Fast tree-based algorithms for DBSCAN on GPUs

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DBSCAN is a well-known density-based clustering algorithm to discover clusters of arbitrary shape. The efforts to parallelize the algorithm on GPUs often suffer from high thread execution divergence (for example, due to asynchronous calls to range queries). In this paper, we propose a new general framework for DBSCAN on GPUs, and propose two tree-based algorithms within that framework. Both algorithms fuse neighbor search with updating clustering information, and differ in their treatment of dense regions of the data. We show that the cost of computing clusters is at most twice the cost of neighbor determination in parallel. We compare the proposed algorithms with existing GPU implementations, and demonstrate their competitiveness and excellent performance in the presence of a fast traversal structure (bounding volume hierarchy). In addition, we show that the memory usage can be reduced by processing the neighbors of an object on the fly without storing them.

1 Introduction

Clustering is a data mining technique that splits a set of objects into disjoint classes, called clusters, each containing similar objects. DBSCAN (Density-Based Spatial Clustering of Applications with Noise) [13] is a density-based clustering algorithm. It is attractive in situations where the number of clusters is not known a priori, or where clusters may be of irregular shape. It is widely used in a diverse set of applications such as bioinformatics [29], noise filtering and outlier detection [5], halos identification in cosmology [36], image segmentation [37], and many others.

The DBSCAN algorithm is based on a notion of the local density of each point, requiring identifying close neighbors of each point in a dataset. Its breadth-first search nature makes parallelization a challenge. Major progress has been made in the last two decades, starting from the master-slave [43, 3] and map-reduced [20, 11] approaches, and transitioning to using shared memory [34, 33, 18, 25] and GPU [6, 39, 2, 42, 41, 27, 15, 9, 16] implementations, and even approximate algorithms [35, 28, 10]. A breakthrough realized in the work [34] introduced using the UNION-FIND technique for cluster labeling. This fundamentally changed the nature of the algorithm, breaking with its breadth-first search nature.

In this work, we first introduce a general parallel algorithm with sufficient degree of parallelism for thousands of cores available on GPUs. All components of the algorithm are executed on a GPU, requiring no transfers of data between a CPU and a GPU. From the moment the data is loaded into the device memory, as long as the data and constructed search index fit into the GPU memory, all operations are executed on a GPU. We then propose two concrete implementations, focusing on low-dimensional (e.g., spatial) data. As neighborhood search plays a crucial role in the overall algorithm performance, our approach prioritizes using an indexing structure with a fast batched neighborhood search. Specifically, we use a bounding volume hierarchy (BVH), a structure predominantly used in computer graphics for ray tracing. BVH was chosen for its good data and thread divergence characteristics. We combine it with a synchronization-free union-find technique introduced in [22]. Our approach allows processing the found neighboring points on-the-fly, reducing the overall memory consumption of the limited memory on a GPU. We introduce several traversal optimization techniques and reduce the number of distance calculations used by the algorithm in the dense regions. Significant performance improvements over available GPU DBSCAN implementations are demonstrated. Since the local DBSCAN implementation is an inherent component of a full distributed algorithm, the proposed algorithm can be easily plugged into most distributed frameworks to improve the overall performance.

The remainder of the paper is organized as follows. Section 2 introduces the DBSCAN algorithm and related work. Section 3 describes a general framework for a GPU DBSCAN implementation allowing for fine-grained

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parallelism. In Section 4, we describe two tree-based algorithms within that framework. Finally, we demonstrate the algorithm performance in Section 5 and derive our conclusions and future work in Section 6.

2 Background

2.1 DBSCAN algorithm

We briefly outline the DBSCAN algorithm in this Section, referring the readers to [13] for more details.

Let $X$ be a set of $n$ points to be clustered. The key idea of the algorithm is that for a point to be in a cluster, the density in its neighborhood has to exceed some threshold, i.e., its neighborhood has to contain at least a minimum number of points. This is formalized using two user-provided parameters: $\text{minpts} \in \mathbb{N}^+$ and $\varepsilon \in \mathbb{R}^+$.

An $\varepsilon$-neighborhood of a point $x$ is defined as $N_{\varepsilon}(x) = \{y \in X \mid \text{dist}(x, y) \leq \varepsilon\}$, with $\text{dist}(\cdot, \cdot)$ being a distance metric for the set $X$ (e.g., Euclidean). The $\text{minpts}$ parameter defines the minimum number of points for a point to be considered inside a cluster, and a point $x$ is called a core point if $|N_{\varepsilon}(x)| \geq \text{minpts}$. A point $y$ is directly density-reachable from a point $x$ if $x$ is a core point and $y \in N_{\varepsilon}(x)$. A point $y$ is density-reachable from a point $x$ if there is a chain of points $x_1, \ldots, x_n$, $x_1 = x$, $x_n = y$, such that $x_{i+1}$ is directly density-reachable from $x_i$. Points $x$ and $y$ are called density-connected if there exists a point $z$ in $X$ such that both $x$ and $y$ are density-reachable from $z$. Finally, a point $x$ is called a border point if it is density-reachable from a core point, but is not a core point itself. The points that are not core or border points are called noise and are considered to be outliers not belonging to any cluster. Any cluster then consists of a combination of core points (at least one) and border points (possibly, none). Note, that as a border point may be density-reachable from multiple core points, it could potentially belong to multiple clusters. Implementations of the algorithm may differ in their handling of such border points, but typically assign them to a single cluster.

The special case of $\text{minpts} = 2$ (sometimes called Friends-of-Friends, or halo finding in the cosmology literature) is equivalent to finding strongly connected components in the adjacency graph $G = (V, E)$, where $V = X$ and two vertices $x$ and $y$ have an (undirected) edge between them if $\text{dist}(x, y) \leq \varepsilon$. In this case, there are no boundary points, and a point either belongs to a cluster as a core point, or is in the noise.

The pseudocode for the DBSCAN algorithm is shown in the Algorithm 1. The algorithm starts at an arbitrary point $x \in X$, computing its $\varepsilon$-neighborhood $N$ (line 4). If $x$ is not a core point, i.e., $|N| < \text{minpts}$, $x$ is tentatively marked as noise (line 6), and another point is chosen. Otherwise, the algorithm constructs a new cluster $C$ by incrementally adding points that are density-reachable from $x$ in a breadth-first search manner (lines 8-17), including the points that may have been previously marked as noise. Encountered border points are assigned to the first encountered cluster that they are density-reachable from. The algorithm has a computational complexity of $O(n^2)$, or $O(n \log n)$ if a spatial indexing structure (e.g., k-d tree [4] or R-tree [17]) is used.

This standard form of the DBSCAN algorithms led to several interesting adaptations. Among them, DBSCAN* proposed in [7] simplified the algorithm by removing the notion of border points completely, thereby improving consistency with the statistical interpretation of clustering and serving as a basis for a new hierarchical HDBSCAN algorithm [8, 30]. While not addressed in this work, the algorithms proposed in this paper can be easily adapted for DBSCAN*, with several further optimizations possible.

Algorithm 1 DBSCAN algorithm

1: procedure DBSCAN($X, \text{minpts}, \varepsilon$)
2: for each unvisited point $x \in X$ do
3: mark $x$ as visited
4: $N \leftarrow \text{GetNeighbors}(x, \varepsilon)$
5: if $|N| < \text{minpts}$ then
6: mark $x$ as noise
7: else
8: $C \leftarrow \{x\}$
9: for all $y \in N, D$ do
10: if $y$ is not visited then
11: mark $y$ as visited
12: $N \leftarrow \text{GetNeighbors}(y, \varepsilon)$
13: if $|N| \geq \text{minpts}$ then
14: $N \leftarrow N \cup \bar{N}$
15: if $y$ is not a member of any cluster then
16: $C \leftarrow C \cup \{y\}$
17: end if
end for
end if
end for
end procedure

2.2 Related work

Many papers detail parallelization techniques in distributed [43, 20, 34, 42, 41, 33, 18, 21] and shared memory [34, 33, 25] contexts. Instead, here we focus on the works addressing the algorithm parallelization using GPUs.

[6] proposed two algorithms. CUDA-DChust creates sub-clusters (chains) of points density-reachable from each other. Multiple chains are created simultaneously in parallel on a GPU. The algorithm keeps track of chain
collisions through a collision matrix, which is resolved on the CPU in the final stage. CUDA-DClust* is an extension of CUDA-DClust that uses an indexing technique (based on a constant number of directory level partitions) for the computation of \( N_x(x) \). Two slight modifications of CUDA-DClust, reducing the number of memory transfers between a CPU and a GPU, and identifying core points prior to cluster generation, were proposed in Mr. Scan [42]. [39] offloads the \( N_x(x) \) computation to the GPU by assigning points in \( X \) to different threads, which check the distance to \( x \) in parallel. G-DBSCAN [2] constructs the adjacency graph using an all-to-all computation on the GPU, and then executes a parallel breadth-first search with level synchronization. An extension of CUDA-DClust is realized in CudaSCAN [27], which trims the amount of required distance evaluations by partitioning a data set into subregions and performing local clustering within the sub-regions in parallel. A special case of DBSCAN with \( \text{minpts} = 2 \) was studied in [36], where an implicit graph structure combined with a disjoint-set algorithm was used to find strongly connected components utilizing a cell partitioning of the domain as an indexing structure. [15] utilizes a hybrid CPU-GPU approach in which the neighbors of each point are first identified on the GPU, then the neighbor list is transferred to the host, where the clustering is performed. In [32], the authors compared existing GPU implementations in [39], CUDA-DClust* [6] and G-DBSCAN [2], and found G-DBSCAN to be the fastest but requiring significantly more memory (166x of CUDA-DClust) due to storing the adjacency graph. [14] extended the work [15], addressing the limitations of the GPU memory by using a batched mode to incrementally compute \( N_x(x) \), and explored avoiding distance calculations in the dense regions by superimposing a regular grid over the domain, with a special treatment of the cells containing at least \( \text{minpts} \) points, called dense cells.

This work shares similarities with several of the mentioned algorithms. Similar to [2], our algorithm operates on the adjacency graph. However, in this work, the graph is implicit and is never fully formed, resolving many of the memory constraints of the algorithm identified in [32]. Compared to [36], which can be seen as a precursor, this work implements the full DBSCAN algorithm, uses a synchronization-free non-iterative union-find algorithm, and uses and optimizes a tree-based different indexing structure. Like in this work, [15] identified batched neighbor search as a key to performance; however, that approach produced a full adjacency graph and relied on CPU for the clustering itself. We follow the ideas introduced in [42, 36, 14], and utilize an auxiliary regular grid to reduce the number of distance calculations. Compared to the mentioned works, however, the cells of the grid become primitives used in the construction of the tree, both reducing the size of the tree, and allowing for an easier merge of dense cells. Finally, compared to most of the works mentioned, the algorithm only uses the GPU with no support from a CPU, requiring no data transfer between host and device memories during the execution.

3 Parallel DBSCAN framework for GPUs

In this Section, we describe a disjoint-set based approach to the DBSCAN algorithm as proposed in [34], and reformulate the algorithm to expose fine-grained parallelism required in a GPU implementation.

3.1 Disjoint-set based DBSCAN

The main obstacle to the parallelization of the DBSCAN algorithm in the original form (Algorithm 1) is its breadth-first manner of encountering new points, and the linear time required to update the existing neighbor set \( N \). The algorithm proposed in [34] breaks with its breadth-first nature, and serves as the foundation for this work. Instead of maintaining an explicit list of indices, the authors used the UNION-FIND [38] approach to maintain a disjoint-set data structure. The approach relies on two main operations: UNION and FIND. FIND\((x)\) determines the representative of a set that a point \( x \) belongs to, while UNION\((x, y)\) combines the sets that \( x \) and \( y \) belong to.

The UNION-FIND algorithm is typically implemented using trees. For any point \( x \), its representative, returned by FIND\((x)\), is the root of the tree containing \( x \). The UNION\((x, y)\) operation merges two trees (containing \( x \) and \( y \)) by pointing the parent pointer of one tree root (e.g., FIND\((x)\)) to the other (FIND\((y)\)). If \( x \) and \( y \) belong to the same set, then FIND\((x)\) and FIND\((y)\) return the same index, and no merging is required. The procedure starts with creating a forest of singleton non-overlapping trees, each corresponding to a set consisting of a single data point. The method proceeds by progressively combining pairs of sets through merging corresponding trees.

From the implementation perspective, the trees in the UNION-FIND algorithm are stored using a flat array, which we will refer to as labels. A parent of a node in a tree is then simply the value of the label corresponding to that node. The FIND operation simply follows the values of labels until encountering an index that is the same as its label, which indicates that it is the root of
that tree. Two trees are merged by simply changing the label of the root of one of the trees to that of the other.

Algorithm 2 demonstrates a reproduction of the disjoint-set DBSCAN algorithm (DSDBSCAN) as proposed in [34] (Algorithm 2), shown here for completeness. Each point now only computes its own neighborhood (Line 3). If it is a core point, its neighbors are assigned to the same cluster (Lines 8 and 11).

In the original paper, a thread or an MPI rank executed the algorithm sequentially for a subset of data constructed by partitioning, and merged the results in parallel to obtain the final clusters. For GPUs, however, more available parallelism is desired to improve the efficiency. In the next Section, we reformulate the algorithm in such a way.

3.2 Parallel disjoint-set based DBSCAN

While the amount of the parallelism in Algorithm 2 may be sufficient for shared- or distributed-memory implementations, it is insufficient for GPU implementations with thousands or tens of thousands threads. The goal of this Section is to reformulate the algorithm to accommodate such a high number of threads. Our secondary goal is to reduce thread execution divergence (executing different code) and data divergence (reading or writing disparate locations in memory).

Algorithm 2 consists of two distinct kernels: the neighbor search, and the disjoint-set structure update. It is clear that the former is more computationally demanding than the latter. Without taking appropriate care, calling GetNeighbors asynchronously by different threads will result in high execution and data divergence. This is especially true when an index structure, such as k-d tree or R*-tree, is used. Thus, our first goal is to execute neighbor searches simultaneously by all threads in a batched mode.

Our second goal is to address the limited amount of memory available on a GPU. Storing all the neighbors found on Line 3 for all threads executed at the same time may not be possible, given that the number of such neighbors may be a significant fraction of the overall dataset size. This can be addressed by observing that the neighbor list is being used in two different contexts. For assessing whether a point is a core point on Line 4, the only information required is the number of neighbors, but not the neighbors themselves. In the loop on Line 6, the neighbors are assigned to the same cluster as part of the UNION-FIND algorithm. The key observation here is that the neighbors may be processed independently and in any order. In other words, it is possible to process them as they are determined and execute the UNION operation on-the-fly for each neighbor, discarding the found neighbor after that.

Given these findings, we propose modifying the algorithm by splitting it into two phases. In the first phase, called preprocessing, the algorithm determines the core points. We note that while it is possible to do this by computing \(|N_ε(x)|\), it is not strictly necessary. If the neighbors of a point are discovered incrementally (whether through a tree traversal, or otherwise), it is sufficient to encounter \(\text{minpts}\) neighbors to determine a core point. Searching for any more neighbors after that is excessive unless one wants to execute a sweep over multiple values of \(\text{minpts}\). In the latter case, it may be preferable to compute the full set \(|N_ε(x)|\), since that cost will be amortized for multiple \(\text{minpts}\) values. Such a lightweight approach is often much faster than computing the full neighborhood, particularly for situations where \(|N_ε(x)| \gg \text{minpts}\).

The second phase, called main, proceeds with the knowledge of core points, and executes \(\text{UNION}(x, y)\) for each pair of close neighbors. We note, however, that this general formulation leaves a lot of room for optimizations. For example, many of the distance calculations may be eliminated. We examine this in more detail in Section 4.

The two-phase approach results in dramatic reduction of the consumed memory and in better avoidance of thread and data divergence. The memory consumption is linear with respect to the number of points in a dataset (assuming the used search index obeys this, too), making it possible to execute the algorithm for much larger datasets. As was observed in the earlier works, algorithms like G-DBSCAN, which store full neighbor lists, tend to run out of memory even for smaller datasets, particularly in situations where \(|N_ε(x)| \gg \text{minpts}\) for a significant fraction of points.

An additional advantage of the two-phase approach is that it exposes edge-level parallelism rather than vertex-level parallelism. One could consider using multiple threads collaborating on a single point, with each thread assigned one of the outgoing edges in the adja-
Algorithm 3 Parallel disjoint-set DBSCAN algorithm

1: procedure PDSDBSCAN$(X, \text{minpts}, \varepsilon)$
2: if $\text{minpts} > 2$ then
3: for each point $x \in X$ in parallel do
4: determine whether $x$ is a core point
5: for each pair of points $x, y$ such that $\text{dist}(x, y) \leq \varepsilon$ in parallel do
6: if $x$ is a core point then
7: if $y$ is a core point then
8: \text{Union}(x, y)
9: else if $y$ is not yet a member of any cluster then
10: \text{critical section:}
11: mark $y$ as a member of a cluster
12: \text{Union}(x, y)

4 Tree-based algorithms

In the previous Section, we described a general framework for a GPU-based DBSCAN implementation. This Section is dedicated to providing concrete algorithms implemented in this work.

First, for the Union-Find implementation, we chose the algorithm proposed in [22], since it allows a synchronization-free implementation on GPUs. Like most efficient implementations, it uses pointer jumping, a technique to shorten paths of the trees (associated with disjoint sets) during the FIND operation. Specifically, the work uses “intermediate pointer jumping”, which compresses the path of all elements encountered on a way to the tree root by making every element skip over the next element, halving the path length in each traversal. Because the path compression does not guarantee that all paths are fully compressed at the end of the main phase (in other words, that the label of each point in the same cluster is identical at the end of the main phase), an extra finalization phase is introduced to make each point directly to the representative. Out of the three different kernels considered in that work (based on a node degree), only the first one was utilized in our approach, with a single thread assigned to each vertex.

Next, we discuss the details of two algorithms using trees as a search index. Both algorithms fuse tree traversal with executing Union-Find.

4.1 FDBSCAN

FDBSCAN (“fused” DBSCAN) fuses tree traversal with the Union-Find algorithm. It uses a bounding volume hierarchy (BVH), a structure commonly used in computer graphics for ray tracing, for the search index. While any tree can be used, BVH has been shown to be very efficient for low-dimensional data on GPUs. Linear BVH, such as the algorithm proposed in [23], has been demonstrated to be efficient and has low data and thread divergence.

The parallelization is done over points of the dataset, with each thread assigned a single point. The tree search is executed for every point with the radius $\varepsilon$ in a batched mode, i.e., with all threads launching at the same time. Each thread executes a top-down traversal, finding all the neighbors within distance $\varepsilon$ of its assigned point, and executes Union.

For the determination of the core points in the preprocessing phase, we use the recommendation from the previous Section. Specifically, the tree traversal of a thread is terminated early once a sufficient number of neighbors ($\geq \text{minpts}$) is encountered.
We use an additional optimization in the main phase. In Algorithm 3, the algorithm can be seen as operating on the edges of the adjacency graph. As the results of $\text{UNION}(x, y)$ and $\text{UNION}(y, x)$ are identical, it is sufficient to process each edge only once. To facilitate this, we introduced a new hierarchy traversal algorithm. Given a thread corresponding to a point with index $i$, a part of the tree corresponding to the leaf nodes with indices less than $i$ is hidden from the thread. This way, the thread avoids entering the subtrees with lower leaf indices, guaranteeing that all the found neighbors would have indices $j > i$, thus guaranteeing that each pair of neighboring points is processed exactly once. Figure 1 demonstrates the tree mask for a thread corresponding to index 4. The thread would stay in the right sub-tree of the root, skipping the left sub-tree entirely. The advantages of such an approach include fewer memory accesses used during the traversal, reduced number of distance computations, and reduced number of $\text{UNION}$-$\text{FIND}$ operations.

4.2 FDBSCAN-DenseBox

A given combination of $\text{minpts}$ and $\varepsilon$ often results in the number of neighbors within an $\varepsilon$-neighborhood of a point significantly exceeding the value of $\text{minpts}$. In this case, many of the distance computations may be avoided. In this Section, we propose an alternative approach to FDBSCAN which takes advantage of this fact.

Eliminating extra distance computations has been studied in [42, 14]. The methods operate by superimposing a uniform Cartesian grid and processing cells with at least $\text{minpts}$ points more efficiently. We integrated these ideas into a tree-based search index, which we call FDBSCAN-DenseBox.

The procedure starts with computing the bounds of the data set and imposing a regular grid over the computational domain. The grid cell length is set to be $\varepsilon/\sqrt{d}$, with $d$ being the data dimension. This choice guarantees that the diameter of each cell does not exceed $\varepsilon$. Next, we calculate a cell index for all points in the dataset, and determine the number of points in each cell. The cells with at least $\text{minpts}$ are called dense. Figure 2 demonstrates a grid superimposed over a set of points, with dense cells for $\text{minpts} = 5$ marked in red. It is clear that all the points in the dense cells are core points, and belong to the same cluster. Thus, the distance calculations among the points in the same dense cell can be eliminated.

The number of dense cells and the number of points inside them depend heavily on the dataset data distribution and parameters $\varepsilon$ and $\text{minpts}$. If the value of $\varepsilon$ is small compared to the domain size, the number of grid cells in each dimension may be in thousands or more, resulting in billions of grid cells. The data is then spread across a relatively small population of non-empty cells. Searching for nearby cells in this situation becomes non-trivial. While it is possible to do a series of binary searches over a list of cells to produce a list of neighboring non-empty cells, in this work we use an alternative approach.

To accommodate dense boxes, we modify the BVH construction algorithm of FDBSCAN. In FDBSCAN-DenseBox, the hierarchy is constructed out of a mix of points outside of dense cells and the boxes of the dense cells. This is possible to do as the BVH only requires bounding volumes for a set of objects. Thus, such mixing does not impose any additional constraints. The use of this approach with other trees, such as $k$-d tree, would pose more challenges.

Given the knowledge that all points in dense cells are core points, only the points outside of dense cells have to be examined to identify the remaining core points in the preprocessing phase. For every such point, the algorithm finds all nearby objects within distance $\varepsilon$ using the BVH. If the found object is an isolated point, the neighbor count is incremented by one. If it is a box (corresponding to a dense cell), a linear search over all points in that cell is performed, incrementing the count each time a point is within distance $\varepsilon$. Similar to FDBSCAN, the neighbors are only counted until reaching the $\text{minpts}$ threshold, after which the procedure terminates.
At the beginning of the main phase, the UNION operation is executed for all points in the same dense cell. Then, the tree search is performed for all points in the dataset. During the search, once an object within distance $\epsilon$ is found for an individual point, one of two cases may happen. In the first case, the found object is a dense box. In this case, it is sufficient to determine whether a single point of that dense box is within distance $\epsilon$. A thread checks the distances to all points in that dense cell linearly, until either a point within $\epsilon$ is found, in which case UNION() is called, or all points are exhausted. In the second case, the found object is another point (outside of any dense cell). As the newly found point is within $\epsilon$, the usual resolution depending on the core status of both points is executed.

5 Experimental results

In our implementation, we used the ArborX [26] library for the tree-based implementations and the Kokkos library [12] for a device-independent programming model.

The ArborX library provides several features suitable for our implementation. It allows for an early traversal termination, which is used in the preprocessing phases of both FDBSCAN and FDBSCAN-DENSEBox. The callback functionality of the library allows execution of a user-provided code on a positive match, which is used both in preprocessing for the neighbor count and in the main phase for the UNION-FIND kernels.

The experimental studies presented in this Section were performed on the OLCF Summit system. Each node has two IBM POWER9 AC922 22-core CPUs, each having 4 hardware threads, with 6 Nvidia Volta V100-SXM2 GPUs connected by NVLink 2.0 [40]. In our experiments, we used a single V100 GPU.

5.1 Comparison with existing GPU-based algorithms

In this Section, we compare the performance of FDBSCAN and FDBSCAN-DENSEBox algorithms with the two implementations, CUDA-DClust [6] and G-DBSCAN [2], on three real world 2D datasets studied in [32].

The Next Generation Simulation Vehicle Trajectories dataset [1] (NGSIM) consists of 11,800,000+ points corresponding to car trajectories transcribed from the footage of video cameras using NGVIDEO by NGSIM researchers on three highways.

The Taxi Service Trajectory Prediction Challenge dataset [31] (PortoTaxi) consists of 1,710,000+ trajectories with 81,000,000+ points in total, corresponding to the trajectories of several hundred taxis operating in the city of Porto, Portugal.

The 3D Road Network dataset [24] (3D Road) consists of 400,000+ points of the road network of the North Jutland province in Denmark.

In each dataset, only longitude and latitude are considered as 2D geospatial data. Figure 4 shows a visual representation of data distribution samples for each dataset (NGSIM is zoomed on one of the three locations studied).

We compare four algorithms: CUDA-DClust, G-DBSCAN, FDBSCAN and FDBSCAN-DENSEBox. The implementations of the first two algorithms were kindly provided by the authors of [32], and the parameters of CUDA-DClust were selected in the same manner. The comparisons were performed using a random subsampling of the datasets in order to accommodate memory requirements exhibited by certain codes, such as G-DBSCAN.

Similar to [32], we studied the behavior of the algorithms for each dataset for three variations of the parameters.

Impact of $\text{minpts}$

Figures 4(a)(b)(c) show the effect of varying the $\text{minpts}$ parameter while keeping $\epsilon$ and the problem size fixed. The $\text{minpts}$ parameter range was chosen to include regimes where the clustering changes from a few, large clusters to many small clusters. The problem size was kept at 16,384 sampled points, and the values of $\epsilon$ were set to 0.005, 0.01, and 0.08 for NGSIM, PortoTaxi, and 3D Road, respectively.

We observe that the algorithms exhibit little change in the behavior in these experiments with CUDA-DClust trending slightly upwards for larger $\text{minpts}$ values\footnote{This behavior of CUDA-DClust differs from [32], and is explained by using a V100 GPU. We were able to reproduce the stable behavior with a GTX1070 GPU.}. CUDA-DClust is a clear outlier in terms of performance, running 3-4 times slower than the rest of the algorithms. G-DBSCAN and FDBSCAN-DENSEBox perform similarly for the PortoTaxi datasets. G-DBSCAN is 2.5 times faster than FDBSCAN-DENSEBox for the NGSIM dataset, while for the 3D Road dataset FDBSCAN-DENSEBox outperforms G-DBSCAN by 2.5×. FDBSCAN-DENSEBox is always faster than FDBSCAN as it takes advantage of the overly dense regions found in road networks for all datasets. In fact, we observed that over 95% of points are contained in the dense cells for every dataset even for the largest values of $\text{minpts}$. The difference between the two algorithms is highlighted by the fact that most
of the time in FDBSCAN is spent in the tree search, while in FDBSCAN-DenseBox it is in the dense cells processing.

Impact of $\varepsilon$

Figures 4(d)(e)(f) demonstrate the impact of the parameter $\varepsilon$ on the execution times while keeping $\text{minpts}$ and problem size fixed. Increasing $\varepsilon$ increases the size of each neighborhood $N_\varepsilon(x)$, thus increasing the cluster sizes. The problem size was again fixed at 16,384, and the values of $\text{minpts}$ were to chosen to be 500, 50 and 100 for NGSIM, PortoTaxi, and 3D Road, respectively.

Once again, CUDA-DClust is a clear outlier for all datasets. None of the algorithms are sensitive to the search radius for the NGSIM dataset, which is explained by it being overly dense even for small values of $\varepsilon$. Both FDBSCAN and FDBSCAN-DenseBox show little variation in the runtime while varying $\varepsilon$ in all datasets. G-DBSCAN, however, slows down for larger values of $\varepsilon$ for PortoTaxi and especially for the 3D Road dataset, which can be explained by the increase in the storage size of the adjacency graph.

Impact of the number of points in the dataset

For our final comparison, we varied the size of the problem (by increasing the number of drawn samples) for each dataset while keeping the values of $(\text{minpts}, \varepsilon)$ fixed to $(500, 0.0025)$, $(1000, 0.05)$, and $(100, 0.01)$ for NGSIM, PortoTaxi and 3D Road, respectively.

Figures 4(g)(h)(i) present the results, shown in log-log scale. CUDA-DClust, FDBSCAN and FDBSCAN-DenseBox scale similarly, while G-DBSCAN has a slightly worse scaling for the NGSIM and PortoTaxi datasets. While G-DBSCAN outperforms other algorithms on the NGSIM dataset, its poorer scaling results in a similar performance as FDBSCAN-DenseBox for 131,072 points. For the other two datasets, PortoTaxi and 3D Road, FDBSCAN-DenseBox is a clear winner.

It is important to distinguish the two missing data points$^2$ for the G-DBSCAN algorithm on the PortoTaxi datasets. In these cases, G-DBSCAN ran out of memory to store the neighbors of each point. This is a significant limitation of the algorithm. As both FDBSCAN and FDBSCAN-DenseBox are within a general framework proposed in Section 3.2, the used memory scales linearly with the number of dataset points and not the number of found neighbors, allowing these algorithms to execute for significantly larger datasets.

In summary, FDBSCAN and FDBSCAN-DenseBox prove to be competitive, often outperforming other existing algorithms with FDBSCAN-DenseBox being the (much) faster one of the two for this class of problems. While G-DBSCAN has been shown to perform well, it is at an apparent disadvantage for larger density connectedness graphs, requiring large amounts of memory. Both algorithms proposed in this paper do not suffer from this limitation.

5.2 3D problem

In this section, we evaluate the algorithms on a 3D cosmology problem. The dataset consists of the data taken from a single rank of the 64 MPI ranks cosmology simulation performed with HACC [19]. The simulation was run with 1024$^3$ particles with 256$^3$ Mpc/h volumes. The single rank data consists of the volume data (16,000,000+ particles) combined with halos spanning sub-volume boundaries, bringing the total to 36,000,000+ particles. The snapshot is taken from the last step of the simulation, with clusters clearly formed. Figure 5 shows a visualization of a data sample. Compared to the 2D datasets described in the previous Section, the data is vastly more sparse, and more evenly distributed throughout the domain.

$^2$The third missing data point for the largest PortoTaxi CUDA-DClust is due to an undetermined fault in the code.
From the physics perspective, the meaningful choice for $\varepsilon$ is 0.042, given the problem simulation parameters. Given the size of the computational domain, this value for $\varepsilon$ results in the superimposed Cartesian grid of the FDBSCAN-DenseBox algorithm to have more than 3.5 billion cells, with only about 28 million of them being non-empty. While a typical approach in cosmology is to use $\text{minpts} = 2$, corresponding to strongly connected components (or Friends-of-Friends) in the literature, we explore a range of values.

Figure 6 shows the effect of the choice of the $\text{minpts}$ parameter on the execution time. While FDBSCAN and FDBSCAN-DenseBox perform similarly for lower values of $\text{minpts}$, FDBSCAN clearly is the faster of the two for larger values. While for $\text{minpts} = 5$ about 13% of all particles are in the dense cells, less than 2% of the points are in the dense cells for $\text{minpts} = 50$, and none for $\text{minpts} > 100$. Thus, the difference is stemming from the overhead associated with detecting and analyzing the membership of points in the cells.

Figure 7 compares FDBSCAN and FDBSCAN-DenseBox over a range of values for $\varepsilon$ while keeping $\text{minpts}$ fixed at 5. With increasing $\varepsilon$, the advantages of the dense cells become clear. At $\varepsilon = 1.0$, roughly 91% of all points are in the dense cells, resulting in a 16× performance gap between the two algorithms.

6 Conclusions and future work

In this paper, we have presented a general parallel approach for DBSCAN on GPUs, and introduced two algorithms based on a bounding volume hierarchy tree implementation. These algorithms have been evaluated against the other existing GPU algorithms, demonstrating their competitiveness in many situations. The algorithms were also shown to achieve good performance in clustering the 36M+ data points from a cosmology...
simulation in under a second on a single GPU. We have shown that a special treatment of dense areas by using an auxiliary Cartesian grid is advantageous in many situations.

Algorithmically, we see a number of research directions to pursue. Similar to [14], we envision using a heuristic to switch between FDBSCAN and FDBSCAN-DENSEBOX for a given problem. Other directions of research include combining the proposed approach with distributed computations, lowering memory requirements of the used search index, and incorporating other DBSCAN variants such as DBSCAN*.

CRediT author statement

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