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)

Data distribution in $n$-body problems

- Naive approach: Assign $n/k$ particles to each process
- Other approaches?
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Space-filling curves

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https://en.wikipedia.org/wiki/Z-order_curve
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Data distribution in $n$-body problems

- Let us consider a two-dimensional space with bodies/particles in it
Data distribution in *n*-body problems

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Data distribution in $n$-body problems

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Different parallelization methods

- Tree codes: Barnes-Hut simulations
- Fast multiple methods (FMM): Greengard and Rokhlin
- Particle mesh methods
- Particle-particle particle-mesh (P³M) 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

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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