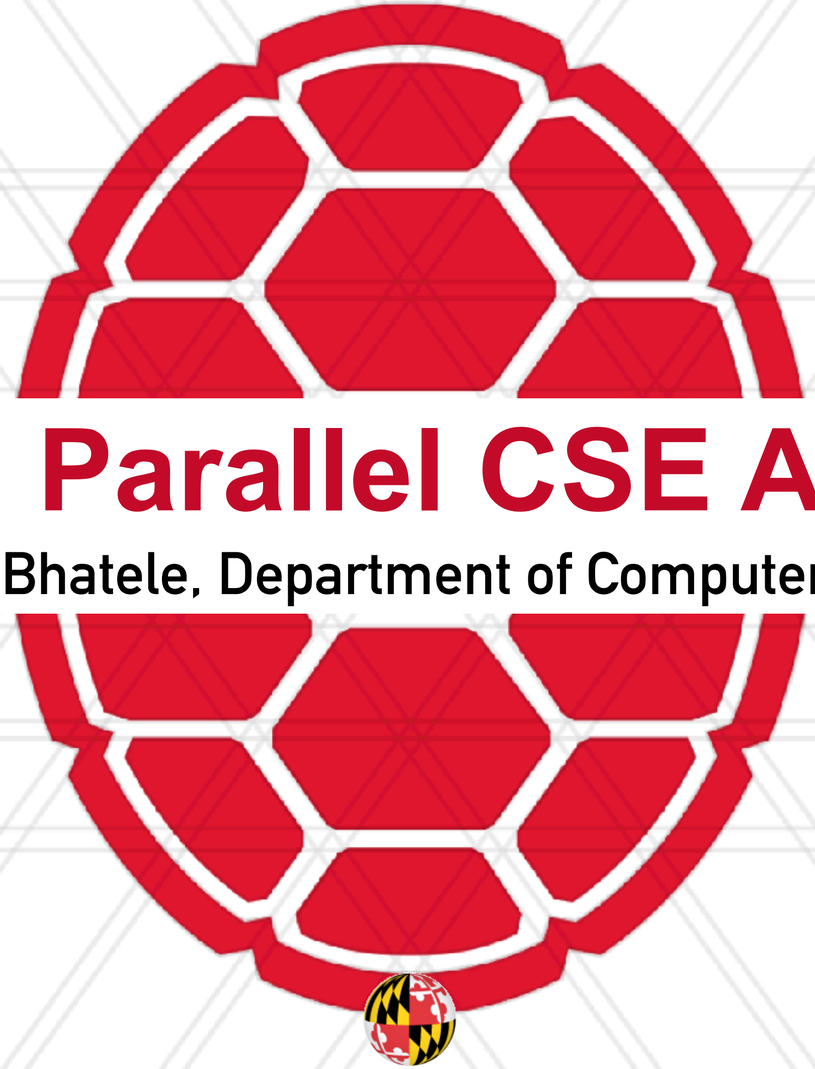
Introduction to Parallel Computing (CMSC498X / CMSC818X)



Lecture 23: Parallel CSE Applications

Abhinav Bhatele, Department of Computer Science

UNIVERSITY OF MARYLAND

Announcements

- Due date for Assignment 4 extended to Nov 24 midnight AoE
- E-mail Abhinav and Shoken with your preferences for the project presentation slot by Nov 25:
  - Provide three options in decreasing order of preference: Dec 3, 8, 10
- Final project and report due on Dec 14

Molecular Dynamics

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

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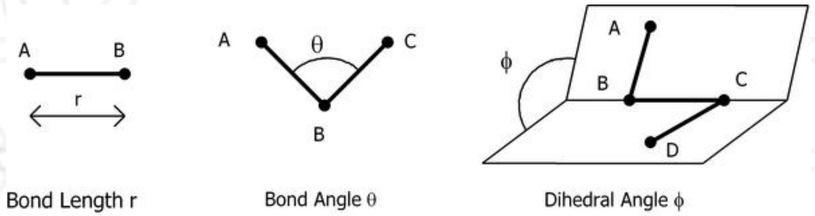
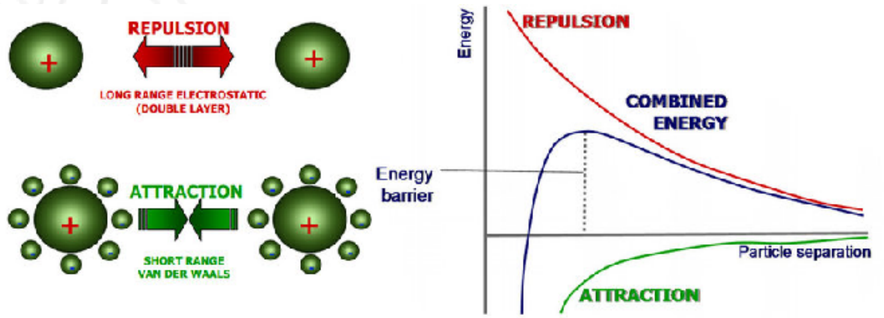
  - Bonded interactions: bonds, angles, dihedrals
  - Non-bonded interactions: van der Waal's and electrostatic forces





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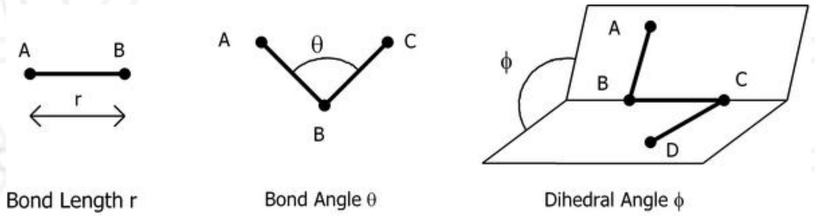
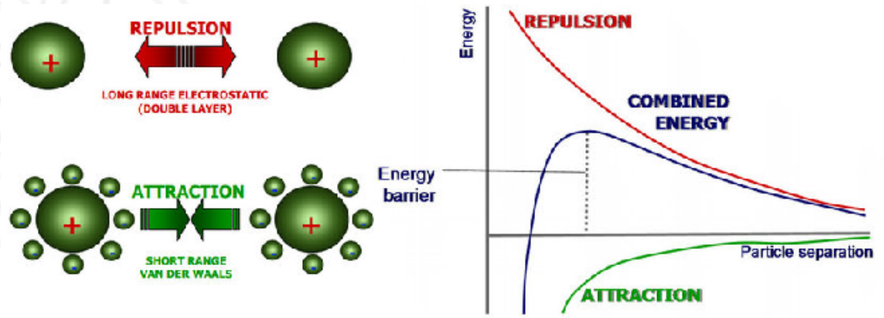
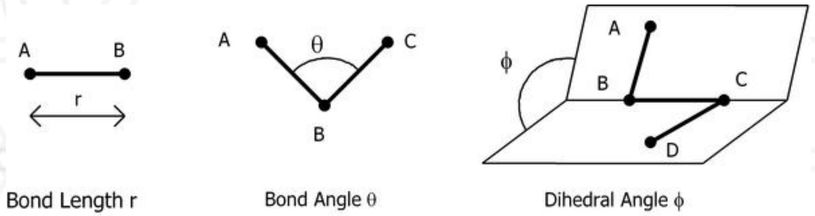
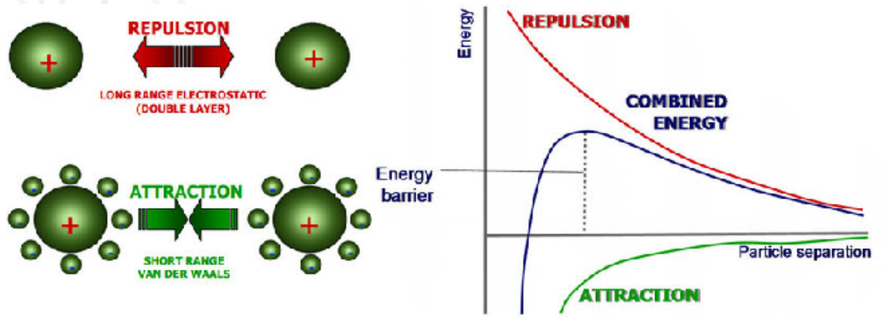




Molecular Dynamics

- 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)





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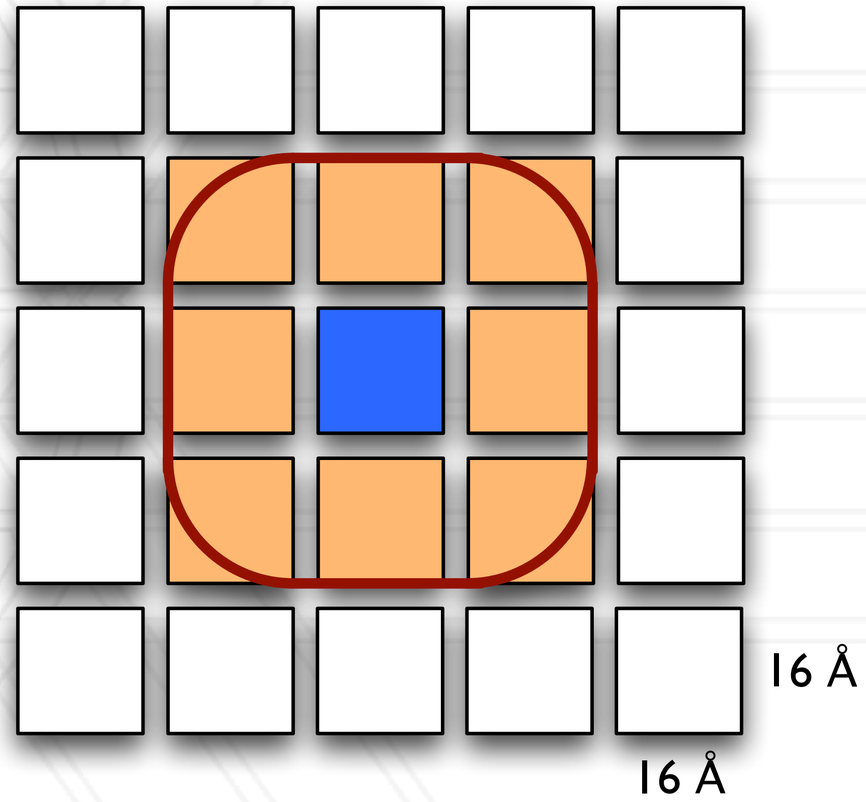
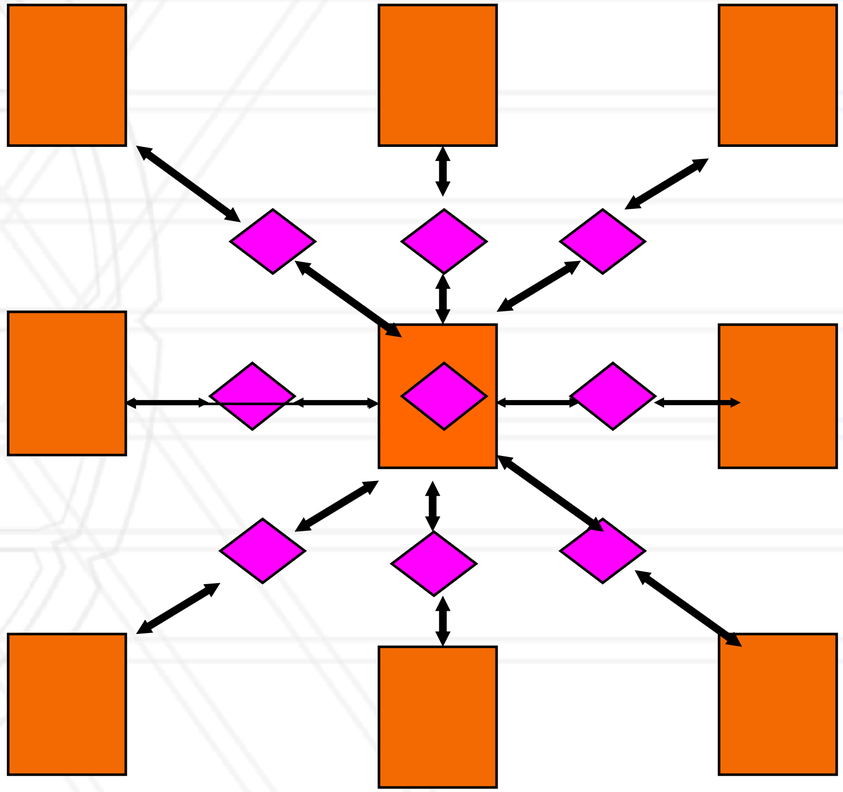
- Force decomposition:
  - Distribute the force matrix to processes
  - Matrix is sparse and non-uniform
- Spatial decomposition:
  - Assign a region of the 3D simulation space to each process



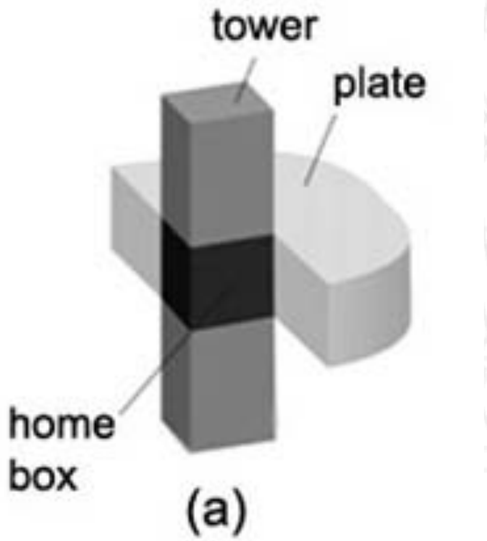
Hybrid parallelization

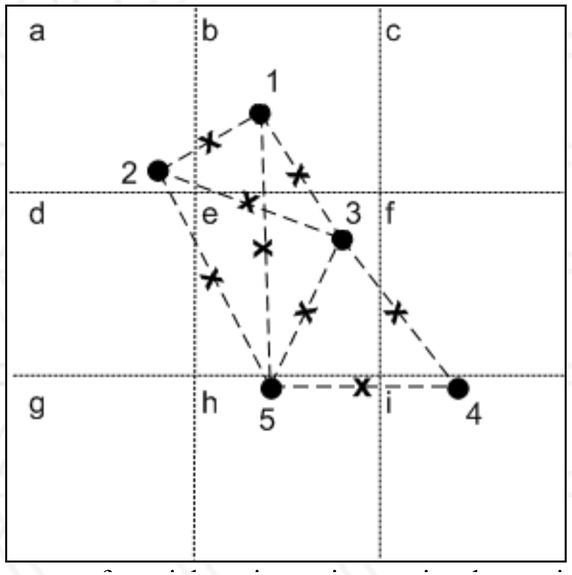
- Hybrid of spatial and force decomposition
- Decouple assignment of data and work to processes
- Distribute both atoms and the force calculations to different processes



Neutral territory (NT) methods

- Desmond's mid-point method





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 to reduce the complexity from $O(N^2)$ to $O(N \log N)$

Parallelization of PME (3D FFT)

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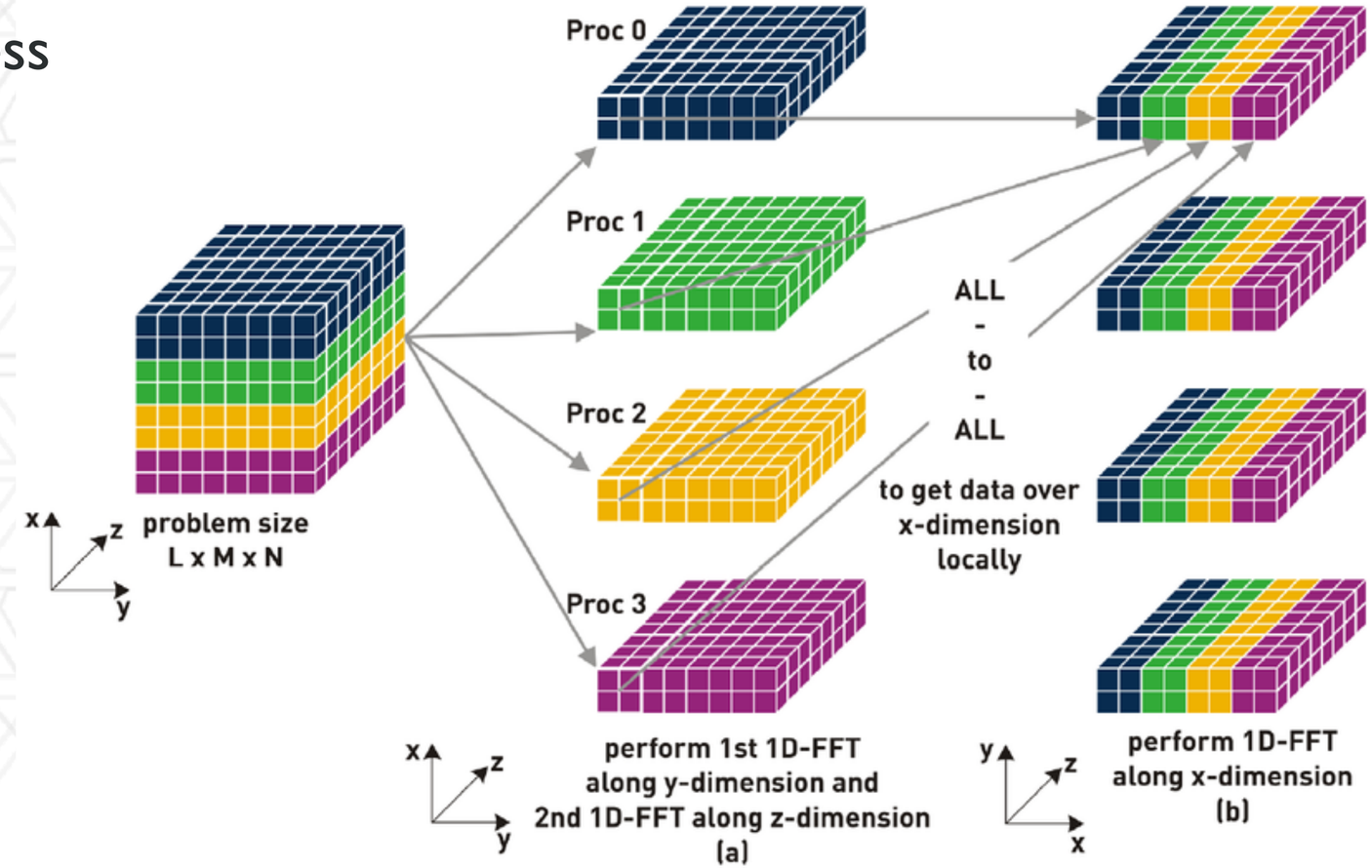
- Bring all the data to one process

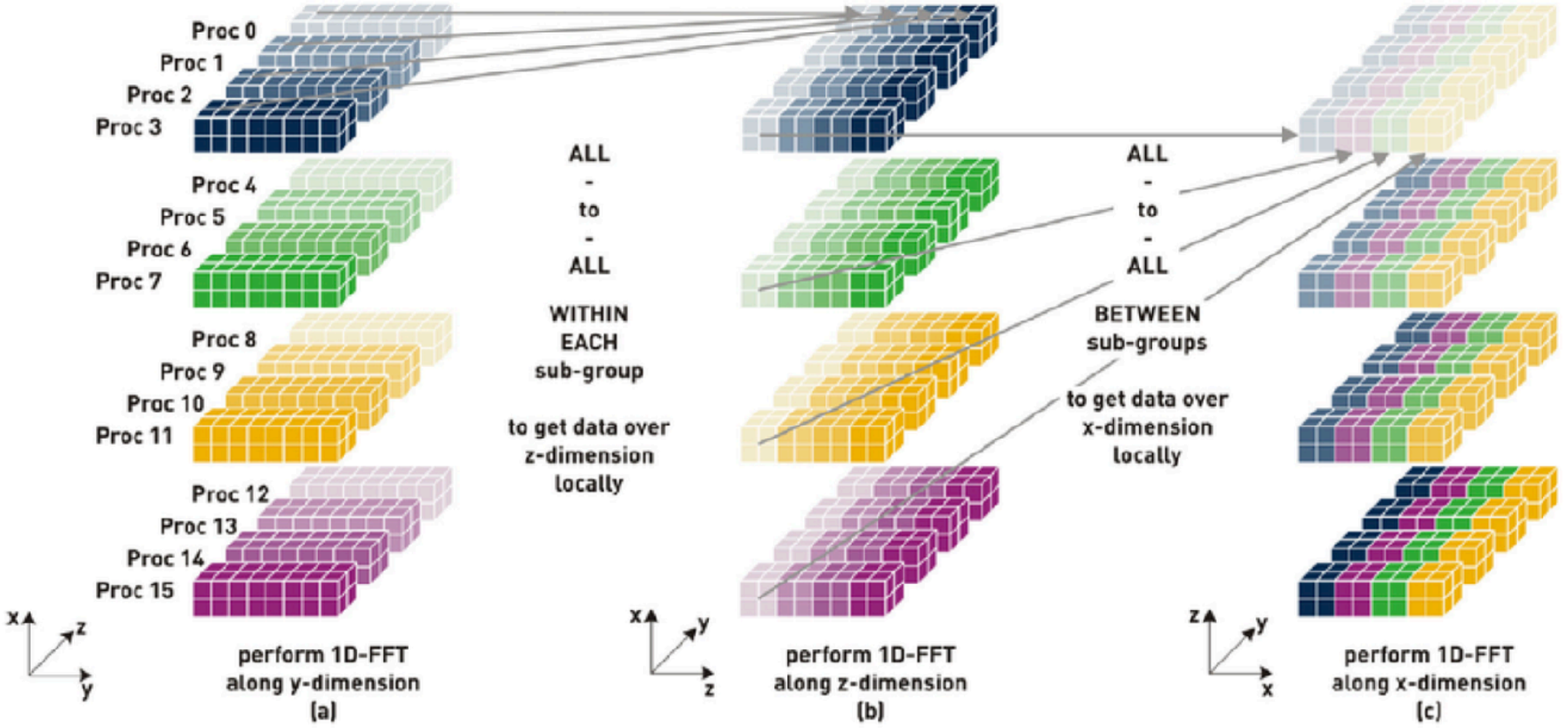
Parallelization of PME (3D FFT)

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



Parallelization of PME (3D FFT)

- 2D or pencil decomposition



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