

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

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

The next generation computing architecture optimized for massive scale.

#### Highlights

- 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 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.

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

## 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

Public research university.

## 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.

# Skills

## Programming

- C/C++ (>7 years)
- Python (>8 years)
- Julia (<1 year)
- Rust (<1 year)

## Parallelism

- OpenMP
- Cilk
- MPI
- CUDA
- VTune
- Perf

## DevOps

- git
- Make
- CMake
- GitHub Actions
- Continuous Integration
- clang-tidy
- Code coverage