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

HPC Software Engineer

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## BACKGROUND

### WORK EXPERIENCE

**Member of the Technical Staff**, Lucata Corporation

Jul, 2022 - Present

Small startup developing custom architecture for sparse graph problems

- Implemented a highly multithreaded version of the GraphBLAS library in C/C++, using C++11/14/17.
- Optimized the multithreaded performance of our version of GraphBLAS and worked closely with the hardware team to improve performance of the Lucata Pathfinder architecture.
- Overhauled the CMake build system for the GraphBLAS 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.

**Flatiron Research Fellow**, Center for Computational Quantum Physics, Flatiron Institute

Sep, 2020 - Jul, 2022 1 year 10 months

Private research institute for high performance computing in basic science research.

- 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.

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

Aug, 2014 - Sep, 2020 6 years 1 month

Public research university.

- 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).

## SKILLS

**Programming**

C/C++ (7+ years) Python (8+ years) Bash (8+ years)

**Parallelism**

OpenMP MPI Cilk CUDA

**Tools**

git CMake gdb perf VTune GitHub Actions

## EDUCATION

**Chemical Physics, Ph.D.**, University of Colorado Boulder

Sep, 2014 - Aug, 2020

**Chemistry, Minor in Mathematics, BS**, Davidson College

Sep, 2010 - May, 2014

## CERTIFICATES

**Software Carpentry Instructor Certificate**, Software Carpentry

Issued on: May 01, 2021

**NVIDIA DLI Certificate - Accelerating CUDA C++ Applications with Multiple GPUs**, NVIDIA

Issued on: Apr 01, 2021

**NVIDIA DLI Certificate - Fundamentals of Accelerated Computing with CUDA C/C++**, NVIDIA

Issued on: Apr 01, 2021

## VOLUNTEER WORK

**Instructor,** Software Carpentry

May, 2021 - Present

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.