Parallel CSE Applications

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Announcements

- Quiz 3 has been posted

Contact me

- CMSC416: If you are an undergrad interested in participating in International Student Cluster Competitions
- bhatele@cs.umd.edu

Molecular Dynamics

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- Calculate trajectories of atoms and molecules by solving Newton's equations of motions

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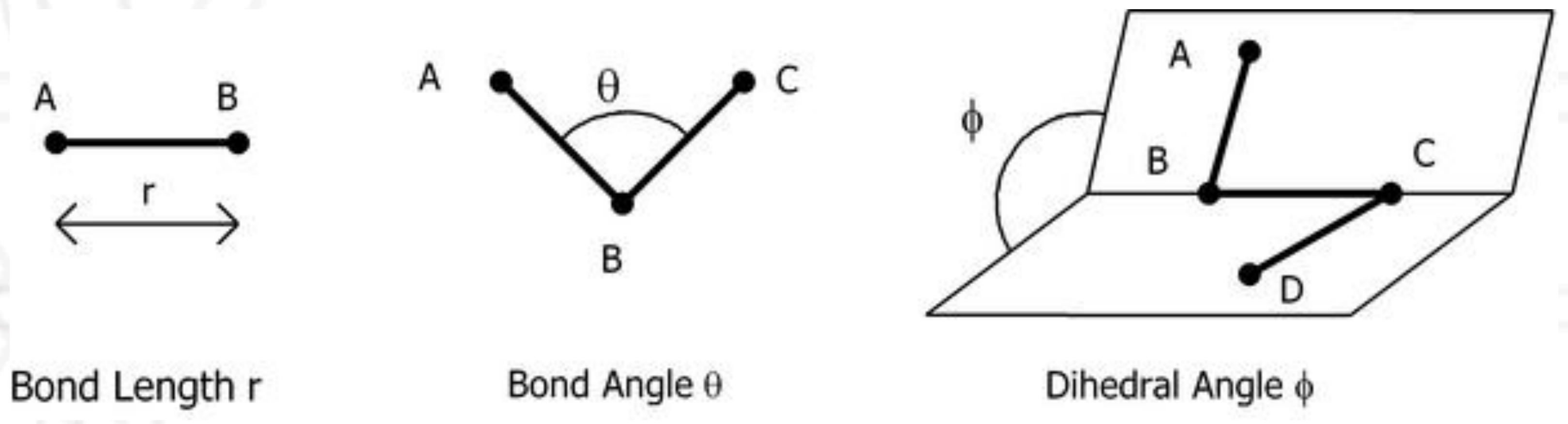
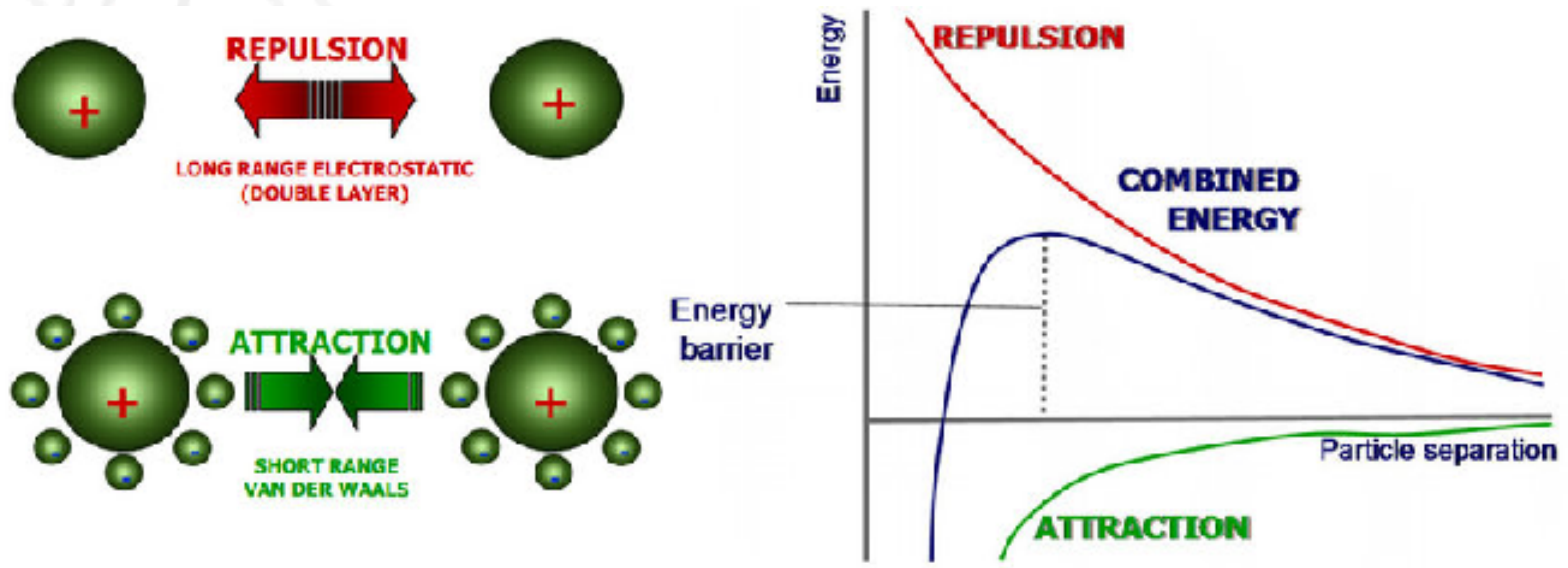
- Force calculations

  - Bonded interactions: bonds, angles, dihedrals

  - Non-bonded interactions: van der Waal's and electrostatic forces





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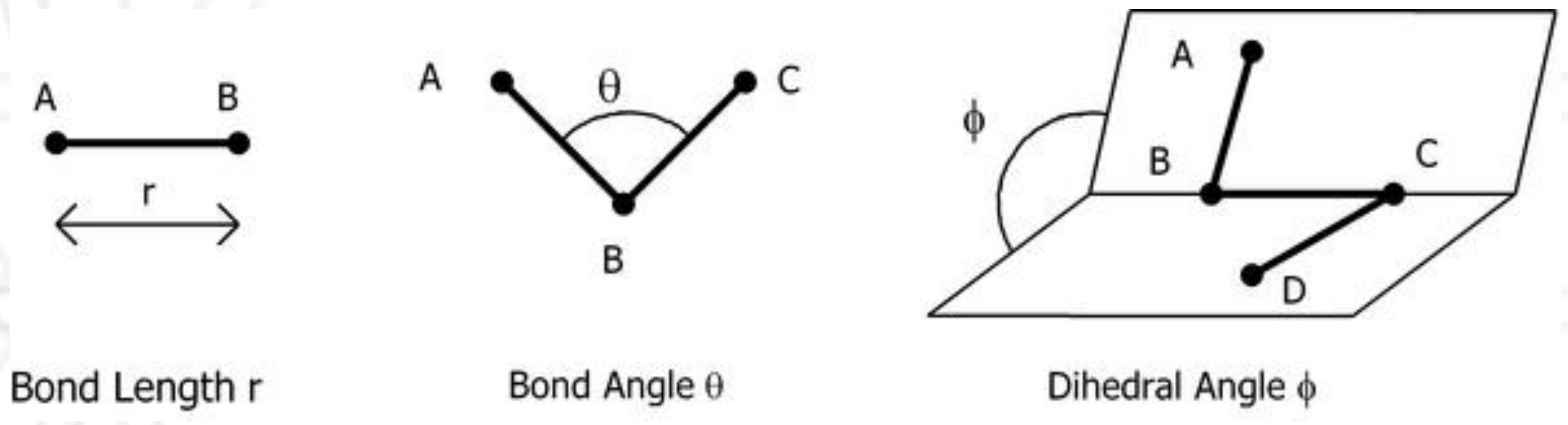

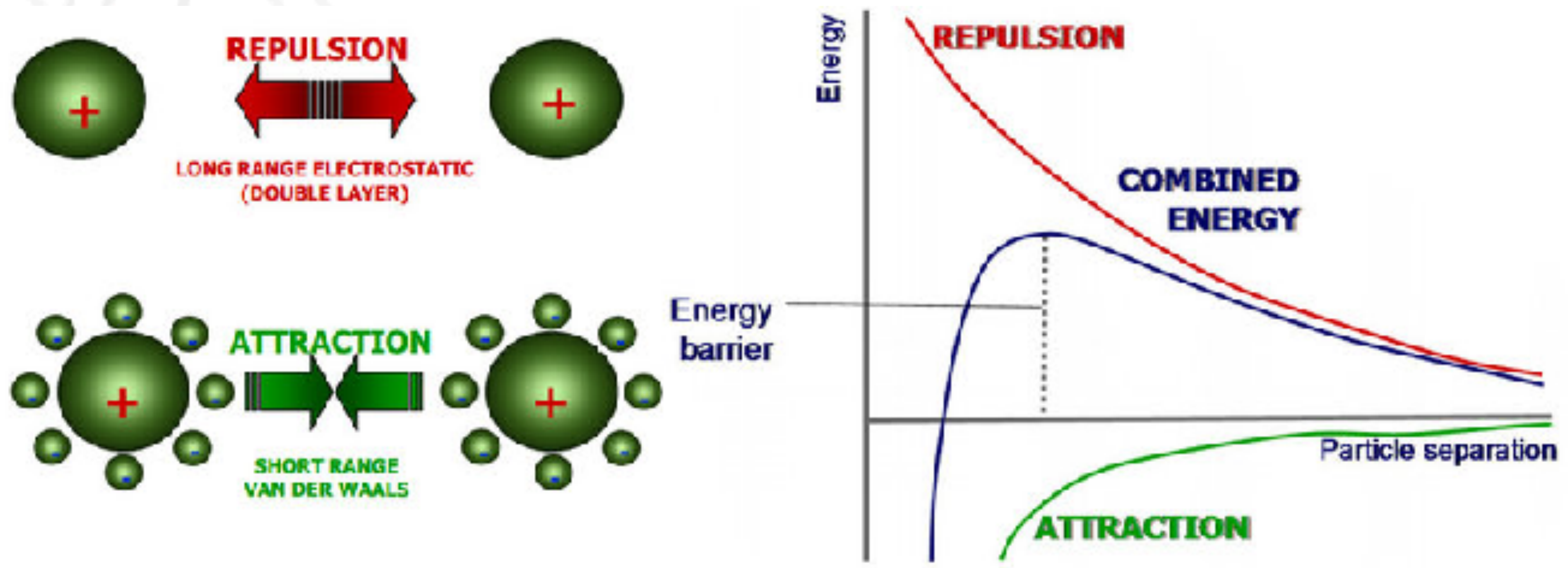

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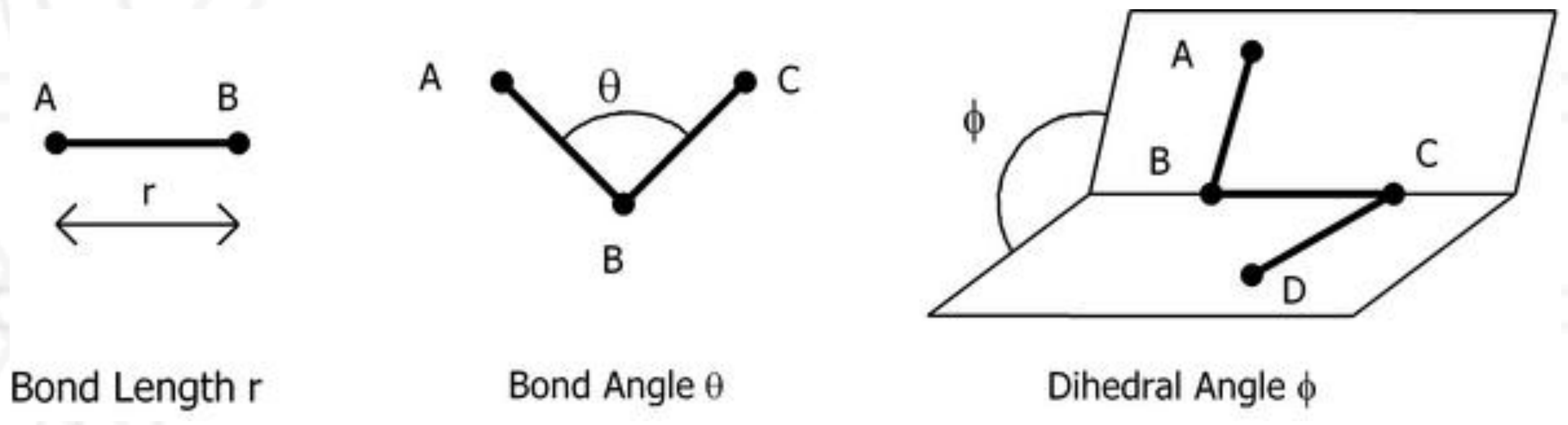

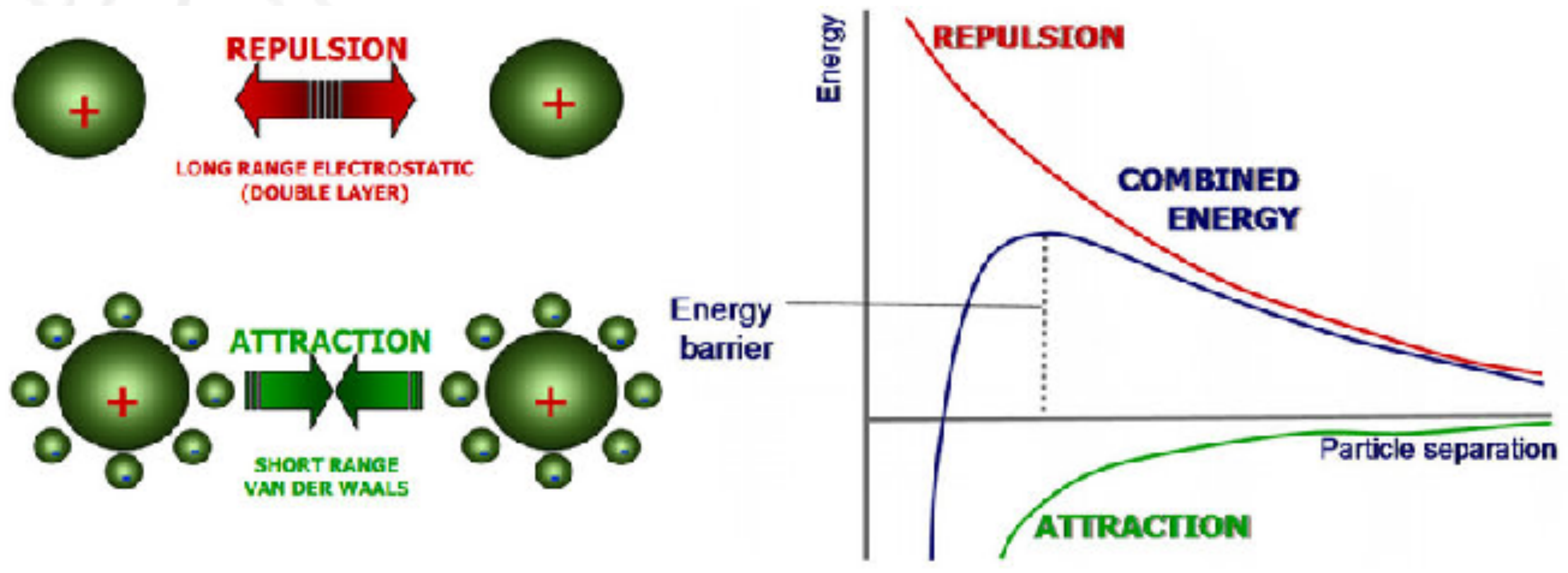

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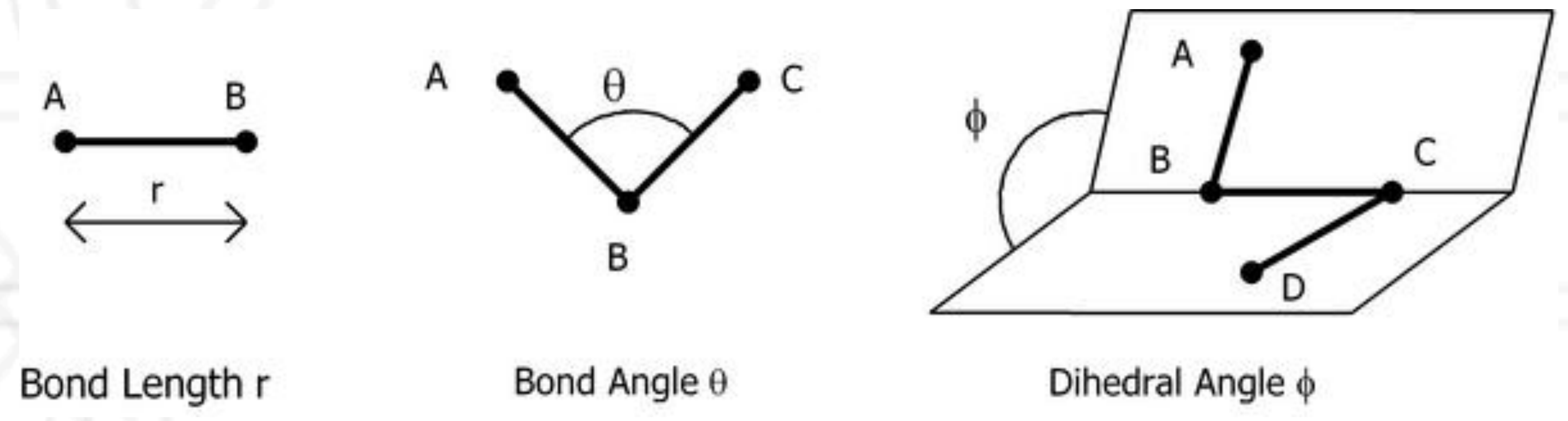
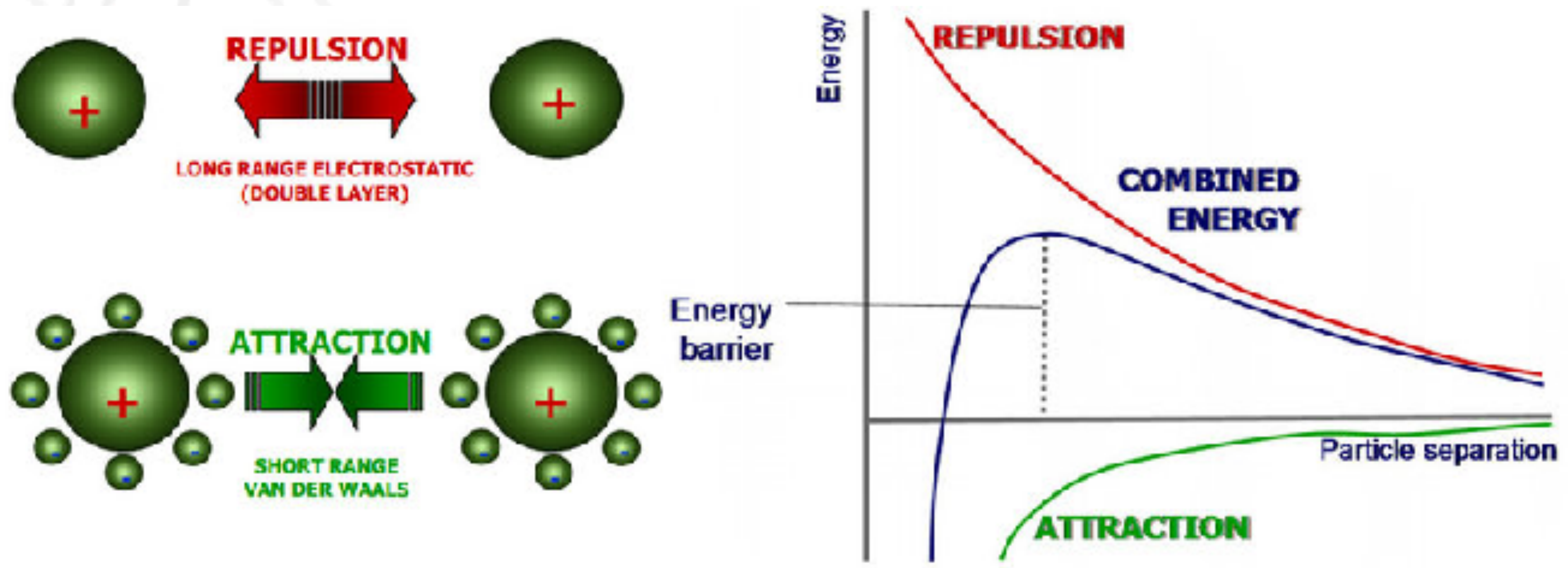
- Used for drug design, materials design





Sequential Algorithm

- At every step, calculate forces on each atom
  - Calculate bonded and short-range forces every step
  - Calculate long-range non-bonded forces every few time steps (using PME or P3M etc.)
- Particle mesh Ewald (PME) summation:
  - Calculate long-range interactions in Fourier space
- Calculate velocities and new positions
- Repeat …

Traditional approaches to parallelization

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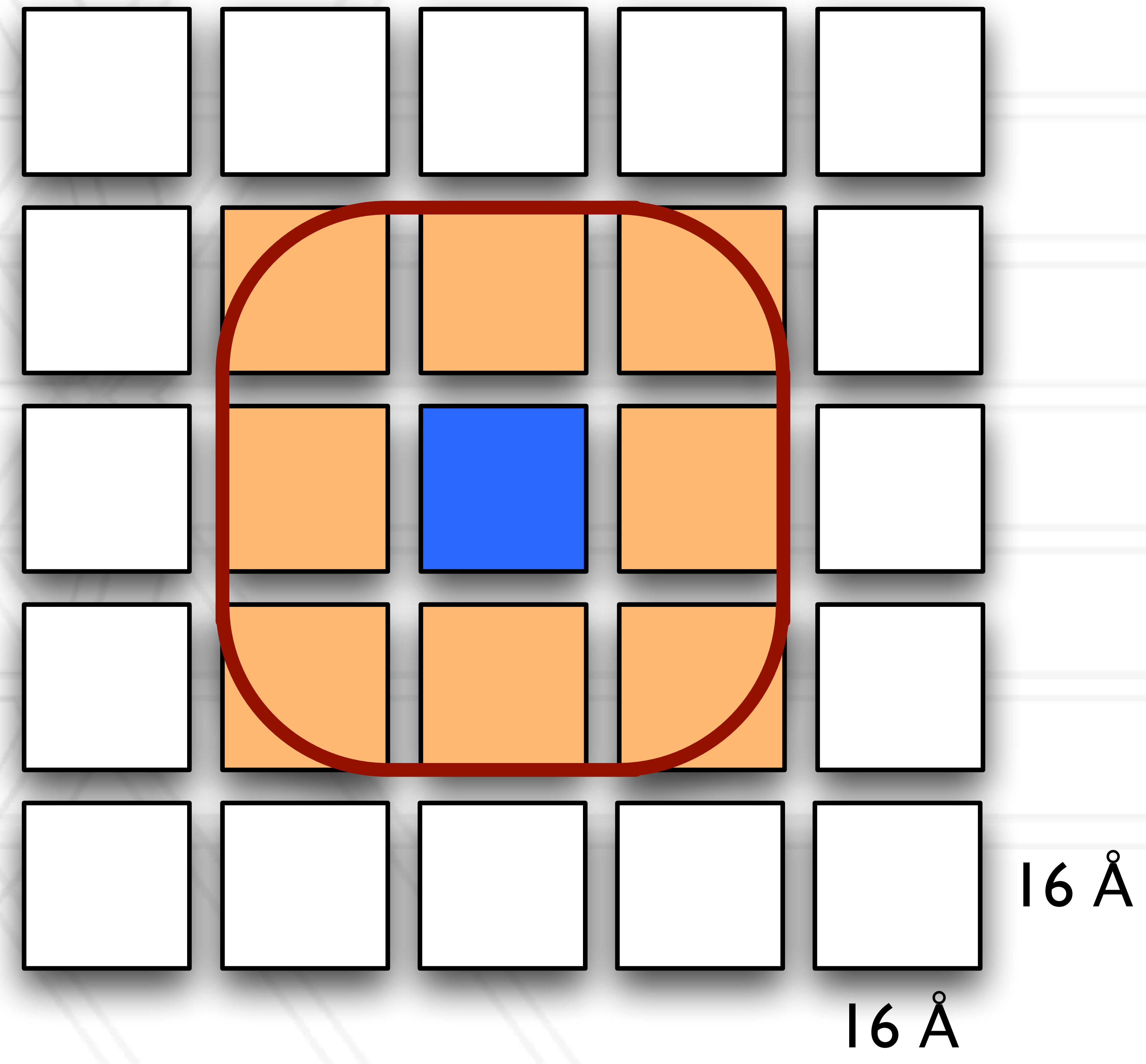
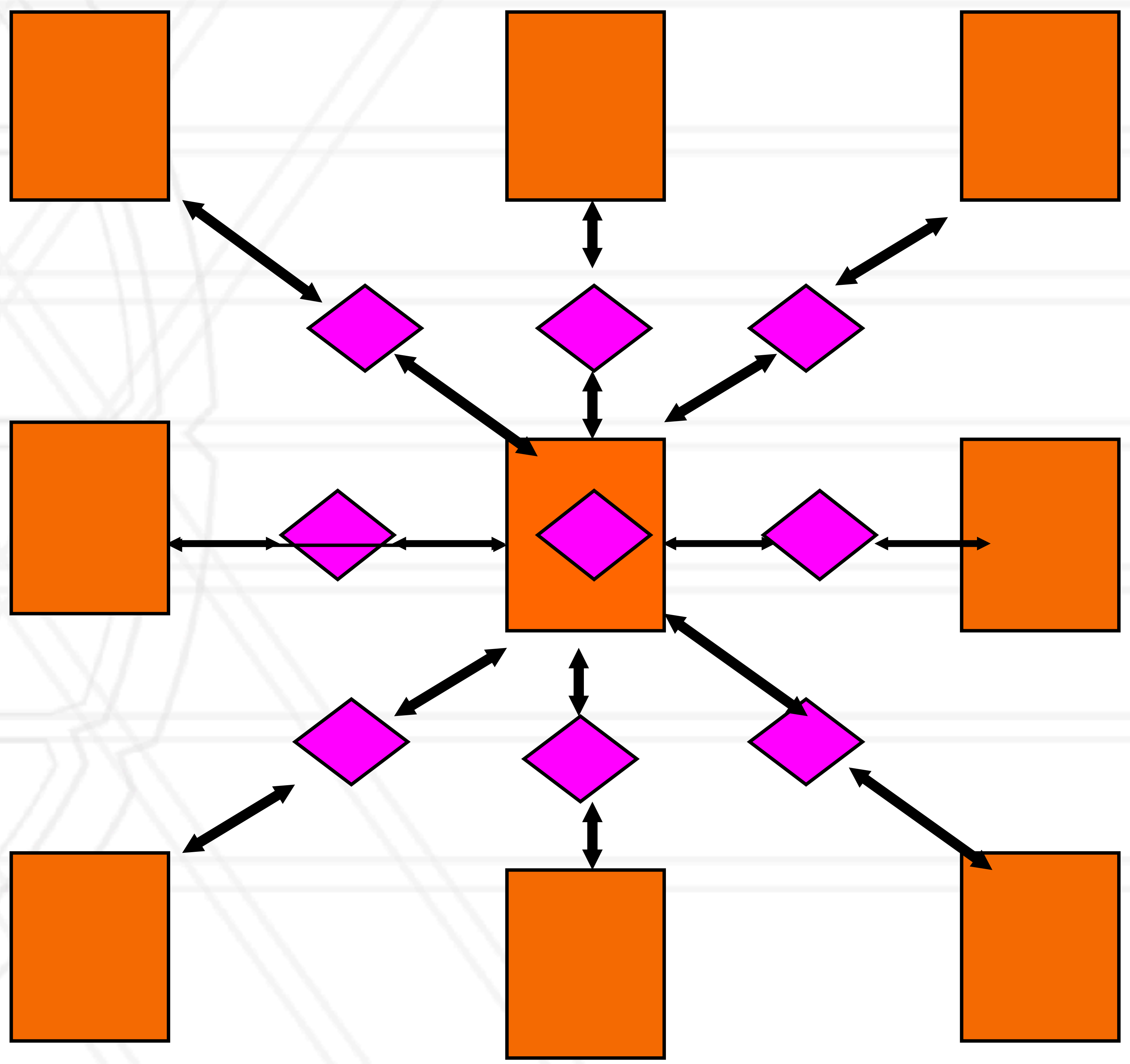
- Atom decomposition:
  - Partition the atoms across processes
- Force decomposition:
  - Distribute the force matrix to processes
  - Matrix is sparse and non-uniform
- Spatial decomposition:
  - Assign a region of the 3D simulation space to each process



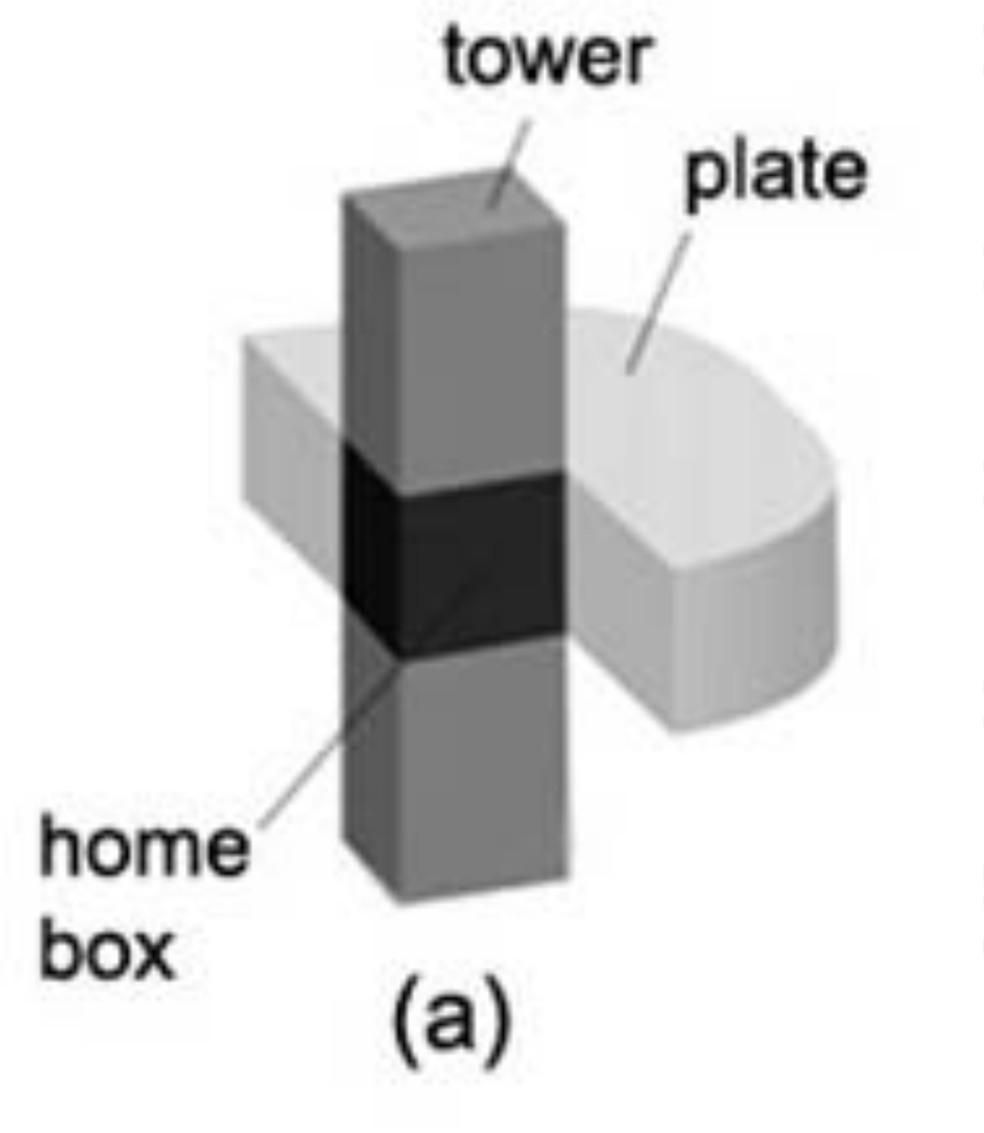
Hybrid parallelization

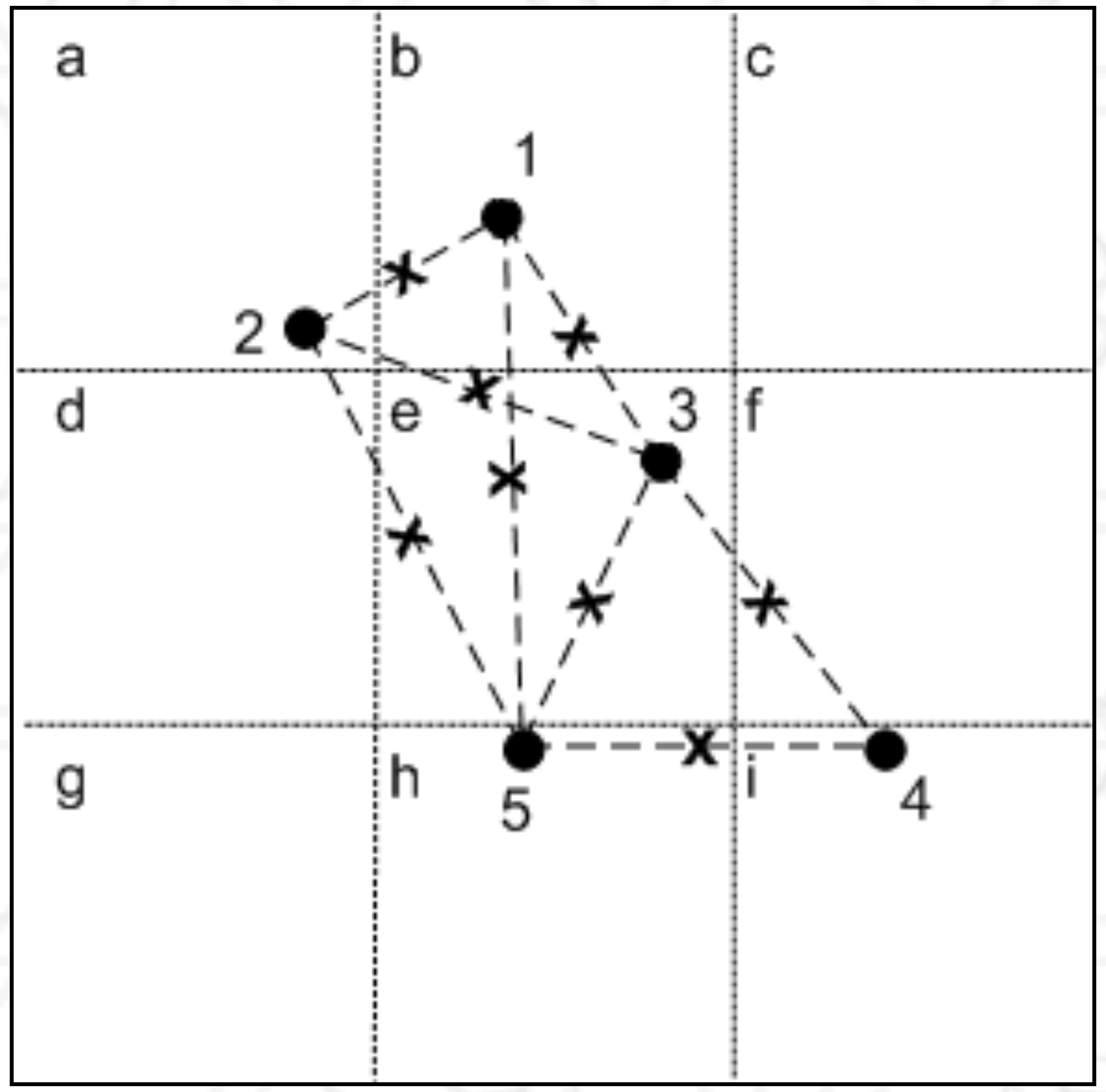
- Hybrid of spatial and force decomposition
- Decouple assignment of data and work to processes
- Distribute both atoms and the force calculations to different processes



Neutral territory (NT) methods

- Desmond's mid-point method





SC23 Test-of-time award:

Shaw DE, RO Dror, JK Salmon, et al. 2009. "Millisecond-scale molecular dynamics simulations on Anton," In *Proceedings of the Conference on High Performance Computing Networking, Storage and Analysis* (*SC09*), Portland, OR, USA, pp. 1-11, doi: 10.1145/1654059.1654126

Particle mesh Ewald

- Replace direct force calculations by:
  - Calculate short-range forces in real space
  - Calculate long-range forces in Fourier space
- Create a 3D mesh/grid representing charge densities of atoms
  - Compute a 3D Fast Fourier Transform (FFT)
- FFT computes the discrete Fourier transform (DFT) or inverse DFT
  - Reduces the complexity from $O(N^2)$ to $O(N \log N)$

Parallelization of PME (3D FFT)

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- Bring all the data to one process

Parallelization of PME (3D FFT)

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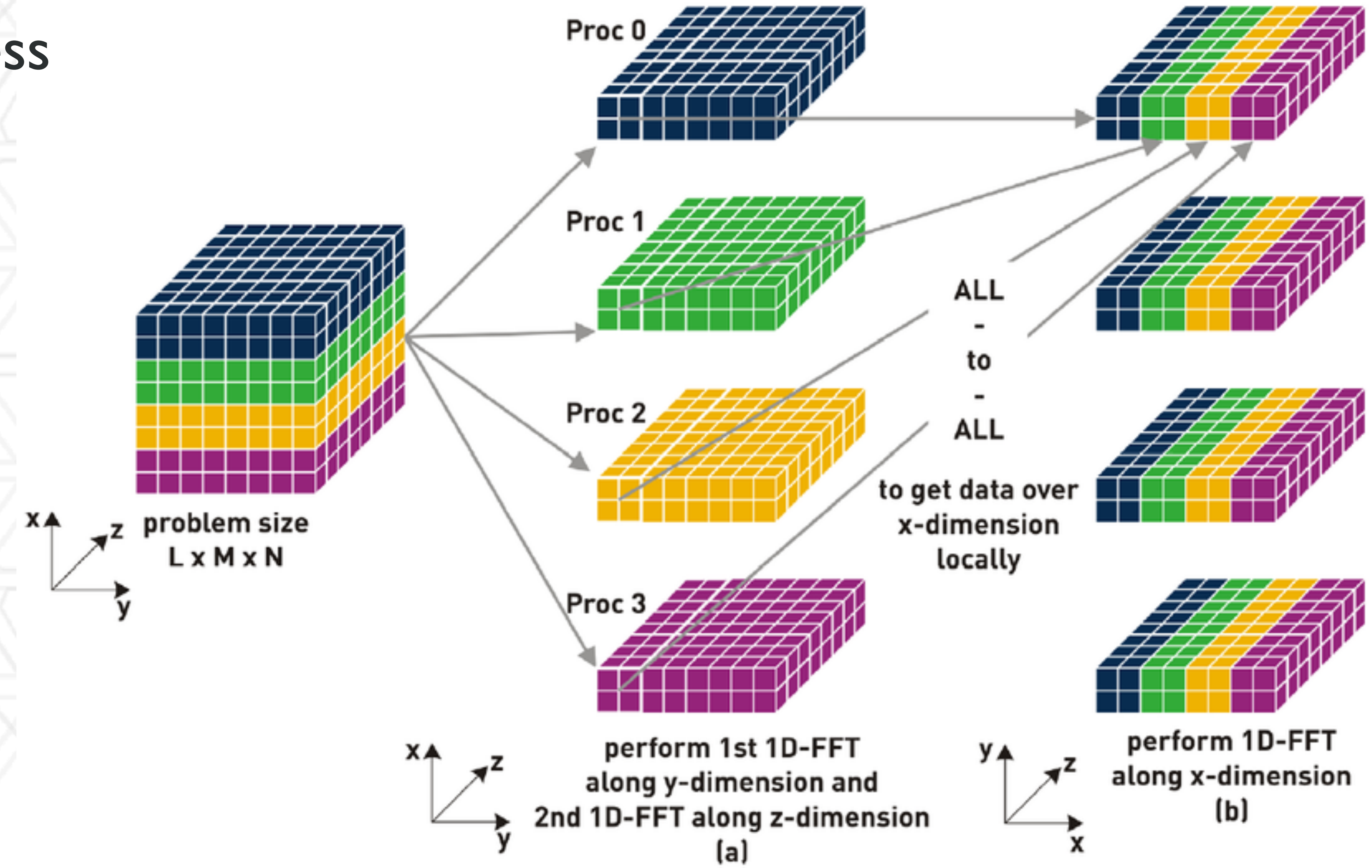
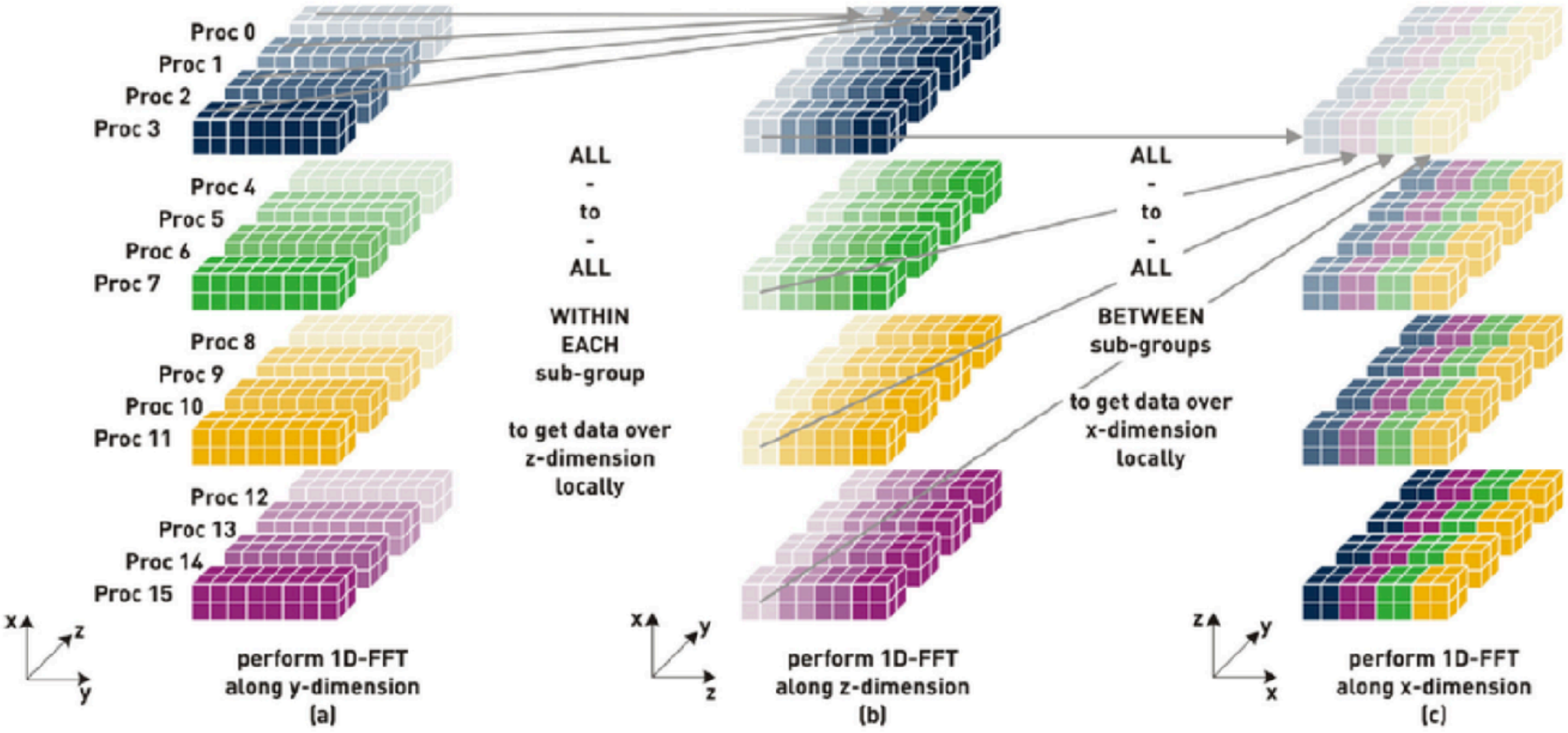
- 1D or slab decomposition

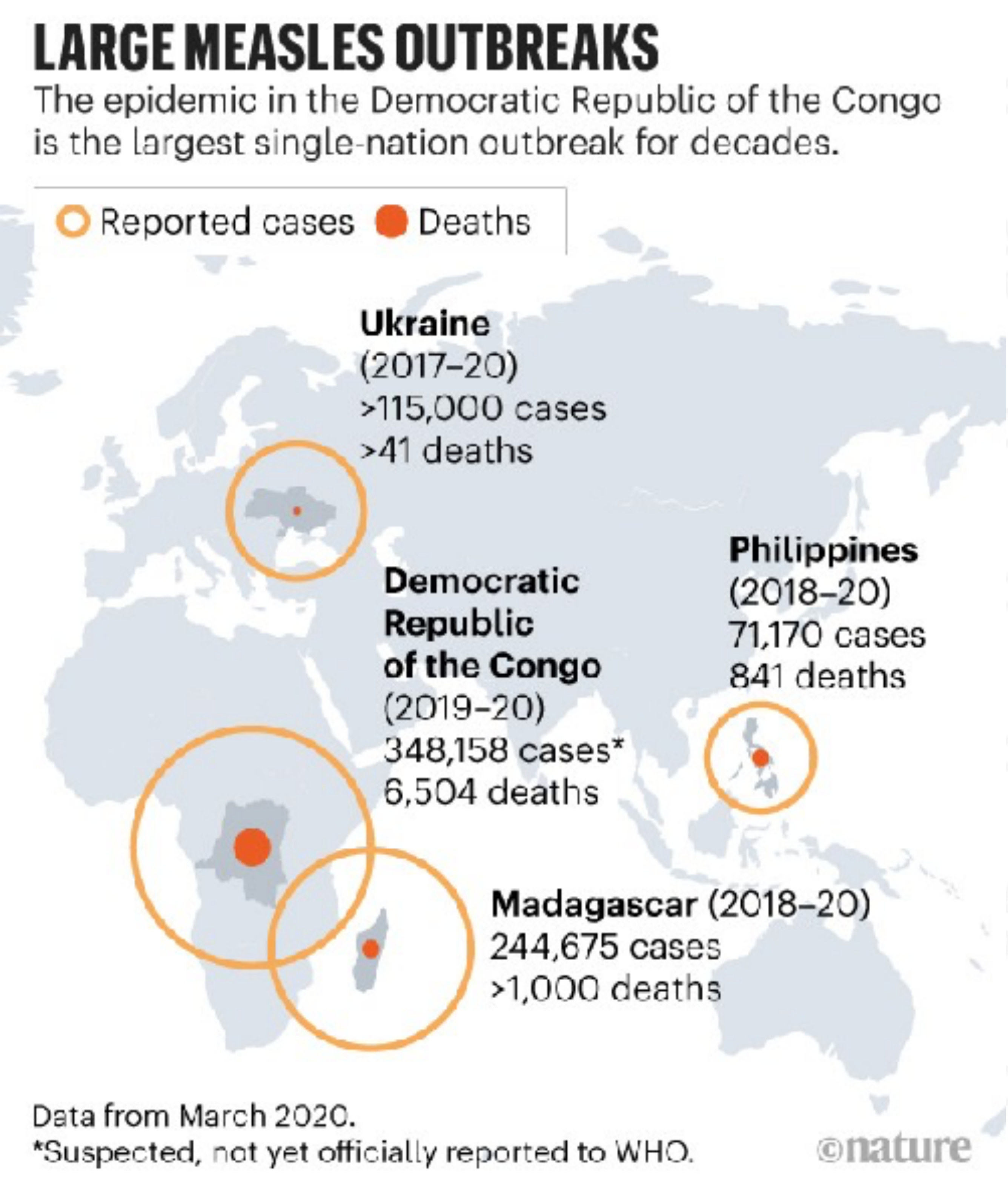


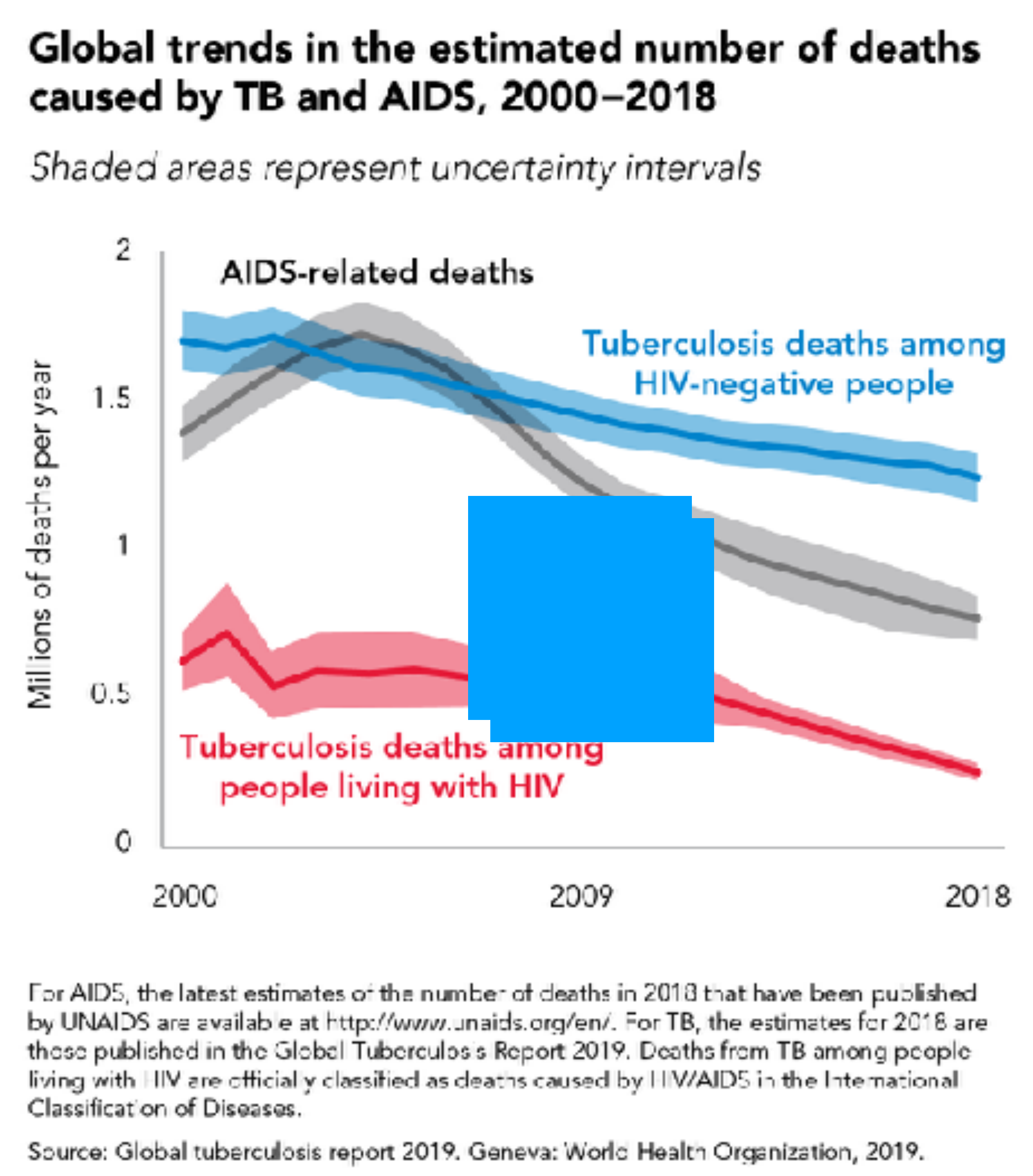
Parallelization of PME (3D FFT)

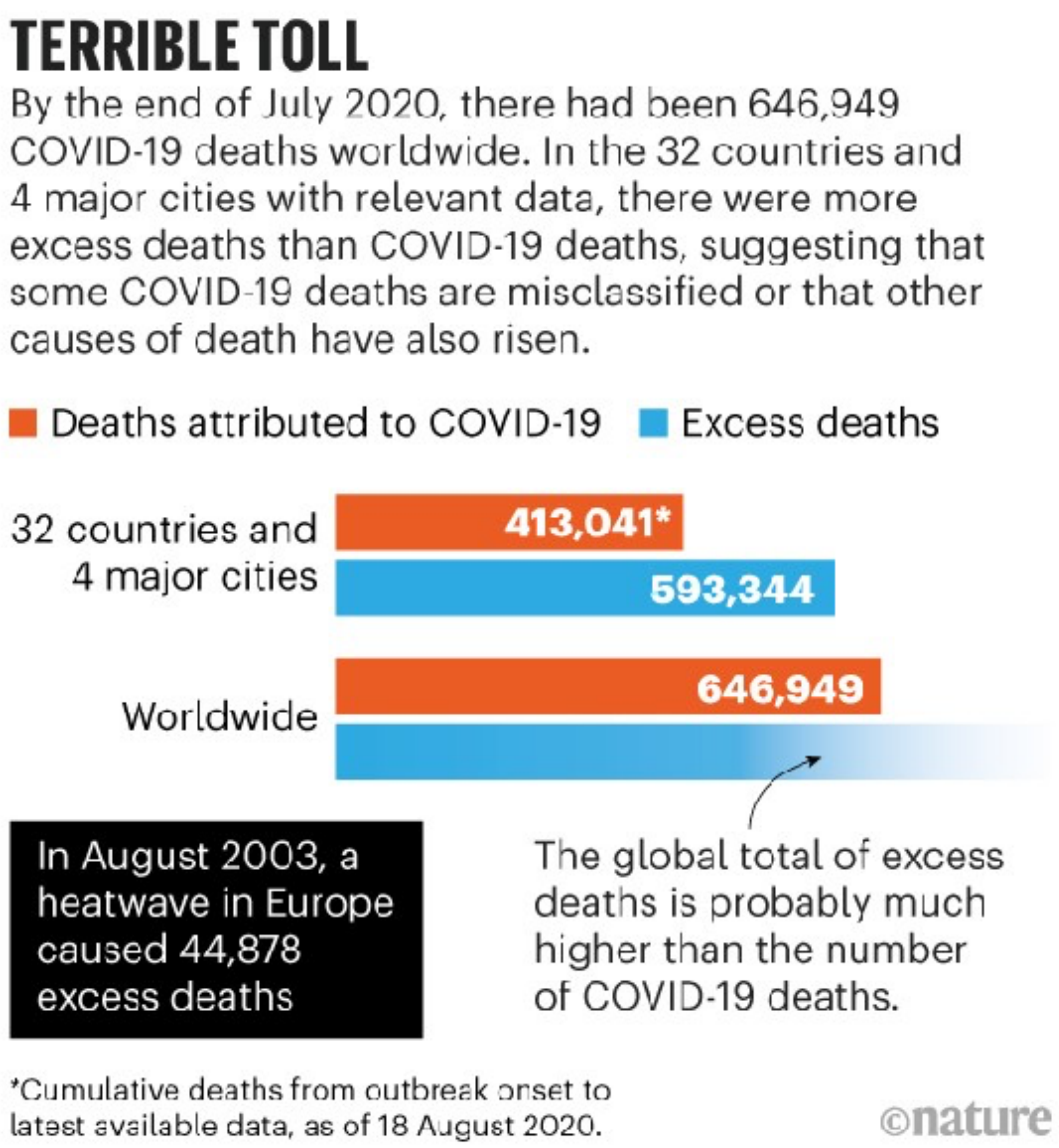
- 2D or pencil decomposition



Measles killed 200,000 in 2020 alone!







Predictions say that 1.66 million people died of tuberculosis in 2020

https://www.nature.com/articles/d41586-020-01011-6

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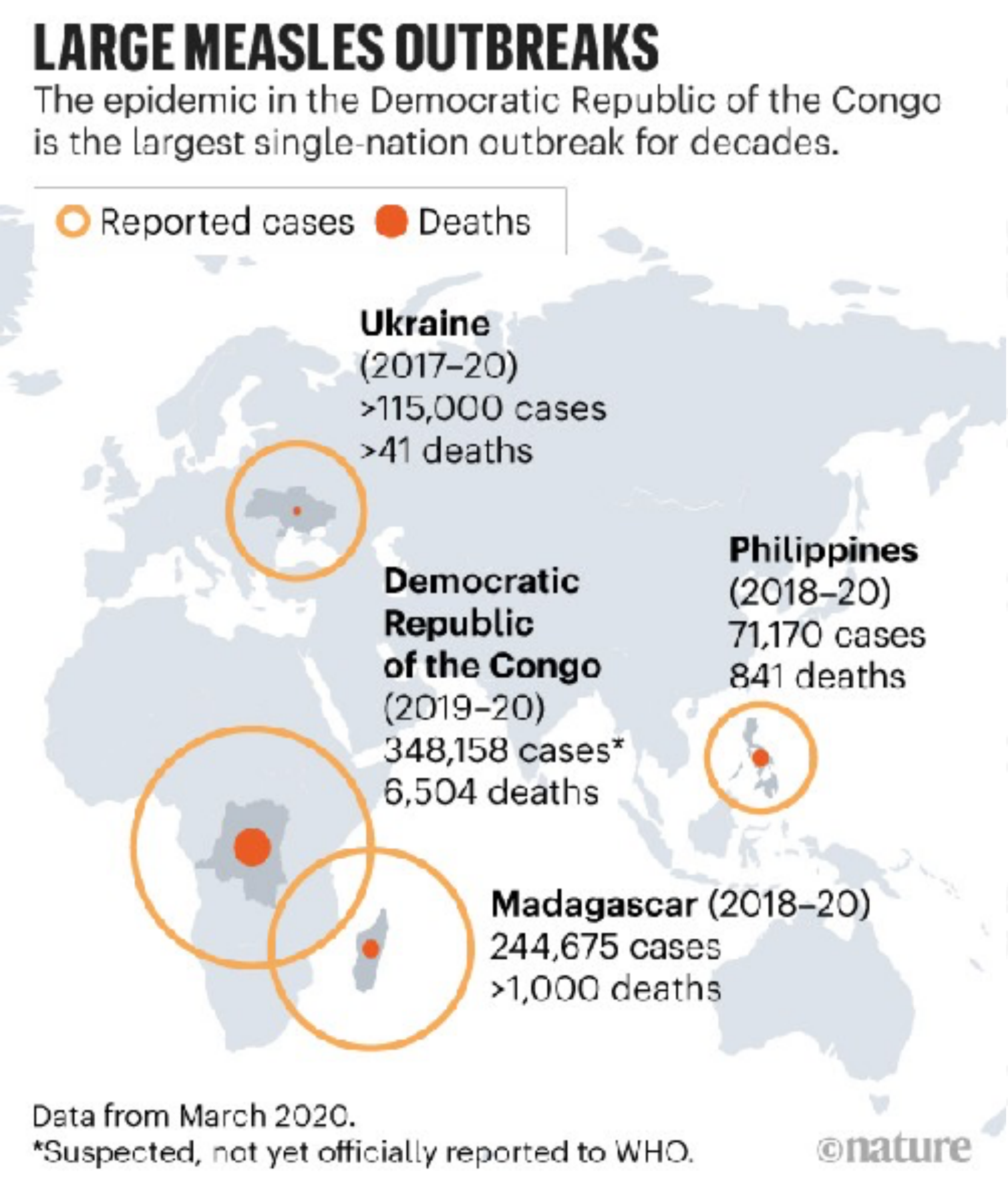

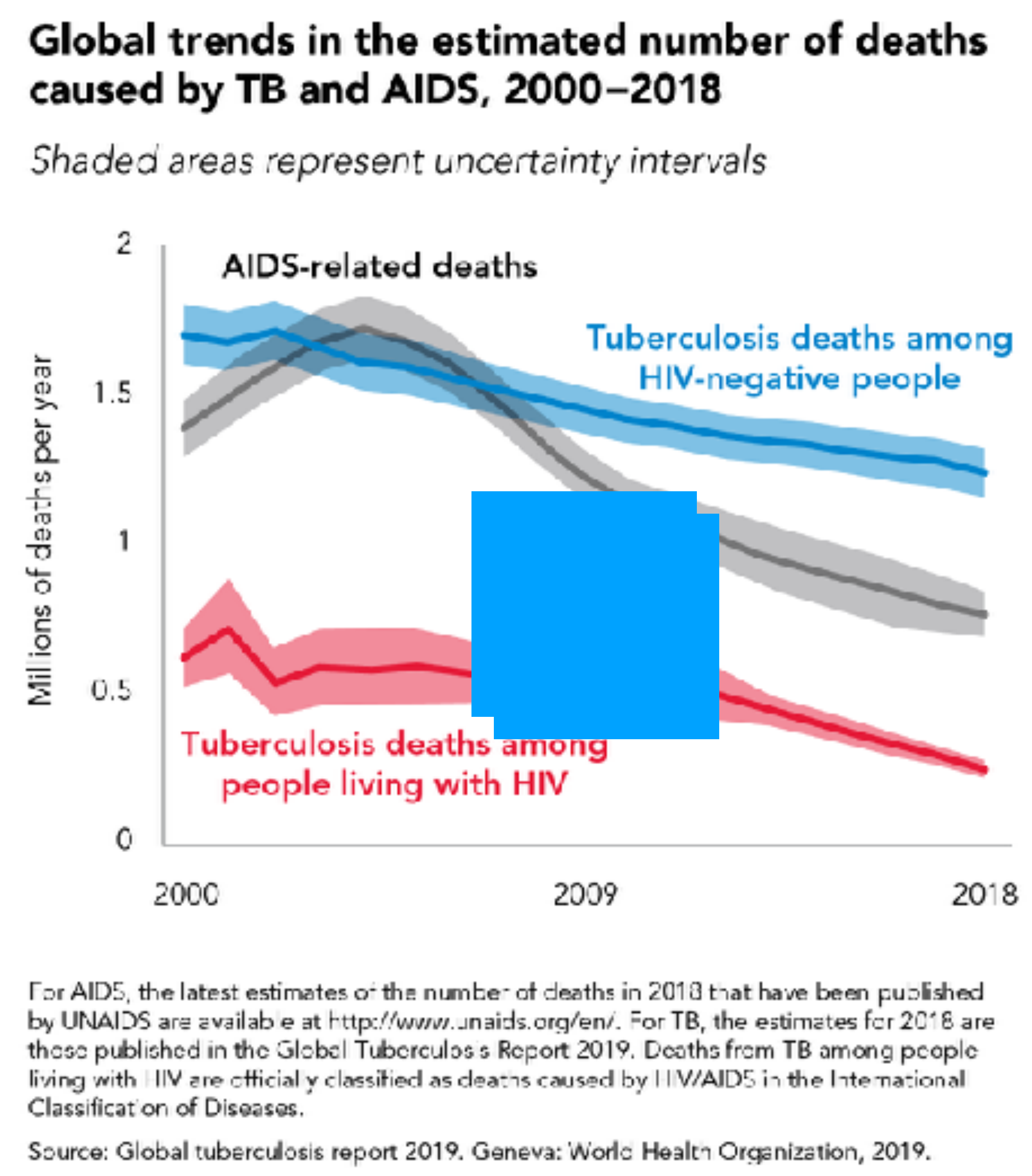

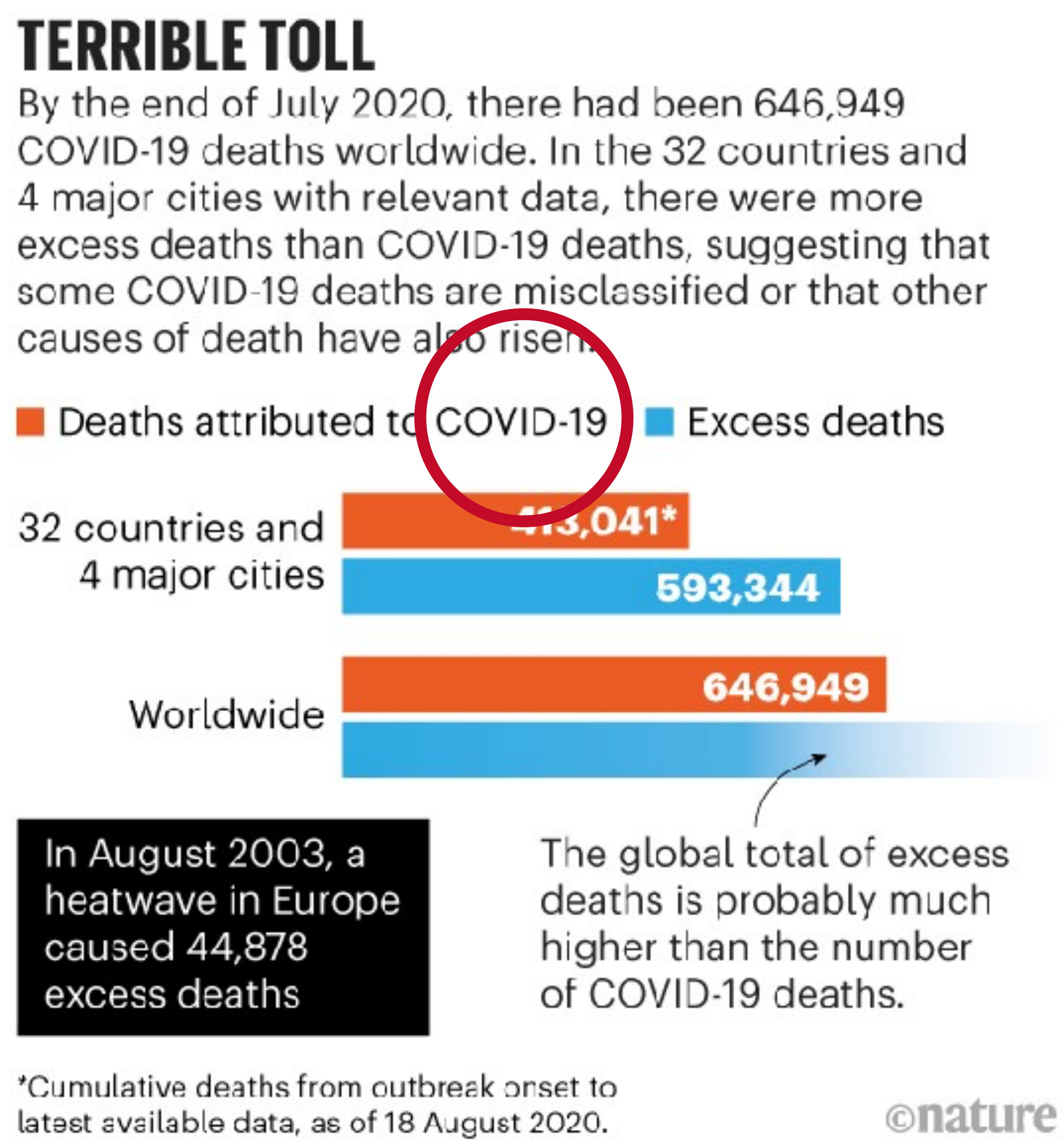

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Societal challenge

- Controlling the spread of infectious diseases is important
- Computational and mathematical modeling of epidemics important to assist governments in responding to outbreaks
- Made challenging due to:
  - increased and denser urbanization
  - increased local and global travel
  - increasingly immuno-comprised population

Approach: individual-based simulation

- Agent-based modeling to simulate epidemic diffusion
- Models agents (people) and interactions between them
- People interact when they visit the same location at the same time
- These "interactions" between pairs of people are represented as "visits" to locations
- Use a bi-partite graph of people and locations or a people-people interactivity graph

Serial algorithm

- At each timestep (typically a day):
  - Determine which people visit which locations
  - “Send” people to those locations
  - At each location “interactions” happen and transmission happens
  - Update people’s states at the end of the day and continue
- Interventions (vaccinations, school closures) can be added on certain days to change people’s susceptibility, movements etc.

Combination of network theory and discrete-event simulations

- Hybrid time-stepped and discrete-event simulation

https://sitn.hms.harvard.edu/flash/special-edition-on-infectious-disease/2014/an-introduction-to-infectious-disease/

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Contact model at each location

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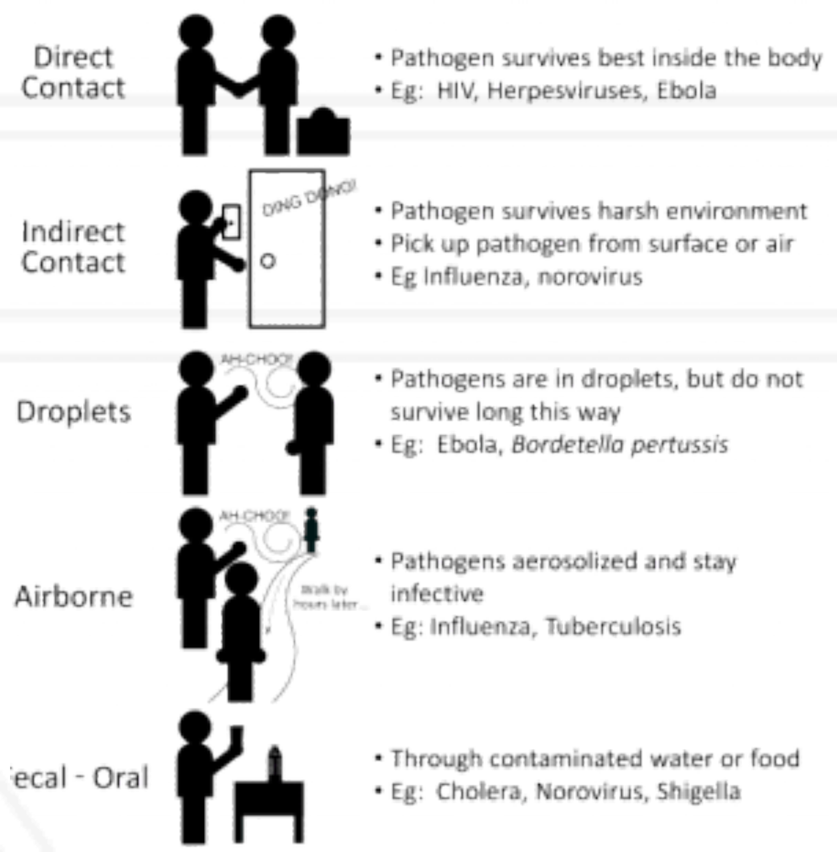
Contact model at each location

Model for human transmission



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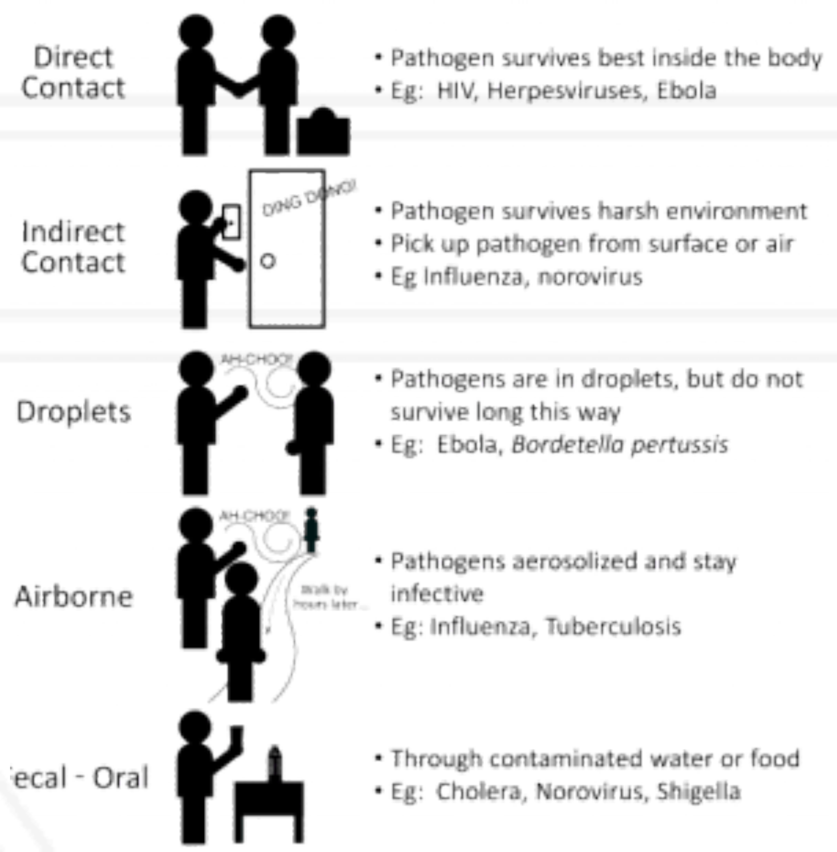
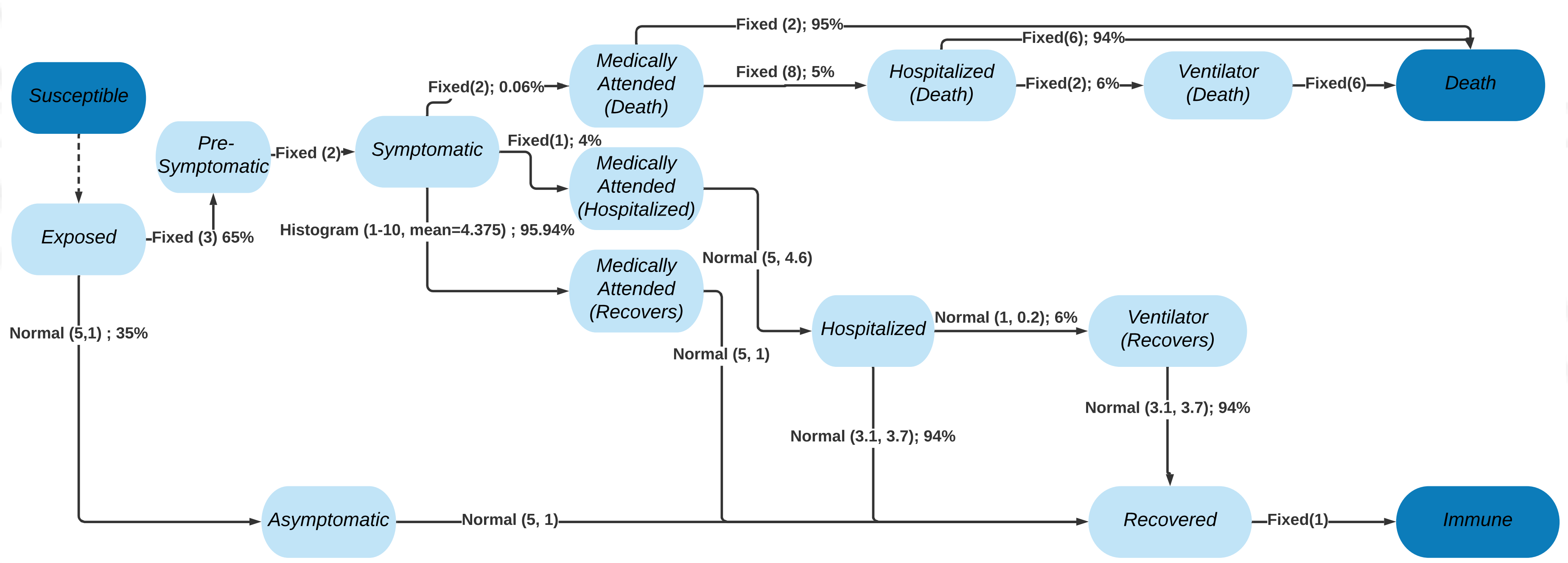


Disease model for each person



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Combination of network theory and discrete-event simulations

- Hybrid time-stepped and discrete-event simulation

```
while d < num_days:
  for each person:
    Send visit messages to locations

  for each location:
    Process all visit messages
    Run discrete event simulation
    Send interaction messages

  for each person:
    Process interactions
    Update disease state
```

Contact model at each location

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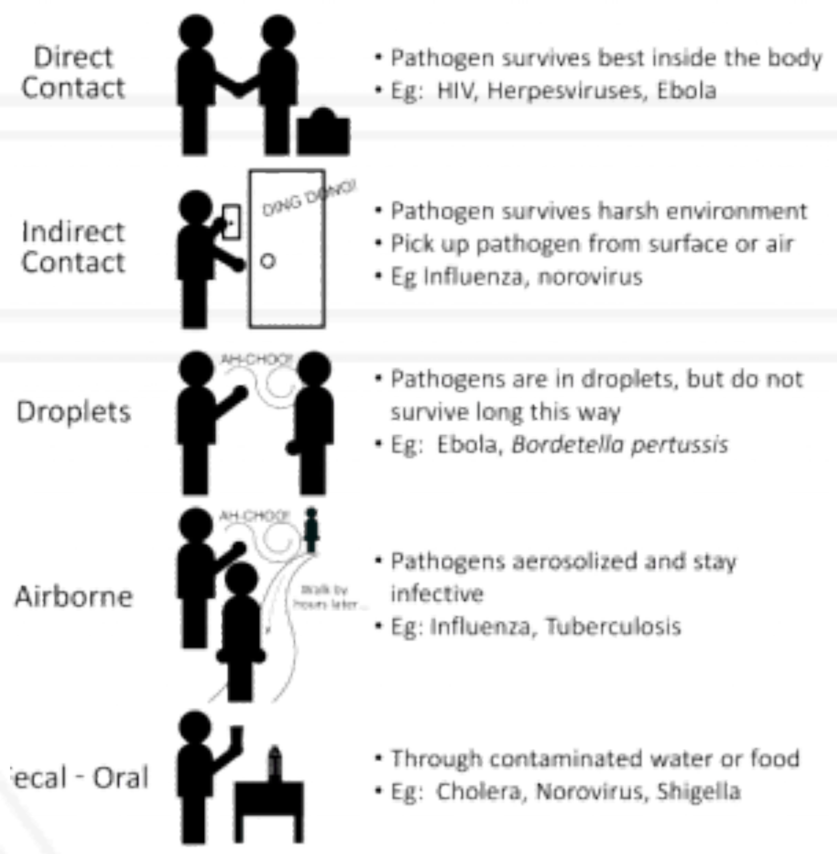

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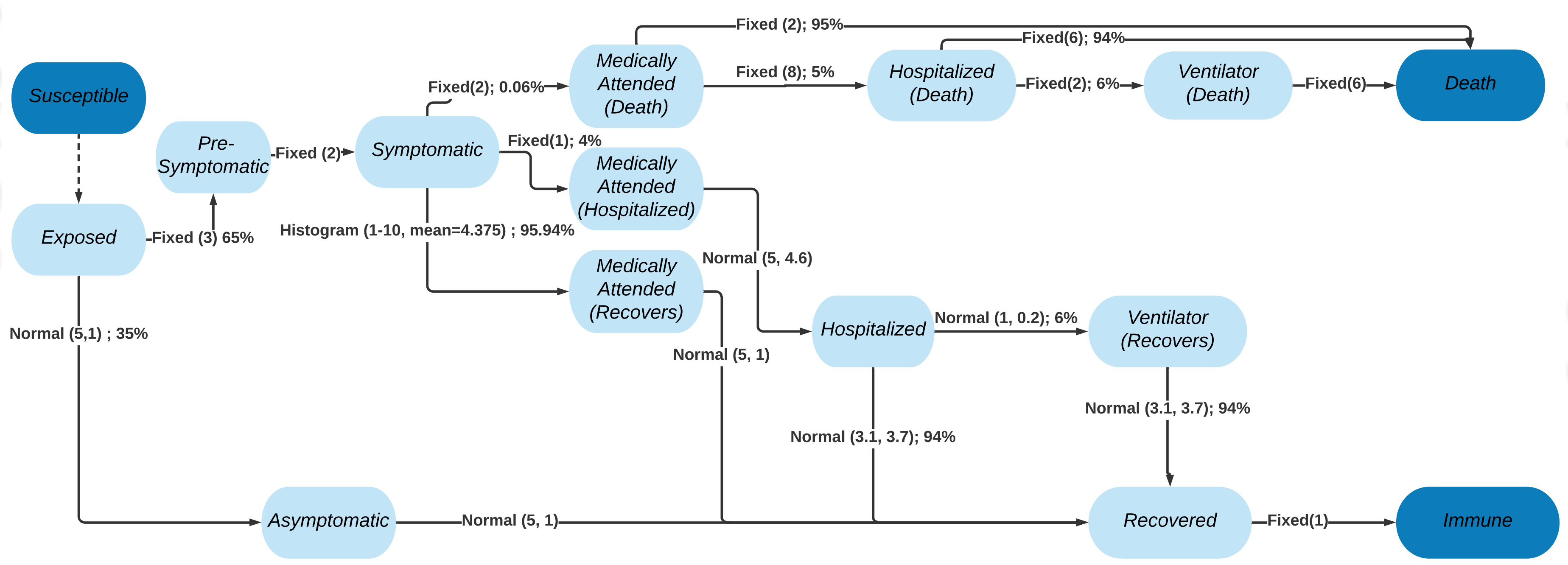

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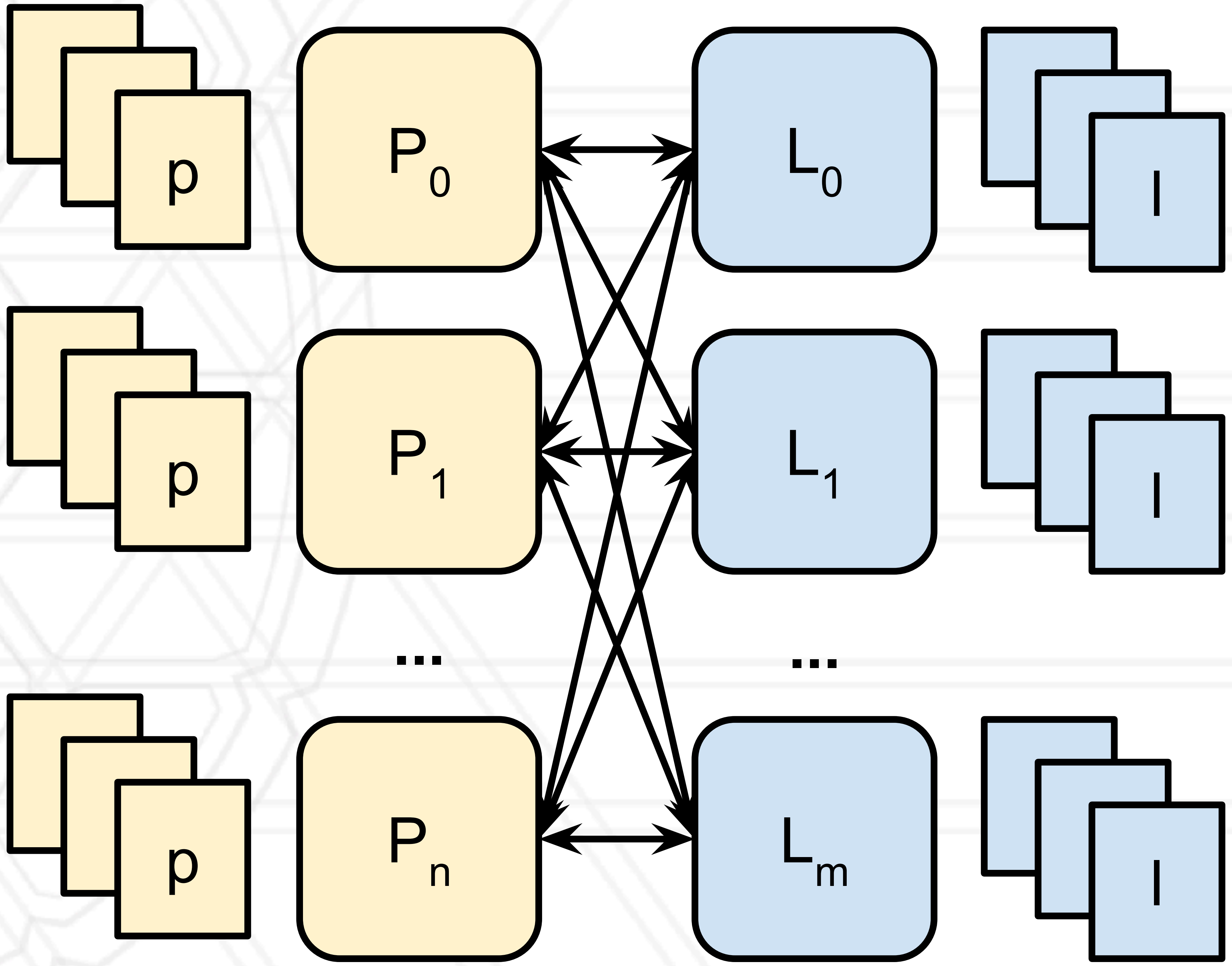
Parallel simulation is challenging

- Size and scale of the social contact network (6 billion agents for a global simulation)
  - Unstructured networks and complicated dependencies lead to high communication cost
- Individuals and their behaviors are not identical
- Co-evolving epidemics, public policies and agent behaviors make it impossible to apply standard model reduction techniques

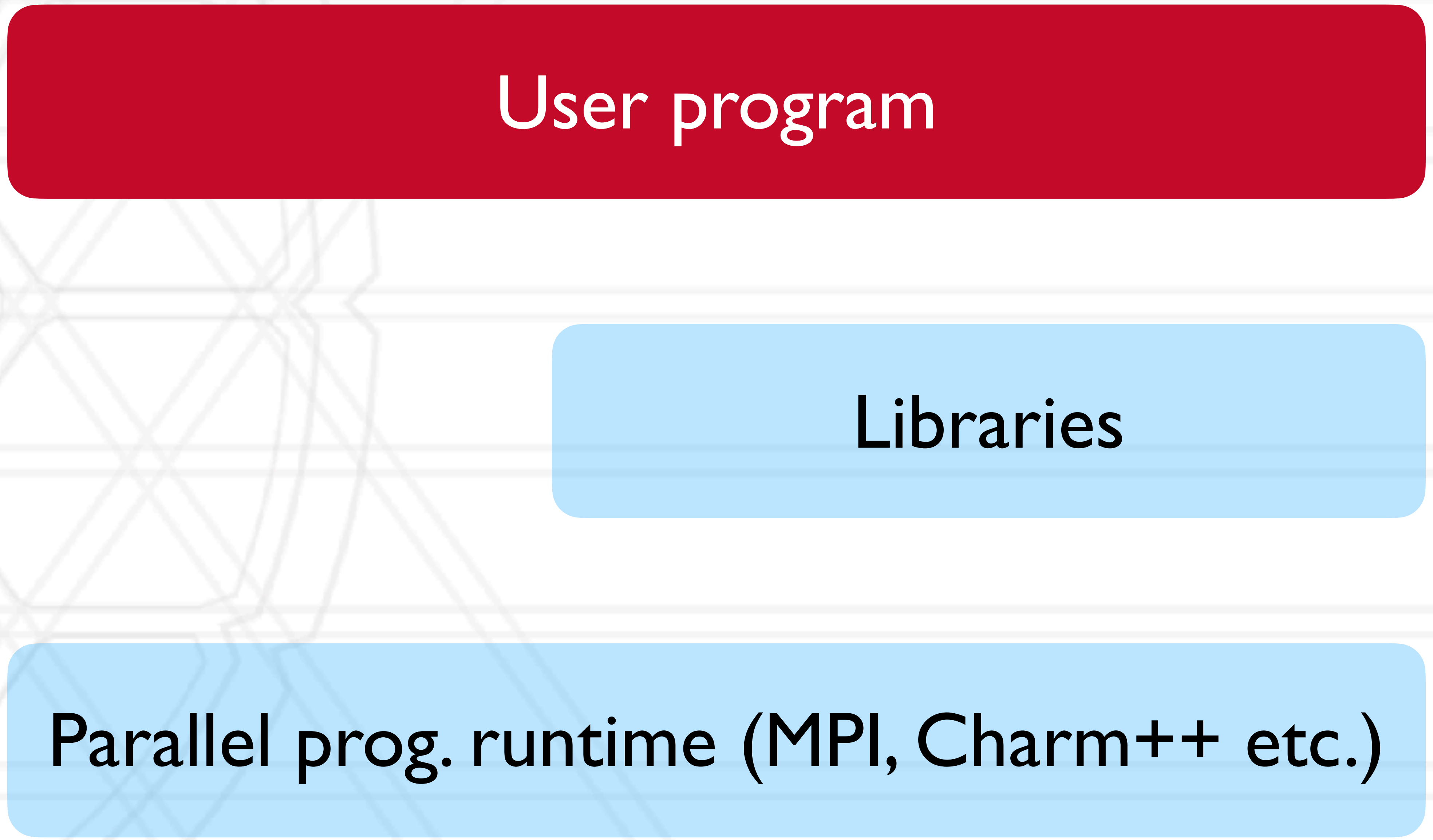
Parallel implementation: Loimos

- All the people and locations are distributed among all processes
- DES computation can be done locally in parallel
- Communication when sending visit and infection messages
- Uses Charm++, a message-driven model



Application software stack

- Parallel programming model / runtime:
  - MPI, OpenMP, Charm++, CUDA, …
- Libraries
  - Data and visualization libraries (mesh management, simulation output)
  - I/O libraries
  - Math/numerical libraries
  - Graph partitioning, load balancing …



Why use libraries?

- No need to reinvent the wheel
  - Libraries are highly optimized, have fewer bugs
- Avoids significant effort to write, optimize and maintain code
- Makes code more portable

Popular Libraries

- Data/visualization and I/O libraries
  - I/O: HDF5, pNetCDF, ADIOS
- Numerical libraries:
  - Fast Fourier transforms: FFTW
  - Dense linear algebra: BLAS, LAPACK, Intel MKL
  - Solvers for sparse systems: Hypre, PETSc, Trilinos
- Graph partitioning/load balancing:
  - METIS, Scotch, Zoltan, Chaco

https://events.prace-ri.eu/event/176/contributions/38/attachments/154/305/HPC_libraries.pdf

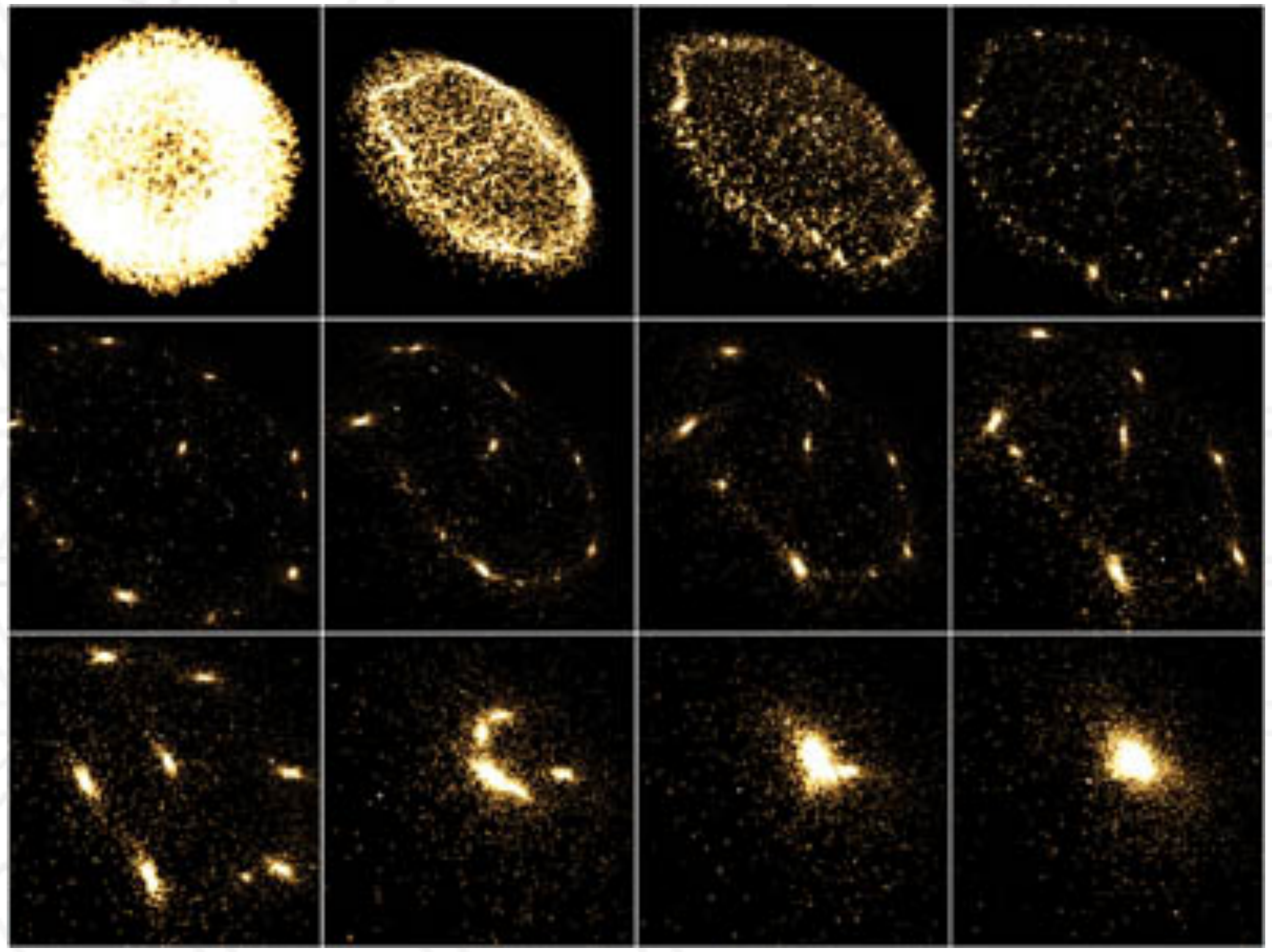
Domain-specific languages/frameworks

- Structured grids: SAMRAI, Chombo, AMREx
- Unstructured grids: MFEM, Quinoa

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/p particles to each process
- Other approaches?

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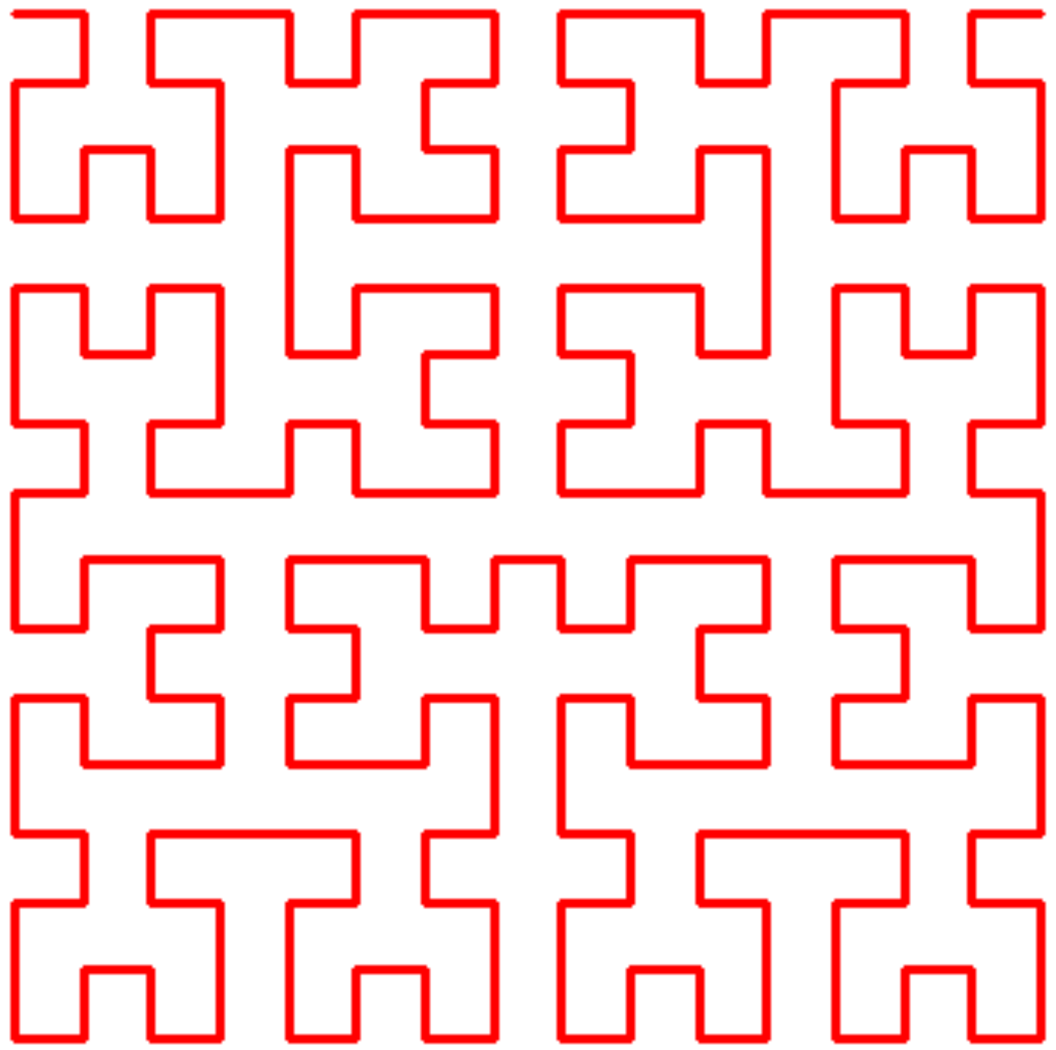

Space-filling curves

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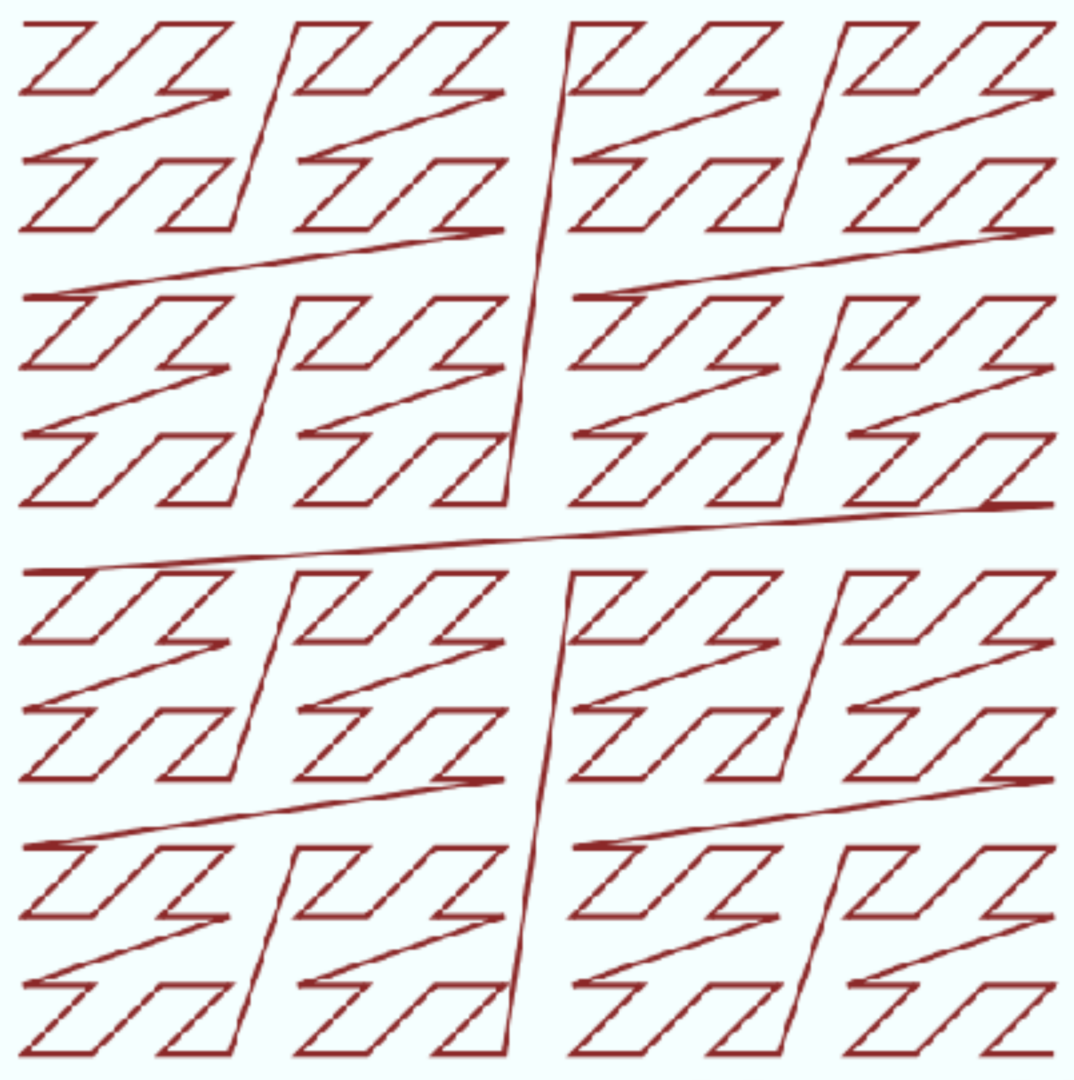

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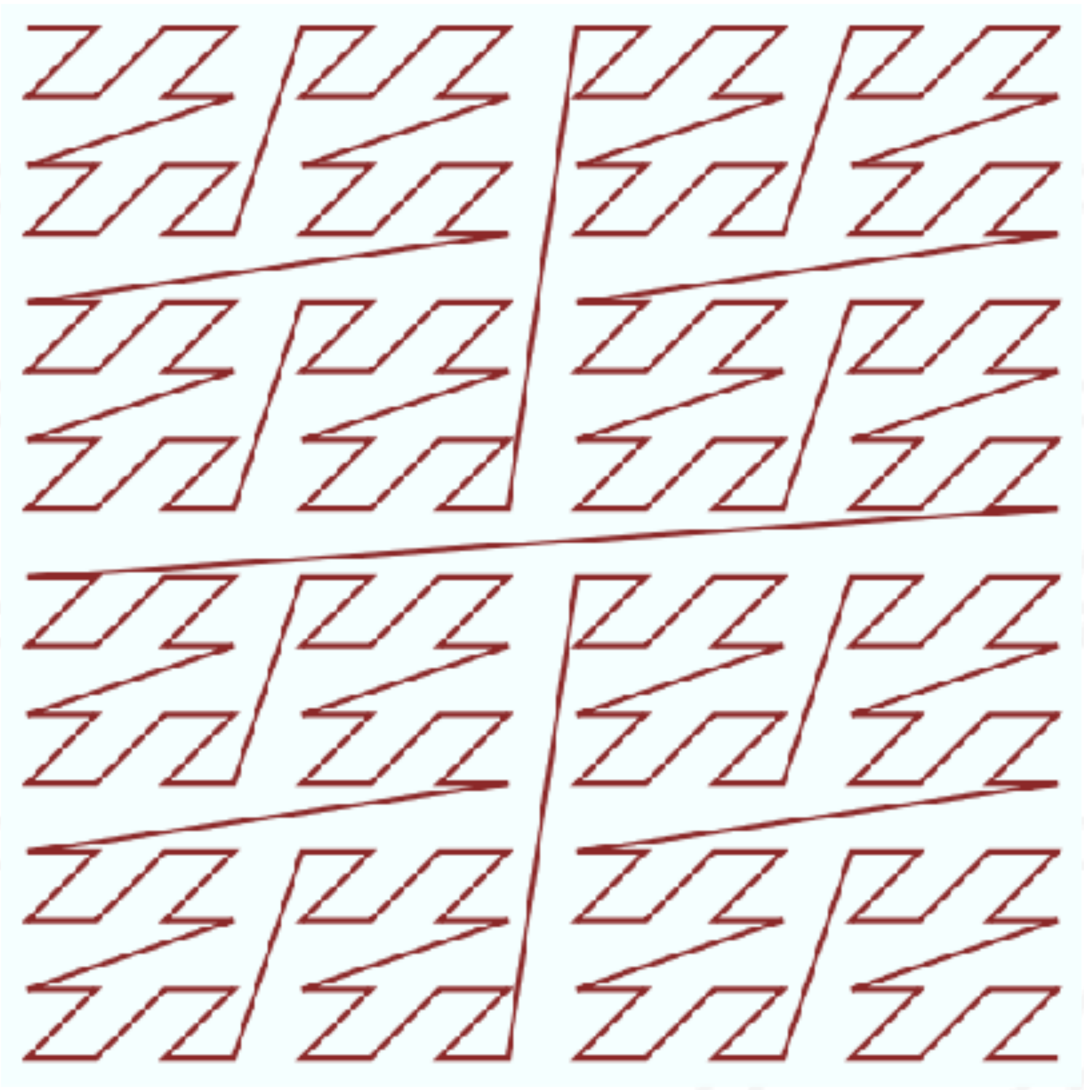

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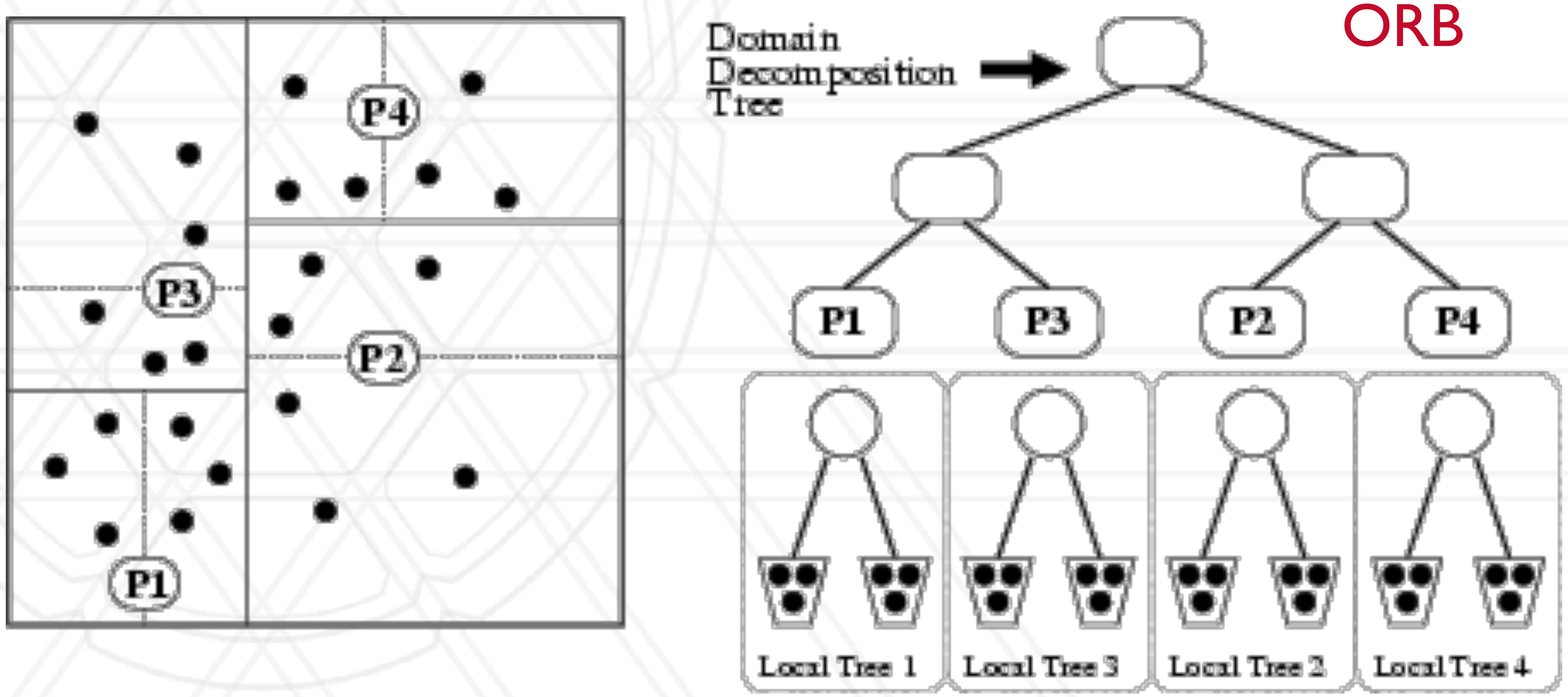
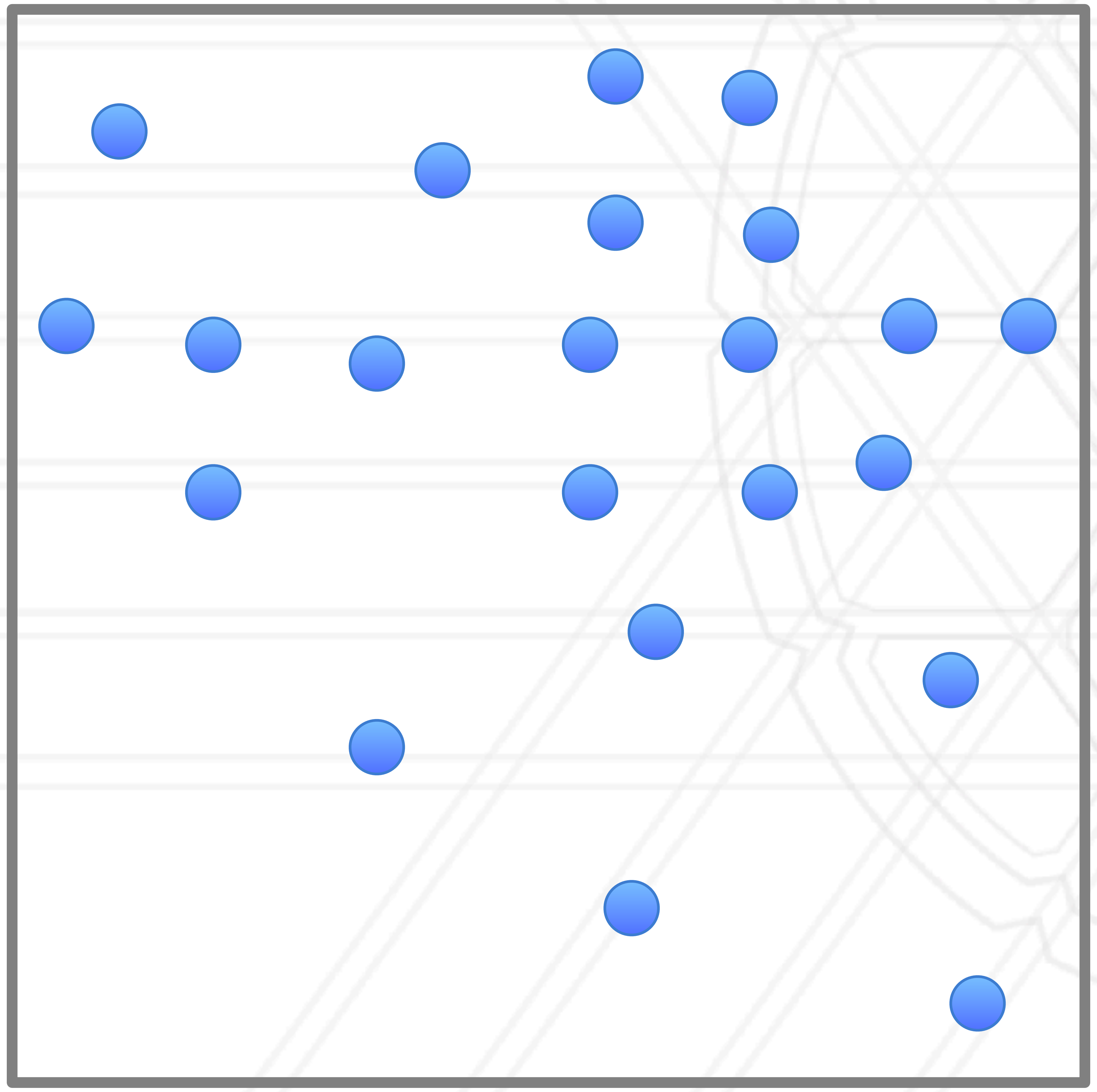


ORB

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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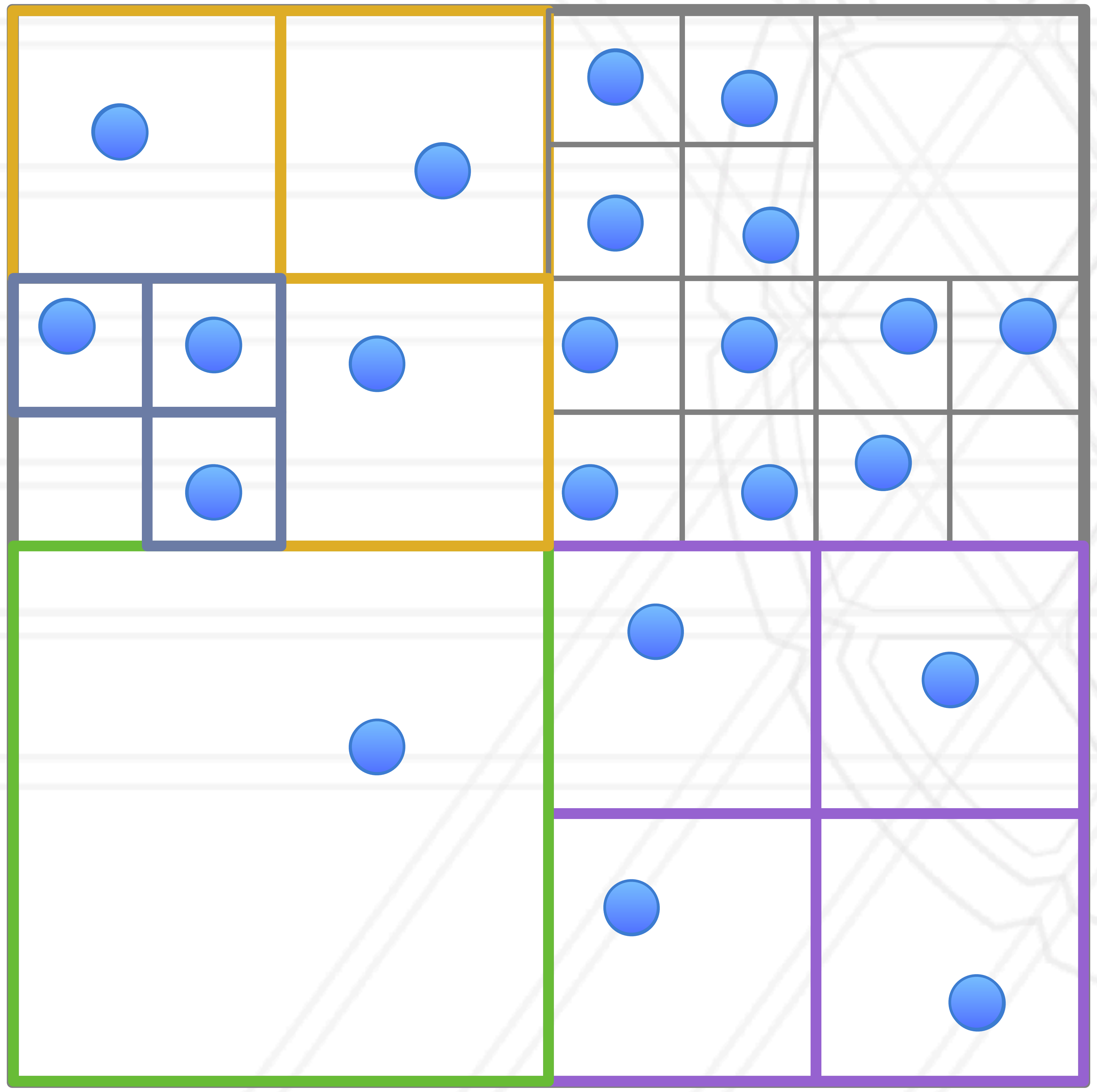

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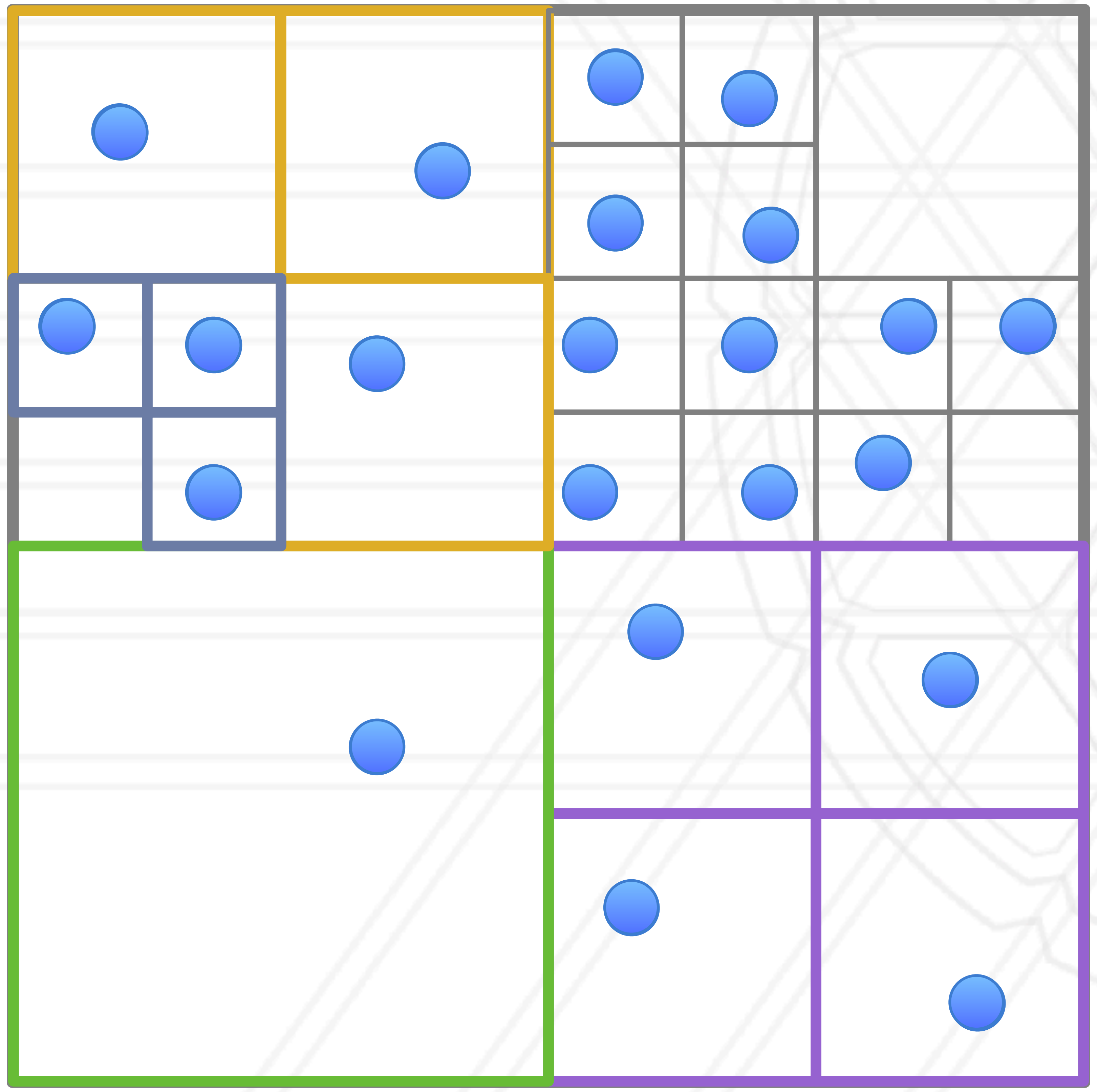
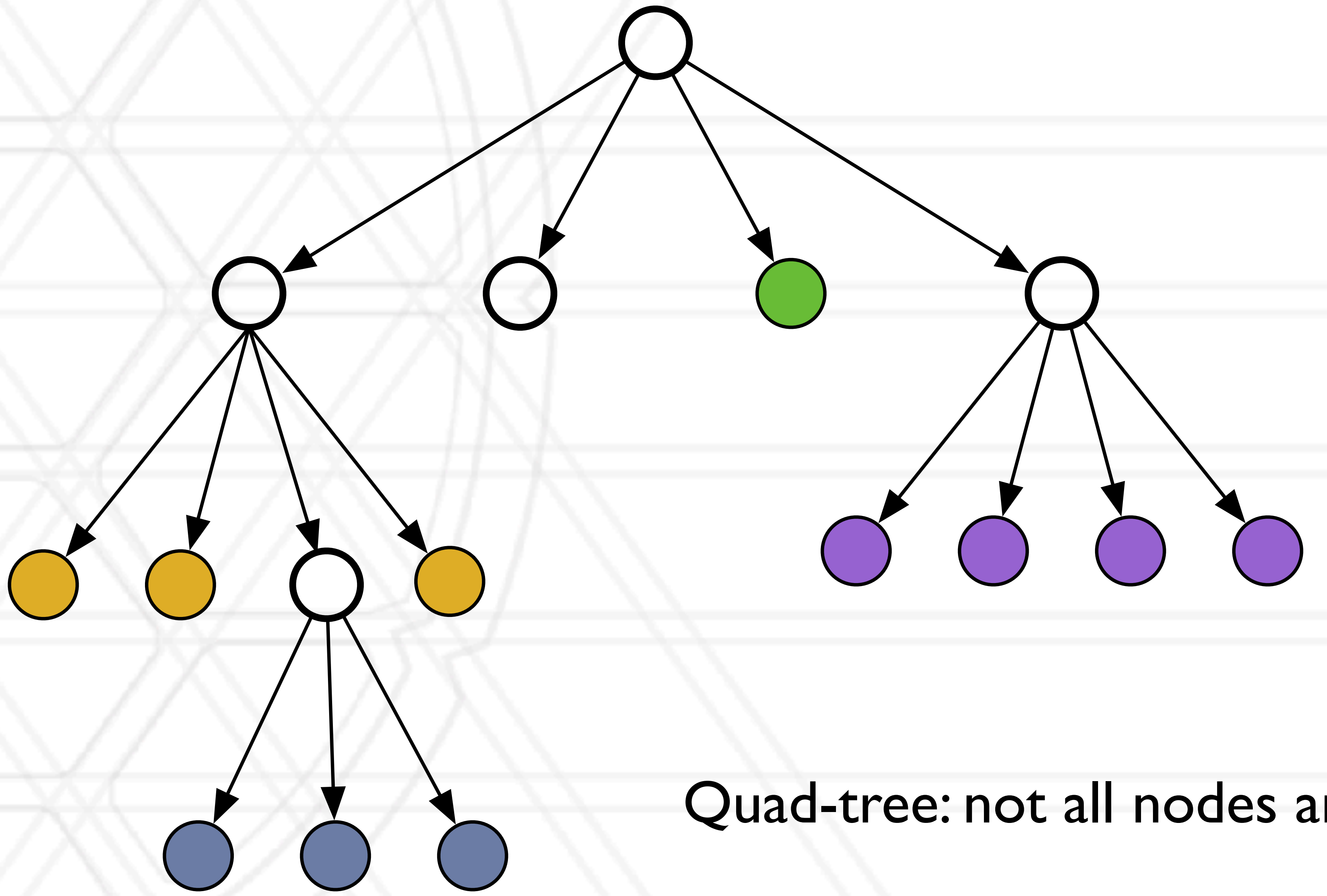




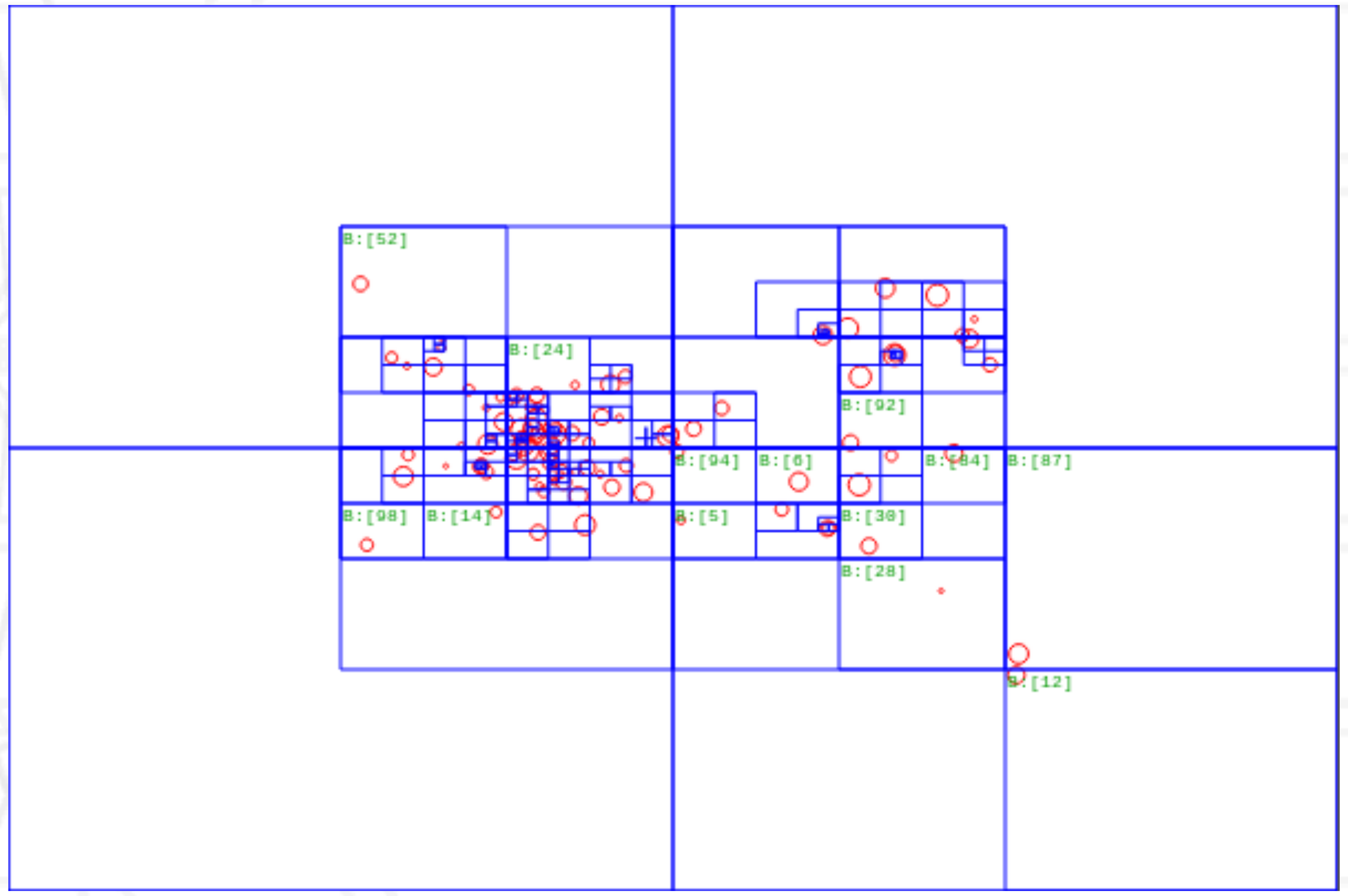
Quad-tree: not all nodes are shown

Different parallelization methods

- Tree codes: Barnes-Hut simulations
- Fast multipole 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
- O(N logN) algorithm



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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

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