CMSC416 4/30 Notes

Molecular Dynamics

Objective: Calculate trajectories of atoms and molecules by solving Newton's equations of motion.

Application: Widely used by pharmaceutical companies to run simulations involving thousands to millions of atoms. Also instrumental in material design, including semiconductor chips and structural engineering.

Force Calculations Used:

Bonded Interactions: Bonds, angles, and dihedrals.

Non-bonded Interactions: Van der Waals forces and electrostatic forces.

Simulation Steps:

Time Scale: 1 femtosecond (10^-15 seconds).

Duration: It requires about 1000 trillion time steps to simulate one second of real time.

Sequential Algorithm

1. Force Calculation: At each time step, calculate the force on each atom.

2. Motion Updates: Using the forces, calculate acceleration and velocity to update positions.

Technique:

Particle Mesh Ewald Summation: Used for calculating long-range electrostatic interactions.

Traditional Parallelization Approaches

1. Atom Decomposition:

- Partitions atoms across processors.
- Challenges: High communication overhead and potential for load imbalance.

2. Force Decomposition:

- Distributes the force matrix among processes, effectively creating a sparse matrix reflecting only local interactions.

3. Spatial Decomposition:

- Assigns a 3D simulation space region to each process. Each cell is 16 angstroms (0.1 nanometers).
- Only neighboring cells are considered in calculations.
- A process typically interacts with 26 neighboring processes in 3D space.

4. Hybrid Decomposition:

- A combination of spatial and force decomposition.
- Divides the space into boxes of 16 angstroms each, with 'diamond' structures facilitating interactions between boxes.
- Assigns both atoms and force calculations to different processes, optimizing load and reducing inter-process communication.

Neutral Territory (NT) Methods

- Diamond Midpoint Method: Performs calculations at midpoints between interacting boxes, reducing the computation load on individual processes.

Particle Mesh Ewald (PME)

- Method:
  - Computes short-range forces in real space and long-range forces via Fourier transform.
  - Utilizes a 3D grid to represent charge densities and applies a 3D Fast Fourier Transform (FFT) for efficient computation.

Parallelization of PME:

- 1D: Decompositions are done within slabs aligned in x, y, or z directions.
- 2D: Uses "pencils" instead of slabs for a more distributed decomposition.

Tracking Disease Outbreaks

- Challenges: Increased urban density, global travel, and a growing immunocompromised population complicate tracking.
- Computational Modeling: Helps simulate disease spread by modeling human interactions and disease transmission dynamics.
- Simulation Examples: Determining the probability of transmission between two people based on interaction duration and conditions.