D. Vale Cofer-Shabica, Ph.D.

Associate Research Scholar, Princeton University

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Professional Summary

Computational scientist and software engineering leader with 10+ years developing high-performance algorithms for classical and quantum mechanical simulations as well as electronic structure calculations. Core contributor to quantum chemistry software, Q-Chem, used by over 50,000 researchers worldwide. Expert in C/C++ and Python programming with proven track record leading distributed software teams, mentoring technical talent, and delivering scalable solutions for CPU and GPU code across DOD, DOE, and NSF super-computing clusters. Domain expert with 10+ peer-reviewed papers and 10+ invited talks; technical mentor with 8+ trainees mentored and multiple successful software project deliveries.

Appointments

Associate Research Scholar — Princeton University, Princeton, NJ, 2024–*Present*

- Led a team of researchers in architecting and developing XEBEES (Python), a framework for numerically exact quantum mechanics simulations. Multiple, transparently-selected backends (NumPy, CuPy, Torch, cuPyNumeric) run on CPUs or GPUs with a single code base. Performant and readable framework enables researchers to easily add new physics.
- Developed and optimized computational algorithms for quantum mechanical simulations, improving performance 60 fold on GPU architectures. Vectorized, iterative solver can diagonalize matrices with over 10^{14} elements.
- Optimized algorithm and implementation to reduce the computational cost of exact quantum mechanical reference calculations from 3.5 hours to 7 seconds.
- Mentored 4 trainees in science, software development, and writing to yield 3 peer-reviewed papers.

Postdoctoral Researcher — University of Pennsylvania, Philadelphia, PA, 2019–2024

- Collaborated in a distributed team of over 100 researchers in the development cycle of the electronic structure code Q-Chem (C/C++/FORTRAN); designed, implemented, tested, and documented new features using version control and ticket system.
- Developed and implemented algorithm based on previously computed states to accelerate excited state geometry optimizations by 50% overall with no approximations in Q-Chem.
- Architected and led development of INAQS (C/C++) connecting Gromacs and Q-Chem, enabling large-scale simulations of non-adiabatic dynamics embedded in a classical environment. Designed minimal API for connection between arbitrary molecular dynamics and electronic structure codes.
- Co-authored proposals securing 8M+ core-hours across national super-computing centers (NERSC and DOD) and efficiently managed a computational campaign to produce data for 6 papers.
- Mentored 5 trainees in science, software development, and paper writing yielding 3 peer-reviewed papers and 6 completed projects.

Director of Education — Harvard University, Banneker Institute, Cambridge, MA, 2019

- Designed and supervised the delivery of technical curriculum on computational and scientific methods for cohort of 10+ students.
- Created hands-on programming workshops to teach practical implementation skills to scientists.

Skills

Programming Languages: C, C++, Python, FORTRAN, Haskell, shell

Frameworks: NumPy, SciPy, JAX, PyTorch, CuPy, cuPyNumeric, asyncio, Armadillo, OpenMP, MPI, CMake

High-Performance Computing: Linux, GPU and distributed computing, portability, dependency management, job scheduling (SLURM/PBS)

Software Development: git/svn, issue tracking (trac/github), debugging (gdb), testing, profiling (gprof, nvsys), API design

Computational Methods: Linear algebra, numerical analysis, optimization, electronic structure theory, quantum and molecular dynamics, statistical mechanics

Education

Ph.D. Theoretical Physical Chemistry — Brown University, Providence, RI, 2018

Potter Prize for Doctoral Thesis of Outstanding Merit; King Teaching Excellence Prize; Chase Leadership and Service Award

Sc.B. Chemical Physics — Brown University, Providence, RI, 2009