RECURSIVE ALGORITHMS FOR DISTRIBUTED FORESTS OF OCTREES

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Abstract. The forest-of-octrees approach to parallel adaptive mesh refinement and coarsening (AMR) has recently been demonstrated in the context of a number of large-scale PDE-based applications. Efficient reference software has been made freely available to the public both in the form of the standalone p4est library and more indirectly by the general-purpose finite element library deal.II, which has been equipped with a p4est backend.

Although linear octrees, which store only leaf octants, have an underlying tree structure by definition, it is not often exploited in previously published mesh-related algorithms. This is because the branches are not explicitly stored, and because the topological relationships in meshes, such as the adjacency between cells, introduce dependencies that do not respect the octree hierarchy. In this work we combine hierarchical and topological relationships between octree branches to design efficient recursive algorithms that operate on distributed forests of octrees.

We present three important algorithms with recursive implementations. The first is a parallel search for leaves matching any of a set of multiple search criteria, such as leaves that contain points or intersect polytopes. The second is a ghost layer construction algorithm that handles arbitrarily refined octrees that are not covered by previous algorithms, which require a 2:1 condition between neighboring leaves. The third is a universal mesh topology iterator. This iterator visits every cell in a domain partition, as well as every interface (face, edge and corner) between these cells. The iterator calculates the local topological information for every interface that it visits, taking into account the nonconforming interfaces that increase the complexity of describing the local topology. To demonstrate the utility of the topology iterator, we use it to compute the numbering and encoding of higher-order C⁰ nodal basis functions used for finite elements.

We analyze the complexity of the new recursive algorithms theoretically, and assess their performance, both in terms of single-processor efficiency and in terms of parallel scalability, demonstrating good weak and strong scaling up to 458k cores of the JUQUEEN supercomputer.

Key words. forest of octrees, parallel adaptive mesh refinement, Morton code, recursive algorithms, large-scale scientific computing

AMS subject classifications. 65M50, 68W10, 65Y05, 65D18

1. Introduction. The development of efficient and scalable parallel algorithms that modify computational meshes is necessary for resolving features in large-scale simulations. These features may vanish and reappear, and/or evolve in shape and location, which stresses the dynamic and in-situ aspects of adaptive mesh refinement and coarsening (AMR). Both stationary and time-dependent simulations benefit from flexible and fast remeshing and repartitioning capabilities, for example when using a-posteriori error estimation, building mesh hierarchies for multilevel solvers for partial differential equations (PDEs), or tracking of non-uniformly distributed particles by using an underlying adaptive mesh.

Three main algorithmic approaches to AMR have emerged over time, which we may call unstructured (U), block-structured (S), and hierarchical or tree-based (T) AMR. Just some examples that integrate parallel processing are (U) 16, 20, (S) 7, 12, 17, 18, and (T) 24, 26. While these approaches have been developed independently

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of one another, there has been a definite crossover of key technologies. The graph-based partitioning algorithms traditionally used in UAMR have for instance been supplemented by fast algorithms based on coordinate partitioning and space-filling curves (SFCs) [9]. Hierarchical ideas and SFCs have also been applied in SAMR packages to speed up and improve the partitioning [8, 10]. Last but not least, the unstructured meshing paradigm can be employed to create a root mesh of connected trees when a nontrivial geometry needs to be meshed by forest-of-octrees TAMR [14].

The three approaches mentioned above differ in the way that the mesh topology information is passed to applications. With UAMR, the mesh is usually represented in memory as some kind of adjacency graph, and the application traverses the graph to compute residuals, assemble system matrices, etc. This approach has the advantages that local graph traversal operations typically have constant runtime complexity and that the AMR library can remain oblivious of the details of the application, but the disadvantages of less efficient global operations, such as locating the cell containing a point, and unpredictable memory access. On the other hand, the SAMR approach allows for common operations to be optimized and to use regular memory access patterns, but requires more integration between the AMR package and the application, and the application may not have the ability to operate on the topology in a way not anticipated by the AMR package.

Tree-based AMR can be integrated with an application for convenience [22], but can also be kept strictly modular [25]. The data structures in most TAMR packages support logarithmic-complexity algorithms for both global operations, such as point location, and local operations, such as adjacency queries. The paper [6] introduces the `p4est` library, which implements distributed forest-of-octree AMR with an emphasis on geometric and topological flexibility and parallel scalability, and connects with applications through a minimal interface.

The implementation of `p4est` does not explicitly build a tree data structure, so tree-based, recursive algorithms are largely absent from the original presentation [6]. Many topological operations on octrees and quadrees, however, are naturally expressed as recursive algorithms, which have simple descriptions and often have good, cache-oblivious memory access patterns. In this paper, we present, analyze, and demonstrate the efficiency of algorithms for important hierarchical and topological operations: searching for leaves matching multiple criteria in parallel, identifying neighboring domains from minimal information, and iterating over mesh cells and interfaces. Each algorithm has a key recursive component that gives it an advantage over previously developed non-recursive algorithms, such as improved efficiency, coverage of additional use cases, or both. We demonstrate the per-process efficiency of these algorithms, as well as their parallel scalability on JUQUEEN [15], a Blue Gene/Q supercomputer.

2. Preliminaries. Here we present a brief overview of the important concepts on which we build our algorithms. We review data structures that represent a distributed forest of octrees that were presented in [6]: we refer the reader interested in more detail to that work. In particular, that work covers the details of how a branch of an octree, called an octant, may be transformed into a neighboring octant, or an octant in a neighboring octree. The relationships between octants and lower-dimensional interfaces were not explored in much depth in that work, however, so we will define those relationships here, as they will be important in the algorithms that follow.

2.1. A forest of octrees. Essentially, a forest of octrees is a space partition consisting of two layers. The first or macro layer is defined by a conforming mesh of
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hexahedral root elements. This macro mesh is intended to match the topology of a given domain. The geometry can optionally be matched by a piecewise diffeomorphic mapping, which is of no consequence in the context of this article. Example geometries, which we will use in performance tests in Section 7 are illustrated in Figure 2.1. In 2D, we consider each root to be a manifold embedded in 3D space, thus it does not make sense to speak of right- or left-handed orientations. In 3D, we assume that the coordinate system of each root is right-handed. For complex domain shapes, the macro mesh can be created by any mesh generation software that outputs conforming hexahedra. It should be noted that the goal is to create relatively few macro elements and to leave further refinement to the second or micro layer, though in practice we have successfully used up to 10^6 macro elements.

The micro layer refers to the recursive adaptive refinement of each root element, which is interpreted as the root of a d = 2 quadtree or a d = 3 octree. This refinement by subdivision is isotropic: Each leaf element can be refined into 2^d children, where each coordinate direction is divided into two half spaces, all of which intersect in the center of the original leaf. Coarsening is the reversal of refinement and can be used to recursively unify all leaves of an octree until we return to the root element. The micro layer may be frequently modified by parallel refinement or coarsening algorithms during a simulation.

The ordering of leaves within one octree follows from a space-filling curve. The SFC index is not explicitly stored but implicitly derived from the coordinates of each leaf; in p4est we use the so-called z-ordering which corresponds to the Morton curve [19]. Combining first the octree number and then the SFC index imposes a total ordering over all leaves in the forest. In a parallel environment we partition the leaves by assigning consecutive ranges of leaves to the processes in increasing order or rank. In other words, if e_1 ≤ e_2 for the indices of two leaves, we know that the first leaf is assigned to (owned by) a lower or the same rank as the second, and belongs to a lower or the same octree. In p4est, we store only leaf octants, which we implement using per-octree arrays that are sorted in ascending Morton order. This concept is also known as a linear octree [25].
2.2. Data structures for distributed forests of octrees. The data structures that \textit{p4est} uses to describe a forest of octrees were designed to include a nearly minimal amount of replicated data. The salient aspects of that description are reviewed here, along with a few algorithms that were presented in \cite{6} that are reused in this work. The data structures and functions in this subsection are summarized in Table 2.1.

In the remainder of this article, $K$ denotes the number of octrees in the macro layer described above, $N$ the total number of leaves in the forest, and $P$ the number of processes that partition the leaves of the forest according to the space-filling curve. $N_p \geq 0$ is the number of leaves owned by process $p$, $0 \leq p < P$, $N = \sum_p N_p$. Note that the parallel partition is not limited to tree boundaries but may split same-tree leaves between distinct processes. Algorithms are written from the perspective of process $p$.

Because process $p$ owns a contiguous set of SFC indices, its range is contained in a contiguous range of octrees, which we denote $T_p$. For each $t \in T_p$, a process has a sorted array of leaves $O^t_p$, and we denote the union of these arrays $O_p := \cup_{t \in T_p} O^t_p$. We allow any process to be empty, in which case we have $T_p = \{\}$ and $O_p = \{\}$. The octant datatype will be described in the next subsection, but for now we note that each octant has a level of refinement, which is in $[0, \ell_{\text{max}}]$, with 0 being the level of the root of an octree and $\ell_{\text{max}}$ being the most refined. In this work, we call on algorithms \texttt{First\_descendant} and \texttt{Last\_descendant}—halves of the algorithm \texttt{Descendants} \cite{6} Algorithm 4—which construct the first and last level-$\ell_{\text{max}}$ descendants of an octant.

The topology of the macro layer—the adjacency of trees across faces, edges, and corners, and the relative orientation of their local coordinate systems—is replicated on each process. This allows each process to compute the local topological descriptions of octants that might exist outside of its own partition in $O(1)$ time.

Although a process does not have information about the leaves owned by other processes, it does know the region owned by every process. This information is stored as a sorted array $\mathcal{F}$ of level-$\ell_{\text{max}}$ octants, one for each process, which indicates the first such octant that could be owned by that process. With this information, each process can compute the process that owns octant $o$ via an algorithm \texttt{Find\_owner}(o) that runs in $O(\log P)$ time. For any $p$, one can also use $\mathcal{F}$ to compute $(f_p, l_p) := \texttt{Range}(p)$, the first and last level-$\ell_{\text{max}}$ octants in the range of process $p$, in $O(1)$ time. Indeed, $f_p$ is just $\mathcal{F}[p]$, and $l_p$ is just the octant whose SFC index immediately precedes $\mathcal{F}[p+1]$. (In practice, we never compute $l_p$ for empty processes, so we do not need the predecessor
of $F[0]$ to be defined.) We refer to the range $[f_p, l_p]$ as $\Omega_p$. We refer to the closure of the portion of $\mathbb{R}^d$ occupied by octants in the range $[f, l]$ as
\[
[f, l] := \bigcup_{o \in [f, l]} \bar{o}.
\]

(2.1)

2.3. Hierarchical and topological relationships. The algorithms we present involve both the hierarchical aspect of octrees and the topological aspect of the regions of space that they represent. Here, we outline our terminology for referring to octants, to the lower-dimensional interfaces between octants, and to the relationships that they have to each other.

The root, intermediate, and leaf nodes of an octree are all called octants. The root of an octree is identified with the $d$-cube $(0, 2^{\ell_{\text{max}}})^d$. An octant $o$ with level $\ell$ is an open $d$-cube with sides of length $h = 2^{\ell_{\text{max}}-\ell}$. Due to the recursive refinement procedure, the coordinates of the corners of $o$ are integer multiples of $h$; the coordinates of the corner of $o$ closest to the origin are used by \texttt{p4est} to identify $o$ and to define its space-filling curve index. In the algorithms in this work, the level of $o$ is written as $o.l$, its coordinates as the $d$-dimensional array $o.x$, and the index of its octree as $o.t$ (the latter is not stored explicitly, but always available from the context). We refer to the set of children of $o$ as $C(o)$: above, we constructively defined the children in terms of recursive refinement, but we can also define the set of children as
\[
C(o) := \{\text{octants } c \text{ such that } c.1 = o.1 + 1 \text{ and } c \subset o\}. \tag{2.2}
\]

We index $C(o)$ in SFC order, so $C(o)[i] < C(o)[j] \iff i < j$.

The boundary $\partial o$ of octant $o$ has a standard partition into lower-dimensional cubes. We refer to this partition as $B(o)$, the boundary set of $o$: it is a set containing $2^{d-n} \binom{d}{n}$ $n$-cubes. The union $\{o\} \cup B(o)$ is a partition of the closure $\bar{o}$ of $o$. When $d = 3$, we call 2-cubes faces, 1-cubes edges, and 0-cubes corners. When we index cubes in $B(o)$ based on which portion of $o$’s boundary the cubes cover, we use an index set $\mathbf{B}$, illustrated in Figure 2.2, which for $d = 3$ is made of $n_c = 8$ corner indices $\{c_i\}_{i=0}^7$, $n_e = 12$ edge indices $\{e_i\}_{i=0}^{11}$, and $n_f = 6$ face indices $\{f_i\}_{i=0}^5$.

Although only octants are present in the \texttt{p4est} datatypes, the presentation of the algorithms in this work is greatly simplified by treating the lower-dimensional cubes directly as first-class objects in the same manner as octants. To this end, we extend
the concepts that we have defined for octants to lower-dimensional cubes. Let \( c \) be an \( n \)-cube for \( 0 \leq n < d \); we say \( c \) has level \( \ell \) if there is an octant \( o \) with level \( \ell \) such that \( c \in B(o) \). We define \( C(c) \) to be the \( 2^n \) \( n \)-cubes with level \( \ell + 1 \) contained in \( c \), and we define \( B(c) \) to be the lower-dimensional cubes that partition its frontier \( \partial c \). A \( 0 \)-cube can be in the boundary sets of octants with different levels, so we define the level of a \( 0 \)-cube \( c \) to be the smallest such level, which corresponds to the largest octant \( o \) such that \( c \in B(o) \). For a \( 0 \)-cube \( c \), we also define \( C(c) := \{ c \} \) and \( B(c) := \{ \} \).

For \( n > 0 \), the children of an \( n \)-cube \( c \) alone do not partition \( c \), i.e., \( \cup_{e \in C(c)} e \subseteq c \), but we can construct a partition of \( c \), which we call the interior set \( I(c) \), by extending the definition of the set of children to include lower-dimensional cubes:

\[
I(c) := \{ \text{n-cubes } e \text{ such that } e.1 = c.1 + 1 \text{ and } e \subset c \}.
\]  

(2.3)

The interior set \( I(c) \) is dual to the closure set \( \{ c \} \cup B(c) \) in that, for every \( k \)-cube in \( \{ c \} \cup B(c) \), there is a corresponding \( (n - k) \)-cube in \( I(c) \). For an octant \( o \), for example, the corners in \( B(o) \) correspond to the children volumes in \( I(o) \), the edges in \( B(o) \) correspond to faces between children in \( I(o) \), the faces in \( B(o) \) correspond to edges in \( I(o) \), and \( o \) itself corresponds to the corner in the center of \( o \) that is common to all of its children. For completeness, we define the interior set of a \( 0 \)-cube \( c \) to be \( I(c) := \{ c \} \).

The last type of set that we define for every \( n \)-cube \( c \) is the support set \( S \), which is the set of octants that are conformally adjacent to \( c \),

\[
S(c) := \{ \text{octants } o \text{ such that } o.1 = c.1 \text{ and } o \subseteq \partial \}.
\]  

(2.4)

For \( 0 < n < d \), \( n = \dim c \), this can be simply stated as \( c \in B(o) \iff o \in S(c) \), but our definition extends to octants in such a way that \( S(o) = \{ o \} \) and to \( 0 \)-cubes in such a way that the support set of a \( 0 \)-cube includes only the largest adjacent octants. In the interior of an octree, the support sets of \( n \)-cube always contains \( 2^{d-n} \) octants, but \( n \)-cubes contained in the interfaces between octrees have irregular support sets determined by the topology of the forest. Constructing \( S(b) \) may require intra-tree coordinate transformations, as described in [6]. When we index \( S(b) \), we do so in SFC order. For a \( 0 \)-cube \( c \), we also define the set \( S_{\max} \) of level-\( \ell_{\max} \) octants adjacent to \( c \),

\[
S_{\max}(c) := \{ \text{octants } o \text{ such that } o.1 = \ell_{\max} \text{ and } c \in B(o) \}.
\]  

(2.5)

This set is useful because the octants in \( S_{\max}(c) \) are guaranteed to be contained in the leaves that are adjacent to \( c \), and so they can be used as keys to search for those leaves, or for the processes that contain them. We index \( S_{\max}(c) \) like \( S(c) \) so that \( S_{\max}(c)[i] \subseteq S(c)[i] \).

The sets we have defined in this section are illustrated in Table 2.2. As mentioned above, lower-dimensional octants are not among the datatypes used by p4est. In the implementation of the algorithms in this work, a lower-dimensional cube \( c \) is represented by an octant \( o \) and an index \( i \in \mathcal{B} \) such that \( B(o)[i] = c \). This representation is sufficient for all the sets defined in this section to be computed in \( O(1) \) time.

3. Parallel multiple-item search via array splitting. We can optimize the search for a leaf that matches a given condition if we begin at the root of an octree and recursively descend to all children that could possibly be a match. This is a lazy exclusion principle which is motivated by a practical consideration: Often an over-optimistic approximate check can be significantly faster than an exact check, which applies to bounding-box checks in computational geometry or to checking the surrounding sphere of a nonlinearly warped octant volume in space.
3.1. Searching a single octree. In Search (Algorithm 1), we use recursion and lazy exclusion for tracking multiple simultaneous queries during one traversal. At each recursion into child octants we only retain the queries that have returned a possible match on the previous level. We implement this by passing a user-defined callback function Match that is expected to indicate a positive result for an octant with a boolean return value, and to update the calling context with the query results. We also pass a flag to Match that indicates that we have arrived at a leaf, at which point the callback is expected to make a final decision for this query and leaf. This mechanism makes it possible for each query to match multiple leaves, such as when searching for the leaves that intersect a polytope.

3.2. Array splitting. Search requires an algorithm Split array that we have not yet specified. Split array takes a sorted array of leaves A and an octant a such that each leaf A[j] is a descendant of a and returns an array of the children of a, h[i] = C(a)[i], and one sorted array H[i] containing the descendants of h[i] as a subset of A.

Because A is sorted, the subarrays can be indicated by a non-decreasing sequence of indices 0 = k[0] ≤ k[1] ≤ ... ≤ k[n_A] = n_A := #A, such that H[i] = A[k[i]], ..., k[i + 1] − 1]. If C(a)[i] has no descendants in A, this is indicated by k[i] = k[i + 1].
Algorithm 1 Search (octant array $A$, octant $a$, query set $Q$, callback $Match$)

Require: $A$ is sorted, $A[j]$ is a descendant of $a$ for each $j$
1: $R = \{\};$ boolean $b \leftarrow (A = \{a\})$ \{$b = true$ identifies a leaf situation, $b = false$ a recursion\}
2: for all $r \in Q$ do
3: if $Match(a, b, r)$ and not $b$ then
4: \hspace{0.5cm} $R \leftarrow R \cup \{r\}$ \{for the recursion we build a subset $R \subset Q$\}
5: end if
6: end for
7: if $R \neq \{\}$ then
8: $(H, h) \leftarrow Split_array(A, a)$ \{see Section 3.2 for an explanation of this function\}
9: for $i = 0$ to $n_o - 1$ do
10: \hspace{0.5cm} Search$(H[i], h[i], R, Match)$
11: end for
12: end if

Let us assume that the children of $a$ have level $\ell$. If we know that $o$ is a descendant of $C(a)[i]$ for some $i$, then we can compute $i$ from $a.o$ using Algorithm 2 that we call $Ancestor_id$, because it is a simple generalization of the algorithm $Child_id$ [0] Algorithm 1).

Algorithm 2 Ancestor_id (octant $o$, int $\ell$)

Require: $0 < \ell \leq o.l$
1: $i \leftarrow 0;$ $h \leftarrow 2^{\ell_{\text{max}} - \ell}$ \{$h \geq \text{length}(o)$; computing the child id relative to an octant at level $\ell - 1$\}
2: for $0 \leq j < d$ do
3: \hspace{0.5cm} $i \leftarrow i \mid (a.x[j] \& h) ? 2^j : 0$ \{bitwise OR and AND operators are denoted by $\mid$ and $\&$\}
4: end for
5: return $i$

If we applied $Ancestor_id$ to each octant in $A$, we would get a monotonic sequence of integers, so if we search $A$ with the key $i$ and use $Ancestor_id$ to test equality, the lowest matching index will give the first descendant of $C(a)[i]$ in $A$. The split operation, however, is used repeatedly, both by $Search$ and by the algorithm $Iterate$ we will present in Section 5 so to make the procedure as efficient as possible, we combine these searches into one algorithm that we call $Split_indices$ (Algorithm 3), which is essentially an efficient binary search for a sorted list of keys.

Algorithm 3 Split_indices (octant array $A$, octant $a$)

Require: $A$ is sorted, $A[j]$ is a strict descendant of $a$ for each $j$
1: $n_A \leftarrow \#A;$ $\ell_{\text{split}} \leftarrow a.l + 1$
2: $k[0] \leftarrow 0;$ $k[1], \ldots, k[n_A] \leftarrow n_A$ \{invariant 1: $\forall i: j \geq k[i]$ then $Ancestor_id(A[j], \ell_{\text{split}})$\}
3: for all $i = 1$ to $n_o - 1$ do
4: \hspace{0.5cm} $l \leftarrow k[i] - 1$ \{invariant 2: $j < l$, then $Ancestor_id(A[j], \ell_{\text{split}})$\}
5: \hspace{0.5cm} while $l \leq k[i]$ do
6: \hspace{0.5cm} \hspace{0.5cm} $j \leftarrow l + \lfloor (k[i] - l)/2 \rfloor$ \{increase lower bound to maintain invariant 2\}
7: \hspace{0.5cm} \hspace{0.5cm} $c \leftarrow Ancestor_id(A[j], \ell_{\text{split}})$
8: \hspace{0.5cm} \hspace{0.5cm} if $c < i$ then
9: \hspace{0.5cm} \hspace{0.5cm} \hspace{0.5cm} $l \leftarrow j + 1$
10: \hspace{0.5cm} \hspace{0.5cm} else
11: \hspace{0.5cm} \hspace{0.5cm} \hspace{0.5cm} $k[i], \ldots, k[c] \leftarrow j$ \{decrease upper bounds to maintain invariant 1\}
12: \hspace{0.5cm} \hspace{0.5cm} end if
13: \hspace{0.5cm} \hspace{0.5cm} end while
14: \hspace{0.5cm} end for
15: return $k$

Suppose, in using a traditional binary search to determine the value of $k[1]$, we
test an array index \( i \) and find that \( \text{Ancestor\_id} (A[i], a.1 + 1) = 4 \). This information tells us not only that \( k[1] \leq i \), but also that \( k[2], k[3], k[4] \leq i \) as well. If we then began a new binary search for \( k[2] \) after the binary search for \( k[1] \) concludes, we would start with a range \([k[1], n_A]\), instead of \([k[1], i]\). Split\_indices narrows the ranges defined by the \( k[i] \) values whenever possible to save unnecessary search steps.

3.3. Searching a forest. To extend the action of \( \text{Search} \) to the whole forest, it can be called once for each octree with the tree’s leaf array and root octant; see \( \text{Search\_forest} \) (Algorithm 4). \( \text{Search\_forest} \) is communication-free and every leaf is queried on its owner process only, while its ancestors can generally overlap multiple process domains.

Algorithm 4 \text{Search\_forest} (query set \( Q \), callback \( \text{Match} \))

\begin{verbatim}
1: for all \( t \in T_p \) do
2: \( \text{Search}(O^t_p, \text{Root}(t), Q, \text{Match}) \) {pass process-local leaves as possible leaf matches}
3: end for
\end{verbatim}

4. Constructing ghost layers for unbalanced forests. When combining adaptive mesh refinement and distributed parallelism, there is no a-priori knowledge on any given process about what leaves might neighbor a process’s partition. This knowledge, however, is necessary to determine the complete local neighborhoods of leaves that are adjacent to inter-process boundaries, which is crucial to many application-level algorithms. If a forest of octrees obeys a 2:1 balance condition \([6, 14]\), at least it is known that parallel neighbors can differ in size by no more than a factor of two. The previously presented \text{Ghost} algorithm in \text{p4est} [6, Algorithm 20] uses this fact in querying the ownership of hypothetical half-size neighbors and communicating leaves to their owners. This algorithm is short and effective, but not usable for an unbalanced forest. In this section, we present an algorithm for ghost layer construction that works for non-2:1-balanced forests. Its key component is a recursive algorithm that determines when a leaf and a process are adjacent to each other.

4.1. Ghost layer construction using range/boundary intersection tests. Let us define the ghost layer in terms of the relational sets defined in Section 2.3. A leaf on process \( q \neq p \) is in the ghost layer \( G_p \) of process \( p \) if it intersects \( \overline{\Omega}_p \),

\[ G_p := \bigcup_{q \neq p} \{ o \in O_q : \overline{o} \cap \overline{\Omega}_p \neq \{ \} \}. \]  

(4.1)

This definition of \( G_p \) includes leaves whose intersection with \( \overline{\Omega}_p \) is a single point. Some applications, such as discontinuous Galerkin finite element methods, only require a ghost layer to include leaves whose intersections with \( \overline{\Omega}_p \) have codimension 1. The boundary set \( B(o) \) allows us to easily define a ghost layer \( G^k_p \) parameterized by codimension \( k \),

\[ G^k_p := \bigcup_{q \neq p} \{ o \in O_q : \exists b \in B(o) \text{ such that codim}(b) \leq k \text{ and } b \cap \overline{\Omega}_p \neq \{ \} \}. \]  

(4.2)

If \( b \cap \overline{\Omega}_p \neq \{ \} \), then \( \overline{\Omega}_q \) must overlap some octant \( s \) in the support set \( S(b) \) that surrounds \( b \); this fact allows us to limit the number of processes for which the intersection test \( b \cap \overline{\Omega}_p \) must be computed. In Algorithm 5, we present a high-level description of
the construction and communication of the full ghost layer, i.e., of \( G_p^d \) for each process \( p \) simultaneously. To modify Algorithm 5 to construct \( G_p^k \) for \( k < d \), we simply limit the subset of \( B(o) \) for which the intersection test on line 15 is performed.

**Algorithm 5 Ghost**

1: \( R \leftarrow \{ \} \) \{list of neighboring processes\}
2: \( G_p^d \leftarrow \{ \} \) \{ghost layer\}
3: for \( q = 0 \) to \( P - 1 \) do
4: \( S_q \leftarrow \{ \} \) \{array of leaves to send to \( q \)\}
5: end for
6: for all \( a \in P_p \) do
7: for all \( b \in B(o) \) do
8: for all \( a \in S(b) \) do
9: \( q_F \leftarrow \text{Find_owner}(\text{First}\_\text{descendant}(a)) \) \{first process whose range overlaps \( a \)\}
10: \( q_L \leftarrow \text{Find_owner}(\text{Last}\_\text{descendant}(a)) \) \{last process whose range overlaps \( a \)\}
11: for all \( q \in [q_F, q_L], q \neq p \) do
12: \( (f, l) \leftarrow \text{Range}(q) \) \{\( \Omega_q = [f, l] \)\}
13: \( f \leftarrow \max\{\text{First}\_\text{descendant}(a), f_q \} \)
14: \( l \leftarrow \min\{\text{Last}\_\text{descendant}(a), l_q \} \)
15: if \( \lceil f, l \rceil \cap b \neq \{ \} \) then
16: \( S_q \leftarrow S_q \cup \{ \} \) \{\( o \in G_q^d \)\}
17: \( R \leftarrow R \cup \{ q \} \)
18: end if
19: end for
20: end for
21: end for
22: end for
23: for all \( q \in R \) do
24: send \( S_q \) to \( q \)
25: receive \( G_q \) from \( q \) \{communication is symmetric: \( S_q \neq \{ \} \Leftrightarrow G_q \neq \{ \} \)\}
26: \( G_p^d \leftarrow G_p^d \cup G_q \)
27: end for
28: return \( G_p^d \)

**4.2. Finding a range’s boundaries recursively.** The pseudocode in Algorithm 5 does not specify how the intersection test \( \lceil f, l \rceil \cap b \neq \{ \} \) on line 15 is to be performed. We know that the range \( \lceil f, l \rceil \) is contained in \( a \in S(b) \) and \( b \in B(a) \): the intersection test can be considered a specific case of a more general problem, which is to determine the subset \( D(f, l, a) \) of \( B(a) \) that intersects \( \lceil f, l \rceil \),

\[
D(f, l, a) := \{ b \in B(a) : \lceil f, l \rceil \cap b \neq \{ \} \}. \quad (4.3)
\]

We can do this by constructing the index set for \( D(f, l, a) \),

\[
D(f, l, a) := \{ j : B(a)[j] \in D(f, l, a) \}. \quad (4.4)
\]

Recall the indices \( B \) used to index \( B(a) \) shown in Figure 2.2. We define the index set \( B_i \) to be the indices that reference boundary cubes that are adjacent to the \( i \)th child,

\[
B_i := \{ j \in B : C(a)[i] \cap B(a)[j] \neq \{ \} \}. \quad (4.5)
\]

Each index \( j \in B_i \) has an interesting property: if we use it to refer to the boundary set of the child \( C(a)[i] \), the cube it refers to is a child of a cube with the same index in \( B(a) \). Or, put succinctly,

\[
j \in B_i \Leftrightarrow B(C(a)[i])[j] \in C(B(a)[j]). \quad (4.6)
\]
The equivalence in (4.6) allows us to construct \( D(f, l, a) \) by partitioning \([f, l]\) into one range \([f_i, l_i]\) for each child \( C(a)[i] \) and to define \( D(f, l, a) \) in terms of \( D(f_i, l_i, C(a)[i]) \):

\[
D(f, l, a) = \bigcup_{0 \leq i < n_c} D(f_i, l_i, C(a)[i]) \cap B_i. \tag{4.7}
\]

This leads to the recursive algorithm \texttt{Find\_range\_boundaries} (Algorithm 6), which takes as arguments the octants \( f, l, \) and \( a, \) and a subset \( B_{\text{query}} \) of \( B \) for which we would like to determine \( B_{\text{query}} \cap D(f, l, a). \) For the intersection test in Algorithm 5 we choose \( B_{\text{query}} = \{ j : B(a)[j] = b \}. \) A proof of the correctness of Algorithm 6 is given in Appendix A. The recursive procedure is also illustrated in Figure 4.1.

4.3. Notes on implementation. At most one instance of \texttt{Find\_range\_boundaries} will call the two recursive copies of itself on lines[12 and][17, all subsequent instances call at most one recursive copy, because the range will include the first or last descendant of \( a. \) We use this fact to take advantage of tail-recursion optimization.
Algorithm 6 Find_range_boundaries (octants \( f, l, a \), index set \( B_{\text{query}} \))

Require: \( f \) and \( l \) are descendants of \( a; f \leq l; f.l = l.l = \ell_{\text{max}} \)

1: if \( B_{\text{query}} = \{\} \) or \( a.l = \ell_{\text{max}} \) then
  2: return \( B_{\text{query}} \)
  3: end if

4: \( \ell_{\text{split}} \leftarrow a.l + 1 \)

5: \( F \leftarrow ((f = \text{First}_{\text{descendant}}(a)) ? -1 : \text{Ancestor}_{\text{id}}(f, \ell_{\text{split}})) \)

6: \( L \leftarrow ((l = \text{Last}_{\text{descendant}}(a)) ? n_c : \text{Ancestor}_{\text{id}}(l, \ell_{\text{split}})) \)

7: if \( F = L \) then

8: \( D_{\text{query}} \leftarrow \text{Find}_{\text{range}} \text{boundaries}(f, l, C(a)[F], B_{\text{query}} \cap B_F) \) \{recursion inside \( C(a)[F] \}\)

9: else

10: \( D_{\text{query}} \leftarrow \bigcup_{F < i < L} B_{\text{query}} \cap B_i \) \{this set may be empty\}

11: if \( F \geq 0 \) then

12: \( l_F \leftarrow \text{Last}_{\text{descendant}}(C(a)[F]) \)

13: \( D_{\text{query}} \leftarrow D_{\text{query}} \cup \text{Find}_{\text{range}} \text{boundaries}(f, l, C(a)[F], (B_{\text{query}} \cap B_F) \setminus D_{\text{query}}) \)

14: end if

15: if \( L < n_c \) then

16: \( f_L \leftarrow \text{First}_{\text{descendant}}(C(a)[L]) \)

17: \( D_{\text{query}} \leftarrow D_{\text{query}} \cup \text{Find}_{\text{range}} \text{boundaries}(f, l, C(a)[L], (B_{\text{query}} \cap B_L) \setminus D_{\text{query}}) \)

18: end if

19: end if

20: return \( D_{\text{query}} \) \{\( D_{\text{query}} = \text{D}(f, l, a) \cap B_{\text{query}} \)\}

in our implementation. We represent subsets of \( B \) by assigning a bit of an integer to each \( i \in B \) and perform set operations with bitwise arithmetic.

Our implementation of \texttt{Ghost} in \texttt{p4est} contains a few optimizations that are not obvious from the pseudocode in Algorithm 5. The majority of leaves do not touch the boundary of \( \Omega_p \), and so cannot be in \( G_q \) for another process \( q \). To avoid the intersection tests for these interior leaves, our implementation first checks to see if \( o \)'s \( 3 \times 3 \) neighborhood is owned by \( p \): this can be accomplished with two \( O(1) \) checks, each for the first and last position of the neighborhood, against \( F \). We also note that if \( b \) is a 0-cube then a process’s range will intersect \( b \) if and only if there is \( s \in S_{\text{max}}(b) \) such that \( s \in [f, l] \). Because of this, calling \texttt{Find}_{\text{range}} \text{boundaries} is not necessary to perform the intersection test for 0-cubes.

5. A universal topology iterator. The forest is first of all a storage scheme for a mesh refinement topology. Applications use this information in manifold ways that we do not wish to restrict or anticipate. We focus instead on designing an interface that conveys this information to applications in a complete and efficient manner, with the main goal of minimizing the points of contact between \texttt{p4est} on the one hand and the application on the other.

As we will see in our discussion of a specific node numbering algorithm in Section 6 some applications need to perform operations not just on leaves, but also on the lower-dimensional cubes on their boundaries. Our algorithm that facilitates this is called \texttt{Iterate}.

5.1. Definitions. Let us assume that the forest of octrees is 2:1 balanced, and let \( \mathcal{W}_p \) be the union of process \( p \)'s local octants and boundary layer,

\[
\mathcal{W}_p := \mathcal{O}_p \cup \mathcal{G}_p. \tag{5.1}
\]
Fig. 5.1. Suppose process \( p \) owns only octant \( o \) in this (two-dimensional) illustration. The gray octants are the ghost layer \( G_p \), so \( W_p \) is the set of all octants shown. The set \( B_p \setminus H_p \) is the set of all cubes shown. The set \( R_p \) of cubes that overlap \( \Omega_p \) is shown in blue. The 0-cube \( b \) shown in red is not in \( R_p \), but is in its closure, \( \overline{R}_p \).

Define \( B_p \) to be the union of \( W_p \) with the boundary sets of \( W_p \),

\[ B_p := W_p \cup \bigcup_{o \in W_p} B(o). \tag{5.2} \]

The set \( B_p \) covers \( W_p \), but it is not a partition (a partition is a disjoint union), because \( B_p \) may contain hanging cubes: cubes of dimension < \( d \) that are in the interior sets of other cubes in \( B_p \). Define \( H_p \) to be these hanging cubes,

\[ H_p := \{ b \in B_p : \exists c \in B_p \text{ such that } c \neq b \text{ and } b \in I(c) \}. \tag{5.3} \]

The set \( B_p \setminus H_p \) is a partition of \( \overline{W}_p \). If there is just one process, the function \texttt{Iterate} executes a user-supplied callback function for every cube \( b \in B_p \setminus H_p \). For a distributed forest, \texttt{Iterate} executes the callback function only for the subset of \( B_p \setminus H_p \) that is relevant to \( O_p \). In our implementation of \texttt{Iterate}, we allow for two definitions of what is relevant. This first is the set \( R_p \) of cubes that overlap \( \Omega_p \),

\[ R_p := \{ b \in B_p \setminus H_p : \exists o \in O_p \text{ such that } b \cap \overline{o} \neq \{ \} \}. \tag{5.4} \]

One potential problem with \( R_p \) is that, because of hanging cubes, it is not necessarily closed: if \( b \in R_p \), there may be \( c \in B(b) \) such that \( c \notin R_p \). As we will show in Section 6, closedness is necessary for some applications. We therefore define the closure \( \overline{R}_p \) to be the union of \( R_p \) with the boundary sets of its elements,

\[ \overline{R}_p := R_p \cup \bigcup_{b \in R_p} B(b). \tag{5.5} \]

The sets we have defined so far—\( W_p, B_p \setminus H_p, R_p, \) and \( \overline{R}_p \)—are illustrated in Figure 5.1.

If \texttt{Iterate} only supplied \( b \) to the callback function, its utility would be rather limited, because it would say nothing about which leaves in \( W_p \) are adjacent to \( b \). So \texttt{Iterate} also supplies the callback function with the set \( \tilde{S}_p(b) \) of leaves adjacent to \( b \),

\[ \tilde{S}_p(b) := \{ o \in W_p : \overline{o} \cap b \neq \{ \} \}. \tag{5.6} \]

It is important to note that \( \tilde{S}_p(b) \) is different from \( S(b) \): the octants in \( \tilde{S}_p(b) \) are leaves, and may not have the same level as \( b \). \( \tilde{S}_p(b) \) may also be incomplete, because
Algorithm 7 Is_relevant (cube b, set $\tilde{S}_p(b)$)

1: if $R_p$ is the relevant set then
2: return $b \cap R_p \neq \emptyset$ ? true : false
3: else if $\overline{R_p}$ is the relevant set then
4: for all $s \in \tilde{S}_p(b)$ do
5: for all $c \in B(s)$ do
6: if $c \cap \overline{R_p} \neq \emptyset$ then
7: if $b \in B(c)$ then
8: return true
9: end if
10: end if
11: end for
12: end for
13: return false
14: end if

a leaf adjacent to $b$ may not be in $W_p$. With $\tilde{S}_p(b)$, the callback function has a fairly complete description of the local neighborhood of $b$ that is relevant to process $p$. $\tilde{S}_p(b)$ is also used to determine whether $b \in R_p$ or $b \in \overline{R_p}$, using a function Is_relevant (Algorithm 7).

For each octant $o \in \tilde{S}_p(b)$, our implementation of Iterate supplements the usual octant data fields $l$, $x$, and $t$ with additional data. We supply a boolean identifying whether $o \in O_p$, so no searching is necessary to determine if $o$ is local or a ghost. We also supply the index of $o$ within either $O_p^t$ for $t = o.t$ (which is easily converted to $j$ such that $O_p[j] = o$) or within $G_p$. Keeping track of this information to supply it for the callback function does not change the computational complexity of Iterate, but introduces additional bookkeeping that we will omit from our presentation of the algorithm.

5.2. Iterating in the interior of a cube. A simple implementation of Iterate might take each leaf $o \in O_p$ in turn and, for each $b \in B(o)$, compute $\tilde{S}_p(b)$ by searching through $W_p$ to find $o$’s neighbors that are adjacent $b$. A bounded number of binary searches would be performed, so the total iteration time would be $O(N_p \log N_p)$. This is the strategy used by the Nodes algorithm in p4est [6] Algorithm 21 and by other octree libraries [25]. We note two problems with this approach. The first is the large number of searches that must be performed. The second is that this approach needs some way of ensuring that the callback is executed for each relevant cube only once, such as storing the set of cubes for which the callback has executed in a hash table.

Instead, the implementation of Iterate that we present proceeds recursively. We take as inputs to the recursive procedure a cube $b$ that represents a region of the forest and an array $S[i]$ of the leaves contained in $S(b)[i]$ in each octant $b$’s support set. If $b$ is in $B_p$ and is in the relevant set, then the octants in $\tilde{S}_p(b)$ can be found in the $S$ arrays and the callback function can be executed if $b$ is relevant. Otherwise, the subset of $B_p$ that is contained in $b$ can be partitioned by the interior set $I(b)$. Each $c \in I(b)$ takes the place of $b$ in a call to the recursive procedure: to compute the leaf arrays for each octant in the support set $S(c)$, we can use the function Split_array (described in Section 3.2) on the arrays $S$. This is spelled out in Iterate_interior (Algorithm 8).

We provide some figures to illustrate the recursion in Iterate_interior: Figure 5.2 shows the cases when $\dim(b) = d$ and $0 < \dim(b) < d$ and Figure 5.3 shows the case when $\dim(b) = 0$. Correctness of Algorithm 8 is proved in Appendix 13.
An instance of \texttt{Iterate\_interior} may call multiple recursive copies of itself: one for each cube in the interior set $I(b)$ (see the loop starting on line 24). We have not yet specified an order for these recursive calls. In our implementation, we have chosen to order these calls by decreasing dimension. This guarantees that, if $c \in B(b)$, then the callback is executed for $b$ before it is executed for $c$. We take advantage of this order in designing a node-numbering algorithm in Section 6.

5.3. Iterating on a forest. To iterate on the complete forest, we must call \texttt{Iterate\_interior} for the root of every tree in $T_p$, and also for the boundary sets of these root octants. This is shown in Algorithm 8. Asymptotic analysis of the performance of \texttt{Iterate} is presented in Appendix C. It shows that, in general, \texttt{Iterate} executes in $O((O_{\text{max}} + N_p) \log N_p)$ time, but if the refinement pattern of the octrees in the forest is uniform or nearly so, then it executes in $O(\log P + N_p)$ time.

5.4. Implementation. The implementation of \texttt{Iterate} in \texttt{paste} has some differences from the presented algorithm to optimize performance. Instead of reproducing the recursive form of the component algorithms, we write them as iterative while-loops in order to get optimal performance and to keep the stack from growing. All space needed to run the component algorithms (which is proportional to the maximum recursive depth) is pre-allocated on the heap. We also noticed that \texttt{Split\_array} can be called with the same arguments multiple times during a call to \texttt{Iterate}. To
\[ b = S(b)[0] \]

| \( S[0] = \{ S(b)[0] \} ? \) | \( \text{true} \) | \( \text{false} \) |
|-------------------------------|-----------------|------------------|
| \( S[0] = \{ S(b)[0] \} \) | \( \tilde{S}_p(b)[0] \) | \( S(b)[0] \) |
| \( \tilde{S}_p(b)[1] \) | \( \tilde{S}_p(b)[2] \) |

**Legend**

- **IterateInterior** \((b, S, \text{callback})\):
  - \( b \)
  - \( S[i] \) (leaves in \( S(b)[i] \))
  - \((H, h) \leftarrow \text{SplitArray} (S[i], S(b)[i])\)
- **callback** \((b, \tilde{S}_p(b))\):
  - \( b \)
  - \( \tilde{S}_p(b)[i] \)

**Fig. 5.2.** Illustrations of **IterateInterior** for \( \text{dim}(b) = d \) (top) and \( 0 < \text{dim}(b) < d \) (bottom). The color red indicates the argument cube \( b \) of **IterateInterior**. The dotted squares indicate the arrays \( S[i] \) of leaves in \( W_p \) that are descendants of \( S(b)[i] \). If \( S(b)[i] \) is a leaf (which is determined by testing whether \( S[i] = \{ S(b)[i] \} \)), then it is in \( \tilde{S}_p(b) \), which is shown with the color blue; otherwise, \( S[i] \) is split using **SplitArray**. If a leaf has been found, the user-supplied callback function is executed, which we indicate with the color green; otherwise, **IterateInterior** is called for each cube in the interior set \( I(b) \): the support sets for these cubes, and the arrays of leaves contained in them, are found in the children and sets created by **SplitArray**.
Fig. 5.3. An illustration of Iterate\textsubscript{interior} when dim(b) = 0, using the same color conventions as Figure 5.2. The arguments of Iterate\textsubscript{interior} are in the left panel. The yellow squares (middle panel) indicate octants in S\textsubscript{max}(b): these must be contained in the leaves in \( \tilde{S}_p(b) \), so we use \( S_{\text{max}}(b)[i] \) as a key to search for \( \tilde{S}_p(b)[i] \) in S[t]. Once \( \tilde{S}_p(b) \) is found, the callback is executed (right panel).

Algorithm 9 Iterate (callback, ghost layer \( G \))

1: for all \( t \in T_p \) do
2: \( r[t] \leftarrow \text{Root}(t) \)
3: \( G[t] \leftarrow \{ o \in G : o.t = t \} \) \quad \{in \text{p}4est, these subsets of \( G \) are returned by Ghost()\}
4: \( S[t] \leftarrow O_p^t \cup G[t] \) \quad \{\( O_p^t \) and \( G[t] \) are already ordered: on sorting is necessary\}
5: Iterate\textsubscript{interior}(r[t], \{S[t]\}, callback)
6: end for
7: for all \( b \in \cup_{t \in T_p} B(r[t]) \) do
8: for \( i = 0 \) to \#S(b) - 1 do
9: \( t \leftarrow S(b)[i].t \) \quad \{Each \( S(b)[i] \) is necessarily the root of an octree\}
10: \( G[t] \leftarrow \{ o \in G : o.t = t \} \)
11: \( SB[i] \leftarrow O_p^t \cup G[t] \) \quad \{\( O_p^t \) and \( G[t] \) are already ordered: on sorting is necessary\}
12: end for
13: Iterate\textsubscript{interior}(b, SB, callback)
14: end for

avoid some of this recomputation, we keep fixed-size caches of the index sets produced by Split\_indices, one for each level \( \ell \), with a FIFO replacement strategy. We also allow the user to specify a separate callback function for each dimension, so that extra recursion can be avoided. If, for example, the callback only needs to be executed for faces, then an instance of Iterate\textsubscript{interior} operating on \( b \) will only call a recursive copy of itself for \( c \in I(b) \) if \( \text{codim}(c) \leq 1 \).

6. A use case for the iterator: higher-order nodal basis construction.

Up to this point, we have developed algorithms over a parallel mesh topology with no special regard for numerical applications. In this section, we use our framework to perform a classic but complex task necessary for finite element computations, namely the globally unique numbering of degrees of freedom for a continuous finite element space over hanging-node meshes. We call it Nodes in reference to (Gauß-)Lobatto, which means that some nodes are located on element boundaries and are thus shared between multiple elements and/or processes, which presents some interesting challenges.

Hanging-node data structures have been discussed as early as 1980 \cite{21} and adapted effectively for higher-order spectral element computations \cite{11,23}. Special-purpose data structures and interface routines have been defined for many discretization types built on top of octrees, including piecewise linear tensor-product ele-
In a hexahedral \( n \)-order nodal finite element, the Lagrangian basis functions and the degrees of freedom are associated with \( \Pi = (n+1)^3 \) \( \mathbb{Q}^n \)-nodes located on a tensor grid of locations in the element. For our purposes, the exact location of the nodes is not important, as long as there is one node at each corner, \((n-1)\) nodes on the interior of each edge, \((n-1)^2\) nodes on the interior of each face, and \((n-1)^3\) nodes on the interior of the element, as in Figure 6.1. If we endow each leaf in a forest of octrees with \( \mathbb{Q}^n \)-nodes, we get \( N \times \Pi \) element nodes. \( \mathbb{Q}^n \)-nodes are numbered in a well-defined order within an element, for example lexicographically, and element-local nodes are then numbered to match the order of their associated leaves. The basis functions associated with the element nodes span a discontinuous approximation space \( \mathcal{D} \).

We want to create a nodal basis for a \( C^0 \)-conforming approximation space \( \mathcal{C} \) on \( \Omega \) such that the restriction of the space to any leaf is spanned by the \( \mathbb{Q}^n \)-nodes' basis functions. The nodes for the basis functions and degrees of freedom of \( \mathcal{C} \) are called global nodes. Each of the \((n-1)^3\) element nodes on the interior of a leaf can be associated with a unique global node, but on the boundary of a leaf, element nodes from multiple leaves may occupy the same location: in this case, the two element nodes are associated with the same global node, as in Figure 6.2 (a). For non-conforming interfaces, the element nodes of the smaller leaves are not at the same locations as those of the larger leaf, but they cannot introduce new degrees of freedom, elements \( [1, 5] \) and discontinuous spectral elements \( [27] \). The \texttt{deal.II} finite element software \( [3] \) uses yet another mesh interface \( [2] \). In our presentation of \texttt{Lnodes}, we hope to show that the \texttt{Iterate} approach is sufficiently generic that it could be used to efficiently construct any of these data structures.

6.1. Concepts. In a hexahedral \( n \)-order nodal finite element, the Lagrangian basis functions and the degrees of freedom are associated with \( \Pi = (n+1)^3 \) \( \mathbb{Q}^n \)-nodes located on a tensor grid of locations in the element. For our purposes, the exact location of the nodes is not important, as long as there is one node at each corner, \((n-1)\) nodes on the interior of each edge, \((n-1)^2\) nodes on the interior of each face, and \((n-1)^3\) nodes on the interior of the element, as in Figure 6.1. If we endow each leaf in a forest of octrees with \( \mathbb{Q}^n \)-nodes, we get \( N \times \Pi \) element nodes. \( \mathbb{Q}^n \)-nodes are numbered in a well-defined order within an element, for example lexicographically, and element-local nodes are then numbered to match the order of their associated leaves. The basis functions associated with the element nodes span a discontinuous approximation space \( \mathcal{D} \).

We want to create a nodal basis for a \( C^0 \)-conforming approximation space \( \mathcal{C} \) on \( \Omega \) such that the restriction of the space to any leaf is spanned by the \( \mathbb{Q}^n \)-nodes' basis functions. The nodes for the basis functions and degrees of freedom of \( \mathcal{C} \) are called global nodes. Each of the \((n-1)^3\) element nodes on the interior of a leaf can be associated with a unique global node, but on the boundary of a leaf, element nodes from multiple leaves may occupy the same location: in this case, the two element nodes are associated with the same global node, as in Figure 6.2 (a). For non-conforming interfaces, the element nodes of the smaller leaves are not at the same locations as those of the larger leaf, but they cannot introduce new degrees of freedom, elements \( [1, 5] \) and discontinuous spectral elements \( [27] \). The \texttt{deal.II} finite element software \( [3] \) uses yet another mesh interface \( [2] \). In our presentation of \texttt{Lnodes}, we hope to show that the \texttt{Iterate} approach is sufficiently generic that it could be used to efficiently construct any of these data structures.
because every function in $C$, when restricted to the non-conforming interface, must be representable using the larger leaf’s basis functions. Conceptually, we can place the global nodes at the locations of the larger leaf’s nodes and associate each element node from the smaller leaves with a single global node, as shown in Figure 6.2 (b). In reality, the value of a function in $C$ at an element node on a non-conforming interface must be interpolated from the values at multiple global nodes, but the conceptual one-to-one association between a leaf’s element nodes and global nodes is sufficient, in that it identifies all of the global nodes whose basis functions are supported on that leaf.

It is important to note that an element node of a leaf $\omega$ may reference a global node that is contained in a cube $b$ that is outside the closure $\bar{o}$, and that $\omega$ is therefore not in the set of adjacent leaves $S_p(b)$ defined in Section 5. In this situation, we say that $\omega$ remotely references the global nodes in $b$. This is also shown in Figure 6.2 (b). If $\omega$ remotely references $b$, this can only be because one of $\omega$’s boundary cubes is hanging, $B(\omega) \cap H_p \neq \emptyset$, in which case we can say the following: there is another cube $c$, $\dim(c) > \dim(b)$, such that $\omega \in S_p(c)$ and $b \in B(c)$. This means that the global nodes referenced by local leaves will be contained in the set $\overline{S}_p$ define in Section 5.

We note that a cube $b$ can be remotely referenced only if $\text{codim } b > 1$.

6.2. Data structures. On process $p$, we can represent the global nodes that define the approximation space $C$ using an array $N_p$ of global nodes and an array $E_p$ of element nodes, where $E_p[j][k]$ maps the $k$th element node of $O_p[j]$ to its global node. $N_p$ and $E_p$ only reference locally relevant global nodes and thus implement fully distributed parallelism. In presenting the $L\text{nodes}$ algorithm, we consider a global node to have the following data fields:

- **index**: the globally unique index of this node,
- **proc**: the process that owns this node, for the purposes of scatter/gather communication of node values,
- **sharers**: the set of all processes that reference this node.

We include the sharers field so that, in addition to the scatter/gather communication paradigm, the global nodes can also be used in the share-all paradigm, wherein any process that shares a node can send information about that node to all other processes that share that node. If each process generates new information about a node, the former paradigm requires two rounds of communication for information to disseminate, one gather and one scatter, while the latter requires one round, but with an increased number of messages. Each paradigm can be faster than the other, depending on communication latency, bandwidth, and other factors. We tend to place the highest weight on latency, hence our added support for share-all.

In our implementation of the $L\text{nodes}$ algorithm available in $p4est$, the data structures that are returned are equivalent to $\{N_p, E_p\}$ described above, but with a node containing only the index field, and with the proc and sharers information available via the following arrays.

- For each process $q \neq p$, a list $N_{p,q}$ of the global nodes in $N_p \cap N_q$.
- The subset $A_{p}^q \subset N_{p,q}$ of global nodes owned by $p$ that are shared by $q$.
- The subset $A_{q}^p \subset N_{p,q}$ of global nodes owned by $q$ that are shared by $p$. The union of $A_{p}^q$ and $A_{q}^p$ is not necessarily equal to $N_{p,q}$: a third process $r$ may own nodes shared by both $p$ and $q$.

Grouping the inter-process information into these arrays reduces the overall storage requirements and is more convenient when creating buffers for asynchronous communication.
Many applications do not require higher-order finite element nodes, but the Lnodes data structure can be used in much more general settings. In particular, the Lnodes data structures for $n = 2$ assign one unique global index to every cube in $\mathcal{R}_p$, and a map from each leaf to the cubes in its closure. If one symmetrizes these mappings, i.e., if one saves the sets $\tilde{S}_p(b)$ generated by Iterate as maps for each $b \in \mathcal{R}_p$, then one has essentially converted the forest-of-octrees data structures into a graph-based unstructured mesh format with $O(1)$ local topology traversal. This format is typical of generic finite element libraries. Lnodes can therefore serve as the initial step in converting a forest of octrees into the format of an external library, with the remaining steps requiring no communication between processes.

6.3. Assigning global nodes. We want the global nodes to be numbered independently of the partitioning of the leaves across the processes (which as a corollary implies independence of the numbering from $P$). For this reason, it is useful to think of each global node as being owned by a single leaf, because an order is then induced by combining lexicographic ordering of element nodes with the ordering of leaves in the space-filling curve. This computation is shown in Algorithm 10, which assumes that we have already determined which leaf owns each global node, and temporarily stored that leaf’s index in the global node’s index field.

\begin{algorithm}
\caption{Global numbering (node array $N_p$, int array $E_p$)}
\begin{algorithmic}[1]
\Require $\forall g \in N_p[\cdot], 0 \leq r < \#N_p$:
\hspace{1em} $g$.proc is set to its owner process
\hspace{1em} if $g$.proc = $p$, $g$.sharers is set correctly
\hspace{1em} if $g$.proc = $p$, $g$.index is (temporarily abused as) the index of the local leaf that owns $g$
\State Create $N[\#N_p]$ \hspace{1em} \{temporarily stores the local indices of global nodes\}
\State $m \leftarrow 0$ \hspace{1em} \{the number of global nodes owned by $p$\}
\For{$j = 0$ to $\#E_p - 1$}
\For{$l = 0$ to $\Pi - 1$}
\hspace{1em} $g \leftarrow E_p[j][l]$ \hspace{1em} \{global node associated with element node $m$\}
\hspace{1em} if $g$.proc = $p$ and $g$.index = $j$ then
\hspace{1em} $N[g] \leftarrow m$ \hspace{1em} \{$g$’s index among the locally owned nodes\}
\hspace{1em} $m \leftarrow m + 1$
\EndIf
\EndFor
\EndFor
\State $\text{Allgather}(t)$ \hspace{1em} \{$t[q]$ is the number of global nodes owned by $q$\}
\State $\text{Prefix sums}(t)$ \hspace{1em} \{$t[q]$ is now the offset to the first global node owned by $q$\}
\ForAll{$g \in N_p$}
\If{$g$.proc = $p$}
\hspace{1em} $g$.index $\leftarrow N[g] + t[p]$ \hspace{1em} \{all fields of $g$ are now complete\}
\hspace{1em} Send $g$ to each $q \in g$.sharers \hspace{1em} \{in practice, group into one message per process\}
\Else
\hspace{1em} Receive updated $g$ from $g$.proc
\EndIf
\EndFor
\end{algorithmic}
\end{algorithm}

We are left with assigning ownership of nodes to leaves in a partition-independent manner. One could greedily assign the global nodes in cube $b$ to the first leaf $o$ whose element nodes reference them, but this causes a problem if $o \notin \tilde{S}_p(b)$. The problem arises because a process’s knowledge of which leaves exist on other processes is limited to the ghost layer constructed by Ghost (Algorithm 5). If greedy assignment is used, then a process may be unable to determine the assignment of all the nodes that it references without further communication between processes. An example of this
Fig. 6.3. An illustration of the disadvantage of greedily assigning global nodes to leaves. Each color represents a different process; the Morton order proceeds right then up, so that \( s < r < q < p \). The illustration is from the point of view of \( p \): the blue background indicates \( \Omega_p \), while the gray background indicates \( p \)'s ghost layer. The central node is contained in a 0-cube \( b \): all of process \( s \)'s and process \( p \)'s leaves are outside of \( \tilde{S}_p(b) \). If we greedily assigned \( b \)'s node, then in situation (a) it would be assigned to a leaf on process \( s \), whereas in situation (b) it would be assigned to a leaf on process \( r \). Both situations look identical to process \( p \), so additional communication would be required for \( p \) to determine the assignment of \( b \)'s node.

Instead, we assign cube \( b \) and its nodes to the first leaf \( o \) in \( \tilde{S}_p(b) \). If \( o \) is owned by process \( p \), then \( \tilde{S}_p(b) \) is complete: every leaf on any process that intersects \( b \) is in \( W_p \), and is thus in \( \tilde{S}_p(b) \). When \( \tilde{S}_p(b) \) is complete, the octant data—\( x, l, t \)—of any leaf that remotely references \( b \)'s nodes can be reconstructed from \( \tilde{S}_p(b) \). We call this procedure \texttt{Reconstruct}\_\texttt{remote} (Algorithm 11). We have already established that \( o \) remotely references \( b \) only if there is \( c \) such that \( o \in \tilde{S}_p(c) \) and \( b \in B(c) \): because \( c \) is adjacent to \( b \), \( c \) must also be in \( B(s) \) for some \( s \in \tilde{S}_p(b) \). \texttt{Reconstruct}\_\texttt{remote} uses this fact to reconstruct \( o \) from \( b \) and \( \tilde{S}_p(b) \). Using \texttt{Find}\_\texttt{owner} on the set returned by \texttt{Reconstruct}\_\texttt{remote} then allows \( p \) to determine all processes that remotely reference \( b \)'s nodes.

When we assign \( b \) to the first leaf \( o \) in \( \tilde{S}_p(b) \), we also guarantee that \( o \) will be owned by the first process \( q \) such that \( \bigcup \Omega_q \) intersects \( b \). This means that each process that references \( b \) can determine the assignment of all nodes it references, even if \( \tilde{S}_p(b) \) is incomplete for that process. We call the procedure for making this determination \texttt{Determine}\_\texttt{owner} (Algorithm 12). This algorithm determines to process that owns \( b \) by finding a 0-cube \( c \) in the interior of \( b \), and then testing the ownership of the octants in \( S_{\max}(c) \).

The previously presented algorithm \texttt{Nodes} [6] Algorithm 21] produces data structures equivalent to those produced by \texttt{Lnodes} for \( n = 1 \). The ownership rule in \texttt{Nodes}—associating each node with a unique level-\( (l_{\max} + 1) \) octant, and assigning ownership based on the process whose range contains that octant—is in principle the

\[2\]The ability to expand the ghost layer outward, increasing each process’s knowledge of the neighborhood of its partition, has been added to \texttt{piest} by the authors, but at the time of writing this addition is not included in the publicly available stable version [4]. Naturally, expanding the ghost layer implies additional communication that we rather avoid for \texttt{Lnodes}.
same as the ownership rule for $L_nodes$. $Nodes$ does not have symmetric communication, however, because it does not construct the neighborhood $\tilde{S}_p(b)$ when it creates a node at $b$, and so it cannot perform a calculation like $Reconstruct\_remote$. Because it does not deduce the presence of remotely-sharing processes, $Nodes$ requires a handshaking step, where the communication pattern is determined.

6.4. The $L_nodes$ algorithm. The algorithm $Global\_numbering$ (Algorithm 11) assumes that the map $E_p$ is already complete, and that the owning process $g.proc$ of each node $g \in N_p$ is already correctly set. It is further assumed that if $g.proc = p$, then $g.sharers$ is also complete and that $g.index$ is equal to the index of the leaf that owns $g$. In $L_nodes$ (Algorithm 13), we create this information using callback function $L_nodes\_callback$ (Algorithm 14) that is executed by $Iterate$.

Algorithm 11 Reconstruct\_remote (cube $b$, set $\tilde{S}_p(b)$)

1: $R \leftarrow \emptyset$
2: for all $c \in \bigcup_{s \in \tilde{S}_p(b)} B(s)$ do ... 
3: if $b \in B(c)$ then
4: for all $o \in \bigcup_{a \in C(c)} S(a)$ do
5: if there is no $s \in \tilde{S}_p(b)$ such that $o \subseteq s$ then
6: $R \leftarrow R \cup \{o\}$ (by the 2:1 condition, $o$ is a leaf, and it remotely references $b$)
7: end if
8: end for
9: end if
10: end for
11: return $R$

Algorithm 12 Determine\_owner (cube $b$)

1: $c \leftarrow a \in I(b)$ such that $\dim(a) = 0$ ... 
2: return $\min_{s \in S_{max}(c)} \{\text{Find\_owner}(s)\}$

The callback $L_nodes\_callback$ for cube $b$ does three tasks: it creates the global nodes in $b$, assigns the global nodes to a process, and completes the references to those nodes in $E_p$. If the nodes are assigned to the current process, the set of all processes that reference the nodes is also calculated. We have already discussed ownership and sharing processes in Section 6.3, but we have not yet explained how $L_nodes\_callback$ completes the entries in $E_p$.

Because $Iterate$ provides the callback with the local indices for each $o \in \tilde{S}_p(b)$, we can easily complete the entries in $E_p$ for those leaves. To complete the $E_p$ entries for remotely-referencing octants, we take advantage of the order of callback execution within $Iterate$. We know that if $o$ remotely references $b$, then there is another cube $c$ such that $o \in \tilde{S}_p(c)$, $\dim(c) > \dim(b)$ and $b \in B(c)$. The order of execution in $Iterate$ guarantees that the callback for $c$ executes before the callback for $b$. The local index for $o$ can be cached during the callback for $c$, using a function $Cache$ and
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With a cache of size $O(N_p)$, Cache and Recover are each $O(1)$ operations.

Algorithm 14 $\text{Lnodes\_callback}$ (cube $b$, set $\tilde{S}_p(b)$)

1: Create $(n-1)\dim(b)$ global nodes $N_{\text{new}}$
2: $N_p \leftarrow N_p \cup N_{\text{new}}$
3: $q \leftarrow \text{Determine\_owner}(b)$
4: for all $g \in N_{\text{new}}$ do
5: \hspace{1em} $g.\text{proc} \leftarrow q$
6: end for
7: if $q = p$ then
8: \hspace{1em} $R \leftarrow \text{Reconstruct\_remotes}(b, \tilde{S}_p(b))$
9: \hspace{1em} $U \leftarrow \{\}$ \hspace{1em} \{list of processes that reference the nodes inside of $b$\}
10: \hspace{1em} for all $s \in \tilde{S}_p(b) \cup R$ do
11: \hspace{2em} $U \leftarrow U \cup \{\text{Find\_owner}(s)\}$
12: \hspace{1em} end for
13: \hspace{1em} $o \leftarrow \min \tilde{S}_p(b)$ \hspace{1em} \{nodes are assigned to $o$\}
14: \hspace{1em} for all $g \in N_{\text{new}}$ do
15: \hspace{2em} $g.\text{sharers} \leftarrow U$
16: \hspace{2em} $g.\text{index} \leftarrow \{j$ such that $O_p[j] = o\}$
17: \hspace{1em} end for
18: end if
19: $L \leftarrow \tilde{S}_p(b) \cap O_p$
20: $L_{\text{indices}} \leftarrow \cup_{j \in L} \{j$ such that $O_p[j] = s\}$
21: $L_{\text{indices}} \leftarrow L_{\text{indices}} \cup \text{Recover}(b)$ \hspace{1em} \{indices of remotely-referencing leaves\}
22: for all $i \in L_{\text{indices}}$ do
23: \hspace{1em} $E_p[i] \leftarrow E_p[i] \cup N_{\text{new}}$
24: end for
25: for all $c \in B(b)$ do
26: \hspace{1em} $H_{\text{indices}} \leftarrow \{\}$ \hspace{1em} \{indices to cache for $c$\}
27: \hspace{1em} for all $s \in L$ do
28: \hspace{2em} if $s \cap c = \{\}$ then \hspace{1em} \{s remotely references $c$, will not be in $\tilde{S}_p(c)$\}
29: \hspace{2em} $H_{\text{indices}} \leftarrow H_{\text{indices}} \cup \{j$ such that $O_p[j] = s\}$
30: \hspace{2em} end if
31: \hspace{2em} end for
32: \hspace{1em} Cache $(c, H_{\text{indices}})$
33: end for

We note that on line 23 of our presentation of $\text{Lnodes\_callback}$, we fill the entries in $E_p[i]$ as though they are unordered sets, even though we have specified $E_p$ as an array. We omit the necessary steps of matching each element node to its global node, which involves calculations relating the orientation of $b$ to the leaves in $\tilde{S}_p(b)$.

7. Performance evaluation. In this section we evaluate the efficiency and scalability of the algorithms presented in this work as they have been implemented in $\text{p4est}$. The parallel scalability is assessed on the Blue Gene/Q supercomputer JUQUEEN, which is configured with 28,672 compute nodes, each with 16 GB of memory and 16 cores, for a total of 458,752 cores. Although additional concurrency is available through hyperthreading, we examine a 16-way MPI-only approach in this paper to guarantee the most reproducible timings. We have compiled the $\text{p4est}$ library and executables with IBM’s XL C compiler in version 12.1.
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**Fig. 7.1.** Scaling results for searching for \( M \) points in a shell domain using \texttt{Search} as implemented by \texttt{p4est.search}. We examine various values of \( M \), \( P \), and \( N \). Three different values of \( P \) are used: \( P_0 = 64 \), \( P_1 = 64^2 \), and \( P_2 = 64^3 \approx 256,000 \). Three different values of \( N/P = D \) are used: \( D_0 \approx 15k \), \( D_1 \approx 122k \), and \( D_2 \approx 979k \). Left: \( M \) separate calls of \texttt{Search} are used to find the \( M \) points. Right: one call of \texttt{Search} is used to find all \( M \) points. The dotted lines symbolize linear weak scaling; points on top of each other demonstrate the independence of the runtime from the local octant count \( D \). The largest number of octants reached is \( 2.568 \times 10^{11} \).

### 7.1. Search

To test the performance of \texttt{Search} (Algorithm 1), we consider the problem of identifying the leaves that contain a set of randomly generated points. We choose a spherical shell domain typical for simulations of earth’s mantle convection, with inner radius \( r = 0.55 \) and outer radius \( r = 1 \), as illustrated in Figure 2.1 (left). For each test, we generate \( M \) points at random, independently and uniformly distributed in the cube containing the shell, and use \texttt{Search} as implemented by the \texttt{p4est} function \texttt{p8est.search} to identify the leaves that contain them.

Each octree \( k \) has an analytic mapping \( \varphi_k \) from the implicit octree coordinate system to a subset of the shell. In the callback that we provide to \texttt{Search}, we have two tests to determine whether the image \( \varphi_k(o) \) of an octant \( o \) contains a point \( x \), one fast and inaccurate in the sense of allowing false positive matches, the other slower but accurate. In the accurate test, the mapping \( \varphi_k \) is inverted to get the preimage \( \xi \) of \( x \) in the implicit coordinate system of the octree \( k \) containing \( o \), and a bounding box calculation determines whether \( \xi \in o \). In the inaccurate test, the image \( x_o \) of the octant’s center is computed, as well as an upper-bound \( r_o \) on the radius of the bounding sphere of \( \varphi_k(o) \), and we test whether \( |x - x_o| \leq r_o \). In \texttt{Search} the accurate test is performed when \( o \) is a leaf, and the inaccurate test when \( o \) is a branch. We perform our tests on a series of forests with increasing numbers of leaves \( N \), but with each forest refined so that the finest leaves are four levels more refined than the coarsest.

In Figure 7.1, we present the scaling results for our tests. Each of the \( P \) processes must determine which of the \( M \) points are in its partition. This means that each process must perform the inaccurate test at least \( M \) times. This is why, for fixed values of \( P \), we see a scaling with \( O(M) \). Indeed, the fraction of points that fall in a given processes partition is on average \( 1/P \), so for large values of \( P \) the majority of the runtime is spent on points that are not in the partition. This is why, in Figure 7.1, the number of leafs on a node \( N/P \) has so little effect on the runtime. When we...
Fig. 7.2. The scalability of the Ghost algorithm for the mesh of six asymmetrically connected cubes shown in Figure 2.1 (right), as implemented by the p4est function p8est_ghost. The mesh is refined uniformly to a chosen level and then adaptively for four more levels, which determines the total element number \(N\). The horizontal scale shows \(N/P\), the number of leaves per process, and the vertical scale shows the runtime. The total number of MPI processes \(P\) is indicated by the marker type. Two lines indicate one second of runtime and \((N/P)^{2/3}\) scaling. The quality of weak scaling can be estimated by the closeness of data points in the vertical. The topmost data point for the largest run corresponds to \(5.137 \times 10^{11}\) octants.

7.2. Ghost. We test the performance of our ghost layer algorithm Ghost (Algorithm 5), as implemented by the p4est function p8est_ghost, on the irregular geometry shown in Figure 2.1 (right). We again create a series of meshes with increasing \(N\) and four levels of difference between the coarsest and finest leaves. In Ghost, we use Find_range_boundaries (Algorithm 6) as a component that determines which processes’ partitions border an octant \(o\). When a partition \(\Omega_p\) with \(N_p\) leaves is well-shaped, we expect \(O(N_p^{2/3})\) of those leaves to be on the boundary of \(\Omega_p\). The remaining leaves in the interior of the domain can be skipped without calling Find_range_boundaries, and so they should contribute very little to the runtime of Ghost.

In Figure 7.2, we show the runtimes for constructing the full ghost layer \(G^3_p\) for a wide range of process counts and leaf densities. For \(P \leq 8k\), we see that the runtime scales very closely with the predicted \((N/P)^{2/3}\) over almost four orders of magnitude. For larger values of \(P\), the increased latency of communicating the octants in the ghost layer starts to dominate the runtime for small values of \(N/P\).

Both weak and strong scaling analyses are contained in our diagrams starting...
with Figure 7.2. We define weak scaling by keeping $N/P$ fixed and increasing $P$, where a constant run time would be ideal. In the diagram, this would mean that data points of different marker type should not spread in the vertical direction. Strong scaling is defined by increasing $P$ while keeping $N$ fixed, with the runtime reducing proportional to a power of $N/P$. In our diagram, ideal scaling would correspond to stepping to the right on the $x$-axis while choosing the marker type for the next lower process count. Then the data points should follow a diagonal line sloped with the desired exponent. The ghost algorithm satisfies these criteria best between 16 and 65,536 processor cores or a factor of 4,096.

7.3. Serial comparison of Lnodes and Nodes. For polynomial degree $n = 1$, the data structures constructed by Nodes [6, Algorithm 21] and Lnodes (Algorithm 13) are essentially equivalent. For a general forest of octrees on a single process, both have $O(N \log N)$ runtimes. While Nodes uses repeated binary searches and hash table queries and insertions, Lnodes uses Iterate (Algorithm 9) to recursively split the forest and operates on subsets of leaves. This divide-and-conquer approach should make better use of a typical cache hierarchy. In this subsection, we present a small experiment that confirms this fact.

The experiment is conducted on a single octree using a single process. We again create a series of meshes with increasing $N$ and four levels of difference between the coarsest and finest leaves. For each forest in the series, we have three programs: one that calls Nodes, one that calls Lnodes, and one that calls neither. We use the Linux utility perf to estimate the number of instructions, cache misses, and branch prediction misses in each program, calling each program 30 times to compensate for the noise in perf’s sampling. The averages of the events from the program calling neither routine is subtracted from the other two averages, giving an estimate of the events that can be attributed to the two routines.

The experiment is performed on a laptop with two Intel Ivy Bridge Core i7-3517U dual core processors. Each core has a 64 kB on-chip L1 cache, a 256 kB L2 cache, and each processor has a 4 MB L3 cache: perf counts L3 cache misses. The p4est library and the executable are compiled by gcc 4.6.4 with -O3 optimization.

The results of the experiment are given in Table 7.1. The table shows that the advantages of Lnodes over Nodes in terms of the number of instructions and the number of branch misses do not grow much with $N$, but the advantage in terms of cache misses grows from a factor of 2 on the smallest problem size to a factor of 11 on the largest.

7.4. Parallel scalability of Lnodes. In the previous subsection we compared the per-process efficiency of Lnodes and Nodes. Here we compare their parallel scalability on the same series of test forests used to test Ghost above.

In Figure 7.3 we show the runtimes of the two algorithms for the test forests. For all values of $P$, Lnodes is still faster than Nodes for larger values of $N/P$, although the relative advantage is smaller on the Blue Gene/Q architecture of JUQUEEN than on the Ivy Bridge architecture used in the serial test. For large values of $P$, the communication pattern of Lnodes, consisting of one allgather and one round of point-to-point communication, is more scalable than the communication pattern of Nodes, which includes a handshake component. For $P \geq 8k$ and $N/P \leq 1k$, Lnodes is roughly twice as fast as Nodes. For the tests using the full 458k cores of JUQUEEN, the extra communication of Nodes is significant, even with $10^5$ octants per process.

https://perf.wiki.kernel.org
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Table 7.1
Serial performance comparison of Nodes (top) and Lnodes for \( n = 1 \) (bottom), as implemented by the p4est functions p8est_nodes and p8est_lnodes, on a series of single-octree forests.

| \( N \)       | runtime (ms) | instructions | branch misses | cache misses | \( N/P \)       | Lnodes runtime in seconds | Nodes runtime in seconds |
|-------------|--------------|--------------|---------------|--------------|-------------|---------------------------|-------------------------|
| \( 4.6 \times 10^3 \) | \( 9.5 \times 10^0 \) | \( 4.3 \times 10^7 \) | \( 2.1 \times 10^5 \) | \( 2.2 \times 10^4 \) | 2 | \( \times 10^{-2} \) | \( \times 10^1 \) |
| \( 1.0 \times 10^1 \) | \( 3.7 \times 10^7 \) | \( 5.3 \times 10^4 \) | \( 1.1 \times 10^4 \) | \( 2 \times 10^5 \) | 16 | \( \times 10^0 \) | \( \times 10^6 \) |
| \( 3.9 \times 10^4 \) | \( 8.6 \times 10^1 \) | \( 4.2 \times 10^8 \) | \( 1.7 \times 10^6 \) | \( 2.2 \times 10^5 \) | 128 | \( \times 10^{-2} \) | \( \times 10^0 \) |
| \( 4.0 \times 10^1 \) | \( 3.1 \times 10^8 \) | \( 3.6 \times 10^5 \) | \( 5.1 \times 10^4 \) | \( 2 \times 10^5 \) | 1024 | \( \times 10^0 \) | \( \times 10^6 \) |
| \( 3.2 \times 10^5 \) | \( 8.4 \times 10^2 \) | \( 3.7 \times 10^9 \) | \( 1.3 \times 10^7 \) | \( 4.8 \times 10^6 \) | 8192 | \( \times 10^{-2} \) | \( \times 10^0 \) |
| \( 3.5 \times 10^2 \) | \( 2.5 \times 10^9 \) | \( 2.7 \times 10^6 \) | \( 4.5 \times 10^5 \) | \( 2 \times 10^5 \) | 65536 | \( \times 10^0 \) | \( \times 10^6 \) |
| \( 2.6 \times 10^6 \) | \( 8.0 \times 10^3 \) | \( 3.3 \times 10^{10} \) | \( 1.0 \times 10^8 \) | \( 6.1 \times 10^7 \) | 458752 | \( \times 10^{-2} \) | \( \times 10^0 \) |
| \( 2.8 \times 10^3 \) | \( 2.0 \times 10^{10} \) | \( 2.2 \times 10^7 \) | \( 5.4 \times 10^6 \) | \( 2 \times 10^5 \) | |

Fig. 7.3. The parallel scalability of the Lnodes algorithm for \( n = 1 \) (left) and Nodes algorithm (right), as implemented by the p4est functions p8est_lnodes and p8est_nodes. The horizontal scale shows \( N/P \), the number of leaves per process, and the vertical scale shows the runtime. The total number of MPI processes \( P \) is indicated by the marker type.

Following the same reasoning as in analyzing Ghost, we can see that both node numbering algorithms have near linear weak and strong scalability for \( P \) between 2 and 65,536. For the full system size of 478k processor cores, run times do not become much smaller than one second total, this being the case where Lnodes is most significantly faster than Nodes.

In Figure 7.3, we compare the scalability of Lnodes for higher polynomial orders to the scalability for \( n = 1 \). For \( P = 2 \), when the effect of MPI communication is negligible, we see that the runtime to construct 3rd-order nodes is less than twice the runtime for 1st-order nodes, even though there are eight times as many element nodes and roughly 36 times as many global nodes; the runtime to construct 7th-order nodes is roughly four times the runtime for 1st-order nodes, even though there are 64 times as many element nodes and, in our meshes, roughly 500 times as many global nodes. For large values of \( P \) the communication costs, which do not increase significantly with \( n \), dominate the runtime, so that the cost of constructing high-order nodes is
Fig. 7.4. The scalability on the JUQUEEN supercomputer of the \texttt{lnodes} algorithm for $n = 3$ (left) and $n = 7$ (right), as implemented by the \texttt{p4est} function \texttt{p8est\_lnodes}. The horizontal scale shows $N/P$, the number of leaves per process, and the vertical scale shows the runtime as a multiple of the runtime for $n = 1$.

essentially the same as 1st-order nodes.

8. Conclusion. In this work, we introduce new recursive algorithms that operate on the distributed forest-of-octrees data structures that the \texttt{p4est} software defines and uses to support scalable parallel AMR. The algorithms developed here exploit a recursive space partition from a topological point of view. They constitute \texttt{p4est}'s high-level reference interface, which is designed to be used directly from third-party numerical applications.

With the \texttt{Search} algorithm, we demonstrate how to efficiently traverse a linear octree downward from the root, even though the flat storage of leaves has no explicit tree structure. This search operation is in some sense purely hierarchical: a similar search could be performed even if the branches and leaves of the tree were not interpreted as a space partition in $\mathbb{R}^d$.

As a component of the \texttt{Ghost} algorithm, we propose a recursive algorithm for determining the intersections between lower-dimensional boundary cubes and ranges of leaves that are specified only by the first and last leaves in the range. This algorithm is notable in that, while the procedure is recursive on the implicit octree structure, the result that it computes—a set of intersections—is purely topological in nature.

In the \texttt{Iterate} algorithm, we present a method of performing callback-based iteration over leaves and leaf boundaries that construct local topological information for the callback on the fly. This procedure combines aspects of the two previous algorithms: it involves recursion over the octree hierarchy and recursion over topological dimension. The divide-and-conquer nature of the algorithm makes better use of the cache hierarchy than approaches to iteration that rely on repeated searches through the array of leaves, as we demonstrate in practice.

We use \texttt{Iterate} in the construction of fully-distributed higher-order $C^0$ finite

\footnote{The number of global nodes depends on the forest topology and the refinement pattern. For a single octree with uniform refinement, the number of global nodes is asymptotically equivalent to $n^3 N$, in which case the number of 7th-order nodes would be 343 times the number of 1st-order nodes. Because of non-conforming elements, however, we see a higher ratio.}
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element nodes in the algorithm $Lnodes$. The topological information provided by $Iterate$ simplifies the handling of non-conforming interfaces, and provides sufficient information to allow for node assignments to be made without communication, and for the communication pattern between referencing processes to be determined without handshaking. In practice, this gives us good scalability, which we have demonstrated to nearly a half million processes on the JUQUEEN supercomputer, and at granularities ranging from hundreds of nodes per MPI process to millions of nodes per MPI process.

The scalability of $Lnodes$ that we have demonstrated is important for more applications than just higher-order finite element nodes, because the data structures returned by the $Lnodes$ algorithm can also serve as the basis for converting a linear forest of octrees into an unstructured mesh adjacency graph. $Lnodes$ includes all of the communication necessary for this conversion, so the same scalability should be achievable by third-party numerical codes that use $Lnodes$ (or a similar approach based on $Iterate$) to interface $p4est$ with their own mesh formats.

**Reproducibility.** The algorithms presented in this article are implemented in the $p4est$ reference software [4]. $p4est$, including the programs used in the performance analysis presented above, is free and freely downloadable software published under the GNU General Public License version 2, or (at your option) any later version.

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Appendix A. Proof of the correctness of Find_range_boundaries (Algorithm 9).

Theorem A.1. Given a range \([f, l]\), where \(f\) and \(l\) are level-\(\ell_{\text{max}}\) octants with common ancestor \(a\), and given a set of boundary indices \(B_{\text{query}} \subseteq B\), Algorithm 9 returns the indices \(D_{\text{query}} = D(f, l, a) \cap B_{\text{query}}\).

Proof. The proof is inductive on \(a.1\).

If \(a.1 = \ell_{\text{max}}\), then \(a = l = f\), so \([f, l] = \bar{a}\) and \(D = B\), so \(D_{\text{query}} = B_{\text{query}},\) which is correctly returned on line 2.

Now suppose that Algorithm 9 returns the correct set \(D_{\text{query}}\) if \(\ell_{\text{max}} \geq a.1 \geq k\), and suppose \(a.1 = k - 1\). Let \(f\) and \(l\) descend from \(C(a)[F]\) and \(C(a)[L]\), and let \(f_i\) and \(l_i\) be the first and last level-\(\ell_{\text{max}}\) octants in \(C(a)[i] \cap [f, l]\) for \(F \leq i \leq L\). If we intersect \(B_{\text{query}}\) with the expression for \(D(f, l, a)\) in (4.7), we get

\[
D_{\text{query}} = D(f, l, a) \cap B_{\text{query}} = \bigcup_{F \leq i \leq L} D(f_i, l_i, C(a)[i]) \cap (B_i \cap B_{\text{query}}).
\]

By the inductive assumption, each of the sets in the union is correctly constructed by \texttt{Find_range_boundaries}, so

\[
D_{\text{query}} = \bigcup_{F \leq i \leq L} \texttt{Find_range_boundaries}(f_i, l_i, C(a)[i], B_i \cap B_{\text{query}}).
\]

If \(F = L\), then this union of recursively computed indices is the same as the set computed on line 8. If \(F < L\), we can see that the union of recursively computed indices is equal to the set computed by \texttt{Find_range_boundaries} once we accept two facts. The first is that, if \([f_i, l_i] = C(a)[i]\), then there is no need for recursion because \(D(f_i, l_i, C(a)[i]) = B\): this accounts for the indices added to \(D_{\text{query}}\) on line 10. The second is that, if it has already been established that \(b \in D_{\text{query}}\), then \(b\) can be removed from the query set for future recursive calls, as is done on lines 13 and 17. Therefore, \texttt{Find_range_boundaries} correctly computes \(D_{\text{query}}\) for \(a.1 = k\) as well. By induction, the proof is complete.

Appendix B. Proof of the correctness of \texttt{Iterate_interior} (Algorithm 8).

Let the definitions in Section 5 be given. We prove the correctness of \texttt{Iterate_interior} (Algorithm 8) when the relevant set is \(R_p\). The proof for the case when \(R_p\) is the relevant set is very similar.

Theorem B.1. Assume that the requirements for the arguments of Algorithm 8 are met. If \(b \in R_p\), then \(S_p(b)\) is correctly computed. If there is a subset of \(R_p\) that is contained in \(p\), then the callback function is executed for all cubes in that subset.

Proof. We first assert that if \(b \in B_p \setminus H_p\), then \(S_p(b)\) is a subset of \(\bigcup_i S[i]\). If \(b\) is an octant then \(S_p(b) = S(b) = \{b\}\). Because \(S[i]\) is defined as all leaves in \(W_p\) that are contained in \(S(b)[i]\), \(S[0]\) must contain \(b\). Now suppose \(b\) is a lower-dimensional cube and \(o \in S_p(b)\). Because \(B_p \setminus H_p\) is a partition, \(b\) only intersects the boundary of \(o\). Because \(b\) is not hanging, there must be \(c \in B(o)\) such that \(c \subseteq b\). This implies that the level of \(b\) is less than or equal to the level of \(o\). The octants in the support \(S(b)\) cover all octants with a higher level than \(b\) that intersect \(b\), so there must be \(i\) such that \(o \subseteq S(b)[i]\) and thus \(o \in S[i]\).

From here, we split the proof into two cases, \(\dim(b) = 0\), and \(\dim(b) > 0\).

Suppose \(\dim(b) = 0\). If \(o\) is supposed to be in \(S_p(b)\), then there is \(i\) such that \(o \in S[i]\). Any descendant of \(S(b)[i]\) that intersects \(b\) must contain \(S_{\text{max}}(b)[i]\), by
definition. Therefore $o$ is correctly added to $\hat{S}_p(b)$ on line 6. Conversely, if $o$ is added to $\hat{S}_p(b)$ on line 5 then $S_{max}(b)[i] \subset o$. Because $\hat{S}_{max}(b)[i] \cap b \neq \{\}$, it must be that $\partial \cap b \neq \{\}$. Because $o$ must be in $S[i] \subseteq \mathcal{W}_p$, $o$ is a leaf in $\mathcal{W}_p$ whose closure intersects $b$, which matches the definition of $\hat{S}_p(b)$. Therefore $\hat{S}_p(b)$ is correctly computed, and the callback will be executed on line 21 if and only if $b \in \mathcal{R}_p$.

Now suppose $\dim(b) > 0$. Let $L$ be the minimum level of a leaf $o \in \cup_i S[i]$ and let $\ell$ be the level of $b$. The remainder of the proof is inductive on the difference $\delta = L - \ell$.

Suppose $\delta = 0$, and let $o \in S[i]$ be a leaf with level $L = \ell$. Because $o \subseteq S(b)[i]$ and because $S(b)[i]$ is a level $\ell$ octant, $o = S(b)[i]$, which by the definition of $S(b)$ implies $\partial \cap b \neq \{\}$, and that therefore $o \in \hat{S}_p(b)$. Because leaves do not overlap, it must be that $S[i] = \{S(b)[i]\}$. Therefore $o$ is added to $\hat{S}_p(b)$ on line 12.

Because of the 2:1 condition, all remaining leaves in $\hat{S}_p(b)$ have level $\ell + 1$. Let $o \in S[i]$ be a leaf with level $\ell + 1$. This implies that $S[i] \neq \{S(b)[i]\}$, so the children of $S(b)[i]$ are assigned to $h$, on line 14 $o$ must be one of these children. On line 15 $o$ is added to $\hat{S}_p(b)$ if and only if $\partial \cap b \neq \{\}$, which matches the definition $\hat{S}_p(b)$. Therefore $\hat{S}_p(b)$ is correctly constructed, and the callback executes on line 21 if and only if $b \in \mathcal{R}_p$.

Now suppose the algorithm is correct for $\delta < k$, and suppose $\delta = k$. There can be no $i$ such that $S[i] = \{S(b)[i]\}$, so the arrays $H_i$ and octants $h_i$ are computed on line 14 for every $i$. Let $c$ be in the interior set $S(b)$: $c$ has level $\ell + 1$. By definition, $S(c)[i]$ also has level $\ell + 1$ and $S(c)[i] \cap c \neq \{\}$, which implies $S(c)[i] \cap b \neq \{\}$. Because $b$ is surrounded by $S(b)$ this implies there is $j$ such that $S(c)[i] \in C(S(b)[j])$ and $k$ such that that $S(c)[i] = h_j[k]$. Therefore, $S[i] = H_j[k]$ is equal to the subset of $\mathcal{W}_p$ contained in $S(c)[i]$. This means that the arguments of the recursive call on line 29 are correct for each $c \in I(b)$. By the inductive assumption, the callback function is executed for the subset of $\mathcal{R}_p$ in the union of $I(b)$, which is equal to $b$. By the principle of induction, the proof is complete.

**Appendix C. Asymptotic analysis of Iterate (Algorithm 9).**

We first present the asymptotic analysis of the complexity of the algorithm in a single process, single octree setting.

**Theorem C.1.** Ignoring the time taken by the callbacks, Iterate executes in the worst case in $O(N \log N)$ time.

*Proof.* The only operations in each instance of Iterate_interior that are not $O(1)$ and the calls to Split_array. Each of these searches is associated with an octant that is a branch, i.e. the ancestor of a leaf, that is in $S(b)$. A branch $o$ can only be in $S(b)$ if $b \in B(o)$, so Split_array is called for that branch $o$ a bounded number of times. Because an octree has $O(N)$ branches that are not leaves, $O(N)$ searches are conducted. Each array that is split contains a subset of leaves, so each instance must run in $O(\log N)$ time. We conclude that an upper bound on the running time is $O(N \log N)$. \hfill $\square$

**Theorem C.2.** Ignoring callbacks, Iterate executes in $O(N)$ time on a uniformly refined octree.

*Proof.* The leaves are all at level $\ell_{max}$, so $N = 2^{d_{max}}$, and there are $2^{d_{max}}$ branches at level $\ell$. Because leaves are evenly distributed, each branch at level $\ell$ has $2^{d_{max}-\ell}$ leaf descendants. Each branch is associated with a bounded number of binary searches and calls to Split_indices, so if we ignore leading coefficients, the total time spent
searching is
\[
\sum_{\ell=0}^{\ell_{\text{max}}-1} 2^{d\ell} \log 2^{d(\ell_{\text{max}}-\ell)} = d \sum_{\ell=0}^{\ell_{\text{max}}-1} 2^{d\ell} (\ell_{\text{max}} - \ell) \\
= d \sum_{\ell=0}^{\ell_{\text{max}}-1} \frac{2^{d\ell_{\text{max}}}}{2^{d(\ell_{\text{max}}-\ell)}} (\ell_{\text{max}} - \ell) \\
\lfloor \ell_{\text{max}} - \ell \rfloor = d \sum_{\ell=1}^{\ell_{\text{max}}} \frac{\hat{\ell}}{2^{d\ell}} = d2^{d\ell_{\text{max}}} O(1).
\]

Because the dimension \(d\) is fixed, \texttt{Iterate} runs in \(O(N)\) time. \qed

A uniformly refined octree is just a regular grid, so the indices of neighbors follow a predictable rule: a linear-time algorithm can be achieved without a recursive algorithm and without searching through the leaf arrays. We outline a class of octrees which has no rule for neighboring indices, but for which \texttt{Iterate} still runs in linear time.

\textbf{Definition C.3.} The class of \(\Delta\)-uniform octrees are those octrees such that each octree’s leaves vary in level between \(\ell_{\text{min}}\) and \(\ell_{\text{max}}\) in an unpredictable manner, but where the difference \(\Delta = \ell_{\text{max}} - \ell_{\text{min}}\) is bounded as \(\ell_{\text{max}}\) grows.

\textbf{Theorem C.4.} \texttt{Iterate} executes in \(O(N)\) time on a \(\Delta\)-uniform octree.

\textit{Proof.} For \(\ell \geq \ell_{\text{min}}\), \(2^{d\ell}\) is now an upper bound on the number of branches at this level, and for every \(\ell\), \(2^{d(\ell_{\text{max}}-\ell)}\) is an upper bound on the number of descendants of a level \(\ell\) branch. Therefore the \(O(2^{d\ell_{\text{max}}})\) runtime for a uniform \(\ell_{\text{max}}\) octree is an upper bound on the runtime of \texttt{Iterate}, while a lower bound on \(N\) is \(2^{d\ell_{\text{min}}} = 2^{d(\ell_{\text{max}}-\Delta)}\). Therefore \(2^{d\ell_{\text{max}}} \leq 2^{d\Delta N}\), so the runtime of \texttt{Iterate} is \(O(2^{d\Delta N}) = O(N)\). \qed

We now consider the \texttt{Iterate} algorithm in the multiple process, single octree setting, and derive bounds in terms of the local number of leaves \(N_p\) and the number of processes \(P\). A key component of the above analysis for the serial runtime, that the number of branches is \(O(N)\), is no longer true in a parallel setting: the number of ancestors of the leaves in \(W_p\) is not necessarily \(O(N_p)\). Suppose \(a\) is the smallest common ancestor of every leaf in \(W_p\) and \(a.1 = \hat{\ell}\). In \texttt{Iterate}, there are binary searches associated with each ancestor of \(a\), and each of those binary searches will be conducted over the whole of \(W_p\), taking \(O(\log N_p)\) each. The number of branches below \(a\) must be \(O(N_p)\), so the analysis for the runtime after level \(\hat{\ell}\) is the same as for a single process, substituting \(a\) for the root, so the time spent below \(a\) is \(O(N_p \log N_p)\) in general or \(O(N_p)\) for a \(\Delta\)-uniform tree. Thus an upper bound for the runtime is to add \(O(\hat{\ell} \log N_p)\) to that time. We can bound \(\hat{\ell}\) by \(\ell_{\text{max}}\), and in the \(\Delta\)-uniform case \(\ell_{\text{max}} \in O(\log N)\). If we assume an even partitioning of the leaves, \(N = P N_p\), then \(\ell_{\text{max}} \in O(\log P + \log N_p)\). The runtime for \texttt{Iterate} on an evenly distributed octree is thus \(O((\ell_{\text{max}} + N_p) \log N_p)\) in general and \(O(\log P + N_p)\) for \(\Delta\)-uniform octrees.

Introducing multiple trees does not affect the analysis significantly: by maintaining separate arrays for each tree, we split the leaves into subregions without needing to call \texttt{SplitArray}, so dividing a process’s range across multiple trees cannot increase the total search time. Some time is taken to set up the calls to \texttt{Iterate\_interior} for the interfaces between octrees, especially if the forest realizes the common use case \(K \ll N\).