





Karl Pierce, PhD

Postdoctoral Research Scientist

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LinkedIn

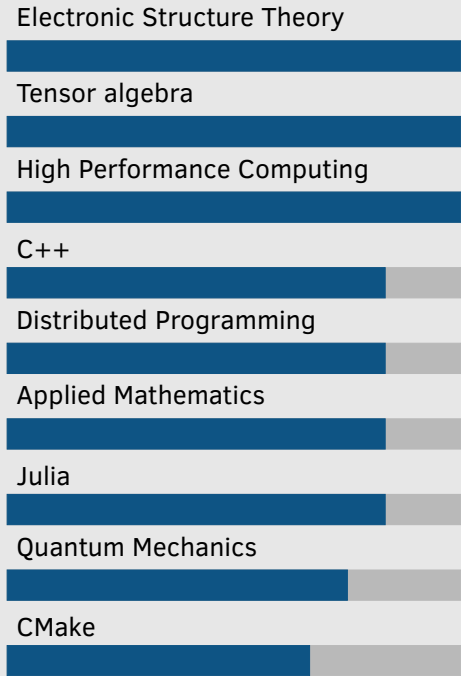
GitHub

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About Me

Results-driven, adaptable scientist with experience in both laboratory and theoretical research. Thrives in independent and group settings with an ambition to collaborate and improve interdisciplinary research.

Skills



Independent Research*
Communication* Experimental
Design* Library and Algorithm
Design*

Objective

Passionate about the application of emerging tensor algebra to physics, chemistry and other computational modeling problems. Dedicated to creating advanced software tools to improve and accelerate the study of applied mathematics on modern distributed computer infrastructures.

Education

2016-2021	PhD Theoretical Chemistry <i>Virginia Tech</i>	Blacksburg, VA
2012-2016	B.S. Chemical Physics <i>Rice University</i>	Houston, TX

Publications

2025	Towards Using Matrix-Free Tensor Decomposition to Systematically Improve Approximate Tensor-Networks. Pierce, K, J. Chem. Theory Comput. 2025, XXXX, XXX, XXX-XXX
2025	Using Matrix-Free Tensor-Network Optimizations to Construct a Reduced-Scaling and Robust Second-Order Møller-Plesset Theory. Pierce, K.; Morales, M J. Chem. Theory Comput. 2025, 21, 12, 5952–5964
2022	Efficient Construction of Canonical Polyadic approximations of Tensor Networks Pierce, K.; Valeev, E. J. Chem. Theory Comput. 2023, 19, 1, 71–81.
2021	Robust Approximation of Tensor Networks: Application to Grid-Free Tensor Factorization of the Coulomb Interaction. Pierce, K.; Rishi, V.; Valeev, E. F. J. Chem. Theory Comput. 2021, 17, 4, 2217–2230.
2021	Breaking the curse of dimensionality in electronic structure methods: towards optimal utilization of the canonical polyadic decomposition. Pierce, K. (2021) [Doctoral dissertation, Virginia Tech, Blacksburg].
2020	Massively Parallel Quantum Chemistry: A high-performance research platform for electronic structure. Peng C; Lewis C; Xiao W; Clement M; Pierce K; Rishi V; Pavošević F; Slattery S; Zhang J; Teke N; Kumar A; Masteran C; Asadchev A; Calvin J; Valeev E. F.; (2020). J. Chem. Phys., 153(4), 44120.

In Preparation

- STTID: High-Performance Sparse Tensor-Train Interpolative Decomposition
Z. Meng; EM. Stoudenmire; K. Pierce; F. Mueller; J. Li
- Effective use of 4-way Canonical Polyadic Decomposition for Accelerating the Coupled-Cluster Perturbative Triples.
Pierce, K.; Bao, Y; Pavošević, F; Valeev, E
- Studying the Efficient Approximation of Lattice Networks using the Canonical Polyadic Decomposition
Pierce, K.; Tindall, J.; Stoudenmire EM.
- The Prediction of Accurate Ground State Energies via Rank-Reduced Periodic Coupled Cluster and the Interpolative Separable Density Fitting Approximation.
Pimpel, F.; Morales, M; Grüneis, A; Pierce, K

Professional Experience

Sept 2022-	Flatiron Software Research Fellow	The Flatiron Institute
	Postdoctoral researcher at the Center for Computational Quantum Physics. Worked with faculty researchers to develop and advance theories in computational quantum physics and chemistry using novel ideas in multilinear algebra. Worked as a lead developer for the ITensors.jl software package. In this package, I created support for heterogeneous CPU/GPU algorithms via the use of state-of-the-art generic programming techniques in the Julia programming language.	
2022	Research Scientist	Virginia Tech
	Worked on developing efficient electronic structure methods for large molecules. Built parallel implementations of these methods using the C++ language for heterogeneous massively parallel computer systems. Planned and conducted research projects requiring independent evaluation, selection, and substantial adaptation or modification from standard published techniques and procedures. Furthermore, I mentored graduate students and postdocs.	
2016-2021	Graduate Research Assistant	Virginia Tech
	PhD supervised under Dr. Edward Valeev Studied electronic structure theory, higher-order tensor algebra, and advanced data compression and algorithmic optimization schemes. Developed production level tools in the software packages BTAS , a higher-order tensor algebra library, TiledArray , a scalable tensor framework for high-performance tensor arithmetic, and MPQC , a platform for ab initio electronic structure methods simulation.	
2015-2016	Research Assistant	Rice University
	Supervised under Dr. Gustavo Scuseria Completed a senior chemistry research project using the Gaussian software package. Using the Generalized Hartree-Fock (GHF) method, I benchmarked the disassociation behavior of diatomic transition metal complexes with the goal of demonstrating the utility of GHF over more expensive electronic structure methods.	
2014-2015	Research Assistant	Rice University
	Supervised under Dr. Emilia Morosan Created novel metallic single and multi-crystals with exotic magnetic properties utilizing techniques such as liquid flux growth, vapor deposition and arc melting. Studied the structure of such metallic crystals using small angle X-Ray Diffractometry. Studied ternary phase diagrams and the underlying physics of superconductivity. Loaded samples onto and probed magnetic properties using a superconducting quantum interference device (SQUID) magnetometer. Mentored younger students on laboratory safety and laboratory methods.	

Invited Presentations and Posters

2025	Toulouse Tensor Workshop 2025	TBD
	Towards the Efficient Approximation of Tensor-Network Contraction via Low-Rank Tensor Decomposition	
2025	Molecular Quantum Mechanics Conference	Seminar
	Application of the Canonical Polyadic Decomposition in the Pursuit of Extremely Low-Scaling Correlation Methods.	
2025	NVIDIA Design, Demos, Ideas, and Research discussions	Seminar
	Studying the effective application of low-rank tensor approximations to electronic structure methods.	
2025	SIAM Conference on Computational Science and Engineering	Seminar
	Towards the Efficient Approximation of Higher-Order, Tensor-Network Contractions Via a Low-Rank, Matrix-Free Tensor Decomposition	
2025	Applied Math Colloquium at Rensselaer Polytechnic Institute	Seminar
	Investigating the Utility of Matrix-Free Tensor Decompositions in Quantum Simulations.	
2024	Juliacon	Seminar
	Improving the life-cycle of tensor algorithm development	
2024	Invited group meeting: Virginia Tech	Seminar
	Approximating tensor contractions via a matrix-free tensor decomposition	
2024	Extreme-scale Mathematically-based Computational Chemistry meeting	Seminar
	Approximating tensor contractions via a matrix-free tensor decomposition	

2024	Invited group meeting: Vienna University of Technology Approximating tensor contractions via a matrix-free tensor decomposition	Seminar
2023	SIAM Conference on Computational Science and Engineering Introduction to the ITensor Software Library for Tensor Network Calculations	Seminar
2021	Colloquium at Vienna University of Technology <i>Utility of the Canonical Polyadic Decomposition and Robust Tensor Network Approximations</i>	Seminar
2019	Virginia Tech Department of Chemistry Internal Seminar <i>Reduced Cost Electronic Structure Theory via the Canonical Polyadic Decomposition</i>	Seminar
2019	American Chemical Society National Meeting <i>Towards Reduced Scaling Higher Order Coupled Cluster Methods via Tensor Decomposition.</i>	Poster
2018	Modern Wavefunction Methods in Electronic Structure Theory <i>Reducing Complexity and Cost of High-Order Coupled-Cluster Method via Canonical Polyadic Decomposition of Hamiltonian</i>	Poster
2018	Penn Conference in Theoretical Chemistry and Electronic Structure Workshop <i>Reducing Complexity and Cost of High-Order Coupled-Cluster Method via Canonical Polyadic Decomposition of Hamiltonian.</i>	Poster
2018	Virginia Tech Department of Chemistry Preliminary Exam <i>Reduced Scaling of Accurate Electronic Structure Methods using Tensor Decompositions</i>	Seminar
2017	Southeast Theoretical Chemistry Association Meeting <i>Toward Efficient Canonical Product Decomposition in TiledArray Framework</i>	Poster

Workshops and Advanced Topic Schools

2025	Research Collaboration Workshop, "Randomized Numerical Linear Algebra" (RNLA) Research Workshop that focuses on developing efficient and practical algorithms for solving problems using numerical linear algebra via randomized techniques. Assigned to work with Dr. Tamara Kolda on a project to study structure-aware randomization for linear algebra.	Los Angeles, CA
2022	Argonne Training Program on Extreme-scale Computing Participated in an intensive two week summer school learning modern key skills, approaches, and about tools to design, implement and execute scientific applications on state of the art, leadership-class computing systems of today and the future.	Chicago, IL
2018	MolSSI Summer School and Workshop Parallel Computing in Molecular Sciences Participated in a three-day lecture series where researchers in academia and from Berkeley national lab. Discussed computational parallelism and communication on homogenous and heterogeneous CPU/GPU computer systems.	Berkely, CA
2018	Modern Wavefunction Methods in Electronic Structure Theory Attended a week-long summer school at the Max-Planck institute in Germany directed towards Ph.D. students and postdocs with aims to teach advanced topics in the field of ab initio electronic structure theory, reduced scaling algorithms, and software implementations on modern hardware.	Gelsenkirchen, Germany

Teaching Experience

Summer 2024	qnumerics : School for Numerical Methods in Quantum Information Science
Spring 2018	Physical Chemistry: Thermodynamics
Fall 2017	General Chemistry Lab
Spring 2017	Physical Chemistry Lab
Fall 2016	General Chemistry Lab

Certificates

2022	NVIDIA Certificate in Scaling CUDA C++ Applications to Multiple Nodes
2022	NVIDIA Certificate in Fundamentals of Accelerated Computing with CUDA C/C++

Professional Affiliations

The American Chemical Society
Society of Industrial and Applied Mathematicians

Extra-curricular Activities

2017-2023	Pole Vault Coach Designed individualized athletic training and programming as a head coach for youth athletes.	Blacksburg High School
2012-2016	Division 1 Athlete Participated in Division 1 athletics at Rice University as a pole vaulter on the track and field team.	Rice University

Awards

2021	Graduate School Doctoral Assistanship Award Award for excellence in research in leadership	Virginia Tech
2012,2014	C-USA Commissioner's Honor Roll	Rice University