Approximation of integral operators by Green quadrature and nested cross approximation

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Received: 8 April 2014 / Revised: 31 January 2015
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Abstract  We present a fast algorithm that constructs a data-sparse approximation of matrices arising in the context of integral equation methods for elliptic partial differential equations. The new algorithm uses Green’s representation formula in combination with quadrature to obtain a first approximation of the kernel function, and then applies nested cross approximation to obtain a more efficient representation. The resulting $H^2$-matrix representation requires $O(nk)$ units of storage for an $n \times n$ matrix, where $k$ depends on the prescribed accuracy.

Mathematics Subject Classification 65N38 · 65N80 · 65D30 · 45B05

1 Introduction

We consider integral equations of the form

$$\int_{\Omega} g(x, y) u(y) \, dy = f(x)$$

for almost all $x \in \Omega$.

In order to solve these equations numerically, we choose a trial space $U_h$ and a test space $V_h$ and look for the Galerkin approximation $u_h \in U_h$ satisfying the variational equation
\[ \int_{\Omega} v_h(x) \int_{\Omega} g(x, y) u_h(y) \, dy \, dx = \int_{\Omega} v_h(x) f(x) \, dx \quad \text{for all} \quad v_h \in V_h. \]

If we fix bases \((\psi_j)_{j \in J}\) of \(U_h\) and \((\phi_i)_{i \in I}\) of \(V_h\), the variational equation translates into a linear system of equations

\[ G \hat{u} = \hat{f} \]

with a matrix \(G \in \mathbb{R}^{I \times J}\) given by

\[ g_{ij} = \int_{\Omega} \phi_i(x) \int_{\Omega} g(x, y) \psi_j(y) \, dy \, dx \quad \text{for all} \quad i \in I, \ j \in J. \quad (1) \]

The matrix \(G\) is typically non-sparse. For standard applications in the field of elliptic partial differential equations, we even have \(g_{ij} \neq 0\) for all \(i \in I, \ j \in J\).

Most techniques proposed to handle matrices of this type fall into one of two categories: kernel-based approximations replace \(g\) by a degenerate approximation \(\tilde{g}\) that can be treated efficiently, while matrix-based approximations work directly with the matrix entries.

The popular multipole method [19,28] relies originally on a special expansion of the kernel function, the panel clustering method [24] uses the more general Taylor expansion or interpolation [11,16], while “multipole methods without multipoles” frequently rely on “replacement sources” located around the domain selected for approximation [1,35]. Wavelet methods [14,15,25] implicitly use an approximation of the kernel function that leads to a sparsification of the matrix due to the vanishing-moment property of wavelet bases, therefore we can also consider them as kernel-based approximations.

Matrix-based approximations, on the other hand, typically evaluate a small number of matrix entries \(g_{ij}\) and use these to construct an approximation. The cross-approximation approach [17,33,34] computes a small number of “crosses” consisting each of one row and one column of submatrices that lead to low-rank approximations. Combining this technique with a pivoting strategy and an error estimator leads to the well-known adaptive cross approximation method [2–5,27,32].

Both kernel- and matrix-based approximations have advantages and disadvantages. Kernel-based approximations can typically be rigorously proven to converge at a certain rate, and they do not depend on the choice of basis functions or the mesh, but they are frequently less efficient than matrix-based approximations. Matrix-based approximations typically lead to very high compression rates and can be used as black-box methods, but error estimates currently depend either on computationally unfeasible pivoting strategies (e.g., computing submatrices of maximal volume) or on heuristics based on currently unproven stability assumptions.

Hybrid methods try to combine kernel- and matrix-based techniques in order to gain all the advantages and avoid most of the disadvantages. An example is the hybrid cross approximation technique [8] that applies cross approximation to a small submatrix resulting from interpolation, thus avoiding the requirement of possibly unreliable error
estimators. Another example is the kernel-independent multipole method [35] that uses replacement sources and solves a regularized linear system to obtain an approximation.

The new algorithm we are presenting in this paper falls into the hybrid category: in a first step, an analytical scheme is used to obtain a kernel approximation that leads to factorized approximation of suitably-chosen matrix blocks. In a second step, this approximation is compressed further by applying a cross approximation method to certain factors appearing in the first step, allowing us to improve the efficiency significantly and to obtain an algebraic interpolation operator that can be used to compute the final matrix approximation very rapidly.

For the first step, we rely on the relatively recent concept of quadrature-based approximations [7] that can be applied to kernel functions resulting from typical boundary integral formulations and takes advantage of Green’s representation formula in order to reduce the number of terms. Compared to standard techniques using Taylor expansion or polynomial interpolation that require $O(m^d)$ terms to obtain an $m$-th order approximation in $d$-dimensional space, the quadrature-based approach requires only $O(m^{d-1})$ terms and therefore has the same asymptotic complexity as the original multipole method. While the original article [7] relies on the Leibniz formula to derive an error estimate for the two-dimensional case, we present a new proof that takes advantage of polynomial best-approximation properties of the quadrature scheme in order to obtain a more general result. We consider the Laplace equation as a model problem, which leads to the kernel function

$$g(x, y) = \frac{1}{4\pi \|x - y\|_2}$$

on a domain or submanifold $\Omega \subseteq \mathbb{R}^3$, but we point out that our approach carries over to other kernel functions connected to representation equations, e.g., it is applicable to the low-frequency Helmholtz equation (cf. [26, eq. (2.1.5)]), the Lamé equation (cf. [26, eq. (2.2.4)]), the Stokes equation (cf. [26, eq. (2.3.8)]), or the biharmonic equation (cf. [26, eq. (2.4.6)]).

2 $\mathcal{H}^2$-matrices

Since we are not able to approximate the entire matrix at once, we consider submatrices. Hierarchical matrix methods [18,21,23] choose these submatrices based on a hierarchy of subsets.

**Definition 1 (Cluster tree)** Let $\mathcal{I}$ denote a finite index set. Let $\mathcal{T}$ be a labeled tree, and denote the label of a node $t \in \mathcal{T}$ by $\hat{t}$. We call $\mathcal{T}$ a cluster tree for $\mathcal{I}$ if

- the root $r \in \mathcal{T}$ has the label $\hat{r} = \mathcal{I}$,
- any node $t \in \mathcal{T}$ with $\text{sons}(t) \neq \emptyset$ satisfies $\hat{t} = \bigcup_{t' \in \text{sons}(t)} \hat{t}'$, and
- any two different sons $t_1, t_2 \in \text{sons}(t)$ of $t \in \mathcal{T}$ satisfy $\hat{t}_1 \cap \hat{t}_2 = \emptyset$.

The nodes of a cluster tree are called clusters. A cluster tree for an index set $\mathcal{I}$ is denoted by $\mathcal{T}_\mathcal{I}$, the corresponding set of leaves by $\mathcal{L}_\mathcal{I} := \{ t \in \mathcal{T}_\mathcal{I} : \text{sons}(t) = \emptyset \}$. 

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Submatrices of a matrix \( G \in \mathbb{R}^{I \times J} \) are represented by pairs of clusters chosen from two cluster trees \( T_I \) and \( T_J \) for the index sets \( I \) and \( J \), respectively. In order to find suitable submatrices efficiently, these pairs are also organized in a tree structure.

**Definition 2** (Block tree) Let \( T_I \) and \( T_J \) be cluster trees for index sets \( I \) and \( J \) with roots \( r^I \) and \( r^J \). Let \( T \) be a labeled tree, and denote the label of a node \( b \in T \) by \( \hat{b} \).

We call \( T \) a block tree for \( T_I \) and \( T_J \) if

- for each \( b \in T \), there are \( t \in T_I \) and \( s \in T_J \) with \( b = (t, s) \) and \( \hat{b} = \hat{t} \times \hat{s} \),
- the root \( r \in T \) satisfies \( r = (r^I, r^J) \),
- for each \( b = (t, s) \in T \) with \( \text{sons}(b) \neq \emptyset \), we have

\[
\text{sons}(b) = \begin{cases} 
\text{sons}(t) \times \{s\} & \text{if } \text{sons}(t) \neq \emptyset \text{ and } \text{sons}(s) = \emptyset, \\
\{t\} \times \text{sons}(s) & \text{if } \text{sons}(t) = \emptyset \text{ and } \text{sons}(s) \neq \emptyset, \\
\text{sons}(t) \times \text{sons}(s) & \text{otherwise}.
\end{cases}
\]

The nodes of a block tree are called blocks. A block tree for cluster trees \( T_I \) and \( T_J \) is denoted by \( T_I \times T_J \), the corresponding set of leaves by \( L_I \times T_J \).

In the following we assume that index sets \( I \) and \( J \) with corresponding cluster trees \( T_I \) and \( T_J \) and a block tree \( T_I \times T_J \) are given.

It is easy to see that \( T_I \times T_J \) is itself a cluster tree for the Cartesian product index set \( I \times J \). A simple induction shows that for any cluster tree, the leaves’ labels form a disjoint partition of the corresponding index set. In particular, the leaves of the block tree \( T_I \times T_J \) correspond to a disjoint partition

\[
\{\hat{t} \times \hat{s} : b = (t, s) \in L_I \times T_J \}
\]

of the product index set \( I \times J \) corresponding to the matrix. This property allows us to define an approximation of a matrix \( G \in \mathbb{R}^{I \times J} \) by choosing approximations for all submatrices \( G|_{\hat{t} \times \hat{s}} \) corresponding to leaf blocks \( b = (t, s) \in L_I \times T_J \).

Since we cannot approximate all blocks equally well, we use an admissibility condition

\[
\text{adm} : T_I \times T_J \to \{\text{true, false}\}
\]

that indicates which blocks can be approximated. A block \((t, s)\) is called admissible if \( \text{adm}(t, s) = \text{true} \) holds.

**Definition 3** (Admissible block tree) The block tree \( T_I \times T_J \) is called admissible if

\[
\text{adm}(t, s) \lor \text{sons}(t) = \emptyset \lor \text{sons}(s) = \emptyset \quad \text{for all leaves } b = (t, s) \in L_I \times T_J.
\]

It is called strictly admissible if

\[
\text{adm}(t, s) \lor (\text{sons}(t) = \emptyset \land \text{sons}(s) = \emptyset) \quad \text{for all leaves } b = (t, s) \in L_I \times T_J.
\]
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Given cluster trees $T_I$ and $T_J$ and an admissibility condition, a minimal admissible (or strictly admissible) block tree can be constructed by starting with the root pair $(r_I, r_J)$ and checking whether it is admissible. If it is, we are done. Otherwise, we recursively check its sons and further descendants [23].

Admissible leaves $b = (t, s) \in L_{I \times J}$ correspond to submatrices $G|_{\hat{t} \times \hat{s}}$ that can be approximated, while inadmissible leaves correspond to submatrices that have to be stored directly. To distinguish between both cases, we let

$$L^+_{I \times J} := \{ b = (t, s) \in L_{I \times J} : \text{adm}(t, s) = \text{true} \}, \quad L^-_{I \times J} := L_{I \times J} \setminus L^+_{I \times J}.$$ 

Defining an approximation of $G$ means defining approximations for all $G|_{\hat{t} \times \hat{s}}$ with $b = (t, s) \in L^+_{I \times J}$.

**Definition 4** (Hierarchical matrix) A matrix $G \in \mathbb{R}^{I \times J}$ is called a hierarchical matrix with local rank $k \in \mathbb{N}$, if for each $b = (t, s) \in L^+_{I \times J}$ we can find $A_b \in \mathbb{R}^{\hat{t} \times k}$ and $B_b \in \mathbb{R}^{\hat{s} \times k}$ such that

$$G|_{\hat{t} \times \hat{s}} = A_b B_b^*,$$

where $B_b^* \in \mathbb{R}^{k \times \hat{s}}$ denotes the transposed of the matrix $B_b$.

In typical applications, representing all admissible submatrices by the factors $A_b$ and $B_b$ reduces the storage requirements for a hierarchical matrix to $O(nk \log(n))$, where $n := \max\{\#I, \#J\}$ [18].

The logarithmic factor can be avoided by refining the representation: we choose sets of basis vectors for all clusters $t \in T_I$ and $s \in T_J$ and represent the admissible blocks in terms of these basis vectors.

**Definition 5** (Cluster basis) A family $\{(V_t)_{t \in T_I}\}$ of matrices $V_t \in \mathbb{R}^{\hat{t} \times k}$ is called a cluster basis of rank $k$.

**Definition 6** (Uniform hierarchical matrix) A matrix $G \in \mathbb{R}^{I \times J}$ is called a uniform hierarchical matrix for cluster bases $\{(V_t)_{t \in T_I}\}$ and $\{(W_s)_{s \in T_J}\}$, if for each $b = (t, s) \in L^+_{I \times J}$ we can find $S_b \in \mathbb{R}^{k \times k}$ such that

$$G|_{\hat{t} \times \hat{s}} = V_t S_b W_s^*.$$ 

The matrices $S_b$ are called coupling matrices.

Although a uniform hierarchical matrix requires only $k^2$ units of storage per block, leading to total storage requirements of $O(nk)$, the cluster bases still need $O(nk \log(n))$ units of storage. In order to obtain linear complexity, we assume that the cluster bases match the hierarchical structure of the cluster trees, i.e., that the bases of father clusters can be expressed in terms of the bases of the sons.
Definition 7 (Nested cluster basis) A cluster basis \((V_t)_{t \in T_I}\) is called nested, if for each \(t \in T_I\) and each \(t' \in \text{sons}(t)\) there is a matrix \(E_{t' \times k} \in \mathbb{R}^{k \times k}\) such that

\[
V_t|_{t' \times k} = V_{t'} E_{t'}.
\]

The matrices \(E_{t'}\) are called transfer matrices.

Definition 8 (\(H^2\)-matrix) Let \(G \in \mathbb{R}^{I \times J}\) be a uniform hierarchical matrix for cluster bases \((V_t)_{t \in T_I}\) and \((W_s)_{s \in T_J}\). If the cluster bases are nested, \(G\) is called an \(H^2\)-matrix.

In typical applications, representing all admissible submatrices by the coupling matrices and the cluster bases by the transfer matrices reduces the storage requirements for an \(H^2\)-matrix to \(O(nk)\).

The remainder of this article is dedicated to the task of finding an efficient algorithm for constructing \(H^2\)-matrix approximations of matrices corresponding to the Galerkin discretization of integral operators.

3 Representation formula and quadrature

Applying cross approximation directly to matrix blocks would lead either to a very high computational complexity (if full pivoting is used) or to a potentially unreliable method (if a heuristic pivoting strategy with a heuristic error estimator is employed).

Since we are interested in constructing a method that is both fast and reliable, we follow the approach of hybrid cross approximation [8]: in a first step, an analytic technique is used to obtain a degenerate approximation of the kernel function. In a second step, an algebraic technique is used to reduce the storage requirements of the approximation obtained in the first step, in our case by a reliable cross approximation constructed with full pivoting. Applying a modification similar to [5], this approach leads to an efficient \(H^2\)-matrix approximation.

We follow the approach described in [7] for the Laplace equation, since it offers optimal-order ranks and is very robust: let \(d \in \{2, 3\}\), let \(\omega \subseteq \mathbb{R}^d\) be a Lipschitz domain, and let \(u : \overline{\omega} \rightarrow \mathbb{R}\) be harmonic in \(\omega\). Green’s representation formula (cf., e.g., [20, Theorem 2.2.2]) states

\[
 u(x) = \int_{\partial \omega} g(x, z) \frac{\partial u}{\partial n}(z) \, dz - \int_{\partial \omega} \frac{\partial g}{\partial n(z)}(x, z) u(z) \, dz \quad \text{for all} \quad x \in \omega,
\]

where

\[
g(x, y) = \begin{cases} 
-\frac{1}{2\pi} \log \|x - y\|_2 & \text{if} \quad d = 2, \\
\frac{1}{4\pi} \frac{1}{\|x - y\|_2} & \text{if} \quad d = 3
\end{cases}
\]

denotes a fundamental solution of the negative Laplace operator \(-\Delta\).
For any \( y \notin \bar{\omega} \), the function \( u(x) = g(x, y) \) is harmonic, so we can apply the formula to obtain
\[
g(x, y) = \int_{\partial \omega} g(x, z) \frac{\partial g}{\partial n(z)}(z, y) \, dz - \int_{\partial \omega} \frac{\partial g}{\partial n(z)}(x, z) g(z, y) \, dz
\]
for all \( x \in \omega, \ y \notin \bar{\omega} \). (3)

On the right-hand side, the variables \( x \) and \( y \) no longer appear together as arguments of \( g \) or \( \frac{\partial g}{\partial n} \), the integrands are tensor products.

If \( x \) and \( y \) are sufficiently far from the boundary \( \partial \omega \), the integrands are smooth, so we can approximate the integrals by an exponentially convergent quadrature rule. Denoting its weights by \((w_v)_{v \in K}\) and its quadrature points by \((z_v)_{v \in K}\), we find the approximation
\[
g(x, y) \approx \sum_{v \in K} w_v g(x, z_v) \frac{\partial g}{\partial n(z_v)}(z_v, y) - w_v \frac{\partial g}{\partial n(z_v)}(x, z_v) g(z_v, y)
\]
for all \( x \in \omega, \ y \notin \bar{\omega} \). (4)

Since this is a degenerate approximation of the kernel function, discretizing the corresponding integral operator directly leads to a hierarchical matrix.

In order to ensure uniform exponential convergence of the approximation, we have to choose a suitable admissibility condition that ensures that \( x \) and \( y \) are sufficiently far from the boundary \( \partial \omega \).

A simple approach relies on bounding boxes: given a cluster \( t \in \mathcal{T}_I \), we assume that there is an axis-parallel box
\[
B_t = [a_{t,1}, b_{t,1}] \times \cdots \times [a_{t,d}, b_{t,d}]
\]
containing the supports of all basis functions corresponding to indices in \( \hat{t} \), i.e., such that
\[
\text{supp } \varphi_i \subseteq B_t \quad \text{for all } i \in \hat{t}.
\]
These bounding boxes can be constructed efficiently by a recursive algorithm [9].

In order to be able to apply the quadrature approximation to a cluster \( t \in \mathcal{T}_I \), we have to ensure that \( x \) and \( y \) are at a “safe distance” from \( \partial \omega \). In view of the error estimates presented in [7], we denote the farfield of \( t \) by
\[
\mathcal{F}_t := \{ y \in \mathbb{R}^d : \text{diam}_\infty(B_t) \leq \text{dist}_\infty(B_t, y) \},
\]
where diameter and distance with respect to the maximum norm are given by
\[
\text{diam}_\infty(B_t) := \max\{ \| x - y \|_\infty : x, y \in B_t \},
\]
\[
\text{dist}_\infty(B_t, y) := \min\{ \| x - y \|_\infty : x \in B_t \}.
\]
We are looking for an approximation that yields a sufficiently small error for all \( x \in B_t \) and all \( y \in F_t \). We apply Green’s representation formula to the domain \( \omega_t \) given by

\[
\delta_t := \text{diam}_\infty(B_t)/2, \quad \omega_t := [a_{t,1} - \delta_t, b_{t,1} + \delta_t] \times \cdots \times [a_{t,d} - \delta_t, b_{t,d} + \delta_t].
\]

It is convenient to represent \( \omega_t \) by means of a reference cube \([-1, 1]^d\) using the affine mapping

\[
\Phi_t : [-1, 1]^d \to \omega_t, \quad \hat{x} \mapsto \frac{b + a}{2} + \frac{1}{2} \begin{pmatrix} b_{t,1} - a_{t,1} + 2\delta_t \\ \vdots \\ b_{t,d} - a_{t,d} + 2\delta_t \end{pmatrix} \hat{x},
\]

and this directly leads to affine parametrizations

\[
\gamma_{2i-1}(\hat{z}) := \Phi_t(\hat{z}_1, \ldots, \hat{z}_{i-1}, -1, \hat{z}_i, \ldots, \hat{z}_{d-1}),
\]

\[
\gamma_{2i}(\hat{z}) := \Phi_t(\hat{z}_1, \ldots, \hat{z}_{i-1}, +1, \hat{z}_i, \ldots, \hat{z}_{d-1})
\]

for all \( i \in \{1, \ldots, d\} \), \( \hat{z} \in Q \),

of the boundary \( \partial \omega_t \), where

\[
Q := [-1, 1]^{d-1}
\]

is the parameter domain for one side of the boundary, such that

\[
\partial \omega_t = \bigcup_{i=1}^{2d} \gamma_i(Q), \quad \int_{\partial \omega_t} f(z) \, dz = \sum_{i=1}^{2d} \int_Q \sqrt{\det D\gamma_i^* D\gamma_i} f(\gamma_i(\hat{z})) \, d\hat{z}.
\]

We approximate the integrals on the right-hand side by a tensor quadrature formula: let \( m \in \mathbb{N} \), let \( \xi_1, \ldots, \xi_m \in [-1, 1] \) denote the points and \( w_1, \ldots, w_m \in \mathbb{R} \) the weights of the one-dimensional \( m \)-point Gauss quadrature formula for the reference interval \([-1, 1]\). If we define

\[
\hat{z}_\mu := (\xi_{\mu 1}, \ldots, \xi_{\mu d-1}), \quad \hat{w}_\mu := w_{\mu 1} \cdots w_{\mu d-1} \quad \text{for all } \mu \in M := \{1, \ldots, m\}^{d-1},
\]

we obtain the tensor quadrature formula

\[
\int_Q \hat{f}(\hat{z}) \, d\hat{z} \approx \sum_{\mu \in M} \hat{w}_\mu \hat{f}(\hat{z}_\mu).
\]

Applying this result to all surfaces of \( \partial \omega_t \) yields

\[
\int_{\partial \omega} f(z) \, dz \approx \sum_{i=1}^{2d} \sum_{\mu \in M} \hat{w}_\mu \sqrt{\det D\gamma_i^* D\gamma_i} f(\gamma_i(\hat{z}_\mu)) = \sum_{(i, \mu) \in K} w_{i \mu} f(z_{i \mu}).
\]
where we define
\[ K := \{1, \ldots, 2d\} \times M, \quad w_{i\mu} := \hat{w}_\mu \sqrt{\det D\gamma_t^* D\gamma_t}, \quad z_{i\mu} := \gamma_t(\hat{z}_\mu). \]

Using this quadrature formula in (4) yields
\[
\tilde{g}_t(x, y) := \sum_{(i, \mu) \in K} w_{i\mu} g(x, z_{i\mu}) \frac{\partial g}{\partial n_i}(z_{i\mu}, y) - w_{i\mu} \frac{\partial g}{\partial n_i}(x, z_{i\mu}) g(z_{i\mu}, y)
\]
\[
= \sum_{(i, \mu) \in K} w_{i\mu} g(x, z_{i\mu}) \frac{\partial g}{\partial n_i}(z_{i\mu}, y) - w_{i\mu} \frac{\partial g}{\partial n_i}(x, z_{i\mu}) \frac{1}{\delta_t} g(z_{i\mu}, y)
\]
for all \( x \in B_t, \ y \in F_t \), (8)

where \( n_i \) denotes the outer normal vector of the face \( \gamma_i(Q) \) of \( \omega_t \). The additional scaling factors in the second row have been added to make the estimate of Lemma 6 more elegant by compensating for the different singularity orders of the integrands.

We use the admissibility condition (cf. 2) given by the relative distance of clusters: a block \( b = (t, s) \) is admissible if \( B_s \) is in the farfield of \( t \), i.e., if \( B_s \subseteq F_t \) holds. Given such an admissible block \( b = (t, s) \), replacing the kernel function \( g \) by \( \tilde{g} \), in (1) leads to the low-rank approximation
\[
G|_{\tilde{t} \times \tilde{s}} \approx A_t B_{ts}^*, \quad A_t = (A_{t+} A_{t-}), \quad B_{ts} = (B_{ts+} B_{ts-}),
\]
where the low-rank factors \( A_{t+}, A_{t-} \in \mathbb{R}^{\tilde{t} \times K} \) and \( B_{ts+}, B_{ts-} \in \mathbb{R}^{\tilde{s} \times K} \) are given by
\[
a_{t+,iv} := \sqrt{w_v} \int_\Omega \varphi_i(x) g(x, z_v) \, dx, \quad b_{ts+,jv} := \sqrt{w_v} \int_\Omega \psi_j(y) \frac{\partial g}{\partial n_i}(z_v, y) \, dy, \quad (10a)
\]
\[
a_{t-,iv} := \delta_t \sqrt{w_v} \int_\Omega \varphi_i(x) \frac{\partial g}{\partial n_i}(x, z_v) \, dx, \quad b_{ts-,jv} := -\sqrt{w_v} \delta_t \int_\Omega \psi_j(y) g(z_v, y) \, dy \quad \text{for all } v = (i, \mu) \in K, \ i \in \tilde{t}, \ j \in \tilde{s}. \quad (10b)
\]

It is important to note that \( A_t \) depends only on \( t \), but not on \( s \). This property allows us to extend our construction to obtain \( H^2 \)-matrices in later sections.

Remark 1 (Complexity) We have \( \#K = 2dm^{d-1} \) by definition, therefore \( A_t B_{ts}^* \) is an approximation of rank \( 4dm^{d-1} \). Standard complexity estimates for hierarchical matrices (cf. [18, Lemma 2.4]) allow us to conclude that the resulting approximation requires \( O(nm^{d-1} \log n) \) units of storage. If we assume that the entries of \( A_t \) and \( B_{ts} \) and the nearfield matrices are computed by constant-order quadrature, the hierarchical matrix representation can be constructed in \( O(nm^{d-1} \log n) \) operations.

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4 Convergence of the quadrature approximation

The error analysis in [7] relies on Leibniz’ formula to obtain estimates of the derivatives of the integrand in (3). Here we present an alternative proof that handles the integrand’s product directly.

The fundamental idea is the following: since the one-dimensional formula yields the exact integral for polynomials of degree $2m - 1$, the tensor formula yields the exact integral for tensor products of polynomials of this degree, i.e., we have

$$
\int_Q \hat{p}(\hat{z}) \, d\hat{z} = \sum_{\nu \in M} \hat{w}_\nu \hat{p}(\hat{z}_\nu) \quad \text{for all } \hat{p} \in Q_{2m-1},
$$

(11)

where $Q_{2m-1}$ denotes the space of $(d-1)$-dimensional tensor products of polynomials of degree $2m - 1$.

Applying (11) to the constant polynomial $\hat{p} = 1$ and taking advantage of the fact that Gauss weights are non-negative, we obtain

$$
\sum_{\nu \in M} |w_\nu| = \sum_{\nu \in M} w_\nu = 2^{d-1}.
$$

(12)

Combining (11) and (12) leads to the following well-known best-approximation estimate.

Lemma 1 (Quadrature error) Let $\hat{\sigma} \in C(Q)$. We have

$$
\left| \int_Q \hat{\sigma}(\hat{z}) \, d\hat{z} - \sum_{\nu \in M} \hat{w}_\nu \hat{\sigma}(\hat{z}_\nu) \right| \leq 2^d \| \hat{\sigma} - \hat{p} \|_{\infty, Q} \quad \text{for all } \hat{p} \in Q_{2m-1}.
$$

Proof Let $\hat{p} \in Q_{2m-1}$. Due to (11) and (12), we have

$$
\left| \int_Q \hat{f}(\hat{z}) \, d\hat{z} - \sum_{\nu \in M} \hat{w}_\nu \hat{f}(\hat{z}_\nu) \right| = \left| \int_Q (\hat{f} - \hat{p})(\hat{z}) \, d\hat{z} - \sum_{\nu \in M} \hat{w}_\nu (\hat{f} - \hat{p})(\hat{z}_\nu) \right|
\leq \left| \int_Q (\hat{f} - \hat{p})(\hat{z}) \, d\hat{z} \right| + \left| \sum_{\nu \in M} \hat{w}_\nu (\hat{f} - \hat{p})(\hat{z}_\nu) \right|
\leq \int_Q \| \hat{f} - \hat{p} \|_{\infty, Q} \, d\hat{z} + \sum_{\nu \in M} |\hat{w}_\nu| \| \hat{f} - \hat{p} \|_{\infty, Q}
= 2^{d-1} \| \hat{f} - \hat{p} \|_{\infty, Q} + 2^{d-1} \| \hat{f} - \hat{p} \|_{\infty, Q}
= 2^d \| \hat{f} - \hat{p} \|_{\infty, Q}.
$$

We are interested in approximating the integrals appearing in (3), where the integrands are products. Fortunately, Lemma 1 can be easily extended to products.
Lemma 2 (Products) Let \( \hat{f}, \hat{g} \in C(Q) \). We have

\[
\left| \int_Q \hat{f}(\hat{z}) \hat{g}(\hat{z}) \, d\hat{z} - \sum_{\nu \in M} \hat{w}_\nu \hat{f}(\hat{\nu}) \hat{g}(\hat{\nu}) \right| \\
\leq 2^d \| \hat{f} - \hat{\rho} \|_\infty, Q \| \hat{g} \|_\infty, Q + \| \hat{f} \|_\infty, Q \| \hat{g} - \hat{q} \|_\infty, Q \\
+ \| \hat{f} - \hat{\rho} \|_\infty, Q \| \hat{g} - \hat{q} \|_\infty, Q \quad \text{for all } \hat{\rho} \in Q_m, \hat{q} \in Q_{m-1}.
\]

Proof Let \( \hat{\rho} \in Q_m \) and \( \hat{q} \in Q_{m-1} \). Then we have \( \hat{\rho} \hat{q} \in Q_{2m-1} \) and Lemma 1 yields

\[
\left| \int_Q \hat{f}(\hat{z}) \hat{g}(\hat{z}) \, d\hat{z} - \sum_{\nu \in M} \hat{w}_\nu \hat{f}(\hat{\nu}) \hat{g}(\hat{\nu}) \right| \leq 2^d \| \hat{f} \hat{g} - \hat{\rho} \hat{q} \|_\infty, Q.
\]

Observing

\[
\| \hat{f} \hat{g} - \hat{\rho} \hat{q} \|_\infty, Q = \| (\hat{f} - \hat{\rho}) \hat{g} + \hat{\rho} (\hat{g} - \hat{q}) \|_\infty, Q \\
= \| (\hat{f} - \hat{\rho}) \hat{g} + \hat{f} (\hat{g} - \hat{q}) - (\hat{f} - \hat{\rho}) (\hat{g} - \hat{q}) \|_\infty, Q \\
\leq \| \hat{f} - \hat{\rho} \|_\infty, Q \| \hat{g} \|_\infty, Q + \| \hat{f} \|_\infty, Q \| \hat{g} - \hat{q} \|_\infty, Q \\
+ \| \hat{f} - \hat{\rho} \|_\infty, Q \| \hat{g} - \hat{q} \|_\infty, Q
\]

completes the proof. \( \square \)

In our application, we want to use quadrature to approximate the integrals

\[
\int_{\partial\omega} g(x, z) \frac{\partial g}{\partial n(z)}(z, y) - \frac{\partial g}{\partial n(z)}(x, z) g(z, y) \, dz \\
= \sum_{i=1}^{2d} \sqrt{\det D\gamma_i^* D\gamma_i} \int_Q g(x, \gamma_i(\hat{z})) \frac{\partial g}{\partial n_i}(\gamma_i(\hat{z}), y) - \frac{\partial g}{\partial n_i}(x, \gamma_i(\hat{z})) g(\gamma_i(\hat{z}), y) \, d\hat{z} \\
= \sum_{i=1}^{2d} \sqrt{\det D\gamma_i^* D\gamma_i} \int_Q \hat{f}_1(\hat{z}) \hat{g}_1(\hat{z}) - \hat{g}_2(\hat{z}) \hat{f}_2(\hat{z}) \, d\hat{z},
\]

where \( \hat{f}_1, \hat{f}_2, \hat{g}_1 \) and \( \hat{g}_2 \) are given by

\[
\hat{f}_1(\hat{z}) := g(x, \gamma_i(\hat{z})), \quad \hat{g}_1(\hat{z}) := \frac{\partial g}{\partial n_i}(\gamma_i(\hat{z}), y), \quad \text{(13a)} \\
\hat{f}_2(\hat{z}) := g(\gamma_i(\hat{z}), y), \quad \hat{g}_2(\hat{z}) := \frac{\partial g}{\partial n_i}(x, \gamma_i(\hat{z})). \quad \text{(13b)}
\]

Therefore we are looking for polynomial approximations of these functions in order to apply Lemma 2. We will look for \( \hat{\rho}_1, \hat{\rho}_2 \in Q_m \) approximating \( \hat{f}_1, \hat{f}_2 \) and for \( \hat{q}_1, \hat{q}_2 \in Q_{m-1} \) approximating \( \hat{g}_1, \hat{g}_2 \). This task can be solved easily using the framework developed in [6, Chapter 4], in particular the following result:
Theorem 1 (Chebyshev interpolation) Let $\mathcal{Q}^m_m : C(Q) \to Q_m$ denote the $m$-th order tensor Chebyshev interpolation operator. Let $f \in C^\infty(Q)$ with $C_f \in \mathbb{R}_{\geq 0}$ and $\gamma_f \in \mathbb{R} > 0$ such that
\[
\left\| \frac{\partial^n}{\partial z_i^n} f \right\|_{\infty, Q} \leq \frac{C_f}{\gamma_f^n} n! \quad \text{for all } i \in \{1, \ldots, d\}, n \in \mathbb{N}_0
\] (14)
holds. Then we have
\[
\| f - \mathcal{Q}^m_m[f] \|_{\infty, Q} \leq 2deC_f(\Lambda_m+1)^d \left( 1 + \frac{\text{diam}_\infty(Q)}{\gamma_f} \right) (m+1)Q \left( \frac{2\gamma_f}{b_{t,i} - a_{t,i}} \right)^{-m},
\]
where $\Lambda_m \leq m + 1$ denotes the stability constant of one-dimensional Chebyshev interpolation and
\[
\varrho(r) := r + \sqrt{1 + r^2} > r + 1.
\]

Proof cf. [6, Theorem 4.20] in the isotropic case with $\sigma = 1$. \qed

If we can satisfy the analyticity condition (14), this theorem provides us with a polynomial in $Q_m$. Since the functions $\hat{f}_1, \hat{f}_2, \hat{g}_1$ and $\hat{g}_2$ directly depend on the kernel function $g$, we cannot proceed without taking the latter’s properties into account.

In particular, we assume that $g$ is asymptotically smooth (cf. [12,13,22]), i.e., that there are constants $C_{as}, c_0 \in \mathbb{R}_{\geq 0}, \sigma \in \mathbb{N}_0$ such that
\[
|\partial^\nu_x \partial^\mu_y g(x, y)| \leq C_{as}(v + \mu)! \frac{c_0^{(|v|+|\mu|)}}{\|x - y\|^{\sigma+|v|+|\mu|}} \quad \text{for all } v, \mu \in \mathbb{N}^d, x, y \in \mathbb{R}^d \text{ with } x \neq y.
\] (15)
The asymptotic smoothness of the fundamental solutions of the Laplace operator $\Delta$ and other important kernel functions is well-established, cf., e.g., [22, Satz E.1.4].

We have to be able to bound the right-hand side of the estimate (15). Since we have chosen the domain $\omega_t$ appropriately, we can easily find the required estimate.

Lemma 3 (Domain and parametrization) The domain $\omega_t$ satisfies the following estimates:
\[
\text{diam}_\infty(\omega_t) = 4\delta_t, \quad \text{dist}_\infty(\mathcal{B}_t, \partial \omega_t) = \delta_t, \quad \text{dist}_\infty(\partial \omega_t, \mathcal{F}_t) \geq \delta_t, \quad |\partial \omega_t| \leq 2d(4\delta_t)^{d-1}.
\] (16)
The parametrizations are bijective and satisfy
\[
\| D\Phi_t \|_2 = 2\delta_t, \quad \| D\gamma_t \|_2 \leq 2\delta_t.
\] (17)
Combining these lower bounds for the distances between $x$ and $\partial \omega_t$ and $y$ and $\partial \omega_t$, respectively, with the estimate (15) allows us to prove that the requirements of Theorem 1 are fulfilled.

**Lemma 4 (Derivatives)** Let $x \in B_t$ and $y \in F_t$. Then we have

$$|\partial^\nu \hat{f}_1(\hat{z})| \leq \frac{C_{as}d}{\delta_{t}^\sigma} (2c_0)^{|\hat{\nu}|}, \quad |\partial^\nu \hat{f}_2(\hat{z})| \leq \frac{C_{as}d}{\delta_{t}^\sigma} (2c_0)^{|\hat{\nu}|}$$

$$|\partial^\nu \hat{g}_1(\hat{z})| \leq \frac{C_{as}d}{\delta_{t}^\sigma+1} (2c_0)^{|\hat{\nu}|}, \quad |\partial^\nu \hat{g}_2(\hat{z})| \leq \frac{C_{as}d}{\delta_{t}^\sigma+1} (2c_0)^{|\hat{\nu}|} \text{ for all } \hat{z} \in Q, \hat{\nu} \in \mathbb{N}_0^{d-1}.$$

**Proof** cf. Appendix A

Due to Lemma 4, the conditions of Theorem 1 are fulfilled, so we can obtain the polynomial approximations required by Lemma 2 and prove that the quadrature approximation converges exponentially.

**Theorem 2 (Quadrature error)** There is a constant $C_{gr} \in \mathbb{R}_{\geq 0}$ depending only on $C_{as}$, $c_0$ and $d$ such that

$$|g(x, y) - \tilde{g}_t(x, y)| \leq \frac{C_{gr}}{\delta_{t}^{2\sigma-d+2}} \left( \frac{2c_0}{2c_0 + 1}\right)^{m-1} \text{ for all } x \in B_t, y \in F_t,$$

i.e., the quadrature approximation $\tilde{g}_t$ given by (8) is exponentially convergent with respect to $m$.

**Proof** In order to apply Lemma 2, we have to construct polynomials approximating $\hat{f}$ and $\hat{g}$.

Let $f \in \{\hat{f}_1, \hat{f}_2\}$. According to Lemma 4, we can apply Theorem 1 to $\hat{f}$ using

$$C_f := \frac{C_{as}}{\delta_{t}^\sigma}, \quad \gamma_f := \frac{1}{2c_0}$$

to obtain

$$\|\hat{f} - \mathcal{Q}_m[\hat{f}]\|_\infty, Q \leq C_{in}(m)C_f \varphi \left( \frac{1}{2c_0} \right)^{-m}$$

with the polynomial $C_{in}(m) := 2de(m+2)^d(m+1)(1+4c_0)$. We fix

$$r := \frac{1}{2c_0}, \quad \zeta := \frac{r + 1}{\varphi(r)} < 1,$$
and find

\[ \| \hat{f} - \mathcal{Q}_m(\hat{f}) \|_{\infty, Q} \leq C_{\text{in}}(m) C_f \rho \left( \frac{1}{2c_0} \right)^{-m} = \frac{C_{\text{in}}(m) C_{\text{as}}}{\delta_t^r} \rho(r)^{-m} = C_{\text{in}}(m) C_{\text{as}} \zeta^m (r + 1)^{-m}. \]

Due to \( \zeta < 1 \), we can find a constant

\[ C_{\text{apx}} := \sup \{ C_{\text{in}}(m) C_{\text{as}} \zeta^m : m \in \mathbb{N}_0 \} \]

independent of \( m, t \) and \( \sigma \) such that

\[ \| \hat{f} - \mathcal{Q}_m(\hat{f}) \|_{\infty, Q} \leq C_{\text{apx}} \delta_t^r (r + 1)^{-m} = \frac{C_{\text{apx}}}{\delta_t^r} \left( \frac{2c_0}{2c_0 + 1} \right)^m \]

for all \( m \in \mathbb{N} \). \( 18a \)

We can apply the same reasoning to \( \hat{g} \in \{ \hat{g}_1, \hat{g}_2 \} \) to obtain

\[ \| \hat{g} - \mathcal{Q}_m-1(\hat{g}) \|_{\infty, Q} \leq C'_{\text{apx}} \delta_t^{\sigma + 1} (r + 1)^{-m+1} = \frac{C'_{\text{apx}}}{\delta_t^{\sigma + 1}} \left( \frac{2c_0}{2c_0 + 1} \right)^{m-1} \]

for all \( m \in \mathbb{N} \). \( 18b \)

with a suitable constant \( C'_{\text{apx}} \in \mathbb{R}_{\geq 0} \).

Now we can focus on the final estimate. We have

\[ |g(x, y) - \tilde{g}_t(x, y)| \leq \left| \int_{\partial \omega_t} g(x, z) \frac{\partial g}{\partial n(z, y)} (z, y) dz - \sum_{v=1}^k w_v g(x, z_v) \frac{\partial g}{\partial n(z_v)} (z_v, y) \right| \]

\[ + \left| \int_{\partial \omega_t} \frac{\partial g}{\partial n(z)} (x, z) g(z, y) dz - \sum_{v=1}^k w_v \frac{\partial g}{\partial n(z_v)} (z_v, y) g(x, z_v) \right| \]

\( 19a \)

\( 19b \)

For the first term, we use

\[ \int_{\partial \omega_t} g(x, z) \frac{\partial g}{\partial n(z, y)} (z, y) dz = \sum_{i=1}^{2d} \sqrt{\text{det}(D\gamma_i^* D\gamma_i)} \int_Q \hat{f}_1(\hat{z}) \hat{g}_1(\hat{z}) d\hat{z}, \]

\[ \sum_{v \in K} w_v g(x, z_v) \frac{\partial g}{\partial n(z_v, y)} (z_v, y) = \sum_{i=1}^{2d} \sqrt{\text{det}(D\gamma_i^* D\gamma_i)} \sum_{\mu \in M} \hat{w}_\mu \hat{f}_1(\hat{x}_\mu) \hat{g}_1(\hat{x}_\mu) \]
to obtain
\[
\begin{align*}
\int_{\partial \omega} g(x, z) \frac{\partial g}{\partial n(z)} (z, y) \, dz - \sum_{v \in K} w_v g(x, z_v) \frac{\partial g}{\partial n(z_v)} (z_v, y) \\
= 2^d \sqrt{\det(D \gamma^*_t D \gamma_t)} \left( \int_Q \hat{f}_1(\hat{\varepsilon}) \hat{g}_1(\hat{\varepsilon}) \, d\hat{z} - \sum_{\mu \in M} \hat{\mu} \hat{f}_1(\hat{\varepsilon}_\mu) \hat{g}_1(\hat{\varepsilon}_\mu) \right).
\end{align*}
\]

Due to (6) and (7), we have
\[
\sqrt{\det(D \gamma^*_t D \gamma_t)} \leq (2\delta_t)^{d-1},
\]
and we can use Lemma 2 to bound the second term and get
\[
\left| \int_{\partial \omega} g(x, z) \frac{\partial g}{\partial n(z)} (z, y) \, dz - \sum_{v \in K} w_v g(x, z_v) \frac{\partial g}{\partial n(z_v)} (z_v, y) \right| \leq (2\delta_t)^{d-1} 2^d \left( \| \hat{f}_1 - \hat{\mu}_1 \|_{\infty,Q} \| \hat{g}_1 \|_{\infty,Q} + \| \hat{f}_1 \|_{\infty,Q} \| \hat{g}_1 - \hat{\mu}_1 \|_{\infty,Q} \right)
\]
for any \( \hat{\mu}_1 \in Q_m \) and \( \hat{\mu}_1 \in Q_{m-1} \). It comes as no surprise that we use the tensor Chebyshev interpolation polynomials \( \hat{\mu}_1 := \hat{Q}_m[\hat{f}_1] \) and \( \hat{\mu}_1 := \hat{Q}_{m-1}[\hat{g}_1] \) investigated before. The inequalities (18) provide us with estimates for the interpolation error, while Lemma 3 in combination with (15) yields
\[
\| \hat{f}_1 \|_{\infty,Q} \leq \frac{C_{\text{as}}}{\delta_t^\sigma}, \quad \| \hat{g}_1 \|_{\infty,Q} \leq \frac{C_{\text{as}}^0}{\delta_t^\sigma + 1}.
\]
Combining both estimates we find
\[
\left| \int_{\partial \omega} g(x, z) \frac{\partial g}{\partial n(z)} (z, y) \, dz - \sum_{v \in K} w_v g(x, z_v) \frac{\partial g}{\partial n(z_v)} (z_v, y) \right| \leq 2^{2d-1} \delta_t^{d-1} \left( \frac{C_{\text{apx}} C_{\text{as}}}{\delta_t^{2\sigma+1}} \left( \frac{2c_0}{2c_0 + 1} \right)^m + \frac{C_{\text{apx}}'}{\delta_t^{2\sigma+1}} \left( \frac{2c_0}{2c_0 + 1} \right)^{m-1} \right)
\]
with the constant
\[
C_{\text{gr.1}} := 2^{2d-1} (C_{\text{apx}} C_{\text{as}} C_0 + C_{\text{apx}}' C_{\text{as}} + C_{\text{apx}} C_{\text{apx}}').
\]
We can obtain similar estimates for the second integrals (19b) by exactly the same arguments and conclude

$$|g(x, y) - \tilde{g}_t(x, y)| \leq C_{gr} \frac{2c_0}{\delta^2 + 2d + 2} (\frac{2c_0}{2c_0 + 1})^{m-1}$$

with the constant $C_{gr} := 4dC_{gr, 1}$. \(\Box\)

5 Cross approximation

The construction outlined in the previous section still offers room for improvement: the matrices $A_{t,+}$ and $A_{t,-}$ appearing in (10) describe the influence of Neumann and Dirichlet values of $g(\cdot, y)$ on $\partial \omega_t$ to the approximation in $\omega_t$. Using the Poincaré-Steklov operator, we can construct the Neumann values from the Dirichlet values, therefore we expect that it should be possible to avoid using $A_{t,+}$ and thus reduce the rank of our approximation by a factor of two. Eliminating $A_{t,+}$ explicitly would require us to approximate the Poincaré-Steklov operator and solve an integral equation on the boundary $\partial \omega_t$, and we would have to reach a fairly high accuracy in order to preserve the exponential convergence of the quadrature approximation.

For the sake of efficiency, we choose an implicit approach: assuming that $A_{t,+}$ can be obtained from $A_{t,-}$ by solving a linear system, we expect that the rank of the matrix $A_t = (A_{t,+} + A_{t,-})$ is lower than the number of its columns. Therefore we use an algebraic procedure to approximate the matrix $A_t$ by a lower-rank matrix. The adaptive cross approximation approach [2, 4, 34] is particularly attractive in this context, since it allows us to construct an algebraic interpolation operator that can be used to approximate matrix blocks based only on a few of their entries.

The adaptive cross approximation of a matrix $X \in \mathbb{R}^{I \times J}$ is constructed as follows: a pair of pivot elements $i_1 \in I$ and $j_1 \in J$ are chosen and the vectors $c^{(1)} \in \mathbb{R}^I$, $d^{(1)} \in \mathbb{R}^J$ given by

$$c_i^{(1)} := x_{i, j_1} / x_{i_1, j_1}, \quad d_j^{(1)} := x_{i_1, j}$$

for all $i \in I$, $j \in J$ are constructed. The matrix

$$\tilde{X}^{(1)} := c^{(1)} (d^{(1)})^*$$

satisfies

$$\tilde{X}_{i, j_1}^{(1)} = x_{i, j_1} x_{i_1, j_1} / x_{i_1, j_1} = x_{i, j_1},$$

$$\tilde{X}_{i_1, j}^{(1)} = x_{i_1, j_1} x_{i_1, j} / x_{i_1, j_1} = x_{i_1, j}$$

for all $i \in I$, $j \in J$, i.e., it is identical to $X$ in the $i$th row and the $j$th column (the eponymous “cross” formed by this row and column). The remainder matrix

$$X^{(1)} := X - \tilde{X}^{(1)}$$

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therefore vanishes in this row and column. If $X^{(1)}$ is considered small enough in a suitable sense, we use $\tilde{X}^{(1)}$ as a rank-one approximation of $X$. Otherwise, we proceed by induction: if $X^{(k)}$ is not sufficiently small for $k \in \mathbb{N}$, we construct a cross approximation $\tilde{X}^{(k+1)} = c^{(k+1)}(d^{(k+1)})^*$ and let

$$X^{(k+1)} := X^{(k)} - \tilde{X}^{(k+1)} = X - \sum_{v=1}^{k+1} \tilde{X}^{(v)}.$$ 

If $X^{(k)}$ is small enough, the matrix

$$\sum_{v=1}^{k} \tilde{X}^{(v)} = \sum_{v=1}^{k} c^{(v)}(d^{(v)})^* = CD^*,$$

with

$$C := (c^{(1)} \ldots c^{(k)}), \quad D := (d^{(1)} \ldots d^{(k)})$$

is a rank-$k$ approximation of $X$.

This approximation can be interpreted in terms of an algebraic interpolation: we introduce the matrix $P \in \mathbb{R}^{k \times I}$ by

$$Pz := \begin{pmatrix} z_{i_1} \\ \vdots \\ z_{i_k} \end{pmatrix}$$

for all $z \in \mathbb{R}^I$.

mapping a vector to the selected pivot elements. The pivot elements play the role of interpolation points in our reformulation of the cross approximation method.

We also need an equivalent of Lagrange polynomials. Since the algorithm introduces zero rows and columns to the remainder matrices

$$X^{(\ell)} = X - \tilde{X}^{(1)} - \cdots - \tilde{X}^{(\ell)}$$

and since the vectors $c^{(1)}, \ldots, c^{(k)}$ and $d^{(1)}, \ldots, d^{(k)}$ are just scaled columns and rows of the remainder matrices, we have

$$c_{i\mu} = c_{i}^{(\mu)} = 0 \quad \text{for all } i \in \{i_1, \ldots, i_{\mu-1}\},$$

$$d_{j\mu} = d_{j}^{(\mu)} = 0 \quad \text{for all } j \in \{j_1, \ldots, j_{\mu-1}\},$$

and since the entries of $PC \in \mathbb{R}^{k \times k}$ are given by

$$(PC)_{v\mu} = c_{i}^{(\mu)} \quad \text{for all } v, \mu \in \{1, \ldots, k\},$$

this matrix is lower triangular. Due to our choice of scaling, its diagonal elements are equal to one, so the matrix is also invertible.
Therefore the matrix

$$V := C (P C)^{-1} \in \mathbb{R}^{I \times k}$$

is well-defined. Its columns play the role of Lagrange polynomials, and the algebraic interpolation operator given by

$$\mathcal{I} := VP$$

satisfies the projection property

$$\mathcal{I} C = V P C = (P C)^{-1} P C = C. \quad (20)$$

Since the rows $i_1, \ldots, i_k$ in $X^{(k)}$ vanish, we have

$$0 = PX^{(k)} = P(X - C D^*)$$

and therefore

$$\mathcal{I} X = V P X = V P C D^* = C D^*, \quad (21)$$

i.e., the low-rank approximation $C D^*$ results from algebraic interpolation.

### 6 Hybrid approximation

The adaptive cross approximation algorithm gives us a powerful heuristic method for constructing low-rank approximations of arbitrary matrices. In our case, we apply it to reduce the rank of the factorization given by (10), i.e., we apply the adaptive cross approximation algorithm to the matrix $A_t \in \mathbb{R}^{t \times 2k}$ and obtain a reduced rank $\ell \in \mathbb{N}$ and matrices $C_t \in \mathbb{R}^{t \times \ell}$, $D_t \in \mathbb{R}^{2k \times \ell}$ and $P_t \in \mathbb{R}^{\ell \times t}$ such that

$$A_t \approx C_t D_t^* = V_t P_t A_t$$

with $V_t := C_t (P_t C_t)^{-1}$. Combining this approximation with (9) yields

$$G|_{t \times \tilde{s}} \approx A_t B_{ts}^* \approx C_t D_t^* B_{ts}^* = C_t (B_{ts} D_t)^*,$$

i.e., we have reduced the rank from $2k$ to $\ell$.

We can avoid computing the matrices $B_{ts}$ entirely by using algebraic interpolation: for $\mathcal{J}_t := V_t P_t$, the projection property (20) yields

$$G|_{t \times \tilde{s}} \approx C_t (B_{ts} D_t)^* = \mathcal{J}_t C_t (B_{ts} D_t)^* \approx \mathcal{J}_t G|_{t \times \tilde{s}}.$$

This approach has the advantage that we can prepare and store the matrices $C_t \in \mathbb{R}^{t \times \ell}$, $P_t \in \mathbb{R}^{\ell \times t}$ and $P_t C_t \in \mathbb{R}^{\ell \times \ell}$ in a setup phase. Since $A_t$ depends only on the cluster.
t, but not on an entire block, this phase involves only a sweep across the cluster tree that does not lead to a large work-load.

Once the matrices have been prepared, an approximation of a block $G|_{\hat{t} \times \hat{s}}$ can be found by computing its pivot rows $P_t G|_{\hat{t} \times \hat{s}}$, obtaining $\tilde{B}_{ts}$ through solving the linear system

$$(P_tC_t)\tilde{B}_{ts}^* = P_t G|_{\hat{t} \times \hat{s}}$$

by forward substitution, and storing the rank-$\ell$-approximation

$$C_t \tilde{B}_{ts}^* = C_t(P_tC_t)^{-1} P_t G|_{\hat{t} \times \hat{s}} = \mathcal{J}_t G|_{\hat{t} \times \hat{s}}.$$ (23)

None of these operations involves the quadrature rank $2k$, the computational work is determined by the reduced rank $\ell$.

**Remark 2 (Complexity)** Computing the rank $\ell$ cross approximation of $A_t \in \mathbb{R}^{\hat{t} \times 2k}$ for one cluster $t \in \mathcal{T}_I$ requires $O(\ell k \#t)$ operations. Similar to [18, Lemma 2.4], we can conclude that the cross approximation for all clusters requires not more than $O(\ell n \log n) \subseteq O(\ell m d^{-1} n \log n)$ operations.

Solving the linear system (22) for one block $b = (t, s) \in \mathcal{L}_I^+ \mathcal{J}$ requires not more than $O(\ell 2\#t)\tilde{s}$ operations, and we can follow the reasoning of [18, Lemma 2.9] to obtain a bound of $O(\ell 2n \log n)$ for the computational work involved in setting up all blocks by the hybrid method.

**Lemma 5 (Hybrid approximation)** Let $b = (t, s) \in \mathcal{T}_I \mathcal{J}$ be an admissible block. Then we have

$$\|G|_{\hat{t} \times \hat{s}} - C_t \tilde{B}_{ts}^*\|_2 \leq (1 + \|\mathcal{J}_t\|_2)\|G|_{\hat{t} \times \hat{s}} - A_t B_{ts}^*\|_2 + \|A_t - C_t D_t^*\|_2 \|B_{ts}^*\|_2.$$ (24)

**Proof** Since (21) implies $C_t D_t^* = \mathcal{J}_t A_t$, we can use (23) to obtain

$$\|G|_{\hat{t} \times \hat{s}} - C_t \tilde{B}_{ts}^*\|_2 \leq \|G|_{\hat{t} \times \hat{s}} - A_t B_{ts}^*\|_2 + \|A_t - C_t D_t^*\|_2 \|B_{ts}^*\|_2 + \|\mathcal{J}_t (A_t B_{ts}^* - G|_{\hat{t} \times \hat{s}})\|_2$$

$$\leq \|G|_{\hat{t} \times \hat{s}} - A_t B_{ts}^*\|_2 + \|A_t - C_t D_t^*\|_2 \|B_{ts}^*\|_2 + \|\mathcal{J}_t\|_2 \|G|_{\hat{t} \times \hat{s}} - A_t B_{ts}^*\|_2$$

$$= (1 + \|\mathcal{J}_t\|_2)\|G|_{\hat{t} \times \hat{s}} - A_t B_{ts}^*\|_2 + \|A_t - C_t D_t^*\|_2 \|B_{ts}^*\|_2.$$ 

The error estimate (24) contains two terms that we can control directly: the error of the analytical approximation

$$\|G|_{\hat{t} \times \hat{s}} - A_t B_{ts}^*\|_2$$

and the error of the cross approximation

$$\|A_t - C_t D_t^*\|_2.$$
The first error depends directly on the error of the kernel approximation (cf. [6, Sect. 4.6] for a detailed analysis), and Theorem 2 allows us to reduce it to any chosen accuracy, using results like [6, Lemma 4.44] to switch from the maximum norm to the spectral norm.

The second error can be controlled directly by monitoring the remainder matrices appearing in the cross approximation algorithm.

Therefore we only have to address the additional factors \(1 + \|J_t\|_2\) and \(\|B^*_ts\|_2\).

The norm \(\|J_t\|_2\) is the algebraic counterpart of the Lebesgue constant of standard interpolation methods. We can monitor this norm explicitly: since \(P_t\) is surjective, we have \(\|J_t\|_2 = \|V_t\|_2\) and can obtain bounds for this matrix during the construction of the cross approximation. Should the product \((1 + \|J_t\|_2)\|G|\hat{t}\|_{s - t} - A_t B^*_ts\|_2\)

become too large, we can increase the accuracy of the analytic approximation of the kernel function to reduce the second term. A common (as far as we know still unproven) assumption in the field of cross approximation methods states that \(\|J_t\|_2 \sim \ell^\alpha\) holds for a small \(\alpha > 0\) if a suitable pivoting strategy is employed, cf. [5, eq. (16)]

For the analysis of the factor \(\|B^*_ts\|_2\), we have to take the choice of basis functions into account. For the sake of simplicity, we assume that the finite element basis is stable in the sense that there is a constant \(C_\psi \in \mathbb{R}_{> 0}\), possibly depending on the underlying grid, such that

\[
\left\| \sum_{j \in J} u_j \psi_j \right\|_{L^2} \leq C_\psi \|u\|_2 \quad \text{for all } u \in \mathbb{R}^J.
\]

\[\text{Lemma 6 (Scaling factor)}\]

There is a constant \(C_{sf} \in \mathbb{R}_{> 0}\) depending only on \(C_{as}, c_0, |\Omega|\) and \(d\) such that

\[
\|B^*_ts\|_2 \leq \frac{C_{sf} C_\psi}{\delta_t^{\sigma - d/2 + 3/2}} \quad \text{for all } (t, s) \in \mathcal{T} I \times \mathcal{T} J \text{ with } B_s \subseteq \mathcal{F}_t.
\]

\[\text{Proof}\]

By definition (9), we have

\[
B_ts = (B^*_ts + B^*_ts-)
\]

and therefore

\[
\|B^*_ts\|_2 = \left\| \begin{pmatrix} B^*_ts+ \\ B^*_ts- \end{pmatrix} \right\|_2 \leq \sqrt{\|B^*_ts+\|_2^2 + \|B^*_ts-\|_2^2}.
\]

We focus on \(B^*_ts+\). A simple application of the Cauchy-Schwarz inequality yields

\[
\|B^*_ts+\|_2 = \sup_{u \in \mathbb{R}^2 \setminus \{0\}, v \in \mathbb{R}^K \setminus \{0\}} \frac{(B^*_ts+ u, v)_2}{\|u\|_2 \|v\|_2}.
\]
Let $u \in \mathbb{R}^\mathring{s}$ and $v \in \mathbb{R}^K$. We use the definition (10) and apply the Cauchy-Schwarz inequality first to the inner product in $L^2(\Omega)$ and then to the Euclidean one to get

\[
\langle B_{ts}^* u, v \rangle_2 = \sum_{j \in \mathring{s}} \sum_{\nu \in K} b_{ts,j \nu} u_j v_{\nu} = \int_\Omega \left( \sum_{j \in \mathring{s}} u_j \psi_j(y) \right) \sum_{\nu \in K} v_{\nu} \sqrt{w_{\nu}} \frac{\partial g}{\partial n(z_{\nu}, y)}(z_{\nu}, y) \,dy
\]

\[
\leq \left( \int_\Omega \left( \sum_{j \in \mathring{s}} u_j \psi_j(y) \right)^2 \,dy \right)^{1/2} \times \left( \int_\Omega \left( \sum_{\nu \in K} v_{\nu} \sqrt{w_{\nu}} \frac{\partial g}{\partial n(z_{\nu}, y)}(z_{\nu}, y) \right)^2 \,dy \right)^{1/2}
\]

\[
= \left\| \sum_{j \in \mathring{s}} u_j \psi_j \right\|_{L^2} \left( \int_\Omega \left( \sum_{\nu \in K} v_{\nu} \sqrt{w_{\nu}} \frac{\partial g}{\partial n(z_{\nu}, y)}(z_{\nu}, y) \right)^2 \,dy \right)^{1/2}
\]

\[
\leq C_\psi \|u\|_2 \left( \int_\Omega \left( \sum_{\nu \in K} v_{\nu}^2 \right) \left( \sum_{\nu \in K} w_{\nu} \left( \frac{\partial g}{\partial n(z_{\nu}, y)} \right)^2 \right) \,dy \right)^{1/2}
\]

\[
= C_\psi \|u\|_2 \|v\|_2 \left( \int_\Omega \sum_{\nu \in K} w_{\nu} \left( \frac{\partial g}{\partial n(z_{\nu}, y)} \right)^2 \,dy \right)^{1/2}.
\]

The asymptotic smoothness (15) in combination with Lemma 3 yields

\[
\left| \frac{\partial g}{\partial n(z_{\nu}, y)} \right| \leq \frac{C_{as} c_0}{\| z_{\nu} - y \|^{\sigma+1}} \leq \frac{C_{as} c_0}{\delta t^{\sigma+1}}.
\]

Since the weights are non-negative and the quadrature rule integrates constants exactly, we have

\[
\sum_{\nu \in K} w_{\nu} \left( \frac{\partial g}{\partial n(z_{\nu}, y)} \right)^2 \leq \sum_{\nu \in K} w_{\nu} \left( \frac{C_{as} c_0}{\delta t^{\sigma+1}} \right)^2 = |\partial \omega_t| \left( \frac{C_{as} c_0}{\delta t^{\sigma+1}} \right)^2.
\]

We conclude

\[
\langle B_{ts}^* u, v \rangle_2 \leq C_\psi \|u\|_2 \|v\|_2 \left( \int_\Omega |\partial \omega_t| \left( \frac{C_{as} c_0}{\delta t^{\sigma+1}} \right)^2 \,dy \right)^{1/2}
\]

\[
= C_\psi \frac{C_{as} c_0}{\delta t^{\sigma+1}} \sqrt{\| \partial \omega_t \| \|u\|_2 \|v\|_2}.
\]
Inserting $|\partial \omega_t| \leq 2d(4\delta_t)^{d-1} = 2^{d-1}d\delta_t^{d-1}$ leads to

$$
\langle B_{ts}^* + u, v \rangle_2 \leq \frac{C_\psi C_{as} c_0}{\delta_t^{\sigma+1}} \sqrt{\Omega |2^{d-1}d^{d/2-1/2}\|u\|_2\|v\|_2}.
$$

For $B_{ts}^*$, we obtain the same result, since the definition (10) includes the scaling factor $1/\delta_t$. Combining both estimates and choosing the constant $C_{sf} := C_{as} c_0 \sqrt{\Omega |2^{d/2}d}}$ completes the proof. \( \square \)

7 Nested cross approximation

Applying the algorithm presented so far to admissible blocks yields a hierarchical matrix approximation of $G$. We would prefer to obtain an $\mathcal{H}^2$-matrix due to its significantly lower complexity.

Since the cluster basis has to be able to handle all blocks connected to a given cluster, we have to approximate the entire farfield. We let

$$
F_t := \{ j \in \mathcal{J} : \text{supp } \psi_j \subseteq \mathcal{F}_t \} \quad \text{for all } t \in \mathcal{T}_I
$$

and use our algorithm to find low-rank interpolation operators $\mathcal{I}_t = V_t P_t$ such that

$$
G|_{i \times F_t} \approx \mathcal{I}_t G|_{i \times F_t} = V_t P_t G|_{i \times F_t}.
$$

Since our construction of $\mathcal{I}_t$ depends only on the matrix $A_t$, this approach does not increase the computational work.

In order to obtain a uniform hierarchical matrix, we also require an approximation of the column clusters. Our algorithm can easily handle this task as well: as before, we let

$$
F_s := \{ i \in \mathcal{I} : \text{supp } \varphi_i \subseteq \mathcal{F}_s \} \quad \text{for all } s \in \mathcal{T}_J
$$

and use our algorithm with the adjoint matrix to find low-rank interpolation operators $\mathcal{J}_s = V_s P_s$ such that

$$
G|_{F_t \times \hat{s}}^* \approx \mathcal{J}_s G|_{F_t \times \hat{s}}^* = V_s P_s G|_{F_t \times \hat{s}}^*.
$$

If a block $b = (t, s)$ satisfies the admissibility condition

$$(t, s) \text{ admissible} \iff (B_s \subseteq \mathcal{F}_t \land B_t \subseteq \mathcal{F}_s) \iff \max\{\text{diam}_\infty(B_t), \text{diam}_\infty(B_s)\} \leq \text{dist}_\infty(B_t, B_s), \quad (26)$$

we have $\hat{s} \subseteq F_t$ and $\hat{t} \subseteq F_s$ and therefore obtain

$$
G|_{\hat{t} \times \hat{s}} \approx \mathcal{J}_t G|_{\hat{t} \times \hat{s}} \approx \mathcal{J}_s G|_{\hat{t} \times \hat{s}} \mathcal{J}_s^* = V_t P_t G|_{\hat{t} \times \hat{s}} P_s^* V_s^* = V_t S_b V_s^* \quad (27)
$$
with \( S_b := P_t G|_{t \times \tilde{s}} P_s^* \). We have found a way to construct a uniform hierarchical matrix. Note that we can compute \( S_b \) by evaluating \( G \) in the small number of pivot elements chosen for the row and column clusters.

In order to obtain an \( \mathcal{H}^2 \)-matrix, the cluster bases have to be nested. Similar to the procedure outlined in [5], we only have to ensure that the pivot elements for clusters with sons are chosen among the sons’ pivot elements.

For the sake of simplicity, we consider only the case of a binary cluster tree and construct the cluster basis recursively. Let \( t \in \mathcal{T} \). If \( t \) is a leaf, i.e., if \( \text{sons}(t) = \emptyset \), we use our algorithm as before and obtain \( \mathcal{I}_t = V_t P_t \).

If \( t \) is not a leaf, we have sons \( t \in T_t \). If \( t \) is a leaf, i.e., if \( \text{sons}(t) = \emptyset \), we have \( \mathcal{I}_t = V_t P_t \) and \( \mathcal{I}_t = V_t P_t \) with

\[
G|_{t_1 \times F_{t_1}} \approx \mathcal{I}_{t_1} G|_{t_1 \times F_{t_1}}, \quad G|_{t_2 \times F_{t_2}} \approx \mathcal{I}_{t_2} G|_{t_1 \times F_{t_1}}
\]

by recursion. Due to \( F_t \subseteq F_{t_1} \cap F_{t_2} \), we have

\[
G|_{\tilde{t} \times F_{\tilde{t}}} = \left( G|_{t_1 \times F_{t_1}} \right) \approx \left( \mathcal{I}_{t_1} G|_{t_1 \times F_{t_1}} \right) = \left( V_{t_1} P_{t_1} G|_{t_1 \times F_{t_1}} \right)
\]

\[
= \left( V_{t_1} P_{t_1} G|_{t_1 \times F_{t_1}} \right) = \left( V_{t_1} P_{t_1} G|_{t_1 \times F_{t_1}} \right)
\]

\[
\approx \left( V_{t_1} P_{t_1} G|_{t_1 \times F_{t_1}} \right) = \mathcal{I}_{t_1} G|_{t_1 \times F_{t_1}}.
\]

where \( A_t \) and \( B_{t,F_t} \) are again the matrices of the quadrature method. By applying the cross approximation algorithm to the two middle factors, we find \( \mathcal{H}_t = \mathcal{V}_t \mathcal{P}_t \) such that

\[
\left( \begin{array}{c}
V_{t_1} \\
P_{t_2}
\end{array} \right) A_t \approx \mathcal{V}_t \mathcal{P}_t \left( \begin{array}{c}
V_{t_1} \\
P_{t_2}
\end{array} \right) A_t.
\]

All we have to do is to let

\[
V_t := \left( \begin{array}{c}
V_{t_1} \\
P_{t_2}
\end{array} \right), \quad P_t := \mathcal{V}_t \mathcal{P}_t
\]

and observe

\[
G|_{\tilde{t} \times F_{\tilde{t}}} \approx \left( \begin{array}{c}
V_{t_1} \\
P_{t_2}
\end{array} \right) A_t B_{t,F_t}^* \approx \left( \begin{array}{c}
V_{t_1} \\
P_{t_2}
\end{array} \right) \mathcal{V}_t \mathcal{P}_t \left( \begin{array}{c}
V_{t_1} \\
P_{t_2}
\end{array} \right) A_t B_{t,F_t}^* = V_t P_t A_t B_{t,F_t}^*.
\]

\[
\approx V_t P_t G|_{t \times F_t} = \mathcal{I}_t G|_{t \times F_t}.
\]
Splitting \( \hat{V}_t \) into an upper and a lower part matching \( V_{t_1} \) and \( V_{t_2} \) yields

\[
\begin{pmatrix}
E_{t_1} \\
E_{t_2}
\end{pmatrix} := \hat{V}_t, \quad V_t = \begin{pmatrix} V_{t_1} \\ V_{t_2} \end{pmatrix} \quad \hat{V}_t = \begin{pmatrix} V_{t_1} \\ V_{t_2} \end{pmatrix} \begin{pmatrix} E_{t_1} \\
E_{t_2}
\end{pmatrix} = \begin{pmatrix} V_{t_1}E_{t_1} \\ V_{t_2}E_{t_2} \end{pmatrix},
\]

so we have indeed found a nested cluster basis.

**Remark 3 (Complexity)** We assume that the ranks obtained by the cross approximation are bounded by \( \ell \).

For a leaf cluster, the construction of \( V_t \) and \( P_t \) requires \( O(\ell k \# t) \) operations. For a non-leaf cluster, the cross approximation is applied to a \( \min\{\# \hat{t}, 2\ell\} \times (2k) \)-matrix and takes no more than \( O(\ell k \min\{\# \hat{t}, 2\ell\}) \) operations. Similar to [10, Remark 4.1], we conclude that \( O(\ell k n) \) operations are sufficient to set up the cluster bases.

The coupling matrices require us to solve two linear systems by forward substitution, one with the matrix \( P_t C_t \) and one with the matrix \( P_s C_s \). The first is of dimension \( \min\{\ell, \# \hat{t}\} \), the second of dimension \( \min\{\ell, \# \bar{s}\} \), therefore solving both systems takes not more than \( O(\min\{\ell, \# \bar{s}\}^2 \ell + \min\{\ell, \# \bar{s}\} \ell^2) \) operations for one block \( b = (t, s) \in L_{+}^{+} \times J_{+}^{+} \). As in [10, Remark 4.1], we conclude that not more than \( O(\ell^2 n) \) operations are required to compute all coupling matrices and that the coupling matrices require not more than \( O(\ell n) \) units of storage.

Since the recursive algorithm applies multiple approximations to the same block, we have to take a closer look at error estimates. The total error in a given cluster is influenced by the errors introduced in its sons, their sons, and so on. In order to handle these connections, we introduce the set of descendents of a cluster \( t \in \mathcal{T}_{F} \) by

\[
\text{sons}^*(t) := \begin{cases} 
\{t\} & \text{if } \text{sons}(t) = \emptyset, \\
\{t\} \cup \text{sons}^*(t_1) \cup \text{sons}^*(t_2) & \text{if } \text{sons}(t) = \{t_1, t_2\}.
\end{cases}
\]

Each step of the algorithm introduces an error for the current cluster: for leaves, we approximate \( G|_{\hat{t} \times F_i} \), while for non-leaves the restriction of \( G|_{\hat{t} \times F_i} \) to the sons’ pivot elements is approximated. We denote the error added by quadrature and cross approximation in each cluster \( t \in \mathcal{T}_{F} \) by

\[
\hat{\epsilon}_t := \begin{cases} 
\| G|_{\hat{t} \times F_i} - \hat{F}_t G|_{\hat{t} \times F_i} \|_2 & \text{if } \text{sons}(t) = \emptyset, \\
\left\| \left( \begin{array}{c}
P_{t_1} G|_{\hat{t} \times F_i} \\ P_{t_2} G|_{\hat{t} \times F_i}
\end{array} \right) - \hat{F}_t \left( \begin{array}{c}
P_{t_1} G|_{\hat{t} \times F_i} \\ P_{t_2} G|_{\hat{t} \times F_i}
\end{array} \right) \right\|_2 & \text{if } \text{sons}(t) = \{t_1, t_2\}.
\end{cases}
\]

We have already seen that we can control these “local” errors by choosing the quadrature order and the error tolerance of the cross approximation appropriately. Combining these estimates with stability estimates yields the following bound for the global error.

**Lemma 7 (Error estimate)** Using the stability constants

\[
\hat{\Lambda}_t := \begin{cases} 
1 & \text{if } \text{sons}(t) = \emptyset, \\
\max\{\| V_{t_1} \|_2, \| V_{t_2} \|_2 \} & \text{if } \text{sons}(t) = \{t_1, t_2\}
\end{cases}
\]

for all \( t \in \mathcal{T}_{F} \).
the total approximation error can be bounded by

\[ \|G|_{i \times F_t} - \mathcal{J}_t G|_{i \times F_t}\|_2 \leq \sum_{r \in \text{sons}^*(t)} \hat{\Lambda}_r \hat{\epsilon}_r \quad \text{for all } t \in T_{\mathcal{I}}. \] (28)

**Proof.** By structural induction.

Let \( t \in T_{\mathcal{I}} \) be a leaf of the cluster tree. Then we have \( \text{sons}^*(t) = \{ t \} \) and (28) holds by definition.

Let now \( t \in T_{\mathcal{I}} \) be a cluster with \( \text{sons}(t) = \{ t_1, t_2 \} \) and assume that (28) holds for \( t_1 \) and \( t_2 \). We have

\[
\|G|_{i \times F_t} - \mathcal{J}_t G|_{i \times F_t}\|_2 = \left\| \left( \begin{array}{c} G|_{i \times F_t} \\ G|_{i_2 \times F_t} \end{array} \right) - \left( \begin{array}{cc} V_{t_1} \\ V_{t_2} \end{array} \right) \tilde{\mathcal{J}}_t \left( \begin{array}{c} P_{t_1} \\ P_{t_2} \end{array} \right) \left( \begin{array}{c} G|_{i_1 \times F_t} \\ G|_{i_2 \times F_t} \end{array} \right) \right\|_2
\]

\[
= \left\| \left( \begin{array}{c} G|_{i_1 \times F_t} \\ G|_{i_2 \times F_t} \end{array} \right) - \left( \begin{array}{cc} V_{t_1} \\ V_{t_2} \end{array} \right) \left( \begin{array}{c} P_{t_1} G|_{i_1 \times F_t} \\ P_{t_2} G|_{i_2 \times F_t} \end{array} \right) \right\|_2
\]

\[
+ \left\| \left( \begin{array}{cc} P_{t_1} G|_{i_1 \times F_t} \\ P_{t_2} G|_{i_2 \times F_t} \end{array} \right) - \tilde{\mathcal{J}}_t \left( \begin{array}{c} P_{t_1} G|_{i_1 \times F_t} \\ P_{t_2} G|_{i_2 \times F_t} \end{array} \right) \right\|_2
\]

\[
\leq \|G|_{i_1 \times F_t} - \mathcal{J}_t G|_{i_1 \times F_t}\|_2
\]

\[
+ \|G|_{i_2 \times F_t} - \mathcal{J}_t G|_{i_2 \times F_t}\|_2 + \hat{\Lambda}_r \hat{\epsilon}_r.
\]

The induction assumption yields

\[
\|G|_{i \times F_t} - \mathcal{J}_t G|_{i \times F_t}\|_2 \leq \sum_{r \in \text{sons}^*(t_1)} \hat{\Lambda}_r \hat{\epsilon}_r + \sum_{r \in \text{sons}^*(t_2)} \hat{\Lambda}_r \hat{\epsilon}_r + \sum_{r \in \text{sons}^*(t)} \hat{\Lambda}_r \hat{\epsilon}_r,
\]

and the induction is complete. \( \square \)

We can find upper bounds for the stability constants during the course of the algorithm: let \( t \in T_{\mathcal{I}} \). If \( \text{sons}(t) = \emptyset \), the matrix \( V_t \) can be constructed explicitly by our algorithm, so we can either find \( \|V_t\|_2 \) by computing a singular value decomposition or obtain a good estimate by using a power iteration.

If \( \text{sons}(t) = \{ t_1, t_2 \} \), we can use

\[
\|V_t\|_2 = \left\| \begin{array}{c} V_{t_1} \\ V_{t_2} \end{array} \right\|_2 \leq \max\{\|V_{t_1}\|_2, \|V_{t_2}\|_2\} \left\| \hat{V}_t \right\|_2
\]

(29)

to compute an estimate of \( \|V_t\|_2 \) based on an estimate of the small matrix \( \hat{V}_t \) that can be treated as before.
This approach allows us to obtain estimates for $\hat{\Lambda}_t$ that can be computed explicitly during the course of the algorithm and used to verify that (28) is bounded.

An alternative approach can be based on the conjecture [5, eq. (16)]: let $\ell \in \mathbb{N}$ denote an upper bound for the rank used in the cross approximation algorithms. If we assume that there is a constant $\Lambda_V \geq 1$ such that

$$\|V_t\| \leq \Lambda_V \ell$$

for all $t \in \mathcal{L}_I$, and

$$\|\hat{V}_t\|_2 \leq \Lambda_V \ell$$

for all $t \in \mathcal{T}_I \setminus \mathcal{L}_I$,

a simple induction using the inequality (29) immediately yields

$$\|V_t\|_2 \leq \Lambda_V^p \ell^p$$

for all $t \in \mathcal{T}_I$, where $p \in \mathbb{N}$ denotes the depth of the cluster tree $\mathcal{T}_I$. Since $\|V_t\|_2$ grows only polynomially with $\ell$ while the error $\hat{\epsilon}_t$ converges exponentially, the right-hand side of the error estimate (28) will also converge exponentially.

8 Numerical experiments

The theoretical properties of the new approximation method, which we will call Green hybrid method (GrH) in the following, have been discussed in detail in the preceding sections. We will now investigate how the new method performs in experiments.

We consider the direct boundary element formulation of the Dirichlet problem: let $f$ be a harmonic function in $\Omega$ and assume that its Dirichlet values $f|_{\partial \Omega}$ are given.

Solving the integral equation

$$\int_{\partial \Omega} g(x, y) \frac{\partial f}{\partial n}(y) \, dy = \frac{1}{2} f(x) + \int_{\partial \Omega} \frac{\partial g}{\partial n}(y) (x, y) f(y) \, dy$$

for almost all $x \in \partial \Omega$

yields the Neumann values $\frac{\partial f}{\partial n}|_{\partial \Omega}$. We set up the Galerkin matrices $V$ and $K$ for the single and double layer potential operators as well as the mass-matrix $M$ and solve the equation

$$V \alpha = \left( K + \frac{1}{2} M \right) \beta,$$

where $\beta$ are the coefficients of the $L^2$-projection for the given Dirichlet data in the piecewise linear basis $(\psi_j)_{j \in \mathcal{J}}$ and $\alpha$ are the coefficients for the desired Neumann data in the piecewise constant basis $(\varphi_i)_{i \in \mathcal{I}}$.

For testing purpose we use the following three harmonic functions:

$$f_1(x) = x_1^2 - x_3^2, \quad f_2(x) = g(x, (1.2, 1.2, 1.2)), \quad f_3(x) = g(x, (1.0, 0.25, 1.0)).$$
Approximation of integral operators by Green quadrature...

Fig. 1 Unit sphere, 32,768 triangles: memory consumption, relative error and setup time for SLP with Green method vs. Green hybrid method vs. Green hybrid method $H^2$. In all cases $\delta_t = \text{diam}_{\infty}(B_t)/2$ was chosen

The approximation quality is measured by the absolute $L^2$-error of the Neumann data

$$\epsilon_j = \left( \int_{\partial \Omega} \left( \frac{\partial}{\partial n} f_j(x) - \sum_{i \in I} \alpha_i \varphi_i(x) \right)^2 \, dx \right)^{1/2}.$$  

The parameters for the Green hybrid method and for the adaptive cross approximation have been chosen manually to ensure that the total error (resulting from quadrature, matrix compression, and discretization) is close to the discretization error for all three harmonic functions.

Nearfield entries are computed using Sauter’s quadrature rule [29,30] with 3 Gauss points per dimension for regular integrals and 5 Gauss points for singular integrals.

All computations are performed on a single AMD Opteron 8431 Core at 2.4 GHz.

Reduced ranks. The pure quadrature approximation (9) produces matrices with local rank of $2k = 12 \, m^2$. This implies that for $m = 10$ the local rank already reaches a value of 1200, leading to a rather unattractive compression rate. As we stated in the beginning of Chapter 6, a rank reduction from $2k$ down to $k$ is at least expected when applying cross approximation to the quadrature approach from (9) due to the linear dependency of Neumann and Dirichlet values. Figure 1 shows that the Green hybrid method (23) performs even better: the storage requirements, given in Fig. 1a, are...
Reduced by approximately 50%, and the $H^2$-matrix version (27) reduces the storage requirements by approximately 75% compared to the $H$-matrix version.

Figure 1b illustrates that the pure Green quadrature approach (9) leads to exponential convergence, as predicted by Theorem 2. The hybrid methods reach a surprisingly high accuracy even for relatively low quadrature orders. We assume that this is due to the algebraic interpolation (23) exactly reproducing the original matrix blocks as soon as their rank is reached.

Figure 1c illustrates that the hybrid method is significantly faster than the pure quadrature method: at comparable accuracies, the hybrid method saves more than 50% of the computation time, and the $H^2$-matrix version saves approximately 50% compared to the $H$-matrix version.

Choice of $\delta_t$. In a second example, we apply the Green hybrid method to different surface meshes on the unit sphere with the admissibility condition (26) and the value $\delta_t = \text{diam}_\infty(B_t)/2$ used in the theoretical investigation as well as the value $\delta_t = \text{diam}_\infty(B_t)$. The latter is not covered by our theory, but Fig. 2 shows that it is superior both with regards to computational work and memory consumption.

Figure 2 also shows the memory and time requirements of the standard ACA technique. We can see that the new method with $\delta_t = \text{diam}_\infty(B_t)$ offers significant advantages in both respects.

Weaker admissibility condition. Another useful modification that is not covered by our theory is the construction of the block tree based on the admissibility condition

$$\max\{\text{diam}_\infty(B_t), \text{diam}_\infty(B_s)\} \leq \eta \text{dist}_\infty(B_t, B_s).$$

If we choose $\eta > 1$, this condition is weaker than the condition (26) used in the theoretical investigation.

Figure 3 shows experimental results for the choices $\eta = 1$ and $\eta = 2$. We can see that both ACA and the new Green hybrid method profit from the weaker admissibility condition.

Linear scaling. In order to demonstrate the linear complexity of the Green hybrid method, we have also computed the single layer potential for the same number of
Approximation of integral operators by Green quadrature…

Fig. 3 Unit sphere: memory consumption and setup time for SLP with the Green hybrid method and adaptive cross approximation. Results are shown with $\delta_t = \text{diam}_\infty(B_t)/2$ for $\eta = 1$ and for $\eta = 2$

Fig. 4 Unit sphere: memory consumption and setup time for SLP with fixed quadrature ranks, cross approximation error tolerances, minimal leafsizes, $\eta = 2$ and $\delta_t = \text{diam}_\infty(B_t)$

degrees of freedom as before but using the same $m$ and $\epsilon_{ACA}$ for all resolutions of the sphere. The results can be seen in Fig. 4.

We can see that both the time and the storage requirements of the new method indeed scale linearly with $n$. Since the standard ACA algorithm [4, Algorithm 4.2] constructs an $H$-matrix instead of an $H^2$-matrix, we observe the expected $O(n \log n)$ complexity.

Combination with algebraic recompression. We have seen that the Green hybrid method works fine with $\delta_t = \text{diam}_\infty(B_t)/2$ as well as with $\delta_t = \text{diam}_\infty(B_t)$. It is also possible to use the weaker admissibility condition (30). In order to obtain the best possible results the new method, we use $\eta = 2$, $\delta_t = \text{diam}_\infty(B_t)$ and apply algebraic $H^2$-recompression (cf. [6, Sect. 6.6]) to further reduce the storage requirements. Table 1 shows the total time and size for different resolutions of the unit sphere as well as the $L_2$-error observed for our test functions. We can see that the error converges at the expected rate for a piecewise constant approximation, i.e., the matrix approximation is sufficiently accurate.

For the ACA method, we also use algebraic recompression based on the blockwise singular value decomposition and truncation. Figure 5 shows memory requirements and compute times per degree of freedom for SLP and DLP matrices. Since the nodal basis used by the DLP matrix requires three local basis functions per triangle, the computational work is approximately three times as high as for the piecewise constant
Table 1  Unit sphere: setup time in seconds, resulting size of SLP and DLP in megabytes and absolute $L_2$-errors for different Dirichlet data using the new hybrid method

| $n$  | $m$  | $\epsilon_{ACA}$ | SLP | DLP | $\epsilon_1$ | $\epsilon_2$ | $\epsilon_3$ |
|------|------|------------------|-----|-----|--------------|--------------|--------------|
|      |      |                  |     |     | Time         | Size         |              |
|      |      |                  |     |     | Time         | Size         |              |
| 2048 | 2    | 5.0e−4           | 5   | 6   | 12           | 5            | 1.3e−1       |
| 8192 | 2    | 1.0e−4           | 23  | 30  | 65           | 25           | 6.3e−2       |
| 32,768 | 2 | 1.0e−5          | 114 | 167 | 309          | 134          | 3.1e−2       |
| 131,072 | 2 | 5.0e−6        | 470 | 751 | 1335         | 596          | 1.6e−2       |
| 524,288 | 2 | 1.0e−6        | 2090| 3692| 6378         | 2936         | 7.8e−3       |

Order of quadrature for Green’s formula is given by $m$ and accuracy used by cross approximation and $H^2$-recompression is given by $\epsilon_{ACA}$, $\delta_t = \text{diam}_\infty(B_t)$, $\eta = 2$ for both SLP and DLP.

Crankshaft. Our new approximation technique is not only capable of handling the simple unit sphere but also of more complex geometries such as the well-known “crankshaft” geometry contained in the netgen package of Joachim Schöberl [31]. We have used the program to create meshes with 1748, 6992, 27,968 and 111,872 triangles.

In order to obtain $O(h)$ convergence of the Neumann data, we have to raise the nearfield quadrature order to 7 Gauss points per dimension for regular integrals and to 9 Gauss points for singular ones. The results are shown in Table 2.

Due to the significantly higher number of nearfield quadrature points, the total computing time is far higher than for the simple unit sphere. We also have to choose $m = 3$ for the Green quadrature method and significantly lower error tolerances for the hybrid method and the recompression in order to recover the discretization error. Except for these changes, the new method works as expected.
Table 2  Crankshaft: setup time in seconds, resulting size of SLP and DLP in megabytes and absolute $L^2$-errors for different Dirichlet data using the new hybrid method

| Dof  | $m$  | $\epsilon_{ACA}$ | SLP | DLP | $\epsilon_1$ | $\epsilon_2$ | $\epsilon_3$ |
|------|------|-------------------|-----|-----|-------------|-------------|-------------|
|      |      |                   | Time | Size | Time | Size |             |
| 1748 | 2    | 1.0e−5            | 149  | 13   | 346  | 9    | 8.8e−2 | 9.5e−3 | 3.6e−2 |
| 6992 | 3    | 1.0e−6            | 1471 | 107  | 3422 | 90   | 3.1e−2 | 4.2e−3 | 1.6e−2 |
| 27,968 | 3    | 1.0e−7            | 10,660 | 633 | 27,410 | 722 | 1.2e−2 | 2.1e−3 | 7.7e−3 |
| 111,872 | 3    | 1.0e−8            | 59,790 | 2985 | 182,200 | 3829 | 4.7e−3 | 1.2e−3 | 3.9e−3 |

Order of quadrature for Green’s formula is given by $m$ and accuracy used by ACA and $H^2$-recompression is given by $\epsilon_{ACA}, \delta_t = \text{diam}_\infty(B_t), \eta = 1$ for both SLP and DLP

Appendix A: Proofs of technical lemmas

Proof of Lemma 3  By definition of the maximum norm, we can find $\iota \in \{1, \ldots, d\}$ such that $2\delta_t = \text{diam}_\infty(B_t) = b_{t,\iota} - a_{t,\iota}$ and $b_{t,\kappa} - a_{t,\kappa} \leq 2\delta_t$ holds for all $\kappa \in \{1, \ldots, d\}$. Most of our claims are direct consequences of this estimate, only the last claim of (16) requires a closer look. Let $x \in \partial\omega_t$ and $y \in F_t$ be given with

$$\|x - y\|_\infty = \text{dist}_\infty(\partial\omega_t, F_t).$$

Let $\hat{x} \in B_t$ be a point in $B_t$ that has minimal distance to $x$. By construction, we have

$$\|x - \hat{x}\|_\infty \leq \delta_t,$$

and the triangle inequality in combination with (5) yields

$$\text{dist}_\infty(\partial\omega_t, F_t) = \|x - y\|_\infty \geq \|\hat{x} - y\|_\infty \geq \|\hat{x} - x\|_\infty \geq \text{dist}_\infty(B_t, B_x) - \delta_t \geq \text{diam}_\infty(B_t) - \text{diam}_\infty(B_t)/2 = \text{diam}_\infty(B_t)/2 = \delta_t,$$

and this is the required estimate. □

Proof of Lemma 4  Let $\kappa \in \mathbb{N}_0^d$ be a multiindex. We consider the function

$$g_x : [-1, 1]^d \rightarrow \mathbb{R}, \quad \hat{\zeta} \mapsto (\partial^\kappa g)(x, \Phi_t(\hat{\zeta}))$$

and aim to prove

$$\partial^\nu g_x(\hat{\zeta}) = s^\nu(\partial^{\nu + \kappa} g)(x, \Phi_t(\hat{\zeta})) \quad \text{for all } \hat{\zeta} \in [-1, 1]^d, \nu \in \mathbb{N}_0^d \quad (31)$$

with the vector

$$s := \begin{pmatrix} (b_{t,1} - a_{t,1} + 2\delta_t)/2 \\ \vdots \\ (b_{t,d} - a_{t,d} + 2\delta_t)/2 \end{pmatrix} \in \mathbb{R}^d.$$

We proceed by induction: for the multiindex $\nu = 0$, the identity (31) is trivial.
Let \( m \in \mathbb{N}_0 \) and assume that (31) has been proven for all multiindices \( \nu \in \mathbb{N}^d_0 \) with \( |\nu| \leq m \).
Let \( \nu \in \mathbb{N}^d_0 \) be a multiindex with \( |\nu| = m + 1 \). Then we can find \( \mu \in \mathbb{N}^d_0 \) with \( |\mu| = m \) and \( i \in \{1, \ldots, d\} \) such that \( \nu = (\mu_1, \ldots, \mu_{i-1}, \mu_i + 1, \mu_{i+1}, \ldots, \mu_d) \).
This implies
\[
\partial^\nu g_x(\hat{z}) = \frac{\partial}{\partial \hat{z}_i}(\partial^{\mu + \kappa} g_x)(\hat{z}) \quad \text{for all } \hat{z} \in [-1, 1]^d.
\]
Applying the induction assumption and the chain rule yields
\[
\partial^\nu g_x(\hat{z}) = \frac{\partial}{\partial \hat{z}_i} s^{\mu} (\partial^{\mu + \kappa} g)(x, \Phi_t(\hat{z})) = \frac{s^{\mu}}{2} (\partial^{\mu + \kappa} g)(x, \Phi_t(\hat{z})) = s^{\nu} (\partial^{\nu + \kappa} g)(x, \Phi_t(\hat{z})) \quad \text{for all } \hat{z} \in [-1, 1]^d
\]
since \( D\Phi_t \) is a diagonal matrix due to (6). The induction is complete.

By definition (7), we have
\[
\gamma_t(\hat{z}) = \Phi_t(\hat{z}_1, \ldots, \hat{z}_{[t/2]} - 1, \pm 1, \hat{z}_{[t/2]}, \ldots, \hat{z}_{d-1}),
\]
therefore (31) implies
\[
\partial^\hat{v} f_1(\hat{z}) = s^{\nu} (\partial^{\nu g})(x, \gamma_t(\hat{z})) \quad \text{for all } \hat{z} \in Q, \hat{v} \in \mathbb{N}^{d-1}_0 \quad (32a)
\]
with
\[
\nu := (\hat{v}_1, \ldots, \hat{v}_{[t/2]} - 1, 0, \hat{v}_{[t/2]}, \ldots, \hat{v}_{d-1}).
\]
The exterior normal vector on the surface \( \gamma_t(Q) \) is the \( t/2 \)th canonical unit vector if \( t \) is even and the negative \( (t + 1)/2 \)th canonical unit vector if it is uneven, so we obtain also
\[
\partial^\hat{v} g_2(\hat{z}) = \pm s^{\nu} (\partial^{\nu + \kappa} g)(x, \gamma_t(\hat{z})) \quad \text{for all } \hat{z} \in Q, \hat{v} \in \mathbb{N}^{d-1}_0, \quad (32b)
\]
where \( \kappa \) is the \( [t/2] \)th canonical unit vector in \( \mathbb{N}^d_0 \).
Exchanging the roles of \( x \) and \( y \) in these arguments yields
\[
\partial^\hat{v} f_2(\hat{z}) = s^{\nu} (\partial^{\nu g})(\gamma_t(\hat{z}), y), \quad (32c)
\]
\[
\partial^\hat{v} g_1(\hat{z}) = \pm s^{\nu} (\partial^{\nu + \kappa} g)(\gamma_t(\hat{z}), y) \quad \text{for all } \hat{z} \in Q, \hat{v} \in \mathbb{N}^{d-1}_0. \quad (32d)
\]
Now we only have to combine the equations (32) with
\[
|s^{\nu}| \leq (2\delta_t)^{|\nu|} \quad \text{for all } \nu \in \mathbb{N}^d_0
\]
and the asymptotic smoothness (15) to obtain

\[
|\partial^\nu \hat{f}_1(\hat{z})| \leq (2\delta_t)^{|\nu|} C_{\text{as}} \hat{v}! \frac{c_0^{\hat{v}}}{\delta_t^{\sigma+1}} \left|\frac{x - y(\hat{z})}{\eta(\hat{z}) - y}\right|^{|\nu|+1}
\]

\[
\leq C_{\text{as}} \hat{v}! \frac{(2\delta_t c_0)^{\hat{v}}}{\delta_t^{\sigma}} \frac{|x - y(\hat{z})|^{\sigma+1+|\nu|}}{\eta(\hat{z}) - y}
\]

\[
|\partial^\nu \hat{f}_2(\hat{z})| \leq (2\delta_t)^{|\nu|} C_{\text{as}} \hat{v}! \frac{c_0^{\hat{v}}}{\delta_t^{\sigma+1}} \left|\frac{x - y(\hat{z})}{\eta(\hat{z}) - y}\right|^{|\nu|+1}
\]

\[
\leq C_{\text{as}} \hat{v}! \frac{(2\delta_t c_0)^{\hat{v}}}{\delta_t^{\sigma+1}} \frac{|x - y(\hat{z})|^{\sigma+1+|\nu|}}{\eta(\hat{z}) - y}
\]

\[
|\partial^\nu \hat{g}_1(\hat{z})| \leq (2\delta_t)^{|\nu|} C_{\text{as}} \hat{v}! \frac{c_0^{\hat{v}}}{\delta_t^{\sigma+1}} \left|\frac{x - y(\hat{z})}{\eta(\hat{z}) - y}\right|^{|\nu|+1}
\]

\[
\leq C_{\text{as}} \hat{v}! \frac{(2\delta_t c_0)^{\hat{v}}}{\delta_t^{\sigma+1}} \frac{|x - y(\hat{z})|^{\sigma+1+|\nu|}}{\eta(\hat{z}) - y}
\]

where Lemma 3 provides the lower bounds \( \delta_t \leq \|x - y(\hat{z})\| \) and \( \delta_t \leq \|y(\hat{z}) - y\| \) and we have taken advantage of \((\nu + \kappa)! = \nu! = \hat{v}!\) due to \(v_{[1/2]} = 0\).

\[ \square \]

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