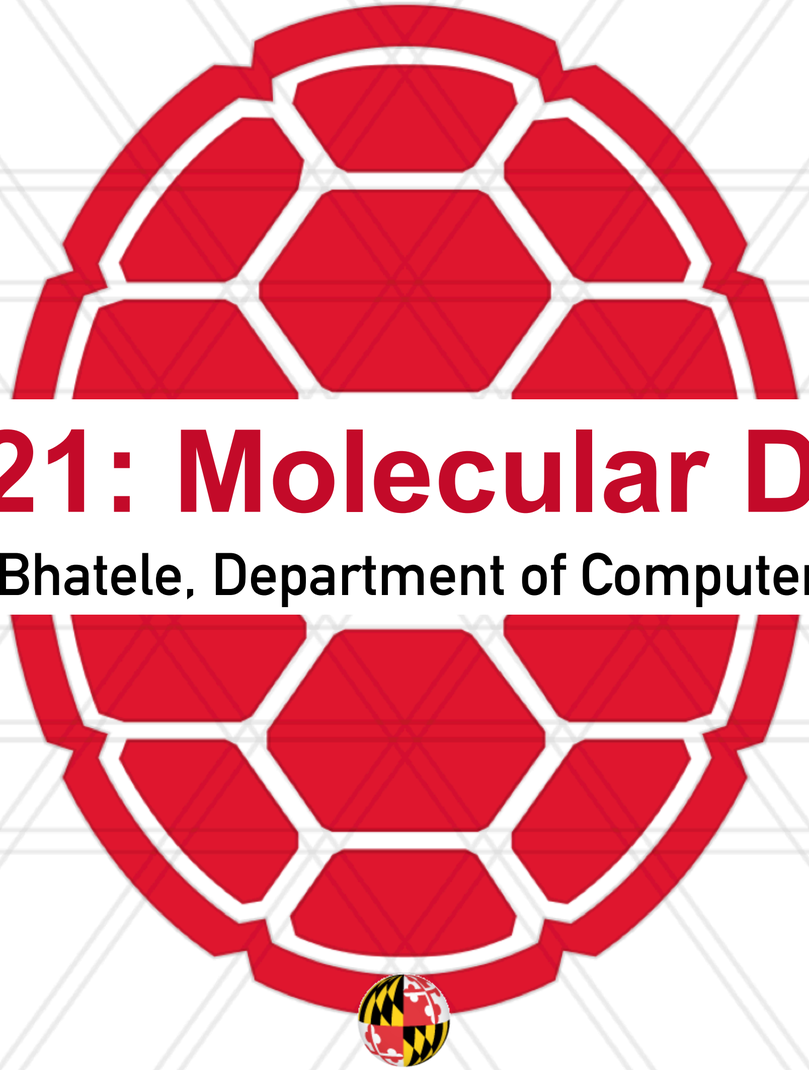
High Performance Computing Systems (CMSC714)



Lecture 21: Molecular Dynamics

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Announcements

- Mid-term on Nov 19 in class: 9:30 am
- No class on Nov 14
- Interim report due on Nov 18: 5:00 pm

Summary of last lecture

- Dense matrix multiplication is another common operation in HPC codes
- Cannon's 2D algorithm
- Agarwal's 3D algorithm

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.)
- Calculate velocities and new positions
- Repeat …

Domain decomposition in parallel MD

Domain decomposition in parallel MD

- Atom decomposition
  - Distribute atoms to processes

Domain decomposition in parallel MD

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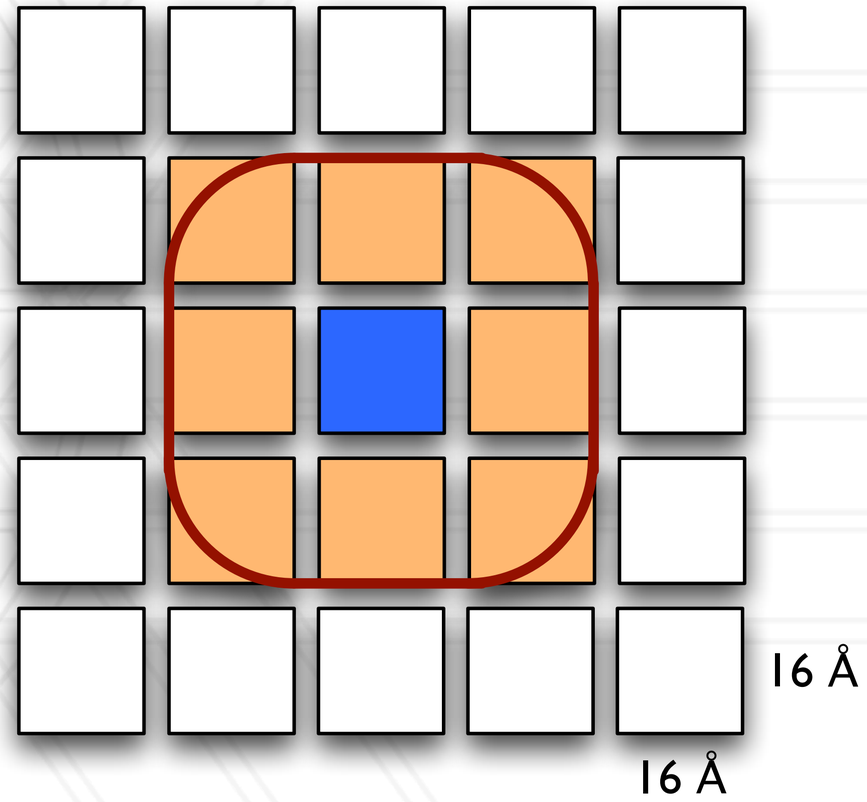
- Force decomposition
  - Assign force calculations to different processes

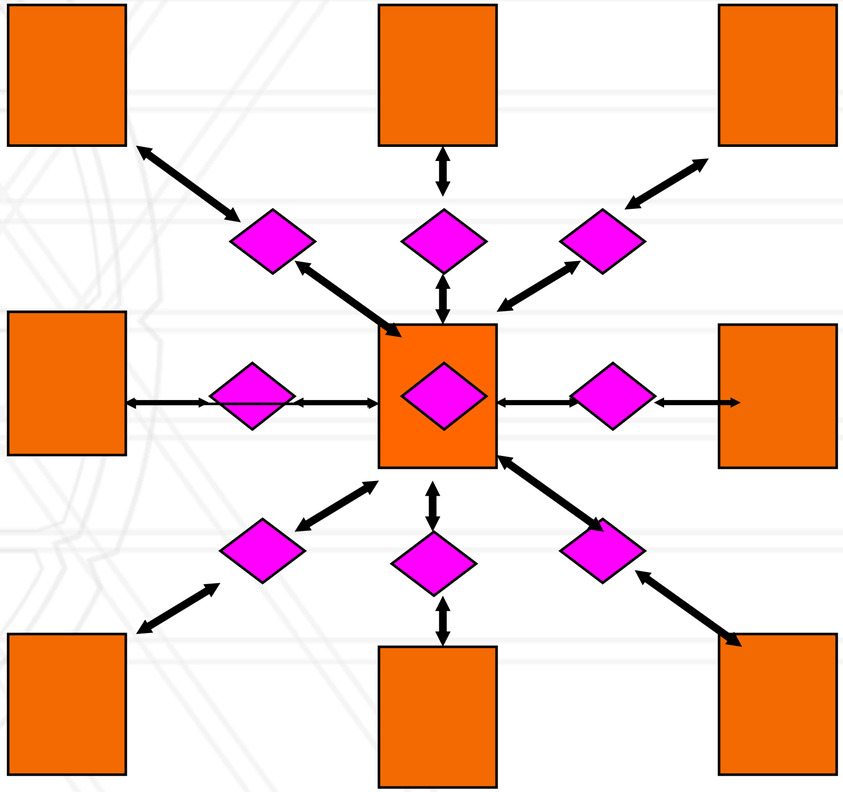
Domain decomposition in parallel MD

- Atom decomposition
  - Distribute atoms to processes
- Force decomposition
  - Assign force calculations to different processes
- Spatial decomposition
  - Assign 3D sub-blocks to each process



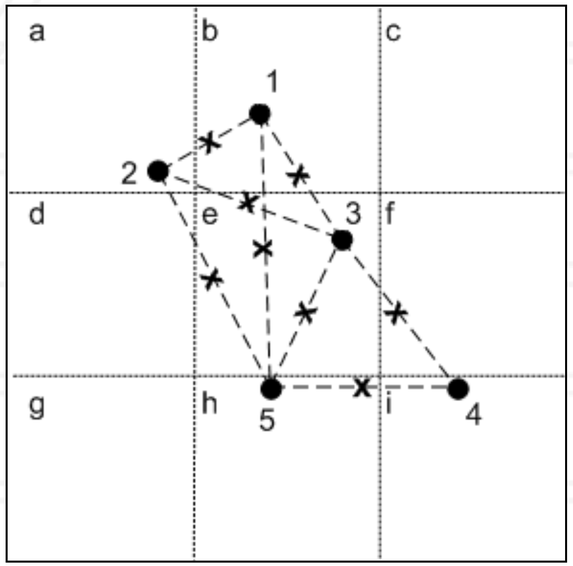
Hybrid parallelization

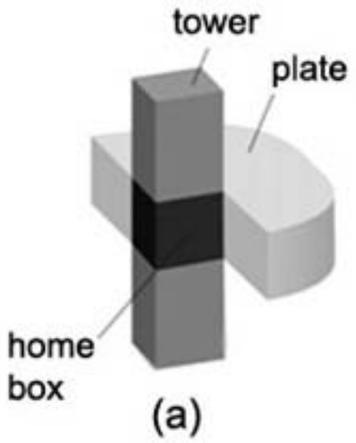
- Hybrid of spatial and force decomposition
- Decouple assignment of data and work to processes
- Distribute both atoms and the force calculations to different processes



Neutral territory (NT) methods

- Desmond's mid-point method





Special purpose hardware

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

Questions

NAMD: Biomolecular Simulation on Thousands of Processors

- What is Ewald electrostatics? (Answered somewhat in paper 2)
- In what ways does Charm++ help with the scalability and load balancing in this particular code
- Is the Elan messaging system commonly used as opposed to MPI? Or are its improvements unique to this particular algorithm? What are the differences?
- Is Charm++ really much more suitable for molecular dynamics simulation comparing to MPI, OpenMP etc?
- NAMD considers rebalancing the computation of interactive forces between patches. Is there any reason not to rebalance the patches (the atom distribution) themselves between processors?
- The paper describes an optimization over a specific computing cluster. Is this a necessary step for general large-scale scientific computing applications?

Questions

Millisecond-Scale Molecular Dynamics Simulations on Anton

- What are some other examples of problems for which people have developed specialized hardware? Are the improvements comparable?
- On non-specialized hardware today how long can MD simulations be run for accurately?
- What is the high throughput interaction subsystem? How does using it change how MD is optimally implemented?
- What is the bottleneck for longer time-scale MD simulation? It is shown in the paper the best time-scale reached on previous papers is 2 us. What factors prevent those experiments from advancing to, say, 10us?
- The PPIP is designed to table-driven function form which is incompatible with SPME. Is it possible to design specialized hardware for SPME?
- It seems that the NT method calculates the interaction of home box with fewer regions. Doesn't this affect the accuracy of simulation comparing to traditional spatial decomposition?

Questions?

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