High Performance Computing Systems (CMSC714)

Lecture 2: Terminology and Definitions

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Announcements

- Slides and video from previous class are now posted online
- Assignments, and midterm dates are also online
- Deepthought2 accounts have been mailed out:
  - http://www.cs.umd.edu/class/spring2021/cmsc714/deepthought2.shtml

Group project timeline

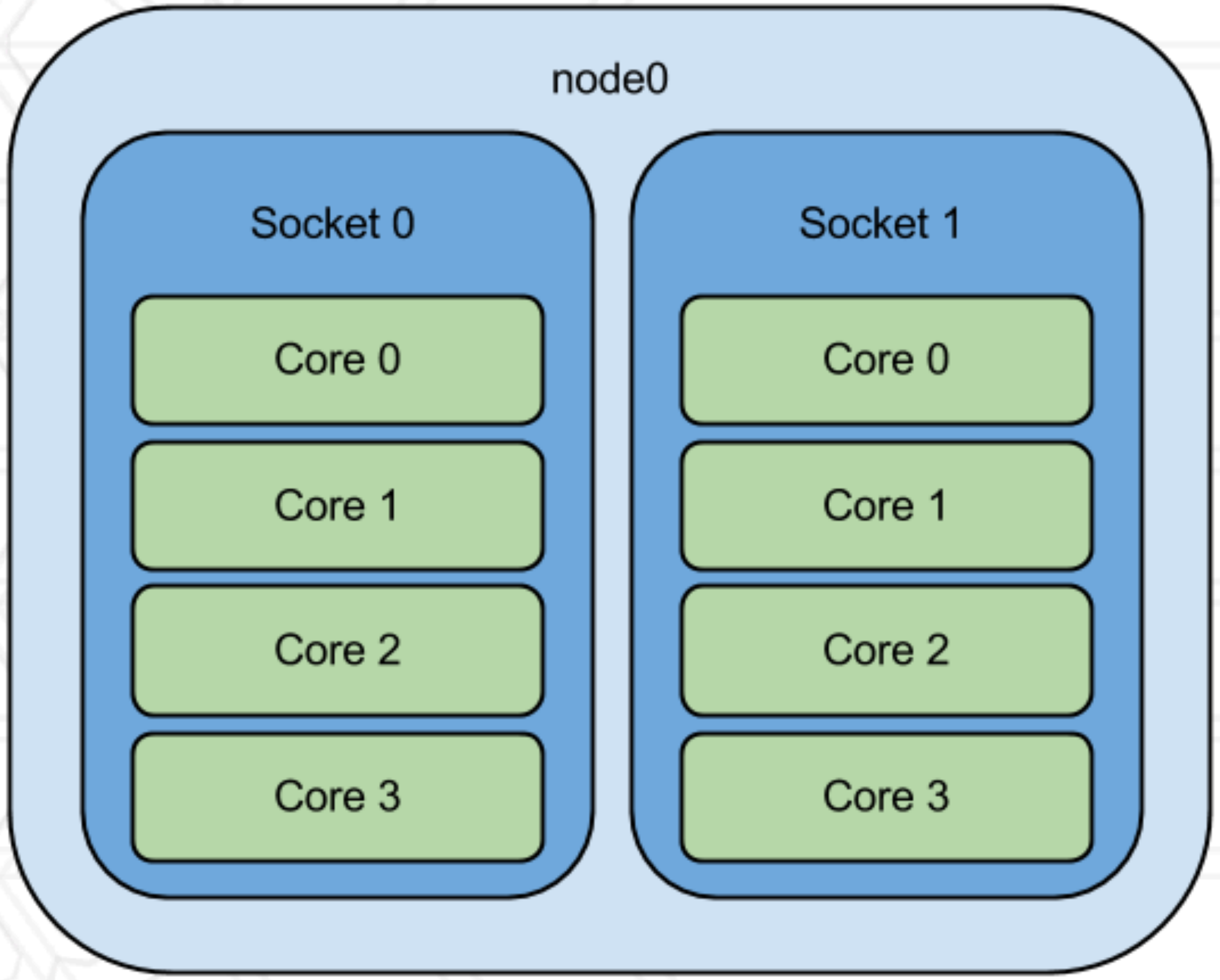
- [Form groups: March 4]
- Finalize project topic: March 11
- Interim report due: April 15
- Project presentations: May 6, 11
- Final project and report due: May 13

Summary of last lecture

- Need for high performance computing
- Parallel architecture: nodes, memory, network, storage
- Programming models: shared memory vs. distributed
- Performance and debugging tools
- Systems issues: job scheduling, routing, parallel I/O, *fault tolerance, power*
- Parallel algorithms and applications

Cores, sockets, nodes

- CPU: processor
  - Single-core or multi-core
  - Core is a processing unit, multiple such units on a single chip make it a multi-core processor
- Socket: same as chip or processor
- Node: packaging of sockets



https://www.glennklockwood.com/hpc-howtos/process-affinity.html

Job scheduling

Job scheduling

- HPC systems use job or batch scheduling
- Each user submits their parallel programs for execution to a "job" scheduler

Job Queue

	#Nodes Requested	Time Requested
1	128	30 mins
2	64	24 hours
3	56	6 hours
4	192	12 hours
5	…	…
6	…	…

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- The scheduler decides:
  - what job to schedule next (based on an algorithm: FCFS, priority-based, ….)
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- Compute nodes: dedicated to each job
- Network, filesystem: shared by all jobs

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Compute nodes vs. login nodes

- Compute nodes: dedicated nodes for running jobs
  - Can only be accessed when they have been allocated to a user by the job scheduler
- Login nodes: nodes shared by all users to compile their programs, submit jobs etc.

Supercomputers vs. commodity clusters

- Supercomputer refers to a large expensive installation, typically using custom hardware
  - High-speed interconnect
  - IBM Blue Gene, Cray XT, Cray XC
- Cluster refers to a cluster of nodes, typically put together using commodity (off-the-shelf) hardware

Serial vs. parallel code

- Thread: a thread or path of execution managed by the OS
  - Share memory
- Process: heavy-weight, processes do not share resources such as memory, file descriptors etc.
- Serial or sequential code: can only run on a single thread or process
- Parallel code: can be run on one or more threads or processes

Scaling and scalable

- Scaling: running a parallel program on 1 to n processes
  - 1, 2, 3, … , n
  - 1, 2, 4, 8, …, n
- Scalable: A program is scalable if it's performance improves when using more resources

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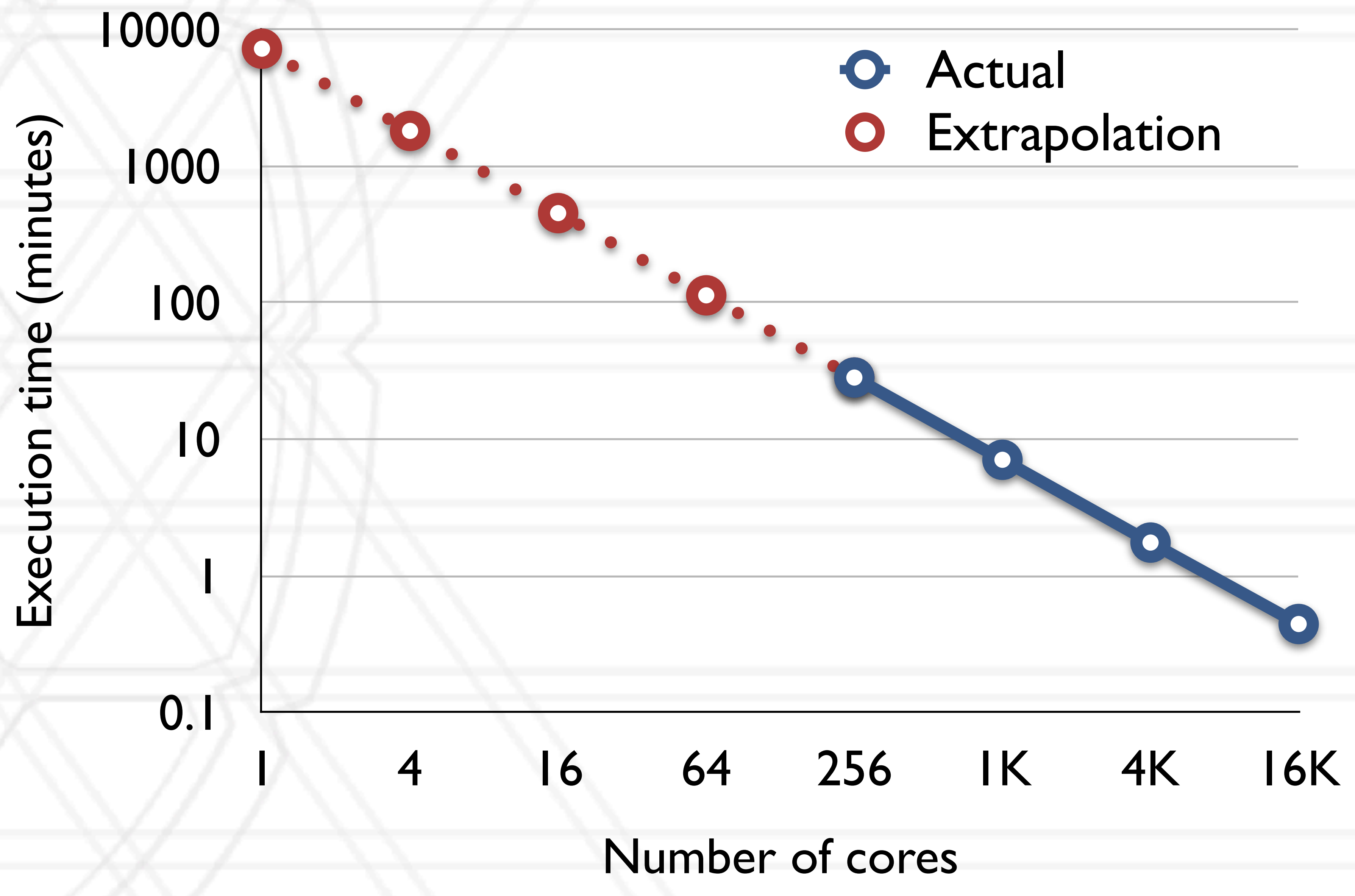

Weak versus strong scaling

- Strong scaling: *Fixed total* problem size as we run on more processes
  - Sorting n numbers on 1 process, 2 processes, 4 processes, …
- Weak scaling: Fixed problem size per process but *increasing total* problem size as we run on more processes
  - Sorting n numbers on 1 process
  - 2n numbers on 2 processes
  - 4n numbers on 4 processes

Speedup and efficiency

- Speedup: Ratio of execution time on one process to that on *n* processes

$$\text{Speedup} = \frac{t_1}{t_n}$$

- Efficiency: Speedup per process

$$\text{Efficiency} = \frac{t_1}{t_n \times n}$$

Amdahl's law

- Speedup is limited by the serial portion of the code
  - Often referred to as the serial "bottleneck"
- Lets say only a fraction f of the code can be parallelized on p processes

$$\text{Speedup} = \frac{1}{(1-f) + f/p}$$

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Amdahl's law

$$\text{Speedup} = \frac{1}{(1-p) + p/n}$$

```
fprintf(stdout,"Process %d of %d is on %s\n",
    myid, numprocs, processor_name);
fflush(stdout);

n = 10000;          /* default # of rectangles */
if (myid == 0)
startwtime = MPI_Wtime();
```

```
MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);

h   = 1.0 / (double) n;
sum = 0.0;
/* A slightly better approach starts from large i and works back */
for (i = myid + 1; i <= n; i += numprocs)
{
x = h * ((double)i - 0.5);
sum += f(x);
}
mypi = h * sum;

MPI_Reduce(&mypi, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
```

100 - p = 40 s on 1 process

$$\text{Speedup} = \frac{1}{(1-0.6) + 0.6/n}$$

p = 60 s on 1 process

Communication and synchronization

- Each physical node might compute independently for a while
- When data is needed from other (remote) nodes, messaging occurs
  - Referred to as communication or synchronization or MPI messages
- Intra-node vs. inter-node communication
- Bulk synchronous programs: All processes compute simultaneously, then synchronize together

Different models of parallel computation

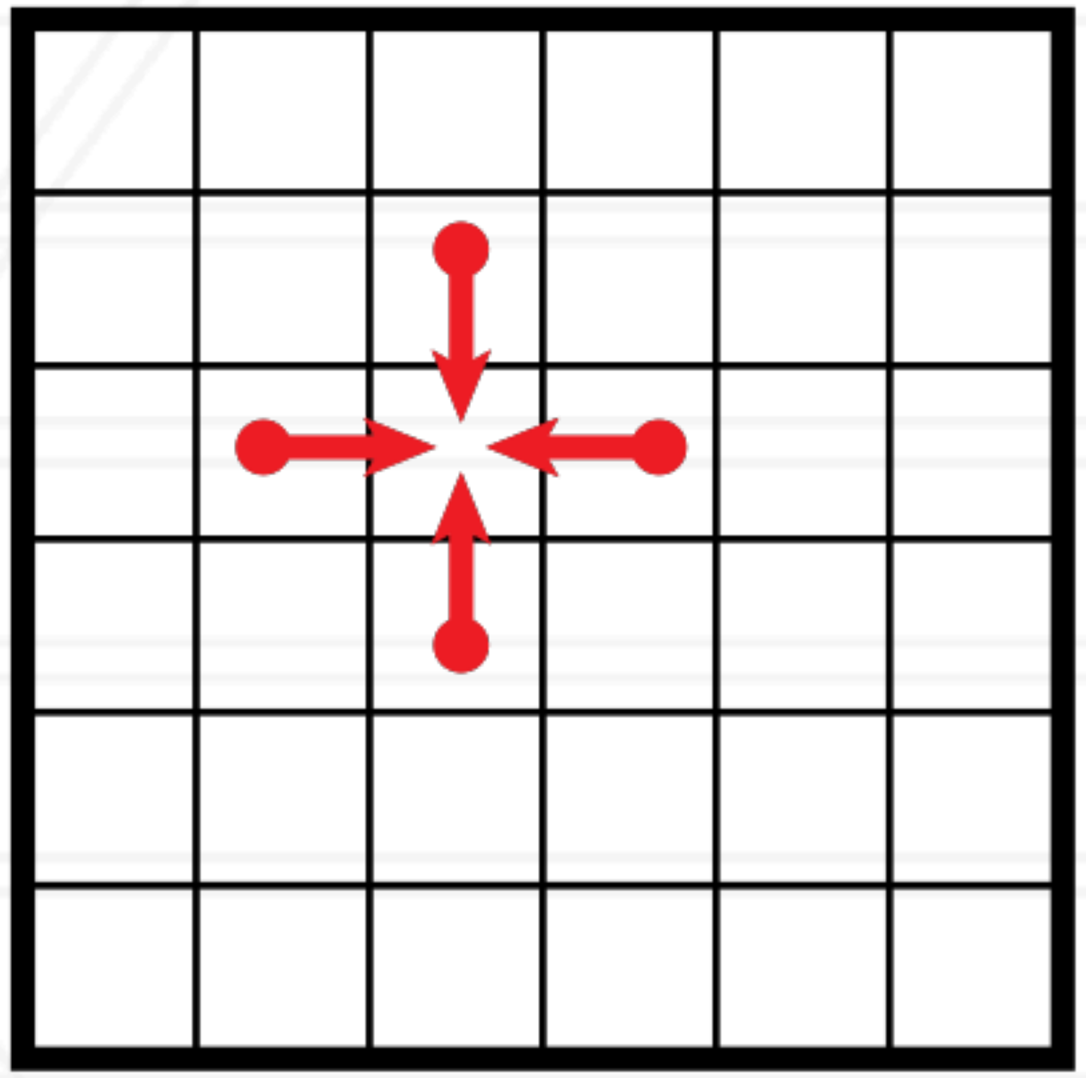
- SIMD: Single Instruction Multiple Data
- MIMD: Multiple Instruction Multiple Data
- SPMD: Single Program Multiple Data
    - Typical in HPC

Writing parallel programs

- Decide the serial algorithm first
- Data: how to distribute data among threads/processes?
  - Data locality: assignment of data to specific processes to minimize data movement
- Computation: how to divide work among threads/processes?
- Figure out how often communication will be needed

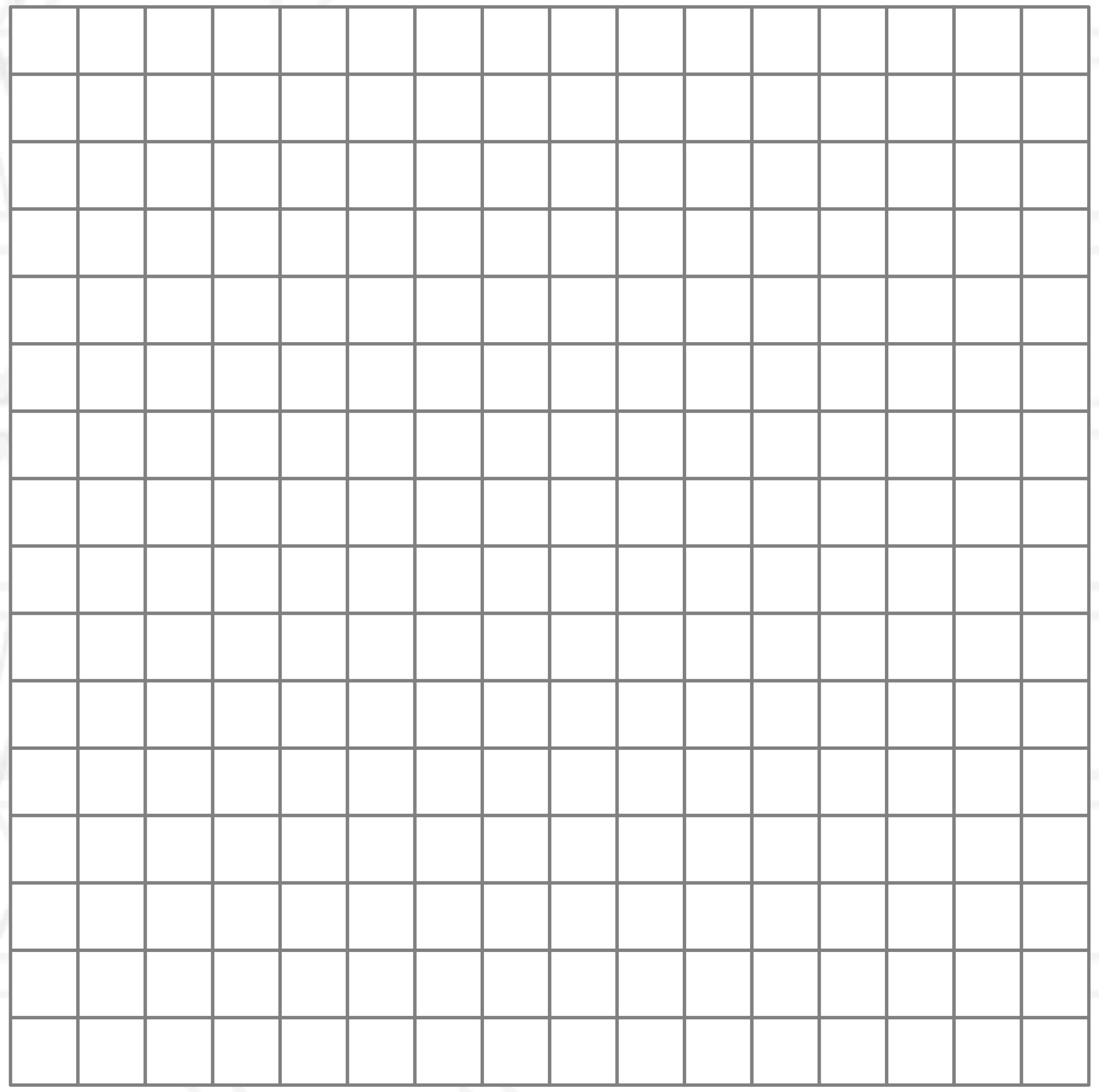
Two-dimensional stencil computation

- Commonly found kernel in computational codes
- Heat diffusion, Jacobi method, Gauss-Seidel method



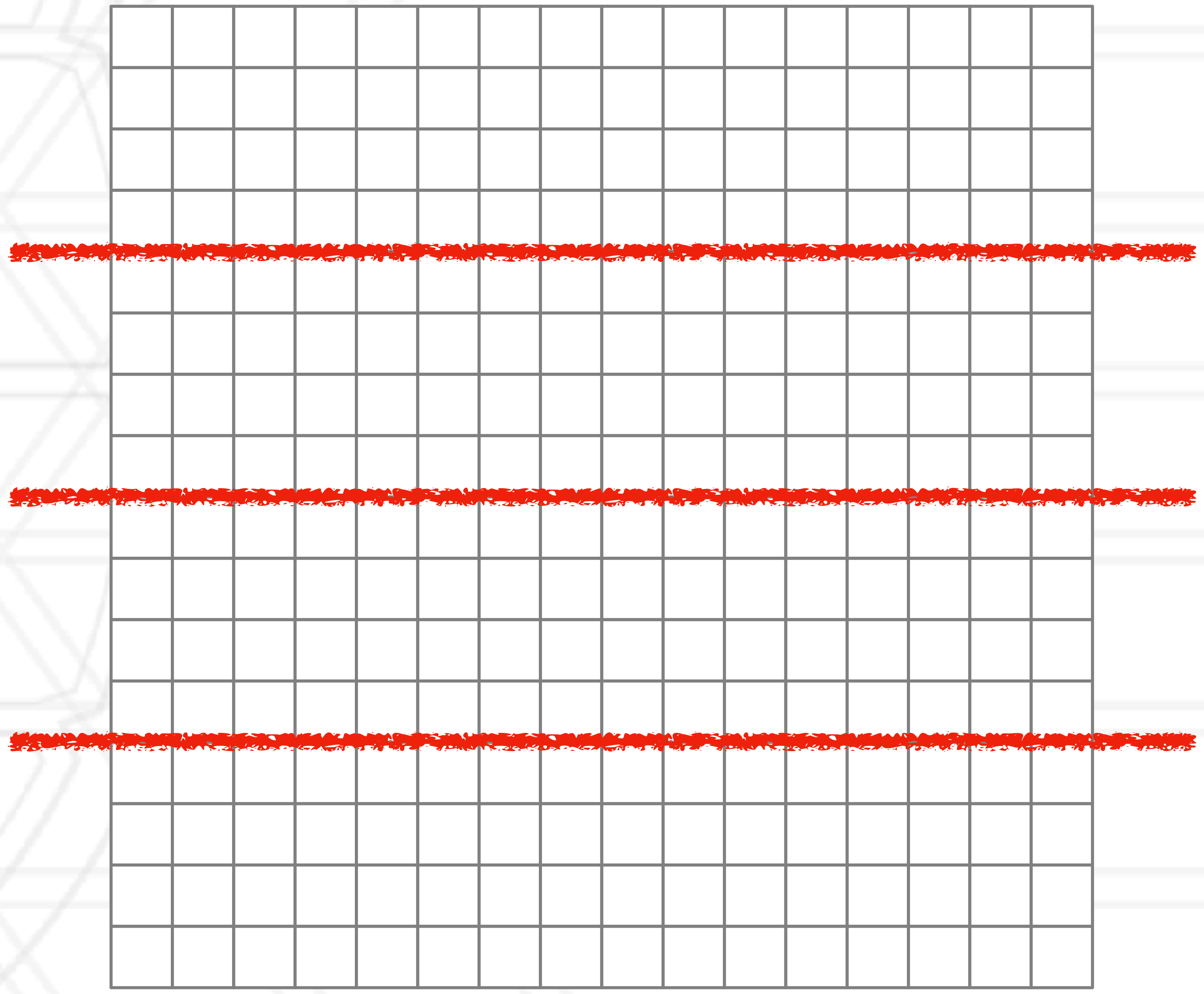
$$A[i,j] = \frac{A[i,j] + A[i-1,j] + A[i+1,j] + A[i,j-1] + A[i,j+1]}{5}$$

2D stencil iteration in parallel



2D stencil iteration in parallel

- 1D decomposition
  - Divide rows (or columns) among processes



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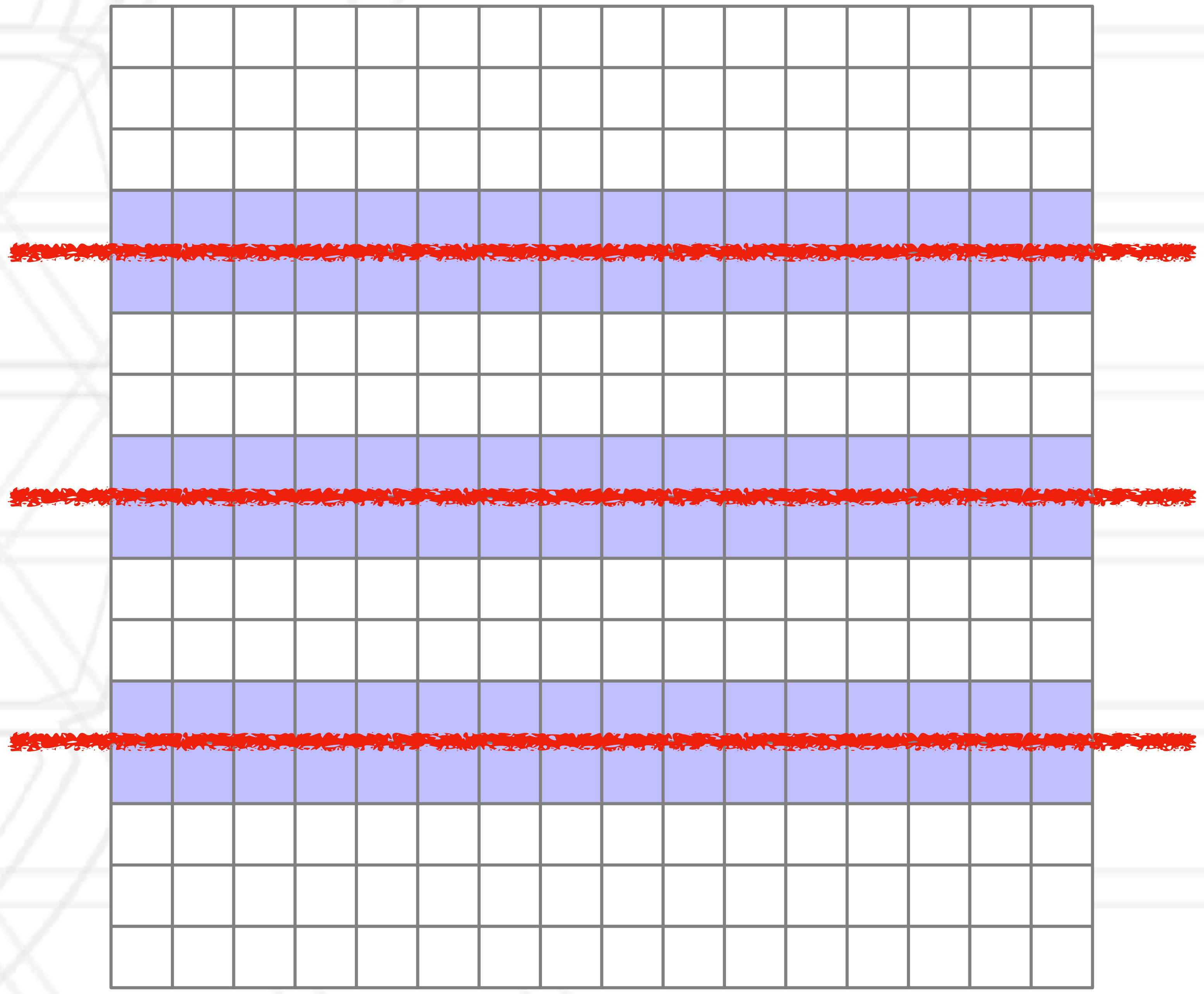

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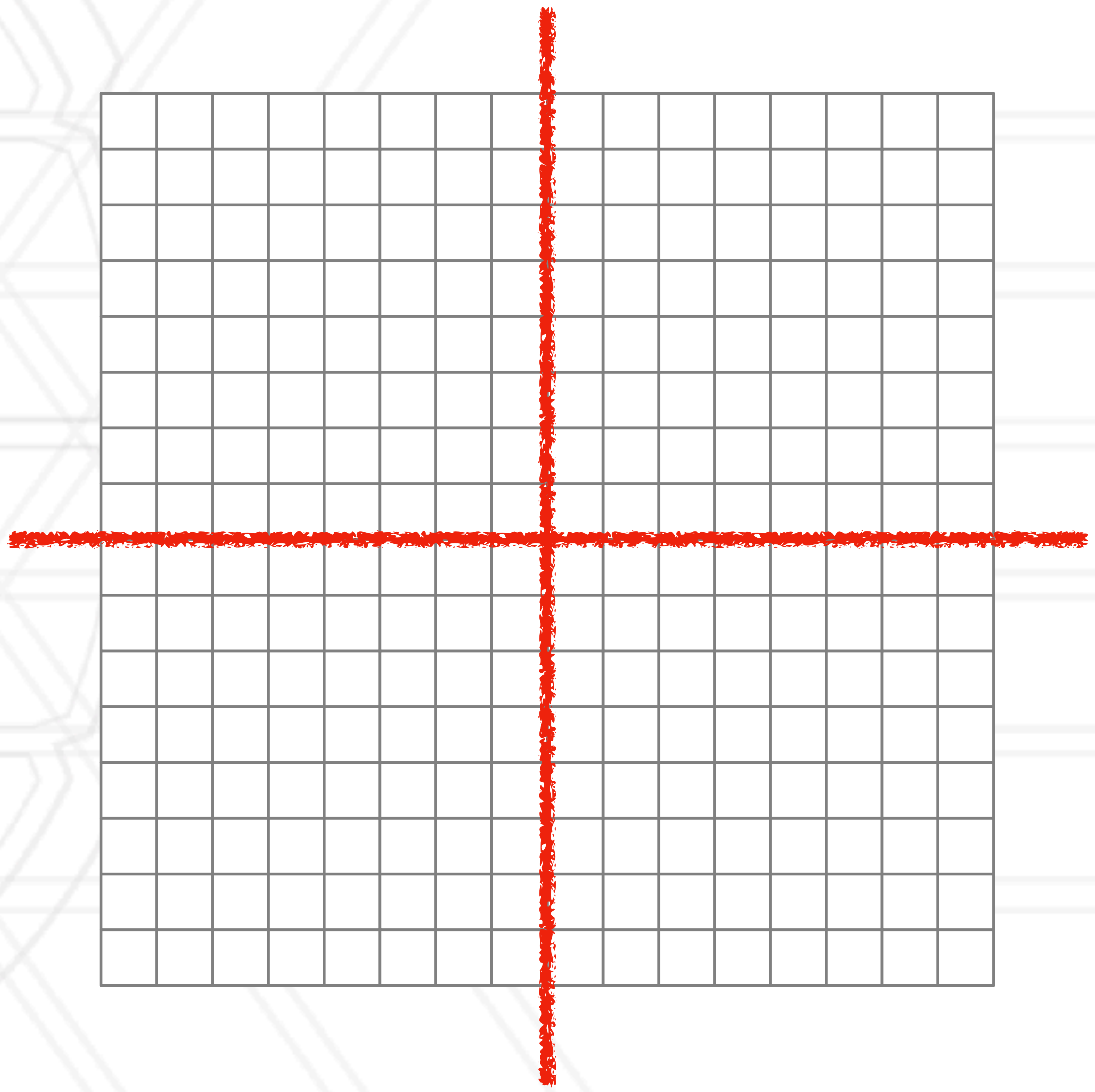

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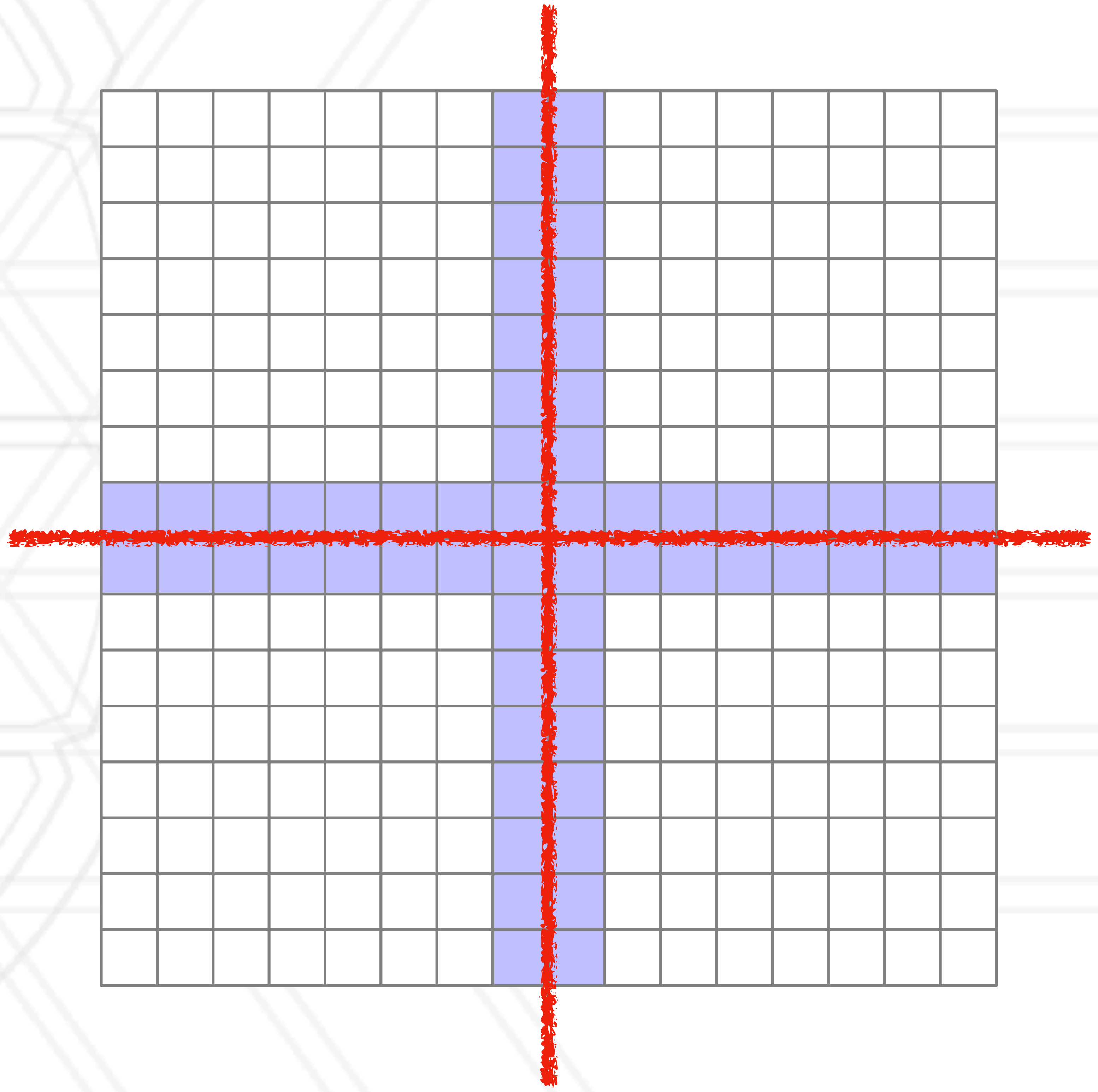
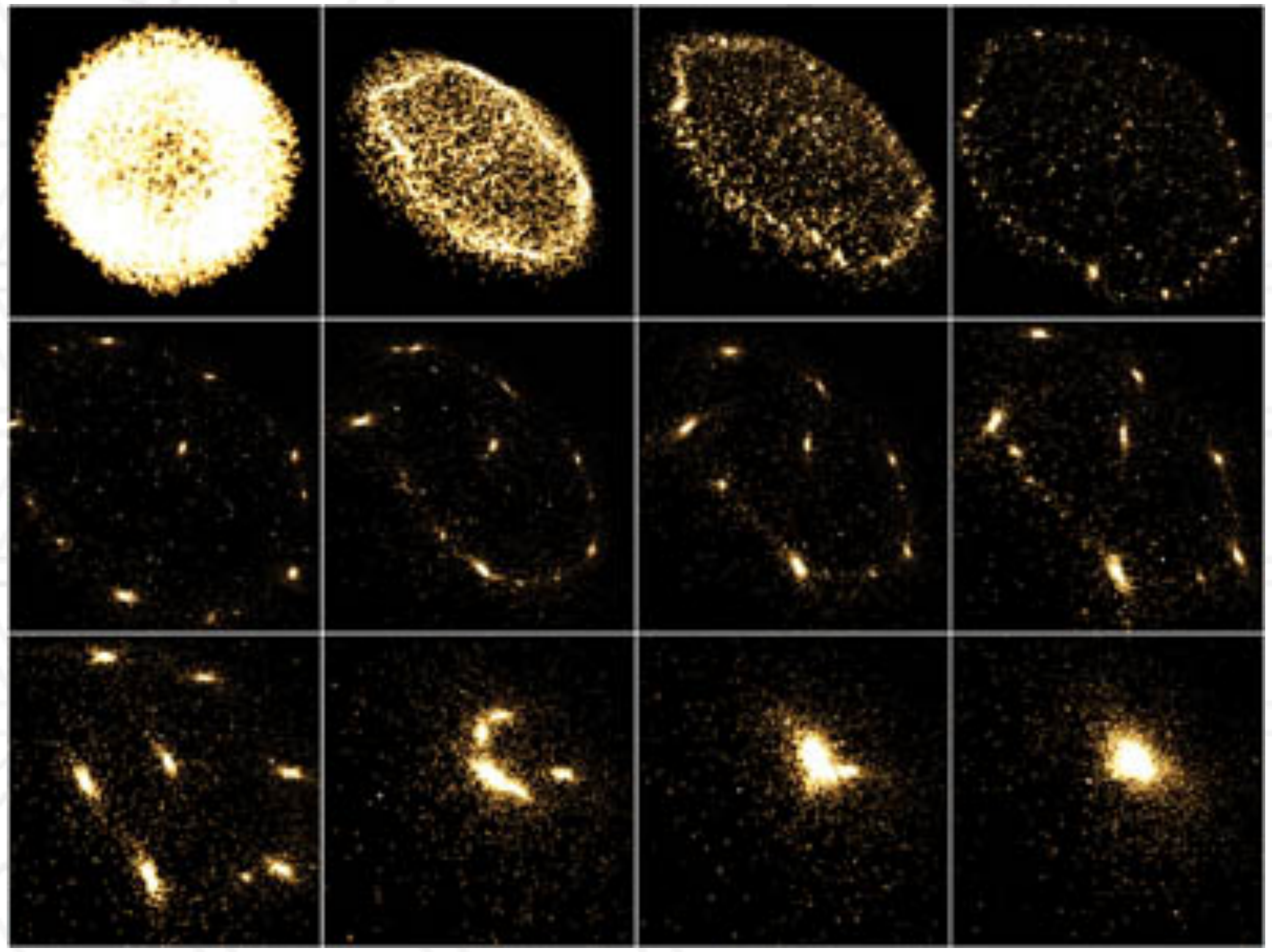


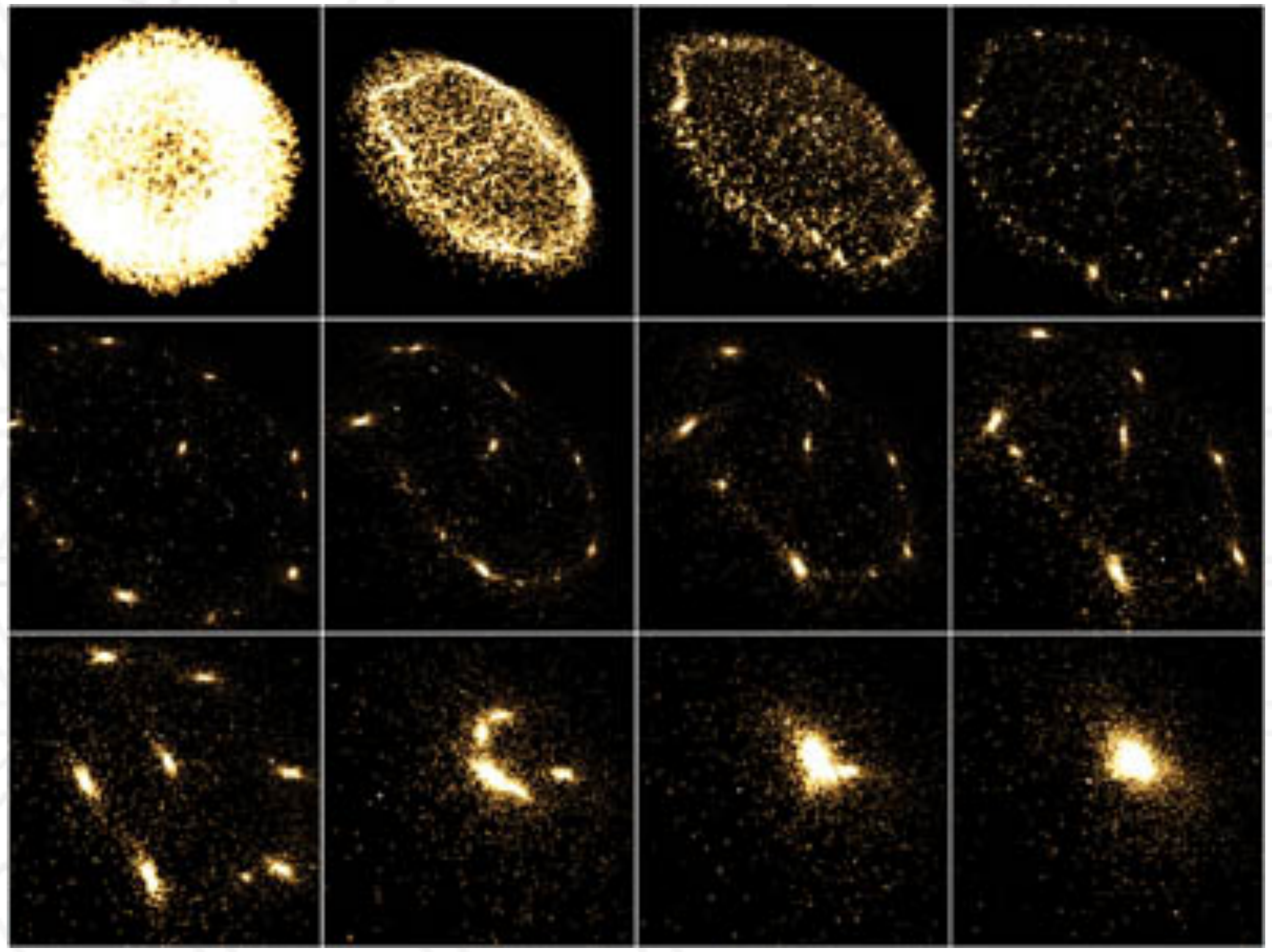
N-body problem



https://developer.nvidia.com/gpugems/gpugems3/part-v-physics-simulation/chapter-31-fast-n-body-simulation-cuda

N-body problem

- Simulating the movement of N-bodies under gravitational forces



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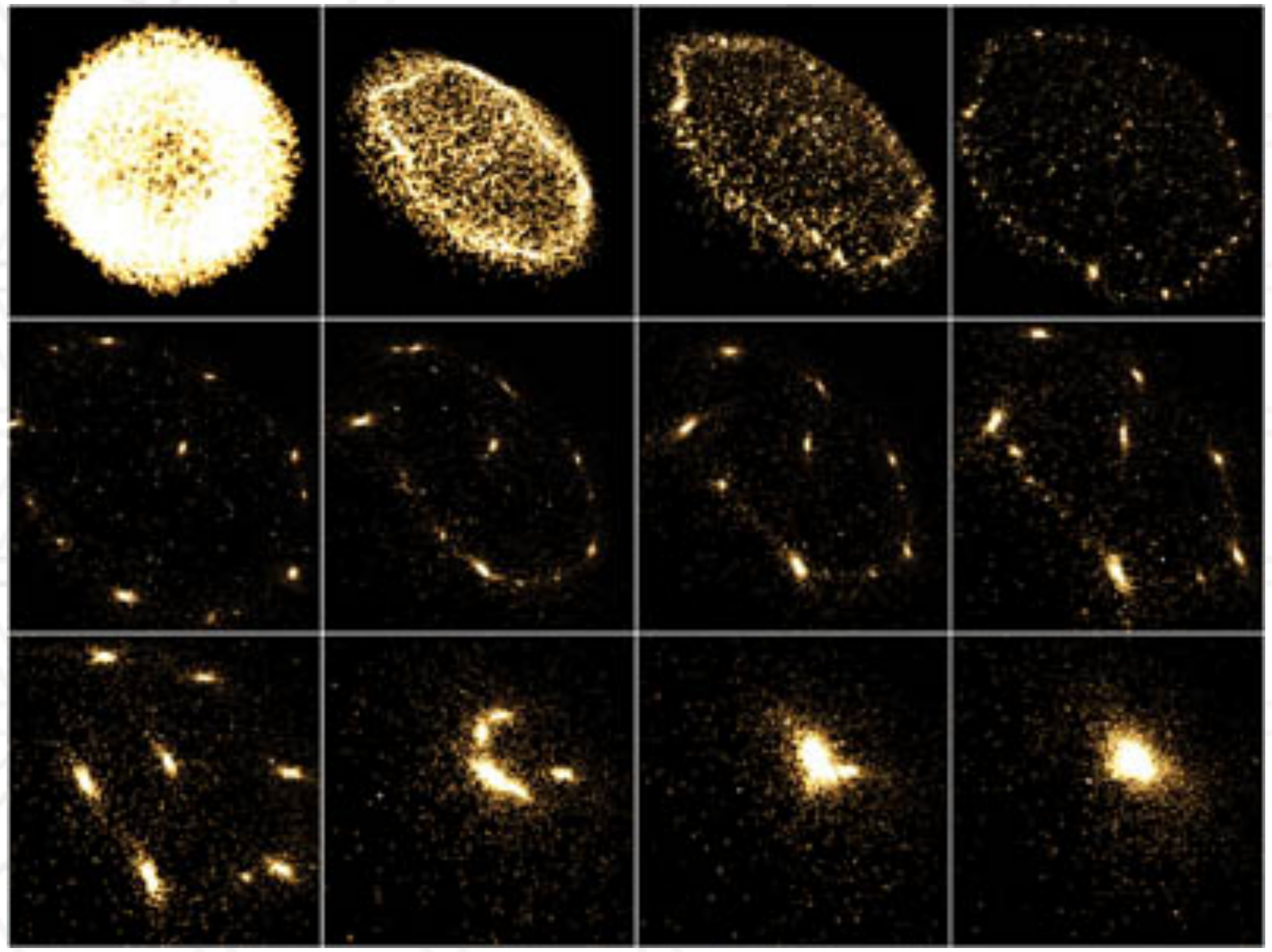
N-body problem

- Simulating the movement of N-bodies under gravitational forces
- Naive algorithm: $O(n^2)$
  - Every body calculates forces pair-wise with every other body (particle)



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Data distribution in N-body problems

- Naive approach: Assign n/k particles to each process
- Other approaches?

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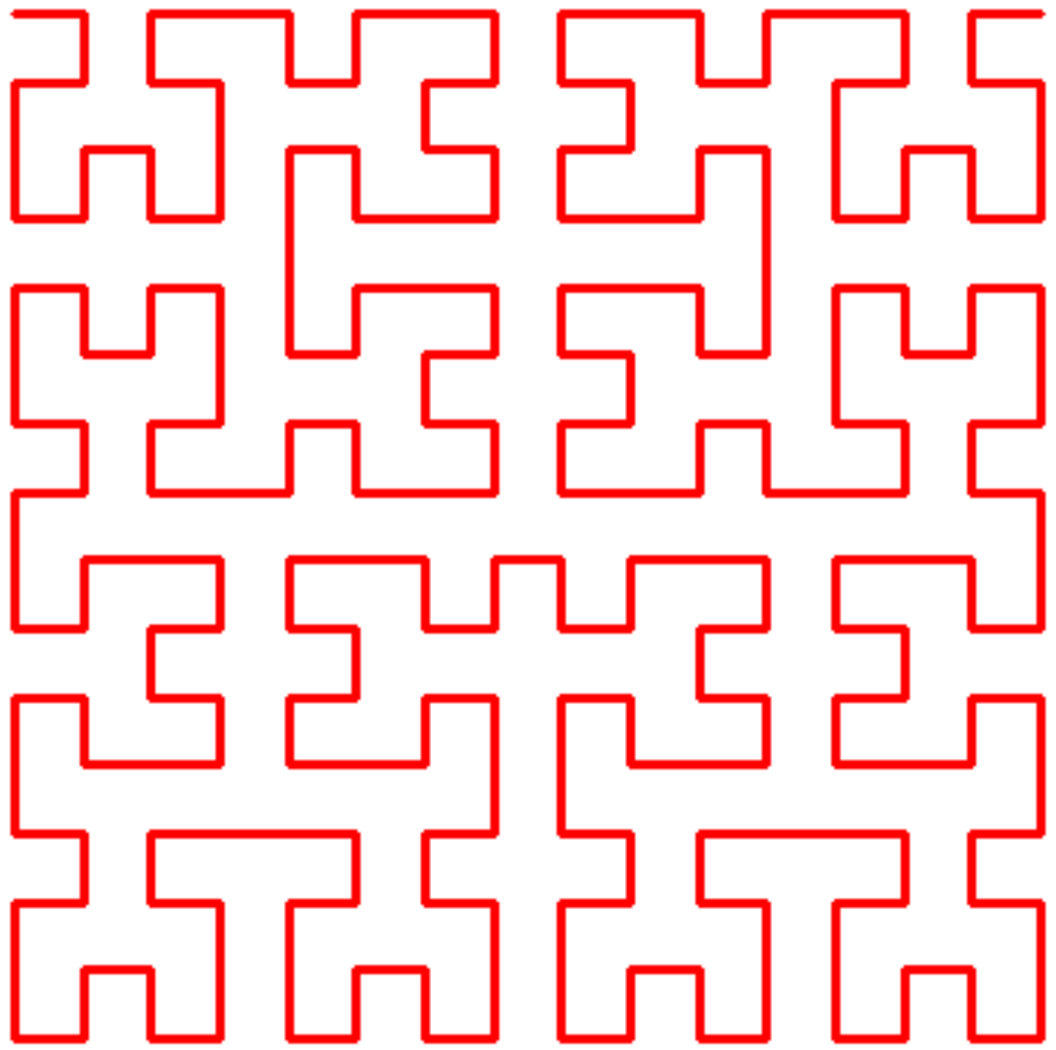

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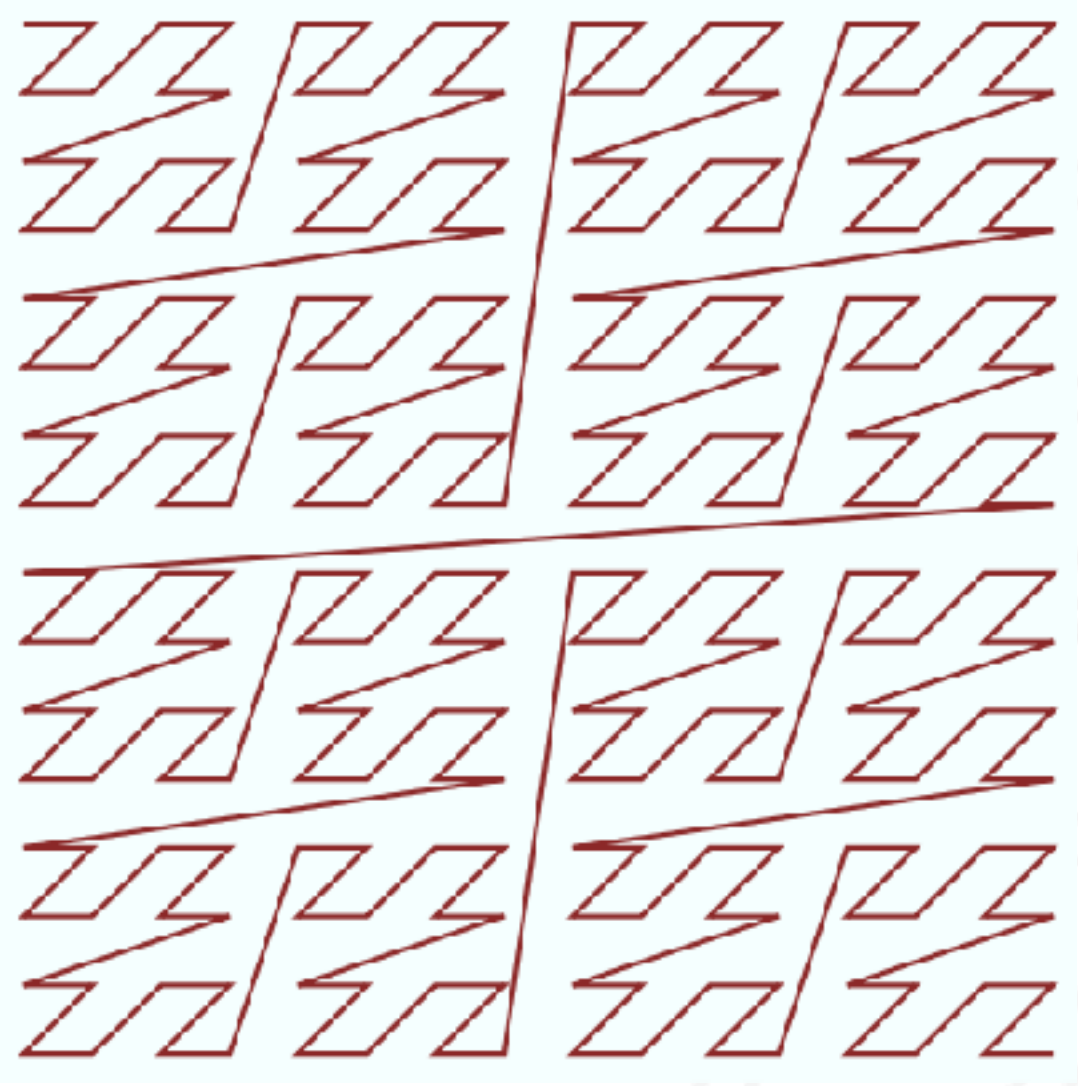

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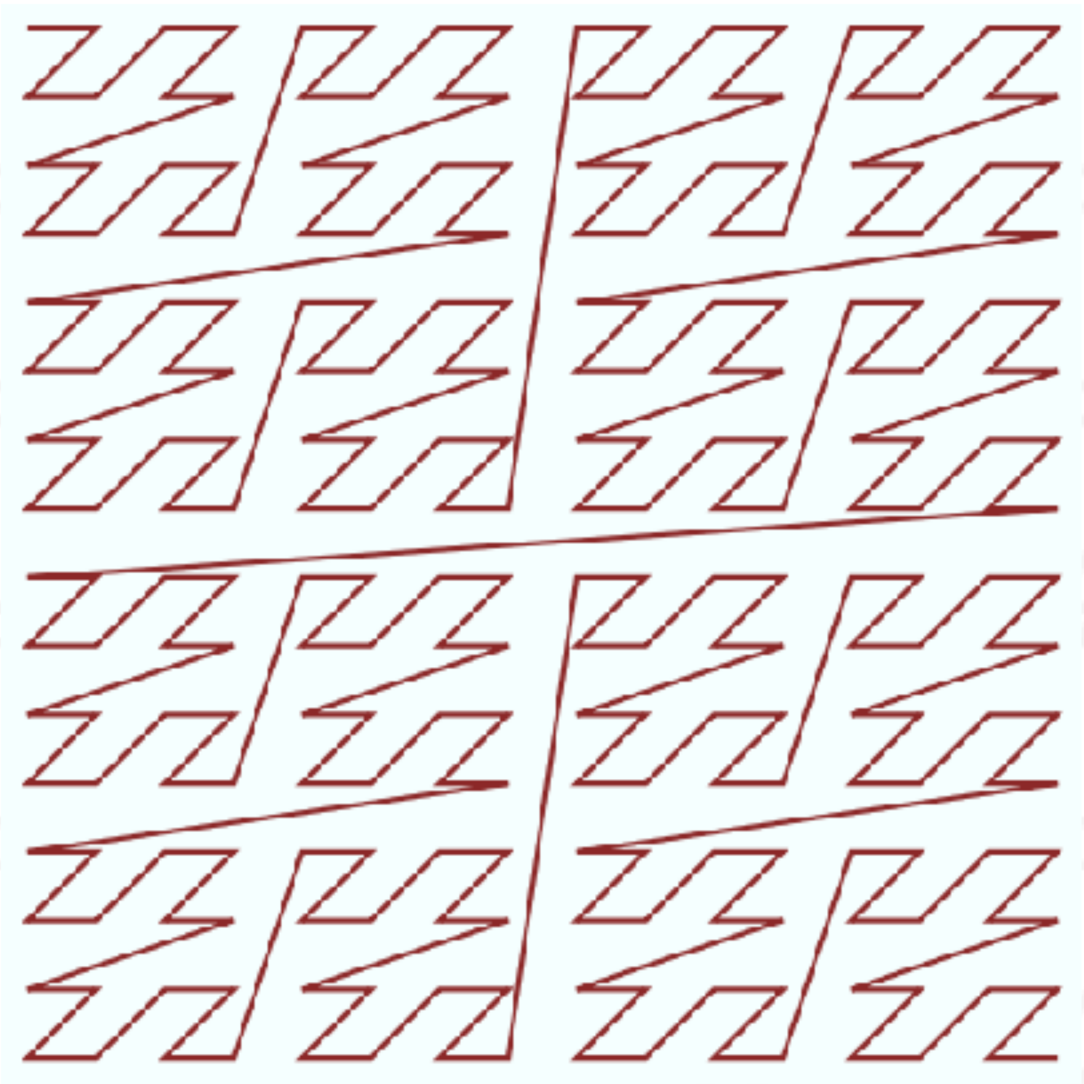

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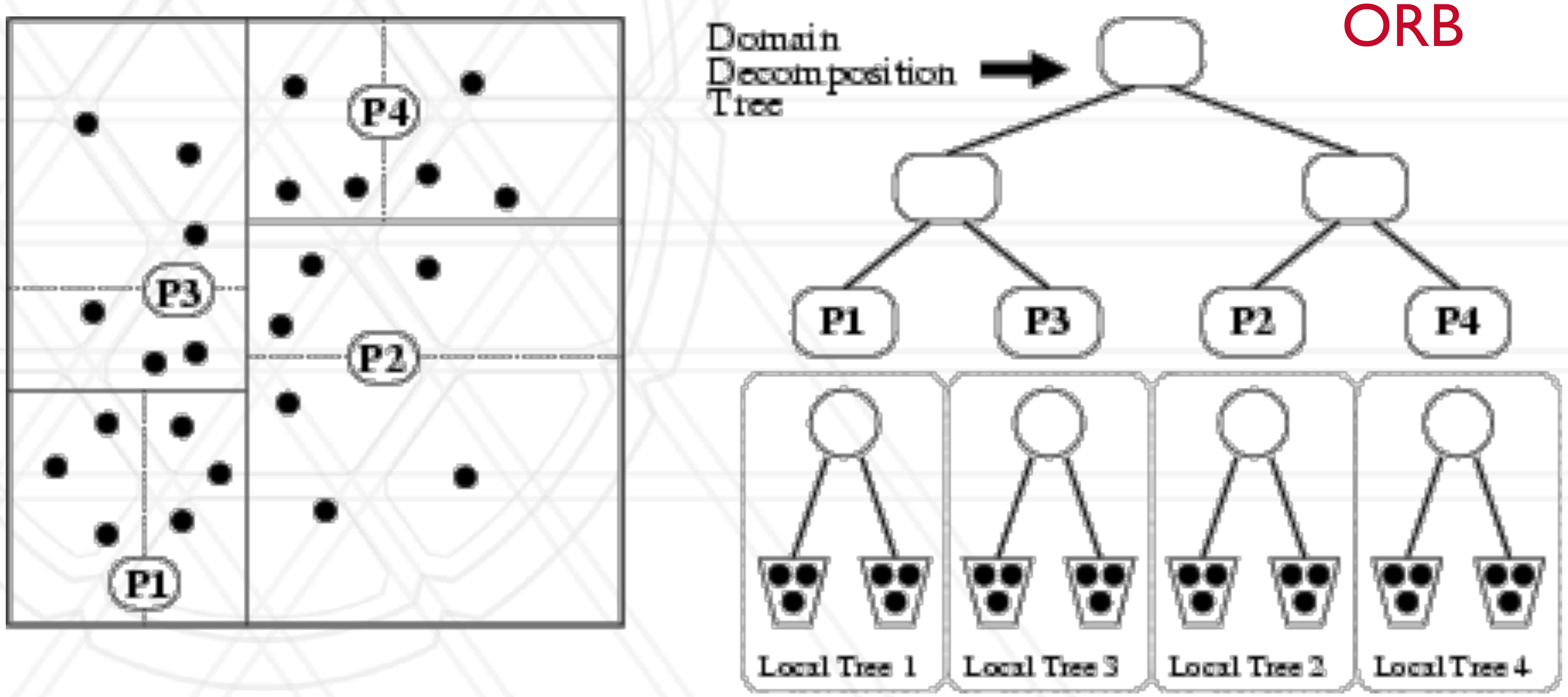
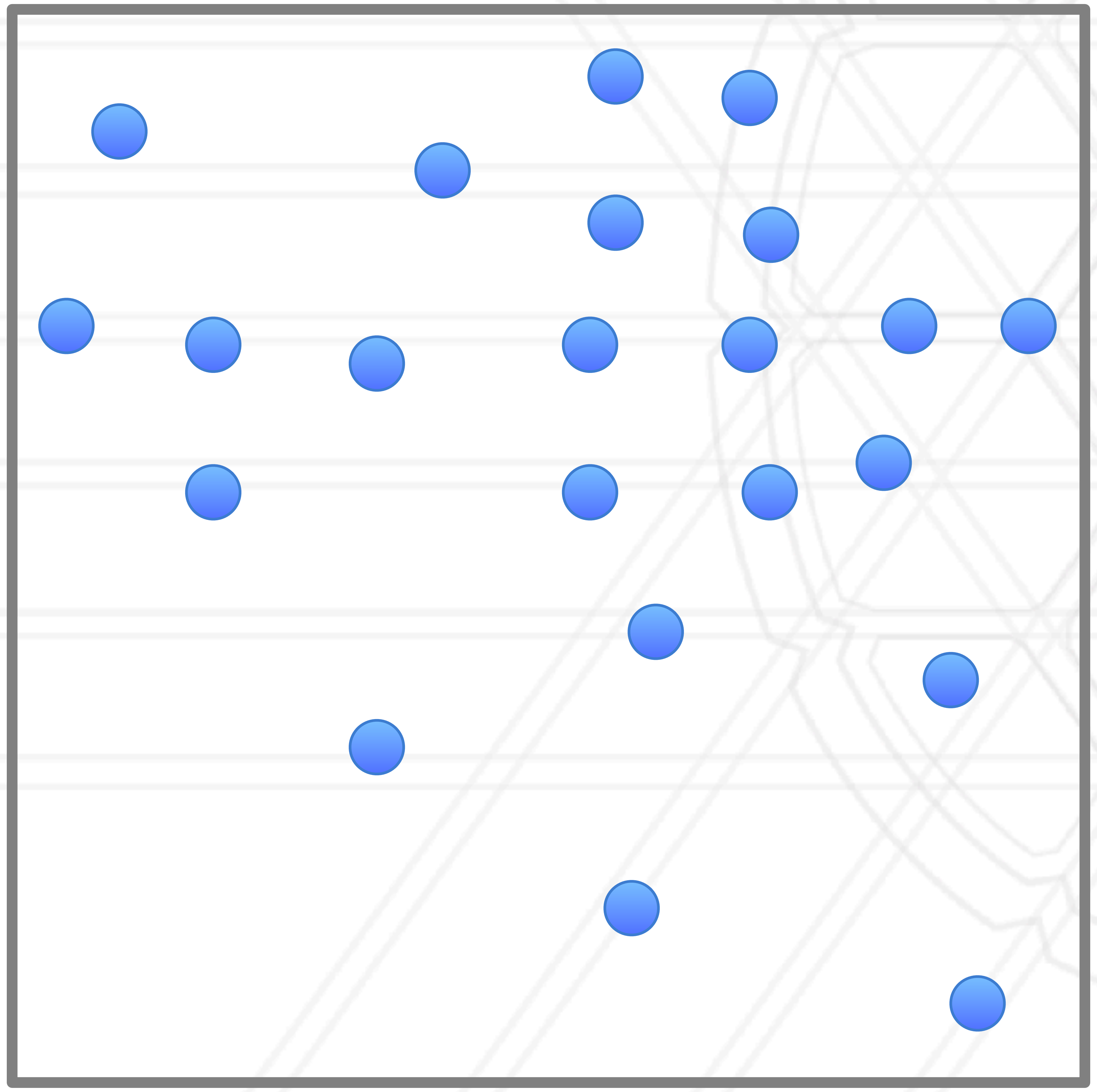


ORB

http://charm.cs.uiuc.edu/workshops/charmWorkshop2011/slides/CharmWorkshop2011_apps_ChaNGa.pdf

Data distribution in N-body problems

- Let us consider a two-dimensional space with bodies/particles in it



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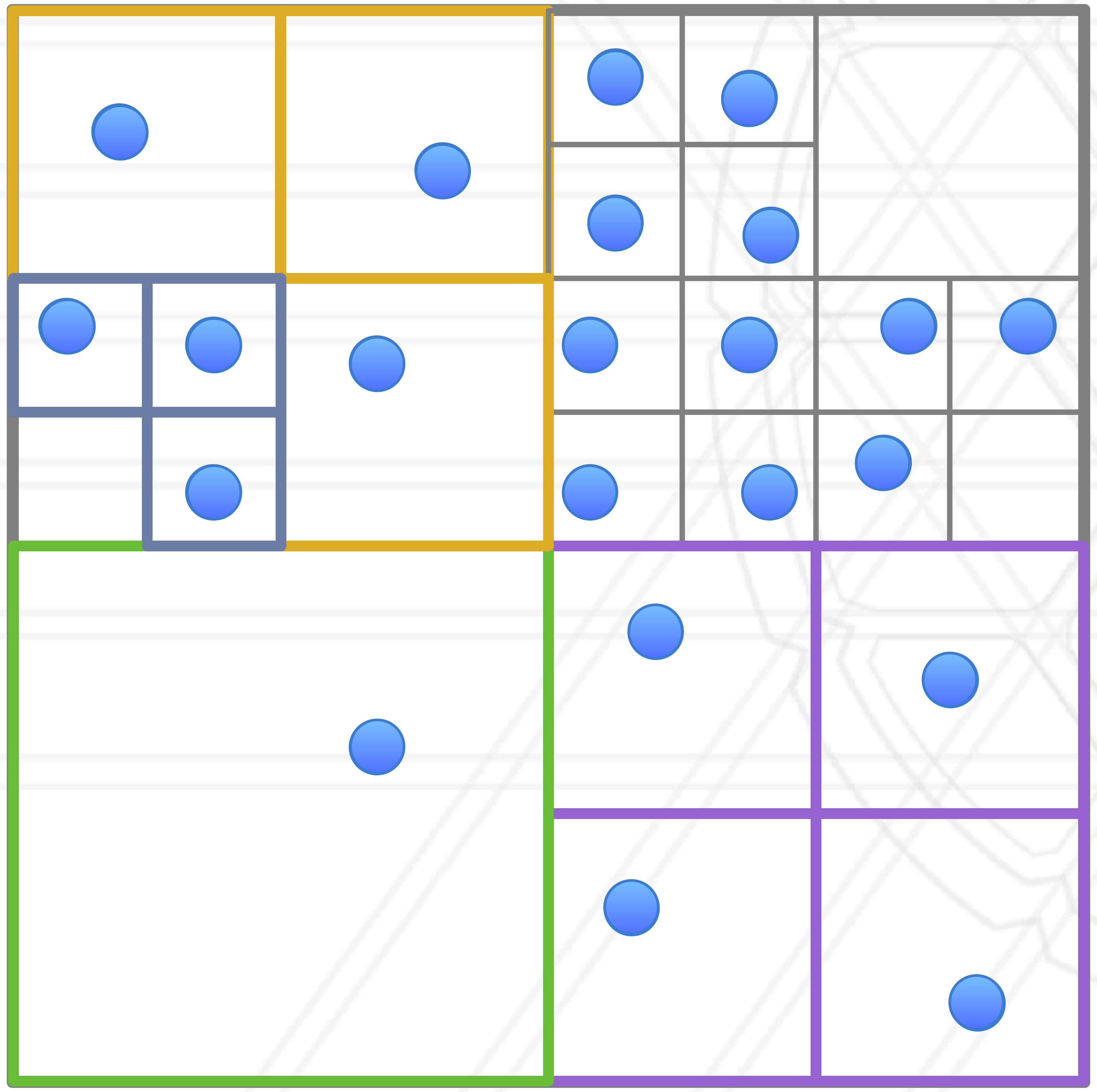

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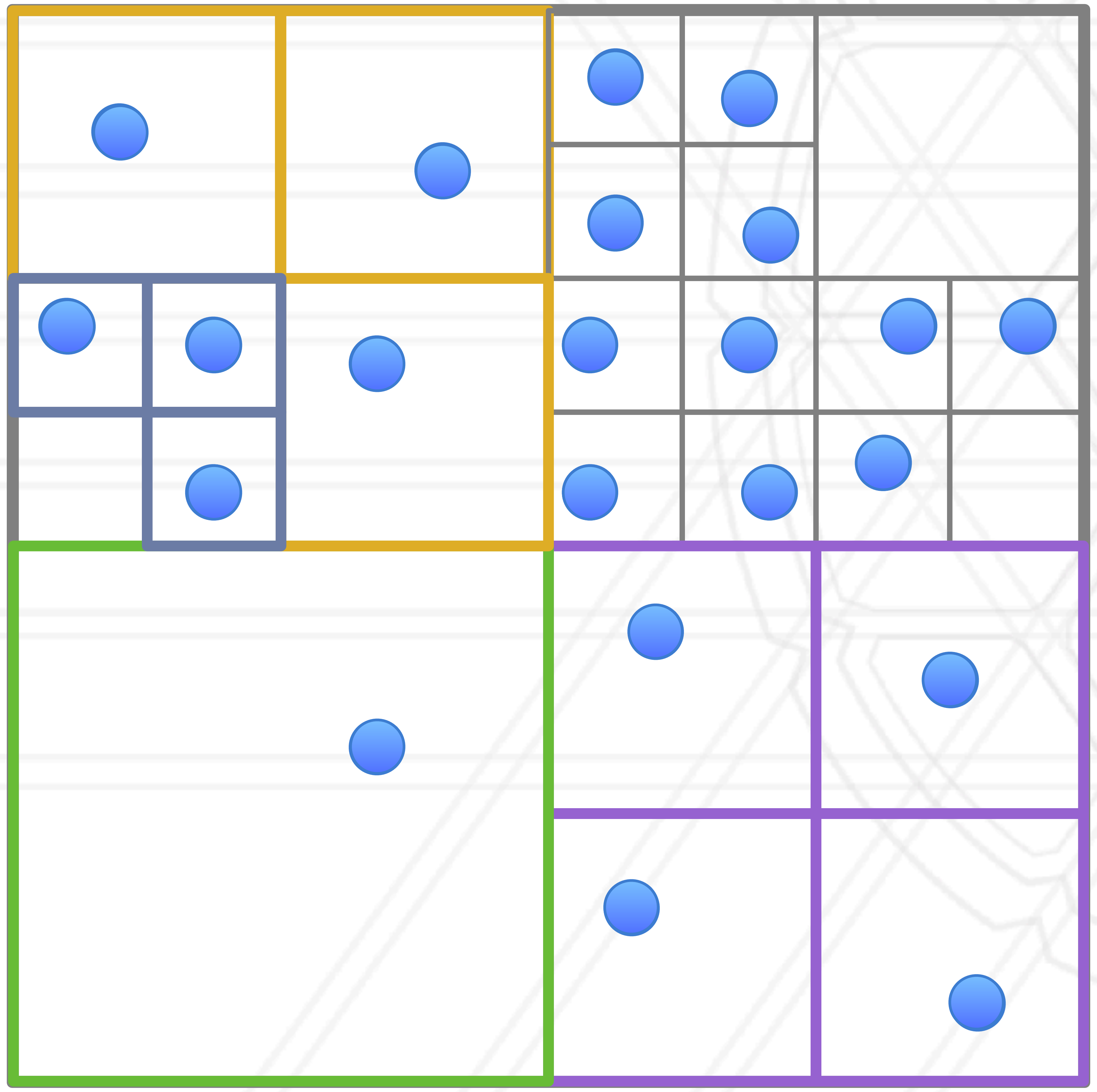

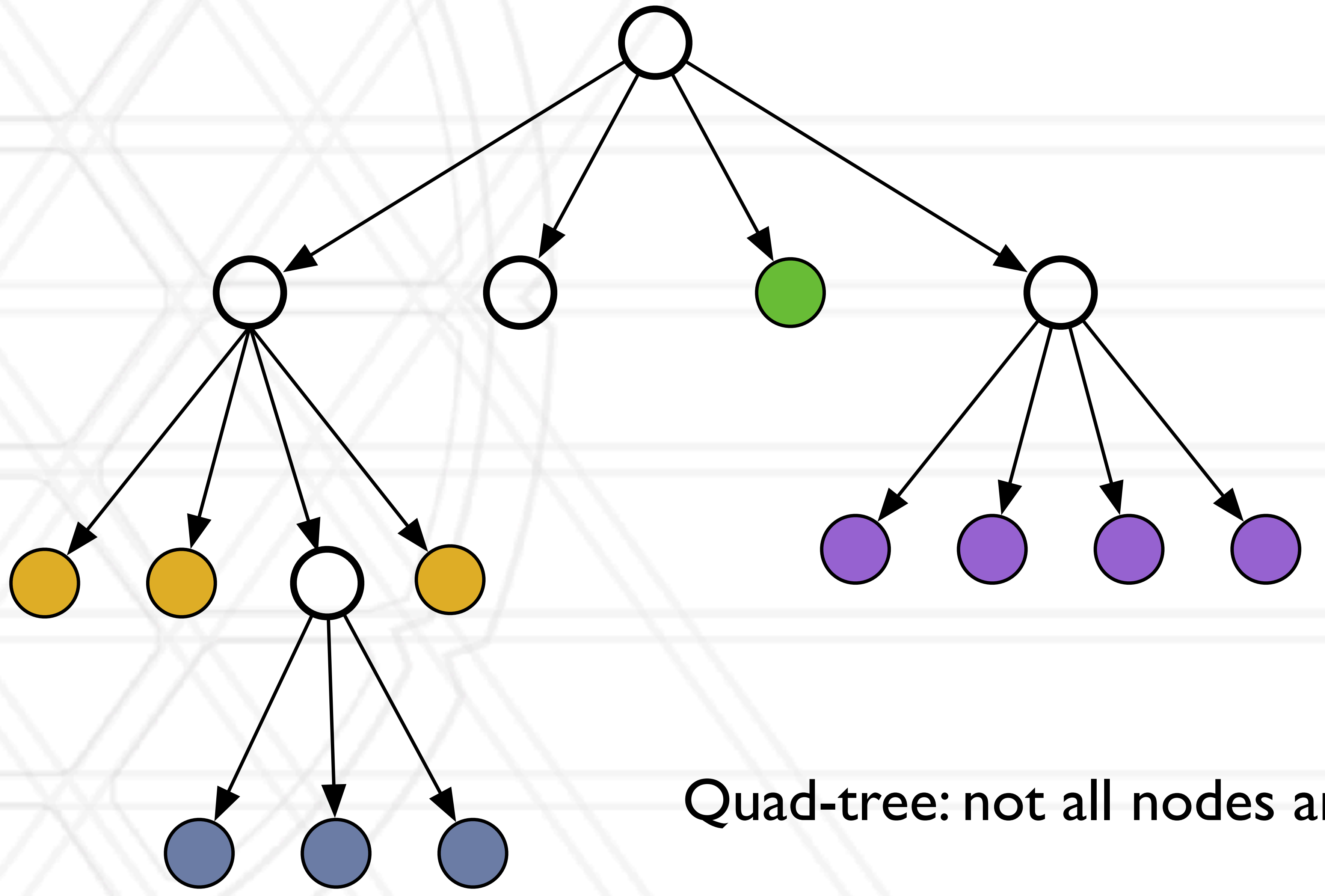

Quad-tree: not all nodes are shown

Load balance and grain size

- Load balance: try to balance the amount of work (computation) assigned to different threads/ processes
  - Bring ratio of maximum to average load as close to 1 as possible
  - Secondary consideration: also load balance amount of communication
- Grain size: ratio of computation-to-communication
  - Coarse-grained (more computation) vs. fine-grained (more communication)

Questions?

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