Optimizing Chebyshev Interaction Model with Parallel Programming: From OpenMP to GPU Acceleration

Rajat Goel[$], Kun-Lin Wu[$], Saurabh Sivakumar[$], Sudheesh Kumar Ethirajan[$], Ambarish Kulkarni

[$]equal contribution

Department of Chemical Engineering, University of California, Davis, CA

Contact Information: rajgoel@ucdavis.edu

UCDAVIS CHEMICAL ENGINEERING

Introduction

ChIMES is a many-body, reactive machine learning potential. The original C++ implementation of ChIMES does not incorporate any parallel computing techniques.

Generate ChIMES parameters

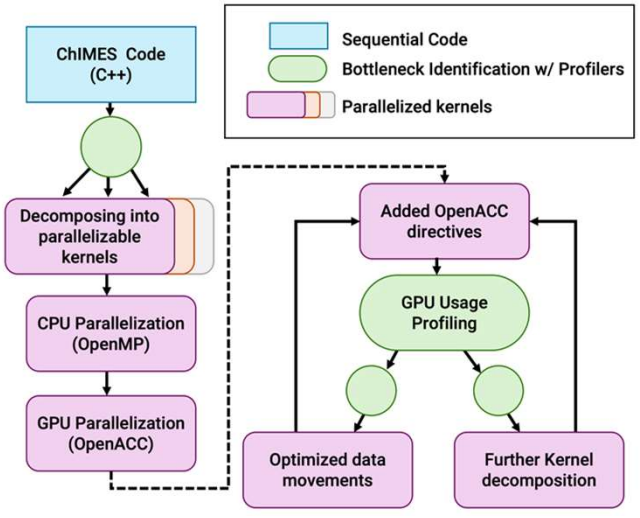
DFT-MD trajectories (forces, energy, stress)

ChIMES Calculator

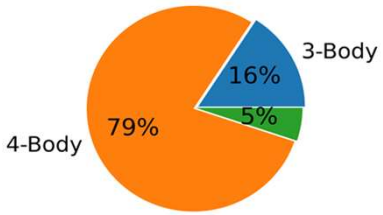
$$E_{ChIMES} = \sum_{i_1}^{n_a} E_{i_1} + \sum_{i_1>i_2}^{n_a} E_{i_1 i_2} + \sum_{i_1>i_2>i_3}^{n_a} E_{i_1 i_2 i_3} + \sum_{i_1>i_2>i_3>i_4}^{n_a} E_{i_1 i_2 i_3 i_4}$$

LAMMPS

Methodology

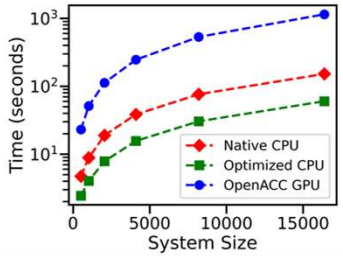


Bottlenecks



- **Problem**
  Higher order interaction terms are **compute intense**
- **Solution**
  Parallelize code with **independent kernels** and **multidimensional arrays**

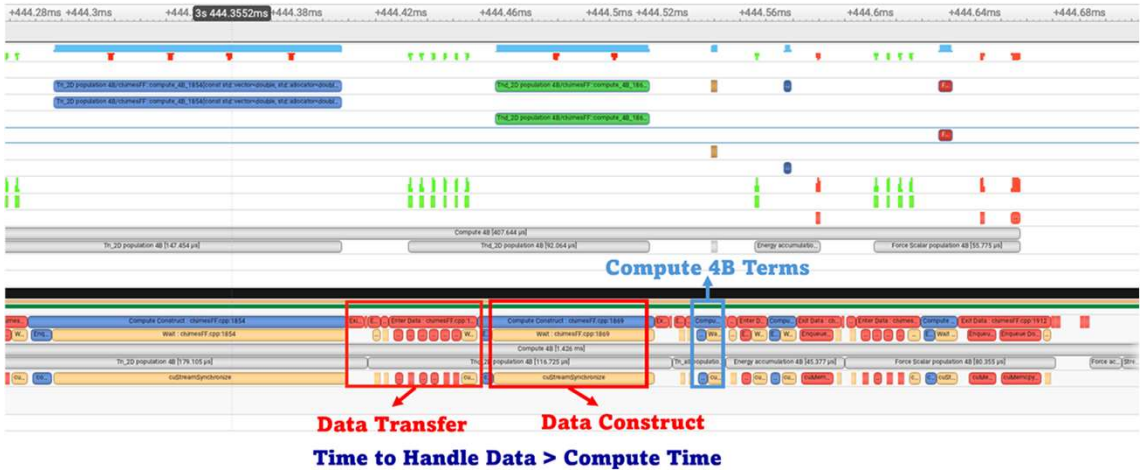
Scalability



- Current **GPU scaling** is limited by **lack of optimization**; future work will address this

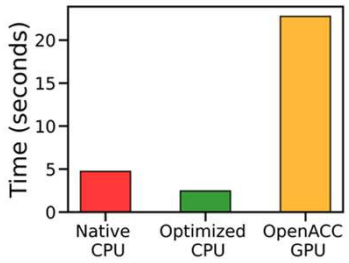
Results

GPU Usage Profile



- Code **ported to GPU** using **OpenACC**
- **Identified** further **bottlenecks** using profiles from Nsight Systems
- **Data** is currently **not preserved on GPU**

Future Roadmap



- **Data Movement**
  Optimize data transfers between host and device by analyzing **variable scope** and **pointer usage**
- **OpenACC Optimization**
  Use **asynchronous transfers** and **data locality**

Acknowledgements

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NERSC OPEN HACKATHONS NVIDIA OpenACC