ArborX: a performance portable geometric search library

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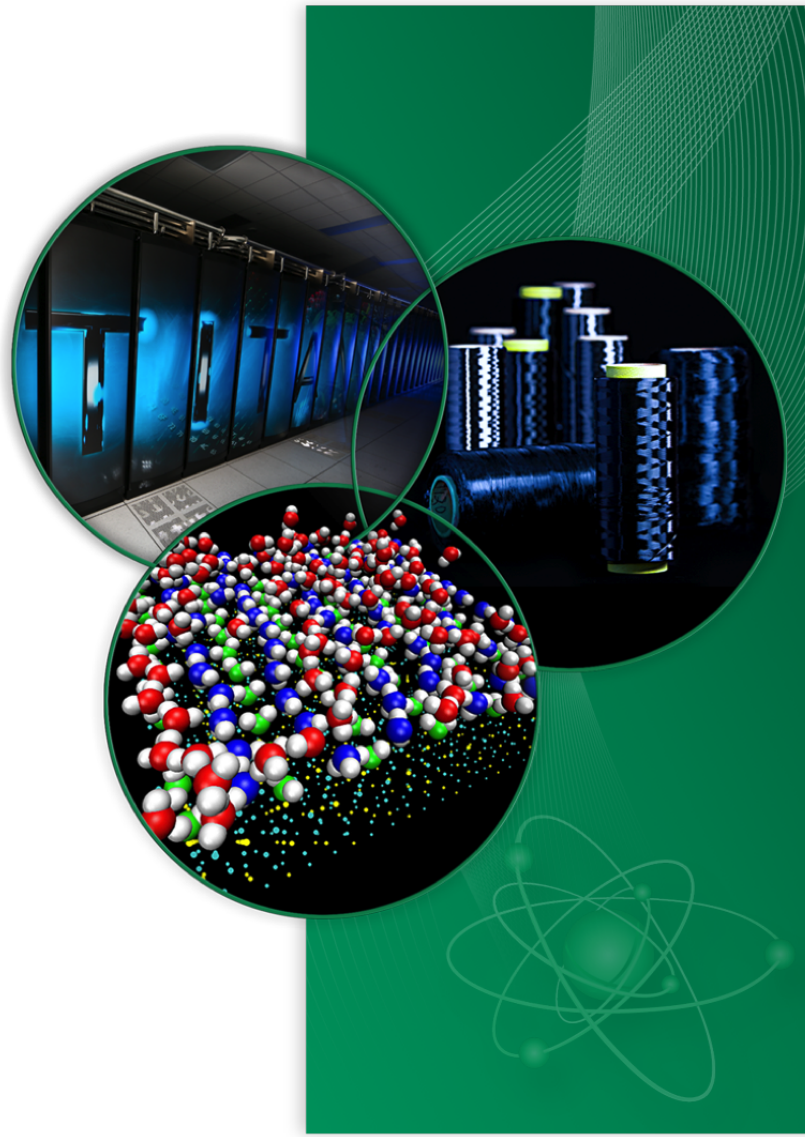

Kokkos tea-time

November 20, 2024

U.S. DEPARTMENT OF ENERGY

Introduction

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What is ArborX?

ArborX is an open-source **performance portable geometric search library** based on MPI+Kokkos.

Geometric search: find geometric objects that are close in some sense.

- **Search**
  - k-nearest neighbors (k-NN)
  - Range (radius search, intersections)
- **Ray Tracing**
- **Clustering algorithms**
  - Minimum spanning tree (Euclidean MST)
  - Density based clustering (DBSCAN, HDBSCAN*)
- **Interpolation**
  - Moving least squares (MLS)

`https://github.com/arborx/ArborX`

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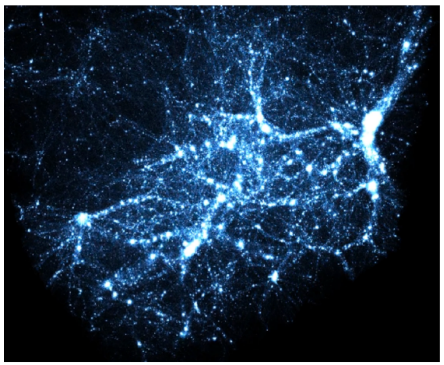
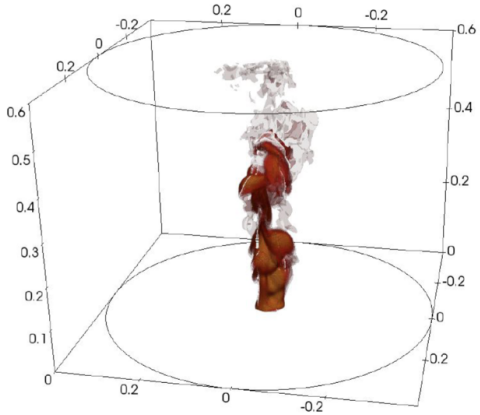
Who uses ArborX?

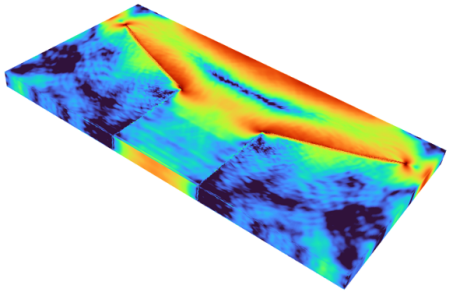
- **NimbleSM** contact mechanics
- **ALEGRA** shock hydrodynamics
- **LGRT** Lagrangian grid reconnection
- **deal.II** finite element library
- **MCRT** thermal radiation
- **Picasso** particle-in-cell
- **HACC/CosmoTools** clustering (dark matter)
- **Cabana** particle-based simulations
- **Adamantine** additive manufacturing
- **STK mesh** SIERRA/Trilinos meshing



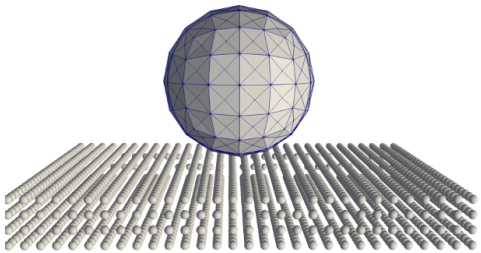
Cosmology (Credits: Nicholas Frontiere, ANL)



Combustion (Credits: Nicolas Tricard, UConn)



Additive manufacturing (Credits: Sam Reeve, ORNL)



Contact mechanicts (Credits: Nicolas Morales, SNL)

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Why use ArborX?

- Fast
- Flexible interface
- Performance portable (Kokkos)
- Modern C++
- Actively developed
- Both on-node and distributed

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Who is developing ArborX?

Core development team

- Daniel Ardnt
- Damien Lebrun-Grandié
- Andrey Prokopenko
- Bruno Turcksin

Most are also Kokkos developers.




Contributors:

- Ana Gainaru
- Wenjun Ge
- Piyush Sao
- Yohann Bosqued

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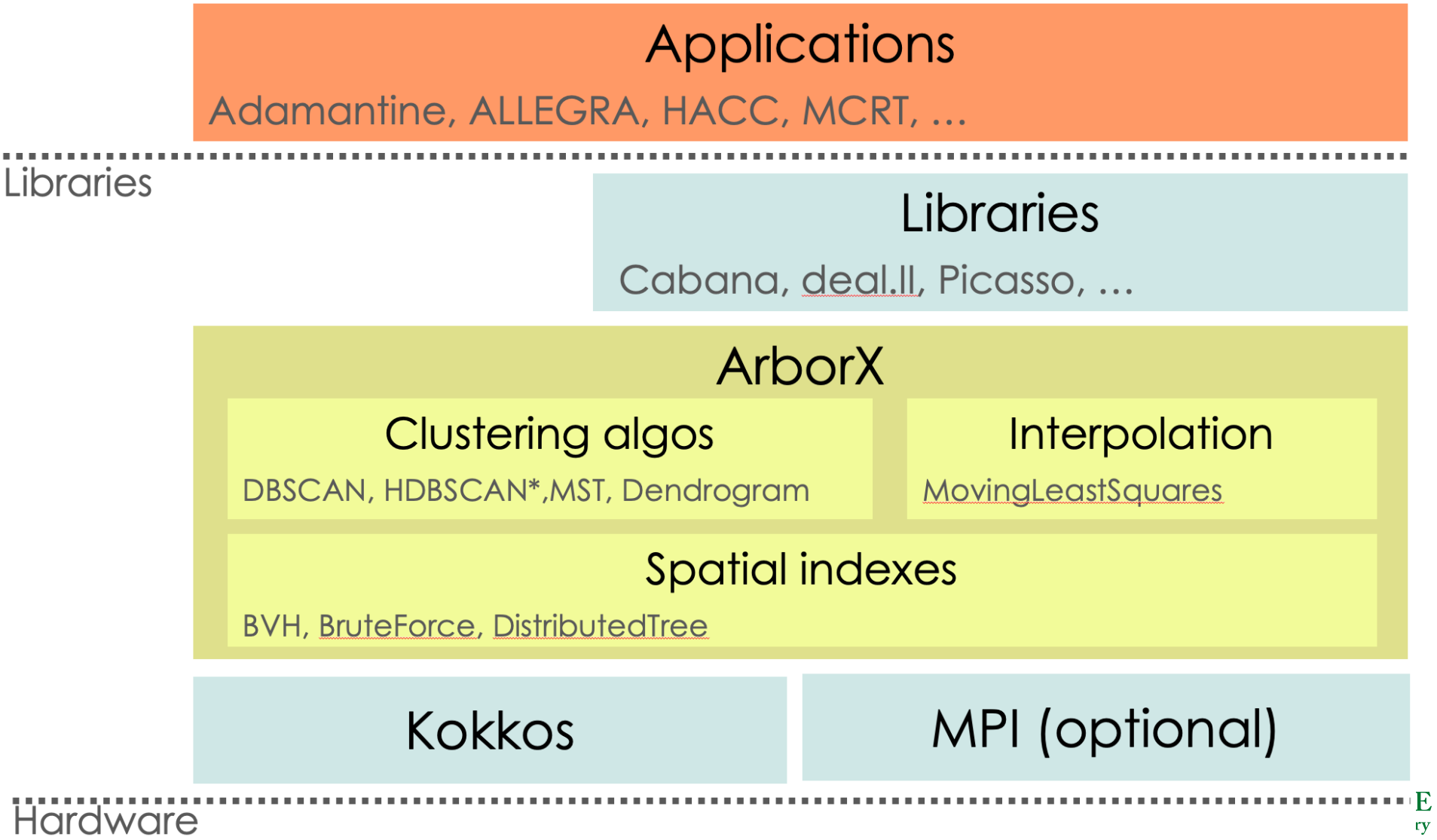
ArborX in the scientific stack



Why Kokkos?

Context: start of US DOE Exascale Computing Project in 2017

- Facing the unknown beyond Summit (Nvidia GPUs)
- SYCL not around a that time
- RAJA? Kokkos? Roll our own?

Join forces with Kokkos

- More than a programming model
- Ecosystem with debugging and profiling tools, math libraries, etc.
- Building a community

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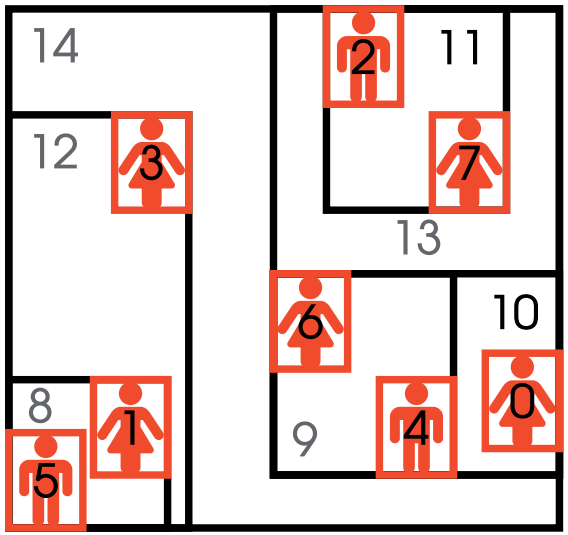
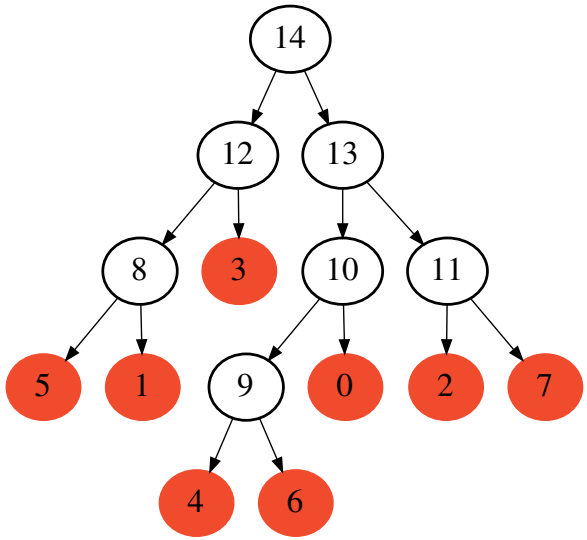
Core concepts

Bounding volume hierarchy (BVH)

Bounding volume hierarchy (BVH) is a tree structure on a set of geometric objects, where each object is associated with a conservative bounding box.





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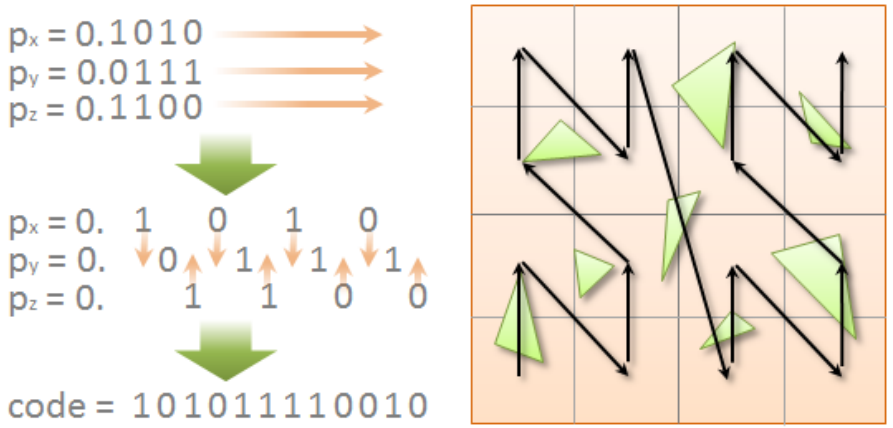
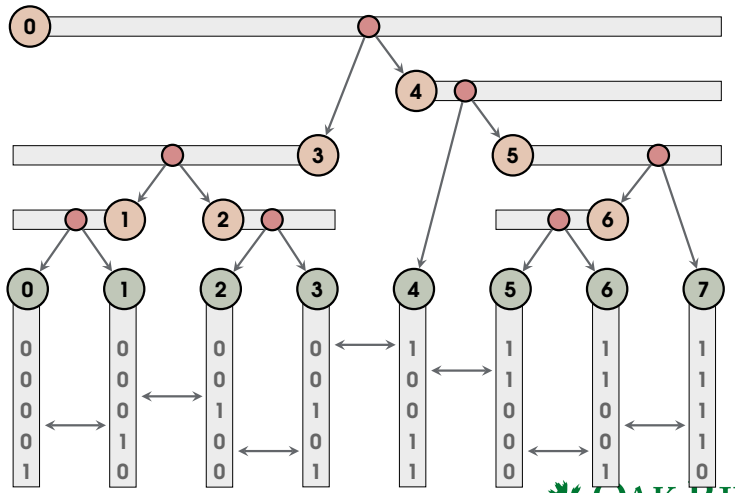
Linear BVH

Impose order in which leaf nodes appear in the tree (Z-curve/Morton codes)



(courtesy of T. Karras, NVidia)

- Each internal node is a linear range over leaf nodes
- The splits are determined according to the highest bit that differs between the Morton codes within the given range
- Can be constructed fully in parallel



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Two flavors of search

Range search

Find all the data that satisfies a criteria (withing certain distance, intersects, etc.)

- Optimized stackless traversal
- Do two passes (count-and-fill) as the number of found object is not known *a priori*
- Multiple knobs to speed things up:
  - Early termination
  - Half traversal for pairs

Nearest search

Find the predefined number of the closest neighbors to a given object.

- Single pass (know in advance how much memory is required)
- Use stack instead of priority queue

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Interface

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Concepts

- Search index is a container of values

  Can be anything (integers, geometries, user types)

- Values are transformed to geometries through indexable getter

  Could be user provided for custom, or default

- Bounding volumes can be customized (AABBs, kDOPs, OBBs)

  AABB by default; could be user provided

```
template<typename MemorySpace,
         typename Value,
         typename IndexableGetter,
         typename BoundingVolume>
class BVH {
  template <typename ExecutionSpace, typename Values>
  BVH(ExecutionSpace const& space,
      Values const& values,
      IndexableGetter const& indexable_getter);

  template <typename ExecutionSpace, typename Predicates,
            typename Callback>
  void query(ExecutionSpace const& space,
             Predicates const& predicates,
             Callback const& callback) const;

  template <typename ExecutionSpace, typename Predicates,
            typename Callback,
            typename Values, typename Offsets>
  void query(ExecutionSpace const& space,
             Predicates const& predicates,
             Callback const& callback,
             Values& values,
             Offsets& offsets) const;
};
```

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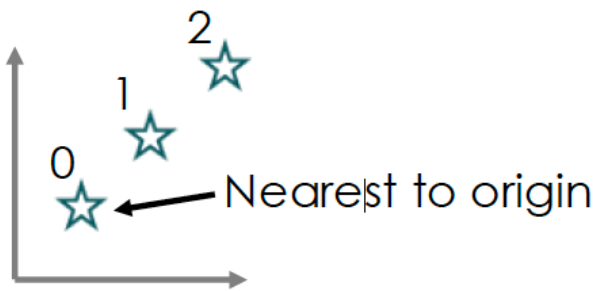
"Hello, world!" in ArborX




```
#include <ArborX.hpp>
#include <Kokkos_Core.hpp>
int main(int argc, charg *argv[]) {
  Kokkos::initialize(argc, argv);
  {
    Kokkos::DefaultExecutionSpace exec;
    // Build data structure
    ArborX::BoundingVolumeHierarchy bvh(
      exec, to-view({
        {1.f, 1.f}, // 0
        {2.f, 2.f}, // 1
        {3.f, 3.f}  // 2
      }));
    // Perform the search
    bvh.query(exec, to-view(
        ArborX::Nearest(ArborX::Point{0.f, 0.f, 0.f})
    ), KOKKOS_LAMBDA(auto /*predicate*/,
                     auto point /*value*/) {
      printf("Nearest to origin is (%f, %f)\n",
        point[0], point[1]);
    });
  }
  Kokkos::finalize();
  return 0;
}
```

Prints "Nearest to origin is (1, 1)"

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Access traits

- Customization point
- Opt-in mechanism to tell ArborX
  - where the data resides
  - how much of it
  - how to access
- Allowed to specialize for user-defined type

```
struct PointCloud {
  float *d_x, *d_y, *d_z;
  int N;
};

template <>
struct ArborX::AccessTraits<PointCloud>
{
  using memory_space = Kokkos::CudaSpace;

  static KOKKOS_FUNCTION
  std::size_t size(PointCloud const &cloud) {
    return cloud.N;
  }
  static KOKKOS_FUNCTION static ArborX::Point
  get(PointCloud const &cloud, std::size_t i) {
    return {{cloud.d_x[i], cloud.d_y[i], cloud.d_z[i]}};
  }
};
```

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User callbacks

Users may not care about the results themselves, or want a subset of the results.

For example:

- Call a function on the results

  May not need to store results, so less memory and single pass for spatial.

  Use case: finding a particle with most neighbors (defined by a length), or particles with a lowest potential (calculated as a function of friends)

- Do results pruning

  Use case: doing fine intersection search with the exact object geometry

- Use processor-local information

  Use case: compute interpolation coefficients for results using mesh parts on a processor

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User callbacks

```
template <typename MemorySpace>
struct Callback {
  template <typename Query, typename Value>
  KOKKOS_FUNCTION
  void operator()(Query const &query, Value const& value) const {
    auto data = ArborX::getData(query);
    // do something
  }
};

template <typename MemorySpace>
struct CallbackWithOutput {
  template <typename Query, typename Value, typename Output>
  KOKKOS_FUNCTION
  void operator()(Query const &query, Value const& value, Output const &out) const {
    auto data = ArborX::getData(query);
    // store something as a result
    out({...});
  }
};
```

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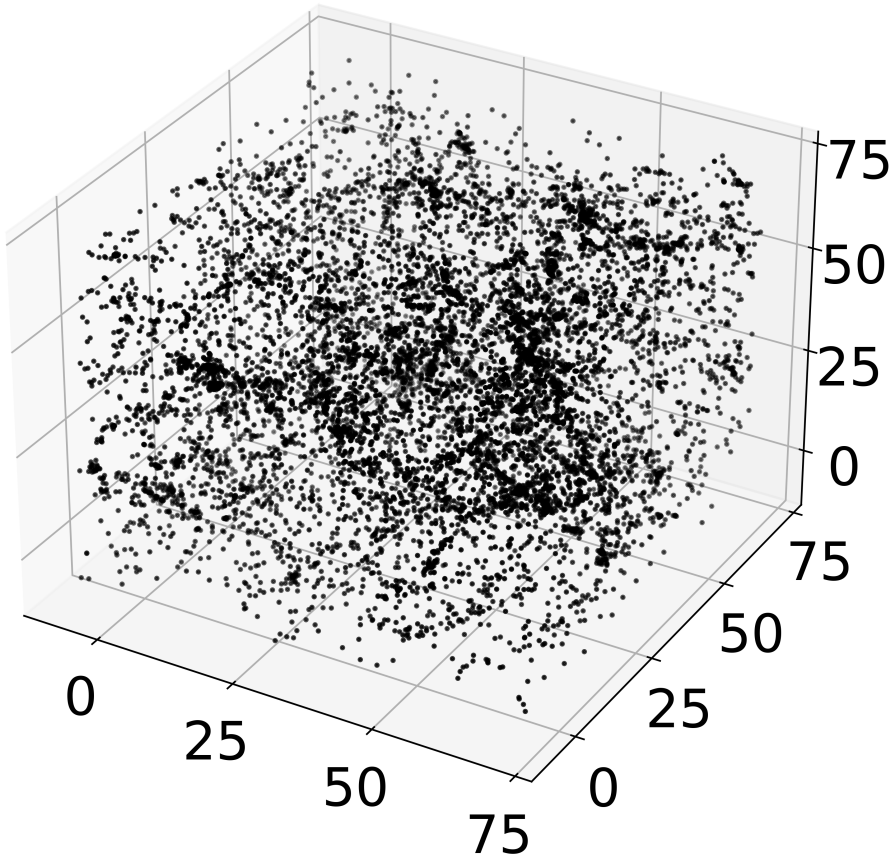
Use case 1: DBSCAN

Application

Cosmological simulation of the universe.

Data is massive. For example, 3096^3 particles running on 64 MPI ranks for a small run. In practice, 500M particles per GPU.

Goal: find dense regions of particles (halos) on each simulation time step.



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DBSCAN algorithm

Clustering: split a set of objects into disjoint classes (clusters), so that objects in each class are more similar to each other than to those in other classes.

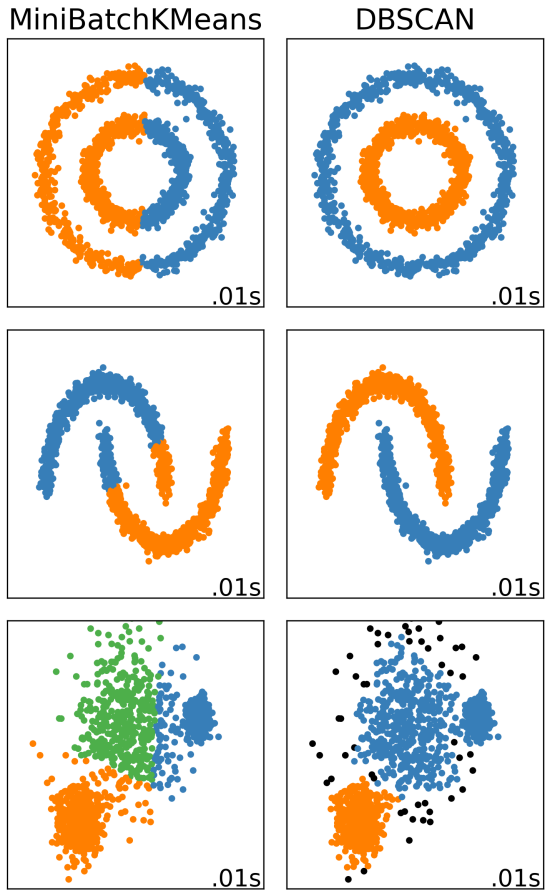
DBSCAN is a clustering algorithm based on density.

Main advantages:

- does not require to specify the number of clusters
- can find arbitrary shaped clusters
- has a notion of noise and is robust to outliers

It also has some disadvantages:

- not fully deterministic (border points)
- does not cope well with clusters of variable density
- choosing its parameters can be difficult



Ester et al. "A density-based algorithm for discovering clusters in large spatial databases with noise." In Kdd, 96(34), pp. 226-231. 1996.

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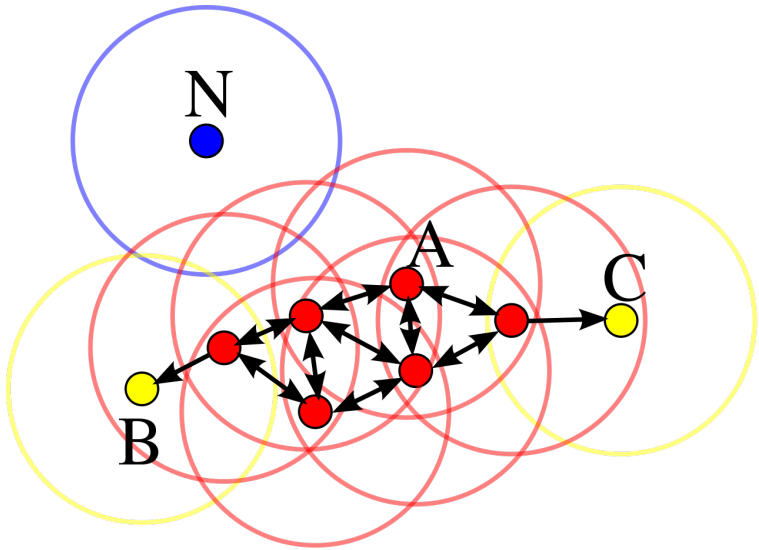
DBSCAN algorithm

Given two parameters, ε and ***minpts***, DBSCAN separates all points into three classes:

- **core points**: have at least *minpts* neighbors within ε
- **border points**: not core points, but have a core point within ε
- **noise**: all other points

Any cluster consists of a combination of core points (at least one) and border points (possibly, none). Example below show *minpts* $= 4$.



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F-DBSCAN (sparse)

Focus: use parallel neighbor computation to minimize data and thread divergence on GPUs. Two phases: *preprocessing* and *main*.

- Use tree structure for search (e.g., kd-tree or BVH)
- Determine core points in preprocessing (terminate early)
- Implicit edges, execute UNION on collision

procedure F-DBSCAN$(X, \mathit{minpts}, \varepsilon)$
if $\mathit{minpts} > 2$ **then**
  for each point $x \in X$ **in parallel do**
    determine whether x is a core point
for each pair of points x, y
  such that $dist(x, y) \leq \varepsilon$ **in parallel do**
  if x is a core point **then**
    if y is a core point **then**
      $Union(x, y)$
    else if y is not yet a member of any cluster **then**
      critical section:
        mark y as a member of a cluster
      mark y as a member of a cluster
      $Union(x, y)$

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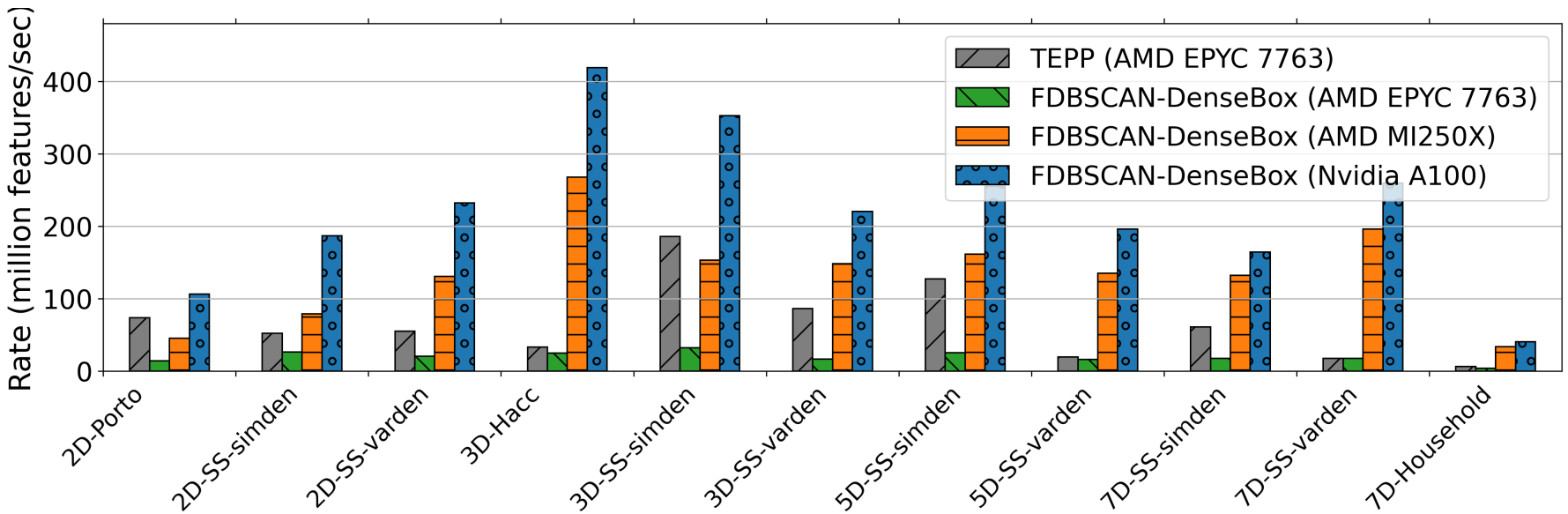
Results: performance portability



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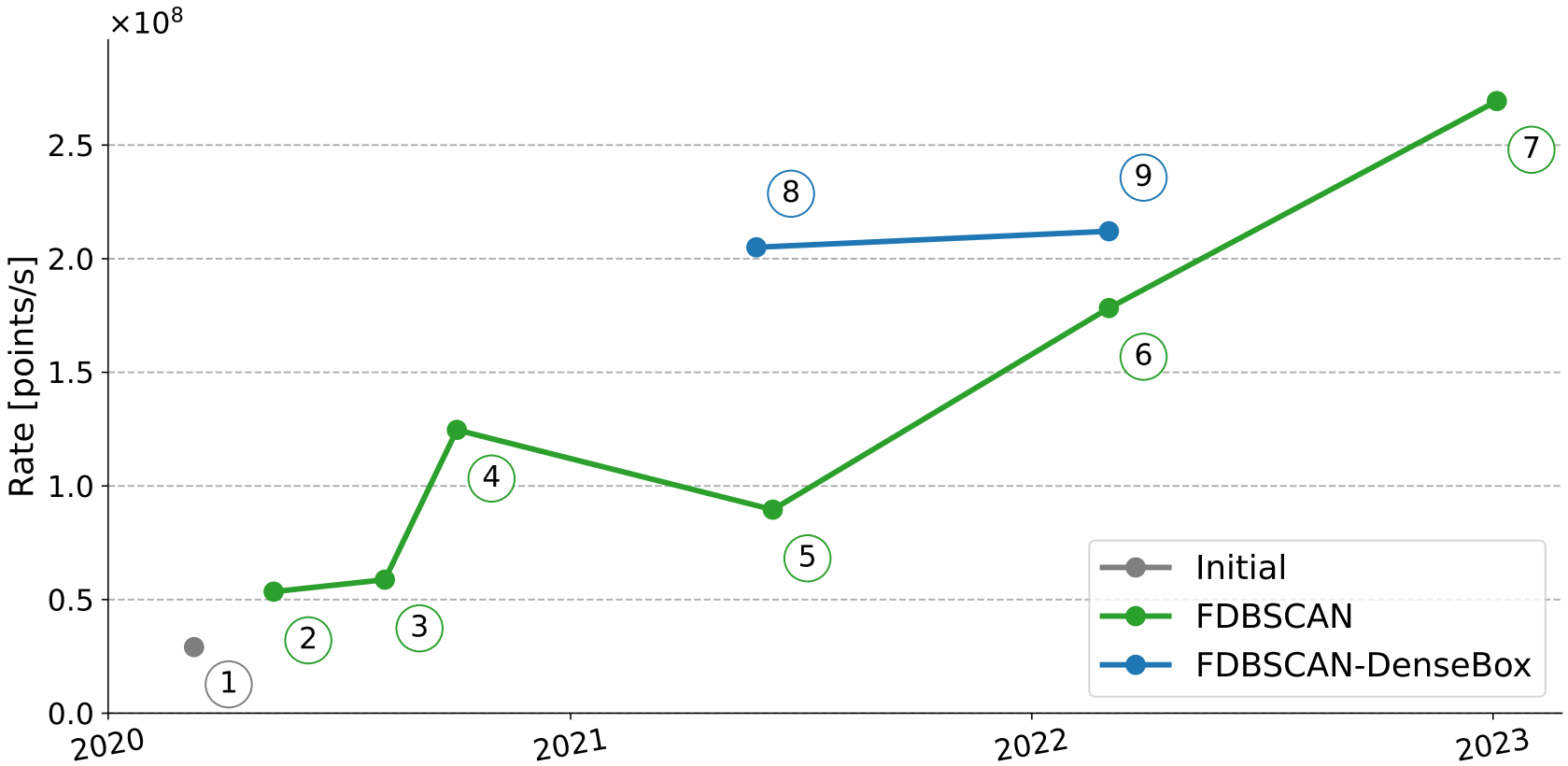
Results: application proxy performance improvement



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Use case 2: Euclidean minimum spanning tree (EMST)

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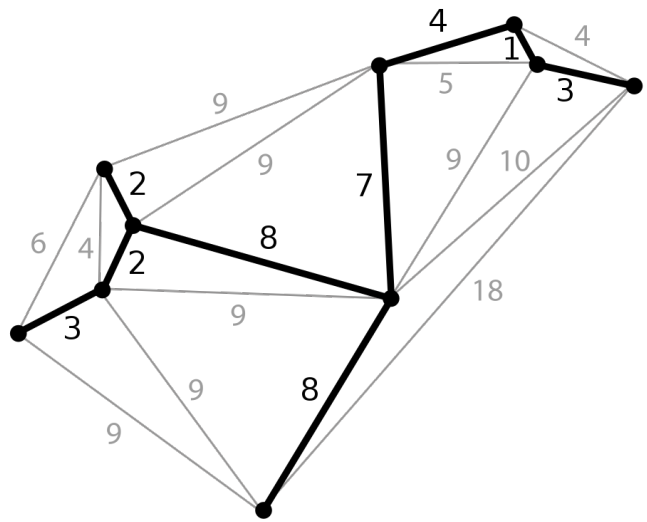
Euclidean minimum spanning tree

A **minimum spanning tree** (**MST**) is a subgraph of a weighted undirected graph that connects all the vertices together, without any cycles and with the minimum possible total edge weight.

A **Euclidean MST** (**EMST**) is a MST of the distance graph of a set of points, *i.e.*, a graph where each pair of vertices are connected by an edge of weight equal to the Euclidean distance between them.

Applications: data clustering (e.g., HDBSCAN*), Euclidean traveling salesman problem, wireless network connectivity, computational fluid dynamics, etc.



c/o Wikipedia

Our goal: fast EMST computation for large (10M+) dataset of low-dimensional data.

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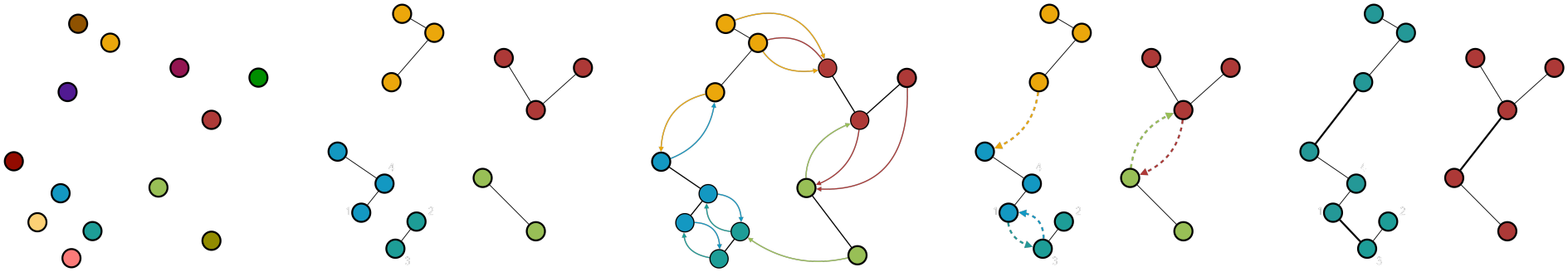
Borůvka's algorithm



a. Initial state (each component having a single vertex).

b. The state after a few Borůvka iterations.

c. Closest neighbors from a different component for each vertex.

d. The shortest outgoing edge for each component.

e. The new components after the merge (the initial state of the next Borůvka iteration).

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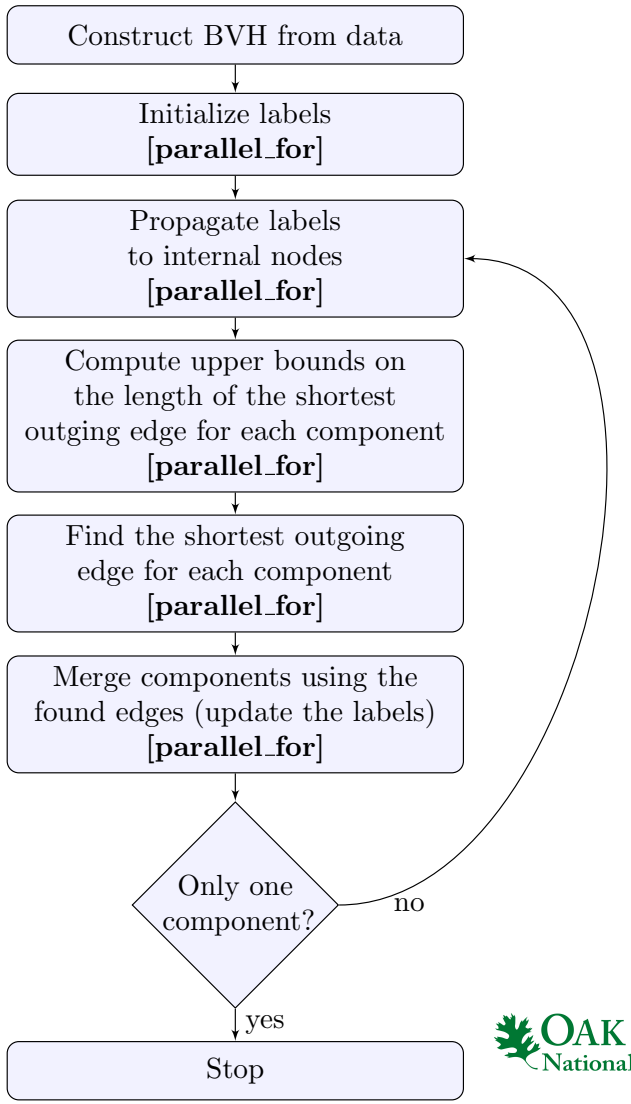
The single-tree algorithm overview

The Borůvka's algorithm is iterative. Each iteration consists of two phases:

1. find the shortest outgoing edge for each component (**expensive!**)
2. merge components

Finding the shortest outgoing edge: a **nearest-neighbor** problem with a **constraint** (the neighbor is from a different component). **Two optimizations** are necessary to prune the number of distance calculations:

- skipping nodes in the same component (**subtree skipping**)
- maintaining an **upper bound** on the distance of the outgoing edge candidates



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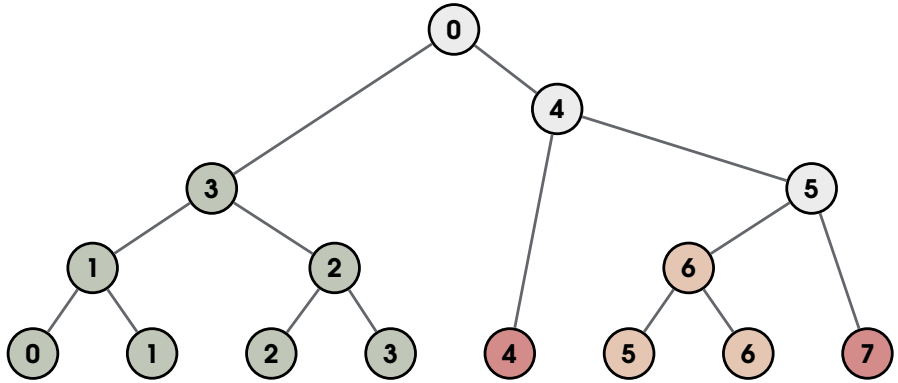
Subtree skipping

Goal: Reduce the number of tree nodes encountered during the traversal.

- Leaf node labels are component membership of the data points.
- Propagate the labels from the leaf nodes to the internal nodes.
  Same labels of children $\rightarrow$ parent label. Different labels of children $\rightarrow$ invalid parent label. Done in a single bottom up traversal
- Skip subtrees of the same label as query during the traversal.



Very important on the **later** Borůvka iterations, when the components are large.

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Datasets

Name	Dim	Size	Description
Ngsim	2	∼12,000,000	Car trajectories on three highways
Ngsimlocation3	2	∼6,400,000	A subset of *Ngsim* (one highway)
PortoTax	2	∼1,710,000	Taxi trajectories in Porto, Portugal
RoadNetwork3	2	∼400,000	Road network of a Denmark province
GeoLife24M3	3	∼24,000,000	User location data
Hacc37M	3	∼37,000,000	Cosmological data from a simulation
Hacc497M	3	∼497,000,000	Cosmological data from a simulation
VisualVar10M2	2	10,000,000	Synthetic data (Gan-Tao generator)
VisualVar10M3	3	10,000,000	Synthetic data (Gan-Tao generator)
Normal100M2	2	100,000,000	Normally distributed points
Normal300M2	2	300,000,000	Normally distributed points
Normal100M2	3	100,000,000	Normally distributed points

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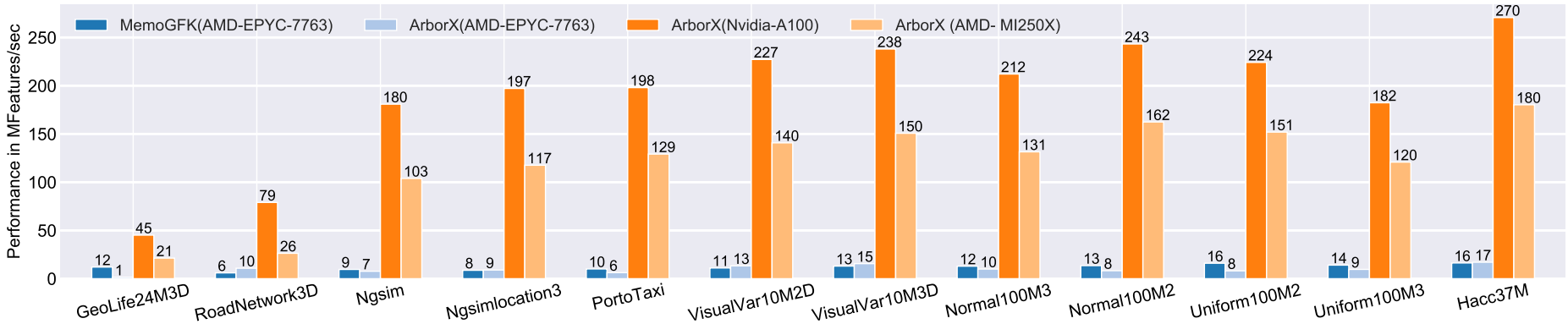
Parallel performance

Performance comparison of the EMST implementations using AMD EPYC 7763 (64 cores), Nvidia A100 and AMD MI250X (single GCD[1]).



- ArborX implementation is faster by 4-24× than MemoGFK on Nvidia A100
- ArborX multi-threaded implementation is within factor 0.5-2× of MemoGFK (the fastest available multi-threaded implementation) (except *GeoLife24M3D*)
- ArborX optimized for Nvidia A100 but not for AMD MI250X

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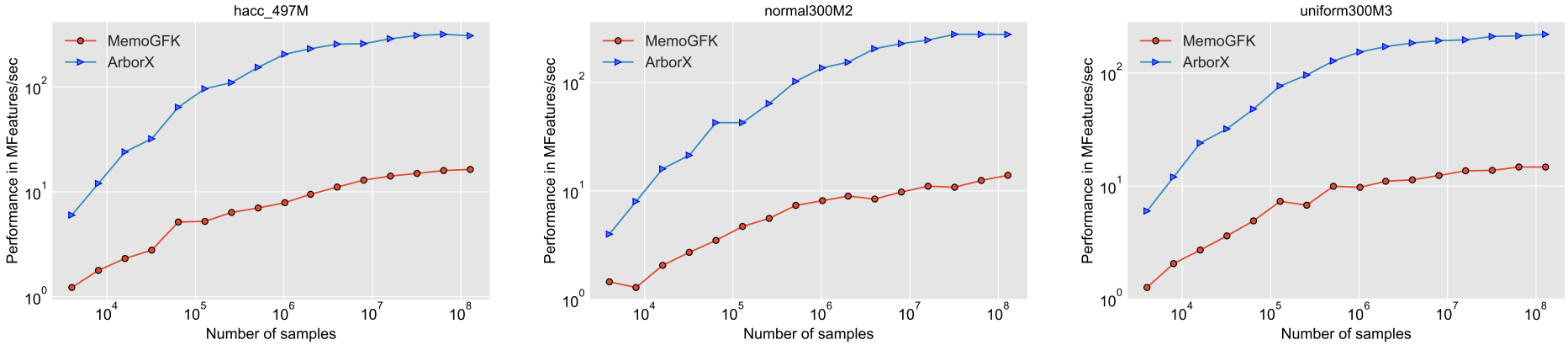
[1] GCD = Graphics Complex Die

Scaling

Effect of the dataset size on the parallel performance using AMD EPYC 7763 and Nvidia A100.



- Performance increases with the number of samples until reaching saturation
- Asymptotically linear complexity of the algorithms

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Future

What does future hold?

- ArborX 2.0 (new interface!)
- Documentation!
- Performance improvements

  OBB hierarchy, hierarchy structure optimization, low precision
- New indexes

  Octree, kd-tree
- Approximate search
- Very high dimensional (dim > 10) search

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Questions?

https://github.com/arborx/ArborX

prokopenkoav@ornl.gov

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