# D. Vale Cofer-Shabica, Ph.D.

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## Professional Summary


Performance engineer and computational scientist with 10+ years building high-performance software for compute-intensive workloads on CPU and GPU architectures. Expert in C/C++, Python, and array computing frameworks (PyTorch, NumPy, CuPy) with proven track record achieving 60×–1800× speedups through profiling, algorithmic optimization, and efficient GPU utilization. Architect of multi-backend frameworks enabling seamless hardware portability; deep current focus on GPU collective communication, NCCL internals, and high-performance interconnects. Contributor to Q-Chem used by 50,000+ researchers. Experienced mentoring technical talent and leading distributed software projects across DOD, DOE, and NSF supercomputing centers. Published researcher with 10+ peer-reviewed papers and 10+ invited talks; technical mentor with 8+ trainees mentored and multiple successful software project deliveries.


## Positions

**Software Engineer III** — Comcast Corporation, Philadelphia, PA, 2026–*Present*

- Designed and delivered automated tooling for network operations including hardware fault monitoring that replaced manual ticketing; identified and implemented SSH connection optimizations that reduced Ansible overheads by 40×.
- Built developer tools and diagnostics adopted across multiple teams and contributed to org-wide platform initiatives.

**Associate Research Scholar** — Princeton University, Princeton, NJ, 2024–2026

- Architected and built XEBEES (Python), a high-performance framework for numerically exact quantum mechanics supporting multiple backends (PyTorch, NumPy, CuPy, cuPyNumeric). Transparent backend selection enables optimized execution on CPUs or GPUs with a single codebase and enables scientists to easily add new physics.
- Built and optimized computational kernels for large-scale numerical computations, achieving 60× performance improvement on GPU architectures through batching, vectorization, and efficient memory management. Built vectorized, iterative solver capable of efficiently diagonalizing matrices with over $10^{15}$ elements.
- Identified critical bottleneck through profiling and optimized computational pipeline to reduce runtime from 3.5 hours to 7 seconds (1800× speedup) through algorithmic and implementation improvements.
- Rapidly acquired new technologies: implemented GPU optimization under CuPy and cuPyNumeric in 1 week.

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

- Architected and built INAQS (C/C++), a framework connecting two large-scale scientific computing codes (Gromacs and Q-Chem) through a clean, minimal API.
- Built algorithm to accelerate excited state geometry optimizations by 50% overall with no approximations in Q-Chem by reusing previously computed wavefunctions.
- Collaborated in a distributed team 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.
- Co-authored proposals securing 8M+ core-hours across national supercomputing centers (NERSC and DOD) and efficiently managed a computational campaign to produce data for 6 papers.

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

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

## Skills

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

**Array, ML, & Parallel Frameworks:** MPI, PyTorch, JAX, NumPy, SciPy, CuPy, cuPyNumeric, asyncio, Armadillo, OpenMP

**High-Performance Computing:** GPU optimization, performance modeling, topology-aware optimization, bottleneck analysis, distributed computing, job scheduling (SLURM/PBS), GPU architecture, compute-communication overlap

**Development & Infrastructure:** atomics, concurrent data structures, memory ordering, git/SVN, Linux, debugging (gdb), testing, profiling (gprof, Nsight Systems), correctness (valgrind, sanitizers), API design, CMake, Docker, Kubernetes, AWS

**Computational Methods:** array computing, linear algebra, iterative algorithms, multivariate optimization, numerical analysis, 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