Introduction to Parallel Computing (CMSC416 / CMSC616)

Parallel CSE Applications

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MARYLAND

Announcements

- Assignment 6 (extra credit) on MPI has been posted
  - Due on Dec 6 11:59 pm
- Final exam is on Dec 16 10:30 am — 12:30 pm
  - In person, closed book/notes

Molecular Dynamics

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

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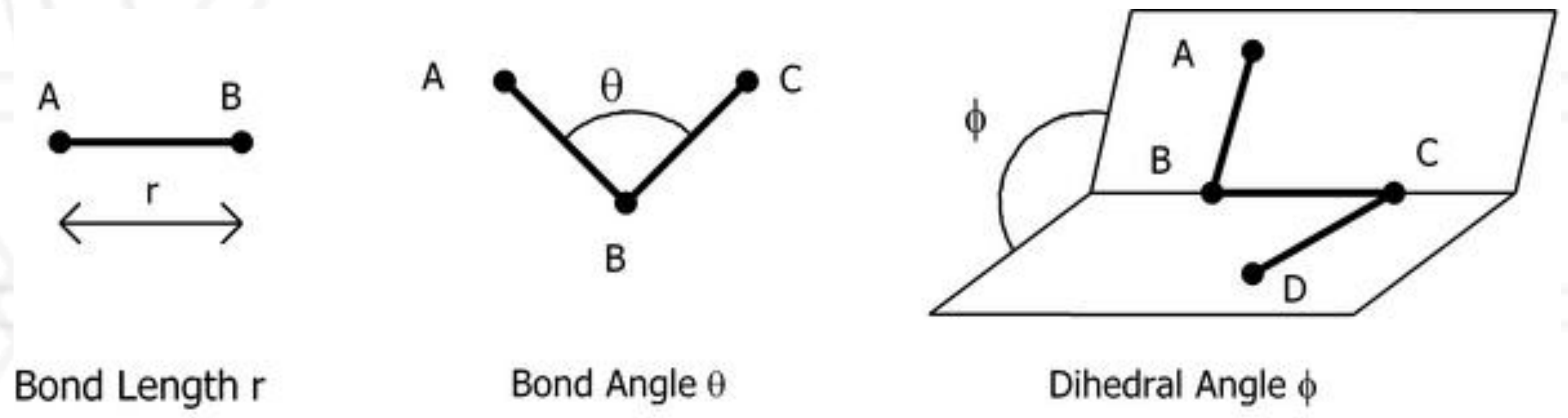
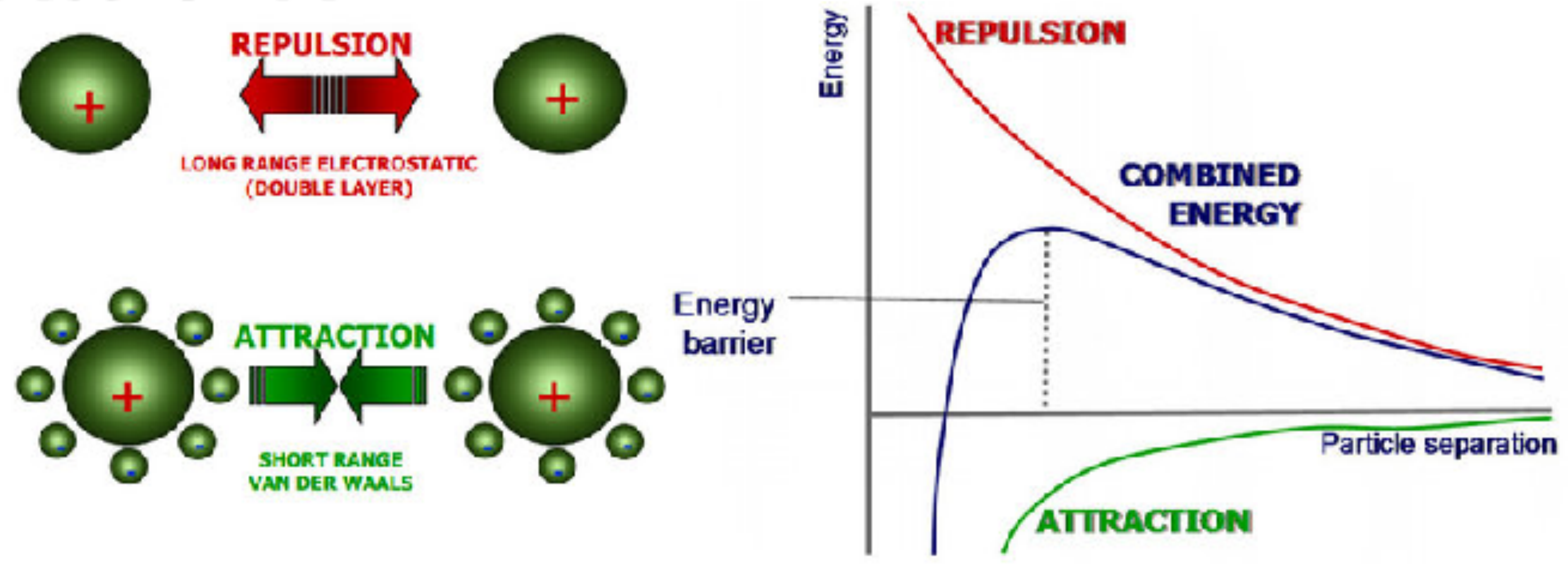
  - Bonded interactions: bonds, angles, dihedrals
  - Non-bonded interactions: van der Waal's and electrostatic forces





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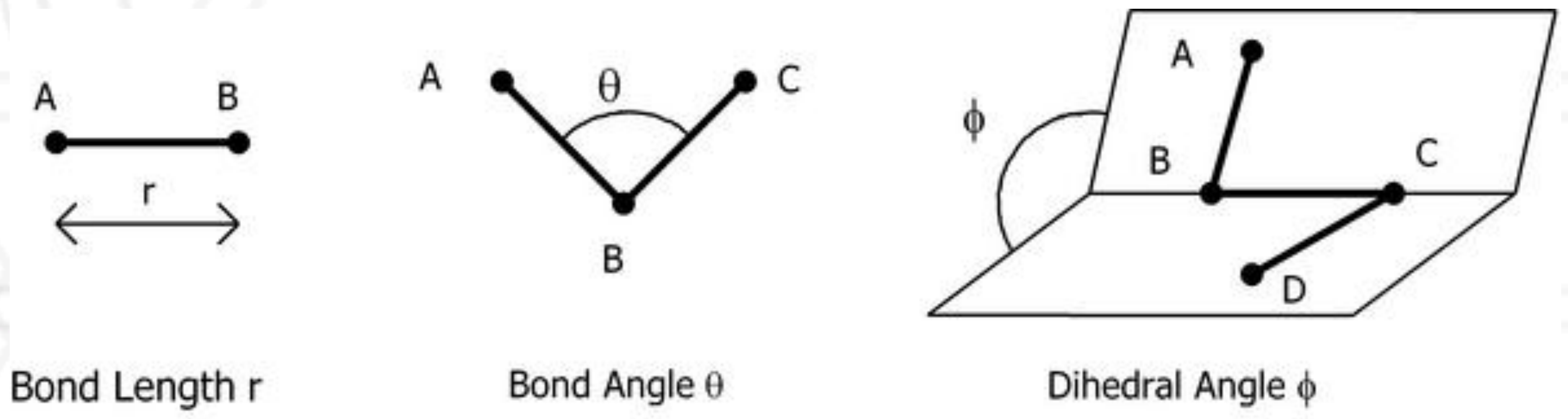

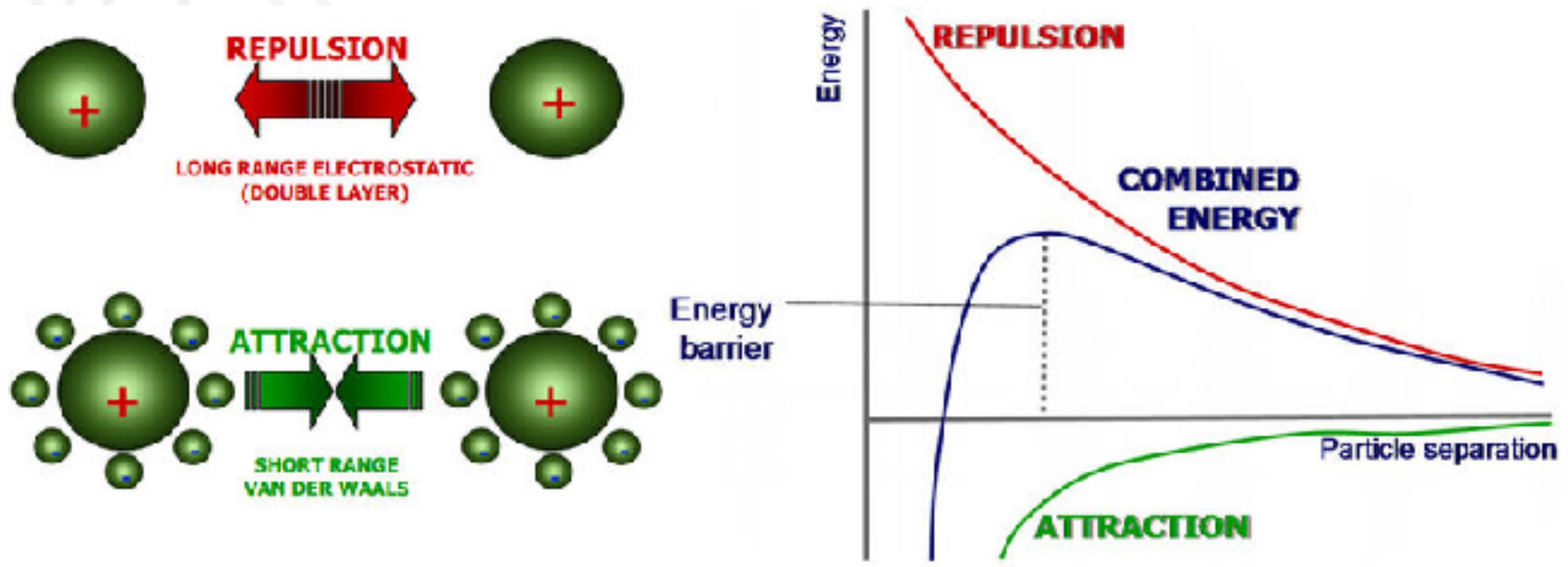

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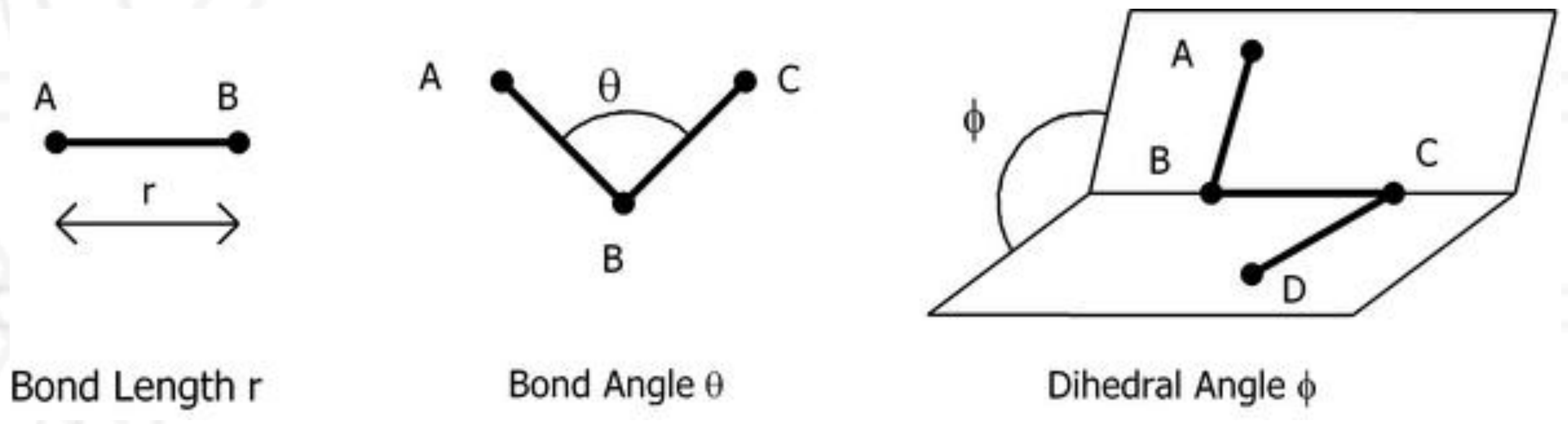

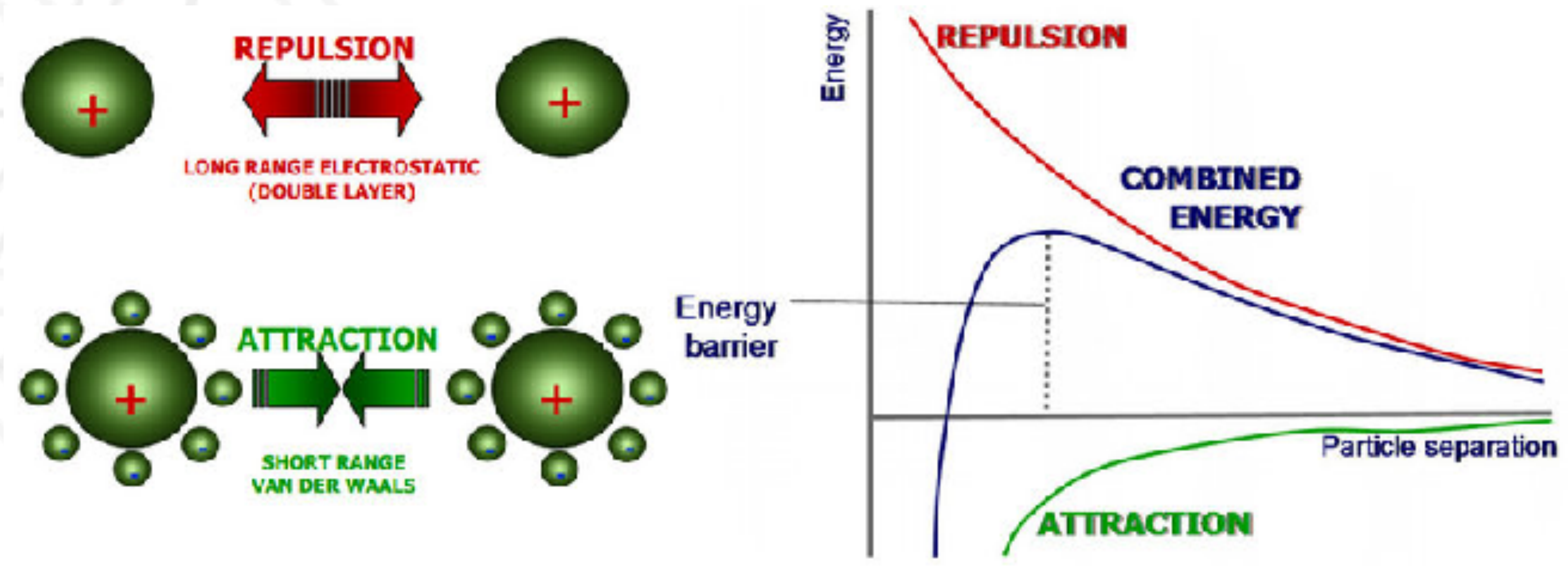

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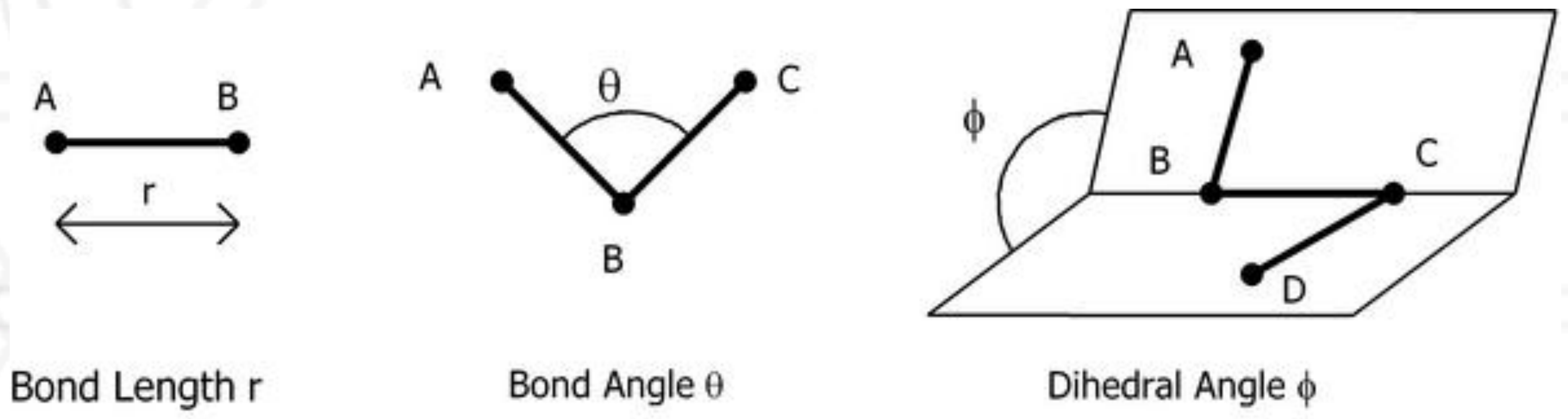
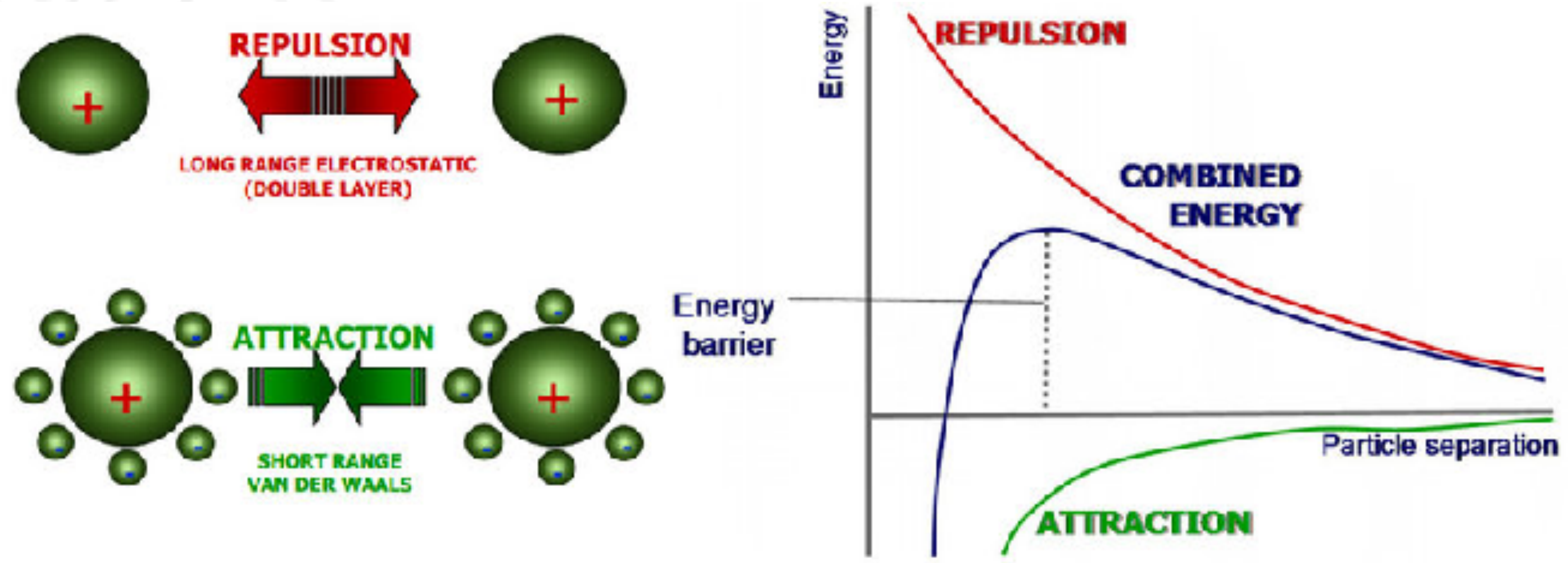
- Simulation step: ~1 femtosecond (10^{-15} s)
- Used for drug design, materials design





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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  - Partition the atoms across processes

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  - Matrix is sparse and non-uniform

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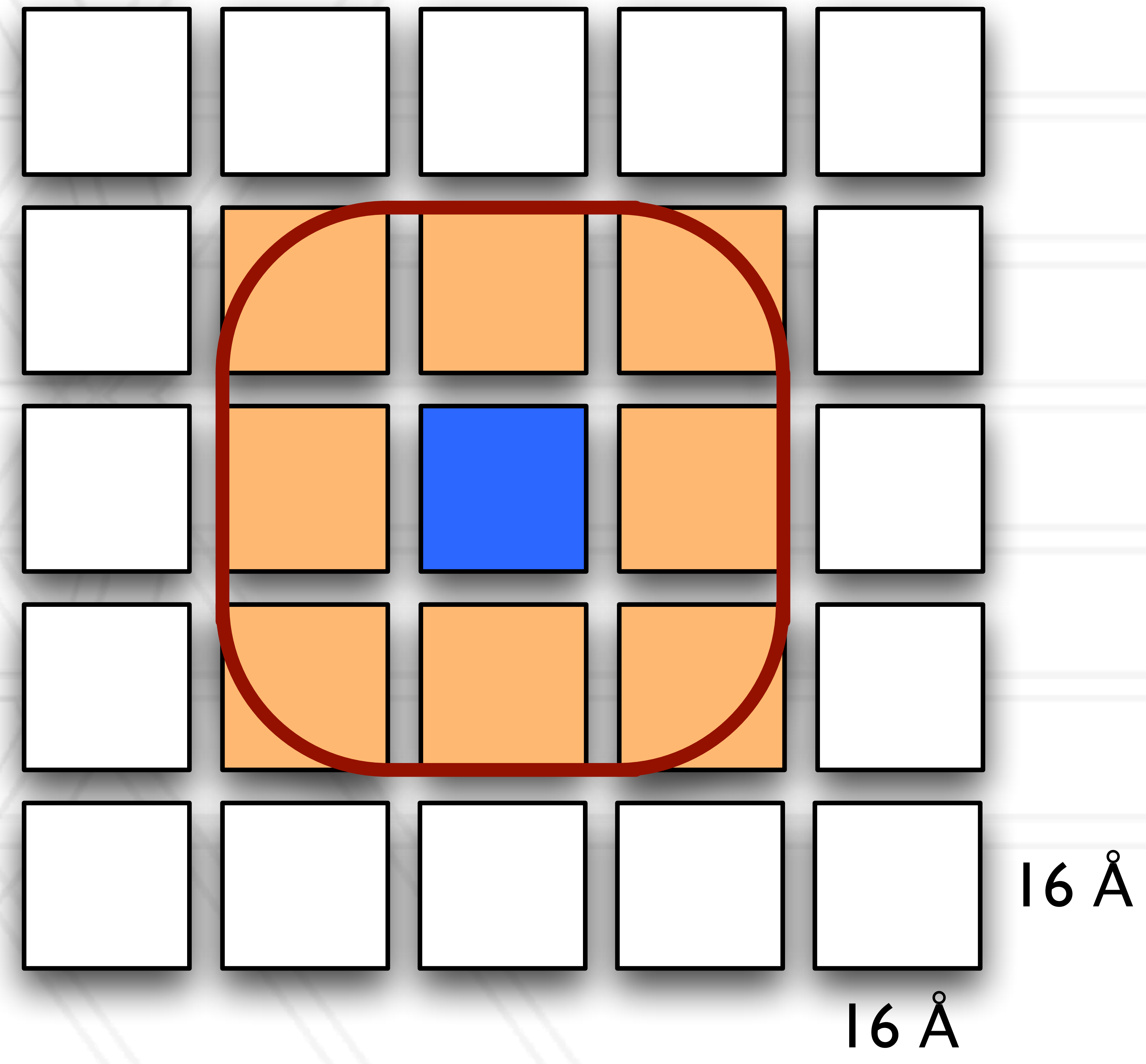
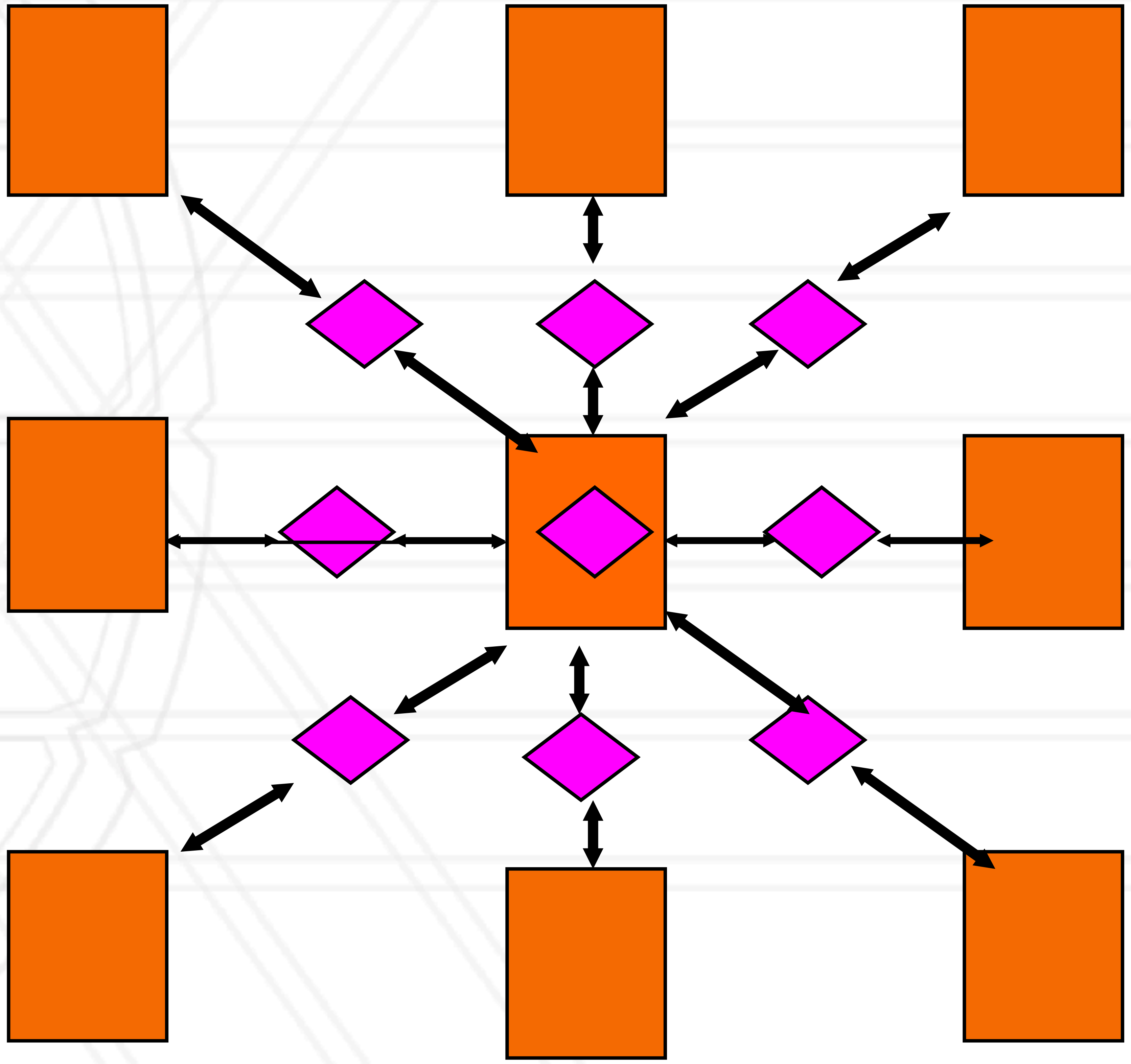
- Force decomposition:
  - Distribute the force matrix to processes
  - Matrix is sparse and non-uniform
- Spatial decomposition:
  - Assign a region of the 3D simulation space to each process



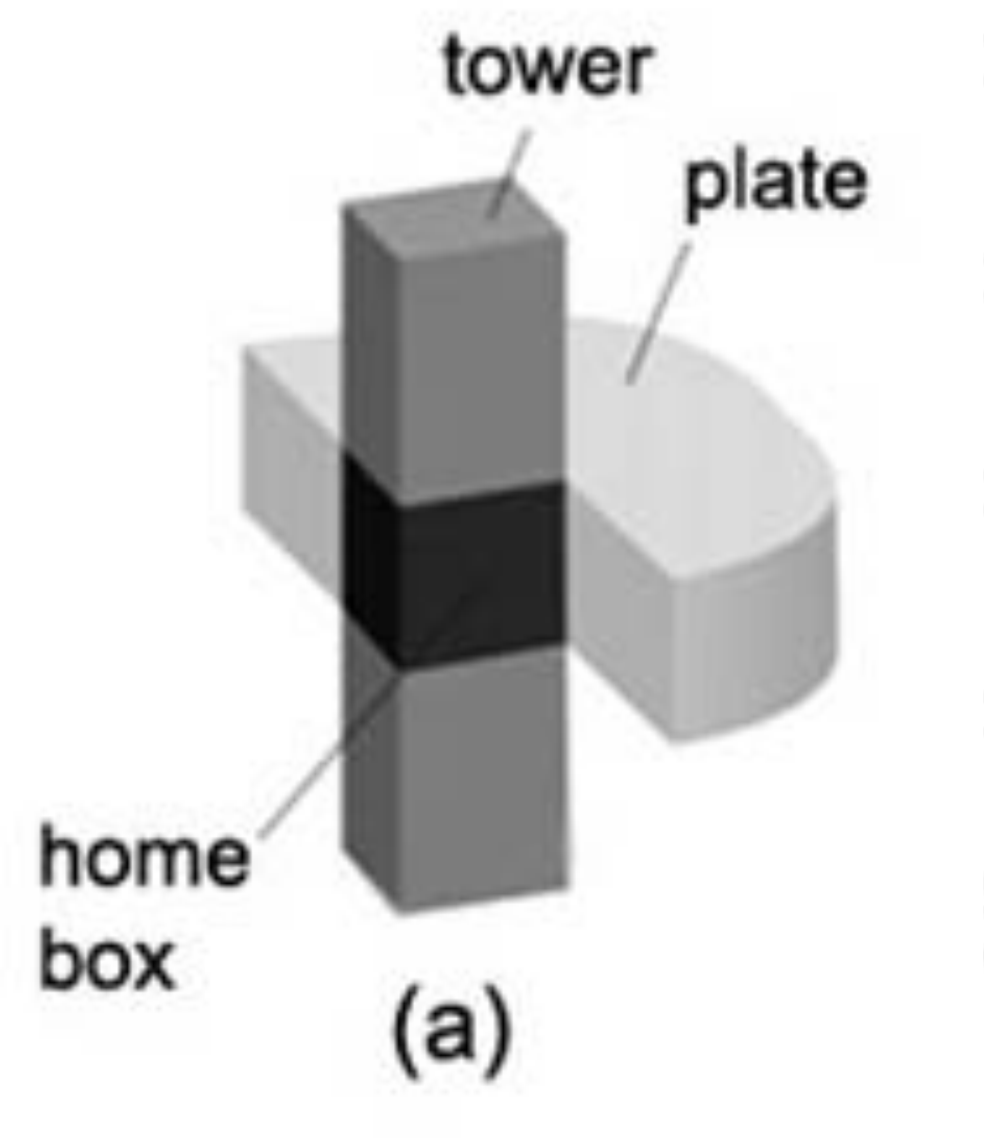
Hybrid parallelization

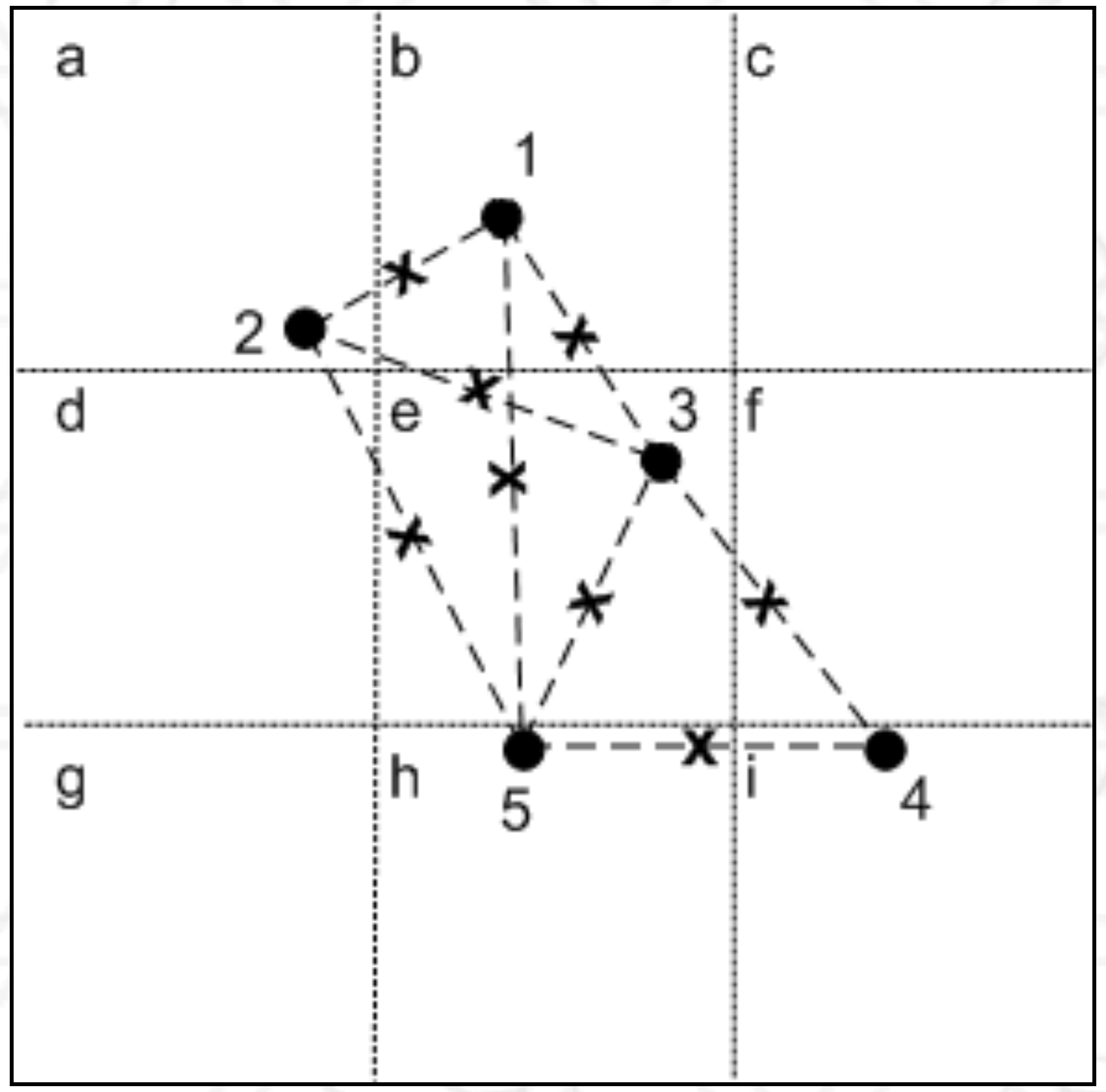
- Hybrid of spatial and force decomposition
- Decouple assignment of data and work to processes
- Distribute both atoms and the force calculations to different processes



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

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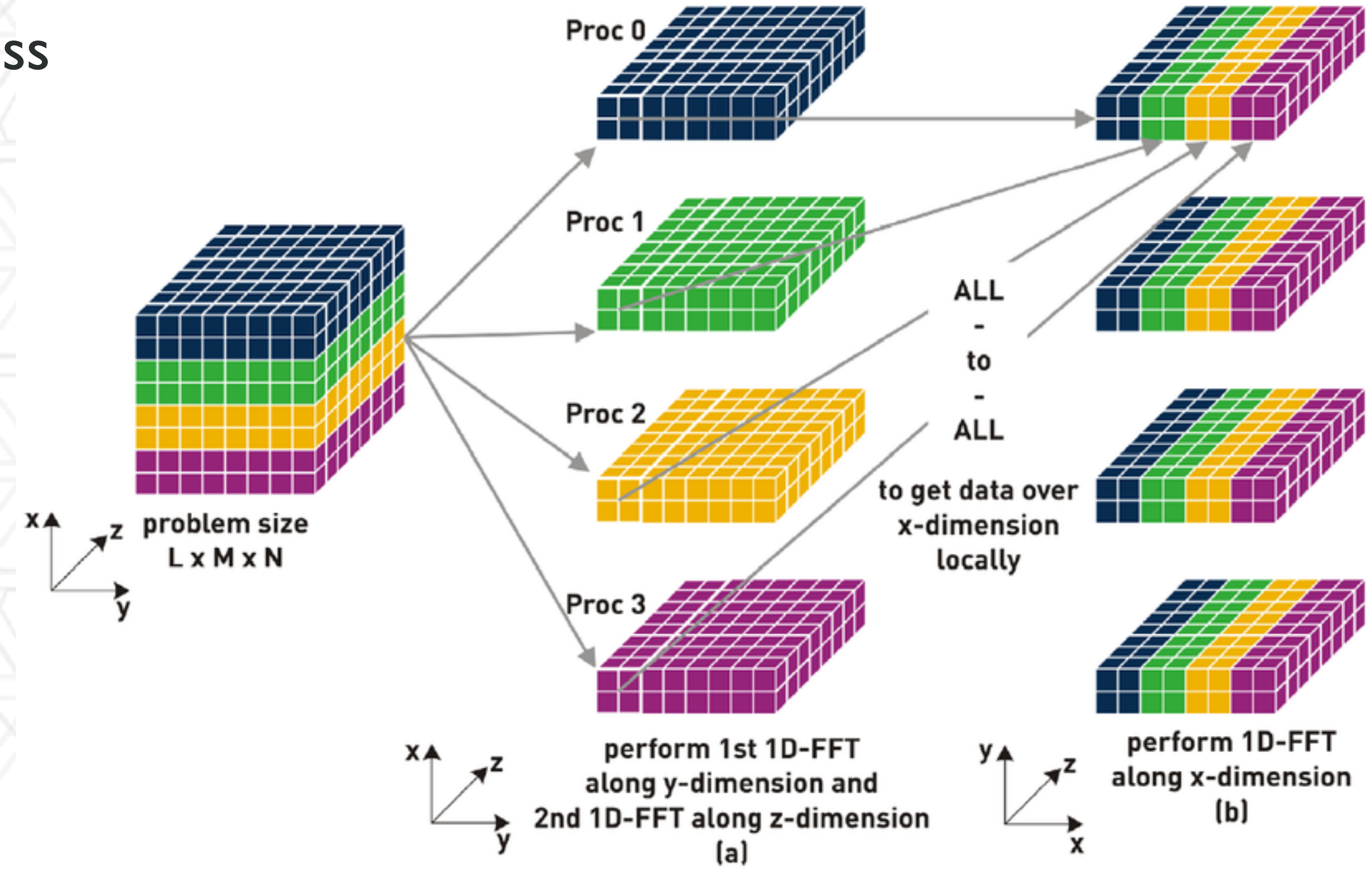
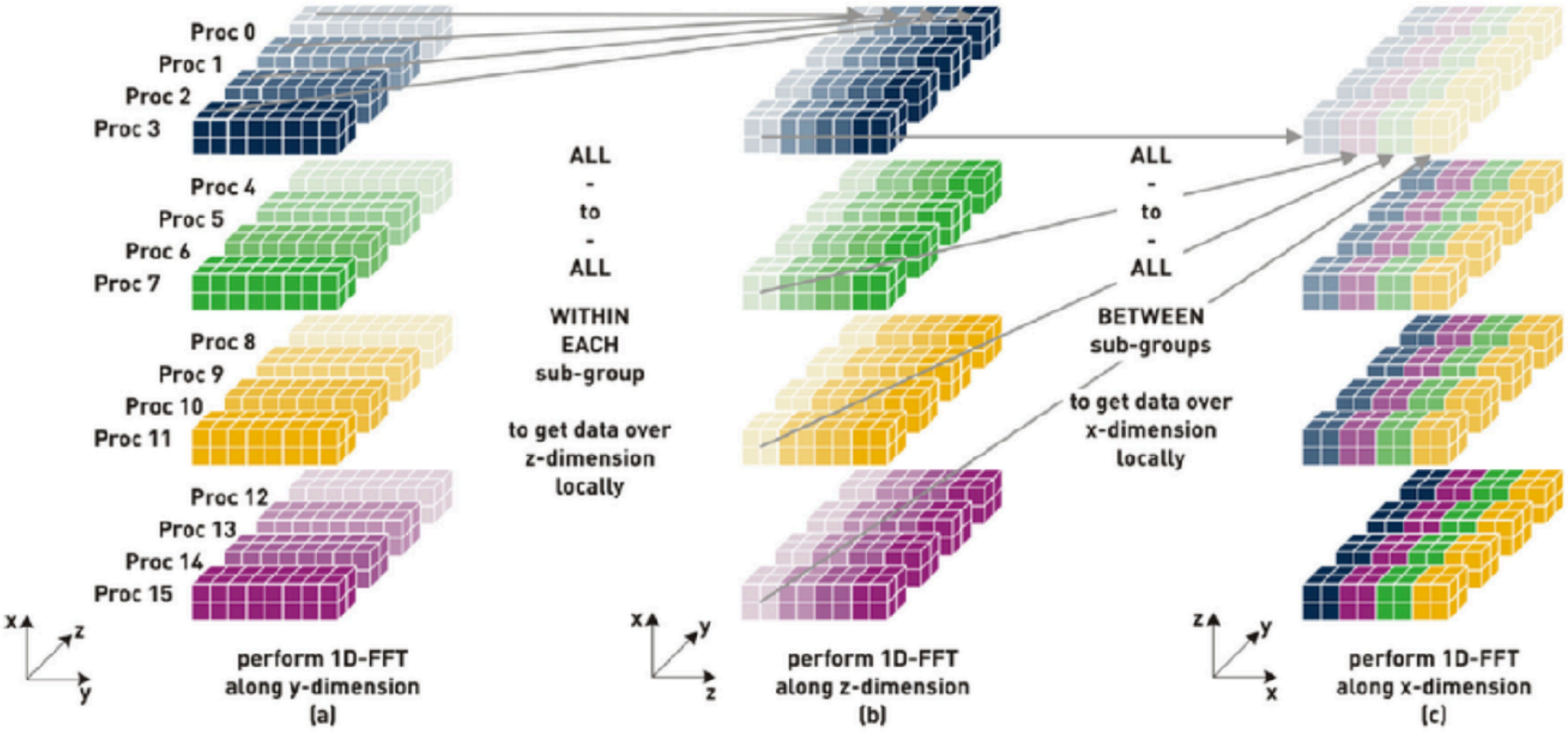
- Bring all the data to one process
- 1D or slab decomposition

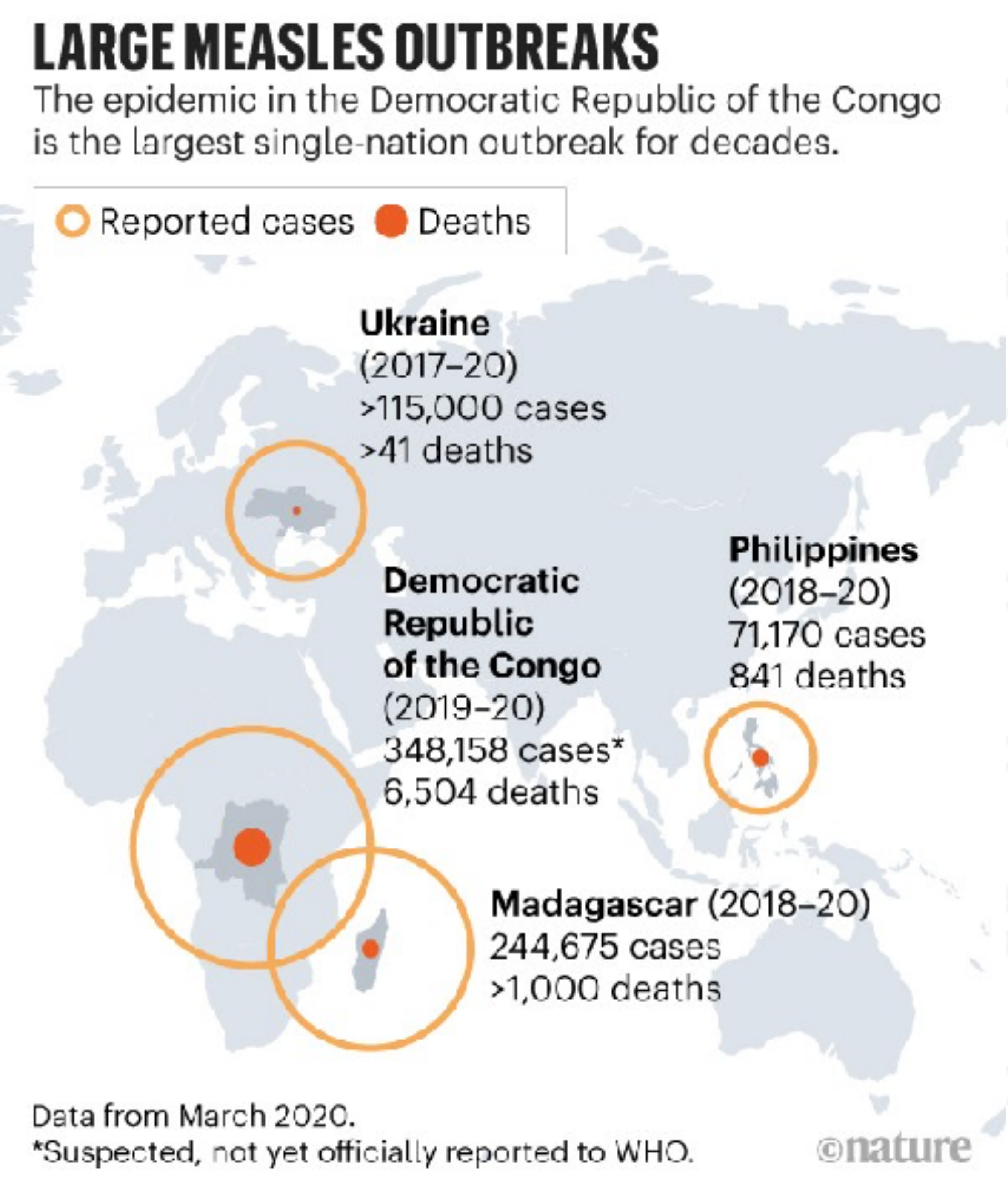


Parallelization of PME (3D FFT)

- 2D or pencil decomposition



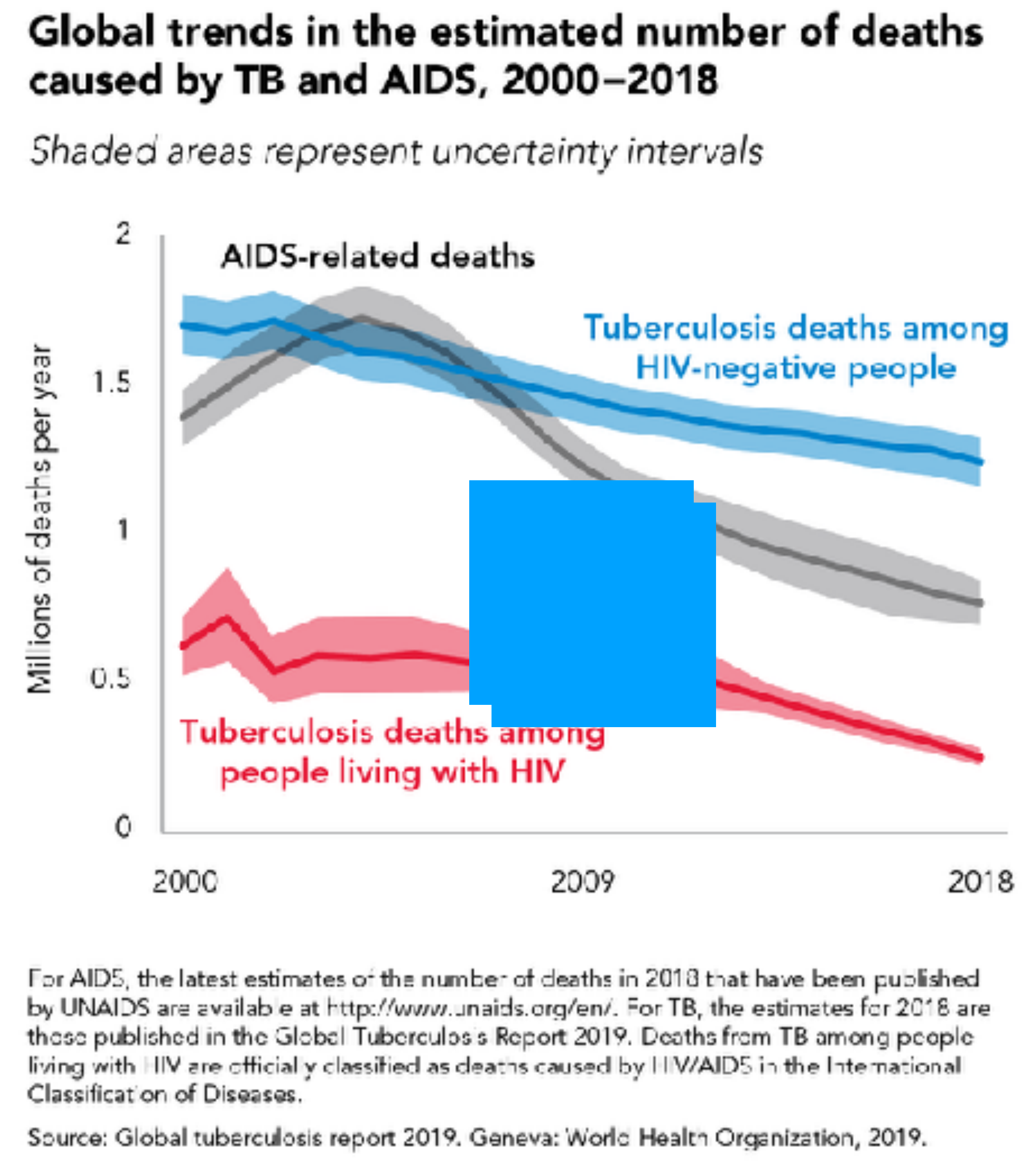
Measles killed 200,000 in 2020 alone!



LARGE MEASLES OUTBREAKS

The epidemic in the Democratic Republic of the Congo is the largest single-nation outbreak for decades.

Data from March 2020.
*Suspected, not yet officially reported to WHO.
©nature

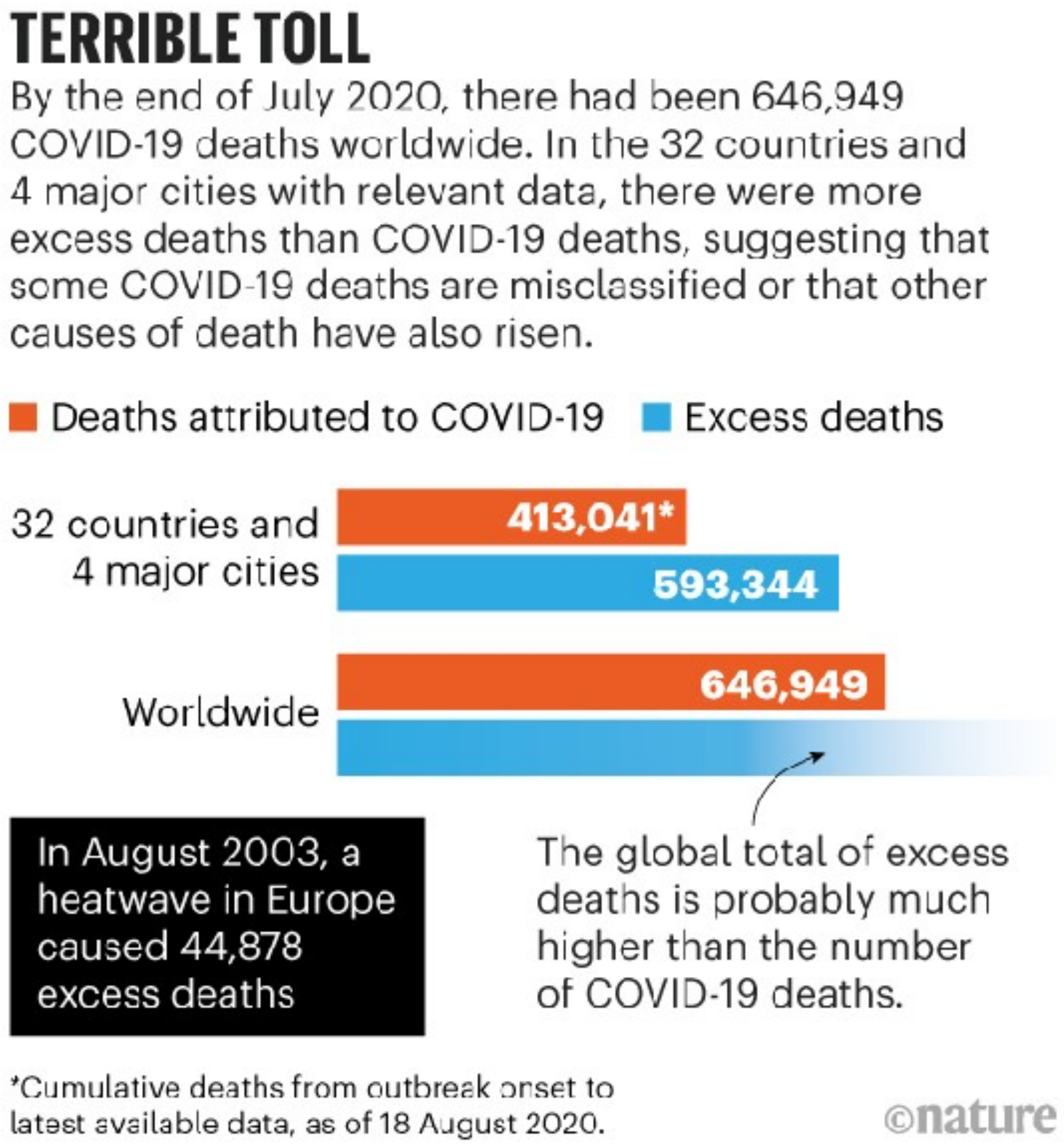


Global trends in the estimated number of deaths caused by TB and AIDS, 2000–2018

Shaded areas represent uncertainty intervals

For AIDS, the latest estimates of the number of deaths in 2018 that have been published by UNAIDS are available at http://www.unaids.org/en/. For TB, the estimates for 2018 are those published in the Global Tuberculosis Report 2019. Deaths from TB among people living with HIV are officially classified as deaths caused by HIV/AIDS in the International Classification of Diseases.

Source: Global tuberculosis report 2019. Geneva: World Health Organization, 2019.



TERRIBLE TOLL

By the end of July 2020, there had been 646,949 COVID-19 deaths worldwide. In the 32 countries and 4 major cities with relevant data, there were more excess deaths than COVID-19 deaths, suggesting that some COVID-19 deaths are misclassified or that other causes of death have also risen.

In August 2003, a heatwave in Europe caused 44,878 excess deaths

The global total of excess deaths is probably much higher than the number of COVID-19 deaths.

*Cumulative deaths from outbreak onset to latest available data, as of 18 August 2020.
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Predictions say that 1.66 million people died of tuberculosis in 2020

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

https://www.nature.com/articles/d41586-020-02497-w

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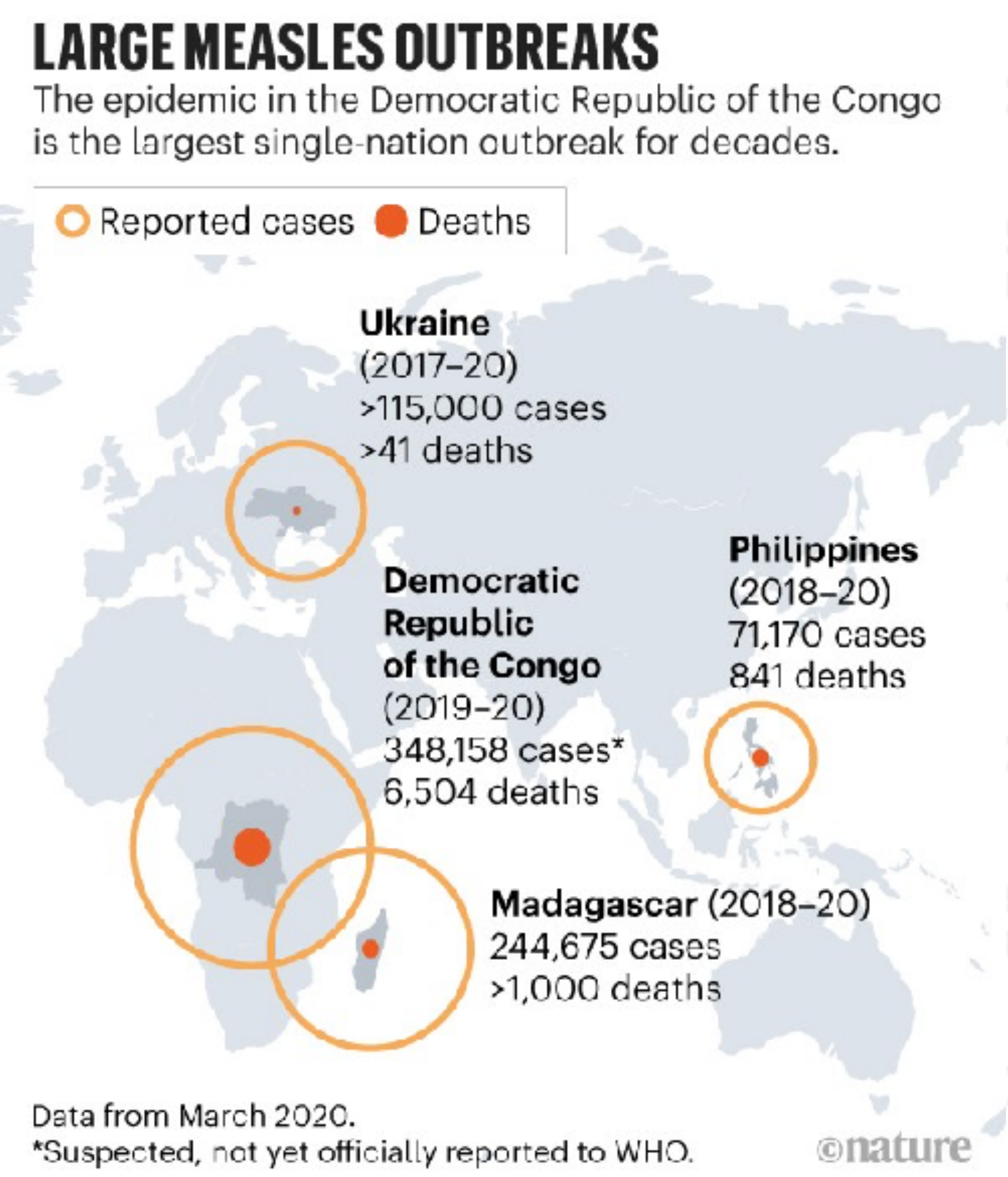

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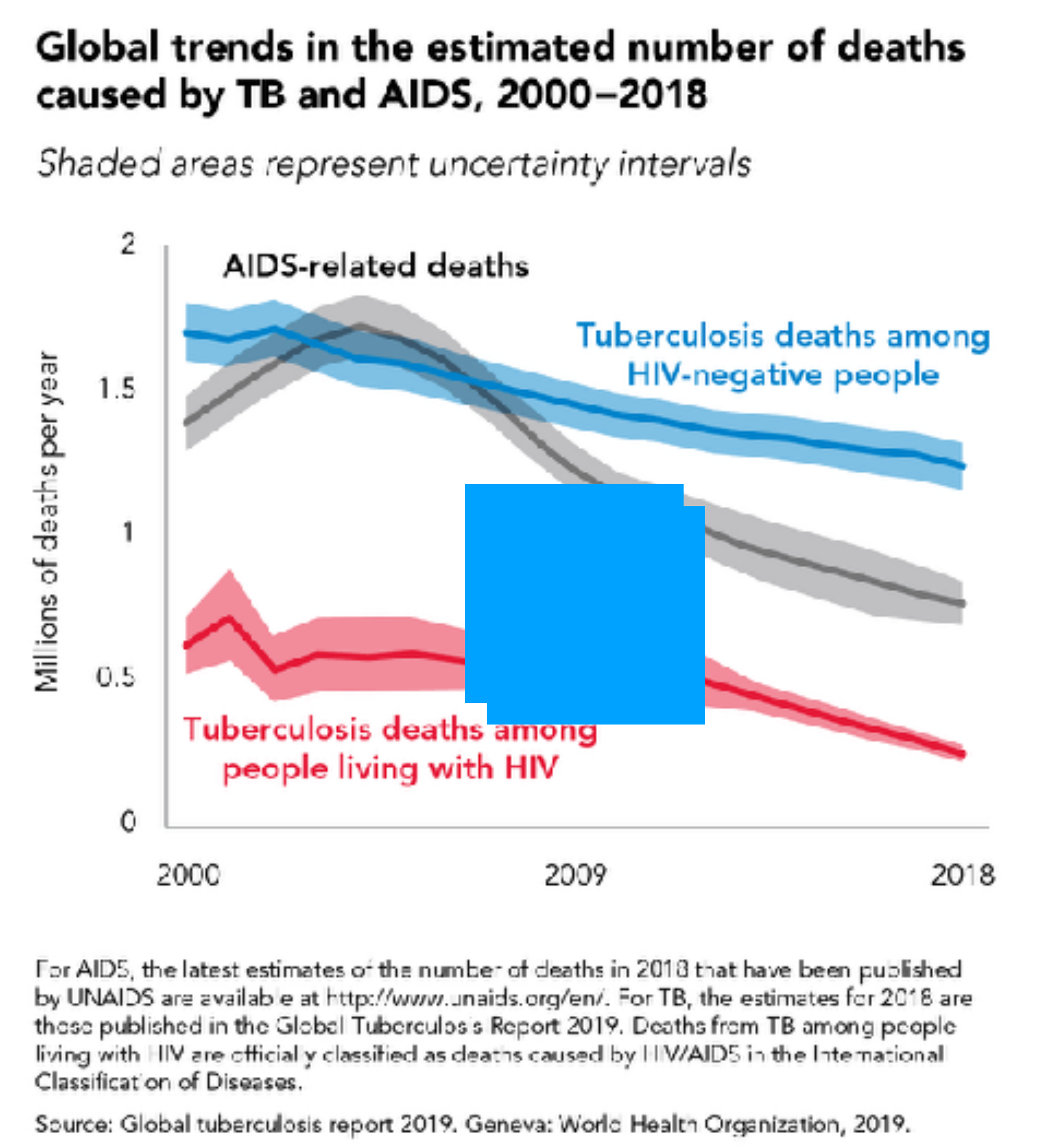

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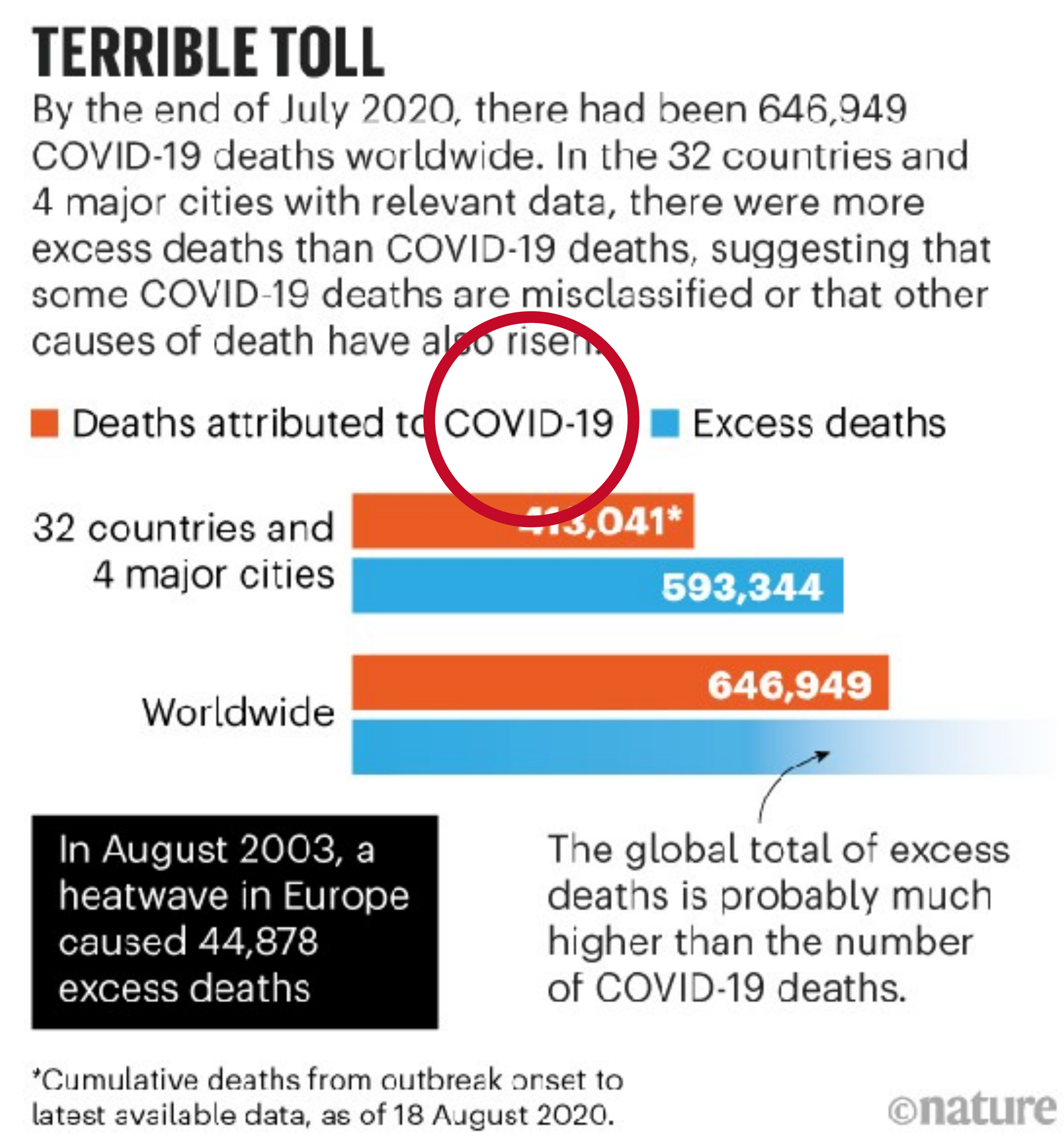

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Societal challenge

- 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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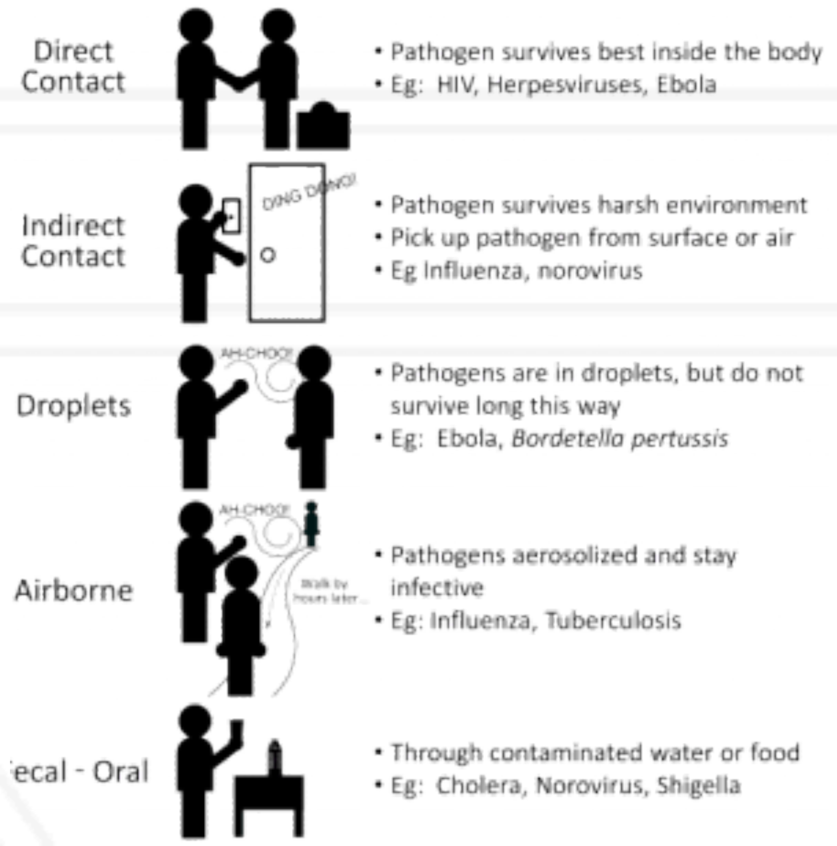
Model for human transmission



Direct Contact	• Pathogen survives best inside the body • Eg: HIV, Herpesviruses, Ebola
Indirect Contact	• Pathogen survives harsh environment • Pick up pathogen from surface or air • Eg Influenza, norovirus
Droplets	• Pathogens are in droplets, but do not survive long this way • Eg: Ebola, *Bordetella pertussis*
Airborne	• Pathogens aerosolized and stay infective • Eg: Influenza, Tuberculosis
ecal - Oral	• Through contaminated water or food • Eg: Cholera, Norovirus, Shigella

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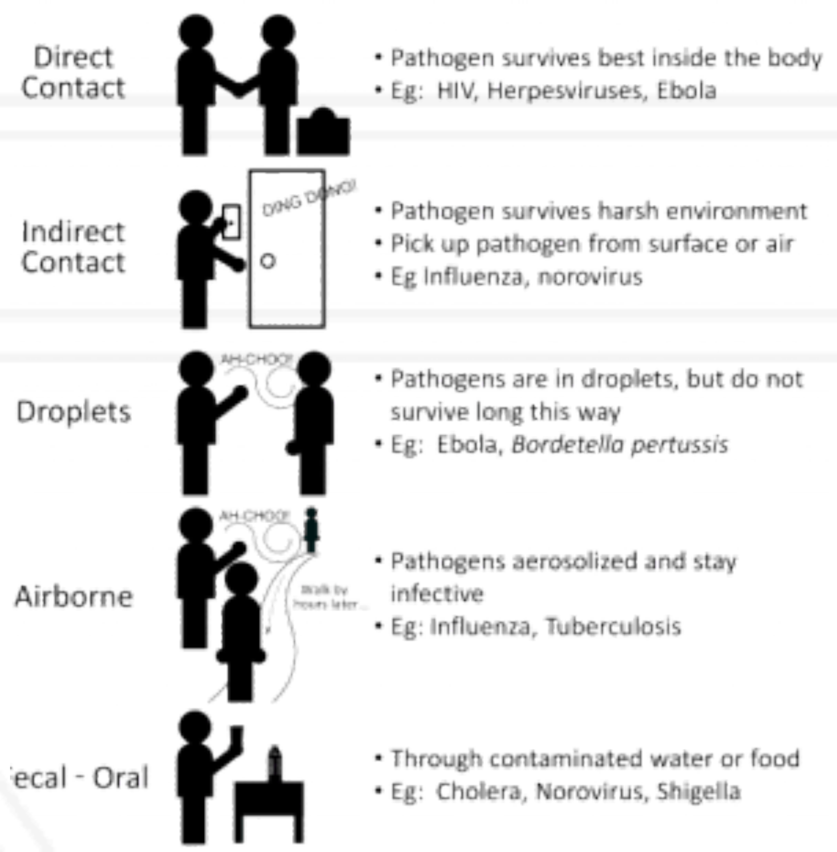

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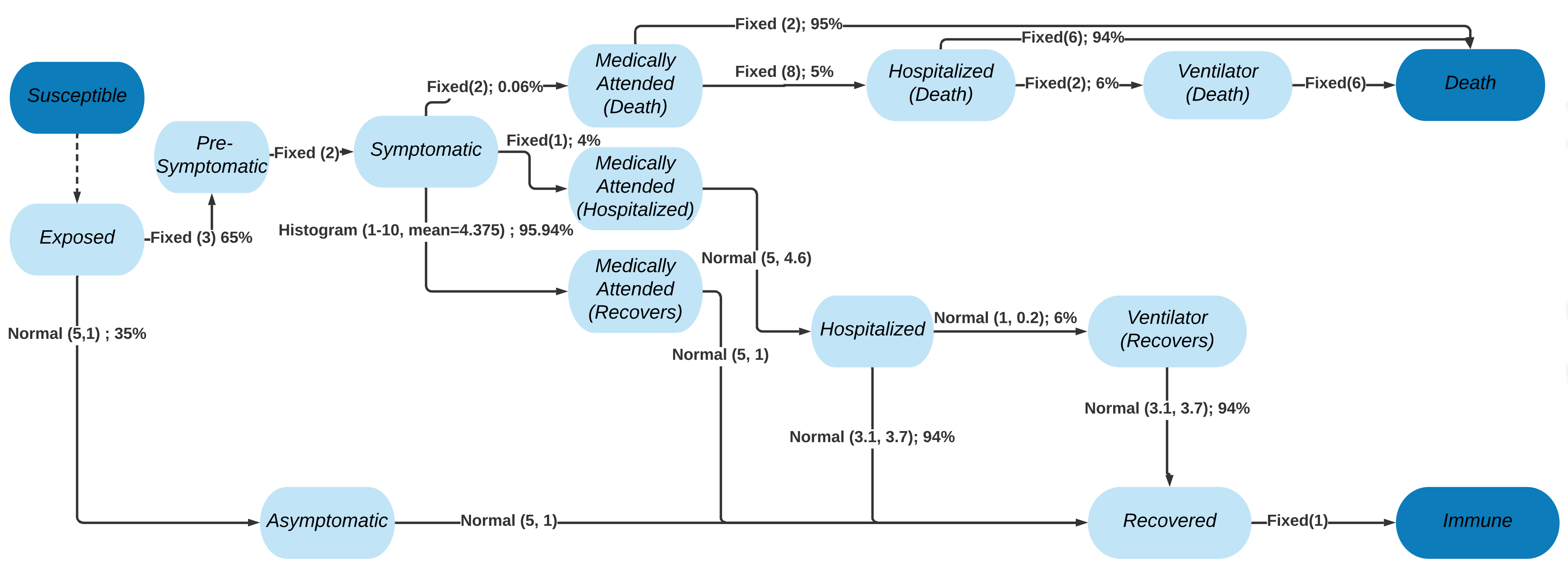
Disease model for each person



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Combination of network theory and discrete-event simulations

- Hybrid time-stepped and discrete-event simulation

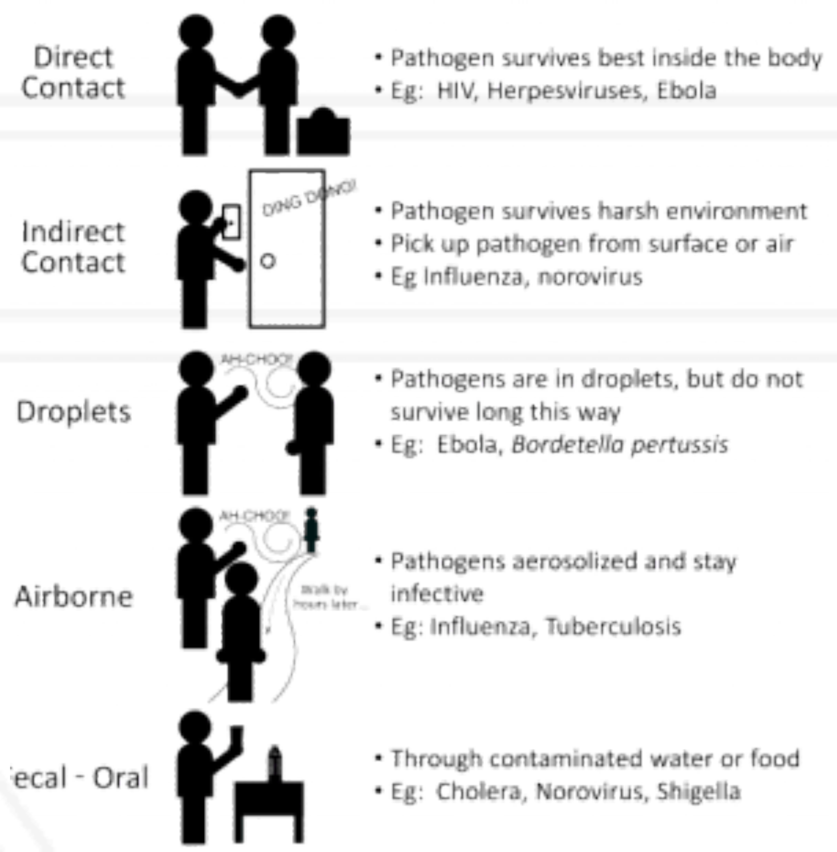
```
while d < num_days:
  for each person:
    Send visit messages to locations

  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

Model for human transmission



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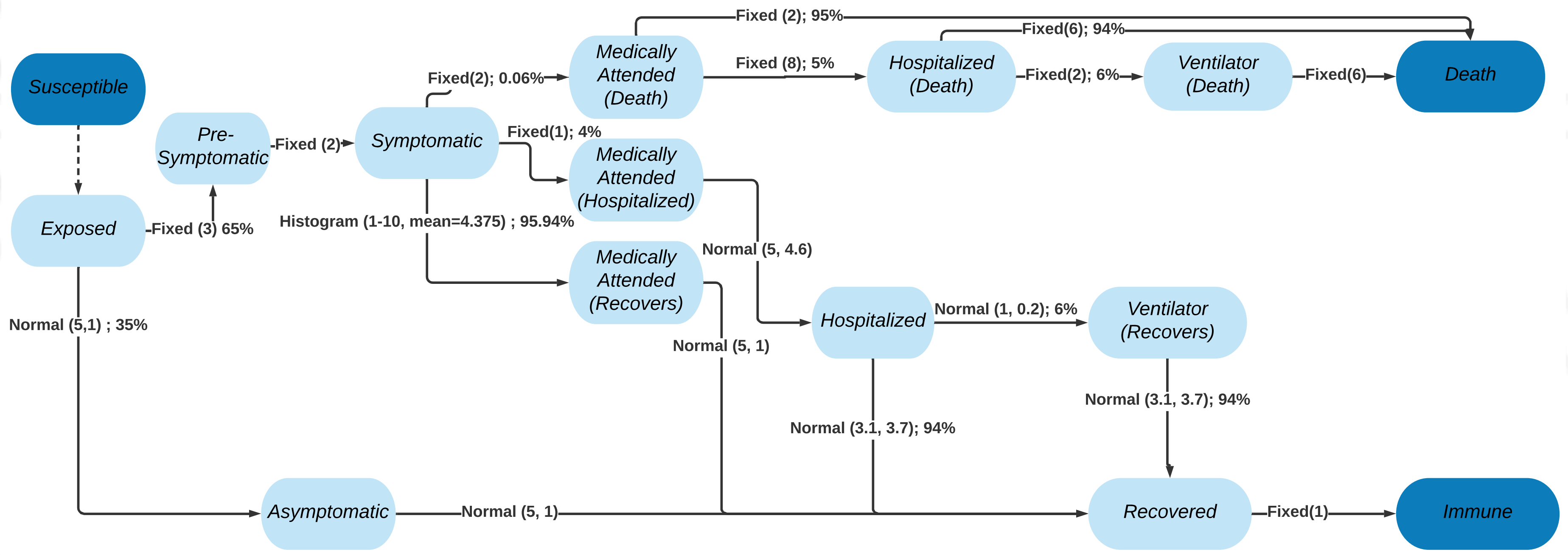

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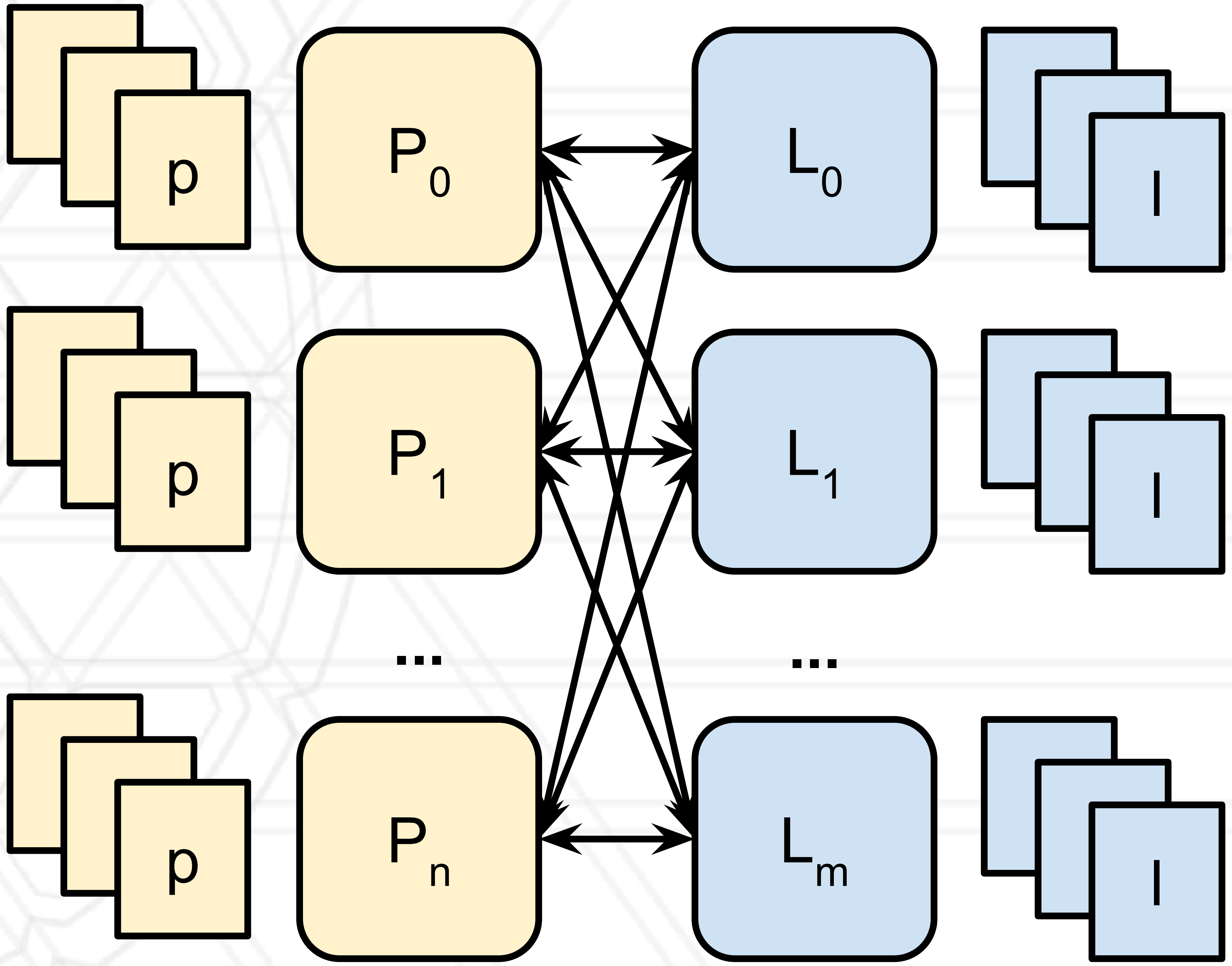
Parallel simulation is challenging

- 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

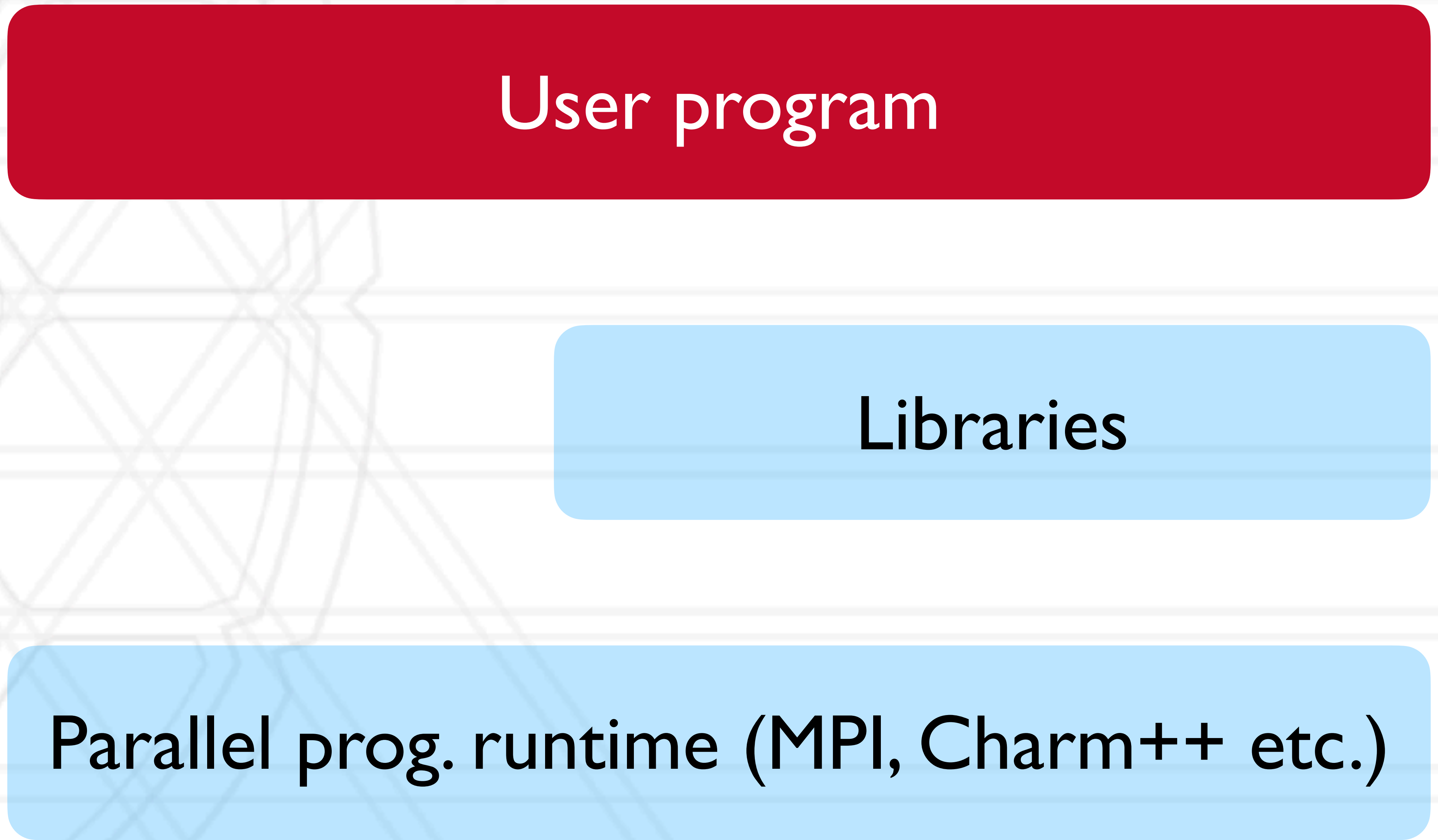
Parallel implementation: Loimos

- 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 …


User program

Libraries

Parallel prog. runtime (MPI, Charm++ etc.)

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

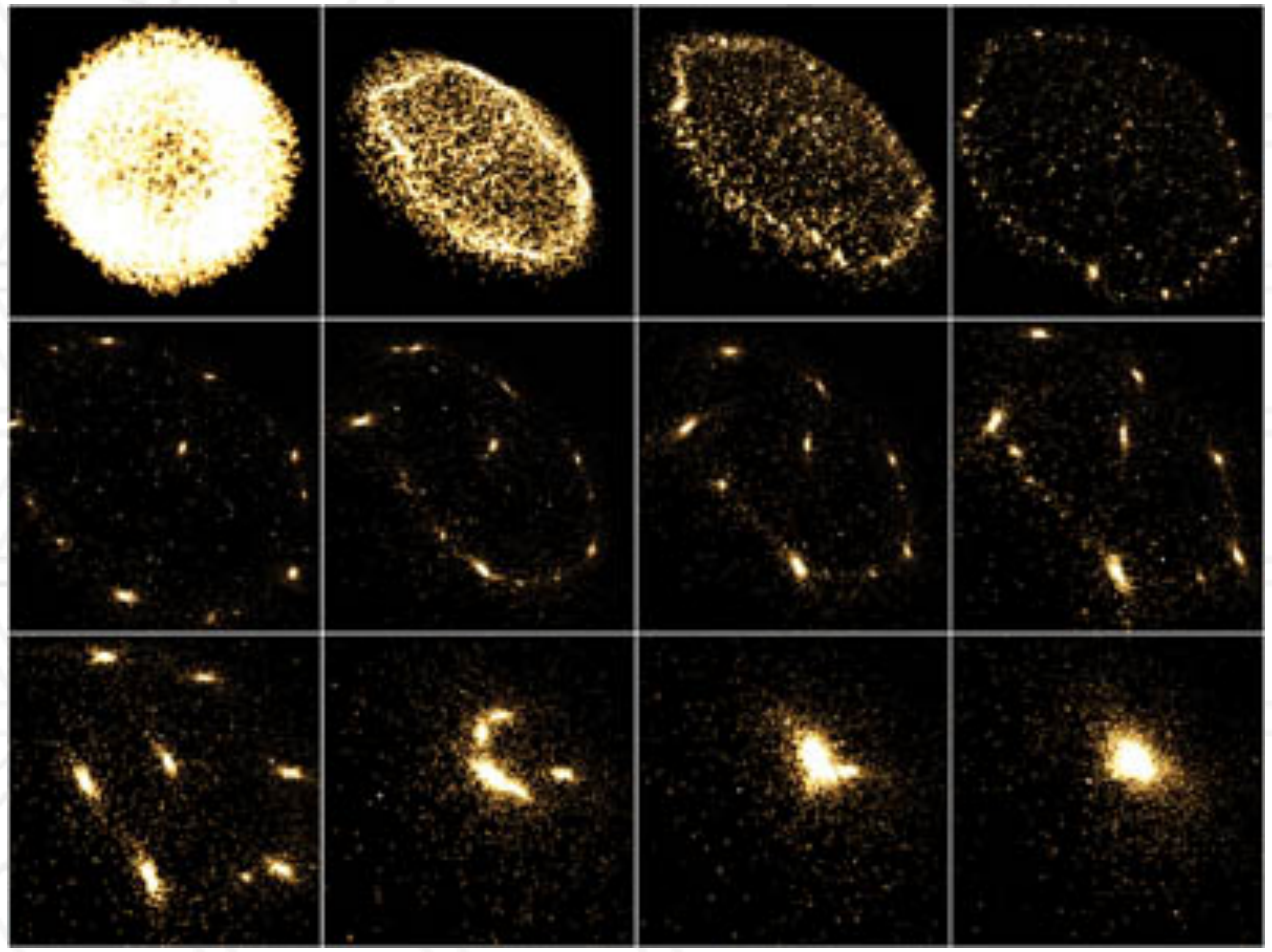
https://events.prace-ri.eu/event/176/contributions/38/attachments/154/305/HPC_libraries.pdf

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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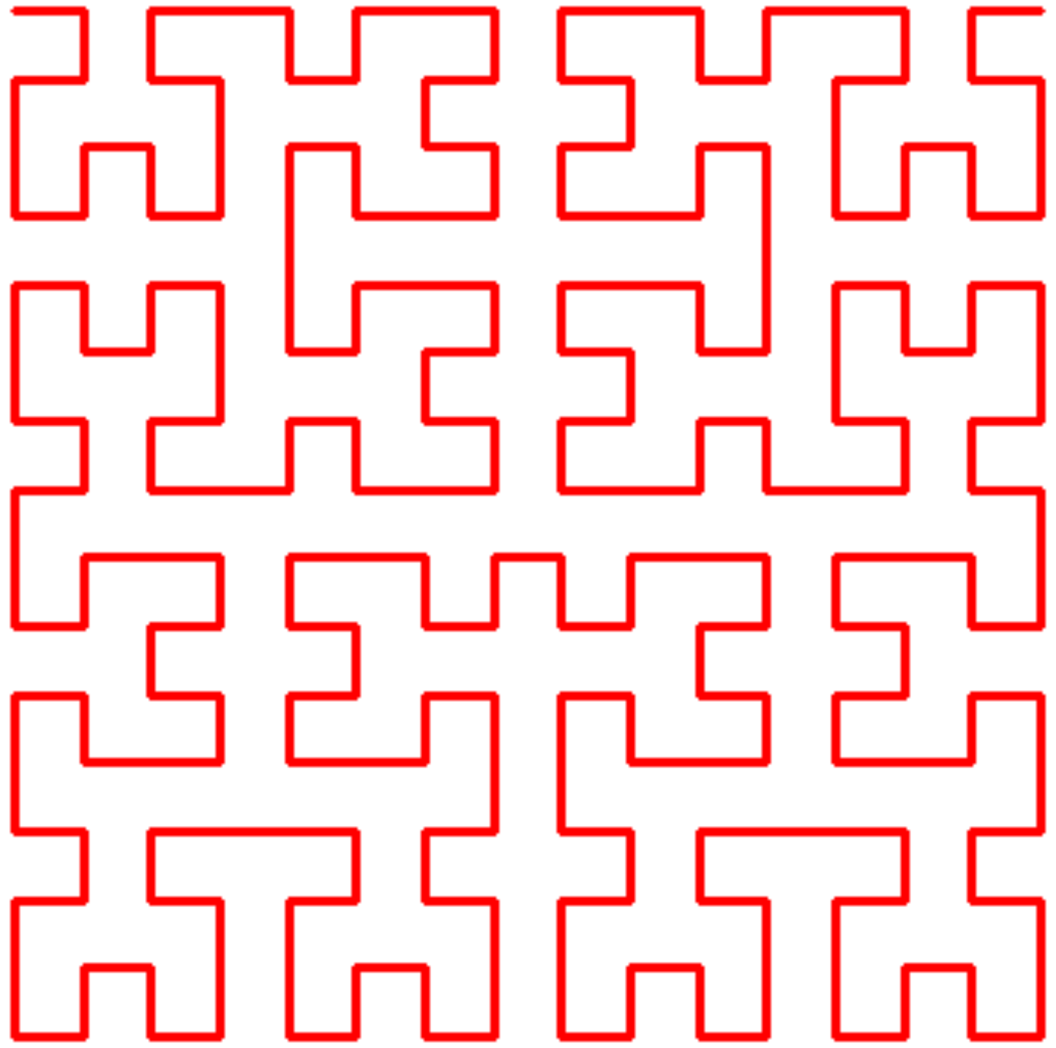

Space-filling curves

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

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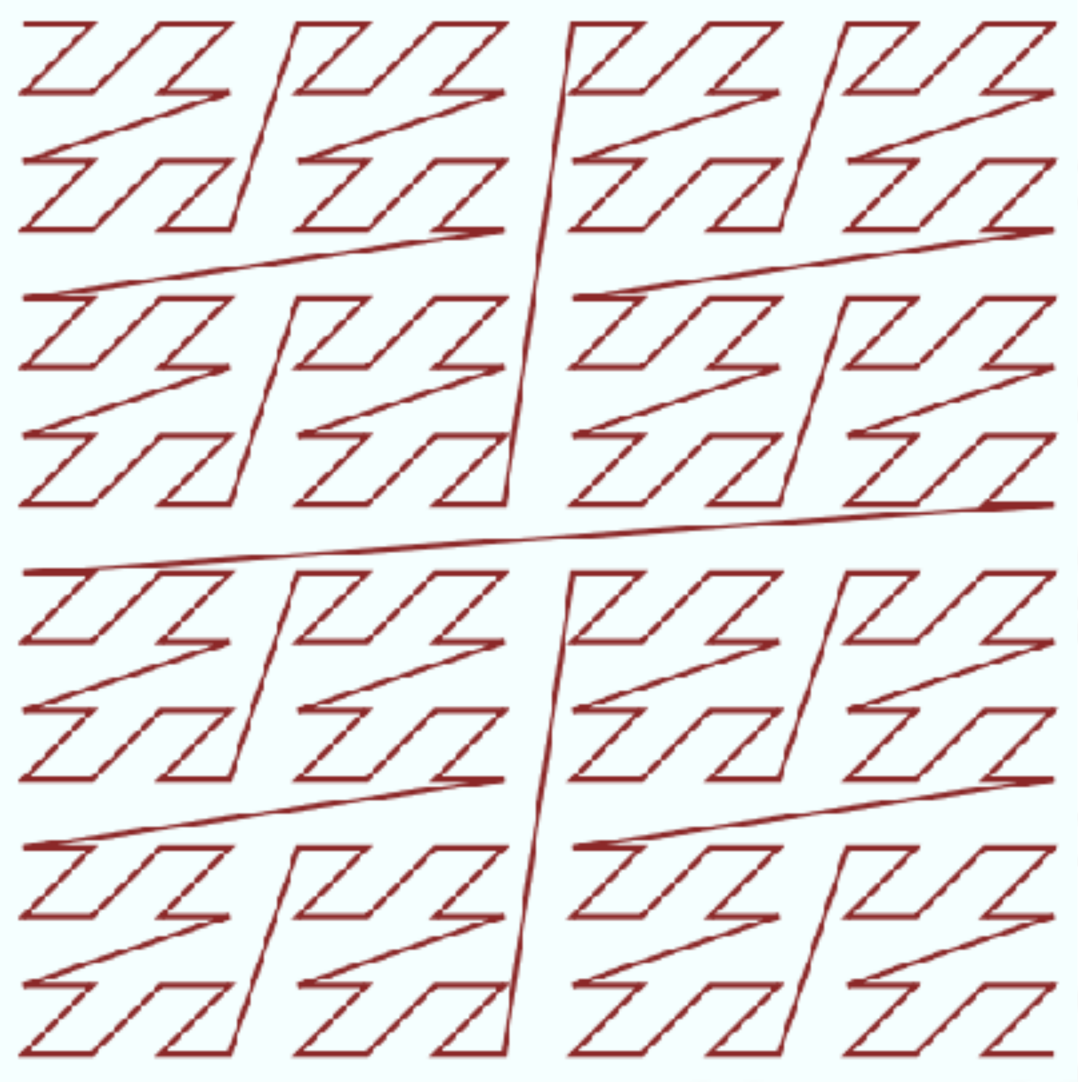

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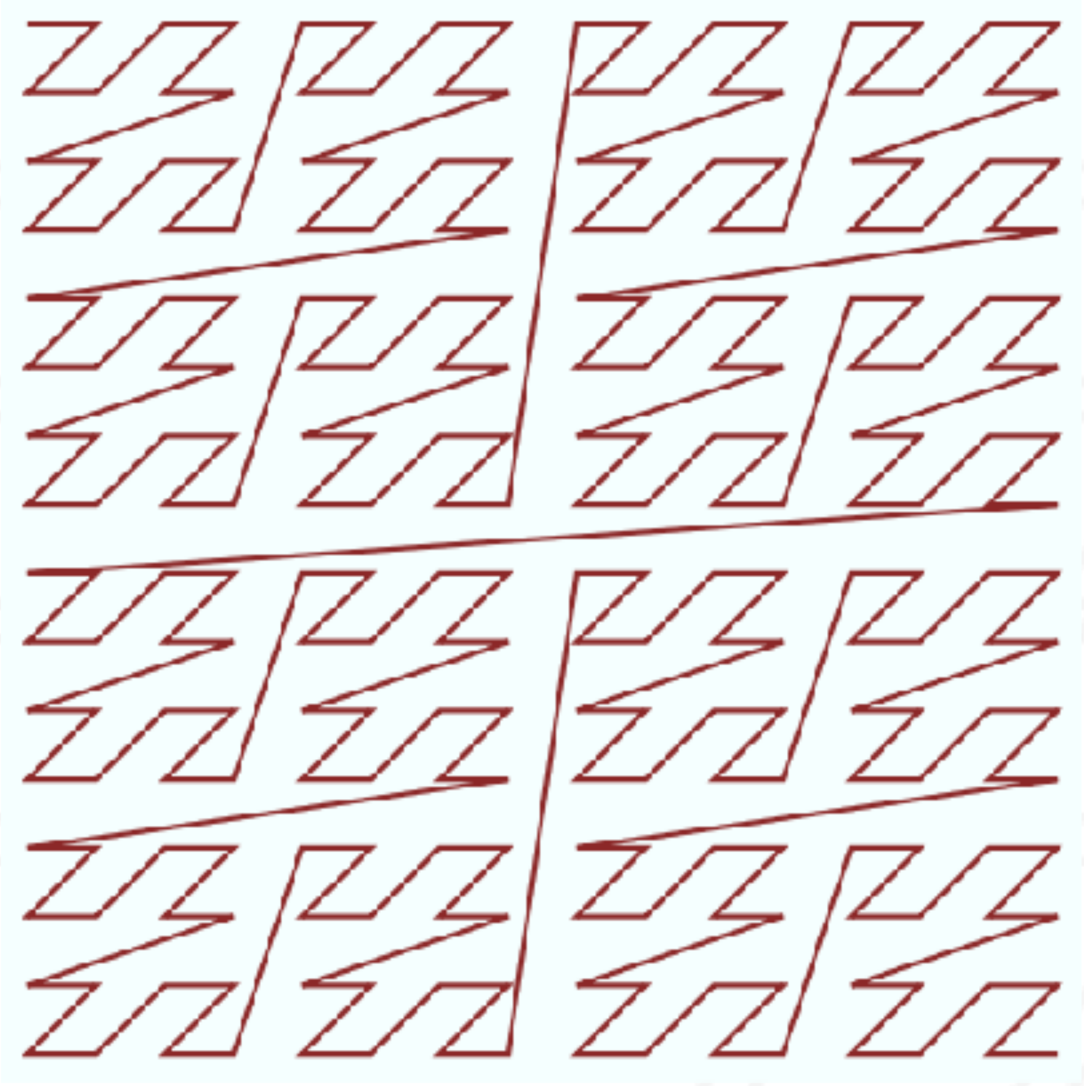

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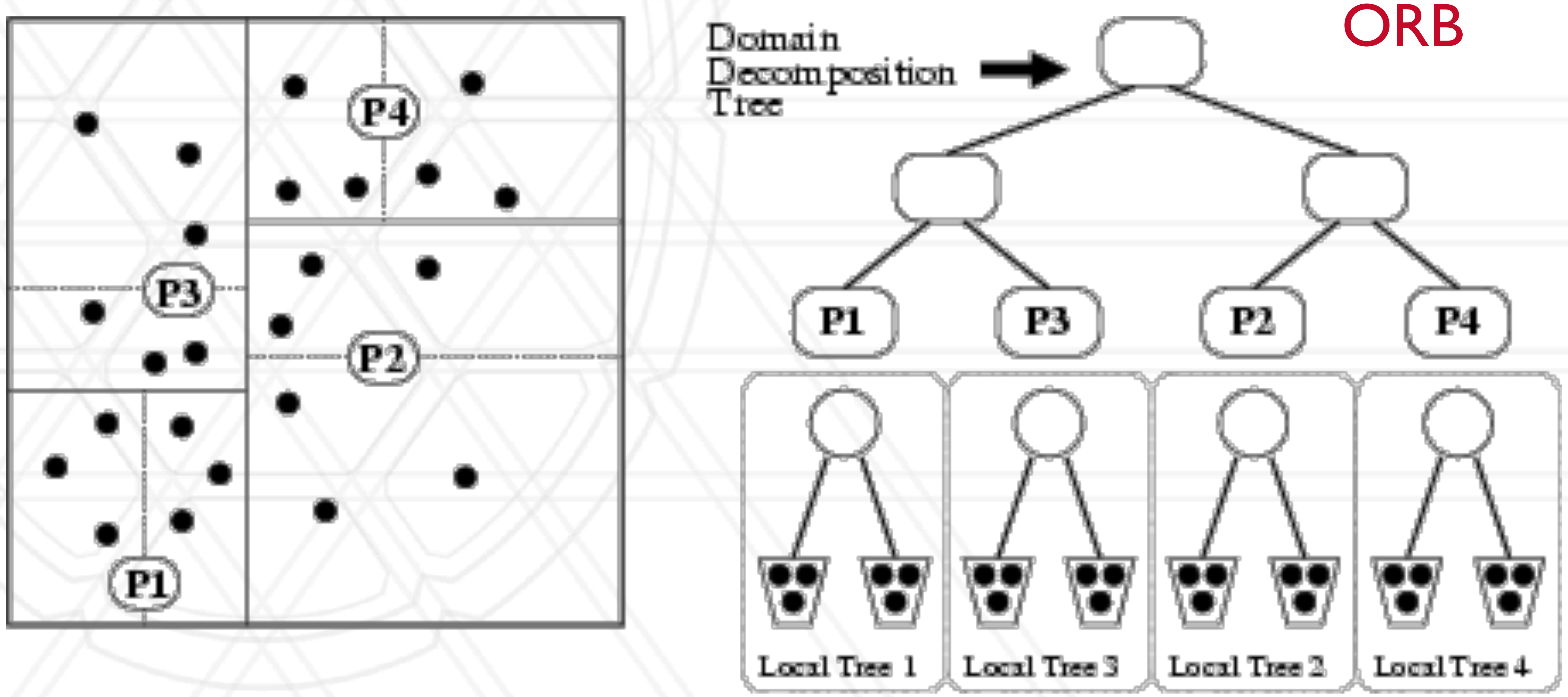
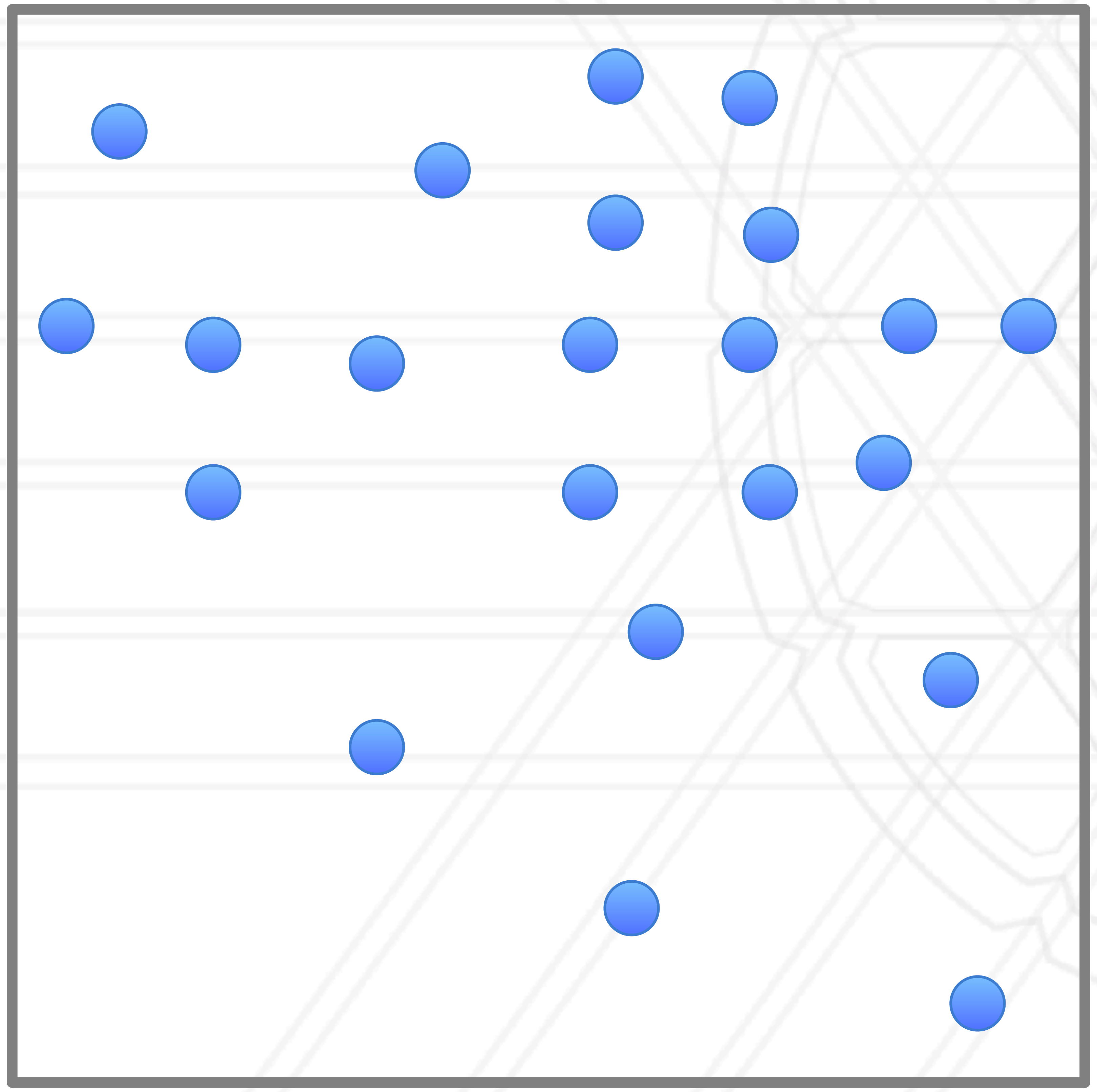


ORB

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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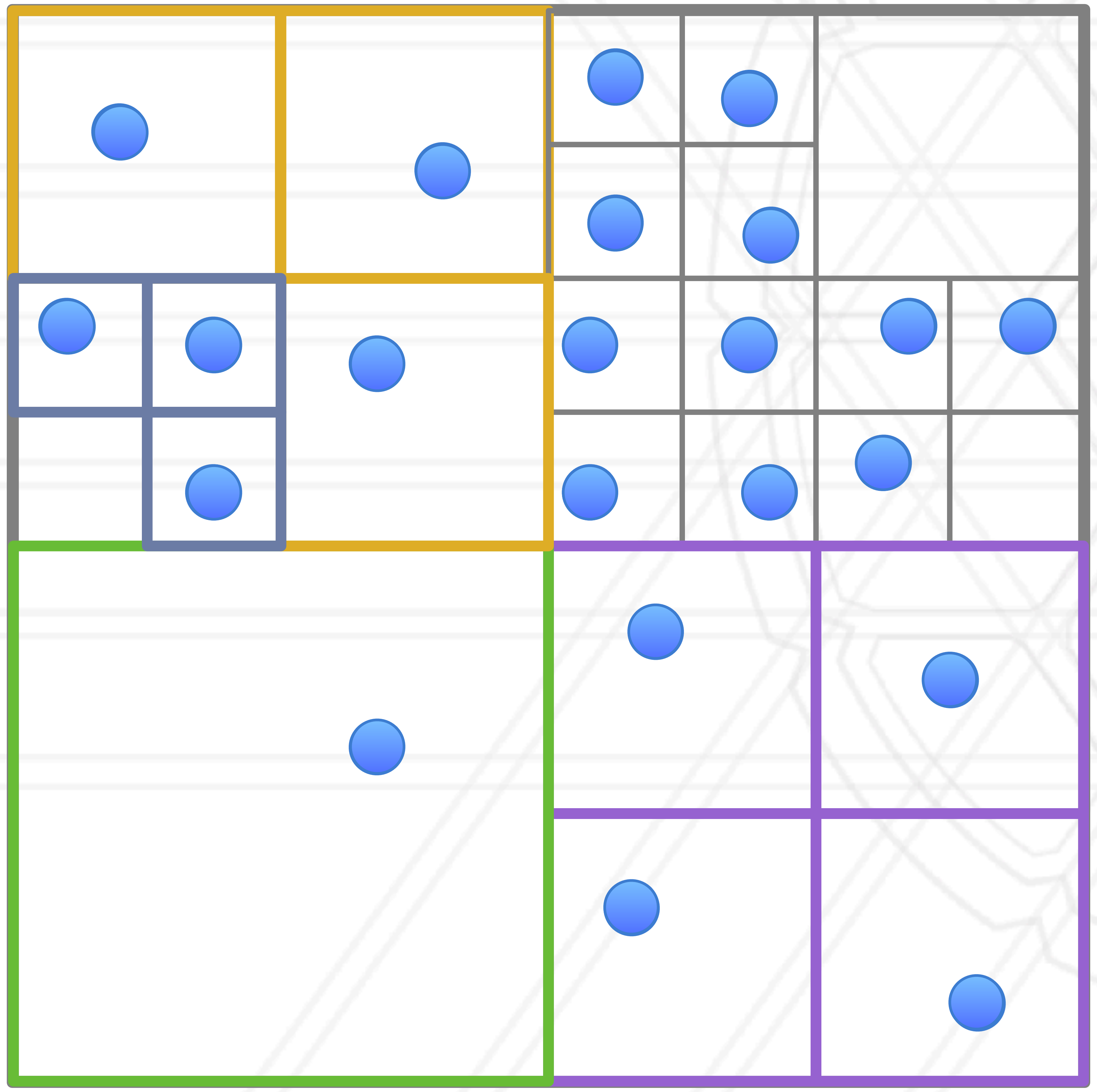

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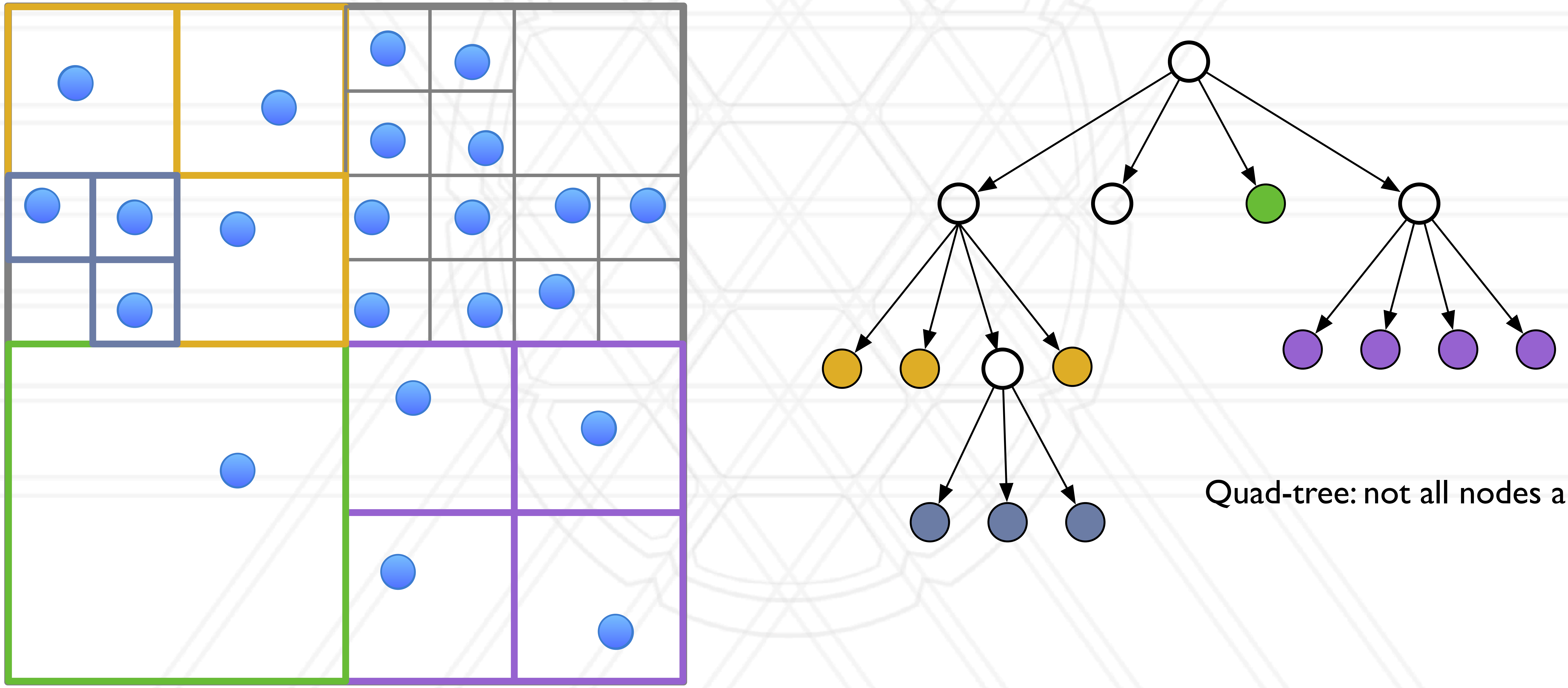


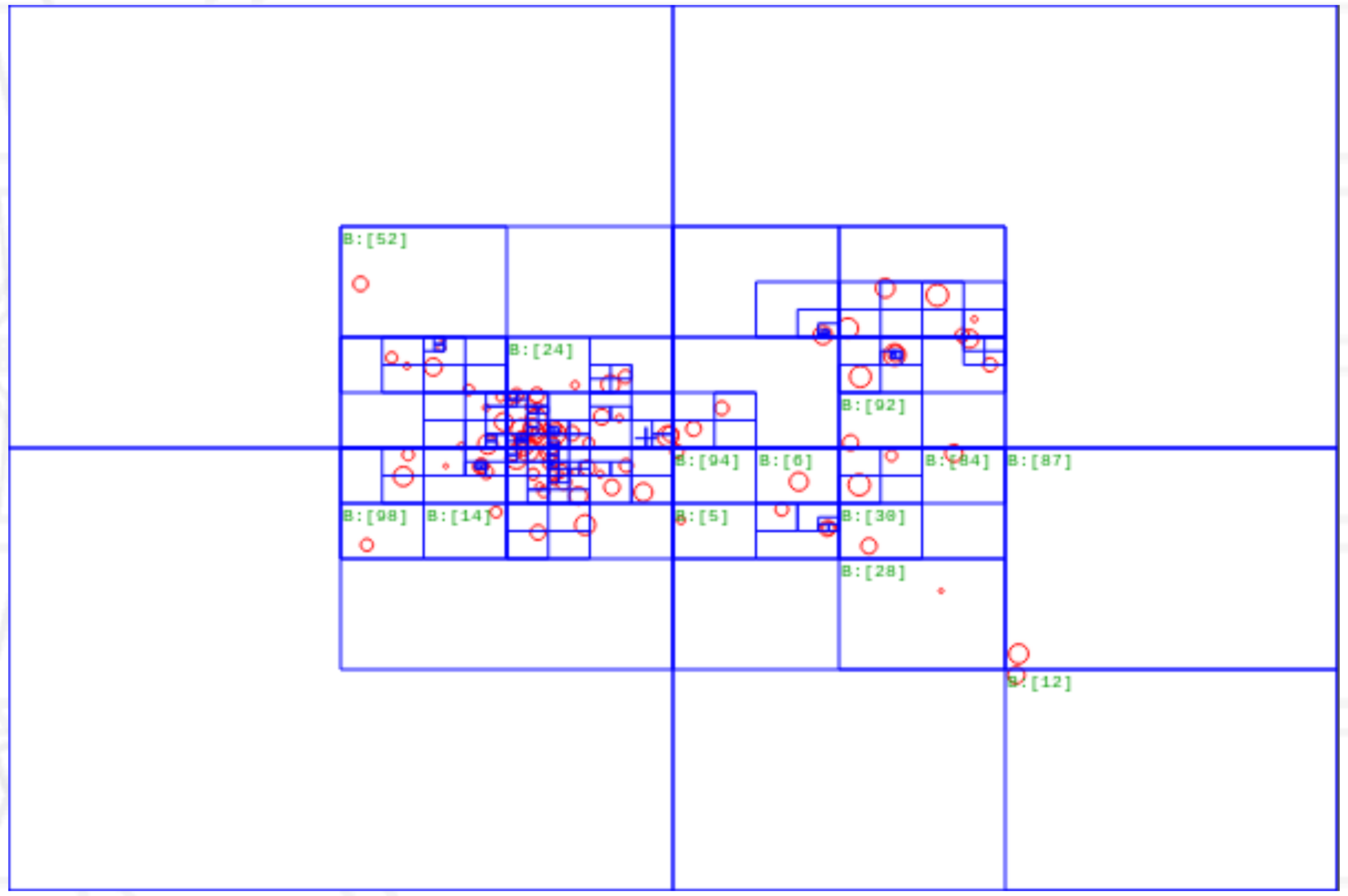
Quad-tree: not all nodes are shown

Different parallelization methods

- Tree codes: Barnes-Hut simulations
- Fast 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



https://en.wikipedia.org/wiki/Barnes–Hut_simulation

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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