CSCS
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Introduction to GPUs in HPC

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Implementing non-trivially parallel problems on GPUs: tree data structures

Why focus on tree data structures?

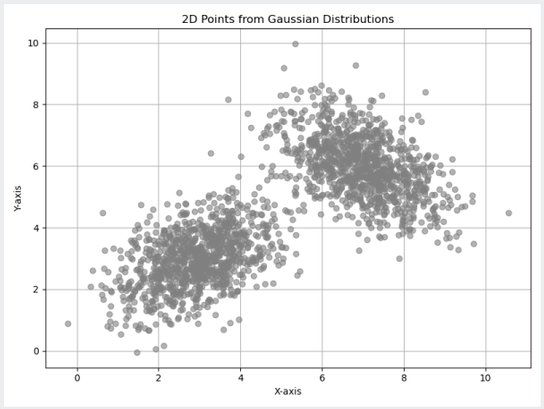
Tree-based data structures have many uses in HPC. That includes binary radix trees, quadtrees and octrees:

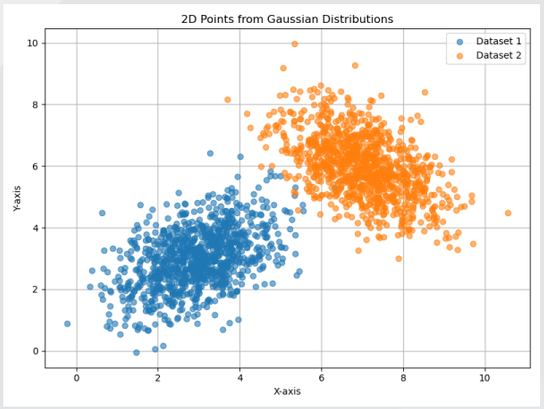
- Neighbor searches for particles in 2D/3D point clouds
- Collision detection in 3D computer graphics
- Adaptive mesh refinement (AMR)
- Domain decomposition to run on multiple compute nodes
- Fast Multipole Method (FMM) for N-body problems

Many naive parallel approaches to trees that work on few-core CPUs do not translate well to GPUs.

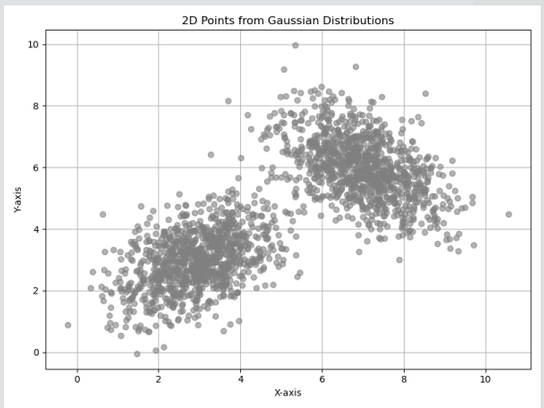
First an example: Neighbor search

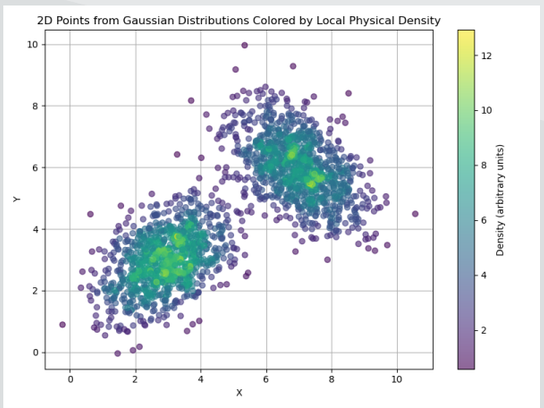
- Finding data which are "close" to each other is a common problem in science.
- Machine Learning: Finding groups of similar characteristics for classification.





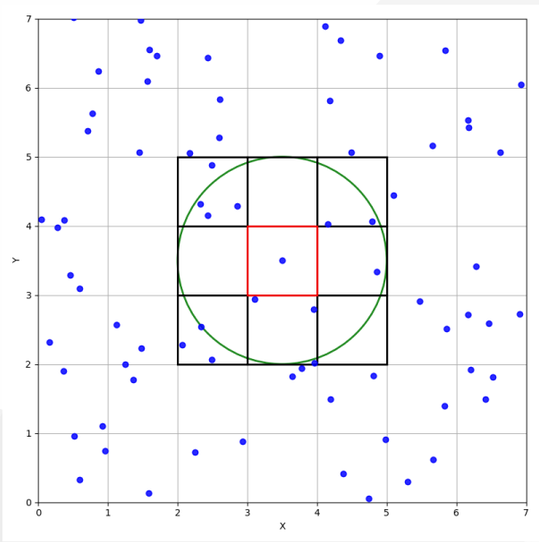
- Physics: Density estimates in particle-based models based on the distribution of N closest neighbors.





How could we find the neighbors of all the particles within a cutoff?

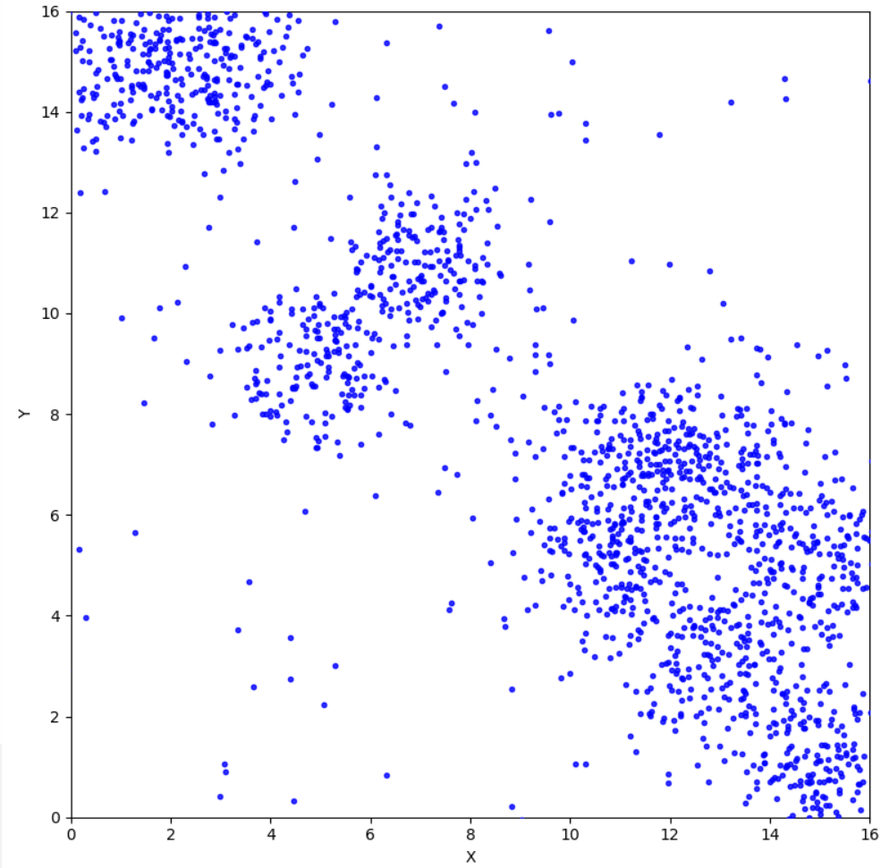
1. For each particle: compute the distance to each other particle, accept/reject. $O(n^2)$
2. Could use Verlet lists (popular in molecular dynamics) to reduce $n \to m$ with a fixed resolution grid, but we need to partition the particles first. $O(mn)$



3. Hierarchical space partitioning (kd-tree, ORB, octree, etc.). $O(n \log n)$

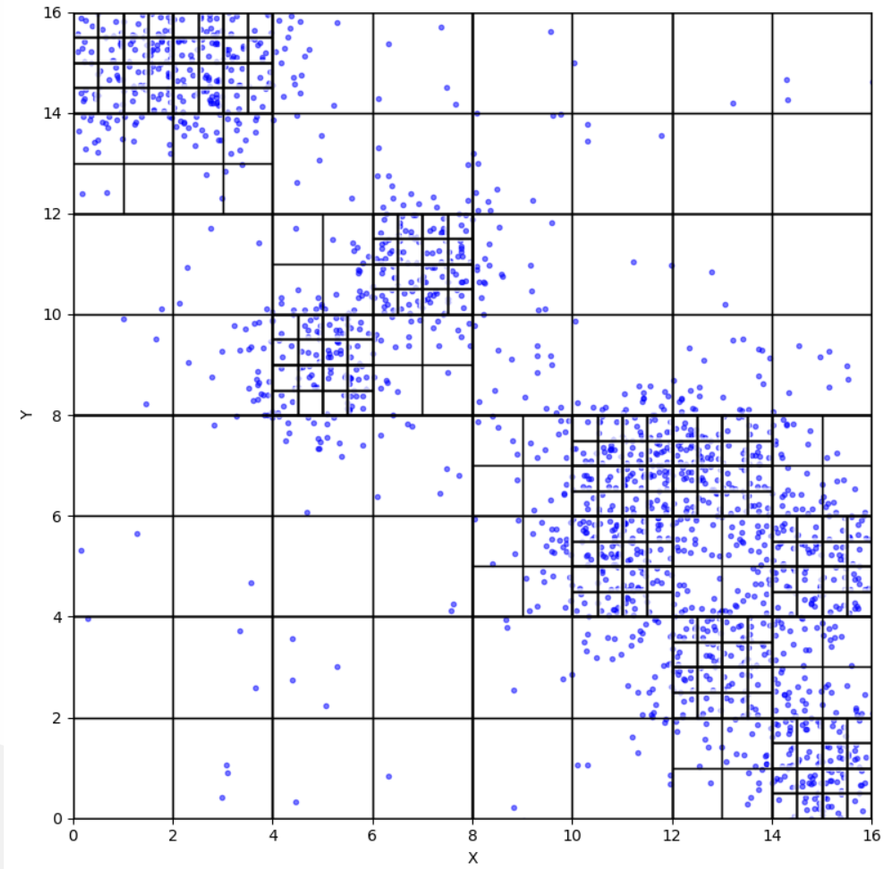
Hierarchical space partitioning

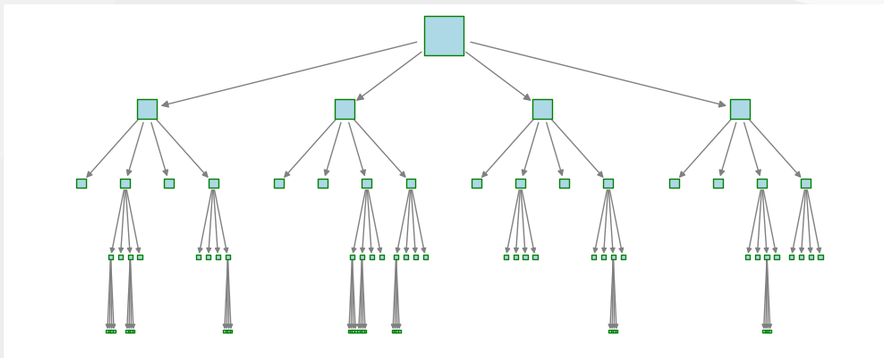
In 2D, let's consider the Quadtree:



Hierarchical space partitioning

In 2D, let's consider the Quadtree. The Octree is the natural 3D extension.





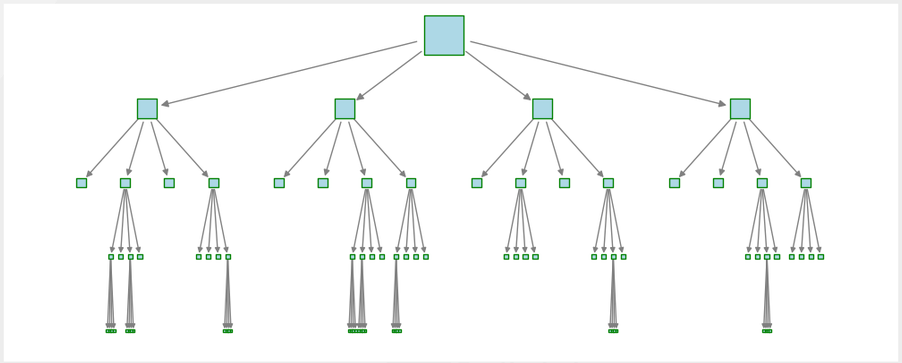
Tree Data Structure

A straight-forward tree data layout with pointers:

```
struct TreeNode
{
    // connectivity
    int numChildren;
    TreeNode* children[numChildren];
    TreeNode* parent;

    // location in space
    std::array<double, 3> nodeCenter;
    std::array<double, 3> nodeSize;

    // additional node properities, e.g.
    int numParticles;
    // etc...
};
```



All Neighbors within R using trees

Basic algorithmic idea:

For each particle at position r,

1. Push the root node onto a work stack.
2. Pop the top most node from the work stack.
3. Is the node completely within a sphere of radius R at r?
   - If yes, accept all particles. Goto 2.
4. Is the node a leaf node?
   - If yes, accept each particle in the node for which $|R - r| < R$. Goto 2.
5. Does the node's bounding box intersect with a sphere of radius R at r?
   - If yes, push all the child nodes onto the stack.
6. Goto 2.

Can this be efficiently implemented on GPUs? Answer: depends on data layout.

What doesn't work

Let's assume the following parallization strategy:

one GPU thread -> neighbor search for one particle.

A straight-forward tree data layout with pointers won't work on the GPU:

- **Tree node** pointers do not ensure that sequentially accessed nodes are local to each other in memory.
- **Particles** in a leaf node are also not guaranteed to be grouped in memory.
- Both scenarios cause memory to be accessed very inefficiently by jumping around.
- If particles of two consecutive GPU threads are far away from each other, paths down the tree will diverge early, causing thread(warp) divergence
- Putting all properties together in a node can lead to poor cacheline usage.

What does work

For the tree:

- Storing tree nodes in arrays (linear buffer)
- A separate array for each node property (-> **struct of arrays** instead of array of structs)

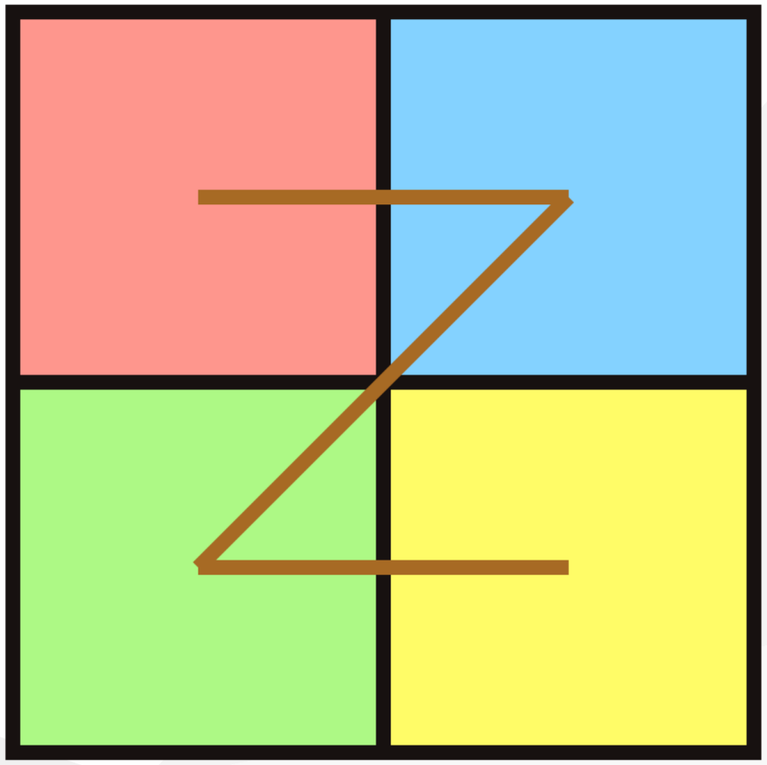
For the particles:

- Particles close in space should be close in memory. This can be achieved for example with **Space Filling Curves (SFCs)**, e.g. Z-curve or Hilbert curve to encode the location in space

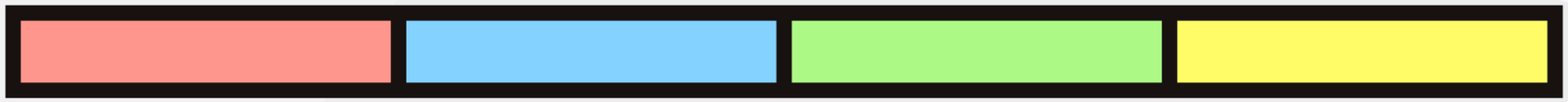
References: Binary radix trees

Space Filling Curves: Intuition

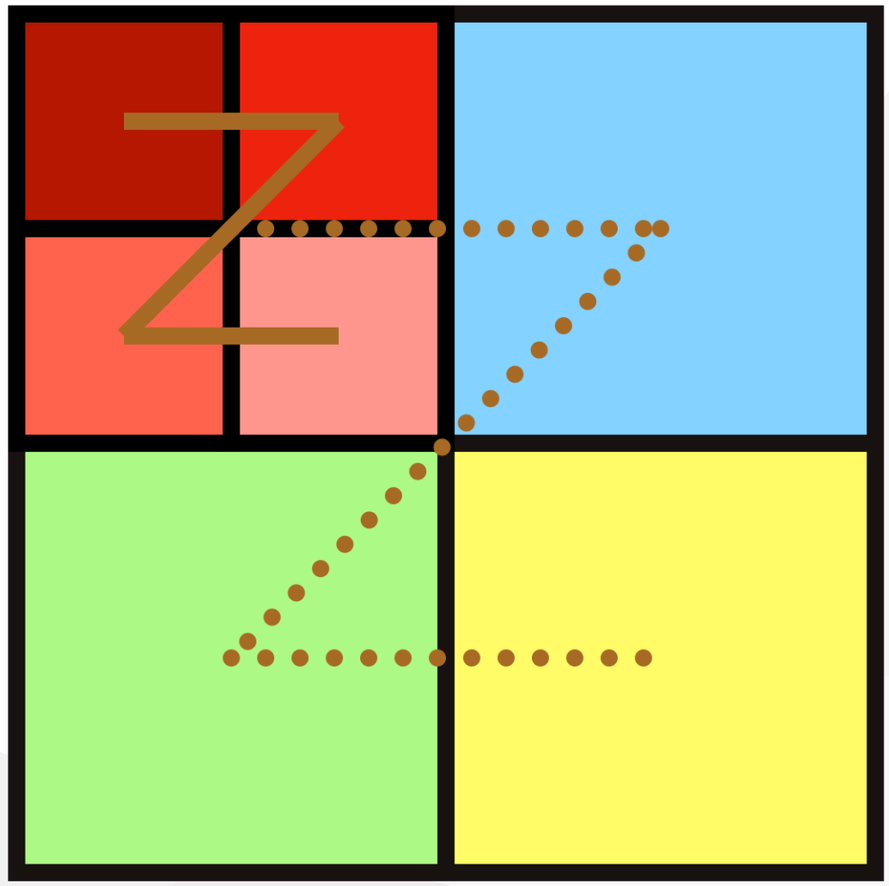
SFCs are mathematical functions that map points in 2D/3D ...

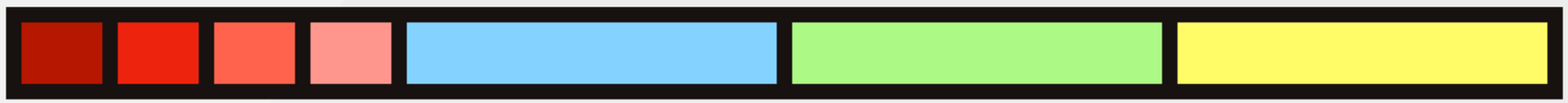


... into the unit interval $[0, 1]$. Areas/volumes into sub-intervals.

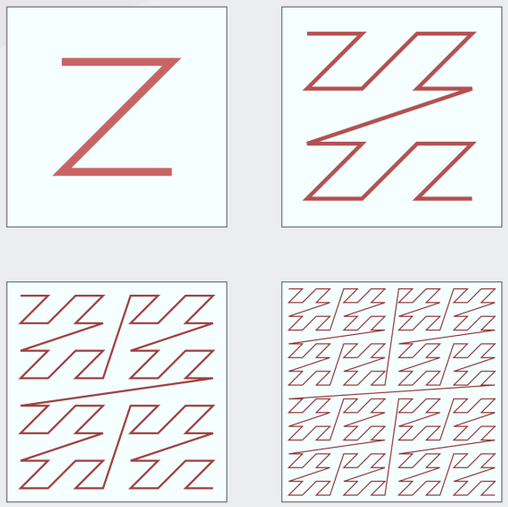
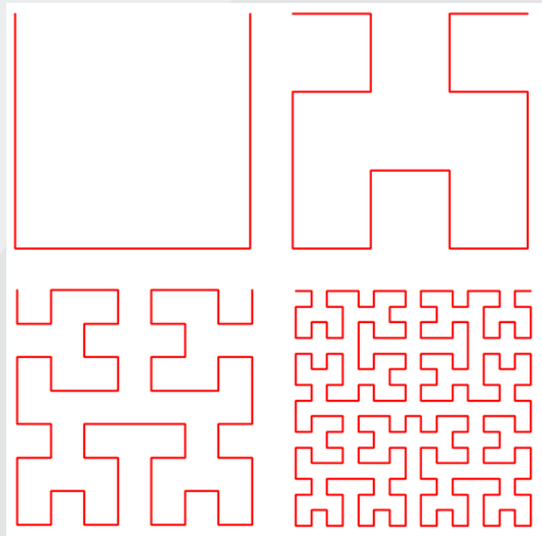


Space Filling Curves: self-similarity





Space Filling Curves: Discretization

Z-curve	Hilbert-curve
	

On a computer, **areas/volumes** are represented as **grids** with M^2 or M^3 grid-points and the **1D interval** or **key-space** is $[0, \ldots, M^{2,3} - 1]$.

- SFC enumerates the grid-points
- M has to be a power of 2: $M = 2^L \rightarrow$ key-space fits in `2L` or `3L` bits
- Grid points align with quad/octree cells at tree-depth L
- Higher tree nodes correspond to ranges in the key-space

Data layout: particles

array	type	dimenions	description
`x`	`FP32/64`	`[numParticles]`	x-coordinates
`y`	`FP32/64`	`[numParticles]`	y-coordinates
`z`	`FP32/64`	`[numParticles]`	z-coordinates
`keys`	`uint64`	`[numParticles]`	SFC keys

- particle `x,y,z` arrays are ordered such that `keys` is sorted

Data layout: octrees

Node geometry:

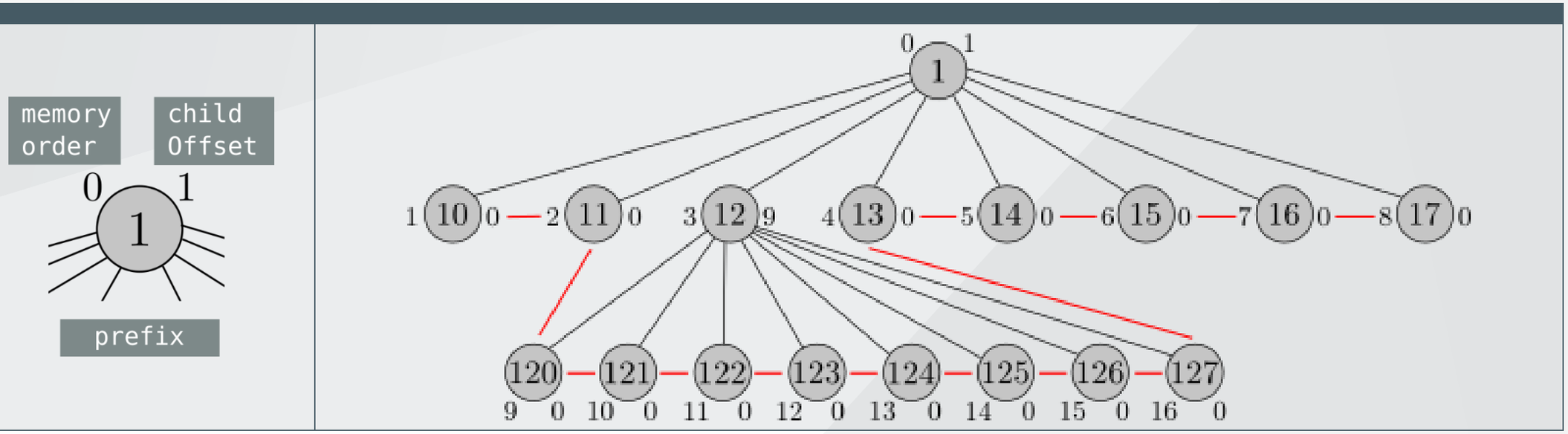
array	type	dimenions	description
`prefixes`	`uint64`	`[numNodes]`	node SFC key
`nodeCenters`	`Vec3<FP32/64>`	`[numNodes]`	3D center coordinate
`nodeSizes`	`Vec3<FP32/64>`	`[numNodes]`	3D node size

- `prefixes` can be decoded into `nodeCenters` and `nodeSizes`

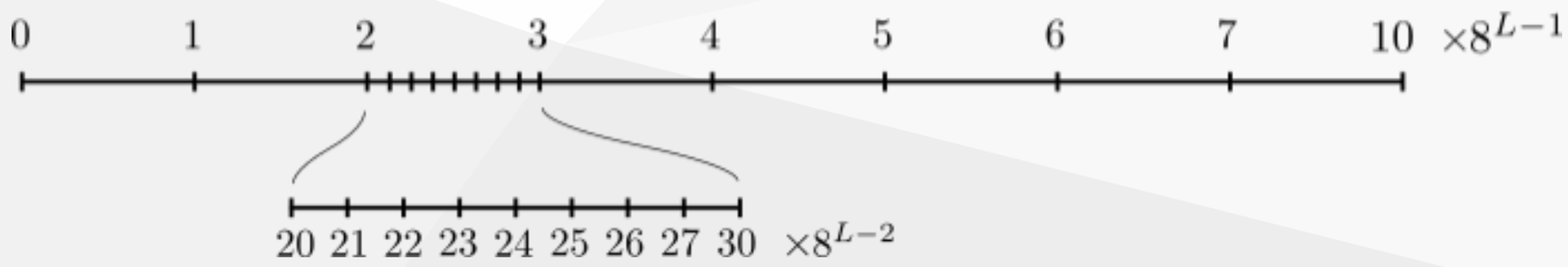
Node connectivity:

array	type	dimenions	description
`childOffsets`	`int32`	`[numNodes]`	first child node
`internalToLeaf`	`int32`	`[numNodes]`	enumeration of leaf nodes
`layout`	`uint32`	`[numLeafNodes]`	index of first particle in `x,y,z`

Data layout: octrees



Just the leaf nodes as they appear in `internaToLeaf` (the red line above):



Example: particles of node `9`: `internalToLeaf[9] = 2`, so from `layout[2]` to `layout[3]`

Octree mini-app repository

We provide a mini-app repository with the following features:

- **Octree construction** from 3D particle point clouds on CPUs and GPUs
- Portable **neighbor search** implementation with depth-first traversal
- Highly optimized explicitly warp-convergent neighbor search with breadth-first traversal

We use the mini-app as a basis for the next exercise, but we won't have time to work through all features. **You're invited to explore!**
For further study, you may also read the paper below.

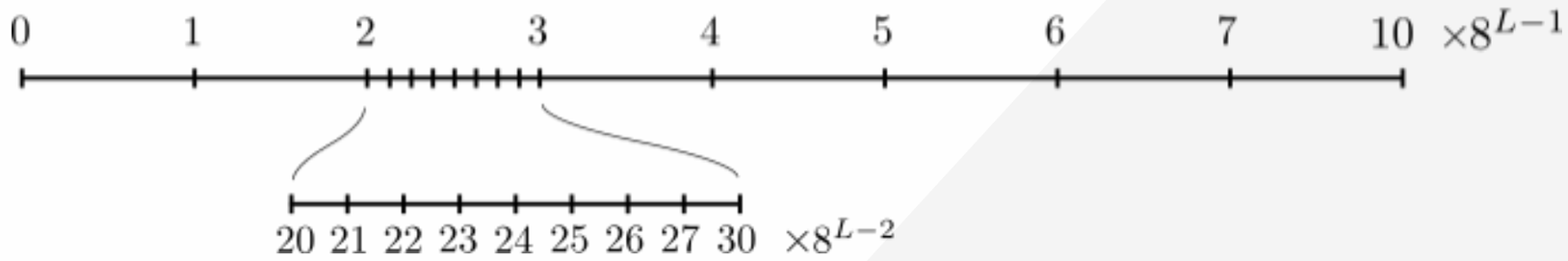
References: Cornerstone octree

Exercise 1: tree traversal for neighbor searching

1. Implementation of neighbor search on CPUs (`findneighbors.hpp`).
   - compile with
     `nvcc -std=c++17 -O3 -Xcompiler -fopenmp neighbor_search.cu`
   - follow the hints given in the file
   - can you make the `all2all` test pass?
2. Implementation of neighbor search on GPUs
   - implement the CUDA kernel in `neighbor_search.cu`
   - which CPU functions can we also use on the GPU?
   - can you make the CPU reference test pass?
   - how much speed-up do you get for 2 million particles?
   - activate the warp-level optimized version, how much faster is it?

Exercise 2: from the root node to a balanced tree

Building the leaves of a balanced octree as a histogram over the SFC key-range:



- Each leaf node covers a section of the space filling curve
- Leaf nodes are like buckets of a histogram
- Each bucket contains the particles whose SFC keys fall into it's range
- Balanced tree: choose the biggest possible buckets such that no bucket contains more than N_{crit} particles.

Exercise 2: from the root node to a balanced tree

1. Study the CPU version and port it to GPU (`tree/csarray_gpu.cuh`)
   - compile the CPU version with `g++ -std=c++17 -O3 -fopenmp octree.cpp`
   - compile the GPU version with
     `nvcc -std=c++17 -O3 -Xcompiler -fopenmp octree.cu`
   - functions to be ported:
     - `computeNodeCountsGpu`
     - `rebalanceDecision`
     - `rebalanceTree`
2. Correctness: does the GPU output match the CPU version?
3. Speedup of the GPU version over the CPU?

Important porting considerations

- Memory access pattern: consecutive threads need to load consecutive addresses in memory
- SIMT and warp-divergence: threads in a warp need to execute the same instructions, branching divergence leads to loss of performance
- CUDA offers several technical features to aid in parallelization and optimization:
  - shared memory and block synchronization
  - intra-warp communication
  - cooperative groups
  - streams and graphs
- Parallel building blocks often serve as a stepping stone. These can be extremely efficient in parallel:
  - reductions ($1 + 2 + 3 + 4 \rightarrow 10$)
  - prefix sums (Blelloch scan) ($1 + 2 + 3 + 4 \rightarrow \{1,3,6,10\}$)
  - sorting (radix sort)

Take-home Message

Massive parallelism may need new algorithms

- Often, a fundamentally new algorithm is needed to expose parallelism
- If your app is inherently sequential or the data layout is not suitable, the technical features of CUDA won't allow you to run efficiently!