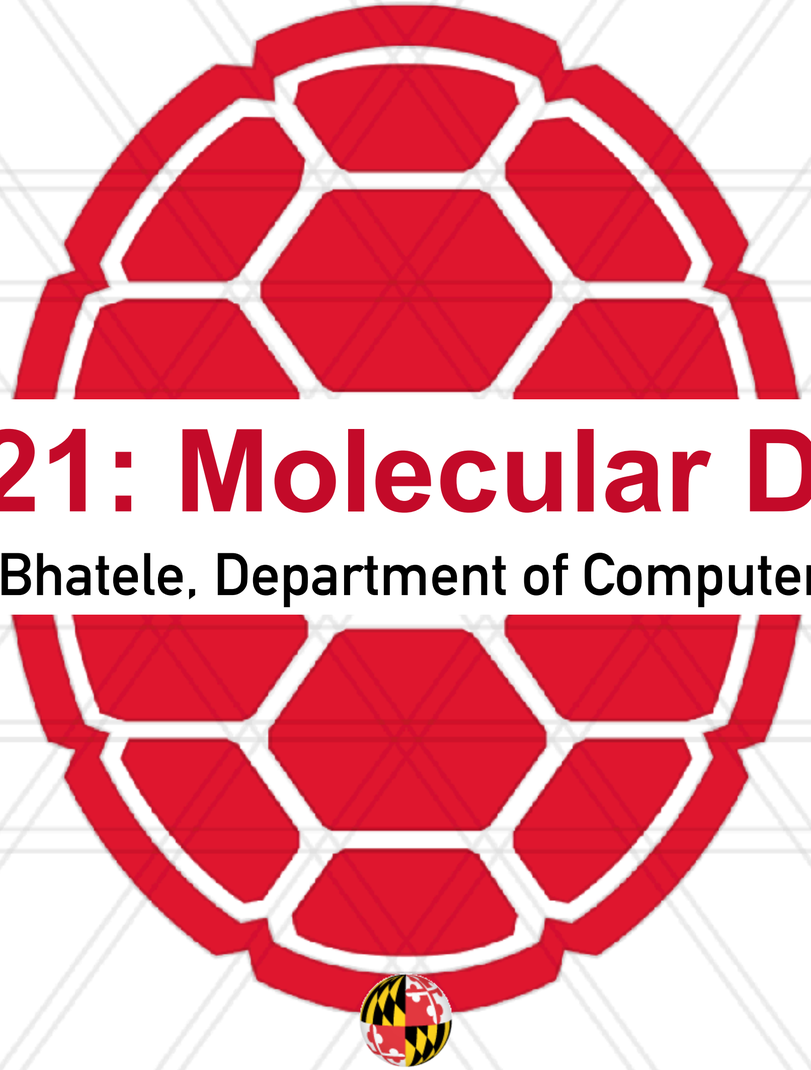
High Performance Computing Systems (CMSC714)



Lecture 21: Molecular Dynamics

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Summary of last lecture

- I/O can become a bottleneck when other portions of the code scale well
  - Reading input datasets, writing numerical/scientific output, checkpointing
- Parallel file system required for high performance
- Different approaches to file I/O:
  - One process per file, shared file, shared files for subsets of processes
- Contention for metadata server and OSTs/disks

Molecular Dynamics

- Calculate trajectories of atoms and molecules by solving Newton's equations of motions
- Force calculations
  - Bonded interactions: bonds, angles, dihedrals
  - Non-bonded interactions: van der Waal's and electrostatic forces
- Number of atoms: thousands to millions
- Simulation step: ~1 femtosecond (10^{-15} s)

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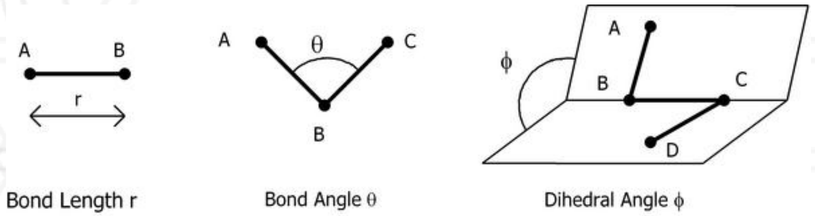

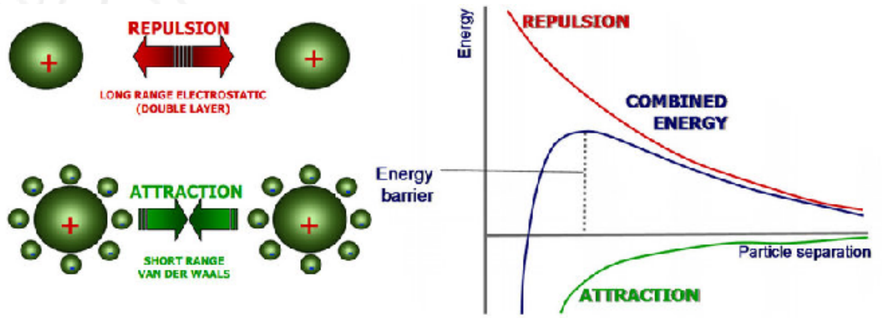

Sequential Algorithm

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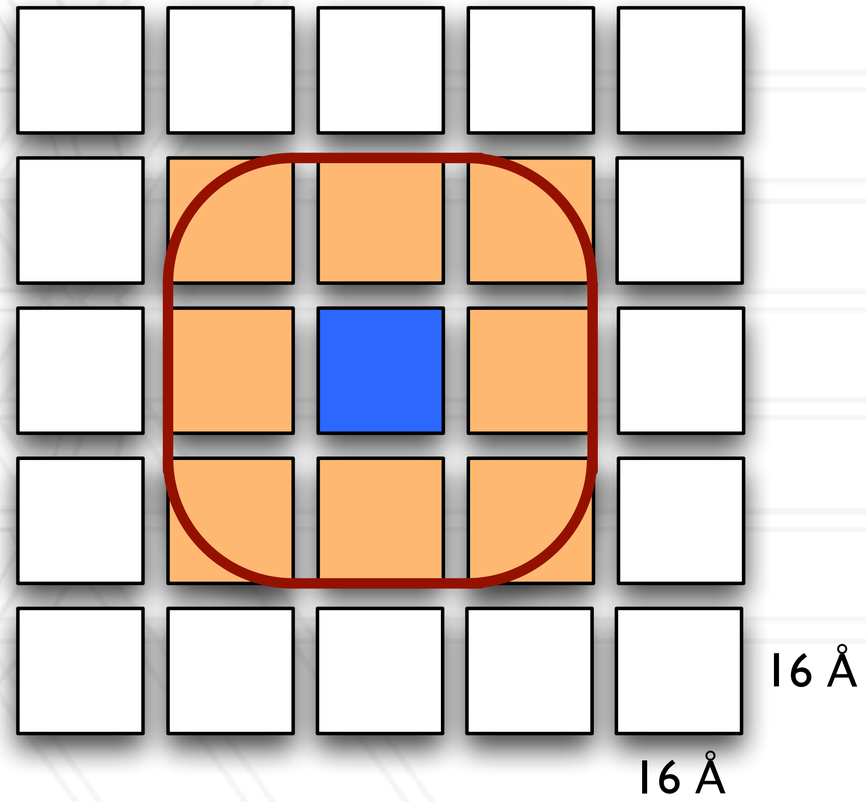
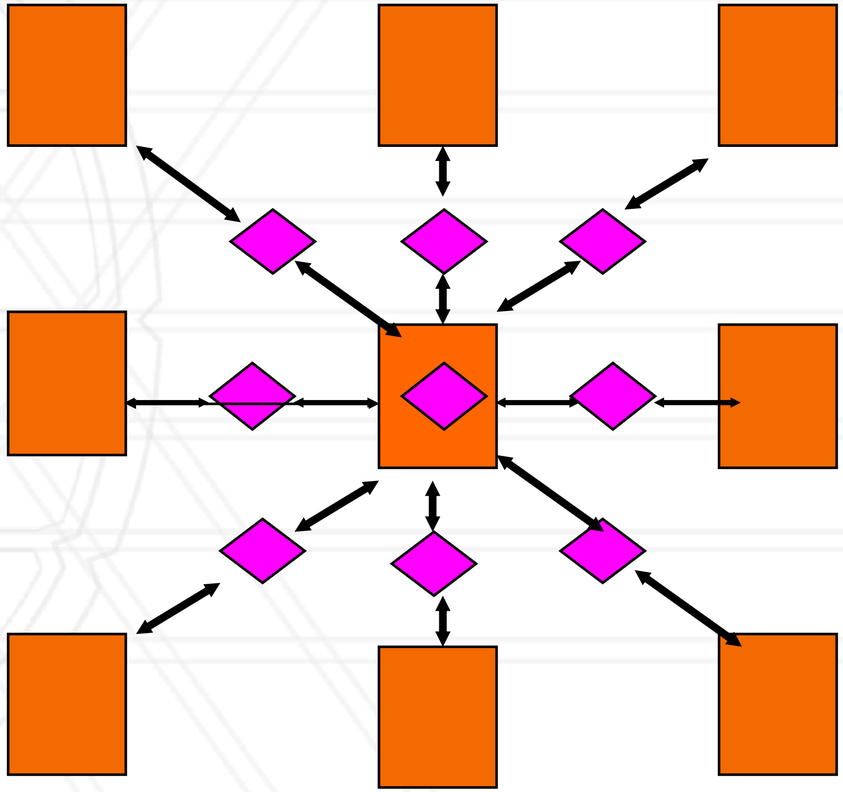
  - Partition the atoms across processes
- Force decomposition:
  - Distribute the force matrix to processes
  - Matrix is sparse and non-uniform
- Spatial decomposition:
  - Assign a region of the 3D simulation space to each process



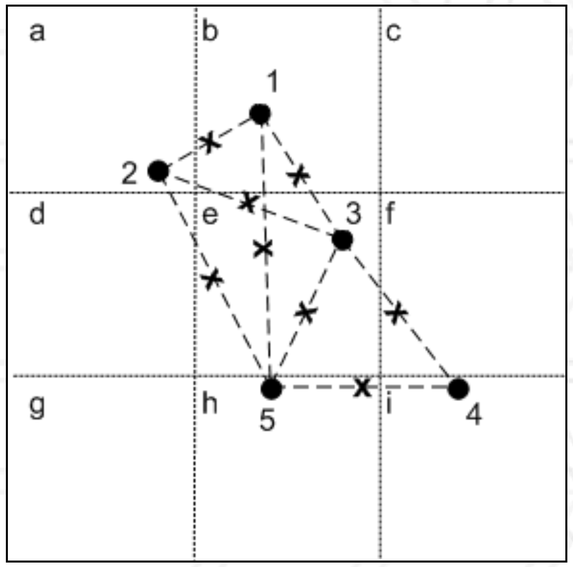
Hybrid parallelization

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

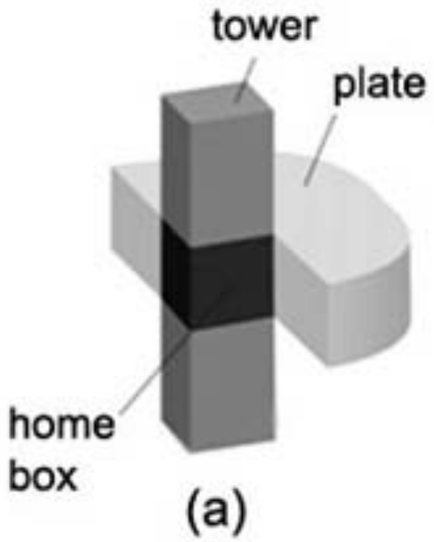


Neutral territory (NT) methods

- Desmond's mid-point method



Midpoint method



NT method

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)

- 1D or slab decomposition

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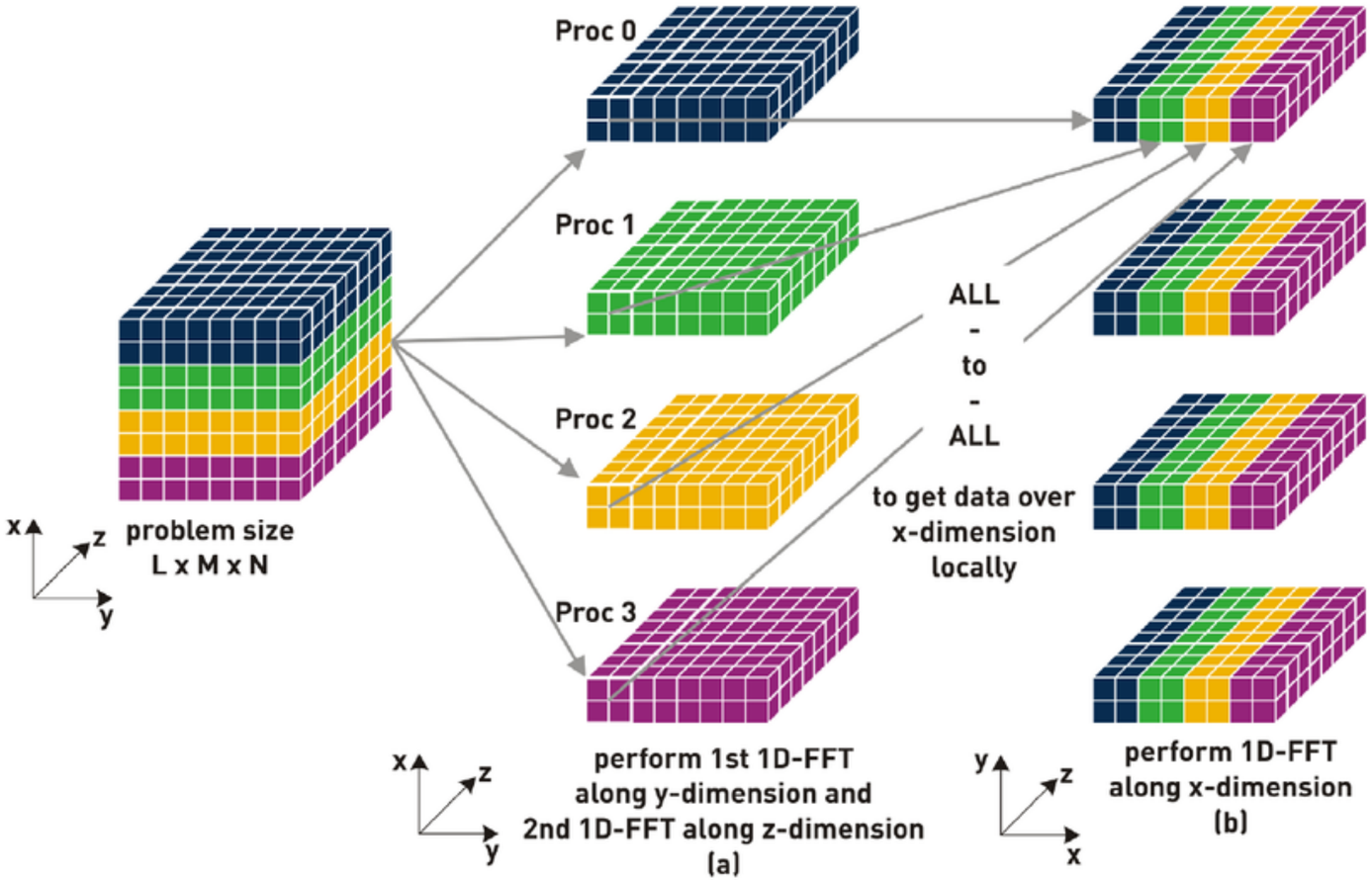
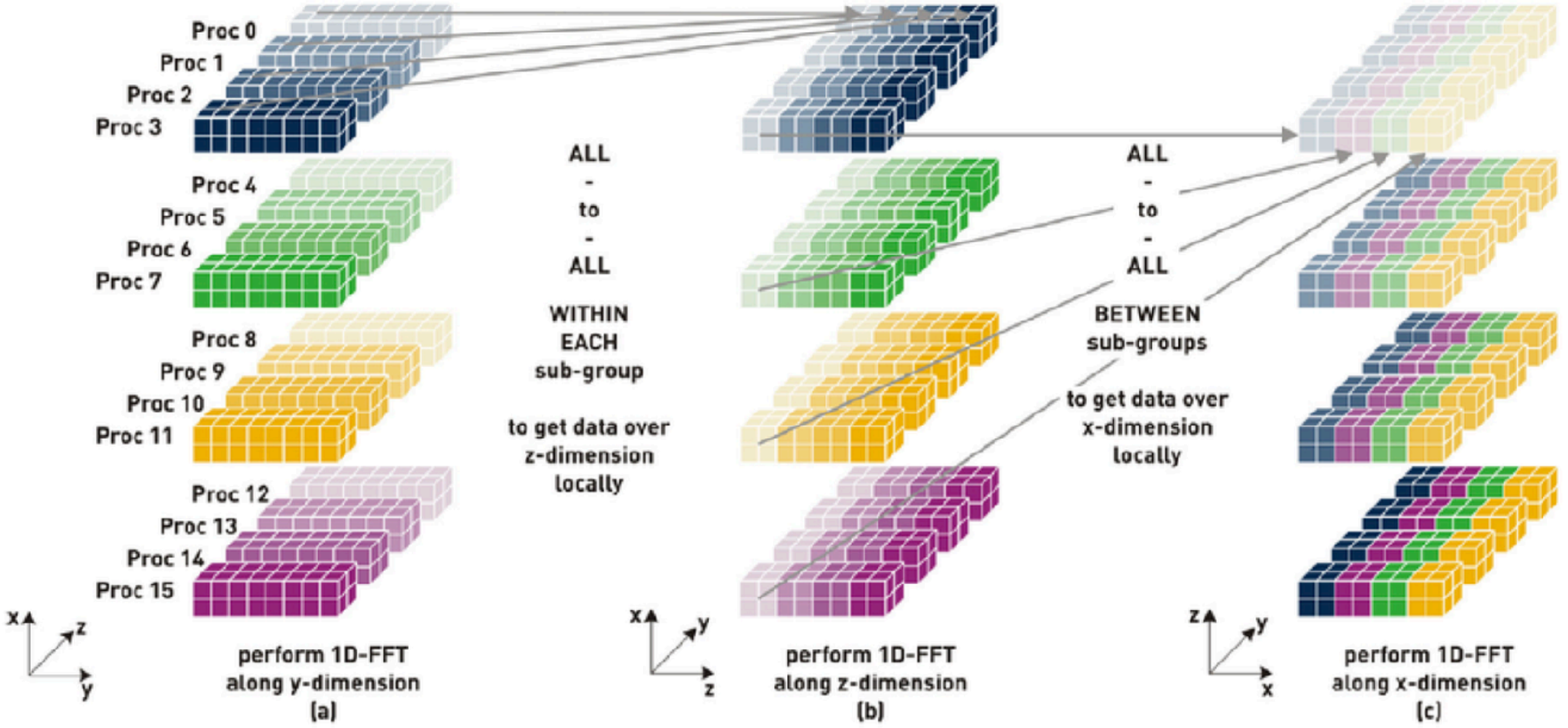


Parallelization of PME (3D FFT)

- 2D or pencil decomposition



Special purpose hardware

- Anton: 512 nodes arranged in a 8x8x8 torus
- Special hardware (HTIS) for calculating short-range pairwise force interactions

Questions?

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