The Variable Order Fast Multipole Method for Boundary Integral Equations of the Second Kind. *

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Abstract

We discuss the variable order Fast Multipole Method (FMM) applied to piecewise constant Galerkin discretizations of boundary integral equations. In this version of the FMM low-order expansions are employed in the finest level and orders are increased in the coarser levels. Two versions will be discussed, the first version computes exact moments, the second is based on approximated moments. When applied to integral equations of the second kind, both versions retain the asymptotic error of the direct method. The complexity estimate of the first version contains a logarithmic term while the second version is \(O(N)\) where \(N\) is the number of panels.

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1 Introduction

Elliptic boundary value problems can often be written in the form of a boundary integral equation of the second kind

\[ \lambda u + \mathcal{W}u = f \quad (1.1) \]

where \(\mathcal{W}\) denotes the double layer operator

\[ (\mathcal{W}u)(x) = \int_S \frac{\partial}{\partial n'} G(|x - x'|)u(x')\,ds(x'). \quad (1.2) \]

Here, \(G(\cdot)\) is the Green’s function of the differential operator, \(S\) is the boundary surface whose normal at \(x' \in S\) is denoted by \(n'\). An equation in the form of (1.1) arises when the solution of a Dirichlet boundary value problem

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is represented with the double layer potential or when the Neumann problem is solved using Green's representation formula. In the latter case the right hand side is of the form $f = \mathcal{V}\partial u/\partial n$ where $\mathcal{V}$ the single layer operator

$$\mathcal{V}q(x) = \int_S G(|x - x'|)q(x') \, ds(x').$$

(1.3)

A common discretization scheme for (1.1) is the Galerkin method using piecewise constant elements. To that end, consider a triangulation of the boundary surface and the finite element space $X_h$ of functions which are piecewise constant on the triangulation. The Galerkin discretization of the layer potential $\mathcal{K}$ (which can be the single or double layer operator) is a matrix with coefficients

$$K_{i,j} = \langle \chi_i, \mathcal{K}\chi_j \rangle,$$

where $\chi_i$ is the characteristic function of the $i$-th triangle. Since integral operators are non-local $K$ is a dense matrix. Therefore the complexity for storage and matrix-vector multiplication is $O(N^2)$, where $N$ is the number of panels.

The Fast Multipole Method (FMM) is an effective tool to overcome $O(N^2)$-complexity. The method was originally developed by Greengard and Rokhlin [7, 6] for particle simulations but its importance for boundary element methods was soon recognized. The FMM accelerates the computation of well separated panel interactions by approximating them with truncated multipole expansions. The original version of the 3D-FMM [6] reduces the complexity of a matrix vector multiplication to $O(p^2 N)$, where $p$ is the order of the multipole expansion. Since $N$ is increased to reduce the discretization error, the order $p$ must be increased as well to keep the error introduced by multipole approximation of the same magnitude as the discretization error. Thus the FMM is not asymptotically optimal, in the sense that the complexity grows faster than $O(N)$ if the convergence of the discretization scheme is preserved. The dominant cost of the FMM are the multipole-to-local (MtL) translations, which, in the original version of the FMM, have $O(p^4)$ complexity. The new version of the FMM relies on exponential expansions and reduces the cost of an MtL to $O(p^2)$ operations [8], but the complexity of the matrix vector multiplication is still $O(p^2 N)$ with an improved constant factor. Thus the new version of the FMM is also not optimal in the above sense.

A different approach to reduce the computational cost for computing all MtL translations is to adjust the expansion order to the level. In the algorithm considered here, low order expansions (typically $p = 2$ or $p = 3$) are used in the finest level, then the order is incremented in each level. Thus inexpensive translations are employed in the fine levels, where most translations must be computed. Since the number of translations that need to be computed decreases exponentially when coarsening the level, the expensive
translations in the coarse levels do not contribute significantly to the overall cost. The complexity of the interaction phase (i.e., the computation of all MtL's in all levels) can be shown to be $O(N)$. Furthermore, in the case of an integral equations of the second kind discretized with piecewise constant elements the truncation error is $O(h)$.

We will discuss two versions of the variable order FMM. In the first version the order of the MtL's is variable, but the moments are computed in the usual upward pass. Since all fine level moments are needed to compute the coarse level moments, the order in the coarsest level determines the order of all the moments that must be computed, even though some moments may not be used for MtL’s. Therefore the asymptotic complexity of the upward pass is of higher order than the interaction phase, although the constant is much smaller. We will discuss a second version of the variable order FMM where moments are approximated in a variable order upward pass which results in an $O(N)$ algorithm. The convergence of the error with this scheme is still $O(h)$.

Here we will present a version of the FMM which is based on Taylor expansions, rather than Multipole expansions. This allows a unified treatment of a large class of Green's functions associated with elliptic boundary value problems and simplifies the discussion of translation operators. For the Laplace kernel, the variable order FMM could also be implemented with multipole expansions, which would, up to floating point errors, give the same results as the method based on Taylor expansions. Furthermore, the constant in the complexity estimate would be somewhat reduced.

The error introduced by the multipole approximation has been estimated in the original FMM paper [7] as well as in other papers, including [5] and [14], but we are not aware of previously published error estimates for the solution of the integral equation.

To put this paper into the proper perspective it is important to point out some of the other approaches to overcome the $O(N^2)$ complexity of boundary integral methods. Wavelet based compression schemes whose complexity estimates have logarithmic terms have been reported in [22, 12], and optimal wavelet schemes are reported in [18, 19]. Contrary to the FMM, wavelets lead to efficient preconditioners. This however, is not so important for second kind integral equations, because the conditioning of the discretized linear system is known to be independent of the meshwidth. Therefore, the advantage of a reduced number of iterations is often offset by the high computational cost to setup the stiffness matrix in the wavelet basis.

The variable order panel clustering method is another scheme which is optimal for second-kind integral equations [11, 13, 16, 17]. This approach and the more general framework of hierarchical (or $H$) matrices [1] are closely linked to the principle ideas of the FMM. We will show that the linear mapping associated with the FMM is an $H$-matrix, and therefore our analysis of the FMM benefits from the work in [17]. In this paper we will derive
sharper bounds of the error due to the Taylor series approximation of the kernel which will enable us to give realistic estimates for the truncation parameters that ensure optimal convergence of the multipole accelerated Galerkin scheme.

Finally, we mention that the scope of applications we have in mind include potential theory, linear elasticity and Stokes flow. In the case of scattering problems our asymptotic estimates only apply for the situation where the mesh is refined while the frequency is fixed. The FMM is very different if the meshwidth is proportional to the wavelength. Papers that deal with this situation are, for instance, [15, 2].

2 Hierarchical Surface Splitting

We briefly describe the hierarchical surface decomposition that the FMM uses to compute far field interactions efficiently. We follow the original paper [7] with some minor modifications. More general clustering schemes could also be used, see e.g., [1, 4].

The surface is embedded in a top-level cube $C_0$. This cube is uniformly subdivided into eight cubes at level one. These cubes are repeatedly refined until the finest level cubes contain at most a predetermined number of panels. The set of cubes that have a non-empty intersection with $S$ at the $l$-th refinement level is denoted by $C_l$. The collection of panels whose centroid is in cube $\nu$ is $S_{\nu}$ and the restriction of a function $f \in L^2(S)$ on $S_{\nu}$ is denoted by $f_{\nu}$, that is,

$$f_{\nu}(x) = \begin{cases} f(x), & x \in S_{\nu}, \\ 0, & \text{otherwise}. \end{cases}$$

The bounding box $B_{\nu}$ of $S_{\nu}$ is the smallest axiparallel box that contains $S_{\nu}$. We choose a point $x_{\nu}$ on $S_{\nu}$ and let

$$\rho_{\nu} = \max_{v: \text{vertex of } B_{\nu}} |v - x_{\nu}|$$

We note without proof that the data structures for the cube hierarchy and the bounding boxes can be determined in order $N$ operations.

We define the separation ratio of two different cubes in the same level as

$$\eta_{\nu, \nu'} = \frac{\rho_{\nu} + \rho_{\nu'}}{|x_{\nu} - x_{\nu'}|}, \quad \nu \neq \nu', \quad (2.1)$$

and set $\eta_{\nu, \nu} = \infty$. To describe the FMM, the following concepts will be needed.

- The nonempty children of cube $\nu$ are denoted by $\mathcal{K}(\nu)$ and the parent is denoted by $\pi(\nu)$. 

• The neighbors \( \mathcal{N}(\nu) \) of cube \( \nu \in C_l \) consist of the cubes that share at least one vertex with \( \nu \) as well as the cubes for which

\[
\eta_{\nu,\nu'} \geq \eta
\]

holds. The parameter \( \eta \) is predetermined. The smaller \( \eta \), the more cubes are considered neighbors.

• The interaction list consists of cubes whose parents are neighbors but which are not neighbors themselves, i.e.,

\[
\mathcal{I}(\nu) := \{ \nu' \in C_l : \pi(\nu') \in \mathcal{N}(\pi(\nu)) \text{ and } \nu' \notin \mathcal{N}(\nu) \}.
\]

The interaction list is a convenient way to split interactions of neighbors at a given level into neighboring and separated interactions at the next finer level. It follows immediately from the definition that

\[
\bigcup_{\nu' \in \mathcal{N}(\nu)} S_{\nu} \times \mathcal{I}(\nu) = \bigcup_{\mu \in \mathcal{K}(\nu)} \left( \bigcup_{\nu' \in \mathcal{N}(\nu')} S_{\mu} \times S_{\nu'} \cup \bigcup_{\nu' \in \mathcal{I}(\nu)} S_{\mu} \times S_{\nu'} \right)
\]

Using this fact repeatedly, we obtain the splitting which lies at the heart of the FMM

\[
S \times S = \bigcup_{l=2}^{L} \bigcup_{\nu \in C_l} S_{\nu} \times \mathcal{I}(\nu) \cup \bigcup_{\nu \in C_l} S_{\nu} \times S_{\nu'},
\]

and hence

\[
\langle f, Kg \rangle = \sum_{l=2}^{L} \sum_{\nu \in C_l} \langle f_{\nu}, Kg_{\nu} \rangle + \sum_{\nu \in C_l} \langle f_{\nu}, Kg_{\nu'} \rangle
\]

(2.4)

3 The Fast Multipole Method

The key idea of the FMM is to approximate the Green’s function in the interaction of well separated boxes by a truncated series expansion. Let \( \varphi_{\nu,\nu'} \) be potential due to panels in cube \( \nu' \) which is evaluated in the well separated cube \( \nu \). Let \( r_{\nu,\nu'} = x_{\nu} - x_{\nu'} \) and \( p \) be the expansion order, then

\[
\varphi_{\nu,\nu'}(x) = \int_{S_{\nu'}} \left( \frac{\partial}{\partial n'} \right)^{\kappa} G(|x - x'|) g(x') ds(x')
\]

\[
\approx \sum_{|\alpha|\leq p} \sum_{|\beta|\leq p-|\alpha|} \frac{D^{\alpha+\beta} G(|r_{\nu,\nu'}|)}{\alpha!\beta!} (x - x_{\nu})^\alpha \int_{S_{\nu'}} (x_{\nu'} - x')^\beta g(x') ds(x')
\]

\[
= \sum_{|\alpha|\leq p} \lambda_{\nu,\nu'}^\alpha (x - x_{\nu})^\alpha, \quad x \in S_{\nu}
\]

(3.1)
where $\alpha, \beta$ are multiindices and $\kappa = 0$ for the single and $\kappa = 1$ for the double layer operator. Here the local expansion coefficient $\lambda^\alpha_{\nu', \nu}$ is given by

$$
\lambda^\alpha_{\nu', \nu} = \sum_{|\beta| \leq p - |\alpha|} \frac{D^{\alpha + \beta} G(|r_{\nu' \nu}|)}{\alpha!\beta!} (-1)^{|\beta|} m^\beta_{\nu', \nu}(g), \quad |\alpha| \leq p,
$$

(3.2)

where $m^\beta_{\nu', \nu}(g)$ is a moment of the function $g$, which is given by

$$
m^\beta_{\nu', \nu}(g) = \int_{S_{\nu'}} \left( \frac{\partial}{\partial n_x} \right)^\kappa (x - x_{\nu'})^\beta g(x) \, ds(x), \quad |\beta| \leq p.
$$

(3.3)

Thus there are two types of moments, depending on whether $\mathcal{K}$ is the single layer ($\kappa = 0$) or the double layer potential ($\kappa = 1$). Since the translation operators for both types are identical, our notations will ignore this distinction. The computation of the local expansion coefficients from the moments in (3.2) is the MtL translation; in matrix notation this will be written as $\lambda_{\nu} = T(\nu, \nu') m_{\nu'}$.

The moments depend on the center $x_{\nu}$. In order to recursively compute the moments of a cube from the moments of its children, it is necessary to translate the center. This operation is the MtM translation. Its coefficients are derived easily from the multivariate binomial formula

$$
m^\alpha_{\nu}(g) = \sum_{\nu' \in \mathcal{K}(\nu)} \int_{S_{\nu'}} \frac{\partial^\kappa}{\partial n_x^\kappa} (x_{\nu'} - x_{\nu} + x - x_{\nu'})^\alpha g(x) \, ds(x)
$$

$$
= \sum_{\nu' \in \mathcal{K}(\nu)} \sum_{\beta \leq \alpha} \binom{\alpha}{\beta} (x_{\nu'} - x_{\nu})^{\alpha - \beta} m^\beta_{\nu', \nu}(g), \quad |\alpha| \leq p.
$$

(3.4)

In matrix notation (3.4) is $m_{\nu} = \sum_{\nu'} M(\nu, \nu') m_{\nu'}$.

The local expansion coefficients of a cube $\nu'$ are computed from the expansion coefficients of the cube’s parent $\nu$ by translating the expansion center

$$
\sum_{|\alpha| \leq p} \lambda^\alpha_{\nu}(x - x_{\nu})^\alpha = \sum_{\alpha} \lambda^\alpha_{\nu}(x - x_{\nu'} + x_{\nu'} - x_{\nu})^\alpha
$$

$$
= \sum_{|\alpha| \leq p} \lambda^\alpha_{\nu} \sum_{\beta \leq \alpha} \binom{\alpha}{\beta} (x_{\nu'} - x_{\nu})^{\alpha - \beta} (x - x_{\nu'})^\beta
$$

$$
= \sum_{|\beta| \leq p} \left( \sum_{\alpha \geq \beta} \binom{\alpha}{\beta} (x_{\nu'} - x_{\nu})^{\alpha - \beta} \lambda^\alpha_{\nu} \right) (x - x_{\nu'})^\beta
$$

$$
= \sum_{|\beta| \leq p} \lambda^\beta_{\nu'} (x - x_{\nu'})^\beta.
$$

In matrix notation we write $\lambda_{\nu'} = L(\nu', \nu) \lambda_{\nu}$.
For the finest level cube \( \nu \), \( \hat{f}_\nu \) denotes the vector of coefficients of \( f_\nu \) in the nodal basis \( \{ \chi_k \} \). The transformation of \( \hat{f}_\nu \) to the moments \( m_\nu(f) \) is linear and will be written in matrix form as \( m_\nu = Q(\nu) \hat{f}_\nu \). Likewise, the transformation of expansion coefficients \( \lambda_\nu \) to coefficients of the corresponding potential in the nodal basis is linear and is written as \( \hat{\varphi}_\nu = U(\nu) \lambda_\nu \).

The FMM is summarized as follows.

**Step 1.** Nearfield Calculation.
for \( \nu \in C_L \)
\[ \hat{\varphi}_\nu = \sum_{\nu' \in \mathcal{N}(\nu)} K(\nu, \nu') \hat{f}_{\nu'} \]

**Step 2.** Moment Calculation.
for \( \nu \in C_L \)
\[ m_\nu = Q(\nu) \hat{f}_\nu \]

**Step 3.** Upward Pass.
for \( l = L-1, \ldots, 2 \)
for \( \nu \in C_l \)
\[ m_\nu = \sum_{\nu' \in \mathcal{K}(\nu)} M(\nu, \nu') m_{\nu'} \]

**Step 4.** Interaction Phase.
for \( l = L, \ldots, 2 \)
for \( \nu \in C_l \)
\[ \lambda_\nu = \sum_{\nu' \in \mathcal{I}(\nu)} T(\nu, \nu') m_{\nu'} \]

**Step 5.** Downward Pass.
for \( l = 2, \ldots, L-1 \)
for \( \nu \in C_l \)
for \( \nu' \in \mathcal{K}(\nu) \)
\[ \lambda_{\nu'} = \lambda(\nu', \nu) \lambda_\nu \]

**Step 6.** Evaluation Phase.
for \( \nu \in C_L \)
\[ \hat{\varphi}_\nu = U(\nu) \lambda_\nu \]

Here the notation \( a += b \) means that variable \( b \) must be added to the value of variable \( a \). Note that after the downward pass the vectors \( \lambda_\nu \) contain the expansion coefficients of the potential due to panels outside of \( \mathcal{N}(\nu) \).

The operators in the upward and downward pass are related by
\[ M(\nu, \nu') = L(\nu', \nu)^T \quad \text{and} \quad T(\nu, \nu') = T(\nu', \nu)^T, \]

furthermore, in the case of the single layer operator, the additional symmetry relation
\[ Q(\nu) = U(\nu)^T \]
holds. For a large variety of kernels, the derivatives in the MtL translations can be computed by recurrence formulas, see [20].
So far we have not been specific about the choice of the expansion orders. In the original version of the FMM the expansion order is the same in all levels, but variable expansion orders have also been considered, see [5]. In this article we will analyze two versions of the FMM with variable moments.

**Exact Moments.** Choose a decreasing sequence of orders \( p_2, p_3, \ldots, p_L \). Perform the translation operations of Steps 2, 3, 5 and 6 in all levels with the largest order \( p_2 \) and perform the MtL translations of Step 4 with order \( p_l \) in level \( l \). Since high-order moments in the coarse levels depend on the high-order moments in the finer levels, the upward pass is computed with the largest order all levels. Thus all moments in this version are exact. Likewise, the low-order expansion coefficients in the fine levels depend on the high-order expansion coefficients in the coarse levels. Therefore the downward is also performed with order \( p_2 \) in all levels.

**Approximate Moments.** Choose a decreasing sequence of orders \( p_2, p_3, \ldots, p_L \) and compute the moments and expansion coefficients in level \( l \) only up to order \( p_l \). All higher order terms are assumed to vanish. The length of a moment or an expansion coefficient vector is given by \( n_l = (p_l + 1)(p_l + 2)(p_l + 3)/6 \). Thus for \( \nu \in C_l \) we have \( M(\nu, \nu') \in \mathbb{R}^{n_l \times n_l + 1} \), \( L(\nu, \nu) \in \mathbb{R}^{n_l + 1 \times n_l} \), and \( T(\nu, \nu') \in \mathbb{R}^{n_l \times n_l} \).

## 4 Exact Moments

We first discuss the variable order FMM with exact moments. The variable order FMM with approximate moments will be discussed in Section 5.

**Bilinear Form**

When the function \( g \) is applied to the operator using the FMM, the expansion coefficients \( \lambda_\nu \) represent the potential due to \( g \) outside \( \nu \) and its neighbors. For \( f, g \in X_n \), the bilinear form induced by the FMM is given by

\[
\langle f, \mathcal{K}_g \rangle := \sum_{\nu \in C_L} \langle f_\nu, \mathcal{K}_g \varphi_\nu \rangle + \sum_{\nu \in C_L} \langle f_\nu, \varphi_\nu \rangle \quad (4.1)
\]

where \( \varphi_\nu \) is the truncated expansion for cube \( \nu \). The terms in the second sum are of the form

\[
\langle f_\nu, \varphi_\nu \rangle = \sum_{|\alpha| \leq p_L} \langle f_\nu, (\cdot - x_\nu)^\alpha \rangle \lambda_\nu^\alpha = m_\nu^T(f) \lambda_\nu
\]

where \( k = 0 \) in the definition of the moments of \( f \). To bring (4.1) into a form that shows the dependence on \( g \) more clearly we backtrace the computation.
of the expansion coefficients. Because of (3.5) we have

\[
\sum_{\nu \in C_L} \langle f_\nu, \varphi_\nu \rangle = \sum_{\nu \in C_L} m^T_\nu (f) \lambda_\nu = \sum_{\nu \in C_L} \left( \sum_{\nu' \in I(\nu)} m^T_\nu (f) T(\nu, \nu') m_{\nu'} (g) + m^T_\nu (f) L(\nu, \pi(\nu)) \lambda_{\pi(\nu)} \right) = \sum_{\nu \in C_L} m^T_\nu (f) T(\nu, \nu') m_{\nu'} (g) + \sum_{\nu \in C_{L-1}} \sum_{\mu \in K_{\nu}} m^T_{\nu} (f) L(\mu, \nu) \lambda_\nu.
\]

In the case of the single layer operator the moments of \( f \) and \( g \) have \( \kappa = 0 \) in their definition (3.3). When \( K \) is the double layer operator, then we set \( \kappa = 0 \) for the the moments of \( f \) and \( \kappa = 1 \) for the moments of \( g \).

The above argument can be repeated for all coarser levels. The final result is

\[
\langle f, K_{\nu} g \rangle = \sum_{\nu \in C_L} \langle f_\nu, K_{\nu} g_{\nu'} \rangle + \sum_{l=2}^{L} \sum_{\nu \in C_L} \sum_{\nu' \in I(\nu)} m^T_\nu (f) T(\nu, \nu') m_{\nu'} (g).
\]

The interactions in \( I(\nu) \) can be written in terms of integral operators. We set

\[
\langle f_\nu, K_{\nu, \nu'} g_{\nu'} \rangle := m^T_\nu (f) T(\nu, \nu') m_{\nu'} (g) = \int_{S_\nu} \int_{S_{\nu'}} \left( \frac{\partial}{\partial n_\nu'} \right)^\kappa G_{\nu, \nu'} (x, x') f(x) g(x') ds(x) ds(x') dx',
\]

where the kernel of \( K_{\nu, \nu'} \) is the Taylor polynomial of the Green’s function (or its normal derivative in case of the double layer operator). Setting \( t_\nu = x - x_\nu \) and \( t'_{\nu'} = x' - x_{\nu'} \), the kernel can be written as

\[
G_{\nu, \nu'} (x, x') = \sum_{|\alpha| \leq \beta} D^\alpha G(|r_{\nu, \nu'}|) \frac{(t_\nu - t'_{\nu'})^\alpha}{\alpha!}.
\]

The following lemma summarizes the previous considerations.

**Lemma 4.1** The bilinear form induced by the FMM with exact moments is given by

\[
\langle f, K_{\nu} g \rangle = \sum_{\nu \in C_L} \langle f_\nu, K_{\nu} g_{\nu'} \rangle + \sum_{l=2}^{L} \sum_{\nu \in C_L} \sum_{\nu' \in I(\nu)} \langle f_\nu, K_{\nu, \nu'} g_{\nu'} \rangle .
\]
The rank of the matrices associated with \( f_\nu, \mathcal{K}_{\nu', \nu} g_{\nu'} \) is at most \( n_1 \). The
Lemma makes clear that the FMM approximates the matrix of \( \langle f, \mathcal{K} g \rangle \) by a
hierarchy of low-rank matrices. In other words, the decomposition in
Lemma 4.1 is an \( \mathcal{H} \)-matrix, see [1].

**Approximation Theory for Taylor Expansions**

The Green’s function of the Laplacian can be approximated by a
series of spherical harmonics, this is also known as the Addition
Theorem [10]. Taylor expansions involve more terms, but allow a
unified treatment of a large class of Green’s functions. Estimates for
Taylor series approximations of some Green’s functions have been
derived in [9], but the results there are weaker than the estimates
pertaining spherical harmonics approximations. Here we improve the
results of [9] and show that the error bounds for Taylor
polynomials are similar to those of the Addition Theorem. The
improved error bounds will clarify the proper choice for the parameter \( \eta \) in (2.2) and
the expansion orders in (3.1).

We assume that the Green’s function depends only on the distance
of the source and the field point, that is, \( G(x, x') = G(|x - x'|) \). Furthermore,
we assume that \( G(\cdot) \) is analytic except for the origin and that there is a
constant \( C \) such that

\[
|G(\tau)| \leq \frac{C}{|\tau|}, \quad 0 \neq \tau \in \mathbb{C}.
\]

(4.4)

The truncated Taylor series of the Green’s function is given by

\[
G(|r + z|) = \sum_{|\alpha| \leq p} \frac{D^\alpha_G(|r|)}{\alpha!} z^\alpha + R_p(r, z)
\]

(4.5)

**Lemma 4.2** For \( \eta < 1 \) and \( \nu' \in \mathcal{I}(\nu) \), there is a constant \( C > 0 \) such the
remainder of the truncated Taylor series is bounded by

\[
|R_p(r, z)| \leq C \frac{p}{|r|} \left( \frac{|z|}{|r|} \right)^{p+1},
\]

where \( r = x_\nu - x_{\nu'} \) and \( z = x - x' - r \).

**Proof.** We will denote by \(|\cdot|\) the analytic continuation of the real
euclidean norm, \(|r| := (r_1^2 + r_2^2 + r_3^2)^{\frac{1}{2}}\). Let \( r, z \in \mathbb{R}^3 \), \( \varphi \) the angle between \( z \) and \( r \),
\( \zeta = \frac{|z|}{|r|} \) and let \( t \in \mathbb{C} \). We have

\[
|r + tz| = |r| \left( 1 + 2t \zeta \cos \varphi + t^2 \zeta^2 \right)^{\frac{1}{2}} = |r| \left( 1 + t \zeta e^{i\varphi} \right)^{\frac{1}{2}} \left( 1 + t \zeta e^{-i\varphi} \right)^{\frac{1}{2}}.
\]

(4.6)
This factorization makes clear that \( t \mapsto |r + tz| \) is analytic for \( |t| < \frac{1}{\zeta} \). Set \( f(t) := G(|r + tz|) \) and consider the Taylor expansion with remainder in Cauchy integral form

\[
f(t) = \sum_{n=0}^{p} \frac{f^{(n)}(0)}{n!} t^n + \frac{t^{p+1}}{2\pi i} \int_{|\tau|=a} \frac{f(\tau)}{\tau^{p+1}(\tau - t)} d\tau
\]

for some \( a \) that satisfies \( |t| < a < \frac{1}{\zeta} \). It follows from the chain rule that for \( t = 1 \) this series is the Taylor series in (4.5), hence the Cauchy integral is used to estimate the remainder \( R_p(r, z) \). We let

\[
a := \left( 1 - \frac{1}{p} \right) \frac{1}{\zeta}
\]

then for \( |\tau| = a \) we have

\[
\left| (1 + \tau \zeta e^{i\varphi}) (1 + \tau \zeta e^{-i\varphi}) \right|^2 \geq 1 - a \zeta = \frac{1}{p}.
\]

From this estimate and (4.4) it follows that

\[
\max_{\tau=\bar{a}} |f(\tau)| = \max_{\tau=\bar{a}} |G(r + \tau z)| \leq C \max_{\tau=\bar{a}} \frac{1}{|r + \tau z|} \leq C \frac{p}{|r|},
\]

and hence the bound

\[
|R_p(r, z)| = \frac{1}{2\pi} \left| \int_{|\tau|=a} \frac{f(\tau)}{\tau^{p+1}(\tau - 1)} d\tau \right| \leq C \frac{p}{|r|} \frac{1}{a - 1} \frac{1}{a^p}
\]

holds. With the choice of the radius in (4.7) it then follows that

\[
|R_p(r, z)| \leq C \frac{p}{|r|} \frac{1}{1 - \frac{1}{p} - \zeta \left( 1 - \frac{1}{p} \right)^{-p} \zeta^{p+1}} (4.8)
\]

which implies the assertion. \( \square \)

Remark 1. For the Green’s function of the Laplacian \( G(t) = 1/t \) one has, using the notations of the above proof,

\[
G(|r + z|) = \frac{1}{|r|} \frac{1}{(1 + 2 \cos \varphi \zeta + \zeta^2)^{\frac{p}{2}}} = \frac{1}{|r|} \sum_{n=0}^{\infty} P_n(\cos \varphi) \zeta^n (4.9)
\]

where \( P_n \) is the \( n \)-th Legendre polynomial. Since \( P_n(\cos \varphi) \zeta^n \) is a homogeneous polynomial of order \( n \) in \( z \), the \( p \)-th partial sum in (4.9) is the \( p \)-th Taylor polynomial of the Green’s function. It is also the expansion into
spherical harmonics, and therefore the FMM based on Taylor expansions gives in exact arithmetic the same results as the FMM based on multipole expansions. Thus (4.9) can also be used to estimate the remainder. Since 

\[ |P_n(\cos \varphi)| \leq 1 \]

we have the bound

\[ |R_p(r, z)| = \left| \sum_{n=p+1}^{\infty} P_n(\cos \varphi) \zeta^n \right| \leq \frac{1}{|r| \zeta} \left( \frac{\zeta}{1 - \zeta} \right)^p. \]

Thus the factor \( p \) in Lemma 4.2 can be dropped for the Laplacian. This factor however will not be important in the following analysis.

**Remark 2.** Lemma 4.2 also applies to the Helmholtz equation. In this case the Green’s function is \( G(\tau) = \exp(ik\tau)/\tau \) and since \( \tau \) in estimate (4.4) is complex, the constant grows exponentially with \( \text{diam}(S)\kappa \). Therefore the following asymptotic results apply only if the wave number is fixed when the mesh is refined.

**Lemma 4.3** If the surface \( S \) is smooth, \( \eta < 1 \) and \( \nu' \in \mathcal{I}(\nu) \), then there is a constant \( C > 0 \) such that the remainder of the normal derivative of the truncated Taylor series is bounded by

\[
\left| \frac{\partial}{\partial n'} \left( G(|r + z|) - \sum_{|\alpha| \leq p} \frac{D^\alpha G(|r|)}{\alpha!} z^\alpha \right) \right| \leq C \frac{p^3}{|r|} \left( \frac{|z|}{|r|} \right)^p. 
\]

where \( r = x_{\nu} - x_{\nu'} \), \( x, x' \in S \) and \( z = x - x' - r \).

**Proof.** Since the points \( x, x', x_{\nu} \) and \( x_{\nu'} \) are all on the surface it is known that \( r^T n' = O(|r|^2) \) and \( z^T n' = O(|z|^2) \). As in the proof of Lemma 4.2 we will estimate the remainder in Cauchy integral form

\[
\frac{\partial}{\partial n'} R_p(r, z) = \frac{1}{2\pi i} \int_{|r| = a} \frac{\partial}{\partial n'} G(|r + \tau z|) \frac{d\tau}{\tau^{p+1}(\tau - 1)} d\tau 
\]

The normal derivative in the integrand is given by

\[
\frac{\partial}{\partial n'} G(|r + \tau z|) = -F(|r + \tau z|)(r + \tau z)^T n' \tau 
\]

where \( F(t) = G'(t)/t \) satisfies the estimate

\[
|F(t)| \leq \frac{C}{|t|^3}, \quad 0 \neq t \in \mathbb{C}. \quad (4.10)
\]

We let \( \zeta = \frac{|z|}{|r|} \) and choose the radius \( a \) according to (4.7). Then

\[
\max_{|r| = a} |(r + \tau z)^T n'| \leq C \left( |r|^2 + a|z|^2 \right) = C|r|^2 \left( 1 + a\zeta^2 \right) \leq C|r|^2.
\]
It follows from (4.6) and (4.10) that
\[
\max_{|\tau|=a} |F(|r + \tau z|)| \leq C \frac{p^3}{|r|^3}.
\]
Thus
\[
\left| \frac{\partial}{\partial n^l} R_p(r, z) \right| \leq C \frac{p^3}{|r|} \left( \frac{1}{a - 1} \frac{1}{a^{p-1}} \right).
\]
The assertion follows as in estimate (4.8). \(\square\)

Comparing the bilinear forms (2.4) and (4.3) makes clear that the only error introduced by the FMM comes from truncating the series in (3.1). Thus for \(f_h, g_h \in X_h\) the error of the bilinear form is
\[
\langle f_h, (\mathcal{K} - \mathcal{K}_F) g_h \rangle = \sum_{i=2}^{L} \sum_{\nu \in C_i \atop \nu' \in \mathcal{I}(\nu)} \langle f_{\nu}, (\mathcal{K} - \mathcal{K}_{\nu, \nu'}) g_{\nu'} \rangle.
\]

**Lemma 4.4** If \(\nu, \nu' \in C_l\) and \(\nu' \not\in \mathcal{N}(\nu)\) then
\[
| \langle f_{\nu}, (\mathcal{K} - \mathcal{K}_{\nu, \nu'}) g_{\nu'} \rangle | \leq C p^\kappa \eta_{\nu, \nu'}^p 2^{-l} \| f_{\nu} \| \| g_{\nu'} \|,
\]
where \(\kappa = 1\) for the single and \(\kappa = 3\) for the double layer operator. Here \(\| \cdot \|\) is the \(L^2(S)\)-norm.

**Proof.** If \(\mathcal{K}\) is the single layer operator it follows from (2.2), (4.2) and Lemma 4.2 that for \(\nu \in \mathcal{I}(\nu')\) and \(z = x - y - r_{\nu, \nu'}\)
\[
| \langle f_{\nu}, (\mathcal{K} - \mathcal{K}_{\nu, \nu'}) g_{\nu'} \rangle | \leq \max_{x \in S_{\nu}, y \in S_{\nu'}} | R_p(r_{\nu, \nu'}, z) | \int_{S_{\nu}} | f_{\nu}(x) | ds(x) \int_{S_{\nu'}} | g_{\nu'}(x') | ds(x')
\]
\[
\leq C p^\kappa \eta_{\nu, \nu'}^p \frac{|S_{\nu}|^\frac{1}{2} |S_{\nu'}| |r_{\nu, \nu'}|}{|r_{\nu, \nu'}|} \| f_{\nu} \| \| g_{\nu'} \|
\]
Since \(r_{\nu, \nu'} \sim 2^{-l}\) and \(|S_{\nu}| \leq C 2^{-2l}\) estimate (4.12) follows. The proof for the double layer operator is analogous. \(\square\)

To obtain the error of the bilinear form, the contributions of all interactions must be added. Because of the factor \(2^{-l}\) in (4.12), the errors are smaller in the finer levels and it suffices to use a smaller expansion order. We set
\[
p_l = L - l + p_L,
\]
where \(p_L\) is a small number independent of the meshwidth.

**Theorem 4.5** For \(f_h, g_h \in X_h\) and \(\eta < 1/2\) the error due to the FMM with orders given by (4.13) is bounded by
\[
| \langle f_h, (\mathcal{K} - \mathcal{K}_F) g_h \rangle | \leq C 2^{-L} \| f \| \| g \|.
\]
\textbf{Proof.} Since interaction lists have a bounded number of elements, it follows that
\[
\sum_{\nu \in \mathcal{C}_l} \| f_{\nu} \| g_{\nu'} \| \leq \left( \sum_{\nu \in \mathcal{C}_l} \| f_{\nu} \|^2 \right)^{\frac{1}{2}} \left( \sum_{\nu' \in \mathcal{C}_l} \| g_{\nu'} \|^2 \right)^{\frac{1}{2}} \leq C \| f_h \| \| g_h \|.
\]
We estimate (4.11) using (4.12)
\[
\left| \langle f_h, (\mathcal{K} - \mathcal{K}_F) g_h \rangle \right| \leq C \sum_{l=2}^{L} \sum_{\nu \in \mathcal{C}_l} p_{l}^{\kappa} \eta_{l}^{\kappa} R_{l} 2^{-l} \| f_{\nu} \| \| g_{\nu} \|
\]
\[
\leq C \sum_{l=2}^{L} p_{l}^{\kappa} \eta R_{l} 2^{-l} \| f_h \| \| g_h \|
\]
\[
\leq C2^{-L} \| f_h \| \| g_h \| \sum_{l=2}^{L} p_{l}^{\kappa} (2\eta)^{L-l}
\]
Since $\eta < 1/2$, the last sum is bounded independently of $L$, and hence estimate (4.14) follows. $\square$.

\textbf{Remark.} Theorem 4.5 shows that the error is linear in the $L^2$-norm. The choice of orders in (4.13) is not suitable if faster convergence or an estimate in a weaker norm is desired. Thus the described acceleration scheme is limited to integral equations of the second kind discretized with piecewise constant elements.

We turn to the solution of (1.1) with piecewise constant elements and FMM accelerated matrix vector multiplications. To obtain asymptotic estimates we assume that an initial coarse triangulation of the surface is several times quasi-uniformly refined and that with each mesh refinement the number of levels $L$ is incremented.

Let $\mathcal{A} = \lambda + \mathcal{W}$ then (1.1) is well posed in $L^2(S)$ if $\mathcal{A}$ is injective and satisfies the continuity condition
\[
\| \mathcal{A} v \| \leq c \| v \|, \quad v \in L^2(S)
\]
as well as the Gårding condition. That is, there is a compact operator $\mathcal{T}$ and a constant $\alpha > 0$ such that
\[
\text{Re} \langle (\mathcal{A} + \mathcal{T}) v, v \rangle \geq \alpha \| v \|^2, \quad v \in L^2(S).
\]
The approximate solution $u_h$ solves the variational problem
\[
\langle v_h, \mathcal{A} u_h \rangle = f_h(v_h), \quad v_h \in X_h \quad (4.15)
\]
where $X_h$ is the space of the piecewise constants and $f_h$ is a linear functional which can be of the form

$$f_h(v_h) = \langle v_h, f \rangle \quad \text{or} \quad f_h(v_h) = \langle v_h, V_r f \rangle$$

depending on the type of equation to be solved. Because of Theorem 4.5 estimates for the error $u - u_h$ in the $L^2(S)$-norm are standard.

**Theorem 4.6** The error satisfies the estimate

$$\|u - u_h\| \leq Ch\|u\|_1$$

**Proof.** It is well known that the Gårding property implies that $A$ satisfies

$$\|A v_h\| \geq c\|v_h\|, \quad v_h \in X_h$$

where $c > 0$. Theorem 4.5 then implies that the operators $A_r$ are stable as $h \to 0$

$$\|A_r v_h\| \geq \|A v_h\| - ||(A_r - A)v_h|| \geq (c - Ch\|v_h\| \geq c\|v_h\|, \quad v_h \in X_h$$

(4.16)

provided that $h$ is sufficiently small.

The remainder of the proof is a Strang-type argument. Denote the solution of (1.1) by $u$, the solution of (4.15) by $u_h$ and set $w_h = u_h - v_h$ for some $v_h \in X_h$. Then by (4.16) it follows that

$$\frac{1}{c} \|u_h - v_h\|^2 \leq \langle u_h - v_h, A_r w_h \rangle$$

$$= \langle u - v_h, Aw_h \rangle + \langle v_h, (A - A_r)w_h \rangle + \langle u_h, A_r w_h \rangle - \langle u, Aw_h \rangle$$

$$= \langle u - v_h, Aw_h \rangle + \langle v_h, (K - K_r)w_h \rangle + f(w_h) - f_h(w_h)$$

Dividing by $\|w_h\|$ and applying the triangle inequality leads to

$$\|u - u_h\| \leq C \inf_{v_h \in X_h} \left( \|u - v_h\| + \sup_{w_h \in X_h} \frac{\langle v_h, Kw_h \rangle - \langle v_h, K_r w_h \rangle}{\|w_h\|} \right)$$

$$+ C \sup_{w_h \in X_h} \frac{f(w_h) - f_h(w_h)}{\|w_h\|}$$

Since $2^{-L} \sim h$ the assertion is immediate from (4.14). □.

**Complexity Estimates**

In the refinement process considered the number of panels per cube is bounded and furthermore the number of non-empty cubes in the $l$-th level is bounded by

$$\#C_l \leq CN4^{-l-l}.$$
Since the parameter $\eta$ remains fixed as the mesh is refined, the number of neighbors and therefore the number of cubes in an interaction list is uniformly bounded. The number of flops to compute one MtL interaction in (3.2) is $p_l^6$, thus the total complexity for the interaction phase is

$$N_{\text{Inter}} \leq C \sum_{l=2}^{L} \# C_l p_l^6 \leq CN \sum_{l=2}^{L} (L - l + p_L)^6 4^{-(L - l)} \leq CN.$$  \hspace{1cm} (4.17)

Furthermore, the complexities of the nearfield and finest-level moment calculations, as well as the evaluation phase (Steps 1, 2 and 6 in the FMM) are obviously $O(N)$.

In the upward and the downward pass (Steps 3 and 5) there are $O(N)$ translations to be computed. In the FMM with exact moments each translation is evaluated with the same order $p_2$. Since the complexity of one translation is $O(p_2^6)$ and since $p_2 \sim L \sim \log_4(N)$ the complexity of the up-and downward pass is $O(N \log_4^6 N)$.

In the FMM with approximate moments the MtMs and LlLs are computed with order $p_l$ in level $l$. A similar calculation as (4.17) shows that the operation count of the up- and downward pass is reduced to $O(N)$. Thus the total complexity of Steps 1 to 6 is $O(N)$.

5 The variable order FMM with approximate moments

The variable order upward pass does not compute exact moments, therefore Lemma 4.3 does not apply. However, we will show in this section that a similar result applies.

The approximate moments of a function $f$ are denoted by $\tilde{m}_\nu^\alpha(f)$. We write

$$\tilde{m}_\nu^\alpha(f) = \int_{S_\nu} \left( \frac{\partial}{\partial n} \right)^\kappa \psi^\alpha(x) f(x) \, dx$$

where $\kappa$ is as in (3.3). In the finest level the moments are exact and hence $\psi^\alpha(x) = (x - x_\nu)^\alpha$. In the second finest level we find

$$\psi^\alpha(x) = \alpha! \sum_{\beta_\nu + \beta_{L-1} = \alpha} \frac{t_{L-1}^{\beta_{L-1}} i_{L-1}^{\beta_{L-1}}}{\beta_{L-1}! \beta_L!}$$

where $t_L = x - x_\nu$ and $t_{L-1} = x_L - x_{L-1}$ and $x_{L-1}$ denotes the expansion center of the bounding box in level $L - 1$ that contains the point $x$. Inductively, we then obtain for $\nu \in C_l$

$$\psi^\alpha(x) = \alpha! \sum_{\beta_1 + \cdots + \beta_L = \alpha} \frac{t_1^{\beta_1} \cdots t_L^{\beta_L}}{\beta_1! \cdots \beta_L!}$$

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where $t_k = x_{k+1} - x_k$, $k = L - 1, \ldots, l$ and $x_k$ denotes the expansion center of the bounding box in level $k$ that contains the point $x$.

The same computation that lead to Lemma 4.3 proves the next lemma.

**Lemma 5.1** The bilinear form induced by the FMM with approximate moments is given by

\[
\langle f, \tilde{K}_{\nu} g \rangle = \sum_{\nu' \in C_L} \langle f_{\nu'}, \tilde{K}_{\nu} g_{\nu'} \rangle + \sum_{l=2}^{L} \sum_{\nu' \in E(l)} \langle f_{\nu}, \tilde{K}_{\nu,\nu'} g_{\nu'} \rangle.
\]

(5.1)

where

\[
\langle f_{\nu}, \tilde{K}_{\nu,\nu'} g_{\nu'} \rangle = \hat{m}_\nu(f)^T T(\nu, \nu') \hat{m}_{\nu'}(g)
\]

and $\hat{m}_\nu(f)$ is the vector with coefficients $\hat{m}_\nu^\alpha(f), |\alpha| \leq p$.

The last term can also be written as

\[
\langle f_{\nu}, \tilde{K}_{\nu,\nu'} g_{\nu'} \rangle = \int_{S_{\nu'}} \int_{S_{\nu}} \sum_{|\alpha| \leq p} \frac{D^\alpha G(|r|)}{\alpha!} \sum_{\beta+\gamma = \alpha} (-1)^\gamma \psi^\beta_{\nu'}(x) \left( \frac{\partial}{\partial \nu'} \right)^\kappa \psi^\gamma_{\nu'}(x') f(x) g(x') ds(x) ds(x').
\]

Thus the kernel is given by

\[
\tilde{G}_{\nu,\nu'}(x, x') = \sum_{|\alpha| \leq p_k} D^\alpha G(|r|) \sum_{\beta+\gamma = \alpha} \sum_{|\beta_k| \leq p_k} \sum_{|\gamma_k| \leq p_k} (-1)^\gamma \frac{t^\beta_1}{\beta_1!} \cdots \frac{t^\beta_L}{\beta_L!} \frac{(t'^1)^\gamma_1}{\gamma_1!} \cdots \frac{(t'^L)^\gamma_L}{\gamma_L!}
\]

\[
= \sum_{|\alpha| \leq p_k} D^\alpha G(|r|) \sum_{\alpha_1 + \cdots + \alpha_L = \alpha} \frac{z^{\alpha_1}_{L}}{\alpha_1!} \cdots \frac{z^{\alpha_L}_{L}}{\alpha_L!}
\]

\[
= \sum_{\|\alpha_1 + \cdots + \alpha_L\| : k \leq p_k} D^{\alpha_1 + \cdots + \alpha_L} G(|r|) \frac{z^{\alpha_1}_{L}}{\alpha_1!} \cdots \frac{z^{\alpha_L}_{L}}{\alpha_L!}
\]

where $z_k = t_k - t'_{k}$, $k = l, \ldots, L$.

If in the above sum the condition $|\alpha_k| \leq p_k$ would be dropped, then the resulting expression would simplify to the standard Taylor polynomial in (4.5). Our main concern is whether the restrictions on the orders affects the approximation property of the Taylor expansion. The following lemmas answer this question.

**Lemma 5.2** If $p_L$ is such that $2^{-p_L} < \eta$, then

\[
\left| G_{\nu,\nu'}(x, x') - \tilde{G}_{\nu,\nu'}(x, x') \right| \leq C \frac{p_l}{|r|} \eta^p_l
\]

holds for $\nu' \in I(\nu)$, $x \in S_{\nu}$ and $x' \in S_{\nu'}$. 

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Proof. Rearranging indices gives the following equivalent representations

\[
G_{\nu,\nu'}(x, x') - \tilde{G}_{\nu,\nu'}(x, x') = \sum_{|\alpha_1 + \cdots + \alpha_L| \leq p_l \atop \sum_{|\alpha_k| > p_k}} D^{|\alpha_1 + \cdots + \alpha_L|} G(|r|) \frac{z_1^{\alpha_1}}{\alpha_1!} \cdots \frac{z_L^{\alpha_L}}{\alpha_L!}
\]

\[
= \sum_{k=1}^{L} \sum_{|\alpha_1 + \cdots + \alpha_L| \leq p_l} \sum_{|\alpha_k| = p_k+1} \sum_{|\alpha_k| = p_k+1} D^{|\alpha_1 + \cdots + \alpha_L|} G(|r|) \frac{z_1^{\alpha_1}}{\alpha_1!} \cdots \frac{z_L^{\alpha_L}}{\alpha_L!}
\]

\[
= \sum_{k=1}^{L} \sum_{|\alpha_1 + \cdots + \alpha_L| \leq p_l} \sum_{|\alpha_k| = p_k+1} \sum_{|\alpha_k| = p_k+1} \left( \frac{z_1^{\alpha_1}}{\alpha_1!} \cdots \frac{z_L^{\alpha_L}}{\alpha_L!} \right) \sum_{|\alpha_k| = p_k+1} D^{|\alpha_1 + \cdots + \alpha_L|} G(|r|) \frac{z_k^{\alpha_k}}{\alpha_k!}
\]

where the notation \( \{ \cdot \}_k \) means that the expression with index \( k \) must be omitted from the enclosed sum or product. Furthermore, we set \( \hat{z}_k = \{ z_1 + \cdots + z_L \}_k \). From the binomial formula and the Cauchy formula we obtain

\[
G_{\nu,\nu'}(x, x') - \tilde{G}_{\nu,\nu'}(x, x') = \sum_{k=1}^{L} \sum_{|\alpha_1 + \cdots + \alpha_L| \leq p_l} \sum_{|\alpha_k| = p_k+1} \left( \frac{z_1^{\alpha_1}}{\alpha_1!} \cdots \frac{z_L^{\alpha_L}}{\alpha_L!} \right) \sum_{|\alpha_k| = p_k+1} D^{a_k+\alpha_k} G(|r|) \frac{z_k^{\alpha_k}}{\alpha_k!}
\]

\[
= \sum_{k=1}^{L} \sum_{|\alpha_1 + \cdots + \alpha_L| \leq p_l} \sum_{|\alpha_k| = p_k+1} \frac{1}{(2\pi i)^2} \int \int \frac{G(|r + \sigma z_k + \tau \hat{z}_k|)}{\sigma^{n+1} \tau^{m+1}} \, d\sigma d\tau
\]

where the radii \( a_k \) and \( \hat{a}_k \) must be determined such that the function \(( \sigma, \tau ) \mapsto G(|r + \sigma z_k + \tau \hat{z}_k|)\) is analytic inside the enclosed disks. To this end consider the identity

\[
|r + \sigma z_k + \tau \hat{z}_k| = |r| \left( 1 + \sigma \zeta_k e^{i\varphi_k} + \tau \hat{\zeta}_k e^{i\hat{\varphi}_k} \right)^{\frac{1}{2}} \left( 1 + \sigma \zeta_k e^{-i\varphi_k} + \tau \hat{\zeta}_k e^{-i\hat{\varphi}_k} \right)^{\frac{1}{2}}
\]

where \( \zeta_k = \frac{|z_k|}{|r|}, \quad \hat{\zeta}_k = \frac{|z_k|}{|r|}, \) and \( \varphi_k, \hat{\varphi}_k \) are the angles between \( r \) and \( z_k, \hat{z}_k \), respectively. This factorization shows that the radii \( a_k \) and \( \hat{a}_k \) must satisfy

\[
\zeta_k a_k + \hat{\zeta}_k \hat{a}_k = 1 - \delta
\]

for some \( \delta > 0 \). If (5.3) holds, then it follows from (4.4) that

\[
\left| \frac{1}{(2\pi i)^2} \int \int \frac{G(|r + \sigma z_k + \tau \hat{z}_k|)}{\sigma^{n+1} \tau^{m+1}} \, d\sigma d\tau \right| \leq \frac{C}{\delta |r| a_k \hat{a}_k} \frac{1}{a_k \hat{a}_k}
\]

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and hence, because of \( p_l = p_k + k - l \)

\[
\left| G_{\nu, \nu'}(x, x') - \tilde{G}_{\nu, \nu'}(x, x') \right| \leq \frac{C}{\delta |\nu|} \sum_{k=l+1}^{L} \sum_{n+m \leq p_l} \frac{1}{a^n_k} \frac{1}{a^n_m} \sum_{n+m < k-l} \frac{1}{a^n_k} \frac{1}{a^n_m} \tag{5.4}
\]

To estimate (5.4) we set

\[
a_k = \left(1 - \frac{1}{p_l}\right) \frac{1 - \zeta_k}{\zeta_k} \quad \text{and} \quad \tilde{a}_k = 1 - \frac{1}{p_l} \tag{5.5}
\]

Note that this choice satisfies (5.3). Because of \(|z_k| + |\tilde{z}_k| < \rho_{\nu} + \rho_{\nu'}\) it follows that

\[
\frac{\zeta_k}{1 - \zeta_k} \leq \eta \tag{5.6}
\]

and since there are constants \(d_1, d_2 > 0\) such that \(|z_k| \leq d_1 2^{-k}\) and \(|\nu| \geq d_2 2^{-l}\), there is a constant \(\gamma\) such that

\[
\frac{\zeta_k}{1 - \zeta_k} \leq 2^{\gamma - k + \gamma}. \tag{5.7}
\]

Estimate (5.6) implies that

\[
\sum_{n+m < k-l} \frac{1}{a^n_k} \frac{1}{a^n_m} \leq C \left(1 - \frac{1}{p_l}\right)^{i-k} \tag{5.8}
\]

and hence we have for (5.4)

\[
\left| G_{\nu, \nu'}(x, x') - \tilde{G}_{\nu, \nu'}(x, x') \right| \leq C \frac{p_l}{|\nu|} \left(1 - \frac{1}{p_l}\right)^{-p_i} \sum_{k=l+1}^{L} \left(\frac{\zeta_k}{1 - \zeta_k}\right)^{p_k} \tag{5.9}
\]

We first estimate the terms in sum for \(l + d \leq k \leq L\), where \(d\) is the smallest integer such that \(2^{\gamma-d} \leq \eta\). Note that \(d\) is independent of \(l\) and \(L\). It follows from (5.7)

\[
\left(\frac{\zeta_k}{1 - \zeta_k}\right)^{p_k} \leq 2^{(\gamma+l-k)(p_L+L-k)}, \quad l + d \leq k \leq L. \tag{5.10}
\]

Since the exponent is quadratic in \(k\) the largest value occurs at one of the endpoints of the \(k\)-interval. Substituting \(k = l + d\) yields

\[
2^{(\gamma-d)(p_L+L-l-d)} = \left(2^{\gamma-d}\right)^{-d} \left(2^{\gamma-d}\right)^{p_i} \leq C \eta^{p_i}
\]

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where the factor $\eta^{-d}$ is absorbed in the constant. Substituting $k = L$ into (5.10) yields, because of $2^{-p_L} \leq \eta$,
\[ 2^p \gamma^{L+L'} \leq \eta^{p_L - \gamma - p_L} \leq C \eta^{p_L}, \]
where $\eta^{-p_L - \gamma}$ is absorbed in the constant. It then follows that
\[ \sum_{k=1+d}^{L} \left( \frac{\zeta_k}{1 - \zeta_k} \right)^{p_k} \leq C \eta^{p_L} \]
To estimate the terms in the sum of (5.9) for $l + 1 \leq k \leq l + d - 1$ we use estimate (5.6). It follows that
\[ \sum_{k=l+1}^{l+d-1} \left( \frac{\zeta_k}{1 - \zeta_k} \right)^{p_k} \leq \sum_{k=l+1}^{l+d-1} \eta^{p_L - (k-l)} \leq C \eta^{p_L} \]
where the factor $\eta^{-d}$ is absorbed in the constant. Thus the sum in (5.9) is bounded by $\eta^{p_L}$ and the assertion follows. $\square$.

**Lemma 5.3** If $S$ is smooth and $p_L$ is such that $2^{-p_L} < \eta$, then
\[ \left| \frac{\partial}{\partial \nu'} \left( G_{\nu,\nu}(x, x') - \tilde{G}_{\nu,\nu}(x, x') \right) \right| \leq C \frac{p^3}{|\nu'|^2} \eta^{p_L} \]
holds for $\nu' \in I(\nu)$, $x \in S_{\nu}$ and $x' \in S_{\nu'}$.

**Proof.** We begin by taking the normal derivative of (5.2)
\[ \frac{\partial}{\partial \nu'} \left( G_{\nu,\nu}(x, x') - \tilde{G}_{\nu,\nu}(x, x') \right) \]
\[ = \sum_{k=l+1}^{L} \sum_{n+m \leq p_L} \sum_{n, m \geq 1} \frac{1}{(2\pi \hat{t})^2} \int \int \frac{F(|r + \sigma z_k + \tau \hat{z}_k|)(r + \sigma z_k + \tau \hat{z}_k)n'}{\sigma^{n+1} \tau^m} d\sigma d\tau \]
where the radii $a_k$ and $\hat{a}_k$ are chosen as in (5.5). The function $F$ satisfies estimate (4.10). Since the surface is smooth, we have
\[ rn' = O(|r|^2), \quad z_k n' = O(|r||z_k|) \quad \text{and} \quad \hat{z}_k n' = O(|r||\hat{z}_k|). \]
Thus, because of (5.3),
\[ |(r + \sigma z_k + \tau \hat{z}_k)n'| \leq C|\nu|^2(2 - \frac{1}{p_L}). \]
It follows that
\[ \left| \frac{1}{(2\pi \hat{t})^2} \int \int \frac{F(|r + \sigma z_k + \tau \hat{z}_k|)(r + \sigma z_k + \tau \hat{z}_k)n'}{\sigma^{n+1} \tau^m} d\sigma d\tau \right| \leq C \frac{p^3}{|\nu'|} \frac{1}{a_k^n} \frac{1}{\hat{a}_k^{m-1}}. \]
and together with (5.8) that

$$\left| \frac{\partial}{\partial n'} \left( G_{\nu,\nu'}(x, x') - \tilde{G}_{\nu,\nu'}(x, x') \right) \right| \leq C_p^3 \frac{L}{|r|} \sum_{k=1}^{L} \sum_{\sum_{n+m} n > \nu_{k,m} \geq 1} \frac{1}{a_k^{m-1}}.$$

Up to irrelevant factors, this expression is identical to (5.4). Proceeding as in the previous proof leads to the assertion. □.

The estimates of Lemmas 5.2 and 5.3 are of the same form as the ones in Lemmas 4.2 and 4.3. Thus Theorems 4.5 and 4.6 also apply for the FMM with approximate moments.

6 Numerical Examples

We illustrate the complexity and convergence of the variable order FMM with exact and approximate moments. All computations are in core on a single processor of a Compaq ES40 Alpha server with 833MHz clock speed.

The method is applied to solve the integral equation

$$2\pi \sigma(x) + \int_S \frac{1}{|x - x'|} \sigma(x') \, ds(x') + \int_S \frac{1}{|x_0 - x'|} \sigma(x') \, ds(x') = 4\pi, \; x \in S,$$

(6.1)

where $S$ is the ellipsoid $(x_1/2)^2 + x_2^2 + (x_3/3)^2 = 1$ and $x_0$ is a point in the interior of the ellipsoid. The solution $\sigma$ of (6.1) is the equilibrium charge distribution when the ellipsoid has constant potential and can be expressed analytically using ellipsoidal coordinates [21]. Note that the first integral operator in (6.1) is the adjoint of the double layer potential, but it is easy to see that the results developed here also apply for this operator. The second integral operator has rank one and can be evaluated with $O(N)$ complexity without compression.

<table>
<thead>
<tr>
<th>panels</th>
<th>fixed order</th>
<th>exact mom.</th>
<th>approx. mom.</th>
</tr>
</thead>
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<tr>
<td>L</td>
<td>p</td>
<td>L</td>
<td>p_L</td>
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<td>192</td>
<td>2 2</td>
<td>2 3</td>
<td>2 3</td>
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<tr>
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<td>3 3</td>
<td>3 3</td>
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<td>4 3</td>
<td>4 3</td>
</tr>
<tr>
<td>12288</td>
<td>4 4</td>
<td>5 3</td>
<td>5 3</td>
</tr>
<tr>
<td>49152</td>
<td>5 4</td>
<td>6 3</td>
<td>6 3</td>
</tr>
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<td>7 3</td>
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</tr>
<tr>
<td>786432</td>
<td>7 6</td>
<td>8 3</td>
<td>8 3</td>
</tr>
</tbody>
</table>

Table 1: Parameters in Tables 2, 3 and 4, see (4.13).
\begin{table}
\centering
\begin{tabular}{|c|c|c|c|}
\hline
panels & fixed order $e_L$ & $L^2$-err & exact mom. $e_L$ & $L^2$-err & approx. mom. $e_L$ & $L^2$-err \\
\hline
192 & 0.00021 & 0.34471 & 0.00005 & 0.34472 & 0.00005 & 0.34472 \\
768 & 0.00103 & 0.14574 & 0.00121 & 0.14575 & 0.00121 & 0.14575 \\
3072 & 0.00142 & 0.06742 & 0.00263 & 0.06740 & 0.00265 & 0.06738 \\
12288 & 0.00053 & 0.03284 & 0.00148 & 0.03283 & 0.00151 & 0.03283 \\
49152 & 1.001635 & -1 & 0.01638 & -1 & 0.01638 \\
196608 & 1.000816 & -1 & 0.00822 & -1 & 0.00822 \\
786432 & 1.000409 & -1 & 0.00413 & -1 & 0.00413 \\
\hline
\end{tabular}
\caption{Errors, $\eta = 0.4$.}
\end{table}

\begin{table}
\centering
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
panels & fixed order & exact mom. & approx. mom. \\
& iteration & total & iteration & total & iteration & total \\
\hline
192 & $0^2(11)$ & 0 & $0^2(11)$ & 1 & $0^2(11)$ & 1 \\
768 & $0^2(11)$ & 3 & $0^2(11)$ & 2 & $0^2(11)$ & 2 \\
3072 & 0.3(12) & 17 & 0.4(11) & 17 & 0.4(11) & 16 \\
12288 & 3.8(10) & 88 & 2.4(10) & 74 & 2.3(10) & 73 \\
49152 & 16.1(10) & 364 & 11.5(10) & 322 & 10.8(10) & 309 \\
196608 & 116.5(10) & 1993 & 49.7(9) & 1310 & 44.4(9) & 1216 \\
786432 & 821.0(9) & 11033 & 212.2(9) & 5774 & 179.7(9) & 5169 \\
\hline
\end{tabular}
\caption{Time per iteration, number of iterations and total time (in seconds), $\eta = 0.4$.}
\end{table}

The initial discretization of the ellipsoid consists of 192 panels, which is several times uniformly refined. In an optimal scheme, the $L^2$-error is halved and the time and memory usage is quadrupled with each mesh refinement. We compare both versions of the variable order FMM and the FMM with fixed order in all levels; the truncation parameters are shown in Table 1. We store the matrices $K(\nu, \nu')$ for the nearby interactions, and the matrices $Q(\nu)$ and $U(\nu)$ of the multipole algorithm. The MtM, MtL and LtL transformations are computed on the fly. Instead of recomputing the derivatives in the MtL transformation one could also compute them once and store them. In this case the memory usage is roughly doubled whereas the timings are only reduced by about ten percent.

The $L^2$-errors associated with the three versions of the FMM are shown in Table 2. For the fixed-order FMM the order was chosen such that the

\footnote{Not enough memory to compute this quantity.}
\footnote{Time is less than 0.1 seconds.}

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error due to the multipole acceleration appeared to be a magnitude smaller than the discretization error. In the variable order versions this was accomplished with $p_L = 3$. Thus we may assume that the errors in Table 2 are good approximations of errors that one would obtain with the uncompressed Galerkin scheme. Note that arguments similar to those of the proof of Theorem 4.5 lead to the conclusion that the compression error of the fixed-order FMM is $O(n^p)$, hence the values of $p$ in Table 1 are consistent with this estimate.

We also compute the quantity

$$e_L = \sup_{f_h, g_n \in X_h} \frac{\langle f_h, (\mathcal{K} - \mathcal{K}_F) g_n \rangle}{\|f_h\| \|g_n\|}$$

by means of the power iteration. For the coarse meshes this number is much smaller than expected which indicates that the asymptotic estimate of Theorem 4.5 applies only after the mesh has been sufficiently refined.

Timings and memory allocations are displayed in Table 3 and 4. The results for the FMM with approximate moments are in good agreement with the theoretical $O(N)$ estimates. In the case of exact moments storage of QtM operators is dominant, because they must be computed with the highest order. Since the order in the coarsest level in the variable-order FMM is higher than in the fixed-order FMM, the variable-order FMM with exact moments uses the most memory.

The separation ratio strongly influences the behavior of the FMM algorithm. The dependence of error, time and memory allocation for different values $\eta$ are shown in Table 5. These results are again in good agreement with the requirement of Theorem 4.5 that $\eta < 0.5$.

Theorem 4.6 applies for smooth surfaces only, but it is interesting to consider nonsmooth surfaces as well. We solve the exterior Neumann problem with Green’s representation formula for the unit cube $[0, 1]^3$ on a graded mesh. Each face of the cube is subdivided into a rectangular grid where the distance of the $i$-th line from an edge is order $(i/n)^2$. Then the four nearest
rows to an edge are deleted. The remaining rectangles are divided into two triangles each. Elschner shows that on this type of grid the Galerkin scheme is stable in $L^2$ and that in the case of piecewise constant elements the error is $O(1/n)$, see [3].

<table>
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<th>variable order</th>
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<td></td>
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<tr>
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<td>0.00060</td>
<td>6</td>
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</tbody>
</table>

Table 6: $L^2$-errors for the cube.

Table 6 displays results of the variable order FMM with approximate moments and of the fixed-order FMM. The errors of the fixed-order FMM appear to be close to the theoretical $O(1/n)$ error bound of the full Galerkin scheme. The errors of the variable-order FMM are identical for the first two significant digits, though one should not have expected that from the theory. We set $p_L = 3$ and increment $L$ each time $n$ is doubled. Since the mesh is non-uniform the cost for the computation of the nearfield is no longer linear in the number of panels. Timings and memory usage reflect this behavior.

References


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