

Gaurav Harsha

Computational Scientist • Scientific Software & HPC

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Summary

Computational physicist (PhD) developing high-performance scientific software for first-principles electronic-structure simulation. Core developer of a production C++/Python/CUDA codebase implementing many-body methods with GPU acceleration and distributed-memory parallelism that scales from workstations to HPC systems. Expertise in numerical linear algebra, scientific computing, and performance optimization, with a track record of turning advanced computational methods into robust, maintainable software.

Technical Skills

Languages:	Python, C++, Fortran, CUDA
Scientific / Numerical:	NumPy, SciPy, PySCF, BLAS/LAPACK, dense & iterative linear algebra, eigen-value solvers, self-consistent (fixed-point) solvers
HPC & Parallel:	MPI, multi-node / multi-core scaling ($\sim 10^3$ cores), GPU/CUDA acceleration, performance profiling & optimization
Data:	pandas, data analysis, probability & statistics
Tooling:	Git, Linux, CMake, SLURM/HPC clusters, reproducible release engineering

Education

Ph.D. & M.S., Physics & Astronomy <i>Rice University, Houston, TX</i>	2016–2021
B.Tech., Physical Science (Gold Medalist) <i>Indian Institute of Space Science & Technology, India</i>	2011–2015

Experience

Research Area Specialist Senior <i>Department of Chemistry, University of Michigan, Ann Arbor</i> <ul style="list-style-type: none">• Lead developer of the Green-Phys suite; architect and implement new Green's-function methods across a C++/Python code base used by research groups internationally.• Optimize the CUDA GPU accelerator (GREEN-GPU), which sustains $\sim 70\%$ of peak FLOPS per device on average across multi-node A100 systems.• Maintain the release pipeline across 5 packages (~ 9 releases) and train 10–20 users across the group and collaborating institutions, including a workshop tutorial.	2025–present
Postdoctoral Research Fellow <i>Department of Chemistry, University of Michigan, Ann Arbor</i> <ul style="list-style-type: none">• Developed first-principles Green's-function methods for the electronic structure of solid-state systems, targeting relativistic effects, disorder, and topological phases.• Presented 8+ conference talks (including invited seminars) and co-authored 10 papers.	2022–2025
Scientist / Engineer <i>Space Applications Centre, ISRO, Ahmedabad, India</i> <ul style="list-style-type: none">• Managed 24/7 thermal-vacuum laboratory operations, supervised staff, and owned equipment maintenance and budgets.• Contributed to the mechanical/thermal design of a large-scale vacuum chamber for spacecraft testing.	2015–2016

Selected Software

- **GREEN-MBPT** — C++/Python packages for *ab initio* Green's-function simulations; core developer.
- **GREEN-GPU** — CUDA accelerator for many-body methods used within GREEN-MBPT.
- **drudge** / **drudge-exts** — symbolic algebra system for tensor and noncommutative algebras; contributor.
- **TFD-CCSD** / **CANON-TFD** — thermal coupled-cluster & perturbation theory (Python/Fortran).

Selected Publications

Selected to span production software, core method development, and highest-impact first-author work (including quantum-computing-relevant algorithms). Full list (15 papers, 9 first-author) at gauravharsha.github.io.

- Iskakov, S., **Harsha, G.** *et al.* **Green/WeakCoupling**: fully self-consistent finite-temperature many-body perturbation theory for molecules and solids. *Comput. Phys. Commun.* **306**, 109380 (2025).
- **Harsha, G.**, Abraham, V. & Zgid, D. Quasiparticle and fully self-consistent *GW* methods using Gaussian orbitals. *Phys. Rev. B* **110**, 235146 (2024).
- **Harsha, G.**, Henderson, T. M. & Scuseria, G. E. Thermofield theory for finite-temperature quantum chemistry. *J. Chem. Phys.* **150**, 154109 (2019). (*Editor's Choice.*)
- **Harsha, G.**, Shiozaki, T. & Scuseria, G. E. On the difference between variational and unitary coupled cluster theories. *J. Chem. Phys.* **148**, 044107 (2018).