Molecular Dynamics

Improving Neighbor Map

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Problem Statement

- Molecular dynamics systems = very common model
  - Two-body interatomic interactions (Lennard-Jones potential function)
  - Periodic boundaries to represent “infinite” space
- Brute Force -> $O(N^2)$ performance when comparing atom pairs
- Improvement: Verlet Table Algorithm / Cell Linked List Algorithm
- Further improvement: https://arxiv.org/pdf/physics/0311055.pdf
  - Combines above techniques
  - Uses additional techniques to improve table update frequency/memory organization
- How does parallelization of system work?

Tasks

1. Research/study molecular dynamics model and algorithms
2. Implement/source code that can be used to create model.
3. Make improvements to model by:
    a. Parallelizing
    b. Following methods described in https://arxiv.org/pdf/physics/0311055.pdf
4. Demonstrate improvements/errors in system

Goals

- Demonstrate parallelization of simulation
- Show the progressive improvement between conventional methods/combined methods
- Understand the use of graph algorithm in solving a complex problem