N-body Simulations

Mar 26, 2021

Parallelization of Irregular Application – Cosmology Application

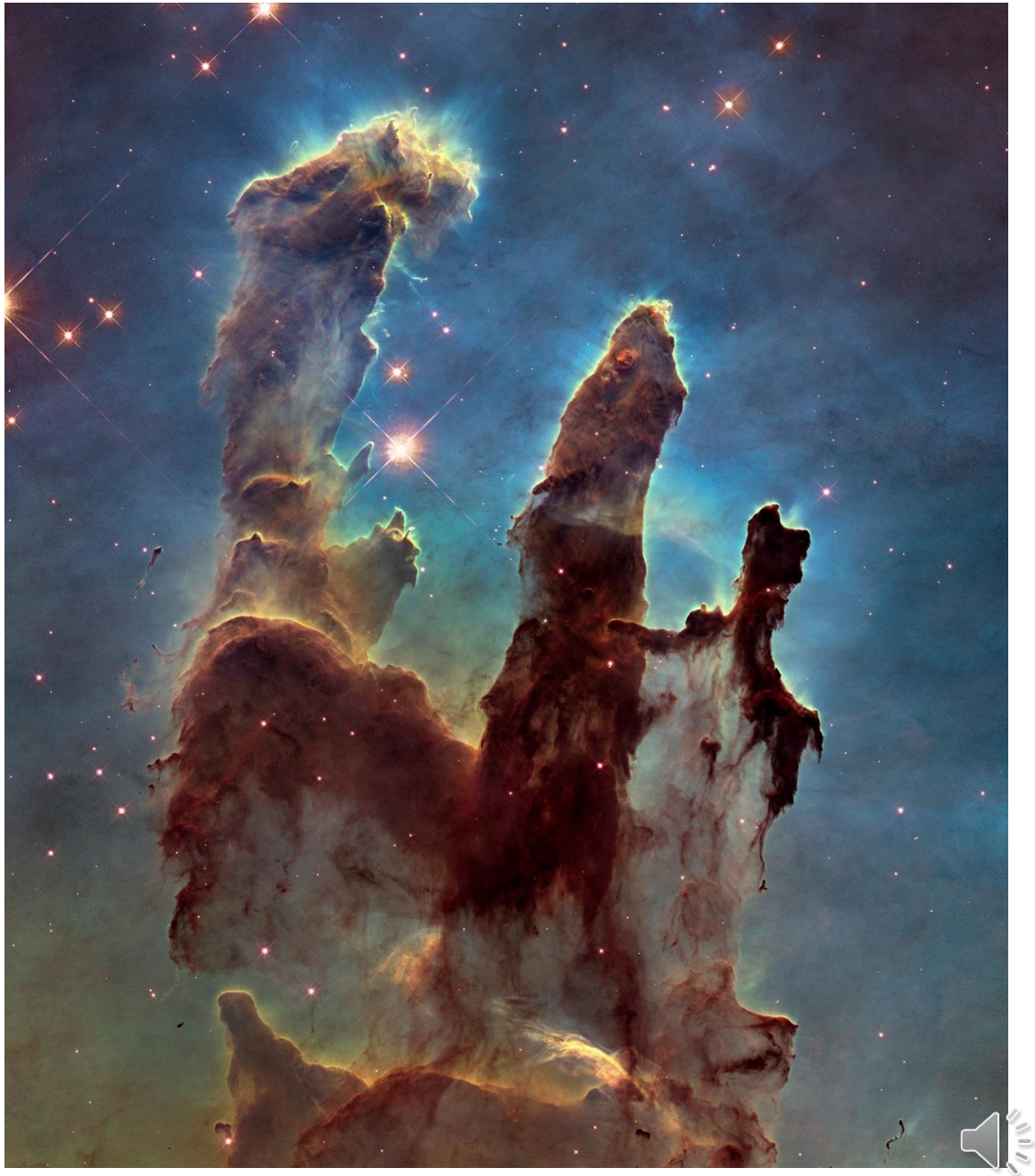
The Chinese Sky

[Source: IDP]

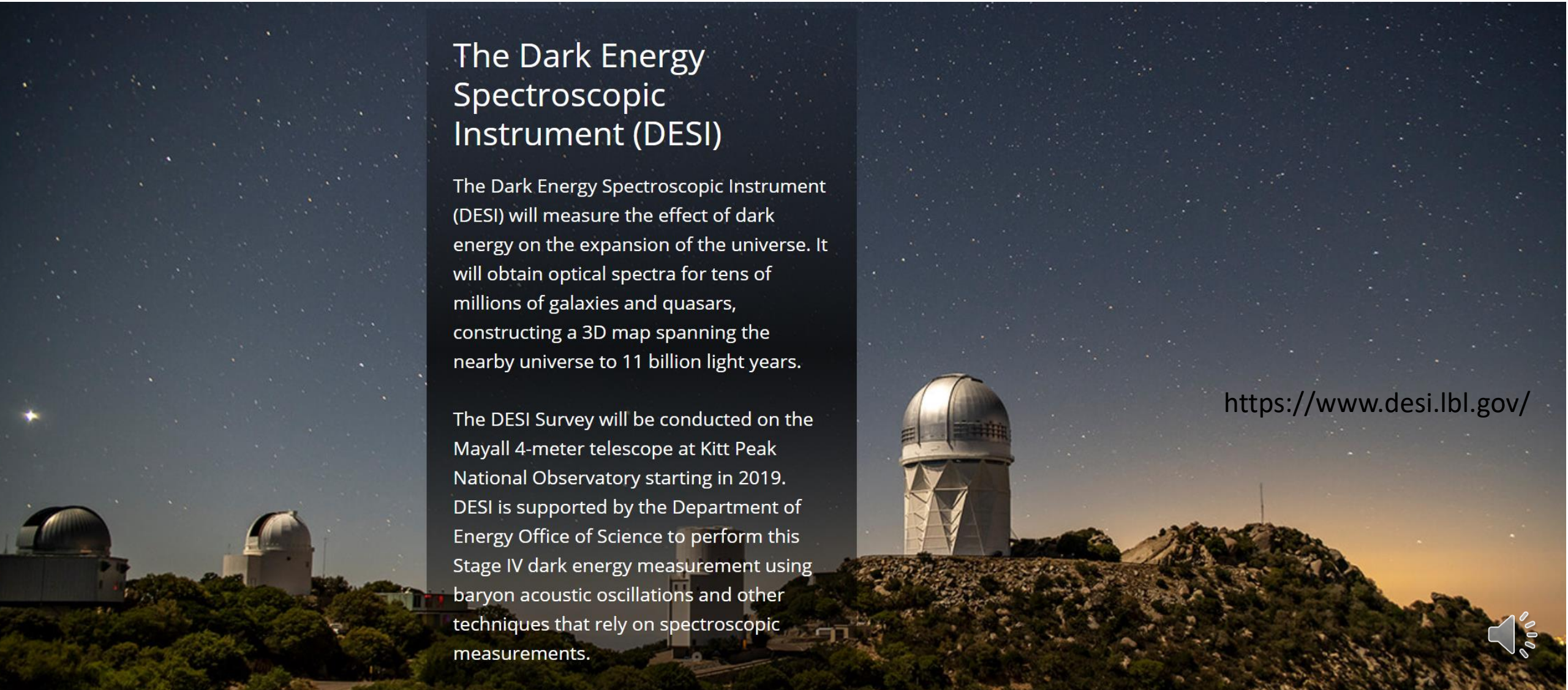
Today

“Hubble has transformed our understanding of the universe, its view from orbit unleashing a flood of cosmic discoveries that have changed astronomy forever. From its explorations of dark matter to its quest to determine the age of the universe, Hubble has helped answer some of the most compelling astronomical questions of our time, and revealed enigmas that we never knew existed. Throughout history, humanity’s eyes on the universe have never seen with more clarity or focus; find out how Hubble has opened the window to the grandeur and mystery of space.”

https://www.nasa.gov/mission_pages/hubble/main/index.html



2020



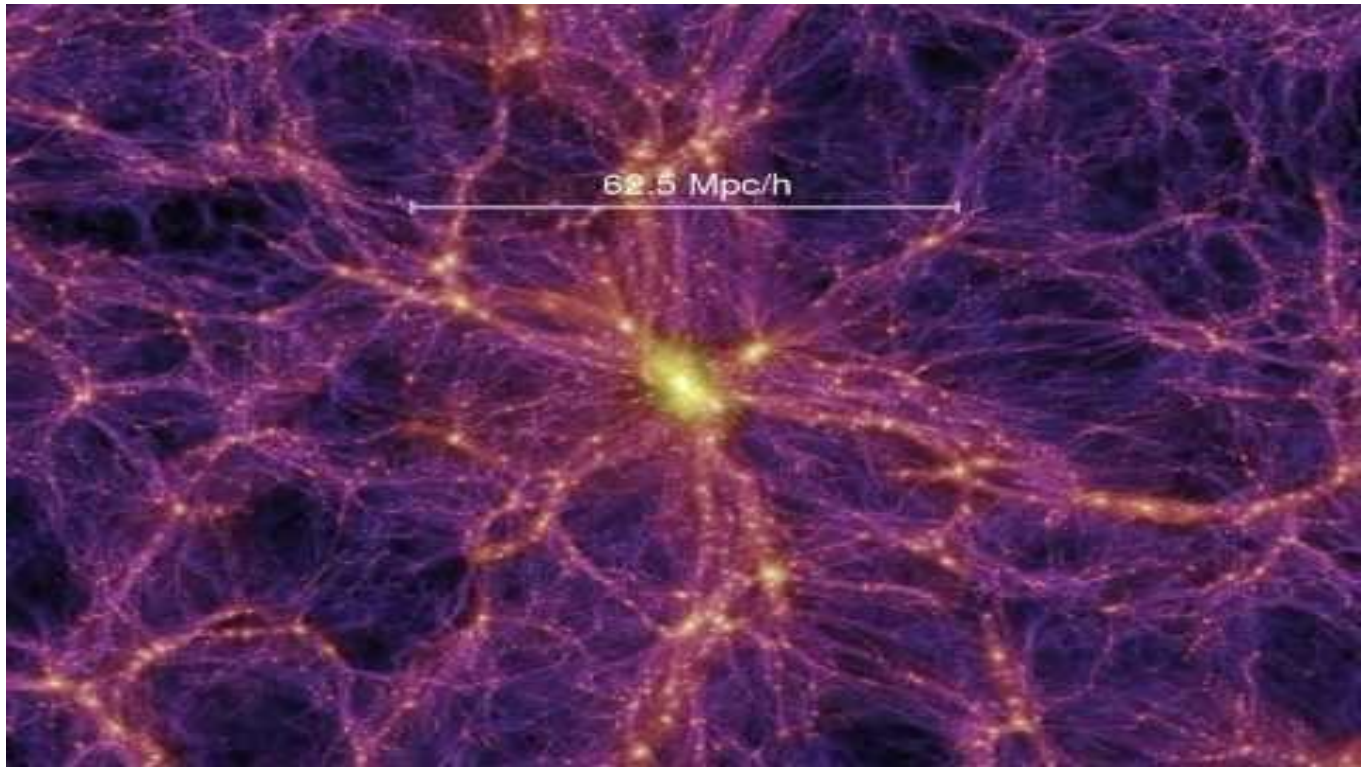
The Dark Energy Spectroscopic Instrument (DESI)

The Dark Energy Spectroscopic Instrument (DESI) will measure the effect of dark energy on the expansion of the universe. It will obtain optical spectra for tens of millions of galaxies and quasars, constructing a 3D map spanning the nearby universe to 11 billion light years.

The DESI Survey will be conducted on the Mayall 4-meter telescope at Kitt Peak National Observatory starting in 2019. DESI is supported by the Department of Energy Office of Science to perform this Stage IV dark energy measurement using baryon acoustic oscillations and other techniques that rely on spectroscopic measurements.

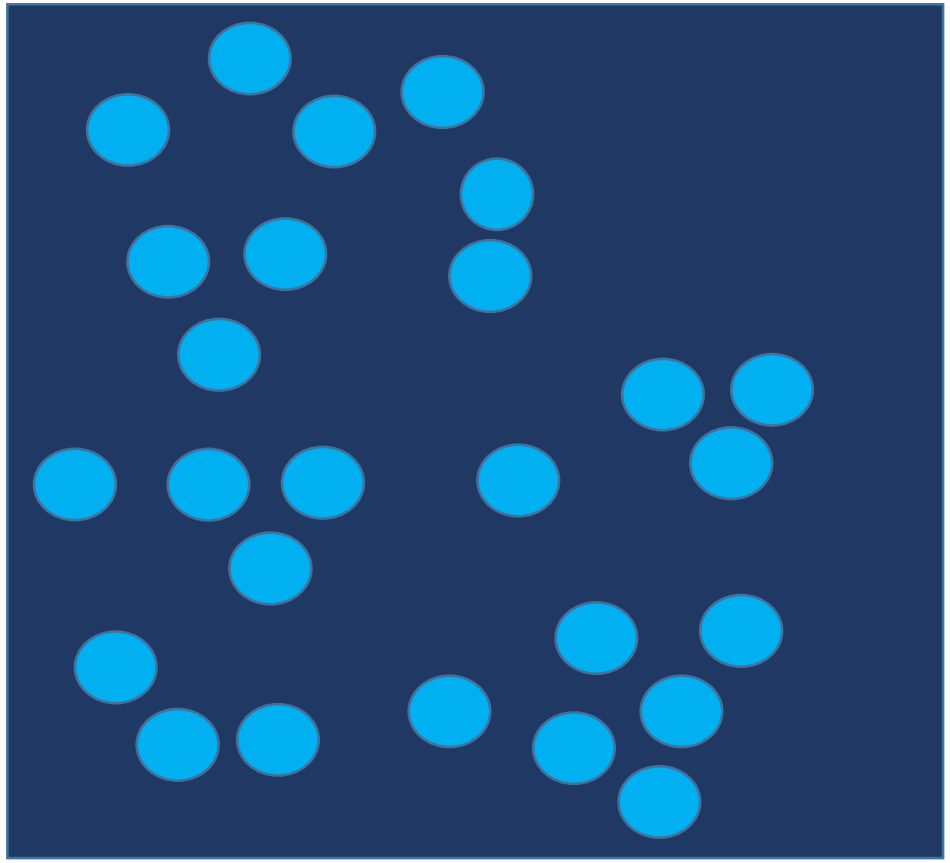
https://www.desi.lbl.gov/

The Millennium Simulation (MPA)



https://wwwmpa.mpa-garching.mpg.de/galform/virgo/millennium/

N-body Simulation



Problem

- N bodies exert force on each other
- Model positions of the particles over time

Applications

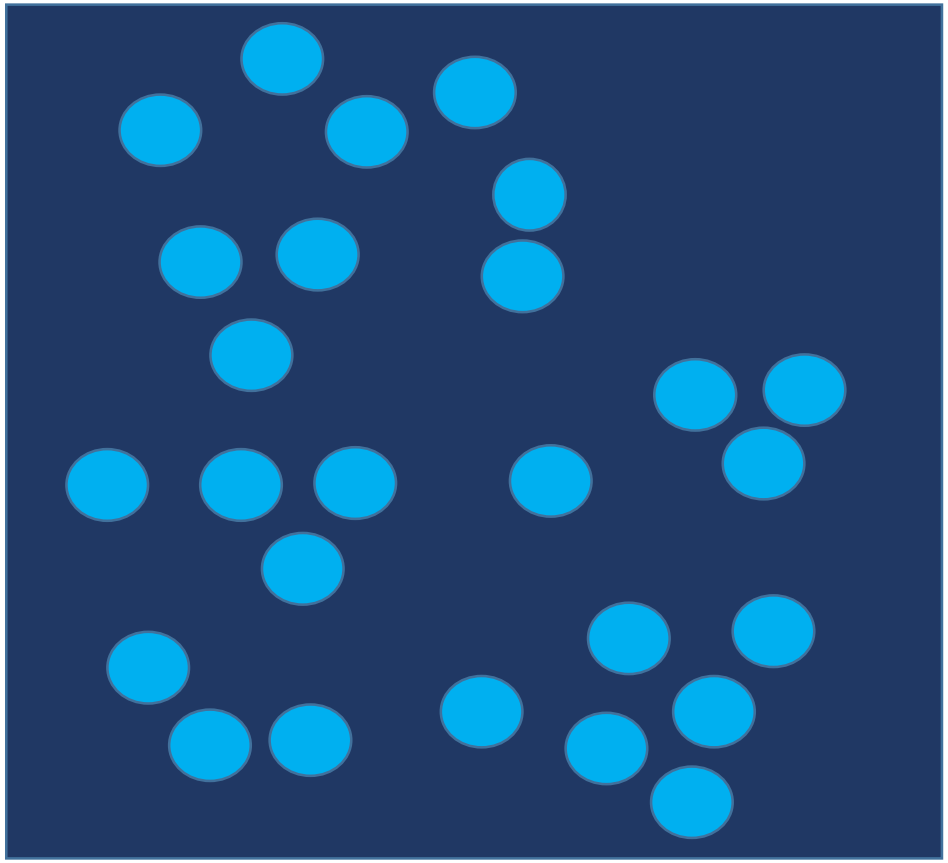
- Evolution of the universe
- Crack propagation in a material

Evolution of Universe

- Understand the evolution of stars over time
  - What if galaxies collide?
- Simulate motion of stars under external forces (N-body problem)
- Compute gravitational forces exerted on each other
  - Pairwise interactions $O(n^2)$ is prohibitively expensive
  - Influence of farther stars are less

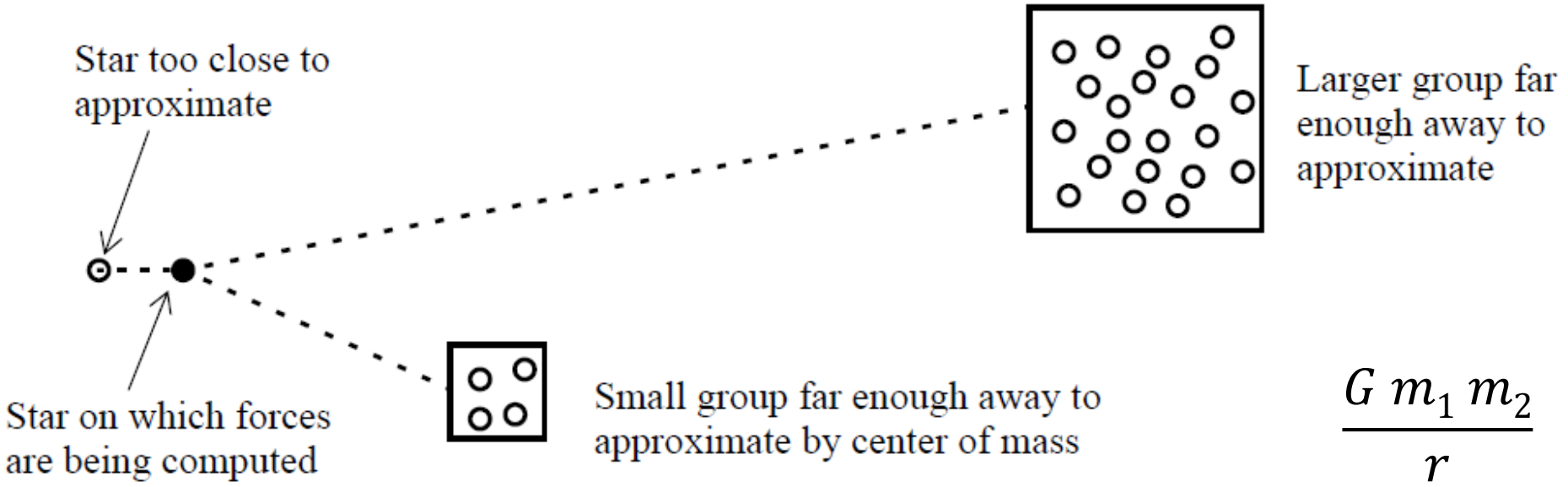
$$\frac{G\, m_1\, m_2}{r}$$

Cosmological Simulation



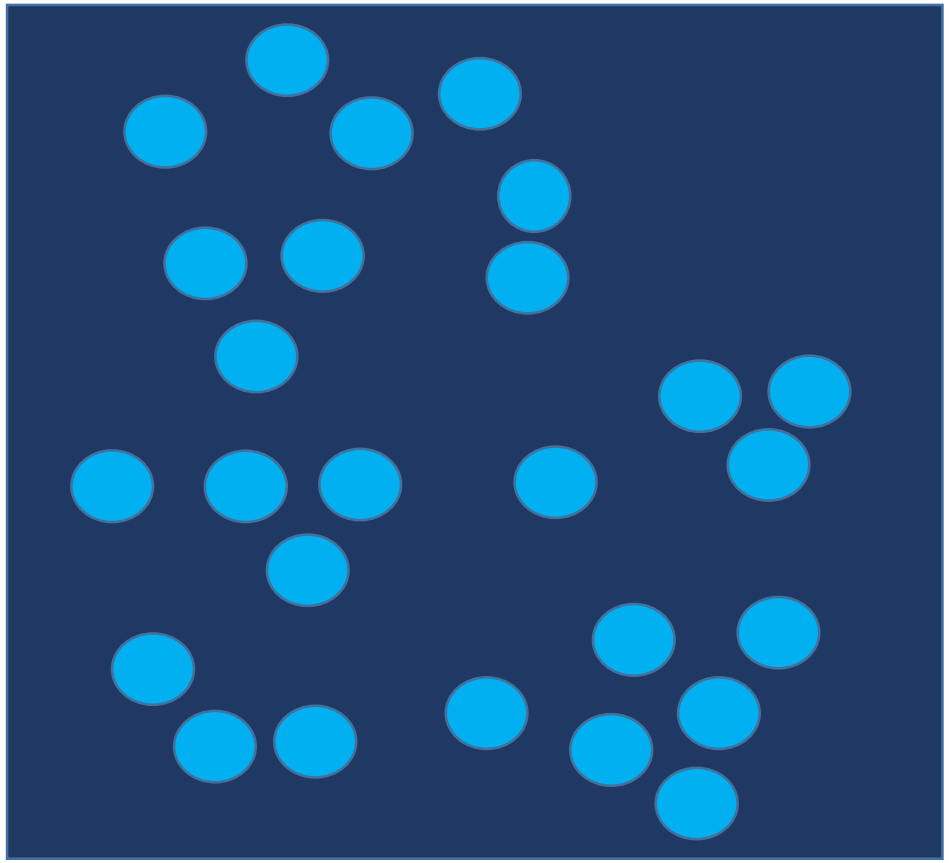
- Net force on every celestial object estimated
- Fields – three-dimensional position, velocity, acceleration, and mass
- Thousands of time steps
- Positions updated, evolving system
- Spatial distribution is irregular
- 8000 hrs → 20 hrs [Appel et al., 1985]

Approximation



$$\frac{G\ m_1\ m_2}{r}$$

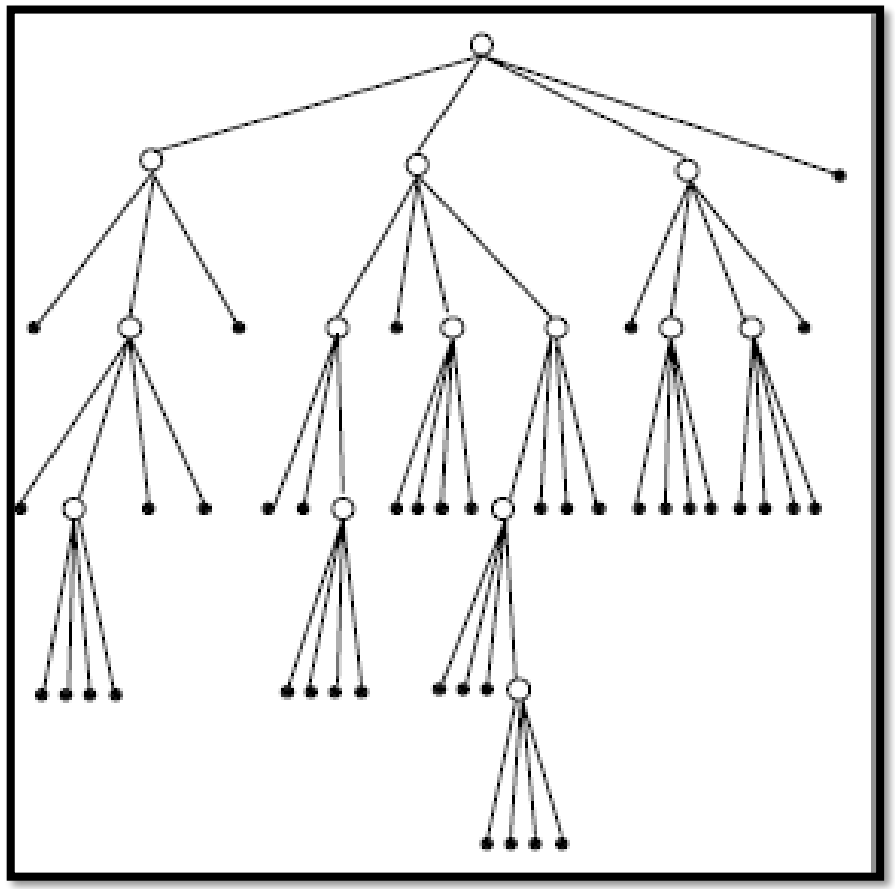
Barnes-Hut – Hierarchical Decomposition



[1986] Barnes-Hut method

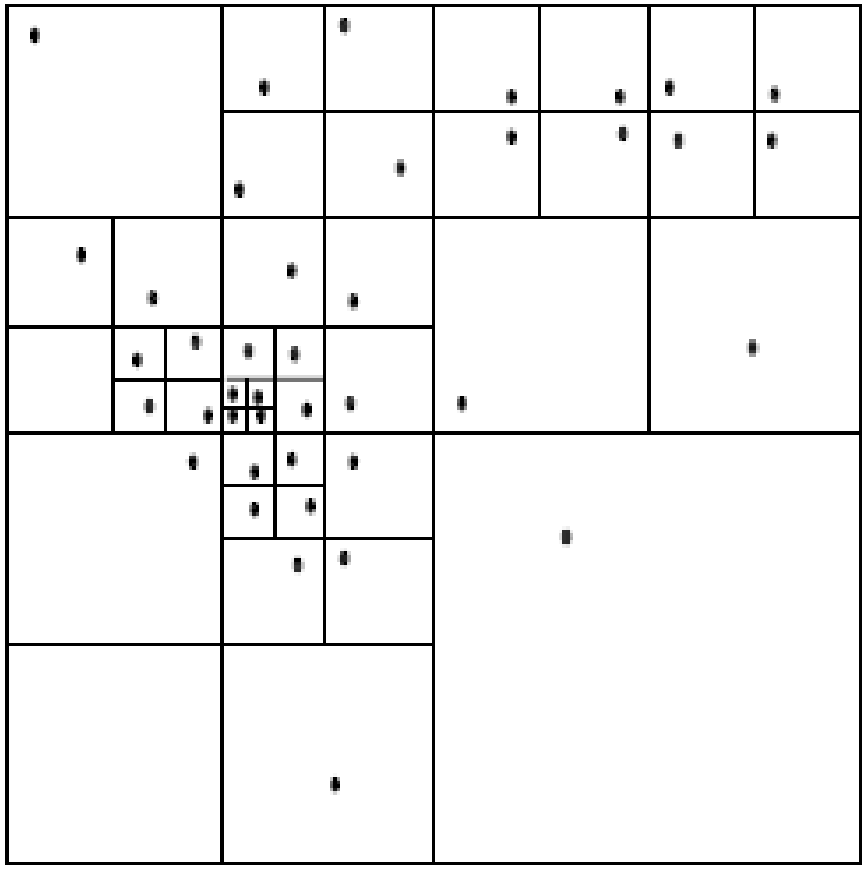
- Effect of a large group of bodies may be approximated by a single equivalent body
- Center of mass (CoM) approximation for distant bodies
- Sub-divide the space into 8 sub-regions
- Sub-divide each region based on the number of bodies

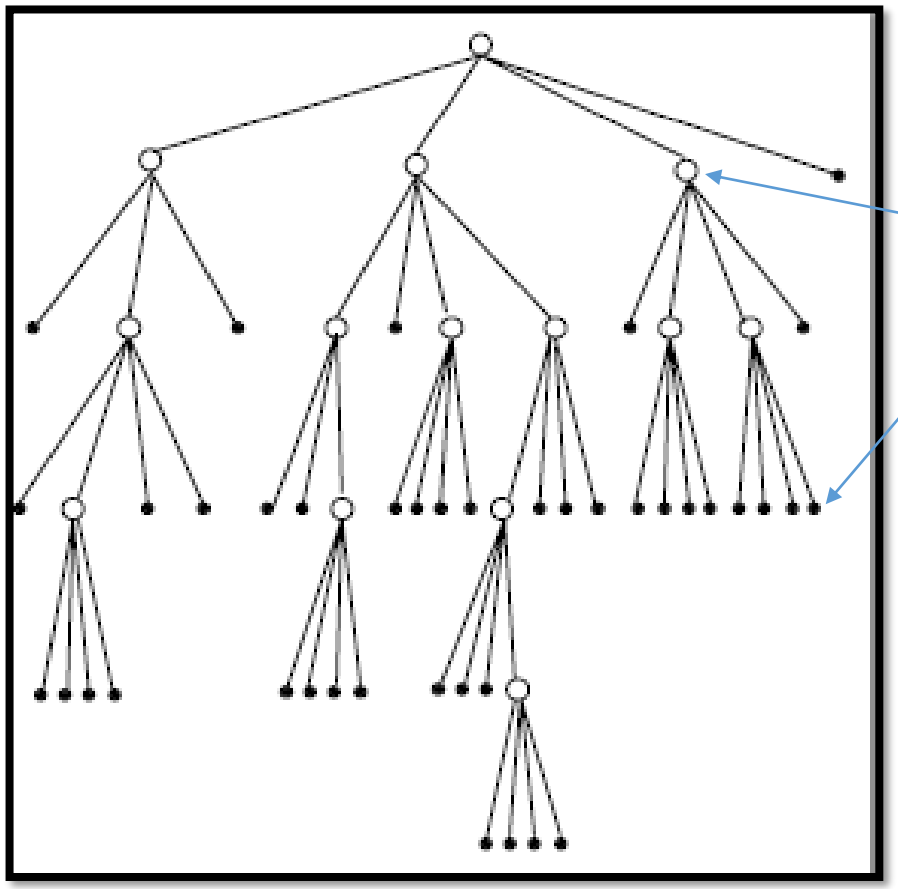
N-body Simulation – Oct-tree formation



- Initially empty root cell
- If #particles > threshold
  - Divide into 8 children
- Internal nodes are cells
- Leaves are individual particles

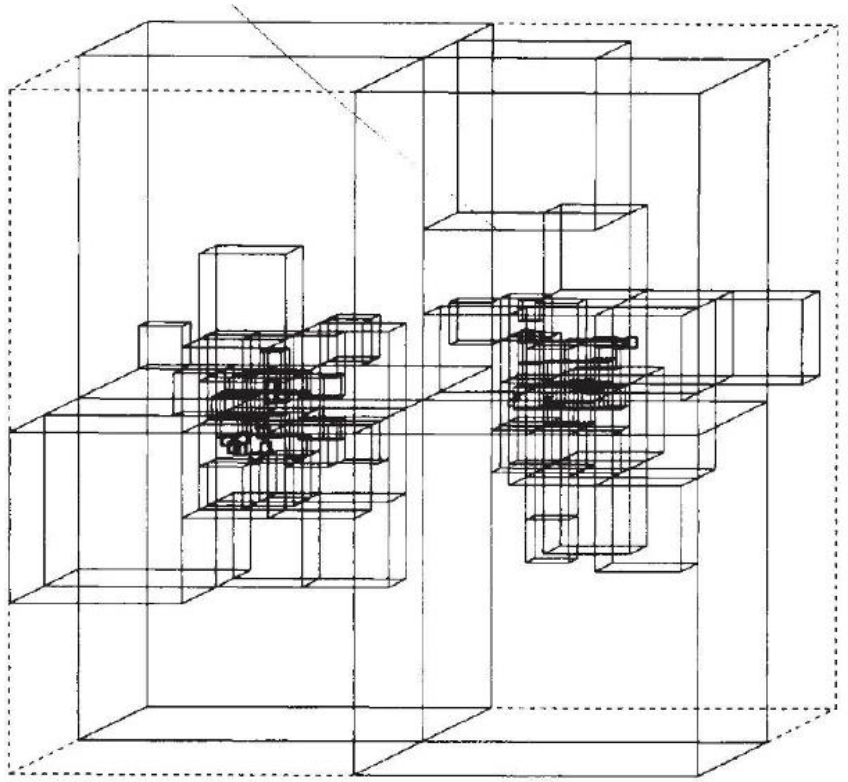
Spatial Domain





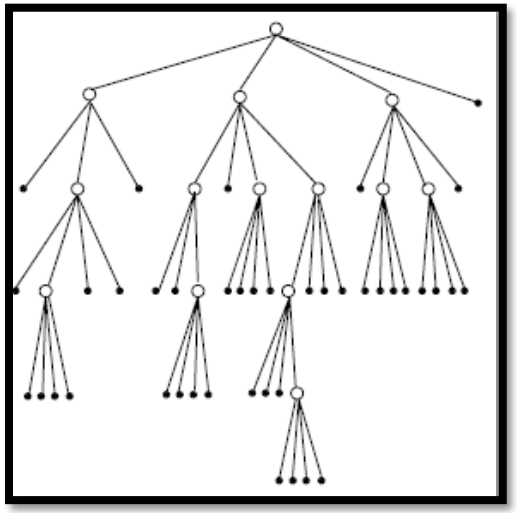
Source: Culler et al.

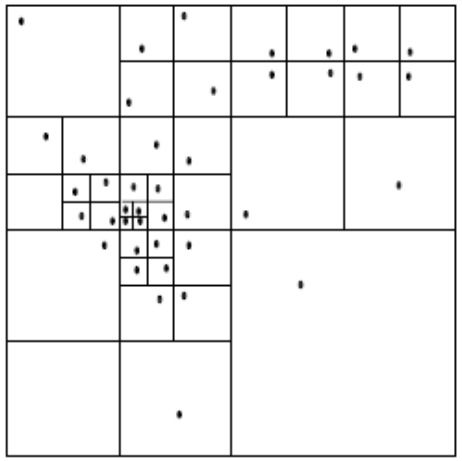
Induced Box Structure



Barnes and Hut, “A Hierarchical O(N log N) Force-calculation Algorithm”

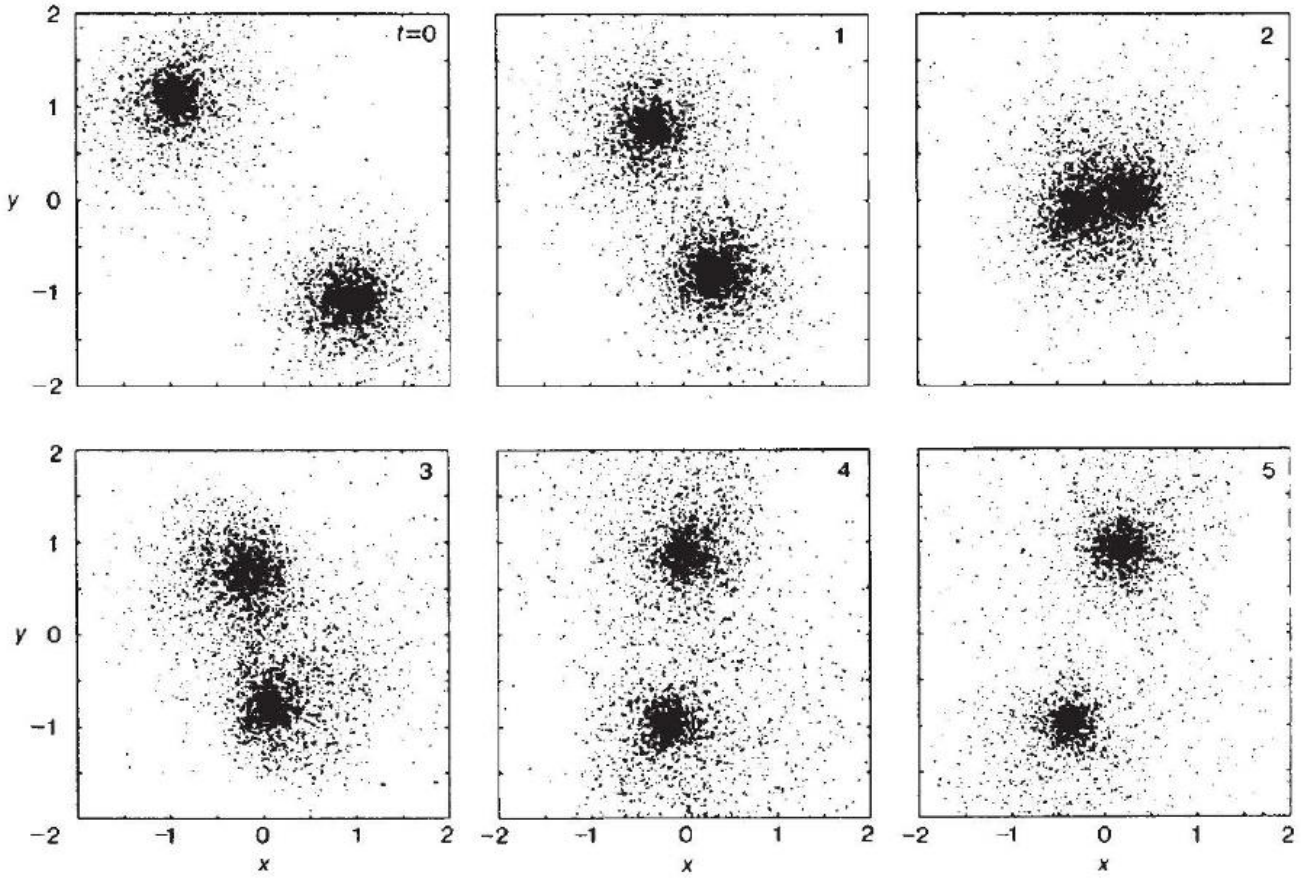
Force Computations





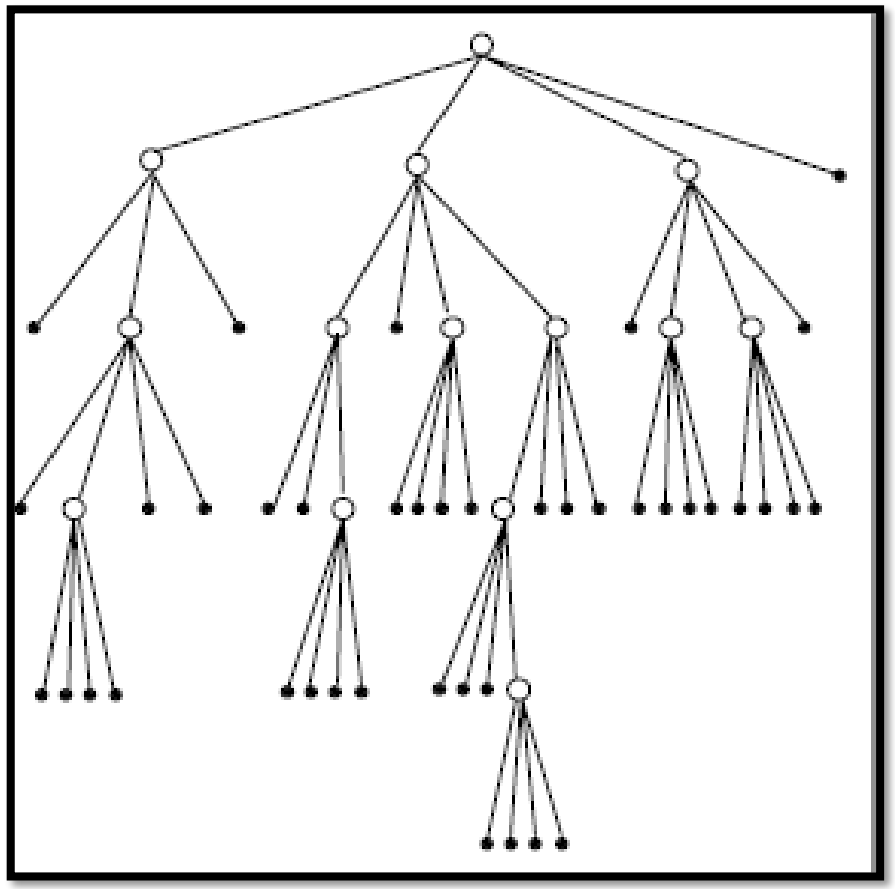
- Traverse the oct-tree for every body
- If the CoM is far away, approximate by a single body
  - Length of cell / distance < Θ
  - Sub-tree need not be expanded
- O(N log N) force computations per time step
- Structure of tree evolves
  - Distribution of bodies change
- Irregular communication pattern
- Global synchronization barrier after each time step

Two Spherical Systems



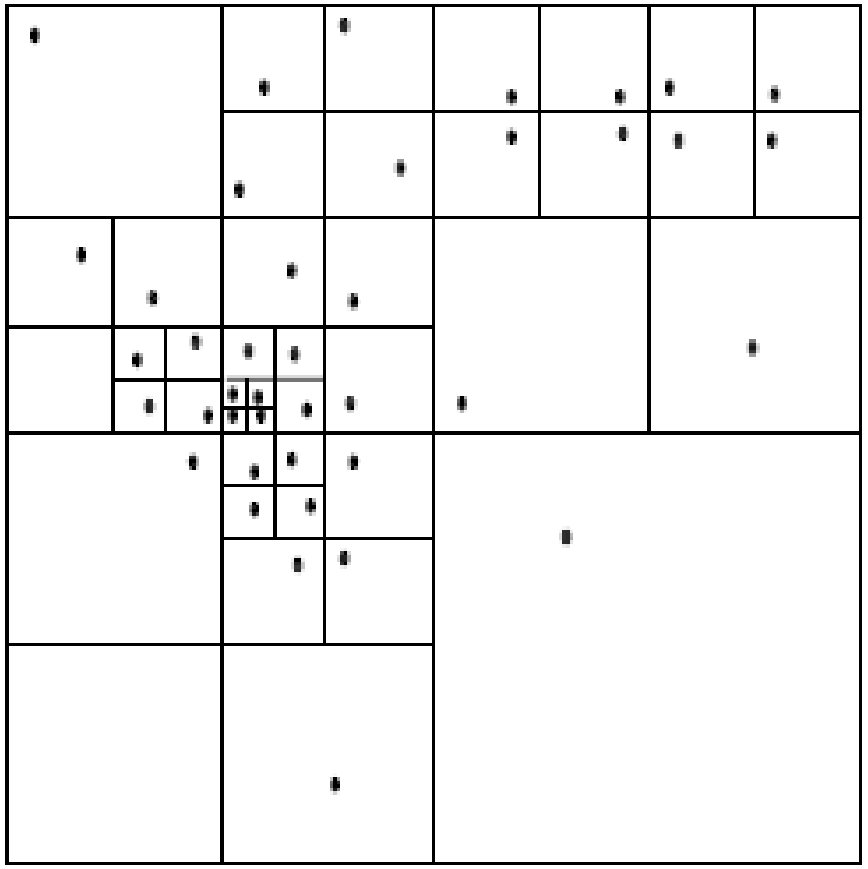
0.1 of the total interactions were required using the hierarchical algorithm

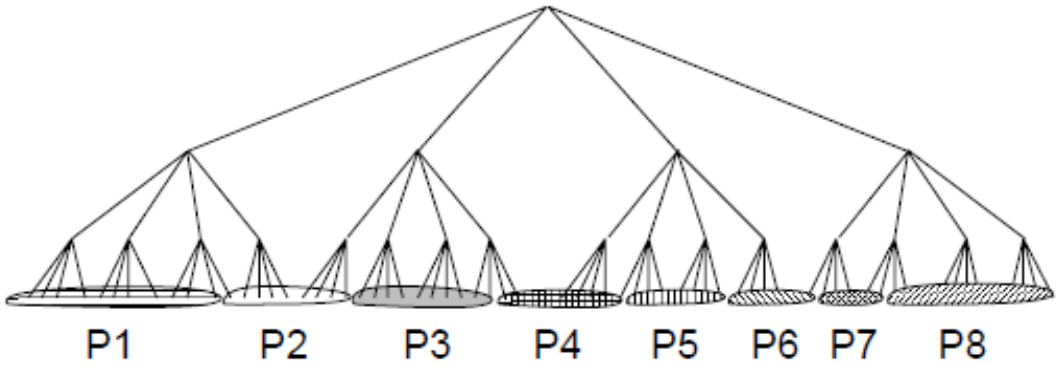
Data Structures



- Array of bodies
  - 3D position, velocity, acceleration, mass
- Array of cells
  - Pointers to children and CoM
- Array of pointers to bodies
- Array of pointers to cells

Assignment and Partitioning



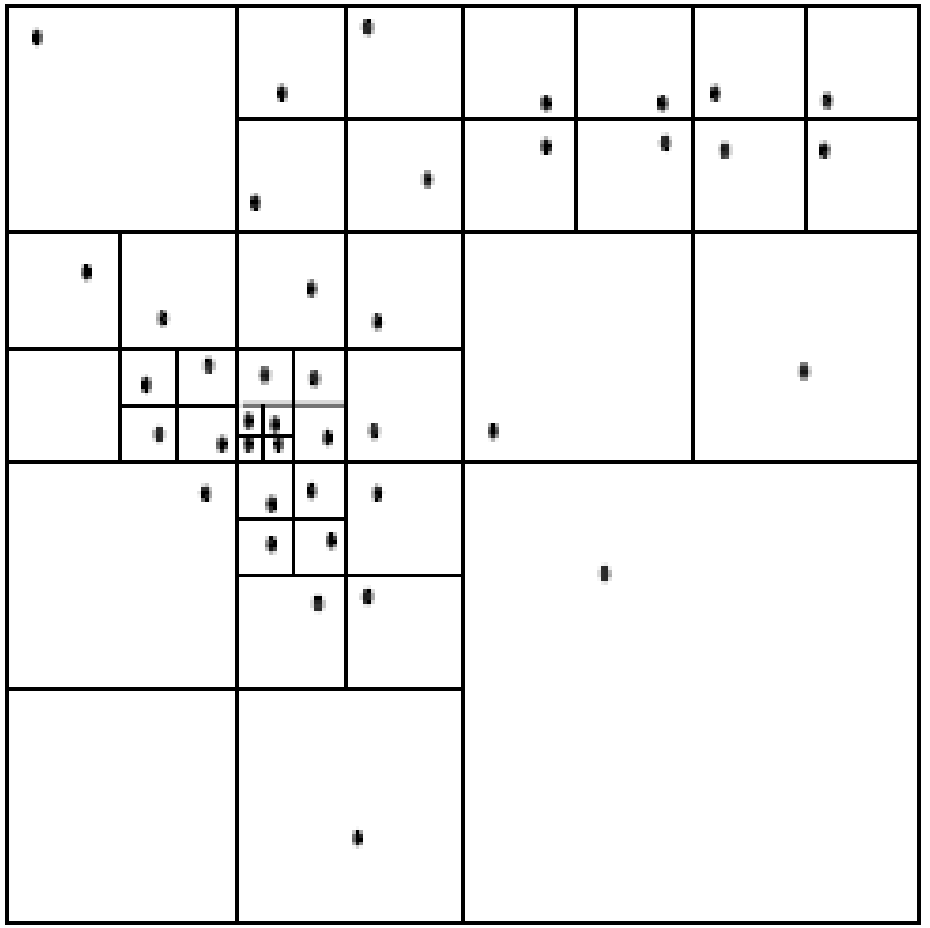


Costzones

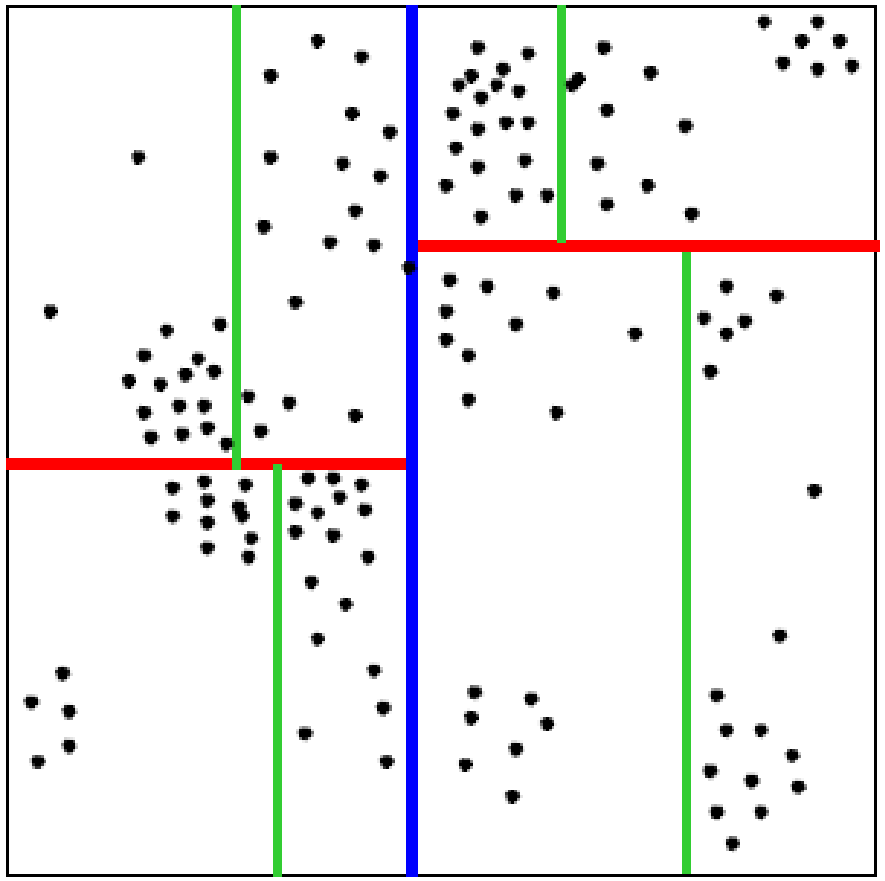
Barnes-Hut – Performance Considerations

- Positions change across time steps
  - Dynamic decomposition
  - Rebuild the tree every time step
  - Repartitioning almost every time step
- Irregular communication pattern
  - Logical process neighbors may own spatially dis-contiguous chunks
- Synchronization between steps
- Partitions are not contiguous in space

We achieved a good domain decomposition but …



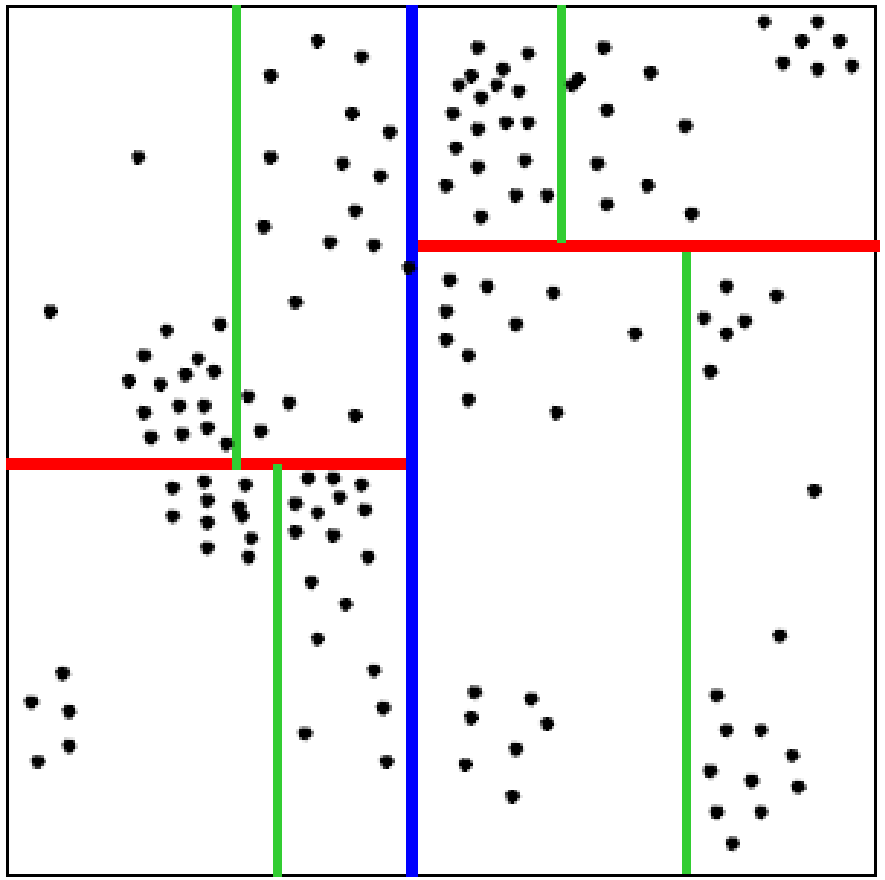
Orthogonal Recursive Bisection (ORB)

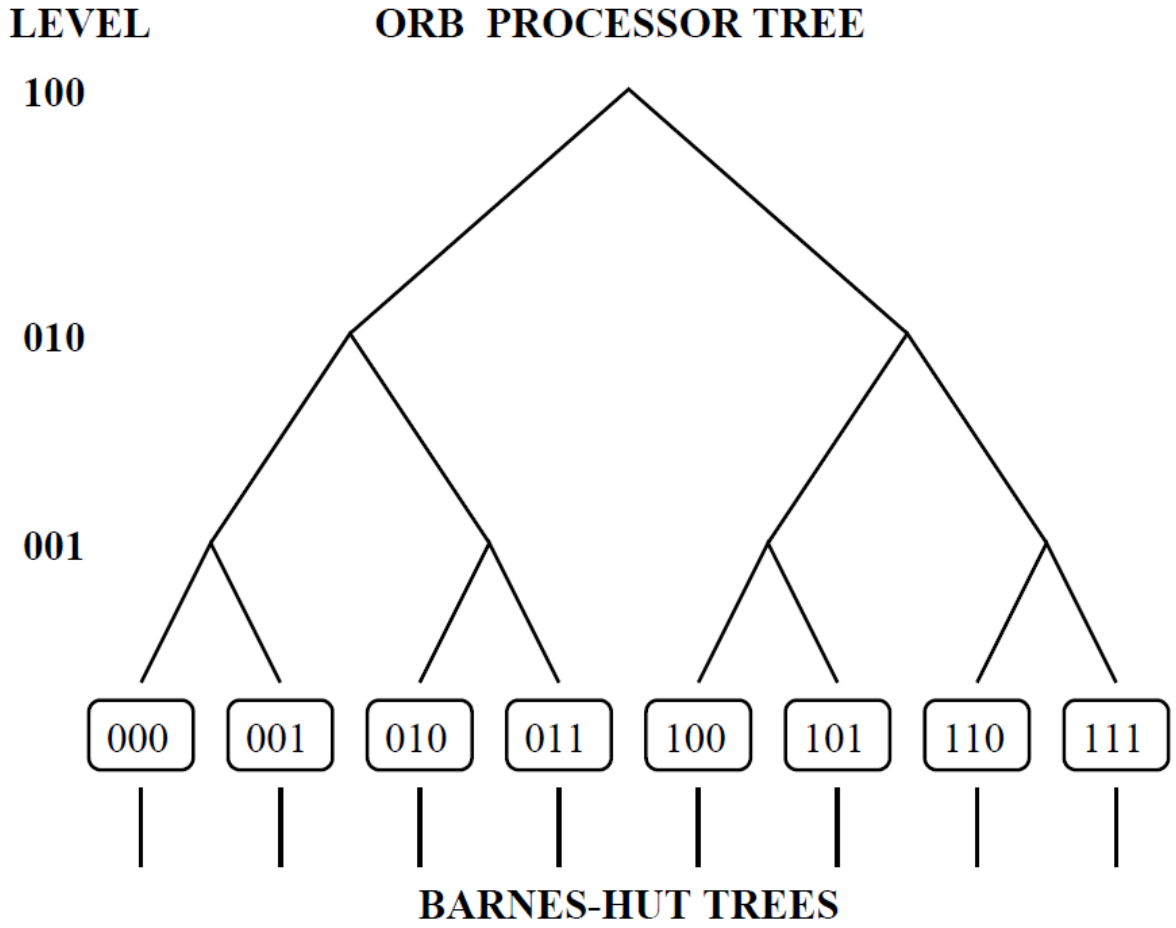


Source: Culler et al.

- Alternate division along the dimensions
  - Partition along the longer dimension first
- ORB binary tree
  - n-level tree represents 2^n sub-volumes
- Preserves physical locality
- Parallel median finder
  - Work: sum of cell-particle interactions
  - First step may be imbalanced

Linking the Trees





Dubinski et al., “A Parallel Tree Code”