Massively Parallelized Interpolated Factored Green Function Method

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Abstract

This paper presents the first parallel implementation of the novel “Interpolated Factored Green Function” (IFGF) method introduced recently for the accelerated evaluation of discrete integral operators arising in wave scattering and other areas (Bauinger and Bruno, Jour. Computat. Phys., 2021). On the basis of the hierarchical IFGF interpolation strategy, the proposed (hybrid MPI-OpenMP) parallel implementation results in highly efficient data communication, and it exhibits in practice excellent parallel scaling up to large numbers of cores—without any hard limitations on the number of cores concurrently employed with high efficiency. Moreover, on any given number of cores, the proposed parallel approach preserves the $O(N \log N)$ computing cost inherent in the sequential version of the IFGF algorithm. Unlike other approaches, the IFGF method does not utilize the Fast Fourier Transform (FFT), and it is thus better suited than other methods for efficient parallelization in distributed-memory computer systems. In particular, the IFGF method relies on a “peer-to-peer” strategy wherein, at every level, field propagation is directly enacted via “exchanges” between “peer” polynomials of low and constant degree, without data accumulation in large-scale “telephone-central” mathematical constructs such as those in the Fast Multipole Method (FMM) or pure FFT-based approaches. A variety of numerical results presented in this paper illustrate the character of the proposed parallel algorithm, including excellent weak and strong parallel scaling properties in all cases considered—for problems of up to 4,096 wavelengths in acoustic size, and scaling tests spanning from 1 compute core to all 1,680 cores available in the High Performance Computing cluster used.

Keywords: Parallelization, Green Function, Integral Equations, Acceleration, OpenMP, MPI, Distributed Memory Systems, High Performance Computing

1 Introduction

This paper presents a parallel implementation of the “Interpolated Factored Green Function” (IFGF) method introduced recently for the accelerated evaluation of discrete integral operators arising in wave scattering and other areas [1]. The proposed implementation, which is structured as a hybrid MPI-OpenMP computer program suitable for instantiation in modern high-performance computing systems (HPC), demonstrates in practice excellent parallel scaling up to large numbers of cores, without any hard limitations on the number of cores concurrently employed with high efficiency, while preserving the linearithmic complexity (namely, $O(N \log N)$ computing cost) inherent in the sequential IFGF algorithm. The IFGF method accelerates the evaluation of discrete integral operators by relying on a certain factorization of the Green function into two factors, a “centered factor” that is incorporated easily as a common factor in the calculation, and an “analytic factor” which enjoys a property of analyticity up to and including infinity—and which thus motivates the IFGF strategy, namely, evaluation of a given discrete integral operator by means of a hierarchical interpolation approach which relies on use of a large

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number of small and independent interpolation procedures. In particular, the IFGF method does not utilize acceleration elements commonly used by other acceleration methods [2–14] such as the Fast Fourier Transform (FFT), special-function expansions, high-dimensional linear-algebra factorizations, translation operators, equivalent sources, or parabolic scaling; detailed discussions in this regard can be found in [1], below in this section, and indeed, at many points throughout this paper. Roughly speaking, the IFGF method relies on a “peer-to-peer” strategy wherein, at every level, field propagation is directly enacted via “exchanges” between “peer” polynomials of low and constant degree, without data accumulation in large-scale “telephone-central” mathematical constructs which require a “downward pass” through the box octree inherent in the Fast Multipole Method (FMM) [7], or the surface evaluation of equivalent sources in direct FFT-based methods [10]. A variety of numerical results presented in this paper illustrate the character of the proposed parallel method, including excellent weak and strong parallel scaling properties in all cases considered—for problems of up to 4,096 wavelengths in electrical size, and scaling tests spanning from 1 compute core to all 1,680 cores available in the HPC cluster used.

The parallelization of accelerated Green function methods has been the subject of a significant literature, which is mostly devoted to tackling a particular difficulty, namely, the “parallelization bottleneck”—which manifests itself under various related guises [15–23], and which almost invariably concerns uses of the hard-to-parallelize [24] FFT algorithm. (Reference [25, Sec. 7], for example, mentions two alternatives to the use of FFTs in the context of the FMM, which, however, it discards as less efficient than an FFT-based procedure.) In the case of the multilevel Fast Multipole Method (FMM), the parallelization bottleneck arises in the evaluation of translation operators associated with the upper part of the octree structure, which leads to low parallel efficiency [2, 15, 20]. In the “directional” FMM [15] the low efficiency in the upper octree is alleviated as a result of the parabolic scaling utilized; however, the parallelization strategy does suffer from hard limitations in the number of parallel tasks that, in the cases considered in that reference, lead to a “leveling off” of the parallel scaling at 256 or 512 cores [15, Secs. 3.6, 4.2], depending on the geometry under consideration. Reference [16] identifies the part of the FMM relying on FFTs as a parallelization bottleneck which arises from FFT-related “lowest arithmetic intensity” and “bandwidth contention”. In [17,18], in turn, a hybrid octree storage strategy is used, which stores a complete set of tree nodes for a certain number of “full” levels in each process, and which reduces the communication in the upper octree levels. Those articles demonstrate the treatment of problems containing very large numbers of discretization points on up to 2,560 processes, but they restrict their illustration of the algorithm’s parallel efficiency to a limited strong scaling test from 1 process (sequential) to 64 processes. In contrast to this hybrid octree-storage strategy, reference [19] simultaneously partitions boxes (clusters) and field values representing the radiating and incoming fields of each box. This approach leads to increased efficiency compared to a parallelization purely based on the boxes (clusters), but the communication in the translation step still poses a bottleneck, resulting in as little as 30% parallel efficiency from one (sequential) core to 128 cores.

Reference [26], in turn, presents scaling results for the parallel BEMFMM implementation of the FMM algorithm, for wave scattering problems on up to 196,608 cores on 6,144 compute nodes, and for problems with up to 2.3 billion degrees of freedom (DOF) and approximately 1,389 wavelengths in size (or, in the nomenclature of Table 2 in [26], a sphere two-meters in diameter illuminated at the frequency of \( f = 238.086 \) KHz, under the assumption of a 343m/s speed of sound). Like the implementations mentioned above, the results in [26] indicate a deterioration of the strong-scaling for growing numbers of cores, as manifested by a flattening of the strong-scaling speedup curves presented as the numbers of cores increase. The weak scaling curve presented in [26] indicate a high weak-scaling efficiency, however, with up to 95% efficiency for weak scaling between 32 and 131,072 cores. Comparison with BEMFMM and IFGF weak scaling results presents some challenges on a number of counts. On one hand the contribution [26] does not mention a crucial element in judging parallelization quality, namely, memory usage: even though memory duplication may be relied upon in a parallel algorithm to maximize parallel efficiency, no indications are provided in that paper about the amount of memory used in any of the runs presented. Further, under closer examination,
the computing times indicated in these curves appeared to be high, and we thus decided to perform a direct comparison of the performance of our IFGF implementation with the BEMFMM implementation on the basis of the freely available BEMFMM open-source download provided by the authors. By necessity, our tests were limited to a test example consisting of a sphere containing approximately 360,000 DOF, which is the largest test case provided with the BEMFMM test code, and we selected a sphere of acoustic diameter of $16\lambda$ for this experiment. We run both algorithms in the 30 available nodes in our cluster, Wavefield, each one of which contains 56 computing cores. Our observations are as follows. The BEMFMM run for the test case considered required 20 secs. in a single node, and 5 secs. in all 30 nodes, with a speedup factor of 4 going from 1 to thirty nodes. The IFGF run, in turn, required 1.6 secs. in a single node, and 0.122 secs in the thirty node cluster, with a speedup factor of 13 going from 1 to 30 nodes. Thus, the IFGF runs in one and 30 nodes were faster than the BEMFMM runs by factors of 12.5 and 40 in the 1-node and 30-node runs, respectively, with an IFGF speedup over three times higher than that provided by BEMFMM going from 1 to 30 nodes. As an additional point of contact with reference [26], it is worth mentioning that, in our 1,680 core cluster, and on the basis of approximately 4 TB of memory, a sphere $1,389\lambda$ in diameter (reported as $f = 238.086$KHz at a speed of sound of $343m/s$ in [26]; cf. Section SM2.7 for details) with 2.12 billion DOF was run in a computing time of 2,380 seconds (Table SM5 in Section SM2.7), which, with a 0.5% near-field error (which may be compared to the only error indicator reported in [26, Table 2] for this test case, which amounts to 20%, as well as the 3% near-field solution error reported in the same table of that paper for significantly smaller problems), is a factor of approximately 46 times longer than the time reported in [26], for the same number of DOFs and sphere size, on a computer 78 times larger (containing 131,072 cores) and on the basis of an unspecified amount of memory. Additional test cases for large sphere problems are presented in Section SM2.7.

Following a different approach, to avoid the communication bottleneck in the upper multilevel FMM octree entirely, references [20, 21] utilize a single-level Fast Multipole strategy. While this method significantly simplifies the algorithm and minimizes the required communication in a parallel setting, it does give rise to a sub-optimal asymptotic computational cost (e.g. $O(N^{3/2})$ in [21] or, exploiting the FFT, $O(N^{4/3}\log^{2/3}N)$ in [20]), and, while resulting in good parallel scaling up to 512 processes in the $O(N^{3/2})$ algorithm [21], as in the case of [15], the parallel efficiency does level off beyond 512 processes. Direct FFT methods, in turn, present alternatives to the various FMM strategies, including, for example, the Adaptive Integral Method [11] (AIM) and the sparse-FFT method [10]. Like the single-level FMM algorithms, these FFT methods exhibit sub-optimal algorithmic complexity (of orders $O(N^{3/2})$ and $O(N^{4/3})$, respectively, and, owing to their strong reliance on FFTs, they also suffer from reduced parallel efficiency, as shown and discussed for the AIM in e.g. [22, 23]. (A parallel version of the algorithm [10], which has been developed by the authors, has not been published, but we report here that, as may have been expected, the overall parallel efficiency of the method suffers from the typical FFT-related degradation.)

Finally we mention parallel methods proposed for non-singular [27] and low-frequency [28, 29] problems which, albeit important and interesting, do not incur some of the main challenges associated with the singular and high-frequency kernels considered in this paper. Thus, although not applicable to singular Green function kernels such as the ones considered here, the Butterfly Method [27] does provide an acceleration technique for Fourier integral operators which, based on linear-algebra constructs instead of the hierarchical interpolation underlying the IFGF approach, incorporates a parallelization strategy that is somewhat reminiscent of the proposed IFGF parallelization approach. The Blue Gene/Q implementation [27] of the Butterfly parallel algorithm demonstrates excellent results in terms of parallel scaling to a large number of cores. The parallel FMM method presented in [29], which is restricted to box geometries and to the Laplace and low-frequency Helmholtz problems, shows impressive scaling up to 299,008 cores on 18,688 nodes. Similarly, the parallel Barnes-Hut tree code [28] for the low-frequency singular problem provides excellent scaling up to 294,912 cores with up to 2,048,000,000 particles.

The parallel IFGF strategy introduced in this contribution is based on adequate partitioning of the interpolations performed on each level of the underlying octree structure, which facilitates the spatial
decomposition of the surface discretization points. As shown in [1], the number of interpolations performed on each level is large and approximately constant (as a function of the octree level). The decomposition and distribution of the interpolation data is based on a total order in the set of spherical cone segments representing the interpolation domains, which is an extension of a domain decomposition based on a Morton curve to the box-cone data structure inherent in the IFGF approach. The usage of space-filling curves for the representation of octree structures underlying the various acceleration methods is not a novel concept [26,29,30]. However, the extension of space-filling curves to the present box-cone structure of the IFGF method to achieve the desired efficiency has not been reported before. In view of its strong reliance on the IFGF’s box-cone structure, the proposed parallelization strategy is therefore not applicable to other acceleration methods such as the FMM. The present parallel IFGF implementation on a 30-node (1,680-core) HPC cluster with Infiniband interconnect, delivers perfect $O(N \log N)$ performance on all 1,680 cores. And, demonstrating high (albeit imperfect) strong and weak parallel efficiencies, unlike other methods, it does not suffer from scaling limitations, under either weak scaling or strong scaling tests, as the number of processing cores grow—conceivably, as argued in Sections 3.2 and 4, up to arbitrarily large numbers of cores. Note that the presented implementation of the proposed parallelization approach deliberately does not utilize any optimizations tailored to the hardware used for the performance tests. It is therefore reasonable to expect a similar performance to that presented in this paper, without hardware-specific optimizations, on a wide variety of modern cluster systems.

This paper includes five sections in its main body (Sections 1 through 5) and two Supplementary Materials sections (Sections SM1 and SM2). Section 2 briefly summarizes the description [1] of the IFGF method, and it introduces the required notations and nomenclature. Section 3 then introduces the proposed parallelization strategy, including a description of computer systems considered (in the first paragraphs of Section 3, see also Section SM1), the associated OpenMP and MPI parallelization approaches (Sections 3.1 and 3.2, respectively), and a discussion of the IFGF’s linearithmic communication costs (Section 3.3)—which results in preservation of the overall IFGF linearithmic parallel computing cost. A variety of numerical results are presented in Section 4 and, with additional detail, in the supplementary materials Section SM2. A few concluding comments, finally, are presented in Section 5.

2 Review of the IFGF Method

As discussed above, the IFGF method provides an accelerated algorithm, requiring $O(N \log N)$ operations, for the numerical evaluation of discrete integral operators of the form

$$I(x_\ell) := \sum_{m=1}^{N} a_m G(x_\ell, x_m), \quad \ell = 1, \ldots, N,$$

for given points $x_\ell$ on a surface $\Gamma \subset \mathbb{R}^3$, and for given complex coefficients $a_m \in \mathbb{C}$, where the function $G(x,y)$, defined for $x, y \in \mathbb{R}^3$, denotes a Green function for some partial differential equation, such as the acoustic Green function

$$G(x,y) = \frac{e^{i\kappa|x-y|}}{4\pi |x-y|}$$

associated with the Helmholtz equation ($i$ denotes the imaginary unit and $\kappa$ the wavenumber) as well as those associated with the Laplace, Stokes, and elasticity equations, among others. In what follows we denote by $\Gamma_N := \{x_1, \ldots, x_N\} \subset \Gamma$ the set of surface discretization points.

For a given $D \in \mathbb{N}$, the IFGF method is based upon use of a $D$-level octree hierarchical decomposition of a cube $B_{1,1,1}^{1}$ containing the discrete surface $\Gamma_N$, where each level is determined by a set of axis-aligned boxes $B_{k}^{d} \subset \mathbb{R}^3$ (defined as the Cartesian product of three one-dimensional half-open intervals of the form $[a, a + H_d)$ for some $a \in \mathbb{R}$), where $k \in \mathbb{N}^3$ denotes a multi-index describing the three-dimensional position
of the box in the resulting Cartesian grid of boxes, and where \( d \) (\( 1 \leq d \leq D \)) denotes the level in the octree. The octree structure of boxes is defined iteratively starting from a single box \( B_{1,1,1}^1 \supset \Gamma_N \) of side \( H_1 \in \mathbb{R}, H_1 > 0 \), on level \( d = 1 \). (Note that there is no undue expense incurred for, say, an elongated surface \( \Gamma \), for which a cubic box could be mostly empty—since, as indicated in what follows, only certain “relevant” child boxes in the box octree are used by the algorithm.) The boxes on consecutive levels \( d = 2, \ldots, D \) are defined by means of a partition of each of the level \((d-1)\) boxes into eight equi-sized and disjoint boxes of side \( H_d = H_{d-1}/2 \) resulting in the level \( d \) boxes \( B_{d}^k \) \( (k \in \{1, \ldots, 2^{d-1}\}^3 =: I_d^d_B) \). The two-dimensional equivalent of the resulting hierarchical octree structure for an illustrative three-level configuration \((D = 3)\) is depicted in Figure 1a. Clearly, each box \( B_{d}^k \) on level \( d \) \((2 \leq d \leq D)\) admits a unique \((d-1)\)-level parent box \( P_{d}^k \) containing \( B_{d}^k \).

To achieve the desired acceleration, the IFGF method only considers interactions between boxes in a certain set \( R_B \) of relevant boxes, which are defined as the boxes in the octree structure that contain at least one surface discretization point:

\[
R_d^d_B := \{B_{d}^k : \Gamma_N \cap B_{d}^k \neq \emptyset, k \in I_d^d_B\}, \quad d = 1, \ldots, D,
\]

Furthermore, for a given box \( B_{d}^k \) on any level \( d \), the method relies on a number of additional concepts, such as the set of neighboring boxes \( \mathcal{N}d_B^d \) (namely the set of level-\( d \) boxes whose closure have a non-empty intersection with the closure \( \overline{B_{d}^k} \) of \( B_{d}^k \)) and the set of cousin boxes \( \mathcal{M}d_B^d \) (non-neighboring boxes that are children of the parents neighbors), as well as related concepts such as the set of neighboring points \( \mathcal{U}d_B^d \) and the set of cousin points \( \mathcal{V}d_B^d \) (which denote the set of surface discretization points within the
neighboring boxes and the cousin boxes, respectively):
\[ \mathcal{N}B_d^d := \{ B_j^d \in \mathcal{R}_B : ||j - k||_\infty \leq 1 \}, \]
\[ \mathcal{M}B_k^d := \{ B_j^d \in \mathcal{R}_B : B_j^d \notin \mathcal{N}B_k^d \land \mathcal{P}B_j^d \in \mathcal{N}\mathcal{P}B_k^d \}, \]
\[ U B_k^d := \left( \bigcup_{B \in \mathcal{N}B_k^d} B \right) \cap \Gamma_N, \]
\[ V B_k^d := \left( \bigcup_{B \in \mathcal{M}B_k^d} B \right) \cap \Gamma_N. \]
(2)

Figure 1a displays the neighbors and cousins of the box \( B_{3(2,1)} \) in white and gray colors, respectively.

The IFGF algorithm accelerates the evaluation of the operator (1) by exploiting a fast method for computations of pairwise interactions between cousin boxes on every level \( d \), for \( d = D, \ldots, 3 \). (Note that the algorithm ends at level \( d = 3 \)—since at \( d = 3 \), each box is a cousin or a neighbor of all the other boxes, and thus, all remaining surface evaluations are completed at this stage.) The evaluation of these interactions is enacted by means of a simple piecewise interpolation method based on a certain factored form of the Green function in a set of box-centered spherical coordinate systems, with one such spherical-coordinate system centered at each one of the relevant boxes. The use of angular and radial interpolation methods gives rise to so-called cone segments \( C_{k,\gamma}^d \); one for each box \( B_k^d \) and for each multi-index \( \gamma \in I_P^d \subset \mathbb{N}^3 \) characterizing a conical interpolation domain. A set \( \mathcal{X}C_{k,\gamma}^d \) of \( P \in \mathbb{N} \) interpolation points is used within each cone segment \( C_{k,\gamma}^d \), where \( P \) is an arbitrary but fixed number throughout the algorithm. In what follows, cone segments \( C_{k,\gamma}^d \) are called co-centered with a box \( B_k^d \) if and only if the origin of the spherical coordinate system defining the cone segment coincides with the center of the box. Two cone segments are called co-centered if they are co-centered with the same box. Note that the sub- and super indices \( k \) and \( d \) in the cone-segment notation \( C_{k,\gamma}^d \) coincide with the corresponding indices of the co-centered box.

To achieve competitive computation times, a certain factorization of the Green function \( G(x,x') = G(x,x'_{k})g_k^d(x,x') \) into a centered factor \( G(x,x'_{k}) \) (centered at the box-center \( x'_{k} \) of the box \( B_k^d \)) and an analytic factor \( g_k^d(x,x') \), is used. The field \( I_k(x) \) in (1) can be expressed, for each level \( d \), as the sum, over all multi-indices \( k \in I_P^d \), of fields \( I_k^d(x) \) equal to the sum of \( G(x,x') \) for all surface discretization points \( x' \) within the box \( B_k^d \), i.e., for all \( x' \in B_k^d \cap \Gamma_N \). Using the aforementioned factorization centered at \( x'_{k} \) yields
\[ I_k^d(x) = \sum_{x' \in B_k^d \cap \Gamma_N} a(x')G(x,x') = G(x,x'_{k})F_k^d(x), \]
\[ F_k^d(x) := \sum_{x' \in B_k^d \cap \Gamma_N} a(x')g_k^d(x,x'), \]
(3)
where \( a(x') \) denotes the coefficient \( a_m \) in (1) that corresponds to the point \( x' \in \Gamma_N \). The IFGF interpolation procedure is then used to evaluate \( F_k^d \). The generation of the \( P \) coefficients of each one of the degree-\( P \) polynomial interpolants \( I_P C_{k,\gamma}^d \), corresponding to interpolation of the field \( F_k^d \) (cf. (3)) over the cone segment \( C_{k,\gamma}^d \), is achieved on the basis of the field values \( F_k^d(\mathcal{X}C_{k,\gamma}^d) := \{ F_k^d(x) : x \in \mathcal{X}C_{k,\gamma}^d \} \).

In [1] it is shown that the analytic factor is analytic everywhere in \( \mathbb{R}^3 \setminus \mathcal{N}B_k^d \) and up to and including infinity, and it can therefore be interpolated accurately throughout that region on the basis of a small (finite!) number of interpolation points. (It is easy to check that the same is true for most of the relevant kernels arising in applications.) Since \( F_k^d \) equals a linear combination of finitely many analytic-factor functions, it is clear that this function shares the same analytic properties, and it can therefore be interpolated with equal quality and efficiency. The cone segments \( C_{k,\gamma}^d \) are defined by means of an iterative procedure similar to the one used in the definition of the boxes \( B_k^d \), but in reversed order, starting from \( d = D \) and moving upwards the tree to \( d = 3 \). The set of cone segments that is to be used at a given level \( d \) depends strongly on the character of the surface \( \Gamma_N \), the wavenumber \( \kappa \) and, possibly, the Green
A two-dimensional sketch of some illustrative box-centered cone segments for a given box $B^d_k$ and its parent $\mathcal{P}B^d_k$ is provided in Figure 1b.

In order to evaluate the discrete operator (1) in $O(N \log N)$ operations, the IFGF algorithm uses iterated interpolation, as illustrated in Figure 2, to evaluate the analytic factor at the interpolation points of consecutive levels—thus avoiding the cost of re-evaluating the field $I^d_k(x)$ on levels $(d-1), (d-2), \ldots, 3$, and using instead the interpolation data on level $d$ to generate the necessary interpolation data at on the consecutive level $(d-1)$. It is important to note that, in order to further increase the efficiency and achieve the desired $O(N \log N)$ complexity, in analogy to the approach used for boxes, the IFGF method only utilizes the set of relevant cone segments $\mathcal{R}_C B^d_k$ for each box $B^d_k$, namely, the cone segments that are actually needed for interpolation back to cousin surface discretization points or to relevant cone segments on the parent level. In other words, the relevant cone segments $\mathcal{R}_C B^d_k$ are defined by

$$\mathcal{R}_C B^d_k := \emptyset \quad \text{for} \quad d = 1, 2,$$

$$\mathcal{R}_C B^d_k := \left\{ C^d_{k;\gamma} \in I^d_C : C^d_{k;\gamma} \cap \nu B^d_k \neq \emptyset \text{ or } C^d_{k;\gamma} \cap \left( \bigcup_{C \in \mathcal{R}_C \mathcal{P}B^d_k} C \right) \neq \emptyset \right\} \quad \text{for} \quad d \geq 3. \quad (4)$$

The serial IFGF algorithm, introduced in [1], is summarized in Figure 2 and described in what follows. Starting from the given coefficients in equation (1) at the bottom of Figure 2, the IFGF algorithm first performs “LevelDSingularInteractions” (which, while required for the full evaluation of (1), are not, strictly speaking, a part of the IFGF strategy, and would, in the context of a scattering solver, be substituted by an appropriate local integration scheme; see e.g. [31]). This “LevelDSingularInteractions” stage evaluates the field $I^d_k$ at all surface discretization points $x$ in all the neighbor boxes of each box $B^D_k$ (i.e. at all $x \in \bigcup B^D_k$ for all relevant boxes $B^D_k$). Next, the algorithm performs “LevelDEvaluations”, that is, it first evaluates the field $F^D_k(x)$ (see (3)) at every interpolation point in the relevant cone segments co-centered with the box $B^D_k$, and it subsequently generates the necessary level-$D$ interpolants. The IFGF algorithm then proceeds through levels $d = D, \ldots, 3$ by performing, on each level $d$, 1) Interpolations to cousin surface discretization points in the “Interpolation” stage, as well as, 2) Interpolations to level $d-1$ interpolation points, and subsequent generation of the interpolants on level $d-1$, in the “Propagation” stage, just as in the “LevelDEvaluations” stage, but utilizing the interpolants instead of direct field evaluations.

The corresponding pseudo-code is presented in Algorithm 1. Note that this algorithm does not include evaluations of interactions between neighboring boxes on the lowest level $D$ (“LevelDSingularInteractions” in Figure 2), which would generally be produced by means of a separate algorithm, as mentioned above in this section.

3 Parallel IFGF Method

The IFGF parallelization scheme proposed in this paper relies on use of a hybrid MPI-OpenMP approach. As detailed in Section 3.2, the MPI interface plays two distinct roles in the proposed scheme: it is used to 1) Enable distributed-memory parallelization across compute nodes, and 2) In the particular case in which MPI ranks are pinned to NUMA nodes (non-uniform memory access), to distribute work and handle memory access across NUMA nodes within each compute node. Additional details concerning the architecture of the computer used, and, in particular, NUMA nodes, can be found in Section SM1. The strategy in point 2) guarantees that memory held by a certain MPI rank is stored within a single NUMA node and can therefore be accessed quickly by all cores within the NUMA node. Moreover, in case 2), access to memory in a different NUMA node within the same compute node is algorithmically effected through MPI in the same manner as access to memory in a different compute node.

The OpenMP parallelization, described in Section 3.1, is used to further distribute the work assigned to each MPI rank. Hence, in the specific hardware implementation demonstrated in this paper (which
Figure 2: Visual representation of the IFGF algorithm, outlined in Algorithm 1, and also expressed in Algorithm 5 in terms of three fundamental functions called \textit{LevelDEvaluations}, \textit{Propagation} and \textit{Interpolation}. Starting from the given coefficients $a_1, \ldots, a_N$ in equation (1), the \textit{LevelDEvaluations} function generates the first set of interpolants on level $D$. The \textit{Interpolation} function interpolates to the surface discretization points and the \textit{Propagation} function facilitates the upwards traversal of the octree structure. Although they are not part of the IFGF algorithm, the interactions between level-$D$ neighbor boxes are represented here by the \textit{LevelDSingularInteractions} function. Note that, unlike other acceleration methods such as the FMM, contributions to the operator output are made at every level, and without a requirement of a downward pass over the octree.

is based on use of compute nodes containing four fourteen-core NUMA nodes) typically four intra-node MPI ranks are used per compute node, each pinned to a single NUMA node, each one of which spawns fourteen OpenMP threads—which, according to our experiments, leads to the best performance achievable without the adverse impact (on e.g. code complexity, memory requirements, or communication) entailed in pure MPI parallelism within each node. A general discussion on the performance of hybrid MPI-OpenMP approaches can be found in [32–34].

### 3.1 IFGF OpenMP parallelization

Before introducing the proposed OpenMP parallelization scheme, we briefly consider a straightforward OpenMP parallelization strategy which we do not recommend but which we present for reference. This straightforward and easily implemented strategy results by simply implementing the algorithm depicted in Figure 2 by assigning, at each level $d$, the work associated with groups of relevant boxes to various OpenMP threads (e.g. with a “\#pragma omp parallel for” statement), in such a way that each group is handled by a single thread. Equi-distribution of relevant boxes onto the OpenMP threads implies equi-distribution of both the surface discretization points and the computations performed per thread—but only provided 1) The surface discretization points are roughly equi-distributed among the relevant boxes, and, 2) There is a sufficient number of relevant boxes to occupy all OpenMP threads. The difficulties associated with point 1) could be negotiated, in view of the law of large numbers [35, Section 13], provided sufficiently many boxes are used, that is to say, provided point 2) is satisfied. In other words, the feasibility of the approach under consideration hinges on the existence of sufficiently many relevant boxes on each level, as required by point 2). Unfortunately, however, for any given discretized surface $\Gamma_N$, point 2) is not satisfied at certain levels $d$ in the octree structure, unless only a small number of threads is employed. Noting that, for any
Algorithm 1 IFGF Method

1: \Direct evaluations on the lowest level.
2: for $B^D_k \in R_B$ do
3:   for $C^D_{k,\gamma} \in R_C B^D_k$ do \Comment{Evaluate $F$ at all relevant interpolation points}
4:     Evaluate and store $F^D_k (\chi C^D_{k,\gamma})$
5:     Generate interpolant $I_P C^D_{k,\gamma}$
6:   end for
7: end for
8: \Interpolation onto surface discretization points and parent interpolation points.
9: for $d = D, \ldots, 3$ do
10:   for $B^d_k \in R_B$ do \Comment{Interpolate at cousin surface points}
11:     for $x \in V B^d_k$ do
12:       Determine $C^d_{k,\alpha}$ s.t. $x \in C^d_{k,\alpha}$
13:       Evaluate and add to result $I_P C^d_{k,\alpha}(x) \times G(x, x^d_k)\delta$
14:     end for
15:     if $d > 3$ then \Comment{Evaluate $F$ on parent interpolation points}
16:       Determine parent $B^{d-1}_j = \mathcal{P} B^d_k$
17:       for $C^{d-1}_{j,\gamma} \in R_C B^{d-1}_j$ do
18:         for $x \in \chi C^{d-1}_{j,\gamma}$ do
19:           Determine $C^d_{k,\alpha}$ s.t. $x \in C^d_{k,\alpha}$
20:           Evaluate and add $I_P C^d_{k,\alpha}(x) \times G(x, x^d_k)\delta / G(x, x^{d-1}_j)$
21:         end for
22:       end for
23:     end if
24:   end for
25:   end for \Comment{Generate interpolants on parent level}
26: for $B^{d-1}_j \in R_B$ do
27:   for $C^{d-1}_{j,\gamma} \in R_C B^{d-1}_j$ do
28:     Generate interpolant $I_P C^{d-1}_{j,\gamma}$
29:   end for
30: end for
31: end for

surface $\Gamma_N$, there are only sixty-four boxes overall on level $d = 3$ of the algorithm (and, in general, even fewer relevant boxes), we see that a definite limit exists on the parallelism achievable by this approach. The method presented in [15] uses this strategy in an MPI context, and it is therefore subject to such a hard limitation on achievable parallelism (although in a somewhat mitigated form, owing to the characteristics of that algorithm, as discussed in Section 1). To avoid such limitations we consider an alternate OpenMP parallelization strategy specifically enabled by the characteristics of the IFGF algorithm, as described in what follows.

The proposed strategy proceeds via parallelization of the three independent programming functions that comprise the IFGF method, namely the LevelDEvaluations function, the Interpolation function and the Propagation function, as mentioned in Section 2 and illustrated in Figure 2. The first of these functions, the LevelDEvaluations function, which corresponds to the loop in line 2 of Algorithm 1, evaluates, for each relevant level-$D$ box, the field generated by the point sources within the box (given by (3) with $d = D$) at the interpolation points in all relevant cone segments co-centered with the box and generates the required interpolants. The second function, the level-$d$-dependent Interpolation function, which corresponds to line 14 under the loops in lines 12 and 13 and is represented in Figure 2 by rightward lines connecting various levels to the “Operator Output”, performs the necessary interpolations to cousin surface discretization points on level $d$ ($d = 3, \ldots, D$). The third and final programming function, the level-$d$-dependent Prop-
Algorithm 2 LevelDEvaluations
1: for $B^D_k \in \mathcal{R}_B$ do
2: for $C^D_{k;\gamma} \in \mathcal{R}_C B^D_k$ do
3: Evaluate and store $F^D_k (X_{C^D_{k;\gamma}})$
4: Generate interpolant $I_P C^D_{k;\gamma}$
5: end for
6: end for

Algorithm 3 Interpolation(d)
1: for $B^d_k \in \mathcal{R}_B$ do
2: for $x \in V B^d_k$ do
3: Determine $C^d_{k;\alpha}$ s.t. $x \in C^d_{k;\alpha}$
4: Evaluate and add to result $I_P C^d_{k;\alpha} (x) \times G(x, x^d_k)$
5: end for
6: end for

agation function, which corresponds to line 20 under the loops in lines 12, 18, and 19 and is represented
in Figure 2 by means of upward pointing arrows targeting the “Interpolant” boxes, interpolates, for each
relevant level-$d$ box, to interpolation points in the relevant cone segments co-centered with the parent box
on level $(d-1)$ and generates the required interpolants. These three functions are outlined in Algorithms 2,
3, and 4, respectively. Using these three functions, the IFGF algorithm (Algorithm 1) may be re-expressed
as Algorithm 5. In what follows, we present our strategies for efficient parallelization of each one of these
functions separately.

Our approach for an efficient parallelization of the LevelDEvaluations function is based on changing the
viewpoint from iterating through the level-$D$ relevant boxes to iterating through the set $\mathcal{R}_D$ of all relevant
cone segments on level $D$. Since corresponding sets of level-$d$ relevant cone segments for the wider range
$3 \leq d \leq D$ are utilized in the parallelization of the Propagation function, we generalize the definition: the
set of all relevant cone segments on level $d$ is denoted by $\mathcal{R}_d^\alpha$, that is
$$\mathcal{R}_d^\alpha := \bigcup_{k \in I_d^\alpha; B^d_k \in \mathcal{R}_B} \mathcal{R}_C B^d_k,$$ for $3 \leq d \leq D$. (5)

Using (5), a parallel version of Algorithm 2 is presented in Algorithm 6. The aforementioned change in
viewpoint corresponds to collapsing the two outermost nested loops in Algorithm 2, effectively increasing
the number of independent tasks and, consequently, the achievable parallelism. Note that, in a C++
implementation, the “parallel for” construct in Algorithm 6 corresponds to e.g. a “for”-loop preceded by
the pragma directive “omp parallel for”.

The proposed parallelization of the $d$-dependent Propagation function follows a similar idea as the parallel LevelDEvaluations considered above—relying now on iteration over the relevant $(d-1)$ (parent-
level) cone segments, which are targets of the interpolation, instead of the relevant level-$d$ boxes emitting
the field. This strategy addresses the difficulties arising from the straightforward approach described at
the beginning of Section 3.1, for which the number of available tasks to be distributed decreases with the
level $d$ and imposes a hard limit on the achievable parallelism. Indeed, in the context of the oscillatory
Green functions over two-dimensional surfaces $\Gamma \subset \mathbb{R}^3$ considered in this paper, for example, wherein
the number of relevant cone segments on each level is an approximately constant function of $d$ [1, Sec. 3.3.3],
the number of independent tasks available for parallelization remains approximately constant as a function
of $d$. Additionally, the proposed parallel Propagation strategy avoids a significant “thread-safety” [36,37],
predicament, that is ubiquitous in the straightforward approach, whereby multiple writes to the same
target interpolation point on the parent level take place from different threads. In contrast, the proposed
Algorithm 4 Propagation(d)

1: for $B_d^k \in R_B$ do
2: Determine parent $B_{d-1}^j = \mathcal{P} B_d^k$
3: for $C_{j;\gamma}^{d-1} \in R_C B_{d-1}^j$ do
4: for $x \in \mathcal{X}_{j;\gamma}^{d-1}$ do
5: Determine $C_{k;\alpha}^d$ s.t. $x \in C_{k;\alpha}^d$
6: Evaluate and add $I_P C_{k;\alpha}^d(x) \times G(x, x_d^k)/G(x, x_{d-1}^j)$
7: end for
8: end for
9: end for
10: for $B_{d-1}^j \in R_B$ do
11: for $C_{j;\gamma}^{d-1} \in R_C B_{d-1}^j$ do
12: Generate interpolant $I_P C_{j;\gamma}^{d-1}$
13: end for
14: end for

Algorithm 5 IFGF Method

1: LevelDEvaluations()
2:
3: for $d = D, \ldots, 3$ do
4: Interpolation(d)
5: if $d > 3$ then
6: Propagation(d)
7: end if
8: end for

Propagation strategy, is by design thread-safe without any additional considerations, since it distributes the targets of the interpolation to the available threads. Note that the practical implementation of this approach requires the algorithm to first determine the relevant box

$$R_B C_{k;\gamma}^d := B_k^d \quad \text{s.t.} \quad C_{k;\gamma}^d \in R_C B_k^d$$

that is co-centered with a given relevant cone segment $C_{k;\gamma}^d$; then to determine the relevant level-$(d+1)$ child boxes

$$CB_k^d := \left\{ B_{j+1}^d \in R_B : j \in I_B^{d+1}, \mathcal{P} B_{j+1}^d = B_k^d \right\},$$

of a given relevant box $B_k^d$ on level $d$; and, finally, to find all the interpolants $I_P C_{k;\gamma}^d$ on the relevant cone segments (4) co-centered with the child boxes from which the propagation needs to be enacted. Using this notation, the resulting Parallel Propagation algorithm is presented in Algorithm 7.

The proposed parallelization strategy for the third and final IFGF programming function, namely, the Interpolation function, relies once again on the strategy used for the LevelDEvaluations and Propagation functions—which, in the present case, leads to changing the viewpoint from iterating through the relevant boxes to iterating through the surface discretization points that are the target of the interpolation procedure. This approach avoids both, the difficulties mentioned at the beginning of Section 3.1 (concerning

Algorithm 6 Parallel LevelDEvaluations

1: parallel for $C_{k;\gamma}^D \in R_C^D$ do
2: Evaluate and store $F_k^D(\mathcal{X} C_{k;\gamma}^D)$
3: Generate interpolant $I_P C_{k;\gamma}^D$
4: end parallel for
Algorithm 7 Parallel Propagation(d)
1: parallel for $C_{d-1}^{\tilde{j}\gamma} \in R^{d-1}_C$ do
2: for $B^d_k \in C(R_B C_{d-1}^{\tilde{j}\gamma})$ do
3: for $x \in X C_{d-1}^{\tilde{j}\gamma}$ do
4: Determine $C_{k,\alpha}^d$, s.t. $x \in C_{k,\alpha}^d$
5: Evaluate and add $I_P C^d_{k,\alpha}(x) \times G(x, x_k^d)/G(x, x_{j}^{d-1})$
6: end for
7: end for
8: Generate interpolant $I_{P} C_{d-1}^{\tilde{j}\gamma}$
9: end parallel for

Algorithm 8 Parallel Interpolation(d)
1: parallel for $x \in \Gamma_N$ do
2: for $B^d_k \in M^d(x)$ do
3: Determine $C_{k,\gamma}^d$, s.t. $x \in C_{k,\gamma}^d$
4: Evaluate $I_P C^d_{k,\gamma}(x) \times G(x, x_k^d)$
5: end for
6: end parallel for

the existence of a small number of relevant boxes in the upper levels of the octree structure), as well as thread-safety difficulties similar to those discussed above in the context of the Propagation function. For a concise description of the parallel Interpolation function in what follows we denote by

$$M^d(x) := \left\{ B^d_K \in R_B : x \in VB^d_K \right\},$$

the set of cousin boxes of a surface discretization point $x \in \Gamma_N$ on level $d$, $3 \leq d \leq D$, which extends the concept of cousin boxes of a box, introduced in (2) in Section 2. Using the definition (8), the Parallel Interpolation function is stated in Algorithm 8.

In summary, the OpenMP parallelization strategies proposed above for the functions Parallel LevelDE-valuations, Parallel Propagation and Parallel Interpolation are thread-safe by design, and they provide effective work distribution by relying on iteration over items (relevant cone segments or surface discretization points) that exist in a sufficiently large (and essentially constant) quantities for all levels $d$, $3 \leq d \leq D$, in the box-octree structure. As a result, the proposed approach effectively eliminates the hard limitation present in the straightforward OpenMP parallelization scheme mentioned at the beginning of this section. Note that the proposed IFGF box-cone parallelization strategy is in general not applicable to other hierarchical acceleration methods, such as e.g. FMM-type algorithms. Indeed, in contrast to the incremental propagation and surface evaluation approach inherent in the IFGF method, previous acceleration methods rely on the FFT algorithm—which, as discussed in Section 1, leads to inefficiencies in the upper portions of the corresponding octree structures [2,15].

3.2 IFGF MPI parallelization

The proposed MPI parallel IFGF algorithm, which enables both data distribution onto the MPI ranks and efficient communication of data between MPI ranks, is described in detail in Sections 3.2.1 through 3.2.3. The approach mirrors the one proposed in Section 3.1 for the corresponding OpenMP interface. In fact, the MPI parallel scheme is based on slight modifications of the OpenMP parallel Algorithms 6, 7, and 8. As indicated by the theoretical discussion in Section 3.3, the communication overhead is such that the intrinsic IFGF linearithmic complexity previously demonstrated in [1] for a single core implementation is preserved on any fixed number $N_c$ of cores; an illustration of this theoretical result on $N_c = 1,680$ cores.
is presented in the Supplementary Materials Table SM4. Most importantly, as in the OpenMP case (cf. the last paragraph of Section 3.1), for arbitrarily large numbers $D$ of levels, the MPI IFGF algorithm iterates over items (relevant cone segments or surface discretization points) that exist in a sufficiently large (and essentially constant) quantities for all levels $d$, $3 \leq d \leq D$, in the box-octree structure. As a result, the strategy results in an overall MPI-OpenMP IFGF parallel scheme without hard limitations on the achievable parallelism as the number of cores grows.

### 3.2.1 Problem decomposition and data distribution

The distribution of the data required by the IFGF algorithm to the MPI ranks can be summarized as the independent distribution of the set of surface discretization points $\Gamma_N$, which are organized on the basis of boxes induced by an octree structure, and the distribution of the set of relevant cone segments on each level $R_d^B$. Clearly, for an efficient parallel implementation, the distribution used should balance the amount of work performed by each rank while maintaining a minimal memory footprint per rank and while also minimizing the communication between ranks. A concise description of the method used for data distribution to the MPI ranks is presented in what follows, where we let $N_r \in \mathbb{N}$ and $\rho \in \mathbb{N}$ ($1 \leq \rho \leq N_r$) denote the number of MPI ranks and the index of a specific MPI rank, respectively.

The distribution of the surface discretization points is orchestrated on the basis of an ordering of the set of relevant boxes $R_d^B$ on each level $d$, which, in the proposed algorithm, is obtained from a depth-first traversal of the octree structure. This ordering is equivalent to a Morton order of the boxes (as described e.g. in [26, 29, 30, 38] and depicted by the red \$-looking curve in the left panel of Figure 3) which, as indicated in [38], can be generated quickly from the positions $k \in I^D_B$ of the level-$D$ boxes $B^D_k$ through a bit-interleaving procedure. Ordering the surface discretization points according to the Morton order of the containing level-$D$ boxes also guarantees a Morton order on every other level $d$, $1 \leq d \leq D - 1$. More precisely, at every level $d$ the Morton order introduces a total order $\prec$ on the set of boxes. The ordering of the surface discretization points $\Gamma_N$ is facilitated by assigning each point $x \in \Gamma_N$ the Morton order of the containing level-$D$ box, which can be computed through a division operation on the coordinates of the point $x$ to get the index $k \in I^D_B$ of the containing box with a subsequent bit-interleaving procedure, followed by a simple sorting of the points according to their assigned Morton order. Noting that the map which assigns to each point on $\Gamma_N$ the Morton order of the containing level-$D$ box is not injective, in order to obtain a total order on all of $\Gamma_N$ we additionally order in an arbitrary manner subset of points $x \in \Gamma_N$ with the same assigned Morton order. The resulting overall order has the desirable properties that, on every level $d$, surface discretization points within any given box are contiguous in memory, and that boxes close in real space are also close in memory.

The sorted surface discretization points are distributed to the MPI ranks based on their containing level-$D$ boxes, in such a way that the boxes processed by each rank are an “interval” set of the form $\{ B \in R^D_B : B^D_{k_1} \prec B \prec B^D_{k_2} \}$, for suitable choices of $k_1, k_2 \in I^D_B$ designed to guarantee that all the boxes on a given rank contain a number of surface discretization points as close as possible to the average value $N/N_r$. Hence, the smallest boxes in the octree structure represent the smallest “unit” for the distribution of the surface discretization points. The maximum possible deviation in the number of discretization points assigned to a certain MPI rank from the average is therefore given by the maximum number of surface discretization points contained within one level-$D$ box in the octree structure. For reasonable distributions of the discretization points $\Gamma_N$ on the surface $\Gamma$, and for a suitable choice of the number of levels $D$, this deviation between MPI ranks is typically less than 100 surface discretization points.

The set of surface discretization points stored in the $\rho$-th MPI rank, $1 \leq \rho \leq N_r$, is denoted by $\Gamma_{N,\rho}$. By definition, the subsets $\Gamma_{N,\rho}$ of $\Gamma_N$ are pairwise disjoint and their union over all MPI ranks $\rho = 1, \ldots, N_r$ equals $\Gamma_N$. The distribution of the surface discretization points is used to evenly divide between all MPI ranks the work performed in the Interpolation function (OpenMP Algorithm 8). The underlying level-$D$ based distribution of $\Gamma_N$ is utilized throughout all levels $d = D, \ldots, 3$. Thus, the MPI parallel Interpolation
Figure 3: Left panel: Two-dimensional example of an ordering of the cone segments based on the Morton order of the boxes on level $d = 3$ with four cone segments per box. The red line indicates the Morton order of the boxes where the red numbers denote the actual Morton code of the containing box. The green numbers denote the ordering of the cone segments in the proposed Morton-based cone-segment ordering. The blue curve denotes a sketch of a scatterer. Right panel: Sketch of a possible cone-segment memory layout, demonstrating the equi-distribution of cone segments among ranks, and emphasizing a central element of the proposed parallelization strategy, namely, that co-centered cone segments may be assigned to different MPI ranks. Note that only relevant boxes and cone segments are stored in memory resulting in some numbers in the ordering being skipped.

Algorithm 9 MPI Parallel LevelDEvaluations

1: parallel for $C^D_{k;\gamma} \in R^D_{C;\rho}$ do
2: Evaluate and store $F^D_k(\chi C^D_{k;\gamma})$
3: Generate interpolant $I_P C^D_{k;\gamma}$
4: end parallel for

function results from the straightforward and level-independent modification of Line 1 in Algorithm 8, to read $x \in \Gamma_{N,\rho}$ instead of $x \in \Gamma_N$—as shown in Algorithm 10. Naturally, the values of the discrete operator $I(x_l)$ in (1) computed by the $\rho$-th MPI rank correspond to points $x_l \in \Gamma_{N,\rho}$, and they are therefore also stored in the $\rho$-th MPI rank. In other words, the set of resulting field values $I(x_l)$ is partitioned and stored in the MPI ranks according to the partition utilized for the surface discretization points $\Gamma_N$.

The data associated with the level-$d$ relevant cone segments is also distributed to MPI ranks on the basis of a total order—in this case, a total order on the set of level-$d$ cone segments that is based on the Morton order imposed on the level-$d$ boxes, in such a way that co-centered cone segments are close in memory. It should be noted that, for every relevant cone segment $C^d_{k;\gamma} \in R^d_C$, $3 \leq d \leq D$ (see (5)), the set of $P$ coefficients that characterize the polynomial interpolants $I_P C^d_{k;\gamma}$ (Section 2), which approximate the field $F^d_k$ in (3) within the cone segment $C^d_{k;\gamma}$, need to be stored, in appropriately distributed manner, for two consecutive levels. Indeed, for each $d$, these level-$d$ coefficients are utilized to enable two different interpolation procedures, namely interpolation from level $d$ to interpolation points at the parent-level $(d-1)$

Algorithm 10 MPI Parallel Interpolation($d$)

1: parallel for $x \in \Gamma_{N,\rho}$ do
2: for $B^d_k \in M^d(x)$ do
3: Determine $C^d_{k;\gamma}$ s.t. $x \in C^d_{k;\gamma}$
4: Evaluate $I_P C^d_{k;\gamma}(x) \times G(x, x^d_k)$
5: end for
6: end parallel for
in the Propagation function (Line 4 in Algorithm 7), as well as interpolation to the level-\(d\) cousin surface discretization points in the Interpolation function (Line 3 in Algorithm 8).

The set of level-\(d\) relevant cone segments \(\mathcal{R}^d_C\), is sorted on the basis of the Morton order induced by the co-centered level-\(d\) boxes followed by a suitable sorting of cone segments in each spherical coordinate system—resulting in a total order \(\sqsubseteq\) in the set of all level-\(d\) relevant cone segments, as depicted in the left panel of Figure 3. (Each set of co-centered cone segments is ordered using the radial direction first, then elevation and finally azimuth, although any other ordering could be used.) Finally, at each level \(d\) \((d = D, \ldots, 3)\), approximately equi-sized and pair-wise disjoint intervals of relevant cone segments \(C\) of the form \(\{C \in \mathcal{R}^d_C : C_{k_1, \gamma_1} \sqsubseteq C \sqsubseteq C_{k_2, \gamma_2}\}\), for some \(k_1, k_2 \in I^d_B\) and \(\gamma_1, \gamma_2 \in I^d_C\) (i.e., disjoint intervals of contiguous cone segments), are distributed to the MPI ranks, as illustrated in the right panel of Figure 3. Note that the specific assignment of cone segments to MPI ranks is solely determined by the order \(\sqsubseteq\) and the number of MPI ranks and cone segments, and it does not otherwise relate to the underlying box tree. In particular, as suggested in the right panel of Figure 3, co-centered cone segments may be assigned to different MPI ranks—which induces a flexibility that leads to excellent load-balancing and, therefore, high parallelization efficiency. As is the case for the relevant boxes, the proposed ordering of the relevant cone segments implies that cone segments which are close in real space (i.e. co-centered with the same box and pointing in the same direction or co-centered with boxes which are close in real space) are also close in memory, and, in particular, are likely to be stored within the same MPI rank. Analogously to the notation introduced above for the distributed surface discretization points, the relevant level-\(d\) cone segments assigned to a MPI rank with index \(\rho\), \(1 \leq \rho \leq \mathcal{N}_r\), are denoted by \(\mathcal{R}^d_{C, \rho}\). The MPI-capable algorithm is thus obtained by adjusting the loops in the first lines in Algorithms 6 and 7 to only iterate over the level-\(d\) relevant cone segments \(\mathcal{R}^d_{C, \rho}\) stored in the current rank \(\rho\), as shown in the MPI parallel Algorithms 9 and 11, instead of iterating over all relevant cone segments on level \(d\).

### 3.2.2 Practical implementation of the box-cone data structures

A C++ implementation of the parallel IFGF box-cone data structures described above, which enables a linearithmic memory and time complexity, is described in detail in what follows.

In the proposed implementation the geometry \(\Gamma_N\) is stored in three separate arrays \(X_1\), \(X_2\) and \(X_3\) (either C style arrays or std::vector) of size \(N\) for the \(x_1\), \(x_2\), and \(x_3\) components of the surface discretization points \((x_1, x_2, x_3) = x \in \Gamma_N\), resulting in a structure of arrays (SoA) memory layout [39], which is beneficial as it leads to increased floating-point performance under automatic vectorization on the basis of single instruction, multiple data (SIMD) hardware [40, Section 2.7] generally available in modern processors. As mentioned above in Section 3.2.1, each one of the three arrays is sorted according to the Morton order of the boxes. Similarly, the real and imaginary parts of the resulting field values \(I(x_\ell)\), \(1 \leq \ell \leq N\), are stored as two independent arrays, \(I_R\) and \(I_3\), of size \(N\). The order of these field values coincides with the order imposed on the surface discretization points such that \(I(x_\ell) = I_R[k] + \iota I_3[k]\) at a given point \(x_\ell\) is

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**Algorithm 11 MPI Parallel Propagation(\(d\))**

1: parallel for \(C_{d-1, j; \gamma} \in \mathcal{R}^d_{C, \rho}\) do
2: for \(B^d_k \in \mathcal{C}(\mathcal{R}_B C_{d-1, j; \gamma})\) do
3: for \(x \in \mathcal{X}^d_{d-1, j; \gamma}\) do
4: Determine \(C^d_{k, \alpha}\) s.t. \(x \in C^d_{k, \alpha}\)
5: Evaluate and add \(I_P C^d_{k, \alpha}(x) \times G(x, x^d_k)/G(x, x^{d-1}_j)\)
6: end for
7: end for
8: Generate interpolant \(I_P C^{d-1}_{d, j; \gamma}\)
9: end parallel for
stored at the same position \( k \) in the arrays \( I_{\mathbb{R}} \) and \( I_{\mathbb{I}} \) as the corresponding surface discretization point \( x_\ell = (X_1[k], X_2[k], X_3[k]) \) in the arrays \( X_1, X_2 \) and \( X_3 \).

The algorithm enacts the box-octree inherent in the IFGF solver in the form of a linear octree structure (cf. [41,42]). In particular, the proposed linear octree only includes data associated with relevant boxes, and it does not store any information about non-relevant boxes, to avoid \( \mathcal{O}(N^{3/2}) \) memory requirements, as described in detail in what follows. Relevant boxes in the linear octree are represented, on each level \( d = 3, \ldots, D \), by the box index \( k \in I_B^d \) (as described above in Section 2) and the equivalent Morton order. Each box stores the position in the arrays \( X_1, X_2, \) and \( X_3 \) of the first surface discretization point contained in the box in addition to the number of discretization points in the box in a hash map (cf. [41, Section 11]) with average \( \mathcal{O}(1) \) time and memory complexity for read access (e.g. a std::unordered_map), where the Morton order of the box is utilized as the key. Thus, given a Morton order of a box, the discretization points contained within the box can be determined in \( \mathcal{O}(1) \) time and memory complexity. Conversely, given any surface discretization point \( x \in \Gamma_N \), the three-dimensional index \( k \in I_B^d \) (for every level \( d = 3, \ldots, D \)) of the box \( B_k^d \) containing the point \( x \) and the associated Morton order can be determined through simple division and bit-interleaving, as described in Section 3.2.1, in \( \mathcal{O}(1) \) time and memory. Overall, this guarantees a true \( \mathcal{O}(N \log N) \) time and memory implementation by avoiding the storage of any information regarding non-relevant boxes. Note that the linear octree structure described above is essentially the same as the one presented in [38].

Similarly, for each level \( d \), the relevant cone segments \( C^{d}_{k,\gamma} \), or, more precisely, the real and imaginary parts of the \( P \) coefficients representing the interpolants \( I_P C^{d}_{k,\gamma} \) on the relevant cone segments \( C^{d}_{k,\gamma} \), are stored separately in two one-dimensional arrays per rank (following the above partition of the cone segments to the ranks). To associate the three-dimensional cone segment index \( \gamma \in I_C^d \) with the actual coefficients, a hash map for each relevant box \( B_k^d \) is used, where the value of the hash map is an index pointing to the first of the coefficients \( I_P C^{d}_{k,\gamma} \) in the array of coefficients mentioned above, and where \( \gamma \in I_C^d \) is the key of the hash map. (Note that the three-dimensional cone segment index \( \gamma \), which runs over both relevant and non-relevant cone segments, corresponds to the relative position of the cone segment in the spherical coordinate system centered at the box center.) The usage of a hash map circumvents the storage of any non-relevant cone segment data while maintaining the association with the three-dimensional index \( \gamma \) that allows an easy identification of the cone segment based on its relative position in spherical coordinates. Thus, for a given Cartesian point \( x \in \mathbb{R}^3 \), this data structure can be used to locate the interpolant \( I_P C^{d}_{k,\gamma} \) for the relevant cone segment \( C^{d}_{k,\gamma} \in R_C^d \) containing the point \( x \) through a transformation of \( x \) to spherical coordinates centered at the origin of the cone segment \( C^{d}_{k,\gamma} \), a division to get the cone segment index \( \gamma \) and a look-up in the hash map to get the coefficients of the interpolating polynomial. The association of any point with the relevant cone segment containing it can therefore be achieved on average in \( \mathcal{O}(1) \) time and memory. This is required in the Interpolation and Propagation function to facilitate the interpolation to cousin surface discretization points and parent-level interpolation points, respectively.

Note that, for increased performance, the hash maps described above and stored on a given rank \( \rho \) are required to contain all associations between boxes, cone segments, discretization points and interpolation coefficients utilized by the current rank \( \rho \) at any point in the algorithm. In particular, if certain surface discretization points or interpolant coefficients are stored on a different rank \( \hat{\rho} \neq \rho \), but are required in the current rank \( \rho \), the above hash maps are utilized to find the data and, consequently, enable the communication of that data through MPI. While this produces some data duplication, analogously to “halo regions” [40, Sec. 9.6] employed in grid-based methods, the memory duplicated in the parallel IFGF method is limited to surface discretization points and interpolant coefficients of neighbors and cousins.

### 3.2.3 Data communication

Clearly, for an MPI rank to access data stored in a different rank, explicit communication between the ranks must take place. The proposed solution, which we favor due to the decreased complexity of the im-
The implementation it entails, is based on one-sided or remote memory access (RMA) communication introduced in MPI-2 [43, Section 5], [40, Section 8]—which utilizes a single MPI_Get or MPI_Put call on the origin rank instead of a coupled MPI_Recv-MPI_Send call (or similar functionalities) involving both the origin and the target rank.

The data any MPI rank may require from other MPI ranks is limited to certain interpolants $I_{\rho C_{k;\gamma}}$. It is therefore sufficient to store the corresponding coefficients in so-called RMA windows (in MPI given by MPI_Win and allocated with e.g. MPI_Win_allocate), which enable the one-sided communication approach. For increased efficiency, the computations and communications are organized among the ranks on the basis of the following two considerations: 1) For each $\rho$, $1 \leq \rho \leq N_r$, the $\rho$-th rank asynchronously collects from other ranks all the data (i.e. the coefficients of the interpolants) it requires to perform Interpolation or Propagation computations assigned to it; and 2) The communications necessary to collect this data are interleaved with the computations in such a way that while the computations by the Interpolation function take place, the communication for the next Propagation function is performed and vice versa. This approach, which effectively hides the communications behind computations (thus increasing the performance and parallel efficiency), requires every MPI rank to store all data it obtains from other ranks for one full level-$d$ ($3 \leq d \leq D$) Interpolation or Propagation step while it continues to store the coefficients it has itself generated—which effectively increases the peak memory per rank requirements slightly (by e.g. 10% or less).

The level-$d$ dependent CommunicateInterpolationData (resp. CommunicatePropagationData) programming function in Algorithm 12 (resp. Algorithm 13) encapsulates the communications performed by each rank to obtain, from other ranks, the polynomial coefficients it needs to enact the necessary level-$d$ interpolation computations (resp. interpolation computations onto level-$(d-1)$ interpolation points) required by the Interpolation (resp. Propagation) function. The LevelDEvaluations function does not need any communications since the surface discretization points $x \in \Gamma_N$, which are required in the LevelDEvaluations function but which are not stored as part of $\Gamma_N$, $\rho$ (see previous Section 3.2.1), are duplicated to the $\rho$-th MPI rank. The rank that stores a level-$D$ relevant cone segment, as described at the beginning of Section 3.2, facilitates the evaluation of the field at the interpolation points of that cone segment and the generation of the interpolants independently from every other MPI rank.

Using the functions 9 through 13, the pseudo-code for the proposed overall MPI-OpenMP IFGF algorithm is given in Algorithm 14. Note that access to RMA windows is usually asynchronous and requires some form of synchronization to ensure the data transfer is finalized before the communicated data is accessed. Moreover, the call to the CommunicatePropagationData in Algorithm 14 requires for the Propagation function to have completed in all ranks targeted by the communication function.
Algorithm 13 CommunicateInterpolationData(d)

1: parallel for \( x \in \Gamma_{N,\rho} \) do
2: for \( B_d^k \in M^d(x) \) do
3: Find \( \tilde{\gamma} \) such that \( x \in C^d_{k,\tilde{\gamma}} \) \( \in \mathcal{R}_C B_d^k \)
4: Identify the MPI rank \( \rho \) on which \( I_{\rho} C^d_{k,\tilde{\gamma}} \) is stored
5: MPI Get \( I_{\rho} C^d_{k,\tilde{\gamma}} \) from rank \( \rho \)
6: end for
7: end parallel for

3.3 Parallel linearithmic complexity analysis

Reference [1, Sec. 3.3.3] shows that the basic IFGF algorithm runs on a linearithmic \( (\mathcal{O}(N \log N)) \) number of arithmetic operations. The present section, in turn, shows that the communication cost additionally required by the proposed MPI-OpenMP parallel IFGF algorithm also grows linearithmically—thus, establishing that, on a fixed number of cores, the parallel algorithm runs on an linearithmic overall computing time.

To do this, in view of the data distribution strategy described in Section 3.2.1, it suffices to ensure that both the Interpolation and Propagation functions require a linearithmic communication cost. Inspection of the corresponding Algorithms 10 and 11 (specifically, lines 4 and 5, respectively) shows that these functions, and, thus, the overall parallel IFGF algorithm, only require communication of certain polynomial coefficients—a task that is effected via the communication Algorithms 13 and 12, respectively. Thus, the analysis of the communication cost amounts to counting the number of coefficients that are communicated, including multiple counts for coefficients that are communicated to multiple ranks, as a result of the application of these two communication algorithms within the overall IFGF algorithm.

In order to count the number of communications effected by each one of these algorithms we proceed as follows. Noting that, since, 1) As indicated in [1, Sec. 3.3.3], there are \( \mathcal{O}(N) \) relevant cone segments per level, each one of which contains \( \mathcal{O}(1) \) data (namely, the \( P \) coefficients of a single polynomial interpolant); 2) Each cone-segment data is stored in exactly one MPI rank (Section 3.2.1); and, as discussed below for both communication algorithms, 3) Each relevant cone segment is communicated to a uniformly bounded number of MPI ranks at each level \( d = 3, \ldots, D \); it follows that for each level \( d \) \( (3 \leq d \leq D) \) a total of \( \mathcal{O}(N) \) coefficients are communicated by each of the communication algorithms 12 and 13 for each one of the \( D = \log N \) levels, at a total communication cost of \( \mathcal{O}(N \log N) \) coefficients by this algorithm, as desired.

It remains for us to show that point 3) above holds for both communication algorithms. In the case of the propagation communication we note that each relevant cone segment on any level \( d = D, \ldots, 4 \) is split into eight smaller cone segments on the parent level \( (d - 1) \). Thus, for each level-\( d \) relevant cone segment, this results in at most \( K \) parent-level cone segments (usually \( K = 8 \), or possibly a slightly higher number owing to the re-centering procedure associated with the Propagation function, but most often \( K = 1 \) that could be targets for the interpolation procedure in the Propagation function. In view of point 2) above, each level-\( d \) relevant cone segment must thus communicate coefficients to no more than \( \mathcal{O}(1) \) ranks, and point 3) follows in this case.

In the case of the interpolation communication, finally, relevant cone-segment coefficients need to be communicated to ranks that store surface discretization points included in boxes that are cousins of the box co-centered with the relevant cone segment. First, on the lowest level \( D \), each relevant box has at most \( K = 189 \) cousin boxes and since, by design, the surface discretization points contained within each one of the smallest boxes are stored in a single MPI rank (Section 3.2.1), it follows that \( \mathcal{O}(1) \) (at most \( 189 \)) different MPI ranks require coefficients contained in each relevant cone segment. Further, since each cone segment is partitioned into eight in the transition from a given level \( d \) to a subsequent level \( (d - 1) \) (so that the number of relevant level-\( D \) boxes contained within a level-\( (d - 1) \) cone equals approximately
Algorithm 14 IFGF Method

1: LevelDEvaluations()
2: CommunicatePropagationData(D)
3:
4: for d = D, . . . , 3 do
5: \hspace{1em} CommunicateInterpolationData(d)
6: \hspace{1em} if d > 3 then
7: \hspace{2em} Propagation(d)
8: \hspace{1em} if d > 4 then
9: \hspace{2em} CommunicatePropagationData(d − 1)
10: \hspace{1em} end if
11: \hspace{1em} end if
12: \hspace{1em} Interpolation(d)
13: end for

one-fourth of the corresponding number for level-\(d\) cone segments, since \(\Gamma_N\) is a discretization of a 2D surface), and since, conversely, the number of MPI ranks storing surface discretization points within a cousin box increases by approximately a factor four in the same \(d\)-to-(\(d−1\)) transition, the number of communications per relevant cone segment remains essentially constant as a result of the \(d\)-to-(\(d−1\)) level transition. It follows that each relevant cone segment is communicated to a \(\mathcal{O}(1)\) number of MPI ranks for all levels \(d\), thus establishing the validity of point 3) for the interpolation communication function, and completing the proof of linearithmic complexity of the proposed parallel IFGF algorithm.

4 Numerical Results

Our numerical examples focus on three simple geometries which coincide with the test cases presented in [1]: a sphere of radius \(a\), the oblate spheroid \(x^2 + y^2 + (z/0.1)^2 = a^2\) and the prolate spheroid \(x^2 + y^2 + (z/10)^2 = a^2\). The latter two geometries are depicted in Figure 4. In what follows the diameter (also referred to as the “size”) of a geometry \(\Gamma\) is denoted by

\[
d := d(\Gamma) := \max_{x,y \in \Gamma} |x − y|,
\]

(not to be confused with the level index \(d\) introduced in Section 2); clearly we have \(d = 2a\) in the case of the sphere and the oblate spheroid geometries and \(d = 20a\) for the prolate spheroid geometry. These relatively simple geometries present the same kinds of challenges, in the context of the IFGF method, that arise in a wide range of real-world problems, including aircraft, lenses and meta-materials (with a point distribution somewhat similar to that in an oblate spheroid), submarines (prolate spheroid), etc. For example, even though the problem of finding a scattering solution for a submarine is much more challenging than the corresponding problem for a spheroid of the same size, in view of the need for accurate integration of singular kernels and adequate representation of the surface Jacobians, the performance of the IFGF method for the evaluation of the discrete operator (1) for a submarine should not differ significantly from the corresponding performance on a prolate spheroid of a comparable discretization, point distribution and electromagnetic size.

In what follows we present IFGF performance data based on various runs for these geometries. For our examples we utilize discretizations \(\Gamma_N\) obtained from use of parametrized surface patches covering \(\Gamma\) and equispaced partitioning of the corresponding parameter spaces. The computer used is described briefly prior to the beginning of Section 3.1 and, in more detail, in the Supplementary Materials Section SM2.1. The strong and weak efficiency and speedup scalability concepts are detailed in Section SM2.4; briefly, relative to a base core-number \(N_0^c\), the \(N_c\)-core run speedup \(S_{N_0^c,N_c}\) and the weak and strong efficiencies \(E_{N_0^c,N_c}^w\)
and $E_{N_c}^{s_0}$ are used to characterize the effectiveness of the proposed parallelization schemes by relating computing times and core numbers under weak-scaling tests (in which $N_c$ is increased proportionally to the size $N$ of the discretization $\Gamma_N$) and strong-scaling tests (wherein $N_c$ is increased as $N$ is held fixed).

| $\Gamma$         | $N$           | $d$        | Nodes $N_c$ | $\varepsilon$ | $T$ (s)   | $E_{N_c}^{w} (\%)$ | $E_{N_c}^{w}^{s_0,N_c}$ |
|-------------------|---------------|------------|-------------|--------------|-----------|-------------------|------------------------|
| Sphere            | 1,572,864     | 128$\lambda$ | 1           | 56           | $2 \times 10^{-3}$ | $7.77 \times 10^1$ | 100                    | -                      |
|                   | 6,291,456     | 256$\lambda$ | 4           | 224          | $2 \times 10^{-3}$ | $9.78 \times 10^1$ | 87                     | 87                     |
|                   | 25,165,824    | 512$\lambda$ | 16          | 896          | $2 \times 10^{-3}$ | $1.34 \times 10^2$ | 69                     | 79                     |
| Oblate Spheroid   | 1,572,864     | 128$\lambda$ | 1           | 56           | $7 \times 10^{-4}$ | $2.99 \times 10^1$ | 100                    | -                      |
|                   | 6,291,456     | 256$\lambda$ | 4           | 224          | $6 \times 10^{-4}$ | $4.17 \times 10^1$ | 79                     | 79                     |
|                   | 25,165,824    | 512$\lambda$ | 16          | 896          | $8 \times 10^{-4}$ | $5.74 \times 10^1$ | 62                     | 79                     |
| Prolate Spheroid  | 6,291,456     | 256$\lambda$ | 1           | 56           | $5 \times 10^{-4}$ | $4.97 \times 10^1$ | 100                    | -                      |
|                   | 25,165,824    | 512$\lambda$ | 4           | 224          | $6 \times 10^{-4}$ | $6.83 \times 10^1$ | 79                     | 79                     |
|                   | 100,663,296   | 1,024$\lambda$ | 16         | 896          | $7 \times 10^{-4}$ | $9.29 \times 10^1$ | 63                     | 79                     |

Table 1: Weak scaling test transitioning from 1 to 4 nodes, and then from 4 to 16 nodes, for three different geometries. The number of nodes, each one containing $N_c = 56$ cores, is kept proportional to the number of surface discretization points, as required by the weak-scaling paradigm.

Table 1 demonstrates the weak IFGF parallel efficiency, for all three geometries considered, from a single compute node ($N_c^0 = 56$) to 4 and 16 compute nodes ($N_c = 224$ and 896, respectively). We find that the efficiency relative to the base $N_c^0 = 56$ case steadily decreases, but, importantly, the weak relative efficiency $E_{N_c}^{w}$ remains essentially constant as $N_c$ increases. Thus, under the assumption that this trend is maintained for arbitrarily large numbers of nodes (as is expected in view of the discussion in the first paragraph of Section 3.2 concerning absence of hard limitations on achievable parallelism), the parallel IFGF method is applicable to arbitrarily large problems—provided correspondingly large hardware is used—with a constant $\approx 80\%$ efficiency factor (cf. Table 1) as the problem and hardware sizes are both quadrupled from a given point of reference. Section SM2.5 demonstrates a similar quality of the proposed algorithm under strong-scaling tests.

The observed speedups under strong scaling tests, in turn, are displayed in Figure 5; additional details concerning these results are provided in Section SM2.5. This figure presents speedup tests for three test cases: a sphere of diameter $d = 128\lambda$ (where $\lambda = \frac{2\pi}{\kappa}$ denotes the wavelength and $d$ is given in (9)), and oblate and prolate spheroids (Figure 4) of large diameters $d = 128\lambda$ and $d = 256\lambda$, respectively. The curves in Figure 5 display, in each case, the observed speedup $S_{1,N_c}$ for $1 \leq N_c \leq 1,680$. In view of the requirements of the strong-scaling setup, test problems were selected that can be run in a reasonable time on a single core and with the memory available in the corresponding compute node. Clearly, such test problems tend to be too small to admit a perfect distribution onto large numbers of cores. As illustrated in Figure 5, however, in spite of this constraint, excellent scaling is observed in the complete range going from 1 core to 1,680 cores (30 nodes). As in the weak-scaling tests, further, there is no hard limitation on
scaling, even for such small problems, (once again, in line with the discussion presented in Section 3), and it is reasonable to expect that, unlike other approaches (for which either hard limits arise [15] as described in the first paragraph of Section 3.1, or which rely on memory duplication [17, 18]), the observed speedup continues to scale with the number of cores, as suggested by Figure 5, up to very large numbers of cores. The computing speedups achieved by the proposed parallel strategy outperform those achieved by other MPI-parallel implementations of FMM and other numerical methods [19, 21, 44], and can be best appreciated by noting that, instead of the e.g. approximately 40 minutes (2.54 × 10³ secs., see first line in Table SM1 in Section SM2.5) required by a single-core IFGF run, a total of 4.5 secs. (4.5 = 2.54 × 10³/S₁₁₆₈₀ secs., where, per Figure 5, S₁₁₆₈₀ = 565) suffices for the corresponding 1,680-core IFGF run. It is interesting to note that an approximately 1.51 second 1,680-core run would have resulted under perfect scaling.

Concluding this section, Figure 6 presents results of an investigation regarding the linearithmic scaling of the parallel IFGF method for the prolate spheroid geometry on a fixed number of nodes, namely, all 30 nodes available in the computer cluster we use, and for N ranging from 6,291,456 to 402,653,184, for corresponding diameters ranging from 512λ to 4,096λ. The data in this figure, which is also presented in tabular form in Table SM4, was generated by pinning a single MPI rank to each compute node, each of which spawns 56 OpenMP threads, with parameters resulting in an IFGF error ε ≈ 1.5 × 10⁻² (cf. equation (SM2)). The results show that the linearithmic algorithmic complexity and memory requirements of the basic IFGF algorithm are maintained in the parallel setting. Indeed, the observed complexity even slightly outperforms the postulated $\mathcal{O}(N \log N)$ within this range of values of N; cf. Table SM4 which suggests convergence to exact linearithmic complexity as N grows.

5 Concluding Remarks

This paper presented a parallel version of the IFGF acceleration method introduced in [1], demonstrating in practice excellent parallel scaling to large core numbers while simultaneously preserving the linearithmic complexity of the sequential IFGF algorithm. The proposed parallelization approach exploits the box-cone octree structure inherent in the IFGF method, resulting in a strategy that, per the theoretical discussion in Section 3.1 and in the first paragraph of Section 3.2, is applicable to arbitrarily large number of processing cores, and it thereby does not suffer from bottlenecks or hard limits inherent in approaches that orchestrate the parallelization on the basis of octree-box partitioning only. A number of additional questions are left for future work, as briefly mentioned in what follows. On one hand, the feasibility of implementations
Figure 6: Illustration of the linearithmic complexity of the parallel IFGF method (which had previously been demonstrated [1] for the serial version of the algorithm), for the prolate spheroid geometry, on 30 compute nodes, with error $\varepsilon \approx 1.5 \times 10^{-2}$. The acoustic diameter of the ellipsoid is kept proportional to $\sqrt{N}$, and it ranges from $512\lambda$ to $4,096\lambda$. Clearly, the parallel implementation preserves (and, in fact, slightly improves upon) the ideal linearithmic scaling. For this test one MPI rank per node and 56 OpenMP threads per MPI rank were used (resulting in 1680 cores). The peak IFGF memory used per MPI rank (excluding the memory required to store the initial geometry) as well as other additional data in tabular form are presented in Table SM4.

on heterogeneous architectures such as, e.g., computer systems that incorporate general purpose graphical processing units (GPUs), is currently under study. In particular, the use of GPUs to accelerate the interpolation processes, which represent the most time consuming part of the IFGF method, appears as highly promising avenue of inquiry. Additionally, minor modifications to the data-decomposition strategy introduced in Section 3.2.1 could be introduced to not only (approximately) equipartition the surface discretization points and cone segments among MPI ranks, but also incorporate the number of actual computations and the amount of data required from other MPI ranks in the partitioning scheme. Such an improved data-decomposition design could indeed be obtained by relying on minor adjustments to the cone and box intervals introduced in Section 3.2.1 leading to improved load-balancing, and, thus, improved parallel efficiency.

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SM1 Background: computing cluster systems

The proposed IFGF parallelization strategy is designed for implementation in modern high performance computing (HPC) cluster systems. The present section reviews relevant hardware and software concepts and nomenclature utilized throughout this paper; more detailed descriptions and alternative hardware designs can be found e.g. in [3, 4]. A modern computer cluster consists of multiple compute nodes. Each node contains its own memory space, and thus the memory in the cluster is distributed between the nodes. In particular, access to memory in other compute nodes requires explicit data communication, which is typically performed via the message passing interface (MPI) [4, Section 8]; the performance of algorithmic implementations for cluster systems can therefore significantly benefit from careful engineering of MPI-based inter-process data communications.

Each node typically comprises one or a few multi-core processors, each one of which, as the name suggests, contains multiple computing cores. The compute nodes typically are so-called shared memory machines (SMMs), where each core within the node can access all of the memory in the node. To efficiently make use of more than a single core, certain specialized programming techniques are required, e.g. the Intel Threading Building Blocks (TBB) library, the C++ standard threading model, MPI, or the OpenMP programming interface. Modern compute nodes usually follow a non-uniform memory access (NUMA) design (in contrast to uniform memory access (UMA)), where the access times to the shared memory depend on the locality of the memory with respect to the multi-core processor accessing it. This design typically results in one or more NUMA nodes per compute node, where memory access to other NUMA nodes on the same compute node is usually significantly slower than access to memory local to the processor. All of the tests presented in this paper were conducted on a small cluster consisting of thirty nodes connected via an InfiniBand interconnect, each one of which contains four fourteen-core NUMA nodes; additional details concerning the hardware used are provided in Section 4 and Supplementary Materials Sections SM2.1 and SM2.2.

On the basis of the functions and synchronization capabilities provided by MPI, a program can be launched as a set of multiple processes (which are identified in what follows by their corresponding integer-valued rank within the group of all processes launched by a given program). One of the main roles of the MPI standard is to allow the programmer to orchestrate the data communications between the ranks. Note that, at runtime, an MPI rank can be assigned, or pinned, to various kinds...
SM2 Supplementary Numerical Results

The present supplementary numerical results section expands on Section 4 in various ways. In particular, this section provides details on the hardware employed and the manner in which it is used (Sections SM2.1 and SM2.2, respectively), and, after detailing the method used for error evaluation (Section SM2.3) and the concepts used to evaluate strong and weak parallel efficiency (Section SM2.4), it presents detailed strong parallel scaling results in Section SM2.5 and data regarding the linearithmic ($O(N \log N)$) scaling tests in Section SM2.6.

SM2.1 Compiler and hardware

The proposed parallel IFGF program was implemented in C++, and the resulting code was compiled with the Intel mpiicpc compiler, version 2021.1, and the Intel MPI library. The following performance-relevant compiler flags were used: -std=c++20, -O3, -ffast-math, -qopt-zmm-usage=high, -no-prec-sqrt, -no-prec-div. All tests were run on our internal Wavefield cluster which consists of 30 dual-socket nodes. Each node consists of two Intel Xeon Platinum 8276 processors with 28 cores per processor, i.e. 56 cores per node, and 384 GB of GDDR4 RAM per node. (The Xeon processors we use support hyper-threading, but this capability was not exploited in any of our tests presented in this paper.) The nodes are connected with HDR Infiniband.

SM2.2 Hardware pinning

As indicated in Section 3, since each compute node in the Wavefield cluster consists of four NUMA nodes, we run four MPI ranks per node each pinned to one of these four NUMA nodes through setting the environment variable “I_MPI_PIN_DOMAIN=cache3”. The shared memory parallelization with OpenMP is then used for the parallelization within each MPI rank, i.e., within a NUMA node. The parallel scaling within a NUMA node from 1 to 14 cores is investigated below using the OpenMP specific environment variables “OMP_NUM_THREADS=[1-14]”, “OMP_PLACES=cores”, and “OMP_PROC_BIND=true”. The continued scaling, which is achieved with the MPI parallelization when exceeding 14 cores, is investigated going from one to four MPI ranks (each rank pinned to one NUMA node in the same compute node), which corresponds to the MPI scaling on a single, shared-memory node. Finally, the scaling of the MPI based distributed-memory parallelization is investigated starting from a single node to 16 nodes, where each node is fully utilized with four MPI ranks per node and fourteen cores per rank, as described above. A different hardware pinning used for the test cases presented in Section SM2.6 is described separately in that section.

SM2.3 Numerical error estimation

The errors reported in what follows were computed as indicated in [2], that is, the relative $L_2$ difference $\varepsilon_M$ between the full, non-accelerated evaluation of the field $I(x)$, as stated in (1), and the IFGF-accelerated evaluation $I_{\text{acc}}(x)$ of (1) computed on a randomly chosen subset of $M$ surface
discretization points. More precisely, the error is given by
\[ \varepsilon_M = \sqrt{\sum_{i=1}^{M} |I(x_{\sigma(i)}) - I_{\text{acc}}(x_{\sigma(i)})|^2 / \sum_{i=1}^{M} |I(x_{\sigma(i)})|^2}, \]  
where \( \sigma \) is a random permutation and \( x_\ell \in \Gamma_N \) denote the surface discretization points. The method used in [2] is suitably extended to the present MPI parallel implementation by using a set of test points \( x_\ell \) that contains a number \( M = 1000 \) of randomly chosen points on each MPI rank. (In [2] it was shown for sufficiently small examples that an error evaluation on a subset of 1000 points produces an error estimation close to the actual error.) More precisely, 1000 surface discretization points are randomly chosen on each MPI rank from the distinct set of surface discretization points \( \Gamma_{N,\rho} \) each MPI rank \( \rho (1 \leq \rho \leq N_r) \) is responsible for based on the distribution introduced in Section 3.2. The final errors are then accumulated resulting in the overall error estimate
\[ \varepsilon := \varepsilon_M \text{ at } M = 1000 \times N_r \text{ points.} \]  
As a result, the errors are dependent on the number \( N_r \) of MPI ranks, which is the reason the shown errors vary slightly as the number of MPI ranks varies (cf. Tables SM2 and SM3). All tests were set up in such a way that an error of approximately \( 10^{-3} \) is achieved, although, the IFGF method can achieve arbitrarily small errors.

**SM2.4 Weak and strong parallel efficiency concepts**

Let \( T(N_c, N) \) denote the time required by a run of the parallel IFGF algorithm on an \( N \)-point discretization \( \Gamma_N \), with a given and fixed discretization scheme, of a given surface \( \Gamma \) using \( N_c \) cores. Using this notation, for a given \( N \), the strong parallel efficiency \( E_{N_0^0,N_c}^s \) that results as the number of cores is increased from \( N_0^0 \) to \( N_c \) is defined as the quotient of the resulting speedup \( S_{N_0^0,N_c} \) to the corresponding ideal speedup value \( S_{N_0^0,N_c}^{\text{ideal}} \):
\[ S_{N_0^0,N_c}^{\text{ideal}} := \frac{N_c}{N_0^0}, \quad S_{N_0^0,N_c} := \frac{T(N_0^0, \Gamma_N)}{T(N_c, \Gamma_N)}, \quad E_{N_0^0,N_c}^s := \frac{S_{N_0^0,N_c}}{S_{N_0^0,N_c}^{\text{ideal}}}. \]

Note that the implicit dependence on \( N \) and \( \Gamma_N \) is suppressed in the speedup and efficiency notations.

The weak parallel efficiency \( E_{N_0^0,N_c}^w > 0 \), in turn, concerns the computing costs that are observed as the numbers \( N_c \) of cores are increased proportionally to the problem size \( N \)—effectively keeping the number of surface discretization points per core constant—so that as the numbers of cores and discretization points are simultaneously increased from \( N_0^0 \) to \( N_c \) and from \( N_0^0 \) to \( N \), respectively, the relation
\[ N/N_0^0 = N_c/N_0 \]  
is satisfied. Since the weak scaling concerns varying numbers \( N \) of surface discretization points, however, the weak parallel-efficiency concept must correctly account for the linearithmic theoretical scaling of the IFGF algorithm. To do this, we consider the computing time \( T(N_c, N) \) required for a run of the algorithm on \( N_c \) cores for an \( N \)-point discretization of a given, fixed, surface \( \Gamma \). In view
of the linearithmic complexity of the algorithm, perfect weak parallel efficiency would be observed if, for a certain constant \( K \), we had

\[
T(N_c, N) = \frac{K}{N_c} N \log N.
\]

Thus is to say, under perfect weak parallel scaling, in view of (SM3) we would have

\[
\frac{T(N_c, N)}{T(N_c^0, N^0)} = \frac{N^0_c N \log N}{N_c N^0 \log N^0} = \frac{\log N}{\log N^0}.
\]

We therefore define the \textit{weak parallel efficiency} that results as the number of cores is increased from \( N_c^0 \) to to \( N_c \) by

\[
E_{N_c^0, N_c}^{w} := \frac{T(N_c^0, N^0) \log N}{T(N_c, N) \log N^0}.
\]

Note that \( E_{N_c^0, N_c}^{w} = 1 \) corresponds to perfect weak parallel efficiency, or a weak parallel efficiency of 100%.

| \( \Gamma \) | \( N \) | \( d \) | \( N_c \) | \( \varepsilon \) | \( T \) (s) | \( E_{1,N_c}^w \) (%) | \( S_{1,N_c} \) |
|----------------|--------|--------|--------|--------|--------|----------------|--------|
| Sphere         | 1,572,864 | 128\( \lambda \) | 1      | \( 2 \times 10^{-3} \) | \( 2.54 \times 10^3 \) | 100  | 1.00        |
|                |         |        | 2      |                      | \( 1.29 \times 10^3 \) | 98   | 1.95        |
|                |         |        | 4      |                      | \( 6.91 \times 10^2 \) | 92   | 3.67        |
|                |         |        | 8      |                      | \( 3.63 \times 10^2 \) | 87   | 6.98        |
|                |         |        | 14     |                      | \( 2.31 \times 10^2 \) | 78   | 10.98       |
| Oblate Spheroid| 1,572,864 | 128\( \lambda \) | 1      | \( 5 \times 10^{-4} \) | \( 9.42 \times 10^2 \) | 100  | 1.00        |
|                |         |        | 2      |                      | \( 4.86 \times 10^2 \) | 97   | 1.94        |
|                |         |        | 4      |                      | \( 2.60 \times 10^2 \) | 91   | 3.62        |
|                |         |        | 8      |                      | \( 1.40 \times 10^2 \) | 84   | 6.69        |
|                |         |        | 14     |                      | \( 8.76 \times 10^1 \) | 77   | 10.75       |
| Prolate Spheroid| 6,291,456 | 256\( \lambda \) | 1      | \( 6 \times 10^{-4} \) | \( 1.42 \times 10^3 \) | 100  | 1.00        |
|                |         |        | 2      |                      | \( 7.29 \times 10^2 \) | 97   | 1.95        |
|                |         |        | 4      |                      | \( 4.33 \times 10^2 \) | 82   | 3.28        |
|                |         |        | 8      |                      | \( 2.37 \times 10^2 \) | 75   | 5.99        |
|                |         |        | 14     |                      | \( 1.49 \times 10^2 \) | 68   | 9.49        |

Table SM1: Strong parallel scaling test of the OpenMP IFGF implementation from \( N_c = 1 \) to \( N_c = 14 \) cores in a single node for three different geometries \( \Gamma \).

**SM2.5 Strong parallel efficiency tests**

Tables SM1, SM2, and SM3 present the strong parallel efficiencies achieved by the proposed parallel IFGF method under OpenMP, shared-memory MPI, and distributed-memory MPI parallelization strategies, respectively, each one for all three test geometries considered in this section. In detail, these tables display the main two strong parallel performance quantifiers, namely the observed
strong parallel efficiency $E_{N_0, N_c}^s$ and speedup $S_{N_0, N_c}$, along with the computing times $T$, the obtained accuracy $\varepsilon$, and details concerning the geometry and the discretizations. The tables clearly show that, in all cases, the IFGF parallel efficiencies are essentially independent of the geometry type. With reference to Section SM2.2 above, the ranges of the parameter $N_c$ considered in these tables span all of the available cores in each one of the relevant hardware units used: 14 cores in a single NUMA node, 56 cores (4 NUMA nodes) in a single compute node, and 16 nodes in the complete cluster (the largest number of nodes which equals a power of 2 in the cluster used).

| $\Gamma$      | $N$          | $d$  | $N_r$ | $N_c$ | $\varepsilon$ | $T$ (s)  | $E_{14,N_c}^s$ (%) | $S_{14,N_c}$ |
|---------------|--------------|------|-------|-------|---------------|---------|-------------------|-------------|
| Sphere        | 1,572,864    | 128$\lambda$ | 1     | 14    | $2 \times 10^{-3}$ | 2.31 $\times 10^2$ | 100               | 1.00        |
|               |              |       | 2     | 28    | $2 \times 10^{-3}$ | 1.49 $\times 10^2$ | 77                | 1.54        |
|               |              |       | 4     | 56    | $2 \times 10^{-3}$ | 7.77 $\times 10^1$ | 74                | 2.97        |
| Oblate Spheroid | 1,572,864    | 128$\lambda$ | 1     | 14    | $5 \times 10^{-4}$ | 8.76 $\times 10^1$ | 100               | 1.00        |
|               |              |       | 2     | 28    | $6 \times 10^{-4}$ | 5.71 $\times 10^1$ | 77                | 1.53        |
|               |              |       | 4     | 56    | $6 \times 10^{-4}$ | 2.99 $\times 10^1$ | 73                | 2.93        |
| Prolate Spheroid | 6,291,456    | 256$\lambda$ | 1     | 14    | $6 \times 10^{-4}$ | 1.49 $\times 10^2$ | 100               | 1.00        |
|               |              |       | 2     | 28    | $6 \times 10^{-4}$ | 9.10 $\times 10^1$ | 82                | 1.65        |
|               |              |       | 4     | 56    | $5 \times 10^{-4}$ | 4.97 $\times 10^1$ | 75                | 3.01        |

Table SM2: Strong parallel scaling test of the shared-memory MPI implementation on a single node, transitioning from $N_c = 14$ cores to $N_c = 56$ (all cores available in one compute node) by increasing the number $N_r$ of MPI ranks from 1 to 4, for three different geometries $\Gamma$.

The largest efficiency deficit observed as a result of a hardware-doubling transition is the decrease by a full 23% (from 100% to 77%) shown in Table SM2, which results from the transition from one to two MPI ranks (that is, from one to two 14-core NUMA nodes). We argue that this deficit, which takes place precisely as an MPI communication between NUMA nodes is first introduced, is not a sole reflection of the character of the algorithm in presence of the MPI interface, since such large deficits are not observed in any other MPI related hardware-doubling transitions reported in the various tables. As potential additional contributing elements to this deficit we mention notably, MPI overhead (which would only be incurred in the first doubling transition but not in subsequent doubling transitions, in view of the decreasing number of pairwise communications incurred by the algorithm under a doubling transition in a strong scaling test, as indicated by the theoretical discussion in Section 3.3), and the Intel Turbo Boost Technology inherent in the processors used—which achieve maximum turbo frequencies when running under lower loads, and which, when concurrently using larger numbers of cores in a single node, cease to operate.

A variety of other data is presented in these tables. Tables SM1 and SM2, which demonstrate the strong scaling within a single NUMA node, and among all four NUMA nodes within a compute node, are included for completeness, but as discussed below, we attach far greater significance to Table SM3, which demonstrates the scaling of the method under the one hardware element that can truly be increased without bounds, namely, the number of compute nodes. In this table, geometries twice as large than those used for the previous two tables are considered (to reasonably increase the minimum computing times), and the hardware is scaled from one compute node to sixteen compute nodes. Per the description in Section SM2.2, each node is assigned four MPI ranks, each one of
which is pinned to one of the four NUMA nodes present in the compute node. Overall, a strong scaling efficiency of over 60% can be observed in all cases, with the results of the sphere test case even above 70% owing to the symmetry of the geometry and the resulting increased load-balance and minimized communication between ranks. The loss of efficiency can be attributed the load-imbalance induced by our data partitioning strategy, the communication between ranks, and the parallelization overhead introduced by MPI and OpenMP.

Table SM3: Strong parallel scaling test of the distributed-memory MPI implementation from \( N_c = 56 \) to \( N_c = 896 \) cores (1 to 16 compute nodes) with 4 MPI ranks per node for three different geometries \( \Gamma \).

| \( \Gamma \) | \( N \) | \( d \) | \( N_c \) | \( \varepsilon \) | \( T \) (s) \( 10^{-3} \) | \( E_{56,N_c}^{s,*} \) (%) | \( S_{56,N_c} \) | \( E_{N_c,N_c}^{s,*} \) |
|-------------|-----|-----|-----|-----|--------|--------|-------|-------|
| Sphere      | 6,291,456 | 256\( \lambda \) | 56  | \( 2 \times 10^{-3} \) | \( 3.55 \times 10^2 \) | 100 | 1.00 | -    |
|             |       |     | 112 | \( 2 \times 10^{-3} \) | \( 1.80 \times 10^2 \) | 99  | 1.97 | 99   |
|             |       |     | 224 | \( 2 \times 10^{-3} \) | \( 9.78 \times 10^1 \) | 91  | 3.64 | 92   |
|             |       |     | 448 | \( 2 \times 10^{-3} \) | \( 5.52 \times 10^1 \) | 81  | 6.44 | 89   |
|             |       |     | 896 | \( 2 \times 10^{-3} \) | \( 3.12 \times 10^1 \) | 71  | 11.40 | 89 |
| Oblate Spheroid | 6,291,456 | 256\( \lambda \) | 56  | \( 6 \times 10^{-4} \) | \( 1.34 \times 10^2 \) | 100 | 1.00 | -    |
|             |       |     | 112 | \( 6 \times 10^{-4} \) | \( 7.41 \times 10^1 \) | 91  | 1.81 | 91   |
|             |       |     | 224 | \( 6 \times 10^{-4} \) | \( 4.17 \times 10^1 \) | 80  | 3.22 | 89   |
|             |       |     | 448 | \( 6 \times 10^{-4} \) | \( 2.38 \times 10^1 \) | 70  | 5.64 | 88   |
|             |       |     | 896 | \( 6 \times 10^{-4} \) | \( 1.40 \times 10^1 \) | 60  | 9.56 | 85   |
| Prolate Spheroid | 25,165,824 | 512\( \lambda \) | 56  | \( 4 \times 10^{-4} \) | \( 2.23 \times 10^2 \) | 100 | 1.00 | -    |
|             |       |     | 112 | \( 5 \times 10^{-4} \) | \( 1.22 \times 10^2 \) | 92  | 1.83 | 92   |
|             |       |     | 224 | \( 6 \times 10^{-4} \) | \( 6.83 \times 10^1 \) | 82  | 3.28 | 89   |
|             |       |     | 448 | \( 6 \times 10^{-4} \) | \( 3.74 \times 10^1 \) | 75  | 5.97 | 91   |
|             |       |     | 896 | \( 6 \times 10^{-4} \) | \( 2.23 \times 10^1 \) | 63  | 10.01 | 84 |

The most important quality illustrated in these tables is the IFGF’s efficiency performance under strong-scaling hardware-doubling transitions demonstrated in the last column of Table SM3. This performance, which mirrors the corresponding weak-scaling performance presented in the last column of Table 1, shows that, as in the weak scaling case, under the assumption that the displayed trend is maintained for large numbers of nodes (below the obvious limit imposed by the fixed problem size), the parallel IFGF method for a fixed problem can be efficiently run in large numbers of computing cores—with an efficiency factor no worse than a constant \( \approx 80\% \) as the hardware sizes are doubled from a given point of reference.

The character of the IFGF algorithm under weak- and strong-scaling hardware-doubling tests, as discussed above in this section and in Section 3.3, would ensure that, provided the demonstrated trends are maintained (as is expected in view of the discussion in the first paragraph of Section 3.2), the method can be executed successfully in very large hardware infrastructures.
SM2.6 Linearithmic scaling

Table SM4 presents numerical data related to the test case considered in Figure 6, which concerns the linearithmic scaling of the parallel IFGF method on a fixed and large number of cores. As indicated in Section 4, the data in the figure and table were generated by pinning a single MPI rank to each compute node, each of which spawns 56 OpenMP threads on each one of the 30 nodes available in the computer cluster we use, with parameters resulting in an IFGF error $\varepsilon \approx 1.5 \times 10^{-2}$ (cf. equation (SM2)). The observed complexity slightly outperforms the postulated $O(N \log N)$ estimate within this range of values of $N$. Note, in particular, the last column of Table SM4 which suggests rapid convergence to exact linearithmic complexity, with a well defined proportionality constant, as $N$ grows.

| $\Gamma$          | $N$     | $d$     | $N_c$ | $\varepsilon$ | $T$ (s)  | Mem/rank | $T/(N \log N)$ |
|-------------------|---------|---------|-------|---------------|----------|-----------|----------------|
| Prolate Spheroid  | 6,291,456 | 512$\lambda$ | 1,680 | $1.5 \times 10^{-2}$ | 4.09 $\times$ 10^6 | 0.50 GB | 9.56 $\times$ 10^{-8} |
|                   | 25,165,824 | 1,024$\lambda$ |       |               | 1.64 $\times$ 10^1  | 1.89 GB | 8.83 $\times$ 10^{-8} |
|                   | 100,663,296 | 2,048$\lambda$ |       |               | 6.71 $\times$ 10^1  | 7.42 GB | 8.33 $\times$ 10^{-8} |
|                   | 402,653,184 | 4,096$\lambda$ |       |               | 2.90 $\times$ 10^2  | 29.73 GB | 8.37 $\times$ 10^{-8} |

Table SM4: Preservation of the linearithmic IFGF scaling in the parallel context. One MPI rank per node and 56 OpenMP threads per MPI rank on 30 compute nodes for a prolate spheroid geometry were used for this test. The peak memory per MPI rank used by the IFGF method (excluding the memory required to store the initial geometry) is listed in the next-to-last column. The value in the last column suggests convergence to exact $O(N \log N)$ scaling.

SM2.7 Large sphere tests

Table SM5 illustrates the performance of the IFGF method in terms of computing time and memory requirements for several large-sphere configurations, all of them run on our full 30 node, 1,680 core cluster. In particular, Table SM5 shows that, as mentioned in Section 1, on the basis of approximately 4 TB of memory, a sphere 1,389$\lambda$ in diameter (which, as described below, corresponds to the case $f = 238.086$KHz considered in [1]) with 2.12 billion DOF was run in a computing time of 2,380 seconds with a 0.5% near-field error (which may be compared to the only error indicator reported in [1, Table 2] for this test case, which amounts to 20%, and compared to the 3% near-field solution error reported in the same table of that paper for significantly smaller problems). The computing time reported for this test case is a factor of approximately 46 times longer than the time reported in [1], for the same number of DOFs and sphere size, on a computer 78 times larger (containing 131,072 cores) and on the basis of an unspecified amount of memory.
Table SM5: Large sphere test cases run on thirty 56-core compute nodes (for a total of 1,680 cores), utilizing thirty MPI ranks. The sphere of acoustic size 1,389λ in this table coincides with largest sphere test case considered in [1].

As indicated above, the sphere 1,389λ in diameter in this table coincides with largest sphere test case considered in [1], which is cited in Table 2 in that reference as a sphere of two-meters in diameter illuminated at the frequency of \( f = 238.086 \) KHz under the speed of sound \( c = 343 m/s \) assumed in that reference. (The number of wavelengths in this two-meter sphere test case equals \( 2 \) meters/\( \lambda = 2f/c = 2 \cdot 238,086/343 \approx 1,388.26 < 1,389 \).) The largest discretization presented in the present table for this sphere test-case (2,120,640,000 discretization points, a limit induced by the largest number representable by a signed 32-bit integer assumed in our geometry-generation code, which will be avoided in subsequent code implementations by switching to 64-bit integers), is slightly smaller than the 2,300,067,840 discretization considered in [1] under a 131,072 core run.

Other test cases listed in Table SM5 include an example for a much larger sphere, 2,048λ in diameter, as well as other 1,389λ test cases for various accuracies and discretization sizes—and, in all cases, on the basis of memory consumptions ranging between \( \approx 1.2TB \) and \( \approx 4TB \).

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