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

- 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.
- Implemented ranges::iota in LLVM's implementation of the C++ standard library, libc++.

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

Sep, 2020 - Jul, 2022 1 year 10 months

- 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

- 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) CMake (5+ years) Rust (<1 year)

Parallelism

OpenMP MPI Cilk CUDA

Tools

git gdb perf VTune clang-tidy 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.