James E. T. Smith, Ph.D.

HPC Software Engineer

Contact

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About

Profiles

Desktop
https://jamesetsmith.github.io/

GitHub
jamesETsmith

LinkedIn
james-smith-ph-d-8525792b

Work

Lucata Corporation

2022-07-11 —

Member of the Technical Staff

Highlights

- 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

2020-09-01 — 2022-07-11

Flatiron Research Fellow

Highlights

- 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

2014-08-01 — 2020-09-01

Graduate (Ph.D.) Research Assistant

Highlights

- 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).

Volunteer

Software Carpentry

2021-05-01 —

Instructor

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.

Education

University of Colorado Boulder

2014-09-01 — 2020-08-01

🎓 **Chemical Physics**
Ph.D.

Davidson College 2010-09-01 — 2014-05-01

🎓 **Chemistry, Minor in Mathematics**

BS

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