JAMES E. T. SMITH, PH.D.

HPC SOFTWARE ENGINEER

ABOUT

270 W 39TH ST
NEW YORK, NEW YORK NY
10018

JAMES.SMITH9113@GMAIL.COM

+1 (508)-596-7110

JAMESETSMITH.GITHUB.IO/

JAMESETSMITH

IN/JAMES-SMITH-PH-D-8525792B

PROGRAMMING

C/C++ (7+ YEARS)
PYTHON (8+ YEARS)
BASH (8+ YEARS)
RUST (<1 YEAR)

PARALLELISM

OPENMP
MPI
CILK
CUDA

TOOLS

GIT
CMAKE
GDB
PERF
VTUNE
CLANG-TIDY
GITHUB ACTIONS

EXPERIENCE

LUCATA CORPORATION

07/2022 - PRESENT

MEMBER OF THE TECHNICAL STAFF

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 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.

CENTER FOR COMPUTATIONAL QUANTUM PHYSICS

09/2020 - 07/2022

FLATIRON RESEARCH FELLOW

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.

UNIVERSITY OF COLORADO BOULDER

08/2014 - 09/2020

GRADUATE (PH.D.) RESEARCH ASSISTANT

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

SOFTWARE CARPENTRY

05/2021 - PRESENT

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

09/2014 - 08/2020

PH.D. CHEMICAL PHYSICS

DAVIDSON COLLEGE

09/2010 - 05/2014

BS CHEMISTRY, MINOR IN MATHEMATICS