High Performance Computing Systems (CMSC714)

Lecture 22: The *n*-body Problem

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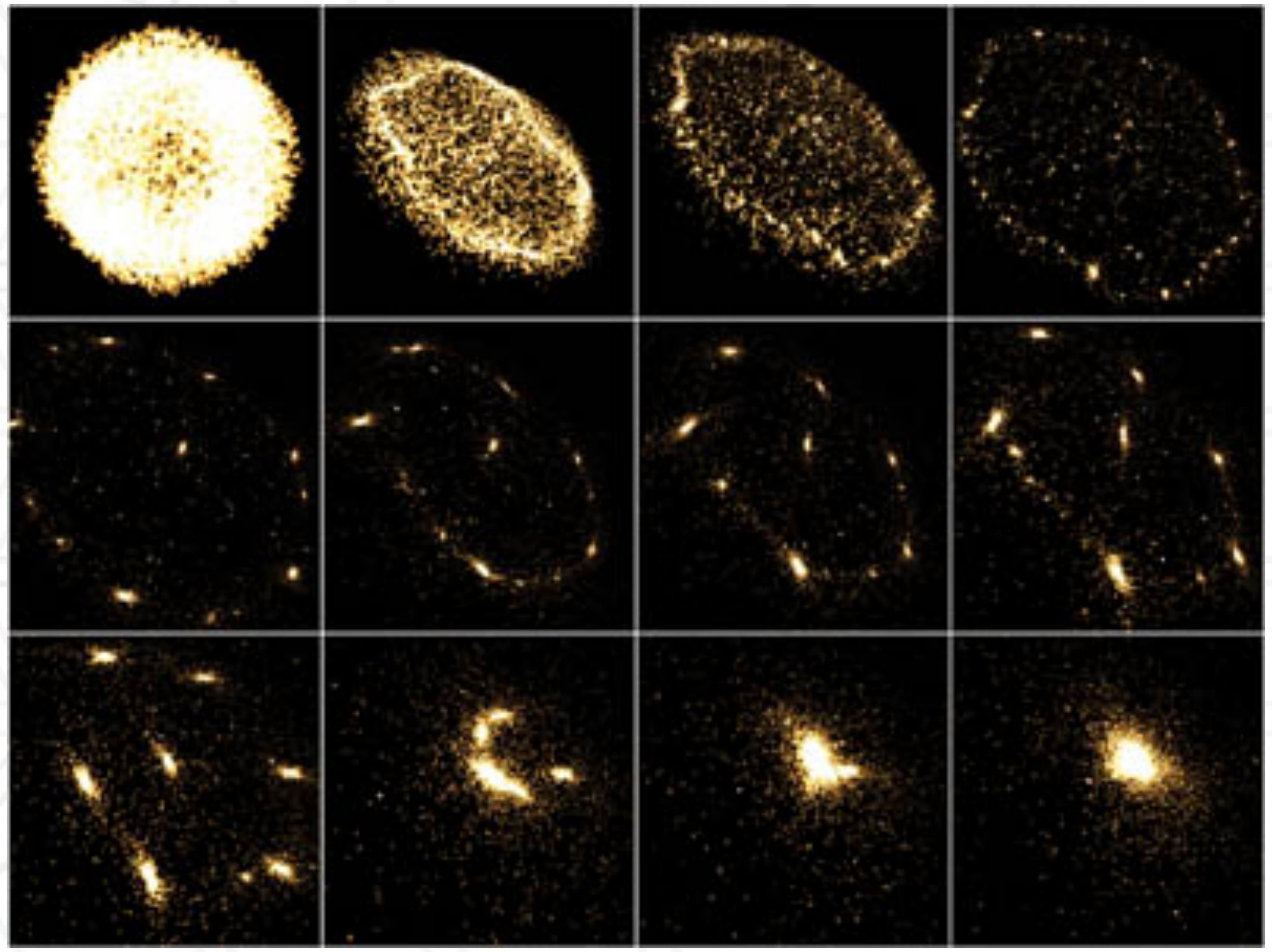
Summary of last lecture

- Molecular dynamics: calculate trajectories of atoms
- Parallelization strategies
  - Atom decomposition
  - Force decomposition
  - Spatial decomposition
  - Hybrid spatial-force decomposition
- Simulation codes: NAMD, Gromacs, Amber, Blue Matter, Desmond

The *n*-body problem

- Simulate the motion of celestial objects interacting with one another due to gravitational forces
- Naive algorithm: $O(n^2)$
  - Every body calculates forces pair-wise with every other body (particle)



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

Data distribution in *n*-body problems

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

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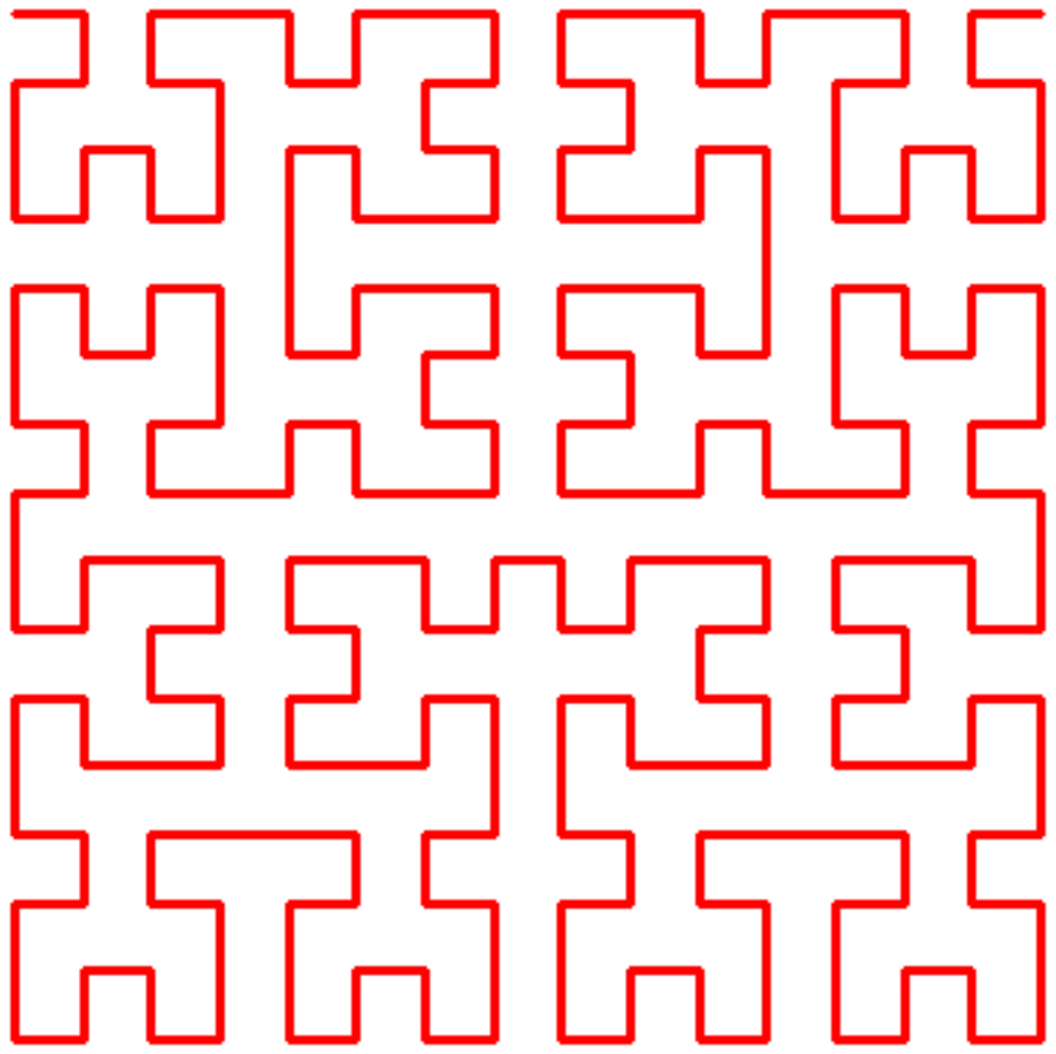

Space-filling curves

http://datagenetics.com/blog/march22013/

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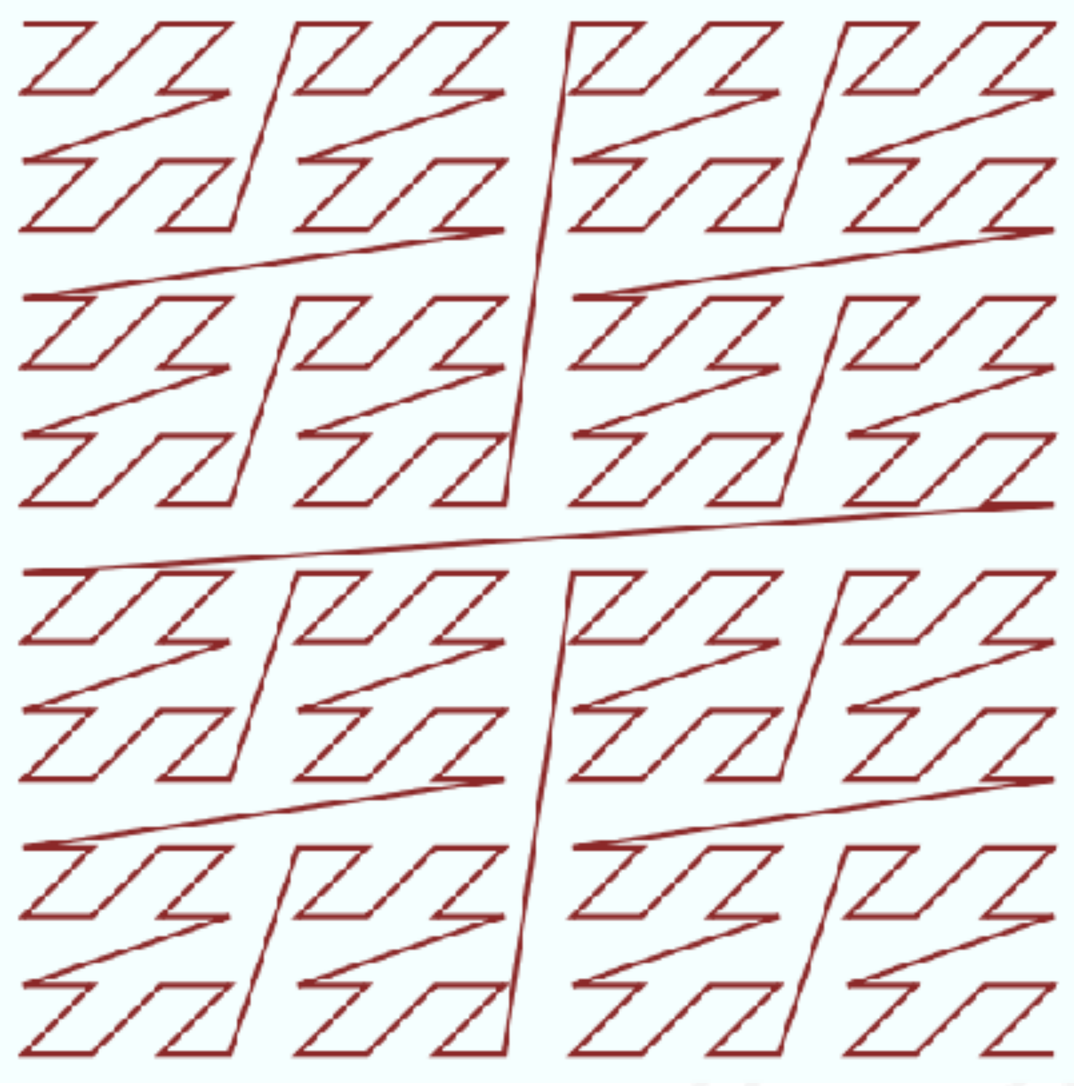

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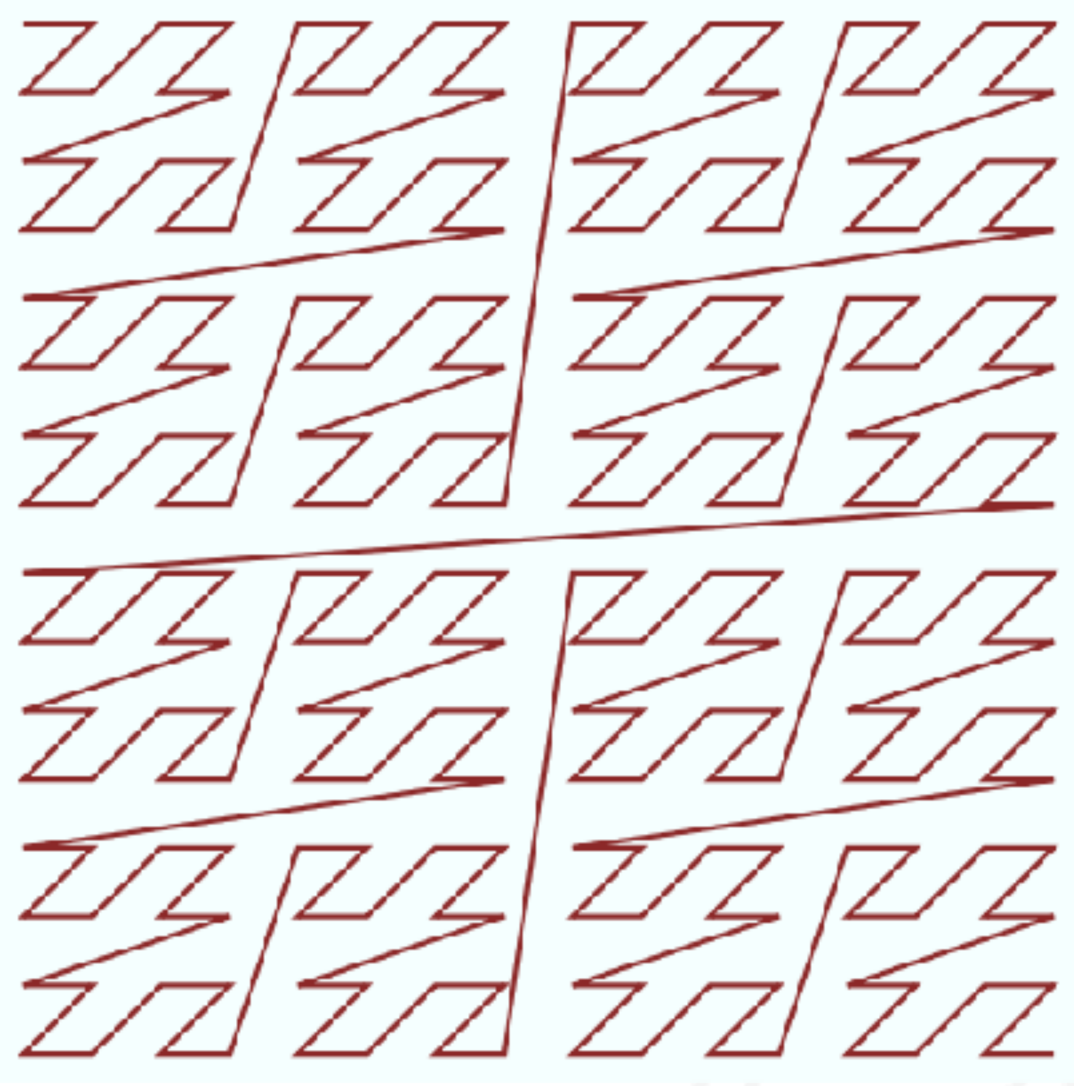

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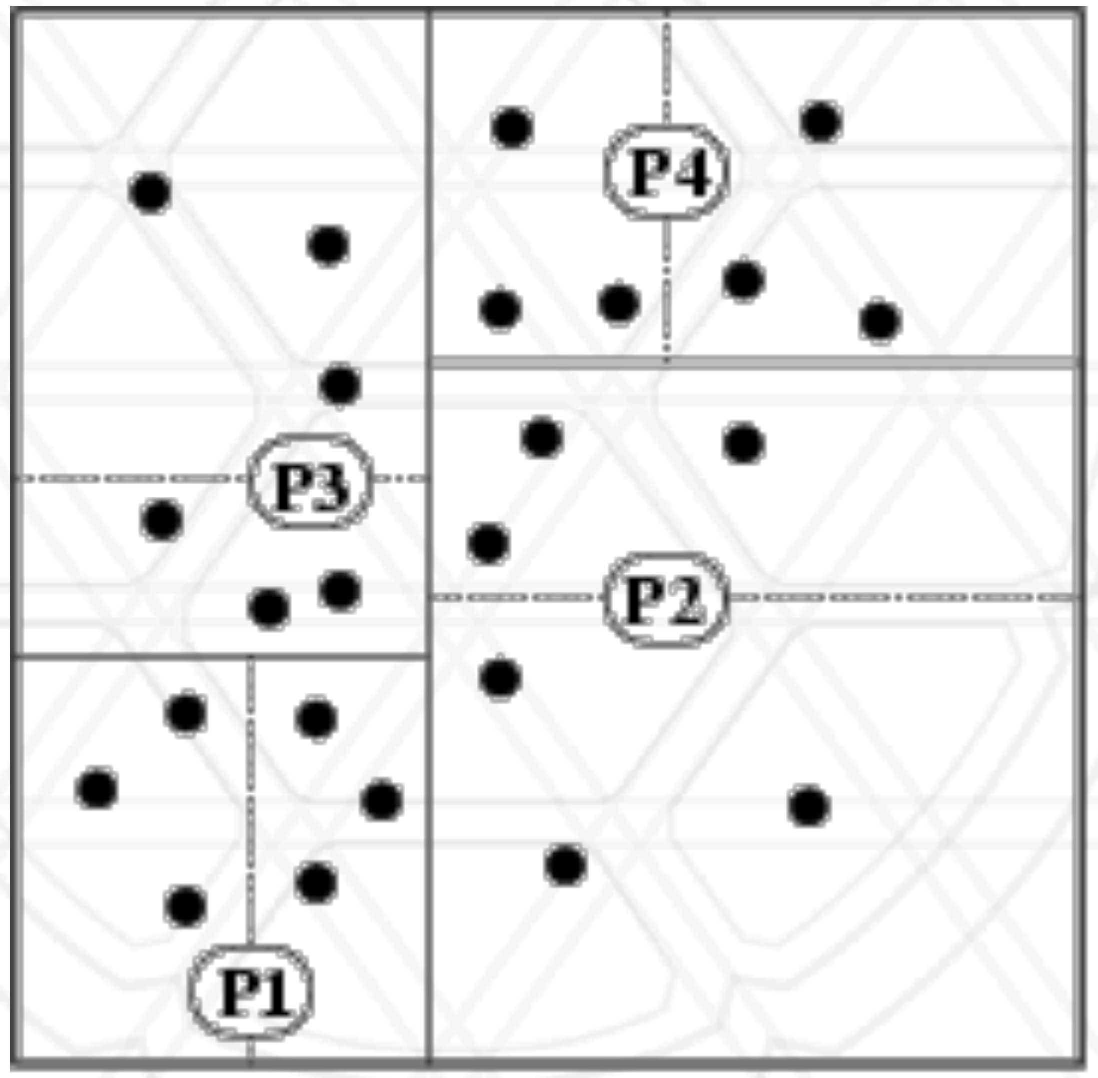
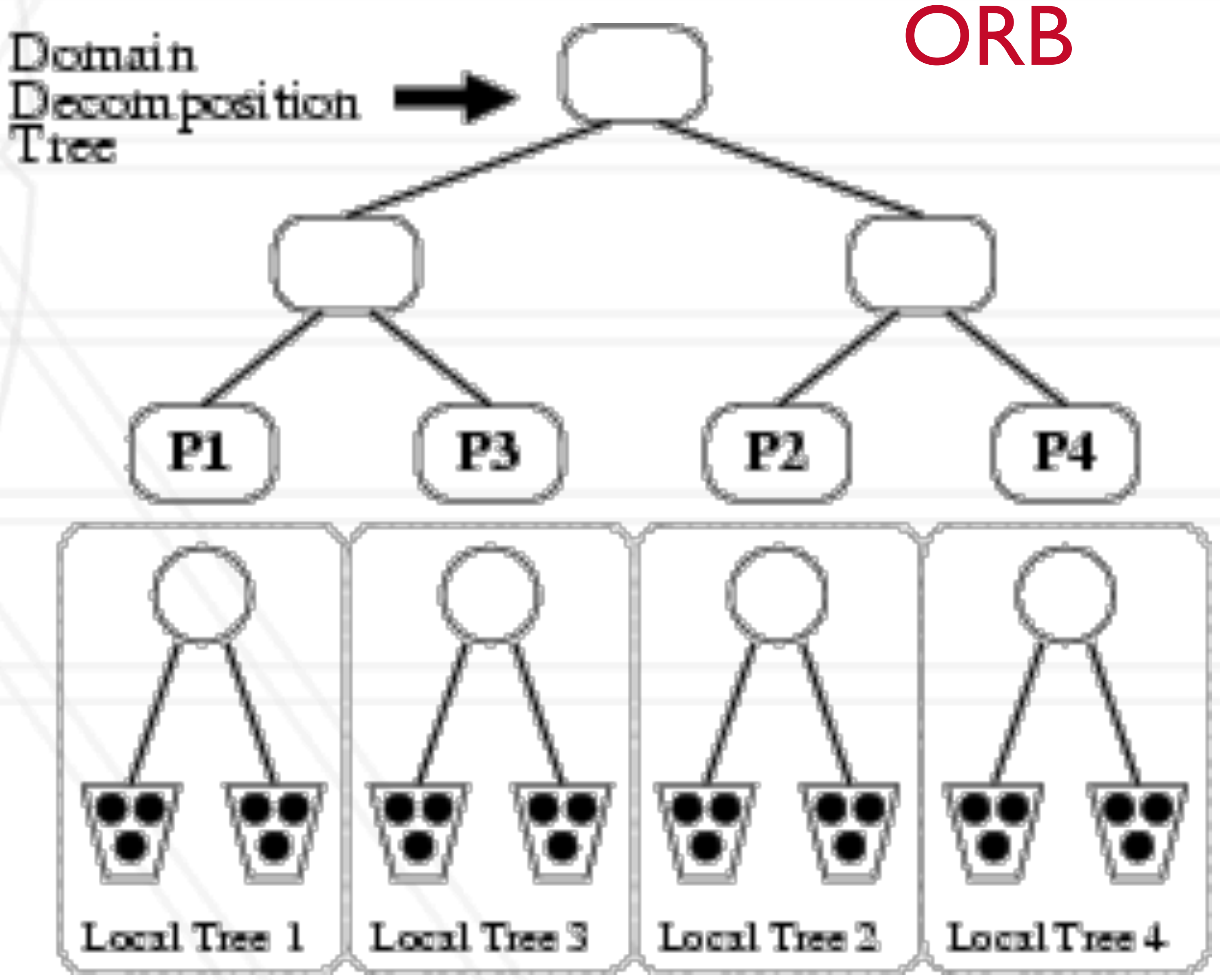


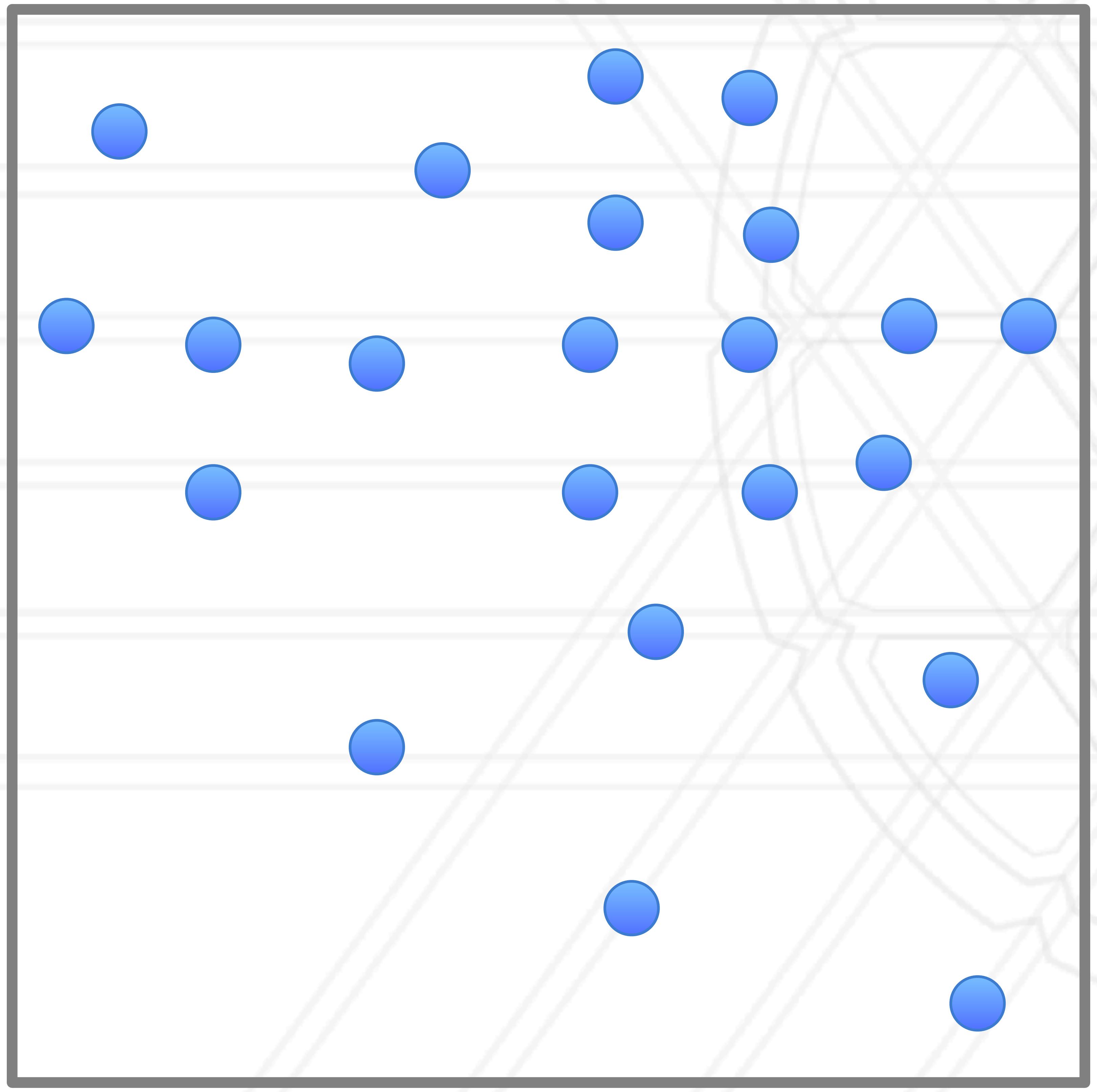


ORB

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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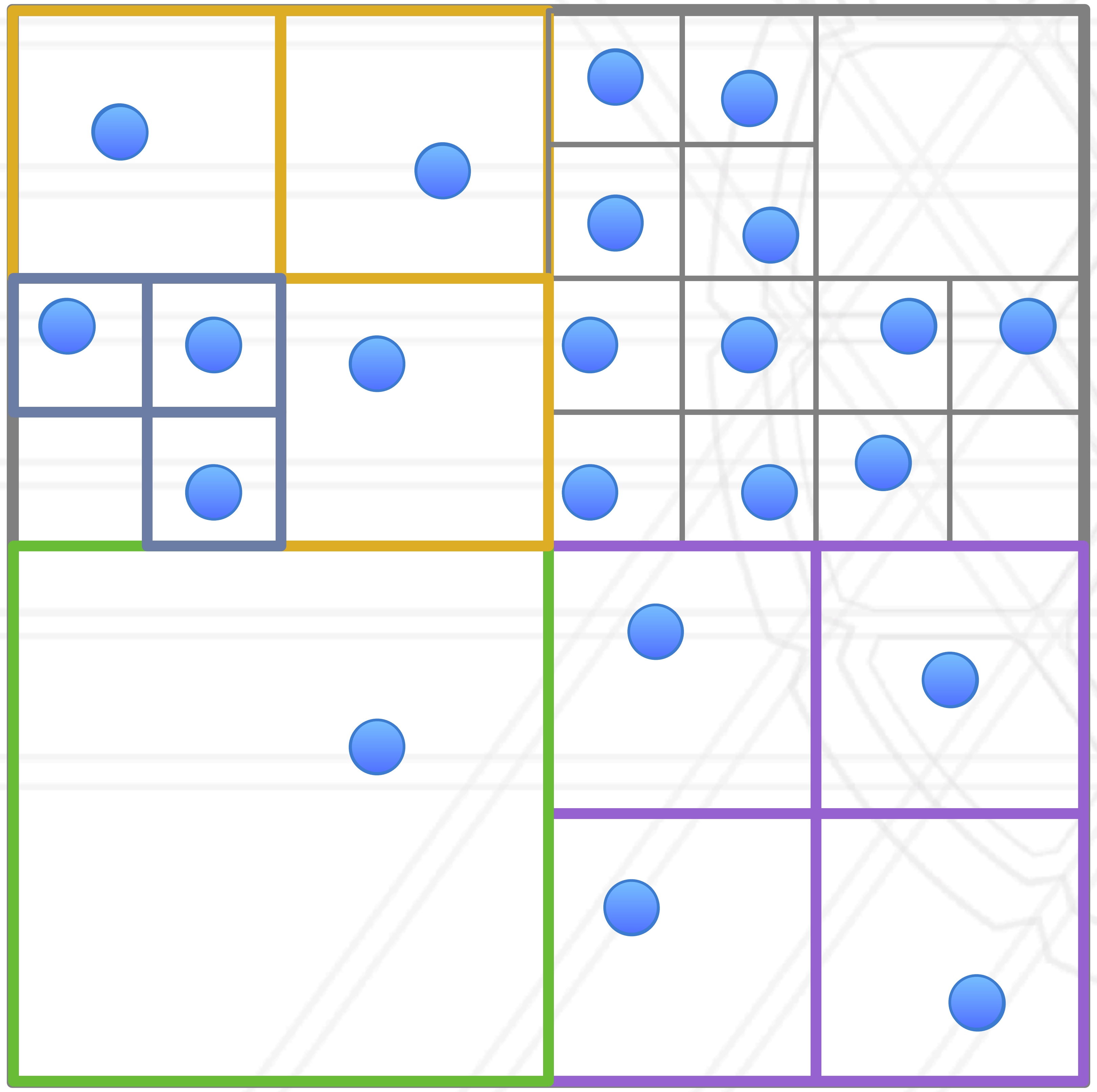

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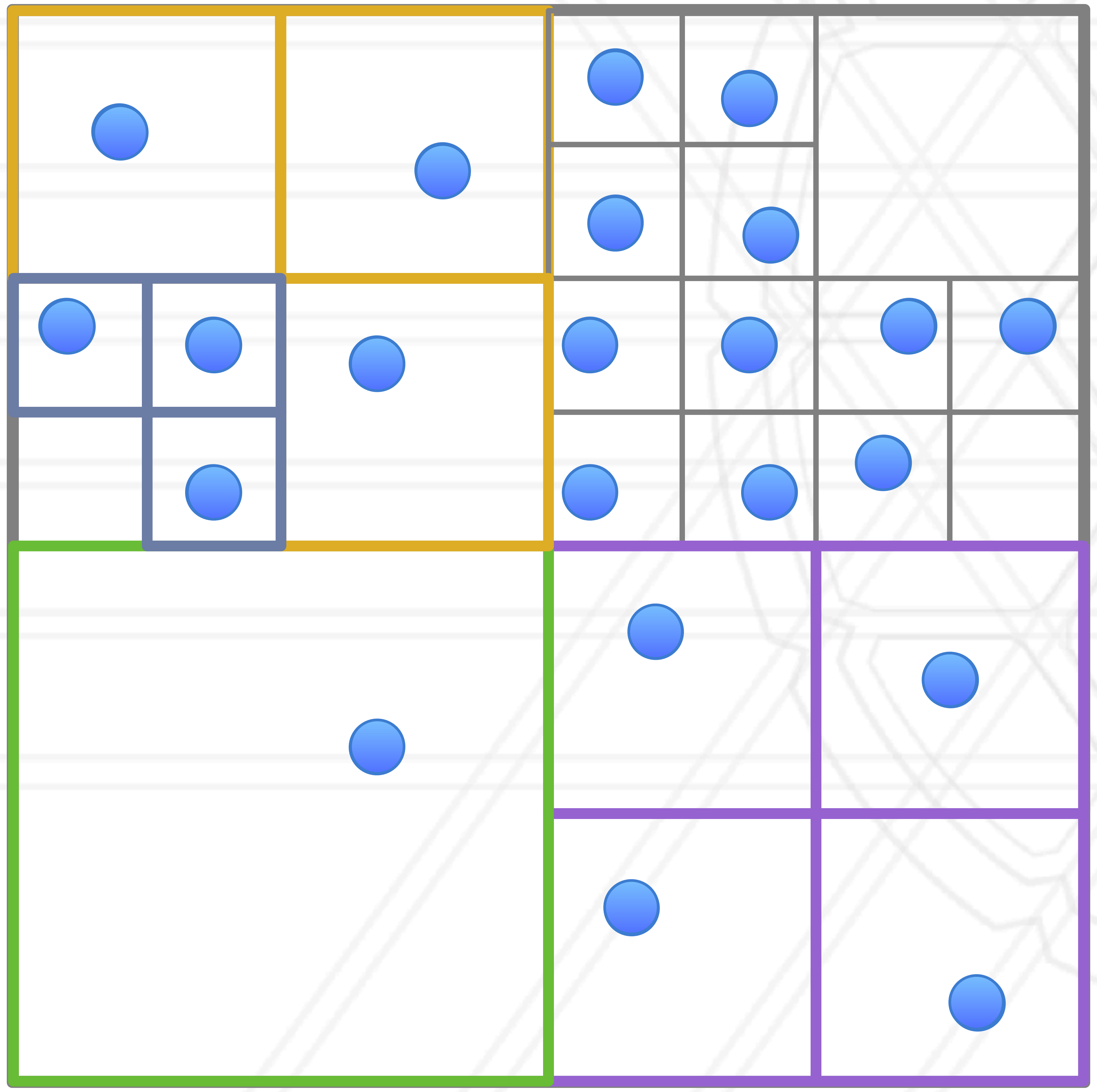
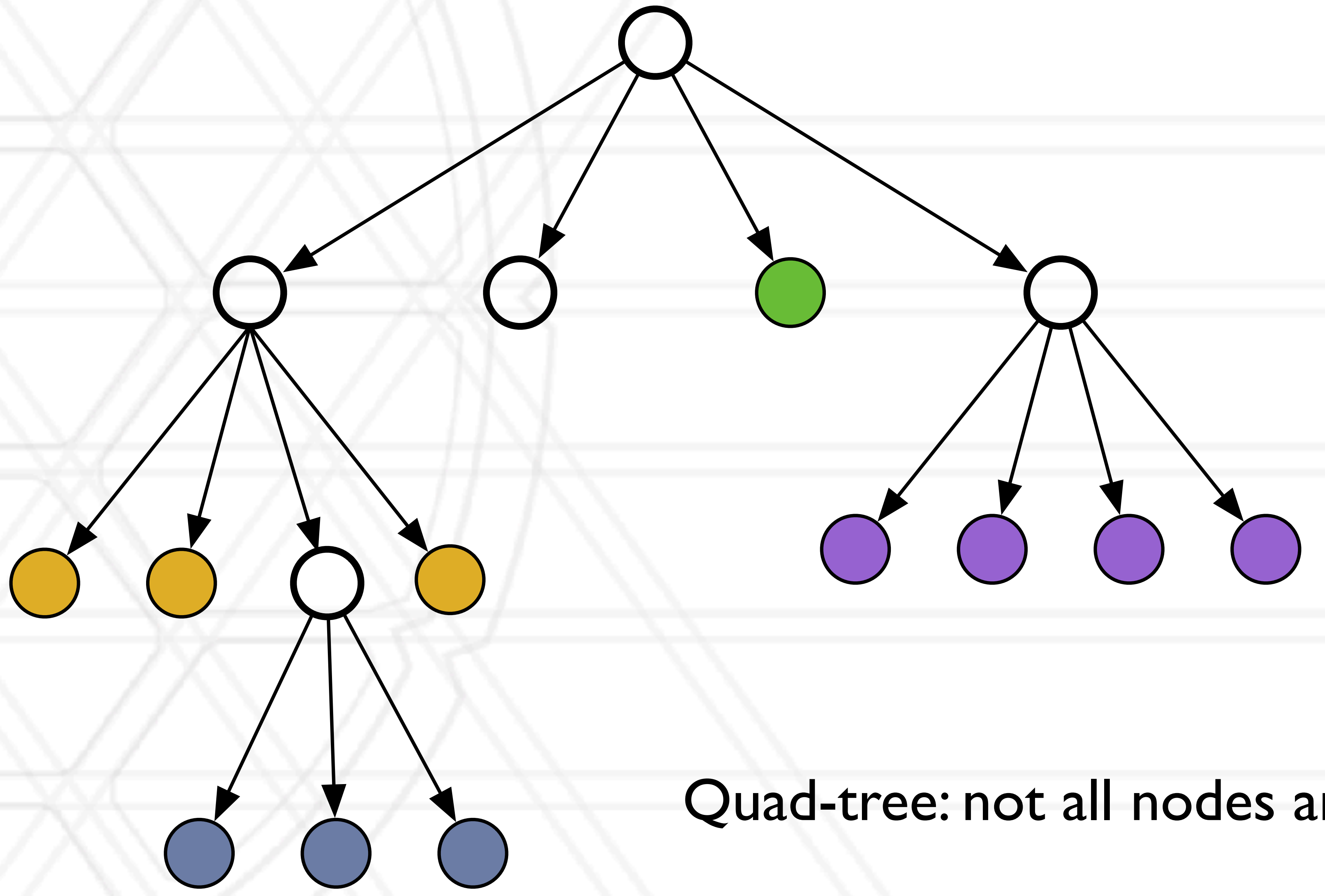




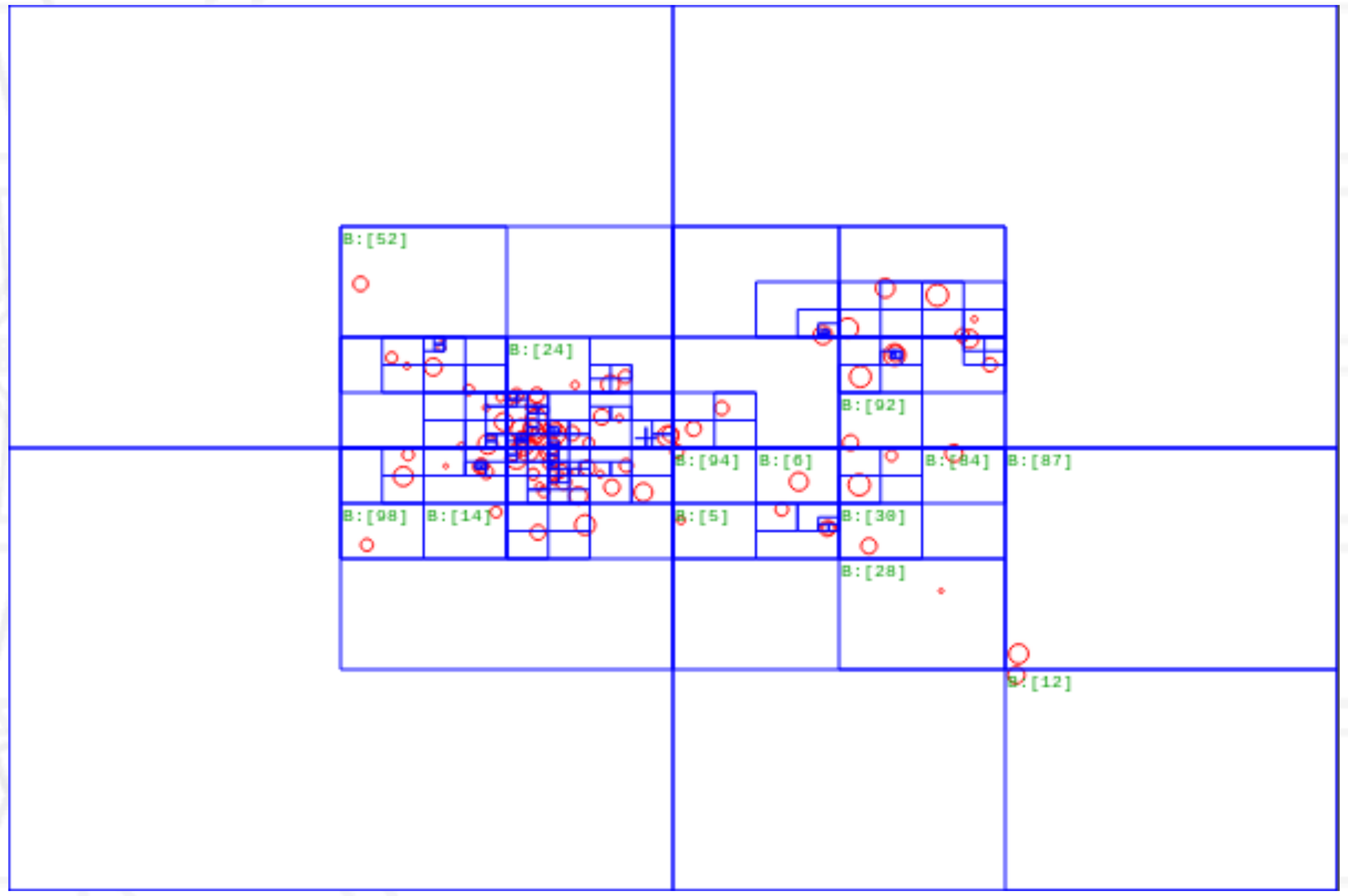
Quad-tree: not all nodes are shown

Different parallelization methods

- Tree codes: Barnes-Hut simulations
- Fast multiple methods (FMM): Greengard and Rokhlin
- Particle mesh methods
- Particle-particle particle-mesh (P^3M) methods

Barnes-Hut simulation

- Represent the space containing the particles as an oct-tree
- Pairwise force calculations for nearby particles
- For tree nodes that are sufficiently far away, approximate the particles in the node by a single large particle at the center of mass



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Fast multipole methods

- Use multipole expansion for distant particles
- Takes advantage of the fact that for nearby particles, multipole-expanded forces from distant particles are similar
- Reduces the time complexity further to O(n)

Particle-particle particle-mesh methods

- Explicit calculation of forces on nearby particles
- Fourier-based Ewald summation for calculating potentials on a grid
- Smoothed particle hydrodynamics

Questions?

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