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\mathcal{H} - and \mathcal{H}^2 -matrices for low and high frequency
Helmholtz equation

by

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Abstract

An approach is presented for the efficient manipulation of matrices arising from the Galerkin discretisation of boundary element operators for the Helmholtz equation. Using \mathcal{H} -matrix and \mathcal{H}^2 -matrix techniques, different methods are proposed for the low frequency and high frequency regimes. In both cases the methods are numerically stable and are proved to have almost linear complexity for the storage and the cost of the matrix-vector multiplication. Problems that have aspects of both regimes pose no difficulty. The efficiency of the methods is demonstrated by numerical examples.

1 Introduction

Many physical problems (e.g. acoustics, electromagnetic scattering) require the solution of the Helmholtz equation; see [20]. We investigate the numerical solution of the Helmholtz equation by the boundary element method (BEM). In such methods the boundary is subdivided into n elements and the problem is reduced to the solution of an $n \times n$ linear system of equations. The system of linear equations arises from the discretisation of integral operators such as

$$(\mathcal{A}u)(x) = \int_{\Gamma} s(x, y)u(y)dy, \quad (1)$$

where Γ is the boundary and $s(x, y)$ is the fundamental solution or a suitable directional derivative of the fundamental solution. The linear system resulting from BEM discretisation is dense making direct methods for the solution of the system prohibitively expensive. To reduce the complexity from $O(n^3)$ for the direct methods, or from $O(n^2)$ for iterative methods, the so-called fast methods can be used (e.g. \mathcal{H} -matrices, panel clustering, FMM, wavelet methods [7, 13, 14, 17]). In this paper we describe how a combination of \mathcal{H} -matrix and \mathcal{H}^2 -matrix techniques can be used to compress matrices arising from the discretisation of integral operators for low or high frequency Helmholtz equation. As for other fast methods (panel clustering and FMM) we make use of a separable expansion of the kernel function

$$s(x, y) \approx \sum_{i,j=0}^K \tilde{s}_{i,j}u_i(x)v_j(y). \quad (2)$$

For the high frequency regime in two dimensions the number of elements n is proportional to the wave number κ , and in three dimensions n is proportional to κ^2 . If h is a parameter controlling the mesh size, this corresponds to $\kappa h = \text{const}$. A further complication is that for a fixed accuracy we can expect the length of expansion K in (2) also to be proportional to κ and hence strongly dependent on n . For a low frequency, κ is a constant with respect to n and hence the length of the expansion is constant for a fixed accuracy. The fast multipole method (FMM) has previously been used to accelerate the solution of the high frequency Helmholtz problem. Initially one or two

level versions were recommended which gave $O(n^{3/2})$ or $O(n^{4/3})$ algorithms [22, 23], but recently a number of multilevel implementations were reported on, both in 2D and 3D, with complexity $O(n \log^a n)$ for some small constant a [1, 8]. Most of these methods suffer from numerical instability at low frequencies. The approach presented in this paper is closest to the approach for the high frequency regime of Amini and Profit [1]. However, we give new error bounds and consider the case of the low frequency regime and problems with aspects of both regimes.

Our method divides the matrices arising from discretisation into admissible parts which are then approximated by an \mathcal{H}^2 -matrix or a low rank matrix. For low frequency all the parts are approximated by low rank matrices, giving rise to an \mathcal{H} -matrix approximation, whereas for high frequency a combination of an \mathcal{H} -matrix and an \mathcal{H}^2 -matrix is used. We will use Graf's addition theorem for Bessel functions and the integral representation of Bessel functions [24] to construct the \mathcal{H}^2 -matrices; this is the standard approach in fast multipole methods. For the construction of low rank matrices we use ACA, see [2], though any other method designed for asymptotically smooth functions is applicable. Only a brief description of \mathcal{H} - and \mathcal{H}^2 -matrix methods will be given, for more detail see [4, 12, 15]. The resulting algorithm has a complexity of $O(n \log^2 n)$. Our method is numerically stable at all frequencies in a very natural way making the implementation relatively simple and allowing small scale details of the boundary in the high frequency regime. We allow for interaction between clusters of different sizes, which is usually not the case in the fast multipole methods for the Helmholtz equation. The combination of \mathcal{H}^2 -matrices with low-rank matrices except from providing stability also allows for a greater control of memory and time requirements of the method. There is a range of frequencies for which both the \mathcal{H} -matrix and the \mathcal{H}^2 -matrix technique are applicable. The optimal choice depends on the memory resources and on the number of times the Galerkin matrix is to be applied to a vector. The efficiency of the method is demonstrated by numerical examples. One of the advantages of hierarchical matrix methods is the possibility of further algebraic recompression [3, 11]. These are directly applicable and effective in the low frequency regime, however the standard recompressions for \mathcal{H}^2 -matrices in the case of the Helmholtz equation are too expensive in the high frequency regime. One of interesting further improvements would be the extension of recompression techniques to the high frequency regime.

1.1 Statement of the problem

Let $\Omega \in \mathbb{R}^d$, $d = 2, 3$, be a bounded domain with boundary Γ and exterior Ω_+ . We are interested in the numerical solution of the exterior Helmholtz equation,

$$\Delta u + \kappa^2 u = 0, \quad x \in \Omega_+, \quad (3)$$

where the wave number κ is a positive real parameter. The boundary conditions can be a combination of Dirichlet and Neumann data:

$$\alpha u(x) + \beta \frac{\partial u}{\partial n}(x) = f(x), \quad x \in \Gamma. \quad (4)$$

To make the solution unique, a condition at infinity is necessary:

$$\left| \frac{\partial u}{\partial r} - i\kappa u \right| \leq \frac{c}{r^2} \quad \text{at } \infty. \quad (5)$$

The unique fundamental solution of the Helmholtz elliptic operator, respecting the condition at infinity, in 2D is the Hankel function of the first kind of order 0,

$$G_\kappa(x, y) = H_0(\kappa \|x - y\|). \quad (6)$$

In 3D the fundamental solution is the zero order spherical Hankel function of the first kind,

$$G_\kappa(x, y) = \frac{e^{i\kappa \|x - y\|}}{\|x - y\|}. \quad (7)$$

To solve this problem numerically using BEM, the boundary elliptic partial differential equation is formulated as a boundary integral equation. To discretise the integral operators which are of the form (1), where the singularity function $s(x, y)$ is the fundamental solution or a suitable derivative, Galerkin's method can be applied. If we use $\{\phi_1, \dots, \phi_n\}$ as both the test and trial bases then the Galerkin matrix has the entries

$$A_{ij} = \int_{\Gamma} \int_{\Gamma} s(x, y) \phi_i(x) \phi_j(y) dx dy. \quad (8)$$

For asymptotically smooth singularity functions $s(\cdot, \cdot)$, \mathcal{H} -matrix techniques have already been successfully applied [16]. A function $s(\cdot, \cdot)$ is said to be *asymptotically smooth* if for multi-indices $\alpha, \beta \in \mathbb{N}^d$

$$|\partial_x^\alpha \partial_y^\beta s(x, y)| \leq C(\alpha + \beta)! c_0^{|\alpha|+|\beta|} \|x - y\|^{-|\alpha|-|\beta|-\sigma} \quad (9)$$

holds for constants $C, c_0, \sigma \in \mathbb{R}_{>0}$, where σ is the degree of the singularity of s . For the Helmholtz kernel G_κ in two and three dimensions the inequality

$$|\partial_x^\alpha \partial_y^\beta G_\kappa(x, y)| \leq C(\alpha + \beta)! c_0^{|\alpha|+|\beta|} e^{\kappa \|x-y\|} \|x - y\|^{-|\alpha|-|\beta|-\sigma} \quad (10)$$

holds for constants $C, c_0, \sigma \in \mathbb{R}_{>0}$ depending on the dimension. Since all integrations in (8) are over a compact set $\partial\Omega$, G_κ restricted to this domain is asymptotically smooth, however with a constant which increases exponentially with κ . This shows that if $\kappa \text{diam}(\partial\Omega)$ is a small constant, we are in the *low frequency regime* and all the usual \mathcal{H} -matrix techniques can be applied. However, in the *high frequency regime* where κh is a constant, the above bound increases exponentially as we demand more accuracy, i.e., as the mesh parameter h is decreased. To the latter problem \mathcal{H} -matrix techniques cannot be applied without the more involved structure of \mathcal{H}^2 -matrices.

We proceed by describing some concepts used to construct both \mathcal{H} - and \mathcal{H}^2 -matrices.

2 \mathcal{H} - and \mathcal{H}^2 -matrices: The basics

2.1 Cluster tree

Let the boundary Γ be subdivided into n disjoint panels π_j , $j \in \mathcal{I} := \{1, \dots, n\}$. We consider piecewise constant basis functions ϕ_j , such that $\text{supp } \phi_j = \pi_j$, $j \in \mathcal{I}$. Let $T_{\mathcal{I}}$ be a tree whose nodes are clusters, i.e., subsets of the index set \mathcal{I} . The root of the tree is the cluster containing all the indices $\tau_{\text{root}} = \mathcal{I}$. $T_{\mathcal{I}}$ is a *cluster tree* if the following conditions hold:

- If $\tau \in T_{\mathcal{I}}$ has sons, then the sons form a partition of the father, i.e., $\tau = \dot{\bigcup} \{\tau' : \tau' \in \text{sons}(\tau)\}$.
- For every $\tau \in T_{\mathcal{I}}$, $\#\text{sons}(\tau) = 2$, and $\#\tau > 0$.
- There exists a constant C_{leaf} such that, for each leaf τ , $\#\tau \leq C_{\text{leaf}}$.

We say that the root of the tree is at level 0, and that if a parent is at level l then its children are at level $l + 1$. We introduce the notation

$$\Omega_\tau := \cup_{i \in \tau} \pi_i \subseteq \Gamma$$

for the subset of Γ corresponding to a cluster $\tau \in T_{\mathcal{I}}$. It is sometimes useful to consider the set of clusters which are at the same level of the cluster tree:

$$T_{\mathcal{I}}^{(l)} := \{\tau \in T_{\mathcal{I}} : \tau \text{ at level } l\}.$$

A couple of simple properties of this tree will be useful for later analysis:

- the number of clusters is bounded by $2n - 1$,
- at level l there are at most 2^l clusters.

2.2 Admissibility condition

Since the fundamental solution is singular on the diagonal, we cannot expect that a separable expansion as in (2) can be valid in all of the domain. So we define *admissible blocks* for which we can expect that such an expansion can be found.

For each $\tau \in T_{\mathcal{I}}$ let a centre $c_\tau \in \mathbb{R}^d$ and a radius $r_\tau > 0$ be given such that $\Omega_\tau \subseteq D(c_\tau, r_\tau) = \{y \in \mathbb{R}^d \mid \|y - c_\tau\|_2 < r_\tau\}$. Then we say that a block $b = \tau \times \sigma \in T_{\mathcal{I}} \times T_{\mathcal{I}}$ is admissible if for some $\eta < 1$

$$r_\tau + r_\sigma \leq \eta \|c_\tau - c_\sigma\|_2. \quad (11)$$

Equivalently we say that the clusters τ and σ are *well-separated*.

2.3 Block cluster tree

To easily access such blocks we create a block cluster tree $T_{\mathcal{I} \times \mathcal{I}}$. The root of the tree is the node $\mathcal{I} \times \mathcal{I}$. Then for $b = \tau \times \sigma \in T_{\mathcal{I} \times \mathcal{I}}$ we proceed as follows:

- If b is admissible add it to the set of admissible leaves \mathcal{L}^+ of $T_{\mathcal{I} \times \mathcal{I}}$.
- If τ and σ are leaves of $T_{\mathcal{I}}$, add b to the set of inadmissible leaves \mathcal{L}^- .
- Otherwise, repeat the procedure for all pairs formed by the sons of τ and σ (if one of the clusters has no sons use the cluster instead), which are then the sons of b in the tree $T_{\mathcal{I} \times \mathcal{I}}$.

The levels of the block cluster tree can be defined as in the case of the cluster tree.

2.4 Low rank approximation

Let $b = \tau \times \sigma \in \mathcal{L}^+$ be an admissible block at level l . Define a matrix $A_{\tau, \sigma}$ corresponding to this block by

$$(A_{\tau, \sigma})_{kj} := \begin{cases} \int_{\Omega_\tau} \int_{\Omega_\sigma} s(x, y) \phi_k(x) \phi_j(y) dx dy, & \text{if } k \in \tau \text{ and } j \in \sigma \\ 0, & \text{otherwise.} \end{cases}$$

We consider next, how such a matrix can be approximated by a matrix of a lower rank.

2.4.1 Singular value decomposition (SVD)

If the fundamental solution $s(\cdot, \cdot)$ is an asymptotically smooth function then it can be shown that the singular values of $A_{\tau, \sigma}$ decay exponentially. Let $A_{\tau, \sigma} = U \Sigma V^T$ be a singular value decomposition of $A_{\tau, \sigma}$ with singular values ordered so that $\Sigma_{11} \geq \Sigma_{22} \cdots \geq \Sigma_{nn} \geq 0$. Then for any $\epsilon > 0$ there exists $k \geq 1$ such that $\Sigma_{k+1, k+1} \leq \epsilon$, with $\Sigma_{n+1, n+1} := 0$. For asymptotically smooth functions $k = O(\log^{d-1}(1/\epsilon))$. As an approximation we can use the rank k *reduced singular value decomposition*

$$A_{\tau, \sigma} \approx U_k \Sigma_k V_k^T,$$

where $\Sigma_k := \text{diag}(\Sigma_{11}, \Sigma_{22}, \dots, \Sigma_{kk})$, and U_k and V_k consist of the first k columns of matrices U and V respectively. The error of the approximation in the spectral norm is bounded by ϵ :

$$\|A_{\tau, \sigma} - U_k \Sigma_k V_k^T\|_2 \leq \epsilon.$$

2.4.2 Adaptive-cross approximation to the SVD

Adaptive cross approximation (ACA) is a rank revealing method. It has been shown in [2] that under suitable conditions for matrices arising from the Galerkin discretisation of the single layer potential for asymptotically smooth kernels an approximation of the reduced SVD can be obtained by ACA in $O(nk)$ time. A hybrid method combining ACA and interpolation is the so-called hybrid

cross approximation (HCA), which can be used for a larger class of operators of asymptotically smooth kernels; see [5].

We do not give details of the ACA algorithm. The reader can think of it as a function that given an accuracy $\epsilon > 0$ and the matrix $A_{\tau,\sigma}$ corresponding to an admissible block $b = \tau \times \sigma \in \mathcal{L}^+$, in time $O(nk)$ returns two rank k matrices $A_k, B_k \in \mathbb{C}^{n \times k}$ such that

$$\|A_{\tau,\sigma} - A_k B_k^T\|_2 < \epsilon.$$

Note that since ACA is not an exact method, it does not produce the optimal rank k . However, in practice it produces results close to the optimum. The optimum can be reached by SVD, but the cost of computing the exact SVD is much higher.

2.4.3 Separable expansion

Let us assume that for all $x \in \Omega_\tau$ and all $y \in \Omega_\sigma$ a separable expansion of the fundamental solution is valid, the expansion being of the following form

$$s(x, y) \approx \sum_{i=1}^{K_\tau} \sum_{j=1}^{K_\sigma} \tilde{s}_{i,j}(c_\tau, c_\sigma) u_i(x, c_\tau) v_j(y, c_\sigma),$$

where c_τ and c_σ are as before the centres of the clusters Ω_τ and Ω_σ . The length of expansion K_τ is defined for each cluster and as we see later depends on the size of the cluster.

We can now approximate the matrix $A_{\tau,\sigma}$ corresponding to the block $\tau \times \sigma$ by a matrix of rank $\min\{K_\tau, K_\sigma\}$ defined by

$$(\tilde{A}_{\tau,\sigma})_{kl} := \begin{cases} \sum_{i=1}^{K_\tau} \sum_{j=1}^{K_\sigma} \tilde{s}_{i,j}(c_\tau, c_\sigma) \int_{\Omega_\tau} u_i(x, c_\tau) \phi_k(x) dx \int_{\Omega_\sigma} v_j(y, c_\sigma) \phi_l(y) dy, & \text{if } k \in \tau \text{ and } l \in \sigma \\ 0, & \text{otherwise.} \end{cases}$$

Hence we have that

$$\tilde{A}_{\tau,\sigma} = U_\tau S_{\tau,\sigma} V_\sigma^T, \quad U_\tau \in \mathbb{C}^{n \times K_\tau}, \quad V_\sigma \in \mathbb{C}^{n \times K_\sigma}, \quad S_{\tau,\sigma} \in \mathbb{C}^{K_\tau \times K_\sigma},$$

where

$$(U_\tau)_{ki} = \begin{cases} \int_{\Omega_\tau} u_i(x, c_\tau) \phi_k(x) dx, & \text{if } k \in \tau \text{ and } i = 1, \dots, K_\tau \\ 0, & \text{if } k \notin \tau, \end{cases}$$

$$(V_\sigma)_{lj} = \begin{cases} \int_{\Omega_\sigma} v_j(y, c_\sigma) \phi_l(y) dy, & \text{if } l \in \sigma \text{ and } j = 1, \dots, K_\sigma \\ 0, & \text{if } l \notin \sigma. \end{cases}$$

We call U_τ the *row cluster basis* for cluster τ and V_σ the *column cluster basis* for cluster σ . The possibly dense *coefficient matrix* $S_{\tau,\sigma}$ is defined by $S_{ij} = \tilde{s}_{i,j}(c_\tau, c_\sigma)$.

Finally we define the sparse matrix corresponding to the inadmissible blocks by

$$(A^\diamond)_{kl} := \begin{cases} A_{kl}, & \text{if } \exists b = \tau \times \sigma \in \mathcal{L}^- \text{ such that } k \in \tau \text{ and } l \in \sigma, \\ 0 & \text{otherwise.} \end{cases}$$

We can now define an approximation to the Galerkin matrix A by

$$\begin{aligned} \tilde{A} &:= A^\diamond + \sum_{\tau \times \sigma \in \mathcal{L}^+} \tilde{A}_{\tau,\sigma} \\ &= A^\diamond + \sum_{\tau \times \sigma \in \mathcal{L}^+} U_\tau S_{\tau,\sigma} V_\sigma^T. \end{aligned} \tag{12}$$

2.5 \mathcal{H} -matrices

Definition 2.1 Let $T_{\mathcal{I} \times \mathcal{I}}$ be a block cluster tree as defined before and let $k : \mathcal{L}^+ \rightarrow \mathbb{N}$ be a rank distribution. We define the set of \mathcal{H} -matrices as

$$\mathcal{H}(T_{\mathcal{I} \times \mathcal{I}}, k(\cdot)) := \{M \in \mathbb{C}^{n \times n} \mid \text{rank}(M_b) \leq k(b) \text{ for all admissible leaves } b = \tau \times \sigma \in \mathcal{L}^+\}.$$

If $k(b) \leq k_{\max}$ for all $b \in \mathcal{L}^+$, it can be shown that the cost of storage and the cost of matrix-vector multiplication of an \mathcal{H} -matrix is $O(nk_{\max}p)$, where $p > 1$ is the depth of the block cluster tree $T_{\mathcal{I} \times \mathcal{I}}$.

Approximations to the Galerkin matrix A from this set can be, for example, obtained by applying ACA to each admissible block of the matrix A . In the low frequency case, we expect $k_{\max} = O(\log^{d-1}(1/\epsilon))$ for a fixed accuracy $\epsilon > 0$, giving almost linear complexity for both the storage and the cost of matrix-vector multiplication. However, in the high frequency regime, we expect $k_{\max} = O(n)$ which gives unacceptable quadratic complexity for the storage and matrix arithmetics. Hence for high frequencies another approach is required.

2.6 \mathcal{H}^2 -matrices

For the construction of low rank approximations of admissible blocks we will use the separable expansion of the kernel; see Section 2.4.3. To optimise the cost of the matrix multiplication by a vector we require a further condition on the matrices U_τ and V_σ described in Section 2.4.3.

2.6.1 Nested bases

Let τ and σ be parent nodes in the cluster tree $T_{\mathcal{I}}$ such that $b = \tau \times \sigma \in \mathcal{L}^+$ and let τ' and τ'' be the children of τ and σ' and σ'' the children of σ . Then assume that

$$\text{there exist } T_{\tau',\tau}^U, T_{\tau'',\tau}^U, T_{\sigma',\sigma}^V, T_{\sigma'',\sigma}^V,$$

such that

$$U_\tau = \begin{pmatrix} U_{\tau'} T_{\tau',\tau}^U \\ U_{\tau''} T_{\tau'',\tau}^U \end{pmatrix} \in \mathbb{C}^{n \times K_\tau} \text{ and } V_\sigma = \begin{pmatrix} V_{\sigma'} T_{\sigma',\sigma}^V \\ V_{\sigma''} T_{\sigma'',\sigma}^V \end{pmatrix} \in \mathbb{C}^{n \times K_\sigma}. \quad (13)$$

The matrices $T_{\tau',\tau}^V$ and $T_{\tau'',\tau}^U$ are called *transfer matrices*.

With this final condition the description of the \mathcal{H}^2 -matrix representation of the discretised integral operator is finished. An approximation of the form (12) with fixed bases U_τ, V_σ , is called a *uniform \mathcal{H} -matrix*. If also the cluster bases are nested, it is called an *\mathcal{H}^2 -matrix*. In the next subsection we show how such a format can be used for fast approximate multiplication of the Galerkin matrix by an arbitrary vector.

2.6.2 Fast matrix-vector multiplication

For an arbitrary vector $u \in \mathbb{C}^n$ we consider the computation of an approximation v to Au . The straightforward method would be to apply the approximation \tilde{A} directly. However, the properties of the \mathcal{H}^2 -matrix representation can be used to construct the approximation more efficiently as described by the following four step procedure:

1. Upward pass from level p to level 0 of the tree $T_{\mathcal{I}}$
 - for all leaves $\sigma \in T_{\mathcal{I}}$, $\hat{u}_\sigma := V_\sigma^T u$
 - for all parents σ on the current level, $\hat{u}_\sigma := (T_{\sigma',\sigma}^V)^T \hat{u}_{\sigma'} + (T_{\sigma'',\sigma}^V)^T \hat{u}_{\sigma''}$
2. Far field interaction
 - for all $\tau \in T_{\mathcal{I}}$, $\hat{v}_\tau := \sum_{\tau \times \sigma \in \mathcal{L}^+} S_{\tau,\sigma} \hat{u}_\sigma$, where $S_{\tau,\sigma}$ is the coefficient matrix; see Section 2.4.3.

3. Downward pass from level 0 to level p of tree $T_{\mathcal{I}}$

- initialise the output vector v to zero
- for all parents τ on the current level, $\hat{v}_{\tau'} := \hat{v}_{\tau'} + T_{\tau',\tau}^U \hat{v}_{\tau}$ and $\hat{v}_{\tau''} := \hat{v}_{\tau''} + T_{\tau'',\tau}^U \hat{v}_{\tau}$
- for every leaf $\tau \in T_{\mathcal{I}}$, $v := v + U_{\tau} \hat{v}_{\tau}$

4. Near field interaction

- $v := v + A^{\diamond} u$.

It is not immediately obvious how efficient is the above method of matrix-vector multiplication in the case of the high frequency Helmholtz equation. The first step of the algorithm (the computation of u_{σ} for all leaves σ) has the cost $\sum_{\tau \in T_{\mathcal{I}}^{(p)}} \#\tau K_{\tau} \leq n \max_{\tau \in T_{\mathcal{I}}^{(p)}} K_{\tau}$. Applying a general interaction matrix $S_{\tau,\sigma}$ to a vector costs $O(K_{\tau} K_{\sigma})$. Hence we need to make sure that the expansion lengths are small (constant) at the lowest level p and that either they are also small at higher levels or that the structure of the interaction matrices (and of the transform matrices T^U and T^V) is particularly simple, e.g. Toeplitz or diagonal. Hence some constraints on the \mathcal{H}^2 -matrix representation are necessary. These constraints influence the choice of the separable expansion. Two possible choices for the two-dimensional problem are described in the next section.

3 The two-dimensional problem

3.1 The low frequency regime: \mathcal{H} -matrix

An \mathcal{H} -matrix approximation to the Galerkin matrix A can be obtained by the following procedure:

- Choose $\epsilon > 0$.
- Construct the cluster tree and the block cluster tree.
- For each admissible leaf $b = \tau \times \sigma \in \mathcal{L}^+$ find the low rank approximation $M_{\tau,\sigma}$ to the matrix $A_{\tau,\sigma}$ using ACA with the prescribed accuracy ϵ .
- For each inadmissible leaf $b = \tau \times \sigma \in \mathcal{L}^-$ set $M_{\tau,\sigma} := A_{\tau,\sigma}$.

The method for constructing the cluster and block cluster trees is not crucial in this procedure.

3.1.1 Complexity estimates

Suppose that the \mathcal{H} -matrix constructed by the above procedure is in the set $\mathcal{H}(T_{\mathcal{I} \times \mathcal{I}}, k(\cdot))$ and define $k_{\max} := \max\{k(b) : b \in \mathcal{L}^+\}$.

To estimate the complexity of the storage and the cost of matrix-vector multiplication, as for sparse matrices, we quantify a sparsity property of the block cluster tree $T_{\mathcal{I} \times \mathcal{I}}$.

Definition 3.1 Define the sparsity constant of $T_{\mathcal{I} \times \mathcal{I}}$ by

$$C_{sp} := \max \left\{ \max_{\tau \in T_{\mathcal{I}}} \#\{\sigma \in T_{\mathcal{I}} \mid \tau \times \sigma \in T_{\mathcal{I} \times \mathcal{I}}\}, \max_{\sigma \in T_{\mathcal{I}}} \#\{\tau \in T_{\mathcal{I}} \mid \tau \times \sigma \in T_{\mathcal{I} \times \mathcal{I}}\} \right\}.$$

We assume that C_{sp} is indeed a constant independent of n , as proved in [12] for standard situations. With this assumption we can prove almost linear complexity estimates.

Lemma 3.1 Let $M \in \mathcal{H}(T_{\mathcal{I} \times \mathcal{I}}, k(\cdot))$ and $k_{\max} := \max\{k(b) : b \in \mathcal{L}^+\}$ and let p be the depth of $T_{\mathcal{I} \times \mathcal{I}}$. Then

$$N_{st} \leq 2C_{sp}(p+1) \max\{k_{\max}, C_{leaf}\}n \text{ and } N_{\mathcal{H}.v} \leq 2N_{st},$$

where N_{st} is the storage requirement and $N_{\mathcal{H}.v}$ the complexity of the matrix-vector multiplication.

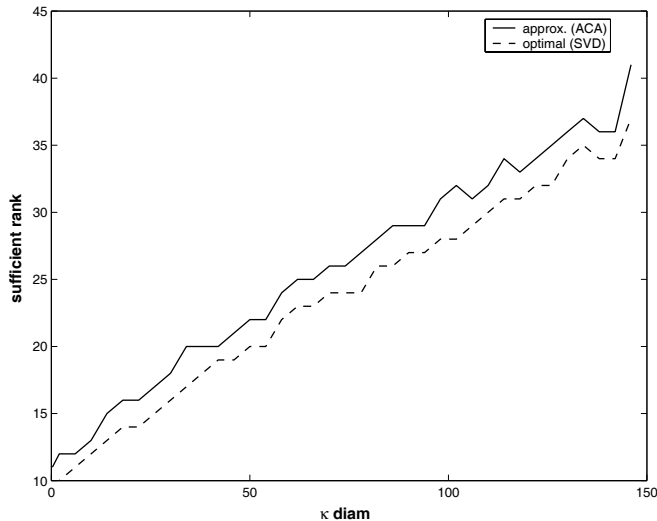


Figure 1: We compute low rank approximations $A_k B_k^T$ to the matrix $A_{\tau, \sigma}$, where $\tau \times \sigma \in \mathcal{L}^+$, by ACA and by SVD. As we increase κ we plot the minimum rank necessary for the two methods such that $\|A_{\tau, \sigma} - A_k B_k^T\|_2 < \epsilon$ for some fixed $\epsilon > 0$.

We recall that C_{leaf} is an upper bound for the number of indices in a leaf cluster; see Section 2.1. The proof of the lemma can be found in [12].

Assuming that the depth of the tree is $O(\log n)$ we obtain almost linear complexity $O(k_{\text{max}} n \log n)$. The difficulty with the Helmholtz problem is that k_{max} can be large. We shall give extensive numerical comparisons in the section on numerical results. Here we discuss the approximation of the matrix corresponding to a single admissible block.

Let $b = \tau \times \sigma$ be an admissible block. Let the clusters Ω_τ and Ω_σ have the same diameter r . We fix an accuracy $\epsilon = 10^{-5}$ and numerically investigate the rank of the approximation produced by ACA as κr is increased. We compare this with the optimal rank obtained by SVD. The results are displayed in Figure 1. As expected the increase in the necessary rank is linear with respect to the increase in $r\kappa$. This highlights the fact that \mathcal{H} -matrices cannot be used in the high frequency regime. Note also that the rank obtained by ACA is quite close to the optimal rank, even for large $r\kappa$. Hence for a low value of $\kappa \text{diam}(\Omega)$ the method is efficient.

3.1.2 Stability and recompression

One fact we would like to note here, is that the construction of \mathcal{H} -matrices using ACA and the subsequent matrix-vector multiplication are numerically stable regardless of accuracy or frequency. This is unlike most of the fast multipole implementations for the Helmholtz equation which become unstable at low frequencies. Depending on the multipole expansion, various techniques, like regularisation, have been applied to combat this instability; see [25]. The procedure described in this section is a simple way of producing an efficient almost linear and completely stable algorithm for the storage and arithmetics of Galerkin matrices for the low frequency problem. Note also that ACA is only one way of constructing the \mathcal{H} -matrix, arguably the simplest. Other possibilities include the already mentioned HCA and interpolation. Further algebraic compressions, which sometimes crucially decrease the computational times, can also be applied to the once constructed \mathcal{H} -matrix; see [11]. These recompressions can compensate for a poor selection of clusters and block cluster trees and also for the difference between the optimal SVD and the approximative ACA.

3.2 The high frequency regime: \mathcal{H}^2 -matrix

In this section we describe two ways of obtaining an \mathcal{H}^2 -matrix representation of the Galerkin matrix in almost linear time allowing for almost linear complexity for the matrix-vector multiplication.

3.2.1 Separable expansions

For the analysis in this section we will need a result due to Graf [24]. For ease of notation, for a vector $x \in \mathbb{R}^2$ we denote its polar coordinates by (ρ_x, θ_x) . In the following, $J_n(\cdot)$ denotes the Bessel function of the first kind of order n and $H_n(\cdot)$ the Hankel function of the first kind of order n .

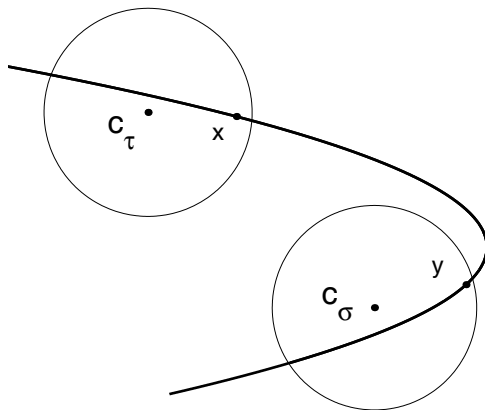
Theorem 3.1 *Let $x, y \in \mathbb{R}^2$ and let $z = x - y$. Then*

$$J_n(\rho_z)e^{\pm in(\theta_z - \theta_x)} = \sum_{m=-\infty}^{\infty} J_{n+m}(\rho_x)J_m(\rho_y)e^{\pm im(\theta_x - \theta_y)}.$$

If $\rho_x > \rho_y$, the following identity holds:

$$H_0(\rho_z) = \sum_{m=-\infty}^{\infty} H_m(\rho_x)J_m(\rho_y)e^{\pm im(\theta_x - \theta_y)}.$$

Let us now consider the situation depicted here:



We will use the following notation in this section:

$$\begin{aligned} x - c_\tau &= \rho_x^\tau (\cos \theta_x^\tau, \sin \theta_x^\tau) \\ y - c_\sigma &= \rho_y^\sigma (\cos \theta_y^\sigma, \sin \theta_y^\sigma) \\ c_\tau - c_\sigma &= \rho^{\tau \times \sigma} (\cos \theta^{\tau \times \sigma}, \sin \theta^{\tau \times \sigma}). \end{aligned} \quad (14)$$

Also let $z := (y - c_\sigma) - (x - c_\tau) \in \mathbb{R}^2$.

Point x is allowed to vary inside the cluster Ω_τ and y inside the cluster Ω_σ . We assume that the clusters are well-separated meaning that there exist $\rho_\tau, \rho_\sigma > 0$ and $0 < \eta < 1$ such that

$$\|x - c_\tau\| \leq \rho_\tau, \quad \|y - c_\sigma\| \leq \rho_\sigma, \quad \text{and} \quad \rho_\tau + \rho_\sigma \leq \eta \rho^{\tau \times \sigma}. \quad (15)$$

In this situation the following expansion is readily obtained from the result of Graf:

$$\begin{aligned} H_0(\kappa \|y - x\|) &= \sum_{m=-\infty}^{\infty} H_m(\kappa \rho^{\tau \times \sigma}) e^{im\theta^{\tau \times \sigma}} J_m(\kappa \rho_z) e^{-im\theta_u} \\ &= \sum_{m=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} \underbrace{J_{l+m}(\kappa \rho_x^\tau) e^{-i(l+m)\theta_x^\tau}}_{u_k(x, c_\tau)} \underbrace{H_m(\kappa \rho^{\tau \times \sigma}) e^{im\theta^{\tau \times \sigma}}}_{\tilde{s}_{k,l}(c_\tau, c_\sigma)} \underbrace{J_l(\kappa \rho_y^\sigma) e^{il\theta_y^\sigma}}_{v_l(y, c_\sigma)}. \end{aligned} \quad (16)$$

Truncating this expansion gives a way of constructing finite approximations necessary for the \mathcal{H}^2 -matrix format. To get an estimate of the error due to the truncation, we give bounds for the Bessel

and Hankel functions. It is helpful to recall that Bessel functions are Fourier coefficients of plane waves:

$$J_n(r) = \frac{1}{2\pi} \int_0^{2\pi} e^{ir \sin \theta} e^{-in\theta} d\theta, \quad n = 0, 1, \dots \quad (17)$$

Note also that $J_{-n} = (-1)^n J_n$. The relationship between Bessel functions and plane waves will be of crucial importance for all the results in this section. For this reason, we also give a bound for the error in the approximation of Bessel functions by a sum of plane waves.

Lemma 3.2 *Let $r_{\max}, r, \rho > 0$ and $n \in \mathbb{Z}$ be such that $r \leq r_{\max}$ and $\rho < |n|$. Then*

$$|J_n(r)| \leq e^{r_{\max} \sinh a - a|n|}, \quad \text{for any } a > 0, \quad (18a)$$

$$|H_n(\rho)| \leq \sqrt{2} + \frac{2}{\pi} e^{-\rho \sinh \delta + \delta(|n|+1)}, \quad \delta = \operatorname{arcosh}((|n|+1)/\rho). \quad (18b)$$

Also,

$$\left| J_n(r) - \frac{1}{K} \sum_{l=1}^K e^{ir \sin(\frac{2\pi l}{K})} e^{-\frac{2\pi i l n}{K}} \right| \leq 2 \frac{e^{r_{\max} \sinh a - (K-n)a}}{1 - e^{-K\sigma}}, \quad \text{for any } K \in \mathbb{N} \text{ and } a > 0. \quad (19)$$

Proof: Since $|J_n(r)| = |J_{-n}(r)|$ and $|H_n(\rho)| = |H_{-n}(\rho)|$, without loss of generality we can assume that $n \geq 0$.

For a fixed r , $c_n := J_n(r)$ is the n th Fourier coefficient of the complex analytic function $f(z) := e^{ir \sin z}$. For any $a > 0$, f is analytic in the horizontal strip $|\operatorname{Im} z| < a$ and hence $g(w) := f(\frac{1}{i} \log w)$ is analytic in the annulus $e^{-a} < |w| < e^a$. The Fourier coefficients of f are just the Laurent coefficients of g which can be bounded by Cauchy's estimate; see [18]. This gives the inequality

$$|c_n| \leq \max_{|\operatorname{Im} z| < a} |f(z)| e^{-an},$$

which in turn gives the inequality

$$|c_n| \leq e^{r \sinh a - an} \leq e^{r_{\max} \sinh a - an}, \quad \text{for any } a > 0.$$

This finishes the proof of (18a). Note that if $n > r_{\max}$, the bound $e^{r_{\max} \sinh a - an}$ reaches its minimum at $a = \operatorname{arcosh}(n/r_{\max})$.

To obtain the bound in (18b) we use the integral representation of $H_n(\cdot)$

$$H_n(\rho) = J_n(\rho) + \frac{i}{\pi} \int_0^\pi \sin(\rho \sin \theta - n\theta) d\theta - \frac{i}{\pi} \int_0^\infty (e^{nt} + (-1)^n e^{-nt}) e^{-\rho \sinh t} dt,$$

which can be found in [10]. From this, we immediately have the bound

$$|H_n(\rho)| \leq \sqrt{2} + \frac{2}{\pi} \int_0^\infty e^{nt - \rho \sinh t} dt.$$

Since $e^{(n+1)t - \rho \sinh t} < e^{(n+1)\delta - \rho \sinh \delta}$, for $\delta = \operatorname{arcosh}((n+1)/\rho)$ and any $t > 0$, we have that

$$\frac{2}{\pi} \int_0^\infty e^{nt - \rho \sinh t} dt \leq \frac{2}{\pi} \int_0^\infty e^{-t} dt e^{(n+1)\delta - \rho \sinh \delta} = \frac{2}{\pi} e^{(n+1)\delta - \rho \sinh \delta}.$$

With this the proof of the second inequality is finished.

The quantity that we want to bound in (19) is the remainder of the composite trapezoidal rule for 2π -periodic functions. The periodic integrand is $f_n(\theta) := \exp(ir \sin \theta) \exp(-in\theta)$. Since $f_n(\cdot)$ is an entire function, the remainder is bounded by the expression

$$2 \max_{|\operatorname{Im} z| < a} |f_n(z)| \frac{e^{-Ka}}{1 - e^{-Ka}}, \quad \text{for any } a > 0;$$

see [9]. The proof is finished by finding a bound for $f_n(\cdot)$:

$$\max_{|\operatorname{Im} z| < a} |f_n(z)| \leq e^{r_{\max} \sinh a + na}, \quad \text{for any } a > 0.$$

□

The bounds in the above lemma are close to optimal and can be effectively used to obtain the number of terms needed in the separable expansion for a particular accuracy $\epsilon > 0$. Instead, for simplicity, in the remaining results we give only the asymptotic dependence on the accuracy ϵ .

Lemma 3.3 *Let $r_{\max} > 0$ and $0 < \eta < 1$. There exists a constant $C(\eta)$ such that for any $\epsilon > 0$, $r, \rho \in \mathbb{R}^+$, and any $M \in \mathbb{N}$ with*

$$r \leq r_{\max} = \eta\rho, \quad M \geq C(\eta)(r_{\max} + \log \frac{1}{\epsilon}),$$

we have

$$\sum_{n=M}^{\infty} |J_n(r)| < \epsilon \quad \text{and} \quad \sum_{n=M}^{\infty} |H_n(\rho)J_n(r)| < \epsilon.$$

Also, for any $K \geq 2M$

$$\sum_{n=0}^M |H_n(\rho)| \left| J_n(r) - \frac{1}{K} \sum_{l=1}^K e^{ir \sin(\frac{2\pi l}{K})} e^{-\frac{2\pi i l n}{K}} \right| < \epsilon.$$

Proof: Let us first prove the second inequality above. From (18a) and (18b) it follows that

$$|H_n(\rho)J_n(r)| \leq \sqrt{2}|J_n(r)| + e^{r_{\max} \sinh a - an - \rho \sinh \delta + \delta(n+1)}, \quad \delta = \operatorname{arcosh}((n+1)/\rho), \quad \text{and any } a > 0.$$

With the choice $a = \delta' := \operatorname{arsinh}(\frac{\rho}{r_{\max}} \sinh \delta)$, the above expression becomes

$$|H_n(\rho)J_n(r)| \leq \sqrt{2}|J_n(r)| + e^{-n(\delta' - \delta) + \delta}.$$

Since $\rho > r_{\max}$ we have that $\delta' > \delta$ for all n . Writing out the definitions of δ' and δ , we see that $\delta' - \delta = \operatorname{arsinh}(\frac{\rho}{r_{\max}} \sinh(\operatorname{arcosh}(\frac{n+1}{\rho}))) - \operatorname{arcosh}(\frac{n+1}{\rho})$ is an increasing function of n for $n > \rho$. Let $C(\eta)$ be such that $C(\eta)\eta > 1$. Then $(n+1)/\rho > M/\rho \geq C(\eta)r_{\max}/\rho = C(\eta)\eta > 1$ and hence by defining $B(\eta) = \operatorname{arsinh}(\frac{1}{\eta} \sinh(\operatorname{arcosh}(C(\eta)\eta))) - \operatorname{arcosh}(C(\eta)\eta)$ and by applying once more the inequality (18a) we obtain that

$$|H_n(\rho)J_n(r)| = O(e^{-B(\eta)n + \delta}).$$

Note also that $e^\delta \leq e^{\operatorname{arcosh}(C(\eta)\eta)} \leq 2C(\eta)\eta$. Hence, by summing the geometric series, we obtain that

$$\sum_{n=M}^{\infty} |H_n(\rho)J_n(r)| = O\left(C(\eta)\eta \frac{e^{-B(\eta)M}}{1 - e^{-B(\eta)}}\right),$$

from which the result follows.

The rest of the proof is obtained in a similar manner by applying inequalities (18a) and (19). □

Next we give a result describing a separable expansion obtained by truncating (16).

Theorem 3.2 *Let (15) hold. Using notation (14), define vectors $u_{M_1} = u(x, c_\tau) \in \mathbb{C}^{K_1}$, $v_{M_2} = v(y, c_\sigma) \in \mathbb{C}^{K_2}$, and a matrix $S_{M_1, M_2} = S(c_\tau, c_\sigma) \in \mathbb{C}^{K_1 \times K_2}$, where $K_1 = 2M_1 + 1$ and $K_2 = 2M_2 + 1$ for some $M_1, M_2 \in \mathbb{N}$, by*

$$\begin{aligned} (u_{M_1})_j &= J_{j-M_1-1}(\kappa\rho_x^\tau) e^{i(j-M_1-1)\theta_x^\tau}, \quad j = 1, \dots, K_1, \\ (v_{M_2})_k &= J_{k-M_2-1}(\kappa\rho_y^\sigma) e^{-i(k-M_2-1)\theta_y^\sigma}, \quad k = 1, \dots, K_2, \end{aligned}$$

$$(S_{M_1, M_2})_{jk} = H_{k-j+M_1-M_2}(\kappa\rho_x) e^{i(k-j+M_1-M_2)\theta_x}, \quad j = 1, \dots, K_1 \quad \text{and} \quad k = 1, \dots, K_2.$$

There exists a constant $C(\eta) > 0$ such that for any $\epsilon > 0$, $\kappa > 0$, and $M_1 \geq C(\eta)(\kappa\rho_\tau + \log(\frac{1}{\epsilon}))$ and $M_2 \geq C(\eta)(\kappa\rho_\sigma + \log(\frac{1}{\epsilon}))$

$$|H_0(\kappa\|x - y\|) - u_{M_1}^T S_{M_1, M_2} v_{M_2}| < \epsilon(M_1 + M_2) |H_{M_1+M_2}(\kappa\rho^{\tau \times \sigma})|.$$

Proof: For the proof we will need three inequalities. From Lemma 3.3 it follows that there exists a constant $C_1(\eta) > 0$ such that if $M_1 \geq C_1(\eta)(\kappa\rho_\tau + \log(\frac{1}{\epsilon}))$ and $M_2 \geq C_1(\eta)(\kappa\rho_\sigma + \log(\frac{1}{\epsilon}))$ then

$$\sum_{|m| > M_1} |J_m(\kappa\rho_x^\tau)| < \epsilon/3 \quad \text{and} \quad \sum_{|m| > M_2} |J_m(\kappa\rho_y^\sigma)| < \epsilon/3.$$

Since $\rho_z = \|y - c_\sigma - x + c_\tau\| \leq \rho_\tau + \rho_\sigma < \rho^{\tau \times \sigma}$ we have that there exists a constant $C_2(\eta) > 0$ such that for $M > C_2(\eta)(\kappa(\rho_\tau + \rho_\sigma) + \log(\frac{1}{\epsilon}))$

$$\sum_{|m| > M} |H_m(\kappa\rho^{\tau \times \sigma}) J_m(\kappa\rho_z)| \leq \epsilon/3.$$

Define $C(\eta) := \max\{C_1(\eta), C_2(\eta)\}$. By truncating the expansion (16) we obtain the following expression for the remainder:

$$\begin{aligned} H_0(\kappa\|x - y\|) - u_{M_1}^T S_{M_1, M_2} v_{M_2} &= \sum_{|m| > M_1+M_2} H_m(\kappa\rho^{\tau \times \sigma}) e^{im\theta^{\tau \times \sigma}} J_m(\kappa\rho_z) e^{-im\theta_u} + \\ &\sum_{|m| \leq M_1+M_2} H_m(\kappa\rho^{\tau \times \sigma}) \sum_{|l+m| > M_1 \vee |l| > M_2} J_{l+m}(\kappa\rho_x^\tau) e^{-i(l+m)\theta_x^\tau} J_l(\kappa\rho_y^\sigma) e^{il\theta_y^\sigma}. \end{aligned}$$

Finally, the result follows from the fact that $H_m(x)$ is a strictly increasing function of m for fixed x . \square

The term $|H_{M_1+M_2}(\kappa\rho^{\tau \times \sigma})|$ can get exponentially large, but as we explain later in the paper, to avoid numerical instability, separable expansions will only be used when for the particular ϵ this term is bounded. Notice that the matrix S is Toeplitz and hence can be applied to a vector using FFT in almost linear time. Alternatively, we can re-write the expansion so that the matrix S is diagonal with the diagonal equal to the discrete Fourier transform of the vector obtained by combining the first row and the first column of the Toeplitz matrix. In this case the basis vectors become the discrete Fourier transforms of the original Bessel basis vectors.

The above result shows that a separable expansion for the fundamental solution $G_\kappa(\cdot) = H_0(\cdot)$ exists, with basis functions $u_l(p - c_\tau) = J_l(\kappa\|p - c_\tau\|) e^{il\theta_{p-c_\tau}}$ and $v_j(q - c_\sigma) = u_j(q - c_\sigma)$. The fact that the Bessel functions are Fourier transforms of plane waves, see (17), can be used to derive an alternative separable expansion, which has the advantage that the coefficient matrix is diagonal. The simple structure of the coefficient matrix is due to the following property of plane waves:

$$e^{i\rho_b \sin(\theta - \theta_b)} e^{i\rho_c \sin(\theta - \theta_c)} = e^{i\rho_{b+c} \sin(\theta - \theta_{b+c})}, \quad \text{for all } b, c \in \mathbb{R}^2. \quad (20)$$

This is a well known property of plane waves that was originally used to prove a special case of Graf's theorem; see [24].

Theorem 3.3 *Let (15) hold. Using notation (14), define vectors $u_M = u(x, c_\tau)$, $v_M = v(y, c_\sigma) \in \mathbb{C}^K$ and a diagonal matrix $S_M = S(c_\tau, c_\sigma) \in \mathbb{C}^{K \times K}$, where $K = 2M + 1$ for some $M \in \mathbb{N}$, by*

$$\begin{aligned} (u_M)_j &= e^{-i\kappa\rho_x^\tau \sin(2\pi j/K - \theta_x^\tau)}, \quad (v_M)_j = e^{i\kappa\rho_y^\sigma \sin(2\pi j/K - \theta_y^\sigma)}, \\ (S_M)_{jj} &= \frac{1}{K} \sum_{n=-M}^M H_n(\kappa\rho^{\tau \times \sigma}) e^{in(\theta^{\tau \times \sigma} - 2\pi j/K)}, \quad j = 1, \dots, K. \end{aligned}$$

There exists a constant $C(\eta) > 0$ such that for any $\epsilon > 0$, $\kappa > 0$ and $M \geq C(\eta)(\kappa(\rho_\tau + \rho_\sigma) + \log(\frac{1}{\epsilon}))$

$$|H_0(\kappa\|x - y\|) - u_M^T S_M v_M| < \epsilon.$$

Proof: The form of the separable expansion is obtained by first applying Theorem 3.1 which gives the expansion

$$H_0(\kappa\|x - y\|) = \sum_{m=-\infty}^{\infty} H_m(\kappa\rho^{\tau\times\sigma})e^{im\theta^{\tau\times\sigma}} J_m(\kappa\rho_z)e^{-im\theta_u}.$$

The next step is to truncate the above expansion and apply the trapezoidal rule to the Bessel functions and use the separability property (20) of plane waves. The proof is completed by noticing that Lemma 3.3 is directly applicable to the remainder of the truncation and of the quadrature. \square

The above form of the separable expansion is the most commonly used diagonal form in fast multipole methods. For a more detailed derivation see [6]. As for the diagonal expansion obtained from the Toeplitz one, the diagonal of S can be computed by a single application of FFT.

The great advantage of the second expansion is that the coefficient matrix is diagonal. However, the first expansion may be advantageous when the diameters of clusters τ and σ are considerably different, since in Theorem 3.2 we can choose $M_1 \propto \rho_\tau$ and $M_2 \propto \rho_\sigma$ whereas in Theorem 3.3 we have only one parameter M that has to be chosen proportionally to the sum $\rho_\tau + \rho_\sigma$. Both expansions are potentially numerically unstable since the coefficient matrix S is in neither case bounded. As is well known, this prevents the use of the diagonal expansion at low frequency, whereas it is possible to regularise the expansion in Bessel functions; see [25]. We will say more about stability later in the paper.

3.2.2 Construction of U_τ, V_σ

We now define the row cluster basis U_τ as before:

$$(\hat{U}_\tau)_{ki} = \begin{cases} \int_{\Omega_\tau} (u(x, c_\tau))_i \phi_k(x) dx, & \text{if } k \in \tau \text{ and } i = 1, \dots, K_\tau \\ 0, & \text{if } k \notin \tau, \end{cases}$$

where we have two choices for $u(x, c_\tau) \in \mathbb{C}^{K_\tau}$, either Bessel functions as given by Theorem 3.2 or plane waves as given by Theorem 3.3. In either case, the condition that the bases are nested (13) will not be satisfied. Hence, instead of defining these matrices for the non-leaf clusters in the same way, we first define the transform matrices $T_{\tau',\tau}^U$ for each child-parent pair τ', τ and then define

$$U_\tau := \hat{U}_\tau, \text{ if } \tau \text{ a leaf, otherwise } U_\tau := \begin{pmatrix} U_{\tau'} T_{\tau',\tau}^U \\ U_{\tau''} T_{\tau'',\tau}^U \end{pmatrix}, \quad (21)$$

where τ' and τ'' are the children of τ . The matrices V_σ are defined in a similar fashion. To simplify the notation slightly we will write $T_{\tau',\tau}$ to denote $T_{\tau',\tau}^U$ for the rest of this section. It is clear that the matrices $T_{\tau',\tau}$ and $T_{\tau'',\tau}$ should be defined so that the nestedness condition holds approximately

$$\hat{U}_\tau \approx \begin{pmatrix} \hat{U}_{\tau'} T_{\tau',\tau} \\ \hat{U}_{\tau''} T_{\tau'',\tau} \end{pmatrix}. \quad (22)$$

Since for an arbitrary vector $\zeta \in \mathbb{C}^{K_\tau}$

$$(\hat{U}_\tau \zeta)_k = \begin{cases} \int_{\Omega_{\tau'}} \phi_k(x) u(x, c_\tau)^\top \zeta dx, & k \in \tau', \\ \int_{\Omega_{\tau''}} \phi_k(x) u(x, c_\tau)^\top \zeta dx, & k \in \tau'', \end{cases}$$

and

$$\begin{pmatrix} \hat{U}_{\tau'} T_{\tau',\tau} \zeta \\ \hat{U}_{\tau''} T_{\tau'',\tau} \zeta \end{pmatrix}_k = \begin{cases} \int_{\Omega_{\tau'}} \phi_k(x) \left(T_{\tau',\tau}^\top u(x, c_{\tau'}) \right)^\top \zeta dx, & k \in \tau', \\ \int_{\Omega_{\tau''}} \phi_k(x) \left(T_{\tau'',\tau}^\top u(x, c_{\tau''}) \right)^\top \zeta dx, & k \in \tau'', \end{cases}$$

we can see that the condition (22) is satisfied if

$$u(x, c_\tau) \approx \begin{cases} T_{\tau',\tau}^\top u(x, c_{\tau'}), & x \in \Omega_{\tau'}. \\ T_{\tau'',\tau}^\top u(x, c_{\tau''}), & x \in \Omega_{\tau''}. \end{cases} \quad (23)$$

3.2.3 Construction of $T_{\tau',\tau}$

Let τ be a parent cluster with child τ' . We wish to construct the transform operator $T_{\tau',\tau}$ so that (23) is satisfied. Since we have two choices for the functions $u(x, c_\tau)$ we need also to construct two transfer operators. First of all we explain how to transform one basis to the other.

Proposition 3.1 *Let $u_1, u_2 \in \mathbb{C}^K$ where $K = 2M + 1$ for some $M \in \mathbb{N}$. If u_1 and u_2 are defined by*

$$(u_1)_j = J_{j-M-1}(\rho_x) e^{i(j-M-1)\theta_x} \text{ and } (u_2)_l = e^{-i\rho_x \sin(2\pi l/K - \theta_x)}, \quad j, l = 1, \dots, K,$$

then

$$u_1 = F_M u_2 + r_M,$$

where $F_M \in \mathbb{C}^{K \times K}$ is a shifted Fourier matrix defined by

$$(F_M)_{jl} = e^{2\pi i l(j-M-1)/K},$$

and there exists a constant $C > 0$ such that for any $\epsilon > 0$ and all $M > C(\rho_x + \log(\frac{1}{\epsilon}))$ we have

$$\|r_M\|_\infty \leq \epsilon.$$

Proof: We proceed as follows:

$$\begin{aligned} J_j(\rho_x) e^{ij\theta_x} &= \frac{1}{2\pi} \int_0^{2\pi} e^{i\rho_x \sin \theta} e^{ij(\theta_x - \theta)} d\theta \\ &= \frac{1}{2\pi} \int_0^{2\pi} e^{-i\rho_x \sin(\theta - \theta_x)} e^{ij\theta} d\theta \\ &= \frac{1}{K} \sum_{l=1}^K e^{-i\rho_x \sin(2\pi l/K - \theta_x)} e^{-2i\pi l j/K} + (r_M)_j, \end{aligned}$$

where $(r_M)_j$ is the remainder of the composite trapezoidal rule for 2π -periodic functions. The rest of the proof goes along the lines of the proofs of Lemma 3.2 and Lemma 3.3. \square

Note that F_M and F_M^{-1} can be applied to a vector using FFT in $O(K \log K)$ time.

The transform operator we wish to construct consists of a translation of the centre of expansion and of interpolation used to change the length of the basis vector. From the fact (20) it is not difficult to see that the translation is simple for the plane wave functions: As in Theorem 3.3, define two basis vectors $u_1 := u(x, c_\tau)$ and $u_2 := u(x, c_{\tau'}) \in \mathbb{C}^K$, $k = 2M + 1$, which have identical lengths K but different centres c_τ and $c_{\tau'}$. So

$$(u_1)_j = e^{-i\kappa \rho_x^\tau \sin(2\pi j/K - \theta_x^\tau)} \text{ and } (u_2)_j = e^{-i\kappa \rho_x^{\tau'} \sin(2\pi j/K - \theta_x^{\tau'})}, \quad j = 1, \dots, K.$$

From (20) we see that $u_1 = D u_2$ for a diagonal matrix D with

$$D_{jj} = e^{i\kappa \|c_\tau - c_{\tau'}\| \sin(2\pi j/K - \theta_{c_\tau - c_{\tau'}})}.$$

For the Bessel functions, the change of the centre is not as simple but the interpolation is trivial. It consists simply of truncation or padding by zeros of the basis vectors. Note that this procedure introduces no additional error.

Combining the change of the centre of the plane waves and the interpolation of the Bessel functions with Proposition 3.1 allows us to easily construct the transform operator for both types of basis functions. The details are given in the next theorem.

Theorem 3.4 *Let $u_1 \in \mathbb{C}^{K_1}$ and $u_2 \in \mathbb{C}^{K_2}$ where $K_1 = 2M_1 + 1$ and $K_2 = 2M_2 + 1$ for some $M_1, M_2 \in \mathbb{N}$. If u_1 and u_2 are defined by*

$$(u_1)_j = e^{-i\kappa \rho_x^\tau \sin(2\pi j/K_1 - \theta_x^\tau)} \text{ and } (u_2)_l = e^{-i\kappa \rho_x^{\tau'} \sin(2\pi l/K_2 - \theta_x^{\tau'})},$$

for $j = 1, \dots, K_1$ and $l = 1, \dots, K_2$ then

$$u_1 = DF_{M_1}^{-1} P_{M_1, M_2} F_{M_2} u_2 + r_{M_1, M_2},$$

where F_{M_1}, F_{M_2} are shifted Fourier matrices as in Proposition 3.1, $D \in \mathbb{C}^{K_1 \times K_1}$ is a diagonal matrix with

$$D_{ll} = e^{i\kappa \|c_\tau - c_{\tau'}\| \sin(2\pi l / K_1 - \theta_{c_\tau - c_{\tau'}})},$$

and P_{M_1, M_2} is an $K_1 \times K_2$ sparse matrix of zeros and ones, which is described by its action on a vector ¹:

$$P_{M_1, M_2} v = \begin{cases} (0, \dots, 0, (v)_1, (v)_2, \dots, (v)_{K_1}, 0, \dots, 0)^T, & \text{if } K_2 > K_1 \\ ((v)_{M_1 - M_2 + 1}, (v)_{M_1 - M_2 + 2}, \dots, (v)_{M_1 + M_2 + 1})^T, & \text{otherwise.} \end{cases}$$

There exists a constant $C > 0$ such that for any $\epsilon > 0$, $M_1 > C(\rho_\tau + \log(\frac{1}{\epsilon}))$, and any $M_2 > C(\rho_\sigma + \log(\frac{1}{\epsilon}))$

$$\|r_{M_1, M_2}\|_\infty < \epsilon.$$

From this result it is clear that we can define the transform operator for plane waves as

$$T_{\tau', \tau}^U := DF_{M_1}^{-1} P_{M_1, M_2} F_{M_2}. \quad (24)$$

From Proposition 3.1, it follows that the transform operator for Bessel functions should be defined as

$$T_{\tau', \tau}^U := F_{M_1} DF_{M_1}^{-1} P_{M_1, M_2}. \quad (25)$$

Since in both cases $V_\sigma = \overline{U_\sigma}$, we have that

$$T_{\sigma', \sigma}^V = \overline{T_{\sigma', \sigma}^U}.$$

Note that it is possible to construct the transform operators in linear time and to apply them to a vector in log-linear time using FFT.

3.2.4 Construction of $S_{\tau, \sigma}$

We consider two cases. In the first case we assume that for each $\tau \times \sigma \in \mathcal{L}^+$ we have $\text{diam}(\Omega_\tau) \approx \text{diam}(\Omega_\sigma)$. For this case we choose to define the row and cluster bases using plane waves. Then we define $S_{\tau, \sigma} := S(c_\tau, c_\sigma) \in \mathbb{C}^{K \times K}$ given by Theorem 3.3. This would be the standard approach in fast multipole methods for the Helmholtz equation.

In the second case we allow for clusters of different sizes. For this case we define the row and cluster bases using Bessel functions. We could now simply define $S_{\tau, \sigma}$ using Theorem 3.2, however, we choose to use the diagonal expansion again. In this case row and cluster bases need to be transformed to plane waves from Bessel functions. Hence, we define the coefficient matrix by

$$S_{\tau, \sigma} := P_{K_\tau, K} F_K S(c_\tau, c_\sigma) F_K^{-1} P_{K, K_\sigma}.$$

This allows us to choose K_τ , K_σ and K independently from each other and as small as possible. We could equally have chosen plane waves as the basis functions, but then the prolongation from K_τ to K would consist of two applications of FFT rather than one, and the same for the restriction from K to K_σ . We should note here that it is possible to perform the prolongation and restriction of plane wave basis in $O(K)$ time by nearest-neighbour approximation; see [19]. It is, however, not clear for how large a value of K is this profitable.

¹ P_{M_1, M_2} simply appends zeros to the beginning and the end of a vector if $M_2 > M_1$, otherwise it truncates entries from the front and the end of the vector.

3.3 Complexity analysis

We now have all the ingredients necessary for the construction of the \mathcal{H}^2 -matrix representation. We construct the \mathcal{H}^2 -matrix approximation by the following procedure:

- Choose $\epsilon > 0$.
- Construct the cluster tree $T_{\mathcal{I}}$ and the block cluster tree $T_{\mathcal{I} \times \mathcal{I}}$.
- For each cluster $\tau \in T_{\mathcal{I}}$ and some constant $C_1 > 0$ set $K_\tau = \lfloor C_1 \kappa \text{diam}(\Omega_\tau) + C_1 \log \frac{1}{\epsilon} \rfloor$. If τ is a leaf, construct the row and cluster bases U_τ and V_τ .
- For each parent cluster τ construct $T_{\tau, \tau'}$ and $T_{\tau, \tau''}$ using (24) or (25).
- For each admissible leaf $b = \tau \times \sigma \in \mathcal{L}^+$ construct the coefficient matrix $S_{\tau, \sigma} \in \mathbb{C}^{K \times K}$ using Theorem 3.3, where $K = K_\tau + K_\sigma$.
- For each inadmissible leaf $b = \tau \times \sigma \in \mathcal{L}^-$ set $M_{\tau, \sigma} := A_{\tau, \sigma}$.

Before we estimate the computational complexity of the construction of the matrix and the cost of matrix-vector multiplication we make a couple of assumptions that hold in standard situations. The first assumption is as before that C_{sp} is a constant. The second assumption, pertinent to the two dimensional problem, is that there exists a constant C_2 , such that for any level l

$$\sum_{\tau \in T_{\mathcal{I}}^{(l)}} \text{diam}(\Omega_\tau) \leq C_2. \quad (26)$$

This condition simply prevents pathological cases, such as the case where each child cluster has the same diameter as its parent cluster. A standard algorithm for the construction of the cluster tree, as described in [12], would prevent such a case from happening. In the best case, when the diameter of each child cluster is exactly half the diameter of its parent, (26) holds for $C_2 = \text{diam}(\Omega)$. The condition is useful since it gives the following inequality:

$$\sum_{\tau \in T_{\mathcal{I}}^{(l)}} K_\tau \leq C_1 (C_2 \kappa + \#T_{\mathcal{I}}^{(l)}).$$

Also, recall that there are at most $2n - 1$ clusters in the cluster tree $T_{\mathcal{I}}$. Hence for any level L ,

$$\sum_{l=0}^L \#T_{\mathcal{I}}^{(l)} \leq 2n - 1.$$

Now we are in a position to give estimates for the storage and the cost of construction and matrix-vector multiplication.

Lemma 3.4 (Storage) *If p is the depth of $T_{\mathcal{I} \times \mathcal{I}}$ and (26) holds, then there exists a constant C depending only on C_1 , C_2 , and C_{sp} such that*

$$N_{\text{st}} \leq C(p\kappa + n) \quad \text{and} \quad N_{\text{con}} \leq C(p\kappa \log \kappa + n \log \kappa),$$

where N_{st} is the storage requirement and N_{con} the cost of the construction of the \mathcal{H}^2 -matrix.

Proof: The cost of storing and constructing the row and column cluster bases for the leaf clusters is the same. It can be estimated as follows:

$$\begin{aligned} \sum_{\tau \in T_{\mathcal{I}}^{(p)}} \# \tau K_\tau &\leq C_{\text{leaf}} \sum_{\tau \in T_{\mathcal{I}}^{(p)}} K_\tau \\ &\leq C_{\text{leaf}} C_1 (C_2 \kappa + \#T_{\mathcal{I}}^{(p)}) \\ &\leq C_{\text{leaf}} C_1 (C_2 \kappa + n). \end{aligned}$$

The cost of storing the coefficient matrices is equal to

$$\begin{aligned}
\sum_{b=\tau \times \sigma \in \mathcal{L}^+} (K_\tau + K_\sigma) &= \sum_{l=0}^p \sum_{\tau \in T_{\mathcal{I}}^{(l)}} K_\tau \#\{\sigma : \tau \times \sigma \in \mathcal{L}^+ \text{ or } \sigma \times \tau \in \mathcal{L}^+\} \\
&\leq C_{\text{sp}} \sum_{l=0}^p \sum_{\tau \in T_{\mathcal{I}}^{(l)}} K_\tau \\
&\leq C_{\text{sp}} C_1 \sum_{l=0}^p (C_2 \kappa + \#T_{\mathcal{I}}^{(l)}) \\
&\leq C_{\text{sp}} C_1 (C_2 \kappa (p+1) + 2n - 1).
\end{aligned}$$

Since for each coefficient matrix we require a single application of FFT, the cost of the construction is larger than the storage cost by a logarithmic factor:

$$C_{\text{sp}} C_1 (C_2 \kappa (p+1) + 2n - 1) \log(\kappa + 1).$$

The cost of the construction and of the storage of transfer matrices is the same and bounded by

$$\sum_{l=0}^{p-1} \sum_{\tau \in T_{\mathcal{I}}^{(l)}} 2K_\tau \leq 2C_1 (C_2 \kappa (p+1) + 2n - 1).$$

Finally, as for \mathcal{H} -matrices, the cost of constructing and storing the matrices corresponding to the inadmissible blocks is $O(n)$. This gives the final result. \square

Lemma 3.5 (Multiplication) *Under the same conditions as in the previous lemma there exists a constant C such that*

$$N_{\mathcal{H} \cdot v} \leq CN_{\text{con}},$$

where $N_{\mathcal{H} \cdot v}$ is the cost of matrix-vector multiplication.

Proof: We compute the cost of matrix-vector multiplication following the steps of the fast algorithm explained in Section 2.6.2. The reasoning is the same as in the proof of the previous lemma.

1. Upward pass.

- (a) The cost of applying the cluster bases to a vector for the leaves is the same as the cost of constructing them. Hence by the proof of Lemma 3.4 the total cost for all leaf clusters is $O(\kappa + n)$.
- (b) The cost of applying the transform matrices to a vector is larger than the cost of constructing them since applications of FFT are necessary. The further logarithmic factor gives the complexity $O(p\kappa \log \kappa + n \log \kappa)$.

2. Far field interaction

- (a) The cost of multiplication is the same as the cost of constructing the coefficient matrices since in both cases FFT is used. Hence the cost is $O(p\kappa \log \kappa + n \log \kappa)$.

3. Downward pass

- (a) Same cost as in 1b.

4. Near field interaction

- (a) Since A^\diamond is sparse, the cost is $O(n)$.

Combining the above estimates gives the result. \square

Since we are interested in the high frequency regime, i.e., $\kappa \propto n$, assuming $p = O(\log n)$ we have that the cost of storage is $O(n \log n)$ and the cost of construction and matrix-vector multiplication is $O(n \log^2 n)$. However, in practical situations κ is considerably smaller than n so that we expect the costs to behave closer to $O(n)$ and $O(n \log n)$ for the storage and matrix-vector complexity respectively.

At this stage we could proceed to the numerical results, however for the sake of better efficiency and numerical stability a closer look needs to be taken at the expansions used in the derivation.

3.4 High and low frequency problems; stability: \mathcal{H} - and \mathcal{H}^2 -matrices

An important deficiency of the presented separable expansions is their numerical instability. In both cases the coefficient matrices $S_{\tau,\sigma}$ cannot be bounded. This is due to the fact that $H_l(\rho)$ diverges to infinity very quickly when $l > \rho$. The expansion in Bessel functions can be regularised by scaling. This is used in [25], however the authors sacrifice the Toeplitz structure for stability. It is possible to preserve the structure and stabilise by scaling, this, however, forces us to use a sum of three \mathcal{H}^2 -matrices instead of a single one which is too great a sacrifice in terms of computational time. Here we propose a much simpler remedy which is easy to implement and has been shown to be effective.

The instability problems of the expansions used in this paper have attracted a lot of attention over the years. We will use one observation only, and that is that for a fixed $\epsilon > 0$ there exists a constant $C(\epsilon, \eta)$ such that $\|S_{\tau,\sigma}\|_\infty$ is bounded for admissible blocks $b = \tau \times \sigma$ for which $\kappa \min\{\text{diam}(\Omega_\tau), \text{diam}(\Omega_\sigma)\} \geq C(\epsilon, \eta)$; see [21]. Accordingly, we divide the set of admissible leaves \mathcal{L}^+ into two disjoint subsets \mathcal{L}_1^+ and \mathcal{L}_2^+ :

$$\mathcal{L}_1^+ := \{\tau \times \sigma \in \mathcal{L}^+ : \kappa \min\{\text{diam}(\Omega_\tau), \text{diam}(\Omega_\sigma)\} \geq C(\epsilon, \eta)\} \text{ and } \mathcal{L}_2^+ := \mathcal{L}^+ / \mathcal{L}_1^+.$$

After choosing the precision and constructing the cluster and block cluster trees, we construct an approximation to the Galerkin matrix by the following procedure:

- For each leaf τ construct the row and cluster bases U_τ and V_τ .
- For each parent cluster τ construct $T_{\tau,\tau'}$ and $T_{\tau,\tau''}$.
- For each $b = \tau \times \sigma \in \mathcal{L}_1^+$ construct the coefficient matrix $S_{\tau,\sigma}$.
- For each $b = \tau \times \sigma \in \mathcal{L}_2^+$ construct a low rank approximation $M_{\tau,\sigma}$ to $A_{\tau,\sigma}$ using ACA.
- For each inadmissible leaf $b = \tau \times \sigma \in \mathcal{L}^-$ set $M_{\tau,\sigma} := A_{\tau,\sigma}$.

Using the complexity estimates developed for the pure \mathcal{H} -matrix and pure \mathcal{H}^2 -matrix formats it is not difficult to see that the complexity proved in the previous section is preserved since the low rank matrices are used only in the domains with size of a bounded number of wavelengths. Separable expansions are used only in domains that are large enough so that the numerical instability is not visible.

With this we have finished our description of an $O(n \log^2 n)$ algorithm. In the next section we give numerical results illustrating the practicability of our method.

4 Numerical results

In this section we demonstrate how our algorithm behaves in practice through numerical examples. We do this by considering the simple example of the discretisation of the single layer potential on an ellipse using a Galerkin method with piecewise constant basis functions. Since eventually we

n	Setup (s)	MV mult. (s)	Mem. (MB)	Mem/ n (kB)
1024	3.6	0.003	4	4.2
2048	7.7	0.006	9	4.6
4096	17.4	0.013	19	4.9
8192	37.3	0.028	41	5.2
16384	81.8	0.062	88	5.7
32768	169.2	0.127	189	6.1
65536	363.1	0.27	398	6.4
131072	785.4	0.545	839	6.7
262144	1735.8	1.44	1762	7.1

Table 1: CPU times and memory consumption in the low frequency regime with $\kappa = 64$.

plan to discretise operators for which the symmetry is lost, we do not make use of the fact that the resulting matrix is symmetric. The ellipse is given by the equation $x^2 + (y/2)^2 = 2^2$. The computations are done on a 3 GHz Intel PC. In all computations the error is controlled so that $\|A - \tilde{A}\|_\infty < 10^{-5}$. This is checked exactly only for matrices of size less than $2^{15} = 32768$. For larger matrices the error is estimated by comparing 100 randomly chosen columns of A and \tilde{A} .

4.1 The low frequency regime

For the low frequency regime we fix $\kappa = 64$ and increase the number of panels n . To approximate the Galerkin matrix we use the \mathcal{H} -matrix obtained by ACA as described in section 3.1. The results are shown in Table 1. As expected both the computational times and memory consumption scale close to linearly. The matrix-vector multiplication is very fast even for a quarter of a million degrees of freedom.

4.2 High frequency regime

For the high frequency regime we increase both n and κ , keeping $n/\kappa = \text{const}$. We apply the mixed format of an \mathcal{H}^2 -matrix with low-rank matrices obtained by ACA as described in section 3.2; the results are shown in Table 2. We allow for clusters of different sizes to be admissible hence we use the variant with Bessel basis functions. As predicted, we see that the storage increases as $O(n)$ and the matrix-vector multiplication as $O(n \log n)$.

For interest, we also apply the method designed for the low frequency regime. Namely, we approximate the Galerkin matrix by a pure \mathcal{H} -matrix obtained using ACA; the results are shown in Table 3. We see that up to $\kappa = 128$ the results are the same for the two methods; this is because for κ of that size no admissible block is of sufficient size to allow for a stable separable expansion. This also explains the sudden jump in the time needed for one matrix-vector multiplication when going from $n = 4096$ to $n = 8192$. For $n > 2^{16} = 65536$ the \mathcal{H} -matrix approach consumes too much memory hence the blank entries in Table 3. Nevertheless, it is an interesting observation that for all other cases the matrix-vector multiplication is considerably faster using the \mathcal{H} -matrix approach, the difference becoming smaller for larger n . The advantage of the \mathcal{H}^2 -matrix approach can be seen in the much lower setup time and memory consumption. Which method is preferable for a particular choice of n and κ depends not only on available memory but also on the convergence of the iterative method that is eventually used for the solution of the linear systems arising from the discretisation.

n	κ	Setup (s)	MV mult. (s)	Mem. (MB)	Mem/ n (kB)
1024	32	3.11	0.003	3	3.8
2048	64	7.66	0.006	9	4.6
4096	128	18.79	0.014	21	5.5
8192	256	42.08	0.166	57	7.4
16384	512	73.53	0.434	99	6.4
32768	1024	148.7	0.878	200	6.4
65536	2048	301.3	2.02	402	6.4
131072	4096	629.7	4.37	806	6.5
262144	8192	1305	9.84	1607	6.4

Table 2: CPU times and memory consumption in the high frequency regime for approximation with an \mathcal{H}^2 -matrix stabilised by low-rank matrices.

n	κ	Setup (s)	MV mult. (s)	Mem. (MB)	Mem/ n (kB)
1024	32	3.11	0.003	3	3.8
2048	64	7.66	0.006	9	4.6
4096	128	18.79	0.014	21	5.5
8192	256	45.86	0.034	53	6.8
16384	512	122.8	0.086	139	8.9
32768	1024	324.7	0.228	385	12.3
65536	2048	939.4	0.664	1141	18.3
131072	4096	–	–	–	–
262144	8192	–	–	–	–

Table 3: CPU times and memory consumption in the high frequency regime for approximation with an \mathcal{H} -matrix.

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