

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

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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)



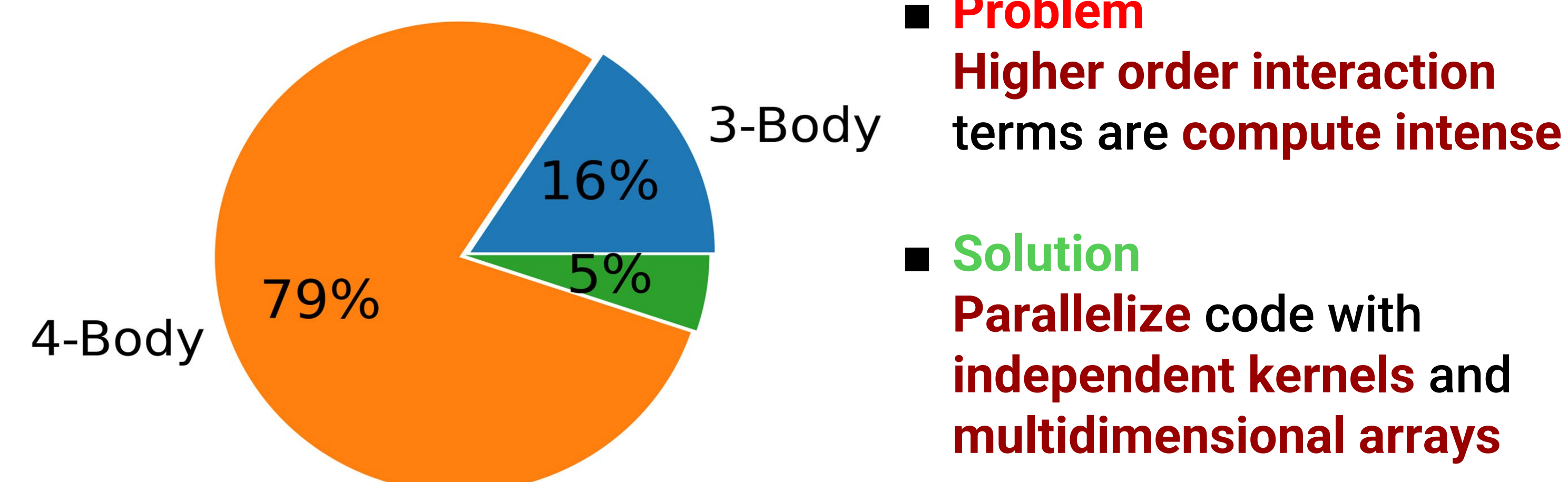
ChIMES Calculator

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



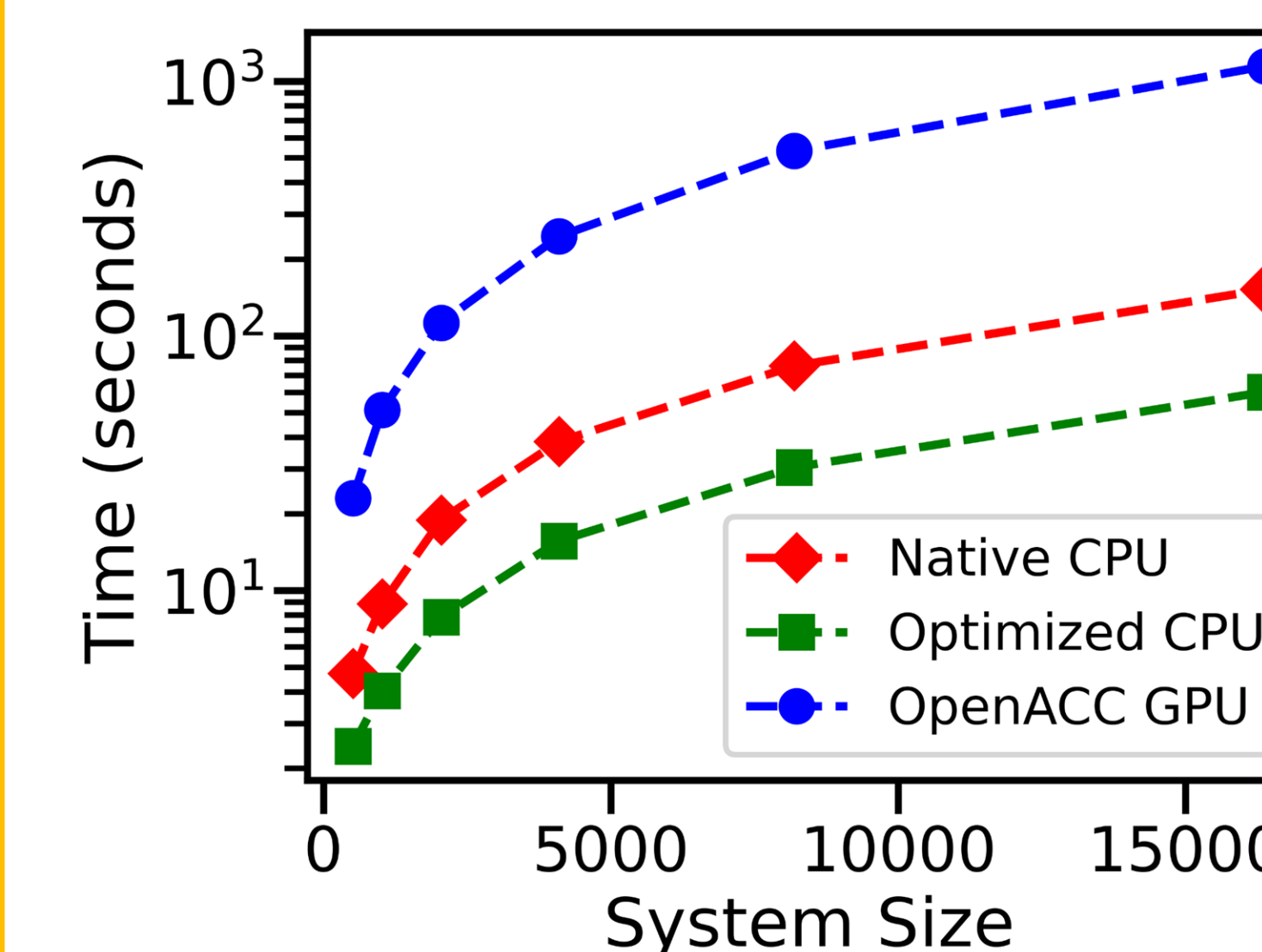
LAMMPS

Bottlenecks



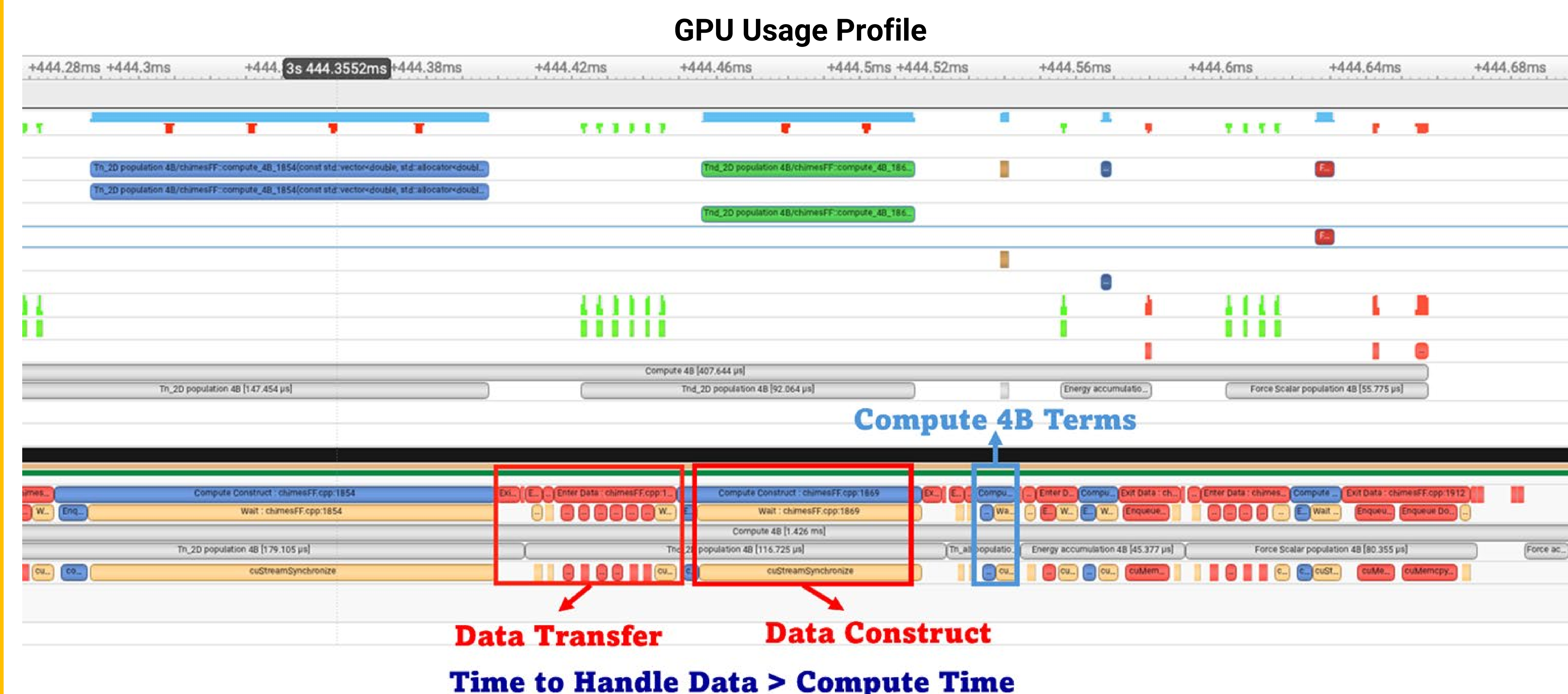
- **Problem**
Higher order interaction terms are **compute intense**
- **Solution**
Parallelize code with **independent kernels** and **multidimensional arrays**

Scalability



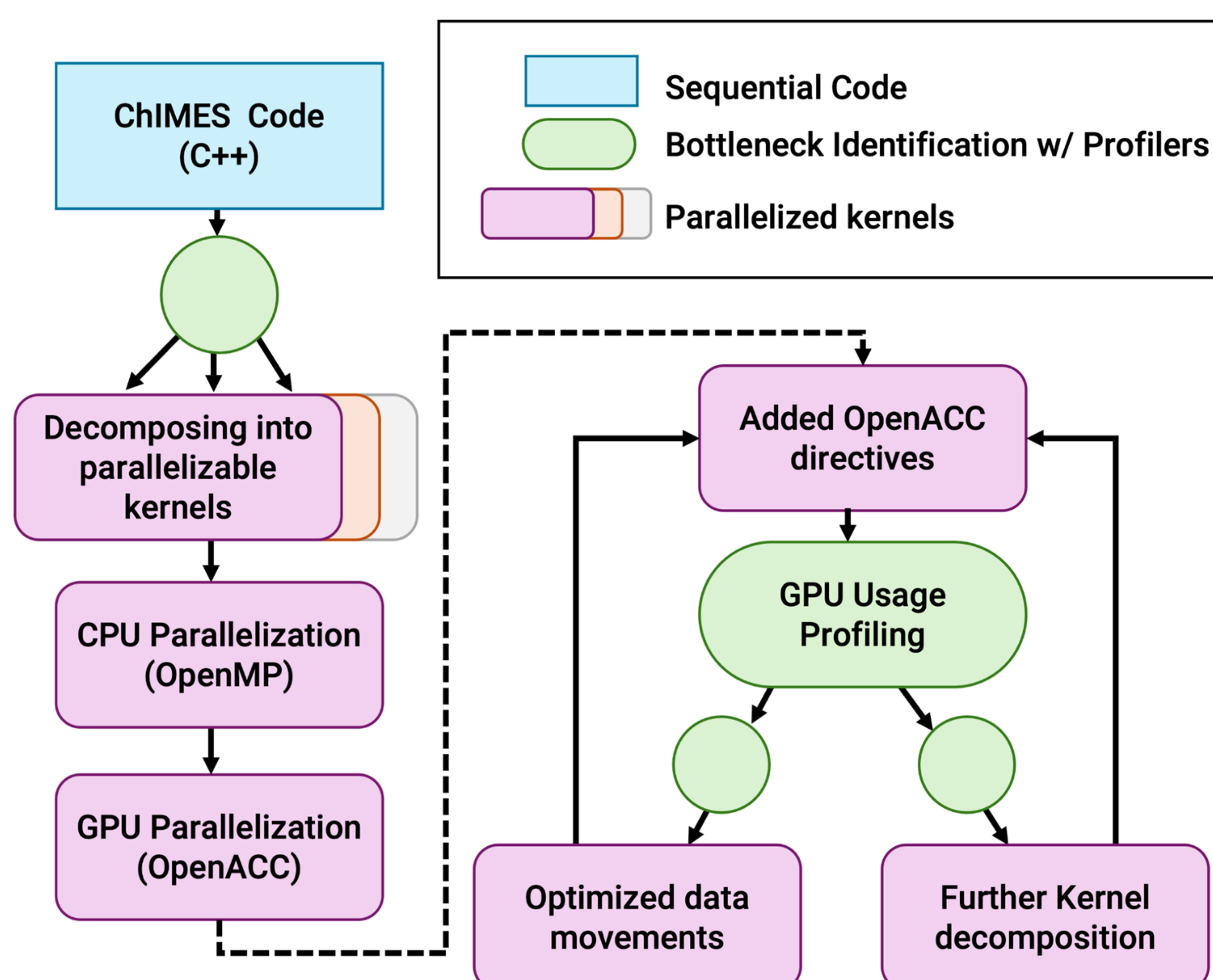
- Current **GPU scaling** is limited by **lack of optimization**; future work will address this

Results

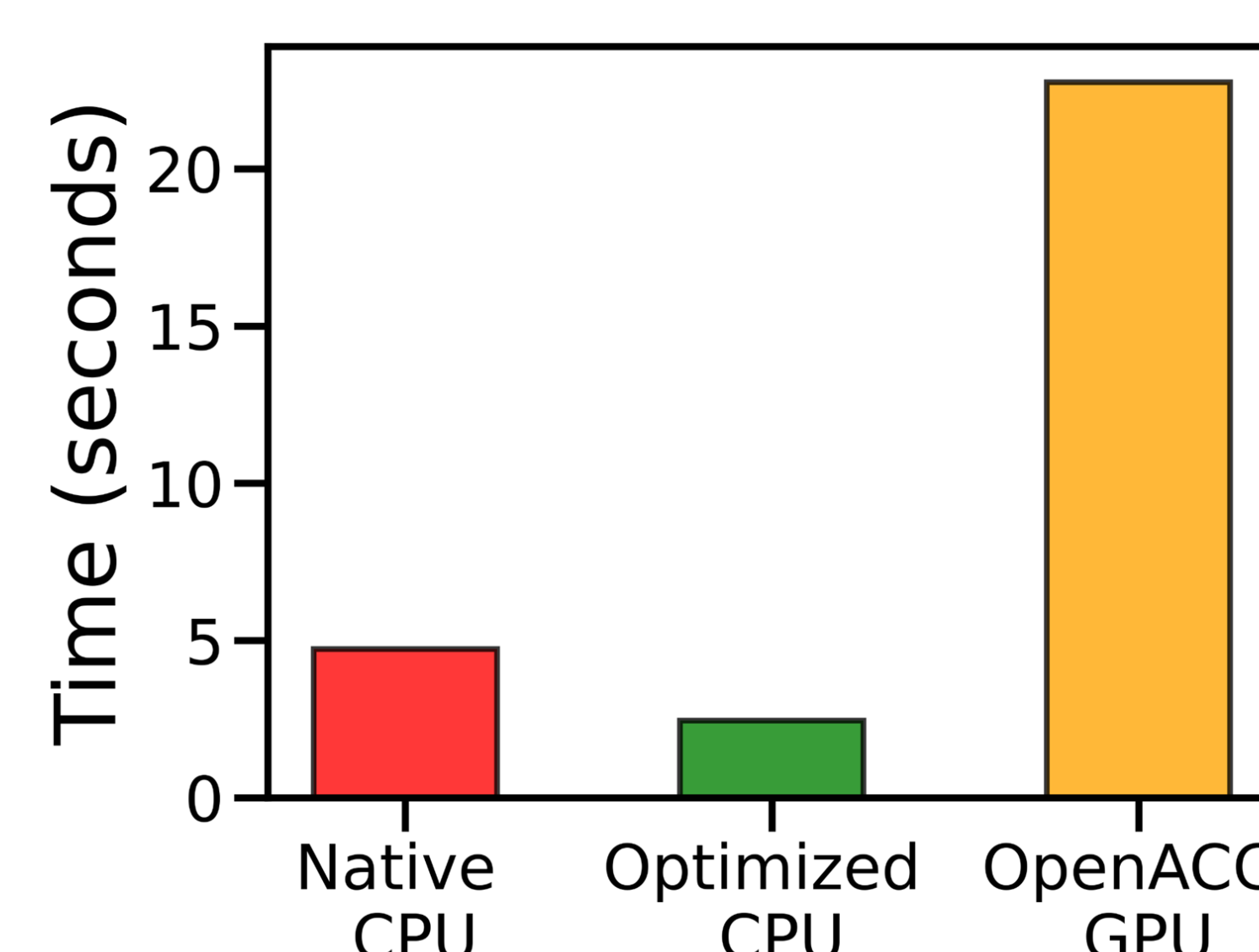


- Code **ported to GPU** using **OpenACC**
- Identified further **bottlenecks** using profiles from Nsight Systems
- Data is currently **not preserved on GPU**

Methodology



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

This work was completed in part at the NERSC GPU Hackathon, part of the Open Hackathons program supported by OpenACC-Standard.org. We thank our mentors, Dr. Phillip Thomas (NERSC) and Dr. Neil Mehta (NERSC), and the NVIDIA mentors for their guidance on Nsight Systems. We also acknowledge Dr. Nir Goldman (LLNL) for his assistance with the ChIMES code. This work used resources of NERSC, a U.S. Department of Energy Office of Science User Facility.