

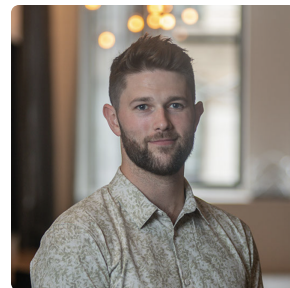
# James E. T. Smith, Ph.D.

## Software Engineer

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<https://jamesetsmith.github.io/> 🔗 [jamesETsmith](#) [james-smith-ph-d-8525792b](#)



### SKILLS

#### Programming

C/C++ (>7 years)

Python (>8 years) Julia (<1 year)

Rust (<1 year)

#### Parallelism

OpenMP

MPI

Cilk

CUDA

#### Tools

git

CMake

VTune

Perf

GitHub Actions

clang-tidy

gcov

### WORK EXPERIENCE (3)

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

**Jul 2022 - Current**

📍 New York, NY,

The next generation computing architecture optimized for massive scale.

- 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** at Center for Computational Quantum Physics, Flatiron Institute

**Sep 2020 - Jul 2022**

📍 New York, NY,

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** at University of Colorado Boulder

**Aug 2014 - Sep 2020**

📍 Boulder, CO,

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).

## VOLUNTEER

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**Instructor** at Software Carpentry

**May 2021 - Current**

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 (2)

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

**2014 - 2020**

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

**2010 - 2014**

## CERTIFICATES

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**Software Carpentry Instructor Certificate**

Software Carpentry

**2021-05-01**

 <https://software-carpentry.org/>

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

NVIDIA

**2021-04-01**

 <https://www.nvidia.com/en-us/training/>

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

NVIDIA

**2021-04-01**

 <https://www.nvidia.com/en-us/training/>