CSE 402 Final Project Proposal

Molecular Dynamics Parallel Optimization

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1 Objective:

Classical Molecular dynamics scales with the system size and handling large numbers of particles becomes computationally intensive. Sequential computing becomes time intensive and cumbersome. Parallel computing is able to speed up the computation significantly making runtimes faster. Thus, the objective of this study is to implement a three dimensional molecular dynamics simulation with three levels of parallelism: sequential, OpenMP (shared memory), and MPI (distributed memory).

2 Approach:

The project will be written in C++ and use the velocity Verlet algorithm in order to update the positions and velocities of each particle. The code will simulate a gas of identical molecules with inter-molecular forces calculated using the Leonard-Jones potential. The boundaries will be implemented as rigid, elastic walls containing the micro-canonical (constant e) ensemble. The code will be profiled at each stage using PAPI.

3 Timeline:

- Week 1: Write proposal and have group meeting to set up plan.
- Week 2: Write basic code and design parallel strategies.
- week 3: Collect result generating by different parallel methods and form visual materials.
- week 4: Wrap up all codes and write final report.

4 Possible Issues:

- Synchronization of the particle velocities and positions, when running on different threads, at the end of every time step especially with MPI.
- Designing communicators in three dimensions with MPI could be difficult.
- Using Blue Waters for GPU parallelization if possible, might also be an issue.

5 Pre Code Version:

Please refer to initial sequential code in our group gitlab repository.
gitlab.engr.illinois.edu:xiuyiqin/molecular-dynamics.git