Karl Pierce, PhD

Postdoctoral Research Scientist

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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

Electronic Structure Theory

Tensor algebra

C++

Distributed Programming

Mathematics

Julia

Quantum Mechanics

LaTeX

CMake

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 — Blacksburg, VA
Virginia Tech

2012-2016 B.S. Chemical Physics — Houston, TX
Rice University

Publications

2022 Efficient Construction of Canonical Polyadic approximations of Tensor Networks
Pierce, K.; Valeev, E. 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. 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). Journal of Chemical Physics, 153(4), 44120.

In Preparation

Effective use of 4-way Canonical Polyadic Decomposition for Accelerating the Coupled-Cluster Perturbative Triples.
Pierce, K.; Bao, Y; Pavošević, F; Valeev, E

Towards Using Matrix-Free Tensor Decomposition to Systematically Improve Approximate Tensor-Networks.
Pierce, K.

Studying the Efficient Approximation of Lattice Networks using the Canaonical Polyadic Decomposition
Pierce, K.; Tindall, J.; Stoudenmire EM.

Professional Experience

Sept 2022- Flatiron Software Research Fellow — The Flatiron Institute
Postdoctoral researcher at the Center for Computational Quantum Physics. I am working with faculty researchers on developing and advancing theories in computational quantum physic using advanced higher order tensor algebra. Additionally I am developing ITensors software package to utilize heterogeneous computer architectures using state of the art generic programming techniques in the language Julia.

2022 Research Scientist — Virginia Tech
In this role I worked on developing efficient electronic structure methods for large molecules and condensed phase. Building parallel implementations of these methods using the standard C++ language for standard and heterogeneous massively parallel computer systems. I planned and conducted research projects requiring independent evaluation, selection, and substantial adaptation or modification from standard published techniques and procedures. Furthermore, I mentor 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 theory approaches.

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.

2013 Visiting Scientist — University of Akron
Supervised under Dr. Shing-Chung "Josh" Wong
Studied polymer development techniques, designed mechanical testing for biomedical devices based on IEEE and FDA testing requirements and built testing apparatus and benchmarked approved industry devices.

2012 Research Assistant — University of Akron
8 weeks part time under Dr. Shing-Chung "Josh" Wong
Lead design project to study polymer microfibers produced using a dry-jet wet spinning technique. Built a device to create polymers using the dry-jet wet spinning technique.

2011 Research Assistant — NASA Glenn
Supervised under Dennis Stocker
Assisted in NASA's advanced combustion via microgravity (ACME) experiments. Generated Volumetric measurements for ignition fuel required on the international space station.

Posters and Presentations

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

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 — Seminar
Approximating tensor contractions via a matrix-free tensor decomposition

2023 SIAM Conference on Computational Science and Engineering — Seminar
Introduction to the ITensor Software Library for Tensor Network Calculations

2021 Colloquim at Vienna University of Technology — Seminar
Utility of the Canonical Polyadic Decomposition and Robust Tensor Network Approximations

2019 Virginia Tech Department of Chemistry Internal Seminar — Seminar
Reduced Cost Electronic Structure Theory via the Canonical Polyadic Decomposition

2019 American Chemical Society National Meeting — Poster
Towards Reduced Scaling Higher Order Coupled Cluster Methods via Tensor Decomposition.

2018 Modern Wavefunction Methods in Electronic Structure Theory — Poster
Reducing Complexity and Cost of High-Order Coupled-Cluster Method via Canonical Polyadic Decomposition of Hamiltonian

2018 Penn Conference in Theoretical Chemistry and Electronic Structure Workshop — Poster
Reducing Complexity and Cost of High-Order Coupled-Cluster Method via Canonical Polyadic Decomposition of Hamiltonian.

2018 Virginia Tech Department of Chemistry Preliminary Exam — Seminar
Reduced Scaling of Accurate Electronic Structure Methods using Tensor Decompositions

2017 Southeast Theoretical Chemistry Association Meeting — Poster
Toward Efficient Canonical Product Decomposition in TiledArray Framework

Summer School

2022 Argonne Training Program on Extreme-scale Computing — Chicago, IL
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.

2018 MolSSI Summer School and Workshop Parallel Computing in Molecular Sciences — Berkely, CA
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.

2018 Modern Wavefunction Methods in Electronic Structure Theory — Gelsenkirchen, Germany
Attended a week-long summer school at the Max-Plank 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.

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 — Blacksburg High School
Designed individualized athletic training and programming as a head coach for youth athletes.

2012-2016 Division 1 Athlete — Rice University
Participated in Division 1 athletics at Rice University as a pole vaulter on the track and field team.

Awards

2021 Graduate School Doctoral Assistanship Award — Virginia Tech
Award for excellence in research in leadership

2012,2014 C-USA Commissioner's Honor Roll — Rice University