CMSC 714
Lecture 26
Anton3 and more Molecular Dynamics

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Notes

• Final group project report due Monday, December 12, 6PM
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 sec)
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 ...
Anton3

• The 3rd generation of special purpose machine built for molecular dynamics simulations, built at D.E. Shaw Research
  • to simulate biological processes that occur on very small time scales ($10^{-15}$ sec), such as protein folding, interaction between proteins, etc.
  • and simulate those processes for a long time, maybe up to 100s of $\mu$sec
Anton3

• Many new features, but still most of the computations are mapped to PPIPs (Pairwise Point Interaction Pipelines)
  • But now there are two types, *Big* and *Small*
  • *Big* are for nearby interactions with higher-precision datapaths (23-bit), and also more programmable
  • *Small* are for farther interactions and 14-bit datapaths, with limited types of interaction computations
  • In chip area, 1 Big is same as 3 Small PPIPs
  • And 2 Geometry Cores per node for computations that don’t map onto the PPIPs
  • And a special *Bond* unit per node for ~90% of the bond force computations

• Tiled chip layout allows for more regular routing across units, and a denser design
  • 12 rows by 24 columns Core Tiles for computations
  • Edge Tiles - 96 total, 48 on left and right edges for (serial) connections to other nodes (that also use compression to increase effective bandwidth)

• Claim is that more than 10x energy efficient on MD, in addition to faster time to solution
Anton3

• Performance results show can run large chemical systems (up to millions of atoms) at much higher rates than any previous system, including previous Anton systems and other conventional (CPU/GPU) and special-purpose systems (e.g., MDGrape)
  • can run up to hundreds of microseconds of simulation time per day of wall clock time
    • Over 100 times faster than any other system, including large GPU clusters and supercomputers, with 10x energy efficiency compared to a GPU
    • have run simulated systems up to well over 1000 μseconds even on large molecules with millions of atoms, which showed interesting behavior
  • Have also run multiple concurrent simulations with varying parameters for high throughput
    • E.g., 8 64-node simulations at the same time for an ensemble