TopoCluster: A Localized Data Structure for Topology-based Visualization

Guoxi Liu, Federico Iuricich, Riccardo Fellegara, and Leila De Floriani

Abstract—Unstructured data are collections of points with irregular topology, often represented through simplicial meshes, such as triangle and tetrahedral meshes. Whenever possible such representations are avoided in visualization since they are computationally demanding if compared with regular grids. In this work, we aim at simplifying the encoding and processing of simplicial meshes. The paper proposes *TopoCluster*, a new localized data structure for tetrahedral meshes. TopoCluster provides efficient computation of the connectivity of the mesh elements with a low memory footprint. The key idea of TopoCluster is to subdivide the simplicial mesh into clusters. Then, the connectivity information is computed locally for each cluster and discarded when it is no longer needed. We define two instances of TopoCluster. The first instance prioritizes time efficiency and provides only a modest savings in memory, while the second instance drastically reduces memory consumption up to an order of magnitude with respect to comparable data structures. Thanks to the simple interface provided by TopoCluster, we have been able to integrate both data structures into the existing Topological Toolkit (TTK) framework. As a result, users can run any plugin of TTK using TopoCluster without changing a single line of code.

Index Terms—Data visualization, data structures, topological data analysis, simplicial meshes, tetrahedral meshes

1 Introduction

Processing irregularly distributed data has always posed challenges in scientific visualization. Most tools (e.g., Paraview [1], VisIt [5], or Inviwo [21]) prioritize the analysis of regularly distributed data (i.e., 2D and 3D images), whose encoding is both simple and efficient. The same tools present relevant overheads when analyzing irregularly distributed data that require more involved data structures to be encoded.

This work focuses on data defined on tetrahedral meshes and aims at simplifying the processing and encoding of such data. Specifically, our goal is to define a data structure that is both compact and easy to integrate into existing visualization tools. We tackle this problem by introducing a new data structure called *TopoCluster*. TopoCluster partitions a simplicial complex into clusters and processes its simplices with a two-level technique. At the global level, only the minimum amount of information is stored. At the local level, the full information is extracted within each cluster and discarded when no longer needed. The result is a data structure capable of self-adjusting its memory consumption at run time.

The main contributions of this work are two instances of TopoCluster designed with opposite intents. While one instance prioritizes time performance, the second instance focuses on reducing the memory footprint with a consequent loss in time efficiency. Both data structures are designed to easily adapt to existing frameworks for mesh processing and visualization. To prove their flexibility, we have integrated our data structures into the Topological Toolkit (TTK) [30]. Such integration is transparent to a user or a developer. That is, TTK plugins can be executed either by using the original data structure provided by TTK, or our proposed structures, without changing a single line of code.

The structure of the paper is organized as follows. In Sections

2 Background

A *simplex* of dimension k, k-simplex for short, is defined as the convex hull of $k+1$ linearly independent points in the Euclidean space. A k-simplex σ is a *(proper) face* of an m-simplex τ, with $k<m$, if σ is a proper subset of τ. In this case, τ is said to be a *coface* of σ. A simplex which is not the proper face of any other simplex in Σ is called *top simplex*. The set of cofaces of a simplex σ forms the *star* of σ.

A simplicial complex Σ is a collection of simplices such that every face of a simplex σ is also in Σ, and the intersection of any two simplices σ and τ is either a face of both, or it is empty. The dimension d of Σ is the largest dimension of its simplices. Even if a simplicial complex can be defined in any dimension, we focus on its 3D instances, called *tetrahedral meshes*.

2.1 Topological relations

In a simplicial complex, simplices are involved in *topological relations*. A boundary relation maps a simplex to its faces, for instance, σ is on the boundary of τ iff σ is a face of τ. Vice versa, τ is said to be on the *coboundary* of σ. Two k-simplices τ_1 and τ_2 are said to be *adjacent* if they share a $(k-1)$-simplex on their boundaries. Informally, we say that two 0-simplices (vertices) are adjacent if they share the same 1-simplex (edge) in their coboundaries. A *relational operator* associates a simplex σ to a set of simplices having a specific topological relation with σ.

In the remainder of this paper, we only consider relational operators for tetrahedral meshes. We use capital letters to indicate whether the operator involves vertices (V), edges (E), triangles (F), or tetrahedra (T), and each operator is specified with a pair of letters. For example, EF indicates the relational operator associating an edge (E) to the triangles (F) on its coboundary. On a tetrahedral

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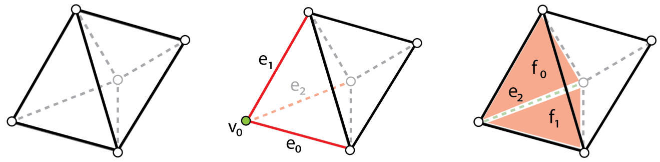

(a) (b) (c)

Fig. 1. (a) Tetrahedral mesh composed by two tetrahedra sharing a triangle. (b) VE relational operator for the vertex v_0 (c) EF relational operator for the edge e_2.

mesh we have six boundary operators (EV, FV, TV, FE, TE, TF), six coboundary operators (VE, VF, VT, EF, ET, FT), and four adjacency operators (VV, EE, FF, TT). Figure

3 Related Work

Generally speaking, data structures differ in the type of simplices and relational operators they encode. Data structures described in Section

3.1 Static data structures

There has been extensive research on topological data structures for simplicial complexes, especially for triangle and tetrahedral meshes [8].

The *incidence graph* [11] encodes explicitly all simplices plus all boundary and coboundary operators, which makes it the most general data structure for simplicial complexes. Multiple data structures have been defined to reduce the extremely large memory requirements of the incidence graph, either by cutting down the number of relational operators or by limiting the simplices encoded. The *Simplex tree* [2] is a variant of the incidence graph which organizes all simplices in a trie [14] and avoids encoding boundary operators. When data size increases, representing all simplices is no longer feasible. For this reason, alternative representations have been designed to prevent encoding simplices of specific dimensions. The *half-edge* [23] is a well-known data structure for triangle meshes, which drastically reduces memory consumption by encoding only the relational operators involving edges.

More recently, compact representations have been developed to maintain the same expressive power of the incidence graph while halving the space required [3], [7], [9]. The novelty of these data structures relies in the encoding of adjacency operators, instead of the more expensive coboundary operators. Examples include the *Indexed data structure with Adjacencies* [24], [25], the *Corner-Table* data structure [27] and its several extensions proposed specifically for triangle meshes [16], [22] and tetrahedral meshes [17]. The *generalized indexed data structure with adjacencies* (*IA**) [4] is the first data structure extending this approach to non-manifold simplicial complexes of arbitrary dimension. Among static data structures for non-manifold simplicial complexes, the *IA** is the most compact [15].

3.2 Stellar decomposition

The Stellar decomposition [12] represents a family of data structures in which relational operators are computed and discarded, at runtime, based on user requests. For this reason, they are called *dynamic* as opposed to the static data structures discussed in Section

The simplicial complex is processed with a *localized approach*. Instead of extracting relational operators altogether in a preprocessing step, the localized approach extracts operators, inside each cluster, at runtime. Given a k-simplex σ and a relational operator o, the simplices in relation with σ (i.e., $o(\sigma)$) will be extracted as follows:

(i) locate the cluster c of Δ containing σ;
(ii) compute the relational operator o for all the k-simplices contained in c;
(iii) return the set of simplices in relation with σ (i.e., $o(\sigma)$);
(iv) discard (delete) o.

The first data structure implementing this model was the *PR-star octree* [32], which was explicitly defined for tetrahedral meshes embedded in $\mathbb{R}^3$. Successively, this has been generalized by the *Stellar tree* [12], which can encode simplicial complexes embedded in any dimension and with arbitrary domain. The Stellar tree uses a hierarchical decomposition $\mathbb{H}$ (an n-dimensional bucketed Point Region quadtree [28]) to organize the mesh vertices. Relational operators are extracted locally to the leaf nodes of such hierarchy, following the Stellar decomposition model. As a result, the Stellar tree is even more compact than adjacent-based data structures like the IA* data structure [4]. On the other hand, simplices in a Stellar tree can only be accessed through a visit of the hierarchy $\mathbb{H}$, which introduces an additional layer of complexity for the developer (see Appendix

Our work aims to maintain the low memory footprint of the Stellar tree while providing an easy interface for implementing and running topological algorithms.

4 TopoCluster

The goal of all data structures for simplicial complexes is that of providing easy access to the relational operators. The proposed data structure, called *TopoCluster*, inherits the localized approach for extracting relational operators from the Stellar decomposition. Different from the Stellar decomposition, it aims at enumerating all the simplices of the simplicial complex Σ through an *enumeration schema*. An explicit enumeration of the simplices of Σ provides multiple benefits from a developer perspective. A practical example is shown in Appendix

In the following, we describe the enumeration schema used by TopoCluster. In the remainder of this paper, σ_i indicates a simplex σ based on its index i; $\bar{\sigma}$ indicates a simplex σ based on its vertices $\{v_0,...,v_k\}$.

Cluster-based enumeration. Given any subdivision Δ that divides the vertices of the simplicial complex Σ into clusters, we define an enumeration schema by assigning each k-simplex to a single cluster. We assume that each vertex v is associated to a single cluster c. We say that v is *internal* to c, and c *contains* v.

For edges, triangles, and tetrahedra we define a k-simplex, with $k>0$, *internal* to a cluster c as follows.

Definition 4.1. Without loss of generality, we assume a total order on the clusters of Δ. Given a cluster $c \in \Delta$ and a k-simplex $\sigma \in \Sigma$, with $0 < k \leq d$, σ is *internal* to c iff. c is the first cluster containing a vertex of σ.

In Figure

The *cluster-based enumeration* is obtained by enforcing the following rules:

- k-simplices internal to a cluster c are enumerated within a closed interval $[l,u]$, where $u-l+1$ is the number of k-simplices internal to c;
- For any pair of clusters, the corresponding intervals do not overlap. As a consequence, for any pair of clusters c_i, c_j, with $i<j$, k-simplices in c_j have indices greater than those in c_i.

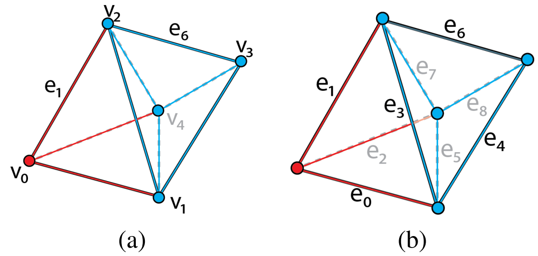

Fig. 2. Tetrahedral mesh Σ formed by two clusters. (a) Subdivision of vertices and edges across two clusters depicted with red and blue colors. (b) Enumeration of the edges of Σ.

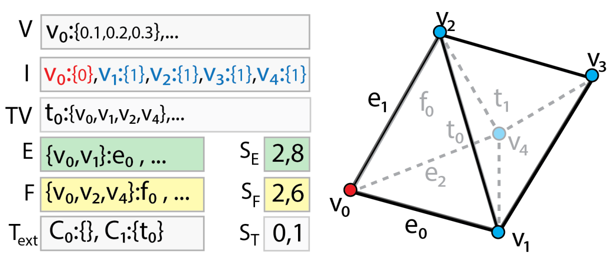

Fig. 3. Table on the left shows the global layer of Explicit TopoCluster for the tetrahedral mesh on the right. V encodes the coordinates of each vertex, I stores the cluster index of each vertex, TV stores the boundary vertices of each tetrahedron, E and F are hash maps encoding indices for edges and triangles respectively, T_{ext} stores indices of external tetrahedra, S_E, S_F, and S_T are arrays storing the enumeration intervals for edges, triangles and tetrahedra respectively.

The result is an explicit enumeration of the simplices of Σ, where each simplex is associated with a unique integer. Figure

Once defined the enumeration schema, we describe how such enumeration is encoded in the data structure. To this end, we have designed two strategies. The first strategy, named *Explicit*, prioritizes the time efficiency (see Section

5 Explicit TopoCluster

The first approach for encoding the enumeration schema is that of explicitly storing the index associated with each simplex of Σ. This is the strategy implemented by the first data structure introduced in this paper called *Explicit TopoCluster*. We recall that the idea behind TopoCluster is that of computing relational operators at runtime. To allow for this interaction, Explicit TopoCluster organizes information into two layers: the *global*, and the *local* layer.

The global layer, described in Section

5.1 Global layer

The global layer of Explicit TopoCluster includes the input tetrahedral mesh Σ, the input subdivision Δ, the enumeration schema, and the list of simplices intersecting each cluster defined in Δ.

Tetrahedral mesh. Mesh Σ is represented through an indexed representation, in which the vertices and tetrahedra are encoded in two arrays, V and TV, respectively. V encodes the coordinates of each vertex, while TV stores the boundary vertices of each tetrahedron (i.e., TV operator). For example, as shown in Figure

Clustering. The subdivision Δ is encoded with an array I, storing the cluster index of each vertex v in the simplicial mesh. For example, in Figure

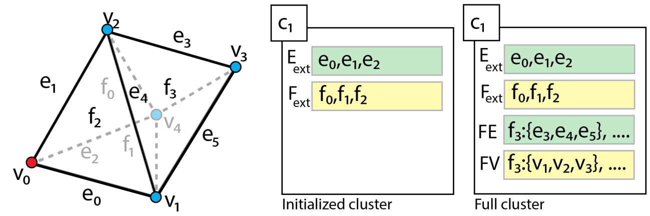

Fig. 4. The local layer of Explicit TopoCluster. An initialized cluster c_1 contains only external edges and triangles denoted by E_{ext} and F_{ext} respectively. The full cluster stores two additional arrays containing FE and FV relational operators.

Enumeration. As described in Section

Internal and external simplices. Finally, we need to encode how simplices are distributed across the clusters of Δ. Specifically, for each cluster c, we encode the simplices internal to c and the tetrahedra intersecting c that are internal to some other cluster. This information provides the full connectivity of the simplicial complex and will be used to compute relational operators (see Section

To retrieve the simplices internal to each cluster c, the number of tetrahedra, triangles, and edges encoded in c are stored in three global arrays named S_T, S_F, and S_E respectively. As mentioned in Section

Finally, an indexed array T_{ext} stores the list of external tetrahedra for each cluster. As shown in Figure

5.1.1 Initializing global structures

All information in the global layer are either received as input, or computed at initialization time. Vertex coordinates (i.e., array V), TV operators (i.e., array TV), and clustering function I are provided as input. Vertices and tetrahedra are reindexed in order to conform with the enumeration property. In practice, this means assigning contiguous indices to vertices(/tetrahedra) contained in the same cluster which takes $O(|V|+|T|)$ time. The array of external tetrahedra T_{ext} and array S_T are populated in $O(|T|)$ time by iterating over the array TV.

Hash tables E and F are initialized by visiting the clusters in any order. For each cluster c, internal edges and triangles are enumerated by checking the list of tetrahedra intersecting c. Since each internal tetrahedron is visited exactly once, and each external tetrahedron is visited at most four times, hash tables E and F are computed in $O(|T|)$. Arrays S_E and S_F are initialized during the same step with no additional cost.

Encoding the input mesh requires $O(|V|+|T|)$ memory. This cost includes the coordinate values of the each point and the TV operator of each tetrahedron. The size of S_E, S_F, and S_T arrays have size linear in the number of clusters (i.e., $O(|C|)$). The size of the hash maps E and F are determined by the number of edges and triangles in the mesh. Then, the global layer requires $O(|V|+|E|+|F|+|T|+|C|)$ memory.

5.2 Local layer: clusters

The local layer is where relational operators are computed and stored. Once a relational operator for a simplex σ is required, TopoCluster locates the cluster c_i containing σ, computes the relational operators of the simplices internal to c_i, and returns the relational operator of σ.

The cluster c_i is considered to be *empty* until a new relational operator is requested. Upon request, the cluster is *initialized* by

Algorithm 1 computeVT(c)

Input: c, cluster
Output: VT, tetrahedra incident in each vertex of cluster c

$VT = \{\}$ *// create empty table*
for each tetrahedron t_i intersecting c *// both internal and external* **do**
  for each v_i in $TV[t_i]$ **do**
    if v_i internal to c **then**
      $VT[v_i] \leftarrow t_i$ *// save t_i in the list associate to v_i*
    end if
  end for
end for
return VT

Algorithm 2 computeFE(c)

Input: c, cluster
Output: FE, edges of each triangle of cluster c

$FV \leftarrow$ **computeFV**(c) *// retrieve local information*
$FE = \{\}$ *// create empty table*
for each internal triangle f_i in c **do**
  for each pair of vertices $\bar{e} = \{v_i, v_j\}$ in $FV[f_i]$ **do**
    e_i = E($\bar{e}$) *// retrieve edge index*
    $FE[f_i] \leftarrow e_i$
  end for
end for
return FE

retrieving the information necessary to compute the relational operator. After a relational operator is computed and stored in c_i, we refer to c_i as *full*.

5.2.1 Initializing clusters

Initializing the cluster c_i means computing the list of internal and external simplices for c_i. Internal simplices are deduced from the arrays S_T, S_F, and S_E. The list of external tetrahedra intersecting the cluster is encoded in the global layer, specifically the array $T_{ext}[i]$. Upon initialization, the cluster c_i creates two arrays, E_{ext} and F_{ext}, encoding the list of external edges and triangles of c. Array E_{ext} is computed by cycling on the list of external tetrahedra $T_{ext}[i]$. For each external tetrahedron $\bar{t} = \{v_1, v_2, v_3, v_4\}$, for each pair of vertices $\bar{e} = \{v_j, v_k\}$ such that $\{v_j, v_k\} \in \bar{t}$ and $v_j \neq v_k$, the index e_j is retrieved from the global hash map E (i.e., $e_j = E(\bar{e})$) and added to E_{ext}. Array F_{ext} is built in a similar fashion by considering triples of vertices for each tetrahedron.

When both E_{ext} and F_{ext} are computed, c_i is said *initialized*. Since the number of vertices per tetrahedron is constant, the initialization of cluster c_i requires $O(|T_{ext}[i]|)$ time. Figure

5.2.2 Computing relational operators

Relational operators for a cluster c_i are computed only after the cluster is initialized. In the following, we describe as an example the extraction of relational operators VT and FE.

VT operator represents the set of tetrahedra incidents in each vertex. Algorithm

Algorithm

Figure

6 Implicit TopoCluster

Explicit TopoCluster fully encodes the enumeration of edges and triangles with the two hash tables E and F. We defined a second data structure, called *Implicit TopoCluster*, implementing a different strategy. Instead of encoding the two hash tables E and F in the global layer, the indexing of edges and triangles is computed on-the-fly when accessing a cluster. This drastically reduces the total cost of the global layer to $O(|V| + |T| + |C|)$.

In the following, we describe the local layer of Implicit TopoCluster since the initialization of the global layer is as in the Explicit TopoCluster (see Section

6.1 Local layer: clusters

The local layer of Implicit TopoCluster resembles that of Explicit TopoCluster. Also in this case, a cluster c_i is said *empty* until a new relational operator is requested. Upon request, the cluster is *initialized* by retrieving the information necessary to compute the relational operator. After a relational operator is computed and stored in c_i, we refer to c_i as *full*.

6.1.1 Initializing clusters

Upon initialization, cluster c_i computes the hash tables of external edges and triangles (i.e., E_{ext} and F_{ext}) as in the Explicit TopoCluster. Additionally, two hash tables are computed associating the enumeration of edges and triangles to their vertices (i.e., hash tables E and F). The latter encodes the same information of the hash tables used by Explicit TopoCluster, but instead of being stored globally, these are stored locally to c_i and encode information limitedly to edges and triangles internal to c_i.

Figure

All structures are generated by iterating the list of tetrahedra intersecting c_i. First, we create hash tables E and F by computing a local enumeration of the internal edges and internal triangles defined over a closed interval $[0, p]$, where p is either the total number of internal edges or the total number of internal triangles. Global indices for the edges are obtained by shifting the local enumeration according to the global enumeration, i.e., $[S_E[i-1]+1, S_E[i]] = [l, u]$. If an edge has local index j, its global index is $j + l$. Global indices for triangles are retrieved in a similar way. The time complexity for computing the local enumeration is $O(|T_{int}|)$, where $|T_{int}| = S_T[i] - S_T[i-1]$ is the number of internal tetrahedra of c_i.

External edges and triangles are retrieved by iterating the list of external tetrahedra $T_{ext}[i]$, similarly to the Explicit TopoCluster. The difference is that the index of each external simplex is no longer provided by global hash maps. To get the index corresponding to an external edge or triangle, we have to access the cluster c_j containing it and compute the internal simplices of c_j. This step requires $O(\sum_{j=0}^{n} |T_{int}^{j}|)$ time, where $|T_{int}^{j}|$ indicates the tetrahedra internal to the cluster c_j, sharing a simplex with cluster c_i. Hence, initializing the cluster c_i requires $O(|T_{int}| + \sum_{j=0}^{n} |T_{int}^{j}|)$ time in total.

6.1.2 Computing relational operators

The strategy for computing relational operators for the Implicit TopoCluster is similar to the Explicit TopoCluster. For example, let us consider the extraction of EF operator (as detailed in Algorithm

Similar to the Explicit TopoCluster, the time complexity of extracting a relational operator is linear to the number of higher dimensional simplices involved. For example, the complexity of

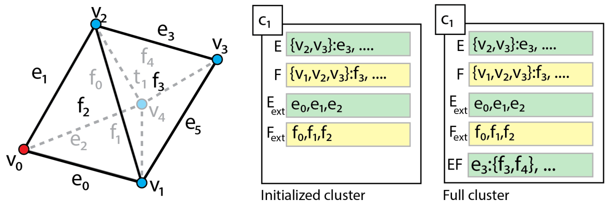

Fig. 5. The local layer of Implicit TopoCluster. An initialized cluster c_1 contains the hash maps for edges and triangles denoted by E and F respectively, and external edges and triangles denoted by E_{ext} and F_{ext} respectively. The full cluster stores and additional array containing the EF relational operator.

Algorithm 3 computeEF(c)

Input: c, cluster
Output: EF, triangles incident in each edge of cluster c

  // Initialize the cluster c
E, F, F_{ext} $\leftarrow$ **initialize**(c)
$EF = \{\}$ *// create empty table*
for each triangle $\bar{f}$ in $(F \cup F_{ext})$ *// both internal and external* **do**
  for each pair of vertices $\bar{e} = \{v_i, v_j\}$ of $\bar{f}$ **do**
    if $\bar{e}$ is internal to c **then**
      if $\bar{f}$ is internal to c **then**
        $f_i = F(\bar{f})$
      else
        $f_i = F_{ext}(\bar{f})$
      end if
      $EF[E[\bar{e}]] \leftarrow f_i$
    end if
  end for
end for
return EF

extracting the EF operator is linear to the number of triangles in the cluster, i.e., $O(|F \cup F_{ext}|)$.

7 Performance Optimization strategies

To optimize memory and time performance, we have defined two strategies: a preconditioning approach, and a cache system.

The first strategy adopts the same preconditioning approach used by TTK [30]. A developer declares the set of relational operators required by an algorithm. Then, clusters will be initialized only with information for those relational operators. For example, suppose we implement an algorithm using only VV and TV operators. The data structure will never enumerate edges and triangles at generation time and it will never compute the associated structures when initializing a cluster. In practice, all structures depicted in green (for edges) and yellow (for triangles) in Figures

Both Explicit and Implicit TopoCluster use the same approach for computing relational operators. Specifically, they compute and discard information each time a cluster is accessed. This introduces a clear drawback when a cluster is accessed multiple times. To tackle this problem, we have defined a second technique inspired by the Stellar tree [12]. This strategy defines a cache system for the clusters based on the Least Recently Used (LRU) replacement strategy. Each time a full cluster c_i is computed, it is saved in the cache. The cluster in the cache will be replaced based on the last time it was accessed. Since the cache size (i.e., the maximum number of clusters that the cache can maintain) is controlled by a user-defined parameter, the memory requirements cannot be estimated theoretically, but we provide an experimental analysis in Section

TABLE 1
Overview of the experimental datasets. For each dataset, we list the type, the number of vertices $|V|$, edges $|E|$, triangles $|F|$ and tetrahedra $|T|$. *Regular* means the dataset comes from 3D regular grids, while *Irregular* means the dataset comes from a tetrahedral mesh with irregularly distributed points.

Data	Type	$\|V\|$	$\|E\|$	$\|F\|$	$\|T\|$
Red Sea	Regular	0.95M	6.33M	10.58M	5.20M
Engine	Regular	1.39M	9.14M	15.18M	7.43M
Cat	Irregular	1.97M	13.24M	22.25M	10.99M
Sphere	Irregular	2.62M	17.54M	29.46M	14.53M
Foot	Regular	4.60M	30.79M	51.51M	25.32M
Shapes	Irregular	7.87M	52.37M	87.63M	43.13M
Hole	Irregular	9.26M	63.70M	108.29M	53.85M
Stent	Regular	17.37M	118.79M	201.40M	99.98M

8 Evaluation of performance

Explicit and Implicit TopoClusters have been implemented as two modules of the Topology Toolkit (TTK version 0.9.7) [30], and use the same interface as the *abstractTriangulation* class of TTK. As a result, all modules implemented in TTK can run seamlessly with TopoCluster.

We recall that TopoCluster requires a clustering for the vertices of the tetrahedral mesh to be provided in input. In the following evaluation, we use a clustering technique based on the Point Region (PR) octree [28]. An octree uses a hierarchical domain decomposition based on a nested refinement of the unit cube. The containment relationship on such cubes defines a hierarchical relationship among the nodes in the octree. The PR octree is constructed by defining the maximum number of vertices allowed in any leaf node of the octree. In the end, vertices belonging to the same leaf node in the PR octree form a cluster in TopoCluster. We select this clustering approach for its generality since any spatially-embedded mesh can be decomposed into clusters using this subdivision.

The following performance analysis is conducted on tetrahedral meshes with the number of vertices between 950K and 17M and with number of tetrahedra between 5.2M and 100M (see Table

8.1 Computing relational operators

In this section, we compare our data structures against the Stellar tree [12] and TTK triangulation [30]. All four data structures use the same encoding for the underlying mesh, that encodes in two arrays the vertex coordinates and the TV operator of each tetrahedron σ, i.e., the list of vertices in the boundary of σ.

TTK Triangulation. TTK triangulation [30] precomputes relational operators at generation time and stores them in multiple lookup tables. Lookup tables, as well as the list of edges and triangles, are extracted in $O(|T|)$ by enumerating all pairs/triplets of vertices. This approach achieves best time performance at

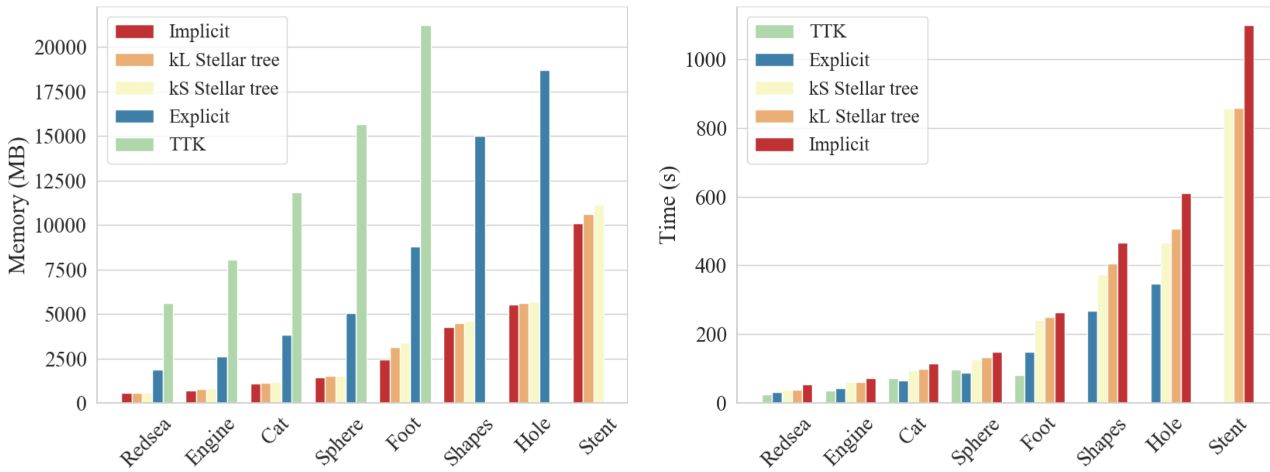

Fig. 6. Memory (in Megabytes) and time (in seconds) required for computing all relation operators with TTK triangulation, Stellar tree, Explicit TopoCluster and Implicit TopoCluster. k_L and k_S indicate a Stellar tree computed with either the larger (800) or smaller (400) bucketing threshold.

runtime since the data structure will provide fast access to all necessary relational operators. At the same time, this strategy is very demanding in terms of memory since relational operators are stored, for the entire execution of the algorithm.

Stellar tree. The Stellar tree is the first data structure defined upon the Stellar decomposition model [12]. It uses a hierarchical decomposition (a Point Region octree [28]) to organize the mesh vertices. The hierarchy $\mathbb{H}$ is encoded through a tree structure used to navigate the mesh. A bucketing threshold is used for limiting the number of vertices per leaf node. In our experiments, we use the bucketing threshold 400 and 800 following the guidelines from the original paper [12]. Another difference compared with TopoCluster is the internal representation of simplices. The Stellar tree enumerates globally only vertices and tetrahedra while it avoids enumerating edges and triangles and represents such simplices as a tuple of vertices.

We compare the performance of the four data structures for extracting relational operators. We start by computing all relational operators involving vertices. Then, we move to edges, triangles, and tetrahedra. Notice that TopoCluster requires two user-defined parameters. The first parameter is the cache size which defines the maximum number of clusters stored in cache (see Section

Figure

Regarding the memory footprint, Explicit TopoCluster provides a good improvement compared to TTK triangulation. Memory usage decreases by three times when using Explicit TopoCluster. Implicit TopoCluster is always the most compact data structure requiring 10% less memory than the Stellar tree.

Considering execution time, Implicit TopoCluster is always the slowest at extracting relational operators. On average, it requires up to 20% time more than the Stellar tree, 70% more time than the Explicit, and it is twice slower than TTK triangulation. TTK triangulation and the Explicit TopoCluster have overall similar performance, even if the latter requires on average 20% more time than TTK triangulation.

Compared to TTK triangulation, the scalability provided by TopoCluster is of practical relevance. Implicit TopoCluster is twice slower than TTK triangulation, but it is also ten times more compact. Explicit TopoCluster is 20% slower than TTK triangulation, but it is also three times more compact.

Compared to the Stellar tree, Implicit TopoCluster is 20% slower, but also 10% more compact. Explicit TopoCluster uses three times the memory than a Stellar tree, but it is also 30% faster. We recall that each simplex is referenced as a unique number in TopoCluster. The generation of such enumeration schema requires more time, which is why TopoCluster is slower than the Stellar tree. Since the enumeration lets us represent each simplex as a single integer, this also explains why Implicit TopoCluster is more compact.

Overall the main advantage of the enumeration strategy implemented in TopoCluster is the easy integration with existing frameworks. In the following sections, we drop the comparison with the Stellar tree, since it does not allow for such integration, and we compare TTK Triangulation and TopoCluster performance by running existing TTK plugins.

8.2 Plugins for topology-based visualization

TTK offers several plugins for topology-based visualization [19]. For the sake of our comparison, we are interested in distinguishing plugins based on how they process the input mesh.

Some plugin visits simplices in a sequential order following the enumeration schema. As a consequence, TopoCluster will access clusters in the same sequential order. We select *TTKScalarFieldCriticalPoints* as an example of a plugin of this kind. Conversely, other plugins visit simplices in a pseudo-random fashion which will force TopoCluster to visit clusters in a random order, possibly initializing the same cluster multiple times. We select *TTKMorseSmaleComplex* as an example of a plugin of this kind.

TTKScalarFieldCriticalPoints. This plugin is used for computing critical points from a given input scalar function. Cluster sizes 5000, and 10000 are chosen for Explicit and Implicit TopoCluster, respectively. Cache size of 1% is selected for both structures.

This plugin requires extracting VV and VT operators. Moreover, VF and FT operators are computed to identify the list of boundary vertices. We recall that a vertex v is on the mesh boundary if at least one of the triangles incident in v has only one tetrahedron on its coboundary.

Figure

TTKMorseSmaleComplex. This plugin is used for computing a Morse-Smale (MS) complex from an input scalar function f defined on a simplicial complex Σ. An *integral line* is a path on

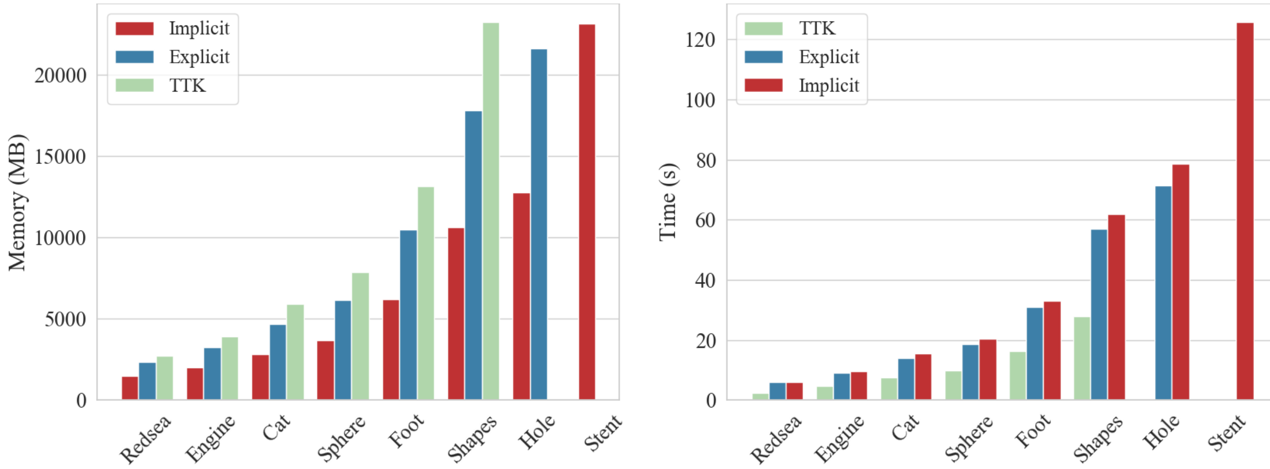

Fig. 7. Memory (in Megabytes) and time (in seconds) required for computing critical points (plugin *ScalarFieldCriticalPoints*) with TTK triangulation (TTK), Explicit TopoCluster (Explicit), and Implicit TopoCluster (Implicit).

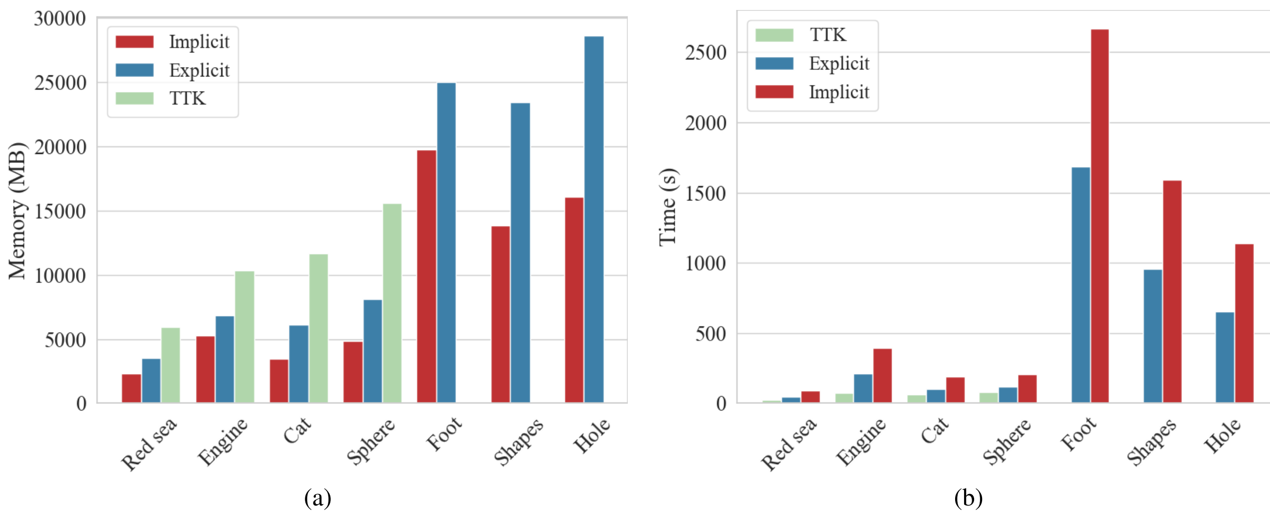

Fig. 8. Memory (in Megabytes) and time (in seconds) required for computing Morse-Smale complex (plugin *MorseSmaleComplex*) with TTK triangulation (TTK), Explicit TopoCluster (Explicit), and Implicit TopoCluster (Implicit).

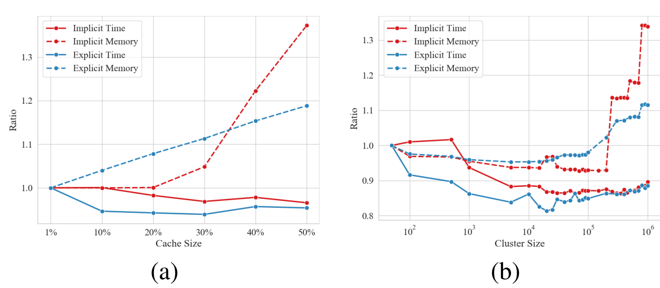

Fig. 9. The changes of memory and time usage on *TTKScalarFieldCriticalPoints* plugin for *Foot* dataset with *Implicit* and *Explicit* TopoCluster when (a) cache rate changes from 1% to 50% and (b) cluster size changes from 10 to 1,000,000.

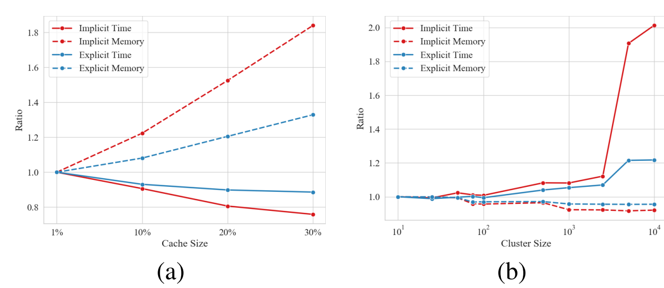

Fig. 10. The changes of memory and time usage on *TTKMorseSmaleComplex* plugin for *Foot* dataset with *Implicit* and *Explicit* TopoCluster when (a) cache rate changes from 1% to 30% and (b) cluster size changes from 10 to 10,000.

Σ which is everywhere tangent to the gradient of f. Integral lines connect pairs of critical points of f. Intuitively, the *MS complex* is a segmentation of the input scalar field in regions where integral lines are connected to the same pair of critical points. Many algorithms have been proposed in the last twenty years [10] to compute MS complexes both in 2D and 3D. Among these, approaches based on discrete Morse theory [13] have proved to be efficient, simpler to implement, and more scalable [18], [26], [33]. The algorithm implemented in TTK, also based on discrete Morse theory, requires almost all relational operators (i.e., VE, VF, VT, EF, ET, FE, FT and TF operators) [30].

First, a discrete gradient is computed by visiting the simplices of the mesh, dimension by dimension, with an embarrassingly parallel process. After all vector pairs have been computed, simplices that are left unpaired are called *critical*. The cells of the MS complex are computed by visiting the discrete gradient starting from the critical simplices.

For the sake of our evaluation, it is important to underline that the extraction of the MS complex requires visiting clusters in a random fashion. That is, starting at a critical simplex σ, the visit is not limited to the cluster containing σ, but it may expand to the surrounding clusters. Then, there is no limit to the number of times each cluster is visited. This represents a worst-case scenario for TopoCluster, which is forced to recompute topological operators multiple times during the plugin execution.

For this experiment, the cluster size is set to 50, while the cache size is set to 10% for both Explicit and Implicit structure (see Section

We can also observe how the memory footprint of TopoCluster does not increase monotonically when using datasets with increasing size. This is a consequence of reducing the memory footprint of relational operators. With only a limited amount of memory dedicated to relational operators, the memory requirement of TopoCluster becomes output-sensitive (i.e., it depends on the size of the MS complex). For this reason, the dataset with a more complicated MS complex, e.g., Foot or Engine datasets, uses more memory than larger datasets.

Figure

8.3 Cache and cluster size

In this section, we discuss the effects that different cache sizes and cluster sizes have on performance. Since a trend has been observed for all datasets, we only show the results about the *Foot* dataset for brevity.

TTKScalarFieldCriticalPoints. For a sequential algorithm, the cache size is of limited importance. Increasing cache size only results in increased memory usage with limited effects on run time. Figure

Different cluster sizes, instead, affect both execution time and memory usage. Figure

TTKMorseSmaleComplex. Unlike the sequential access pattern, the cache size parameter plays an important role in the algorithm that accesses clusters in a pseudo-random way. Figure

Timings increase when increasing the cluster size (see Figure

The lesson learned is that small cluster size is beneficial when an algorithm accesses clusters in a pseudo-random fashion. The available system memory should guide the choice of the optimal cache size since a larger cache size is always beneficial as long as the program does not run out of memory.

8.4 Parallel processing

TTK allows multithread execution by using OpenMP [6]. The main problem in allowing the use of OpenMP with TopoCluster is the cache system. A global LRU cache becomes the main bottleneck since each thread needs exclusive access to it. To address this problem, we have implemented a thread-based caching system. In practice, each thread has a dedicated cache.

If the thread-based cache solves the bottleneck issue, the cache size requires some adjustment since the maximum number of clusters stored in each cache will be multiplied by the number of threads. To this end, TopoCluster provides the functionality of a *dynamic* caching system, which allows the user to specify the size of the cache for a specific subset of the algorithm. In practice, the user can increase the cache size for serial sections, and divide the cache size across multiple threads for parallel sections.

The performance of the new thread-based caching system has been evaluated with *TTKScalarFieldCriticalPoints* and *TTKMorseSmaleComplex* plugins, using the same cluster size of the serial execution and using 12 threads. Since the main goal of TopoCluster is to provide control over memory usage, we balance the cache size requested for multi-thread and single-thread executions. We select a 12% cache size for the single-thread execution, while in parallel sections the cache size is reduced to 1%.

The algorithm implemented in *TTKScalarFieldCriticalPoints* is embarrassingly parallel. Thus, the cache size is maintained at 1% for the entire algorithm. Figure

The memory consumption is roughly the same as the serial execution for all data structures. Among the three data structures, Implicit TopoCluster always uses less memory and is the only data structure that can execute the plugin on all the datasets.

Although the run time improves for all data structures, general trends remain similar to the single-thread run. Implicit TopoCluster uses 50% less memory than the TTK triangulation but is 1.5x slower. Implicit TopoCluster has similar time performance as Explicit TopoCluster, while using only 60% of the memory.

Figure

Finding general trends in the *TTKMorseSmaleComplex* plugin is more challenging since not all steps can be executed in parallel. In this case, we use the dynamic caching system allocating 12% cache size for sequential steps, and 1% cache size for the parallel ones.

Figure

Figure

Since the complexity of the MS complex impacts on the performance of TopoCluster (see Section

In general, TTK triangulation provides best time performance, but it can only be used with meshes of limited size. If the user needs to limit memory consumption while maintaining competitive time performance, Explicit TopoCluster is a satisfactory pick. Implicit TopoCluster is the best choice with very large datasets or when the system has limited memory.

9 Conclusion

In this work, we have designed two new data structures, Explicit and Implicit TopoCluster, based on the Stellar decomposition model [12]. The scope of both data structures is to improve scalability by reducing memory consumption. Both data structures divide the simplicial mesh into clusters in order to process the mesh locally. Explicit TopoCluster encodes more information in the global layer and guarantees run-time efficiency while requiring more memory. On the contrary, Implicit TopoCluster encodes less information in the global layer and guarantees lower memory consumption with limited overhead. We have integrated both data structures in the Topology Toolkit [30], which provides an easy-to-use interface to developers and practitioners in topological data analysis. TopoCluster supports shared memory parallelization based on OpenMP [6], and it can be used with any plugin implemented in TTK.

In our experimental evaluation, we have compared Explicit and Implicit TopoCluster with TTK triangulation [30] and the Stellar tree [12]. Compared to TTK triangulation, Explicit TopoCluster requires half of the memory while still having comparable time

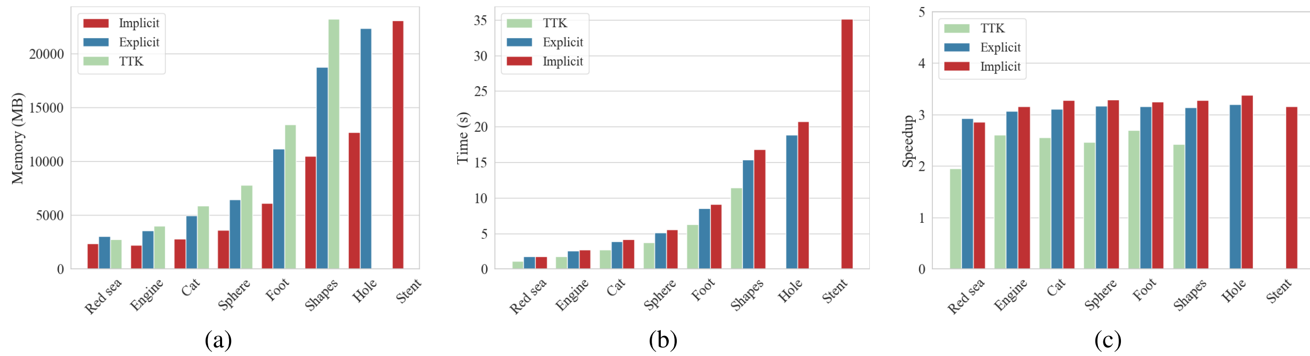

Fig. 11. The results obtained computing critical points (i.e., plugin TTKCriticalPoints) with TTK triangulation (TTK), Explicit TopoCluster (Explicit), and Implicit TopoCluster (Implicit) and enabling OpenMP support. (a) Memory consumption when 1% cache rate is used for TopoCluster. (b) Time usage when 1% cache rate is used for TopoCluster. (c) Speedup for all three data structures compared to serial execution.

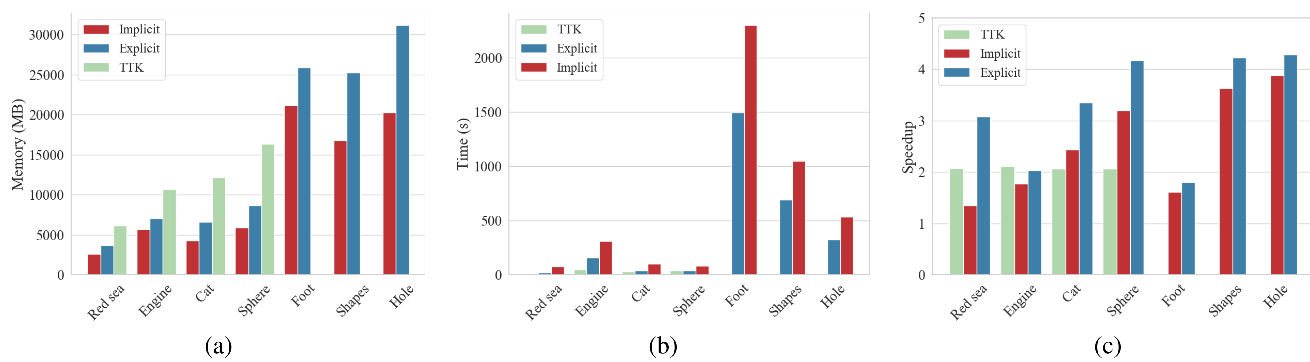

Fig. 12. The results obtained computing Morse-Smale complex (i.e., plugin TTKMorseSmaleComplex) with TTK triangulation (TTK), Explicit TopoCluster (Explicit), and Implicit TopoCluster (Implicit) and enabling OpenMP support. (a) Memory consumption when 1% cache rate is used for TopoCluster. (b) Time usage when 1% cache rate is used for TopoCluster. (c) Speedup for all three data structures compared to serial execution.

performance. When minimal memory usage is crucial, Implicit TopoCluster requires an order of magnitude less memory but is twice slower than TTK triangulation. Compared to the Stellar tree, Explicit TopoCluster uses twice the memory while being 30% faster. Implicit TopoCluster uses 20% less memory while being up to 25% slower than the Stellar tree. However, TopoCluster provides a much easier interface for developers, and it is easier to integrate into existing frameworks for mesh processing.

Even though TopoCluster is currently designed for tetrahedral meshes, it is straightforward to adapt the data structure for triangle meshes. Generalizing TopoCluster to higher dimensions by enumerating all simplices is possible, but this could lead to severe performance decay since the number of simplices grows exponentially with the increase of the complex dimension. This problem affects all data structures that enumerate simplices in full [12].

By enabling OpenMP support in TopoCluster, we have observed that the local processing of the relational operators provides a higher speedup than TTK triangulation. A promising direction of our research is designing a new version of TopoCluster for distributed environments where groups of clusters are distributed across multiple machines.

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Appendix A

Associating unique identifiers to the simplices of a simplicial complex represents a clear advantage for developers.

Figure

The code shown in Figure

```
1 void computeEdgeValues(){
2     int edgeNum = getEdgeNumber();
3     vector<int> values(edgeNum);
4     for(int i=0; i<edgeNum; i++){
5         int v1 = getEdgeVertex(0,i)
6         int v2 = getEdgeVertex(1,i)
7         values[i] = computeValue(v1,v2)
8     }
9 }
```

Fig. 13. Code snippet for the procedure *computeEdgeValues()* implemented in TopoCluster.

```
1  void computeEdgeValues(){
2      map<pair<int,int>, int> values();
3      queue<Node> bfs_visit;
4      bfs_visit.push(getRoot());
5      while(!bfs_visit.empty()){
6          Node node = bfs_visit.head();
7          bfs_visit.pop();
8          if(node.isLeaf()){
9              for(pair<int,int> edge : node.getEdges()){
10                 if(values.find(edge) != values.end()){
11                     values[edge] =
12                     computeValue(edge.first,edge.second);
13                 }
14             }
15         }
16         else{
17             for(Node child : node.getChildren()){
18                 bfs_visit.push(child);
19             }
20         }
21     }
22 }
```

Fig. 14. Code snippet for the procedure *computeEdgeValues()* implemented in the Stellar tree.

The code is simplified thanks to the enumeration provided by TopoCluster. First, results are saved in a simple indexed vector (row 5). Second, each edge is visited by means of a simple for loop (row 6). As a consequence, making a parallel version of the same function would be trivial using OpenMP [6].

Implementing the same procedure without the enumeration property would require more involved code. Figure

The *std::vector* is now replaced by a *std::map* since now each edge is internally represented by a pair of vertices (row 2). The visit of all the edges is replaced by a breadth-first search of the hierarchical decomposition. The visit starts at the root of the hierarchy (row 4) and traverses the entire hierarchy until reaching the leaf nodes, which are the nodes storing the edges (row 8). Moreover, since each edge may appear in multiple nodes, duplicate entries need to be handled accordingly (row 10).