James E. T. Smith, Ph.D.

HPC Software Engineer

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SKILLS

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

WORK EXPERIENCE (3)

Member of the Technical Staff at Lucata Corporation **Jul 2022 - Current**

New York, NY,

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.

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

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)

Ph.D. Chemical Physics at University of Colorado Boulder

2014 - 2020

BS Chemistry, Minor in Mathematics at Davidson College

2010 - 2014

CERTIFICATES

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/