James **E. T. Smith, Ph.D.**

jamesETsmith / +1 508 596 7110 / james.smith9113@gmail.com /
james-smith-ph-d-8525792b / https://jamesetsmith.github.io/

Software engineer with experience in high performance computing, numerical linear algebra, and quantum chemistry.

Skills

Programming C/C++ (7+ years) Python (8+ years) CMake (5+ years) Rust (\<1 year)
Parallelism OpenMP MPI Cilk CUDA
Tools git perf VTune gdb clang-tidy GitHub Actions

Professional Experience

Member of the Technical Staff
Jul. 2022 - Present
Lucata Corporation — *New York, NY*

- Developed 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.
- Collaborated with other teams regularly to address bugs and implement new features in the GraphBLAS library.
- Consolidated and improved the CMake build system for Lucata's custom LLVM 14 compiler.
- Overhauled the CMake infrastructure for the Lucata software ecosystem and set up continuous integration, testing, code coverage, and static linting for nearly all projects.
- Implemented std::ranges::iota in libc++, LLVM's version of the C++ standard library.

C++ C++17 C multithreading Cilk CMake CI LLVM Linux

Flatiron Research Fellow
Sep. 2020 - Jun. 2022
Center for Computation Quantum Physics, Flatiron Institute — *New York, NY*

- 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.

C++ C++20 Python multithreading OpenMP MPI CUDA CMake CI Linux

Graduate (Ph.D.) Researh Assistant
Aug. 2014 - Aug. 2020
University of Colorado Boulder — *New York, NY*

- 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.
- Frequently contributed to the PySCF quantum chemistry package, implementing new features and handling bug reports.
- Wrote a new module for the PySCF package to interface with Dice enabling the investigation previously intractable systems.
- 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).

Python C++ C++11 multithreading OpenMP MPI CMake machine learning scikit-learn Linux

Education

Ph.D. Chemical Physics
Aug. 2014 - Aug. 2020
University of Colorado Boulder — *Boulder, CO, US*

Bachelors of Science in Chemistry, Minor in Math
Aug. 2010 - May 2014
Davidson College — *Davidon, NC, US*

Volunteer

Instructor
May 2021 - Present
Software Carpentry — *New York, NY*

- 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.

Certifications

May 2021 **Software Carpentry Instructor Certificate**, Software Carpentry
Apr. 2021 **NVIDIA DLI Certificate - Accelerating CUDA C++ Applications with Multiple GPUs**, NVIDIA
Apr. 2021 **NVIDIA DLI Certificate - Fundamentals of Accelerated Computing with CUDA C/C++**, NVIDIA