CMSC 714
Lecture 24
Anton3 and more Molecular Dynamics

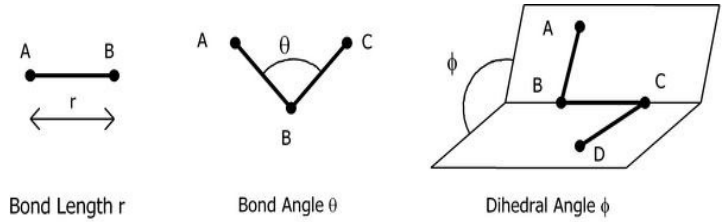
Alan Sussman

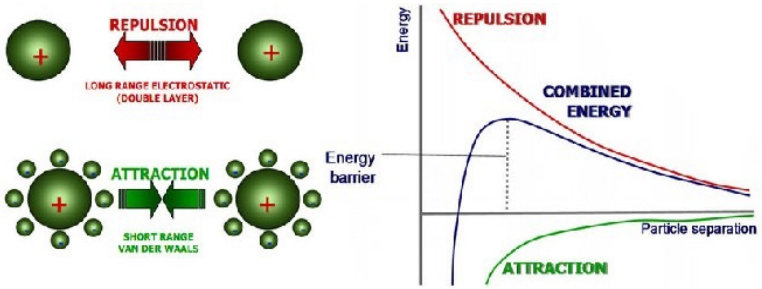
Notes

- Final group project report due Tuesday, December 12, 6PM
- Course evaluation (Student Feedback on Course Experiences) web site open
  - https://www.courseexp.umd.edu

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, up to 100s of μsec

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