James E. T. Smith, Ph.D.

HPC Software Engineer

CONTACT

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TECHNICAL SKILLS

Programming

C/C++ (7+ years), Python (8+ years), Bash (8+ years), CMake (5+ years), Rust (<1 year)

Parallelism

OpenMP, MPI, Cilk, CUDA

Tools

git, gdb, perf, VTune, clang-tidy, GitHub Actions

EDUCATION

Ph.D. in Chemical Physics at University of Colorado Boulder

Sep 2014 - Aug 2020

BS in Chemistry, Minor in Mathematics at Davidson College

Sep 2010 - May 2014

EMPLOYMENT

Lucata Corporation — Member of the Technical Staff

Jul 2022 - Present

- Implemented a highly multithreaded version of the GraphBLAS library in C/C++, using C++11/14/17.
- Optimized the multithreaded performance of Lucata's GraphBLAS implementation and worked closely with the hardware team to improve performance of the Lucata Pathfinder architecture.
- Consolidated and improved the CMake build system for Lucata's custom LLVM 14 compiler.
- Overhauled the CMake build system for the LucataGraphBLAS project and set up continuous integration, testing, code coverage, and static linting.
- Collaborated with other teams regularly to address bugs and implement new features in the GraphBLAS library.
- Implemented ranges::iota in LLVM's implementation of the C++ standard library, libc++.

Center for Computational Quantum Physics — Flatiron Research Fellow

Sep 2020 - Jul 2022

- Implemented OpenMP parallelized stochastic compression methods for quantum chemistry in the open source C++ package FRI-CC.
- Contributed features, bug fixes, and documentation as one of the primary maintainers for the open source Python/C package PySCF.
- Worked closely with the core team of PySCF developers improve the CMake build system and PyPI distribution after the release of PySCF v2.0.0.
- Organized workshops to help members of the Flatiron community better utilize high performance computing resources as part of the Sciware working group.

University of Colorado Boulder — Graduate (Ph.D.) Research Assistant

Aug 2014 - Sep 2020

- Implemented a hybrid MPI-OpenMP parallelized version of the HCI algorithm in the Sharma Group's C++ software Dice
- Built decision tree and graph neural network models to predict etching reaction outcomes and trained these models with experimentally observed data.
- Wrote a new module for the PySCF package to interface with Dice enabling the investigation previously intractable systems.
- Frequently contributed to the PySCF quantum chemistry package, implementing new features and handling bug reports.
- Organized and led a workshop on software best practices for graduate students and post doctoral researchers with staff from the Molecular Sciences Software Institute (MOLSSI).

PROJECTS

Taught regularly about software best practices in scientific computing to learners with a broad programming background. Taught lessons on shell, Git, Python, and data visualization in Python.