CMSC416: Introduction to Parallel Computing

Topic: CSE Applications (Molecular Dynamics)
Date: Tuesday - April, 30, 2024

Correlating Slides: [CSE Applications Slides]

Introduction:

- Over these next 3 lectures, we will look at a variety of domain applications that people develop in HPC (or parallel computing in general)
    - What are some ways to design these applications
    - What are some parallel algorithms people have used when it comes to implementing these apps

Overview of Parallel Computing Applications:

- The diverse applications of parallel computing span from molecular dynamics at the nanoscale to computational astronomy covering cosmic scales.
- Relevance in Various Fields: Parallel computing is pivotal in numerous sectors, including financial trading, epidemiology, climate modeling, and even military applications.

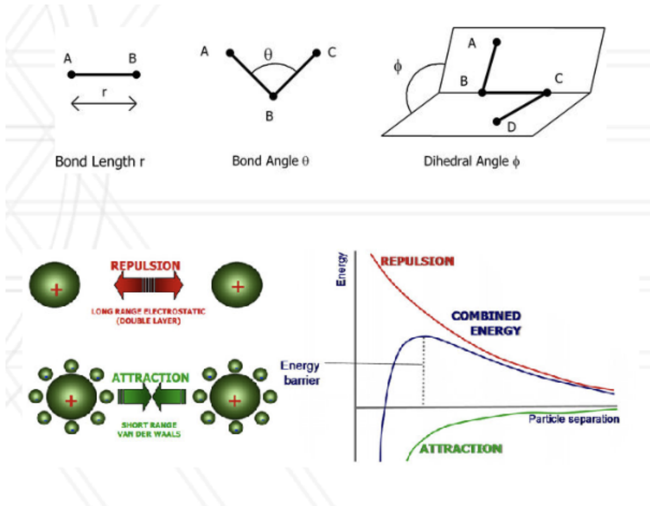
Detailed Exploration of Molecular Dynamics (MD):

- Molecular Dynamics involves the simulation of atomic and molecular interactions to study properties and behaviors under various conditions. It is crucial for the advancement of science in drug design and materials engineering.
- Common Uses:
    - Drug Design: Simulations predict how new drugs can bind to and affect proteins within the human body. This is critical for developing treatments for diseases where no effective drugs currently exist.
    - Materials Design: Used in the creation of new materials with desired properties for use in industries such as electronics and construction.

Computational Techniques in MD:

- Force Calculations:
    - Bonded Interactions: Calculations include bonds (connections between two atoms), angles (connections involving three atoms), and dihedrals (involving four atoms). These are critical for maintaining structural integrity and functionality in molecular simulations.
    - Non-bonded Interactions: Includes forces like Van der Waals (induced electrical interactions between atoms or molecules) and electrostatic (interactions between

charged particles). These forces are crucial for the accurate simulation of molecular dynamics.



(Derived from CSE Applications Slide)

- Simulation Steps:
    - Each simulation step involves recalculating forces affecting each atom, updating their positions based on these forces, and moving forward in simulated time. This iterative process is computationally intensive.

Parallelization Strategies in MD:

- Atom Decomposition: Involves dividing atoms across multiple processors. Each processor handles the computation for its assigned atoms, leading to parallel processing of interactions.
- Force Decomposition: Different processors handle different parts of the force calculations, particularly useful when dealing with sparse interactions.
- Spatial Decomposition: The simulation space is divided among processors. Each processor is responsible for a specific volume of the space, reducing the computation and communication overhead.

Challenges in Molecular Dynamics Simulations:

- Scalability Issues: As the number of atoms increases, the computational load significantly increases, often requiring more sophisticated parallelization strategies.
- Communication Overhead: One of the major bottlenecks in parallel simulations, where processors must frequently exchange data about atom states and forces.
- Load Balancing: Ensuring that each processor has approximately equal amounts of work to prevent some processors from idling while others are overloaded.

Sequential Algorithm for MD:

- Detailed steps for force calculations include calculating bonded and non-bonded forces at each time step, integrating these forces to update atom positions, and iterating over multiple time steps to simulate physical processes over time.
- PME optimizes the calculation of long-range electrostatic forces by transforming them into Fourier space for more efficient computation.