759 Final Project Proposal

Problem statement:

Hybrid Monte Carlo/Molecular Dynamics Simulation:

My research project requires me to write a hybrid Monte Carlo(MC)/Molecular Dynamics(MD) Code to efficiently sample the targeted chemical system. I have already written an interface which uses GPU supported software package OpenMM. The basic idea is using OpenMM to run MD in GPU and generate state information of the system to run a MC in CPU platform. I have written an interface in Python to run MC simulation. With project going further, I realize that there are more and more complicated calculations which need to be done in MC steps. Doing all such calculations in a python interface with one thread is the bottleneck of my code. So I am going to rewrite all the codes in a C++ interface. And more importantly I will use openMP or CUDA to implement the calculations in MC. For example, in MC, I need to fetch the position information of some atoms from GPU and recalculate all distances and use DFS to find the largest cluster. To improve the efficiency, I can create a new plugin in OpenMM and calculate such distances using CUDA.

I realize that fetching information from GPU to run MC would always harm the efficiency. But for now, I do not have the solution to solve that problem.

Motivation/Rationale:

The python interface I am using now is very inefficient.

How you plan to go about it:

Before 20th Nov, rewriting the python interface in C++. This may improve the efficiency a little bit.

21st Nov - 10th Dec, writing OpenMM plugin to do some calculations in MC part at CUDA platform.

10th Dec - 21st Dec, using OpenMP to deal with other complicated calculations.

How you will demonstrate what you accomplished:

I will calculate the efficiency improvement after each step. And make a bar plot of the efficiency to show the progress.

Team members: No

Deliverables:

An PDF which shows what I would implement and what improvement I get compared to the python interface I am using now.

The new interface code and some OpenMM plugin codes.

Participate in Rescale sponsored Final Project competition: No.

Link to your Final Project Repo:

https://github.com/xyli28/759-FinalProject.git

Remarks:
- There's a two-page limit. See if you can make your point without hitting the limit.
- Drop your <u>PDF</u> proposal in the Canvas dropbox `Final Project Proposal 759`.
- Proposal due date: Nov. 3 at 11:59 pm.
- I hope to give feedback within one week.
- The project doesn't necessarily have to be a "ground up" implementation of some large problem, but can be a new parallel implementation of some existing code with the requisite demonstration of the effects of the parallelization (e.g., scaling analysis, correctness, etc.).
- Be bold.