L$, and compute the coefficients $b_n = b(n)$ in (9) by

$$b(n) = \frac{1}{2L+1}\left(\mathcal{F}_{2L+1}u\right)(n), \quad n = -L, \ldots, L. \tag{14}$$

Next we zero-pad the sequence b by adding $sL - L$ zeroes at both ends of b and get the sequence c. The wanted samples $T_L(\alpha_m)$ at the oversampling points α_m in (4) are now obtained by the inverse Fourier transform $\mathcal{F}^{-1}_{2sL+1}$ as

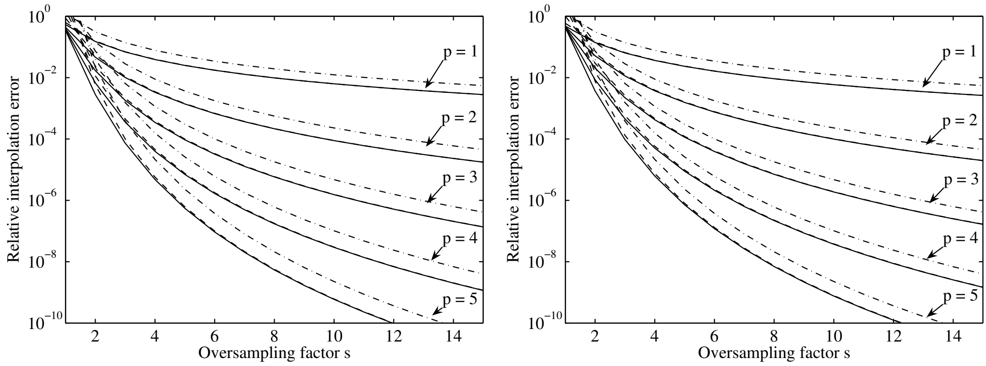
$$T_L(\alpha_m) = (2sL+1)\left(\mathcal{F}^{-1}_{2sL+1}c\right)(m), \tag{15}$$

for $m = -sL, \ldots, sL$. Using FFT in (14) and (15) makes the oversampling very fast with the cost of order $2sL\log(2sL)$.

In estimating the interpolation error by (10) we could use (11) as an upper bound for $\max\left|T_L^{(2p)})\right|$. Though it is quantitatively a good estimate, we get a much more accurate one by numerically computing $\max\left|T_L^{(2p)}\right|$. This can be done easily by using (9), because

$$T_L^{(2p)}(\alpha) = \sum_{m=-L}^{L}(im)^{2p}b_m e^{im\alpha} \tag{16}$$

and we anyway compute the coefficients b_m for oversampling. By using the above oversampling technique with coefficients $(im)^{2p}b_m$, $m = -L, \ldots, L$, we can sample $T_L^{(2p)}(\alpha)$ in a sufficiently dense grid, say with $20L+1$ samples, and find $\max\left|T_L^{(2p)}\right|$ with the computer very accurately.



(a) Level $l = 3$ (b) Level $l = 7$

Figure 1: The relative interpolation error as a function of the oversampling factor s with the number $n = 2p$ of the stencil points, $p = 1, \ldots, 5$, with $L = 65$ on level $l = 3$, and $L = 727$ on level $l = 7$. The solid line (——) marks the actual relative interpolation error, the dashed line (- - - -) the upper bound with $\max \left| T^{(2p)_L} \right|$, and the dash-dotted line ($\cdot - \cdot$—) the Bernstein upper bound.

Fig. 1 compares the actual relative interpolation error (5) with the estimates due to (10) with the computed $\max \left| T_L^{(2p)} \right|$ and with its upper bound (11) for levels $l = 3, 7$ and $L = 65, 727$, respectively, and for $p = 1, \ldots, 5$. As one observes in the Fig. 1, the numerically computed $\max \left| T_L^{(2p)} \right|$ gives us a very good estimate for the actual interpolation error, whereas the upper bound with (11) is clearly a poorer one.

In practical MLFMA computations, the evaluation of the Rokhlin translator T_L is then carried out as follows (also see [6, 8]). Start by choosing q, the number of digits of the target relative accuracy, and for each level l the order L. Notice that the coefficients b_n of $T_L(\alpha)$ in (9) only depend on $D = |\boldsymbol{D}|$ for a fixed L.

Next on each level l for all unique distances D compute and store the coefficients b_n by computing the samples $T_L(\alpha'_m)$ by (2) at the Nyquist sampling points α'_m in (8) and by using (14). Notice that in MLFMA on a fixed level there are 316 different translation vectors $\boldsymbol{D}$ but only 15 unique distances D due to the symmetry. Notice also that $T_L(-\alpha) = T_L(\alpha)$ for all α, $-\pi \leq \alpha \leq \pi$, and therefore only samples $T_L(\alpha'_m)$ for $m = 0, \ldots, L$ need to be computed. It follows that $b_{-n} = b_n$ and only $L + 1$ coefficients b_n for each D need to be stored. Thus one only needs to store $15(L + 1)$ coefficients b_n on each level l.

In carrying out the disaggregation sweeps in the MLFMA, we go through

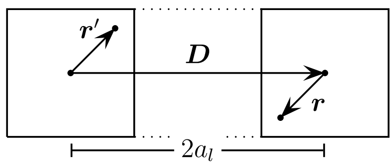


Figure 2: The geometry for finding the maximal relative error $E(l,L)$: the source and the field cube are positioned so that their separation is $2a_l$, and the positions of the source point $\boldsymbol{r}'$ and the field point $\boldsymbol{r}$ are varied inside the cubes.

the levels in the following steps. On a given level l and for a distance D we compute the samples $T_L(\alpha_m)$ at the oversampling points α_m in (4) by using the stored coefficients b_n and FFT as in (15). Thereafter, with these samples, for a vector $\boldsymbol{D}$ of the given length D we evaluate $T_L(\boldsymbol{D},\hat{\boldsymbol{k}})$ by interpolation and obtain the translation matrix. We then apply this translation matrix to all out-to-in translations that use this vector $\boldsymbol{D}$. Next, we evaluate $T_L(\boldsymbol{D},\hat{\boldsymbol{k}})$ for another vector $\boldsymbol{D}$ that has the same length D and compute the out-to-in translations. In this fashion we go through all the vectors $\boldsymbol{D}$ of the given length D. We repeat the process for all the different distances D on the level l.

4 The Field Error Due to the Interpolation of the Rokhlin Translator

Next we study how the the incoming field (1) is affected by the interpolation error in T_L. Because on a division level l the order L controls the truncation error in (1), we must first decide how we choose L so that the maximal relative truncation error $E(l,L)$ in (1) remains less than 10^{-q}, $q=1,\ldots,8$. It is sufficient to find $E(l,L)$ for a point source $\rho(\boldsymbol{r}')=\delta(\boldsymbol{r}')$ for which, with the Green's function G, we obtain

$$F(\boldsymbol{D}+\boldsymbol{r})=\int_S G(\boldsymbol{D}+\boldsymbol{r}-\boldsymbol{r}')\rho(\boldsymbol{r}')\,d\boldsymbol{r}'=\frac{e^{ik|\boldsymbol{D}+\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{D}+\boldsymbol{r}-\boldsymbol{r}'|} \tag{17}$$

and $F_{\max}=\max|F(\boldsymbol{D}+\boldsymbol{r})|=\frac{1}{4\pi a_l}$ with $a_l=2^{l-1}\lambda=2^l\pi/k$ being the side length of a division cube on level l. Here $\boldsymbol{r}\in Q_1$ and $\boldsymbol{r}'\in Q_2$ vary in the pair of the closest non-nearby division cubes Q_1, Q_2 as depicted in the Fig. 2.

It is well-known that $E(l,L)$ can be obtained from the incoming multipole series of the Green's function $G(\boldsymbol{D}+\boldsymbol{r}-\boldsymbol{r}')$, see e.g. [6]. By truncating the series at $n = L$ and dividing by $F_{\max}$ one obtains $E(l, L)$ as

$$E(l, L) = 4\pi a_l \max \left| R_L(\boldsymbol{r} - \boldsymbol{r}') \right|, \tag{18}$$

where $R_L(\boldsymbol{r} - \boldsymbol{r}')$ is the remainder of the series and $\boldsymbol{r} - \boldsymbol{r}'$ varies in a cube with side length $2a_l$ and the center at $\boldsymbol{D}$. The maximum is then easily found numerically. With $E(l, L)$ we then for a given l and q search the least $L = L(l, q)$ so that $E(l, L) \leq 10^{-q}$. In Table 1 we have tabulated $L = L(l, q)$ for $l = -1, \ldots, 10$ and $q = 1, \ldots, 8$. The values with gray background are those for which $\max|T_L| \geq 10^3$. For these values, the interpolation error in $\tilde{T}_L$ becomes high, as (11) suggests, and the estimation of $T_L(\alpha)$ by interpolation is not efficient anymore.

Note that often, instead of the accurate $L(l, q)$, its approximation $N(l, q)$ is used, given by the "excess band-width formula" [6],

$$N(l, q) = kd + 1.8q^{2/3}(kd)^{1/3}, \tag{19}$$

where $d = k\sqrt{3}a_l$. With the Table 1 we can see that this is a rather rough approximation, particularly yielding too low estimates for $L(l, q)$ for lower levels, say $l \leq 3$. An improved approximation has been given by Hastriter et al. [9]. Equation (19) is actually derived for large $|\boldsymbol{D}| \gg a_l$, and it follows, as the derivation in [6] shows, that $N(l-1, q)$ quite accurately gives the truncation order of a multipole series approximating the far field pattern $F_\infty(\hat{\boldsymbol{k}})$ in (1) on a given level l and with the maximal error less than 10^{-q}. In fact, we later use (19) for this purpose.

Because the field integral (1) is evaluated numerically, also the resulting integration error appears in (1). Therefore, to maintain the error control, the numerical integration rule should be chosen so that the integral error remains smaller than the truncation error.

Similarly, the error in the field arising from the interpolation of T_L must be kept smaller than the truncation error. In order to estimate this field error, it is sufficient to consider the field error for a point source at $\boldsymbol{r}'$ with $F_\infty(\hat{\boldsymbol{k}}) = \frac{1}{4\pi} e^{-ik\hat{\boldsymbol{k}}\cdot\boldsymbol{r}'}$.

Let us denote by $F_L(\boldsymbol{D} + \boldsymbol{r})$ the integral on the right-hand side of (1) and by $\tilde{F}_L(\boldsymbol{D} + \boldsymbol{r})$ the same integral when T_L is replaced by the interpolate $\tilde{T}_L$. Then for the field error due to the interpolation error in T_L we get,

$$\left| F_L(\boldsymbol{D} + \boldsymbol{r}) - \tilde{F}_L(\boldsymbol{D} + \boldsymbol{r}) \right| = \left| \int_{|\hat{\boldsymbol{k}}|=1} \left(T_L(\alpha) - \tilde{T}_L(\alpha) \right) \frac{1}{4\pi} e^{ik\hat{\boldsymbol{k}}\cdot(\boldsymbol{r}-\boldsymbol{r}')} \, d\hat{\boldsymbol{k}} \right|, \tag{20}$$

which implies the upper bound

$$\left| F_L(\boldsymbol{D}+\boldsymbol{r}) - \tilde{F}_L(\boldsymbol{D}+\boldsymbol{r}) \right| \leq \frac{1}{4\pi} \int_{|\hat{\boldsymbol{k}}|=1} \left| T_L(\alpha) - \tilde{T}_L(\alpha) \right| \, d\hat{\boldsymbol{k}} \leq \max \left| T_L(\alpha) - \tilde{T}_L(\alpha). \right| \tag{21}$$

Table 1: The orders L for the Rokhlin translator

Level	Accuracy 10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}
−1	6	16	29	45	59	75	91	105
0	7	16	29	45	59	75	91	105
1	13	19	32	46	62	75	91	105
2	23	29	39	49	65	78	92	108
3	46	50	56	65	75	88	101	115
4	89	95	99	105	112	121	131	141
5	176	184	190	194	199	204	210	217
6	349	359	367	373	378	384	388	394
7	697	710	720	727	734	740	747	753
8	1391	1410	1421	1430	1440	1448	1456	1463
9	2780	2805	2821	2834	2844	2854	2864	2874
10	5449	5593	5613	5630	5643	5659	5669	5682

One can check that the upper bound (21) is also valid if $\tilde{F}_L$ and F_L are computed by numerical integration in (1) by one of the two integration rules given below.

By using the upper bound (10) for $\max\left|\tilde{T}_L - T_L\right|$ one immediately gets an estimate for the field error, which could be used for finding optimal pairs (p, s) for the interpolation. However, in practise the field error defined by (20) is from 3 to 10 times smaller than the upper bound given by (21), because the integrand in (20) is highly oscillating around zero and lot of cancellation occurs in the integration, which phenomenon is neglected in (21).

Therefore, a better upper bound for the field error (20) is found on a given level l and with order L by numerically searching the maximum of the right-hand side of (20). To that end we numerically evaluate the integral with $\boldsymbol{r} - \boldsymbol{r}'$ running through the cube with side length $2a_l = 2^l\lambda$ and with the center at $\hat{\boldsymbol{D}}$. We also let $\hat{\boldsymbol{D}}$ vary in the main directions $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$. This search is done below in the Section 5.

We complete this section by reviewing two ways of numerically integrating (1). The first one is the popular way to use the Gauss-Legendre integration over the unit sphere, e.g. see [6], where the sampling grid (θ_m, φ_n) has $(L+1)(2L+1)$ points. The integrand $T_L(\boldsymbol{D}, \hat{\boldsymbol{k}})F_\infty(\hat{\boldsymbol{k}})e^{ik\hat{\boldsymbol{k}}\cdot\boldsymbol{r}}$ in (1) is sampled in this grid with $\hat{\boldsymbol{k}} = \hat{\boldsymbol{k}}(\theta_m, \varphi_m)$ and the samples are multiplied by the proper weights. The summation over the grid yields the field integral.

In the second method, see [10–12], we treat $T_L(\boldsymbol{D}, \hat{\boldsymbol{k}})$ and $F_\infty(\hat{\boldsymbol{k}})$ as trigonometric polynomials of two variables θ and φ. We first sample $F_\infty(\hat{\boldsymbol{k}})$ in a grid, uniform both in θ and φ, with $(N+1)(2N+1)$ sample points where $N = N(l,q)$ as in (19). With these samples $F_\infty(\hat{\boldsymbol{k}})$ is approximated by a trigonometric polynomial $P(\theta,\varphi)$ of order N in both θ and φ. Thereafter, in several steps, the function $\frac{1}{2}T_L|\sin\theta|P$ is anterpolated by FFT down to a trigonometric polynomial $V(\theta,\varphi)$ of order N. Finally, the field integral is obtained by integrating $V(\theta,\varphi)e^{ik\hat{\boldsymbol{k}}\cdot\boldsymbol{r}}$ in the $(N+1)(2N+1)$ uniform grid over $0 \le \theta \le \pi$, $-\pi \le \varphi \le \pi$ using the trapezoidal rule. This method makes the out-to-in translation (1) numerically more efficient than treating it by Gauss-Legendre rule, because $N \simeq \frac{1}{2}L$. Furthermore, the storing and the aggregation of $F_\infty(\hat{\boldsymbol{k}})$ as trigonometric polynomials are less costly and more accurate. Also, the field integral (1) is more accurate for aggregated far field patterns $F_\infty(\hat{\boldsymbol{k}})$ with the second method, see [10].

A thorough numerical testing shows that both above integration methods yield about the same field error given by (20).

5 Optimal (p,s)-Tables

We next seek for the optimized pairs (p,s) for the interpolation of T_L. For a given division level l and target accuracy of q digits we first choose $L = L(l,q)$ as in Section 3. Next we search for the smallest $p \ge 2$ so that the maximal relative field error in (20) is less than 10^{-q} with $s \le 15$. Here, the maximal relative error is the maximum of (20) divided by the maximal field value $F_{\max} = \frac{1}{4\pi a_l}$. Finally for that p we choose the smallest $s \ge 1$ so that the relative field error in (20) remains less than 10^{-q}.

We use two approaches for finding the pairs (p,s). First for fixed p and s we numerically search for the maximum of the field error (20) by letting $\boldsymbol{r} - \boldsymbol{r}'$ vary in a cube Q with side $2a_l$ and center at $\boldsymbol{D}$, and also varying $\boldsymbol{D} = 2a_l\hat{\boldsymbol{e}}$, for $\hat{\boldsymbol{e}} = \hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}$. We used both the two methods reviewed in the Section 4 for the numerical integration in (20). Thereafter, the optimal pairs (p,s) are found for varying levels l and accuracies q. The resulting pairs are presented in the Table 2.

We used MATLAB running on a usual PC workstation for the computations, and due to memory limitations of the PC, we could not compute optimal pairs for levels $l > 7$ with this approach.

Table 2: Numerically computed (p, s) values

	Accuracy							
Level	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}
-1	$(2,4)$	-	-	-	-	-	-	-
0	$(2,2)$	-	-	-	-	-	-	-
1	$(2,2)$	$(2,9)$	-	-	-	-	-	-
2	$(2,2)$	$(2,4)$	-	-	-	-	-	-
3	$(2,2)$	$(2,4)$	$(2,10)$	$(4,8)$	-	-	-	-
4	$(2,2)$	$(2,5)$	$(2,8)$	$(2,12)$	$(3,14)$	-	-	-
5	$(2,2)$	$(2,4)$	$(2,8)$	$(2,13)$	$(3,12)$	$(3,13)$	$(4,12)$	$(5,12)$
6	$(2,3)$	$(2,3)$	$(2,8)$	$(2,15)$	$(3,8)$	$(3,13)$	$(4,11)$	$(4,12)$
7	$(2,2)$	$(2,5)$	$(2,7)$	$(2,14)$	$(3,9)$	$(3,12)$	$(4,10)$	$(4,15)$

Our second approach is computationally much faster and it is based on the upper bound (21) of the field error with the upper bound (10) for $\left|\tilde{T}_L(\alpha) - T_L(\alpha)\right|$. Because the accurate maximal field error is replaced by the upper bound, we do get somewhat less 'optimal pairs' by this approach but now we can reach levels up to $l = 10$. These pairs (p, s) are presented in the Table 3. As the upper bound (21) gives the maximal possible error, the (p, s) values given in the Table 3 are a good check for the Table 2 values since they only rely on a wide numerical search of the maximum of the relative field error in (20). For practical computations we, however, consider the more efficient Table 2 values a safe choice.

Notice also that in the Tables 2 and 3 we have not given (p, s) pairs for cases where in the Table 1 the L values have gray background, i.e. $|T_L| \geq 10^3$, because the interpolation is then not efficient anymore.

6 Conclusions

In this paper, we have improved the previously presented interpolation methods for the Rokhlin translator T_L by introducing a new FFT based oversampling method that is more memory efficient and computationally less costly than directly computing the sample values for local interpolation. As our method also allows the use of higher oversampling factors s, it enables us to use a smaller number of interpolation stencil points, thus yielding a faster algorithm for the interpolation of T_L than before.

We have numerically computed the optimal pairs (p, s) as a function of

Table 3: 'Upper bound' (p, s) values

	Accuracy							
Level	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}
-1	$(2,6)$	-	-	-	-	-	-	-
0	$(2,4)$	-	-	-	-	-	-	-
1	$(2,5)$	$(3,9)$	-	-	-	-	-	-
2	$(2,5)$	$(2,12)$	-	-	-	-	-	-
3	$(2,6)$	$(2,11)$	$(3,10)$	$(5,10)$	-	-	-	-
4	$(2,7)$	$(2,12)$	$(3,9)$	$(3,14)$	$(4,15)$	-	-	-
5	$(2,8)$	$(2,15)$	$(3,10)$	$(3,15)$	$(4,11)$	$(4,15)$	$(5,13)$	$(6,14)$
6	$(2,10)$	$(3,8)$	$(3,11)$	$(4,9)$	$(4,12)$	$(5,10)$	$(5,13)$	$(6,11)$
7	$(2,12)$	$(3,9)$	$(3,13)$	$(4,10)$	$(4,13)$	$(5,11)$	$(5,14)$	$(6,12)$
8	$(2,14)$	$(3,10)$	$(3,14)$	$(4,11)$	$(4,15)$	$(5,12)$	$(5,15)$	$(6,12)$
9	$(3,8)$	$(3,11)$	$(4,9)$	$(4,12)$	$(5,10)$	$(5,13)$	$(6,11)$	$(6,13)$
10	$(3,9)$	$(3,13)$	$(4,10)$	$(4,13)$	$(5,11)$	$(5,14)$	$(6,12)$	$(6,14)$

the target accuracy of q digits and the division level l using the relative error in the translated field as the error criterion, which is a more realistic approach than only using the relative error of the interpolation. These optimal values (p, s) have been tabulated in this paper, and they can be used to obtain optimal accuracy and maximal speed-up in practical computations.

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