

ZACHARY STREETER

PERSONAL INFORMATION

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github <https://github.com/zstreeter>

BRIEF INTRODUCTION

My formal training is in computational physics and chemistry. These fields, in particular, have had limited success because of their massive combinatorial search spaces. This has lead to approximate techniques like density-functional theory (DFT) in quantum chemistry. However, these approximate techniques haven't yielded *ab-initio* understanding which, in some ways, has lead to stagnation. There are two novel solution paths for these statistically daunting areas of study, namely quantum computing and AI. With this in mind I have begun my career after my Ph.D., in AI. With this industry experience, I will create tools that leverage AI for teaching science with an initial objective of teaching physics. As these tools mature, I hope they will lead to *ab initio* understanding of emergent phenomena in physics and other fields like biology. This should keep me busy the rest of my life.

If you would like, please follow the red links above to email me, link up on LinkedIn, and/or check out my github page!

TECHNICAL SKILLS

Software

COMPILED · C(proficient), C++(proficient), Fortran(proficient), Cython(prior experience).

PARALLEL API · MPI(proficient), OpenMP(proficient), Cuda(prior experience), PETSc(proficient), SLEPc(proficient).

SCRIPTING · Posix(prior experience), Bash(proficient), Python(proficient).

BUILD PROCESS · CMake(proficient), Make(proficient).

MARKUP · L^AT_EX(expert), Markdown(proficient), ReStructuredText(proficient).

DEBUGGER · gdb(proficient), lldb(proficient), TotalView(prior experience).

PROFILER · Nsight/visual profiler(prior exexperience), VTune(prior experience).

SCHEDULER · SLURM(proficient).

Workflow

EDITOR · Vim/Neovim.

MULTIPLEXER · Tmux.

VERSION-CONTROL · Git.

RESEARCH INTERESTS

Computer Science High Performance Computing
· Deep Learning.

- Numerical algorithms/methods.
- Finite-Element Methods.
- Computational geometry.
- Computational physics/chemistry.
- Hybrid CPU/GPU Architectures.
- HPC and low level optimization.

Theoretical Physics and Chemistry

- Quantum Information and Computation.
- Deep Learning applied to quantum physics/chemistry.
- Quantum Computers applied to quantum physics/chemistry.
- Nonlinear chemical reaction kinetics.
- Scattering Theory.
- Symplectic Mechanics.
- Underlying Symmetries throughout Physics.

JOBS

September Advanced Micro Devices
2021 to
present

AMD

Part of the Deep Learning Frameworks team. Worked on improving novel AI models with end-to-end specifications for AMD hardware. Used profilers to pin-point bottlenecks and further optimized kernels. Directed projects that contributed to company's AI direction at large. Worked with several large clients in numerous asks. Furthered understanding of AI research directions and advised how AMD can leverage these novel neural-network architectures.
Manager: Peng SUN · Peng.Sun@amd.com

INTERNSHIPS AND RESEARCH POSITIONS

Summer Lawrence Berkeley National Laboratory
2016 to
August
2021

LBNL

Created fully dimensional potential energy surfaces for H_2O^{++} using MOLPRO and Columbus Quantum Chemistry packages. These hypersurfaces were then used in a MPI parallelized classical trajectory simulation of H_2O^{++} breakup following double ionization. This work was essential to deduce the body-frame of the water molecule at the momentum of photo-absorption and resulted in two immediate papers while also providing a benchmark for intense field experimentalist that will be in print shortly. Created a novel suite of high-performance codes that calculate double-ionization cross section for water and can be easily modified to other polyatomics. In general, honed programming skills in C, C++, Fortran, and Python, while becoming a learned software developer devoted to best practices, high performance, and good documentation. Used NERSC supercomputers EDISON and CORI, and also a cluster called Lawrencium, for running large parallel batch jobs (e.g. 40+ physical cores with 3000+ processors). Became proficient in parallel programming using PETSC, MPI, CUDA, and OpenMP.
Reference: Clyde W. McCurdy +1 (510) 486 4283 · cwmccurdy@lbl.gov

	<i>Spring</i> <i>2015</i>	Brookhaven National Laboratory, SULI internship
BNL		Performed experiments with soft X-rays utilizing the Linear Electron Accelerator Facility (LEAF) and the van de Graaff. Prepared samples in glove box and worked on purifying Xenon and CO. This work was essential in studying electron mobility through CO. Once this work was completed, we calculated the quasi-free electron energy resulting in a publication. Understanding the free-electron energy in various liquids is critical in order for those liquids to be used in scattering experiments. Reference: Richard Holroyd +1 (631) 344 4329 · holroydr@optonline.net
	<i>Summer</i> <i>2014</i>	Center for Advanced Microstructures and Devices
CAMD		Became a user in order to continue research from SRC. Reference: Cherice EVANS +1 (718) 997 4216 · cherice.evans@qc.cuny.edu
	<i>2012–2013</i>	Synchrotron Radiation Center
SRC		Built gas handling systems, ran leak checks for high vacuum line, wrote Igor Pro code for data analysis, and worked on calibrating the monochrometer. Also attended lectures in relativistic electrodynamics and worked on electrodynamic problem sets. Reference: Gary FINDLEY +1 (318) 342 1835 · findley@ulm.edu

OPEN SOURCE PROJECTS

	<i>Spring</i> <i>2020</i>	quantumGrid
Author and Maintainer		quantumGrid is a python package for solving a 1-D Schrödinger equation for an arbitrary potential on any interval. The heart of this package is using a Finite Element Method with a Discrete Variable Representation (FEM-DVR) grid to solve the time-dependent or time-independent Schrödinger equation. This grid provides a compact supported foundation for numerically accurate integration and also allows for a natural application of outgoing scattering boundary conditions by adding a complex tail as the last finite element of the FEM-DVR grid, called exterior complex scaling (ECS). This project was created for a graduate course in time-dependent quantum mechanics at UC Davis. Click on the read hyperlink to find out more!

EDUCATION

	<i>2015–</i> <i>August</i> <i>2021</i>	The University of California, Davis
Doctor of Philosophy		GPA: 3.9 · School: Chemistry Description: This degree is a PhD in Theoretical Chemical Physics. Advisors: Prof. Clyde W. McCURDY, Prof. Robert. LUCCHESI (LBNL)
	<i>Fall 2019</i>	The University of California, Berkeley
Notable Course		CS294 – 73 <i>Software Engineering for Scientific Computing</i> School: Computer Science Grade: A+ Description: This graduate course focused on the seven motifs in scientific computing: dense and sparse linear algebra, structured and unstructured grid methods, particle methods, fast Fourier transforms (FFT), and Monte Carlo. Professor: Phillip COLELLA · colella@eecs.berkeley.edu
	<i>Spring</i> <i>2020</i>	The University of California, Berkeley

*Notable Course*CS267 *Applications of Parallel Computers*

School: Computer Science

Grade: A+

Description: Graduate course focused on models for parallel programming.

Overview of parallelism on scientific applications and study of parallel algorithms for linear algebra, particles, meshes, sorting, FFT, graphs, machine learning, etc.

Survey of parallel machines and machine structures. Programming shared- and distributed-memory parallel computers, GPUs, and cloud platforms. Parallel programming languages, compilers, libraries and toolboxes. Data partitioning techniques. Techniques for synchronization and load balancing. Detailed study and algorithm/program development of medium sized applications.

Professor: Katherine A. YELICK · yelick@cs.berkeley.eduProfessor: James DEMMEL · demmel@cs.berkeley.eduProfessor: Aydin BULUÇ · aydin@eecs.berkeley.edu

2007–2009, The University of Louisiana, Monroe

2011–2015

Bachelor of Science

GPA: 3.46 · School: School of Sciences

Major (Concentration): Biology (Chemical Biology)

Personal Courses: Attended formal lectures in Statistical Mechanics, Quantum Mechanics, Electricity and Magnetism, and Relativistic Electrodynamics.

Advisor: Prof. Gary FINDLEY & Prof. Ann FINDLEY

TEACHING

Spring University of California, Davis

2020

Teaching Assistant

Time-Dependent Quantum Mechanics: The first part of this graduate course covers the basic concepts and techniques for solving the time-dependent Schrödinger equation. The initial portion explores the concepts of quantum superpositions, Gaussian wave packets for free and interacting particles, time propagation, the Schrödinger, interaction and Heisenberg representations, time-dependent density matrices, the Wigner phase space distribution, Ehrenfest's theorem, the connection between quantum and classical mechanics in the context of molecular dynamics, the semiclassical wave packet approximation, and time-dependent perturbation theory. The second part of the course turned to applications. Those included absorption and emission of electromagnetic radiation, correlation functions and spectra, molecular dynamics, potential energy surfaces, conical intersections, nonadiabatic transitions and variational transition state theory.

Winter University of California, Davis

2020

Teaching Assistant

Quantum Chemistry: a graduate level discussion of the principles of quantum mechanics and its application to (primarily) stationary state problems in atoms and molecules, including Hartree-Fock calculations of their electronic structure. Using the Psi4 quantum chemistry codes and the Python programming language we performed calculations on small molecules using restricted Hartree-Fock, unrestricted Hartree-Fock, Møller-Plesset perturbation theory (MP2), and configuration interaction (CI) and coupled cluster (CCSD) methods..

2015–2016 University of California, Davis

Teaching Assistant

Taught freshman chemistry for two quarters. My third quarter I taught quantum mechanics for physical chemistry students. This course laid the foundation for quantum mechanics needed later in spectroscopy courses.

Spring Queens College
2015

Teaching Assistant

Taught second semester of freshman chemistry and the corresponding lab. Created lab and recitation quizzes and was the sole arbiter as to how the courses were conducted.

Assisted Professor: Prof. Cherice EVANS

TALKS AND POSTERS PRESENTED AT CONFERENCES

- 2013 SRC Users Meeting Zachary Streeter, Kamil Krynski, C. M. Evans, and G. L. Findley, "Quasi-Free electron in near critical point hydrogen and deuterium," 2013 SRC Users Meeting, University of Wisconsin Synchrotron Radiation Center, Stoughton, WI, September 27 – 28, 2013.
- 2013 SRC Users Meeting Kamil Krynski, Zachary Streeter, C. M. Evans, and G. L. Findley, "Field ionization and photoionization of CH₃I perturbed by diatomic molecules: electron scattering in H₂, HD, D₂, O₂ and CO," 2013 SRC Users Meeting, University of Wisconsin Synchrotron Radiation Center, Stoughton, WI, September 27 – 28, 2013.
- 2014 DAMOP Cherice Evans, Kamil Krynski, Zachary Streeter, and G. L. Findley, "Field Ionization and Photoionization of CH₃I Perturbed by Diatomic Molecules: Electron Scattering in H₂, D₂, O₂, and CO," 45th Annual Meeting of the APS Division of Atomic, Molecular, and Optical Physics, Madison, WI, June 2 – 6, 2014.
- 2014 DAMOP Zachary Streeter, Kamil Krynski, C. M. Evans, and G. L. Findley, "The energy of the quasi-free electron in near critical point H₂, D₂, and O₂," 45th Annual Meeting of the APS Division of Atomic, Molecular, and Optical Physics, Madison, WI, June 2 – 6, 2014.
- 2016 APS Kamil Krynski, Zachary Streeter, C. M. Evans, and G. L. Findley, "Energy of the Quasi-Free Electron in H₂, D₂, and O₂: Probing Intermolecular Potentials within the Local Wigner-Seitz Model," American Physical Society March Meeting, Baltimore, MD, March 14 – 18, 2016.
- 2017 DAMOP Zachary Streeter, Frank Yip, Dylan P. Reedy, Allen Landers, C. William McCurdy, "Classical trajectory studies on the dynamics of one-photon double photionization of H₂O," 48th Annual Meeting of the APS Division of Atomic, Molecular, and Optical Physics, Sacramento, CA, June 5 – 9, 2017.
- 2018 ACS Cherice M. Evans, Jennifer Hare, Baxter Flor, Kamil Krynski, Zachary Streeter, and G. L. Findley, "Energy of the Quasi-Free Electron in CO and HD: Extension of the Local Wigner-Seitz Model to Polar Fluids," 225th ACS National Meeting and Exposition, New Orleans, LA, March 18 – 22, 2018.
- 2019 DAMOP Z. L. Streeter, and C. W. McCurdy, "Sequential dissociation of H₂O⁺⁺ following double photoionization" 50th Annual Meeting of the APS Division of Atomic, Molecular, and Optical Physics, Milwaukee, WI, May 27 – 31, 2019.

PUBLICATIONS

- Published C. M. Evans, Kamil Krynski, Zachary Streeter, and G. L. Findley, "Energy of the Quasi-free Electron in H₂, D₂ and O₂: Probing Intermolecular Potentials within the Local Wigner-Seitz Model," J. Chem. Phys. **143**, 224303 (2015)"
- Published C. M. Evans, Baxter Flor, Kamil Krynski, Zachary Streeter, and G. L. Findley, "Energy of the Quasi-Free Electron in CO and HD: Probing Intermolecular Potentials within the Local Wigner-Seitz model," J. Chem. Phys. **149**, 064307 (2018).
- Published Zachary L. Streeter, Frank L. Yip, Robert R. Lucchese, Benoit Gervais, and C. William McCurdy, "Dissociation dynamics of the water dication following one-photon double ionization I: Theory," Phys. Rev. A, **98**, 053429 (2018).
- Published D. Reedy, J. B. Williams, B. Gaire, A. Gatton, M. Weller, A. Menssen, T. Bauer, K. Henrichs, Ph. Burzynski, B. Berry, Z. L. Streeter, J. Sartor, I. Ben-Itzhak, T. Jahnke, R.

Dörner, Th. Weber, and A. L. Landers, “Dissociation dynamics of the water dication following one-photon double ionization I: Experiment,” *Phys. Rev. A*, **98**, 053430 (2018).

Published

Kirk A. Larsen, Thomas N. Rescigno, Travis Severt, Zachary L. Streeter, Wael Iskandar, Saijoscha Heck, Averell Gatton, Elio G. Champenois, Richard Strom, Bethany Jochim, Dylan Reedy, Dimitri Call, Robert Moshhammer, Reinhard Dörner, Allen L. Landers, Joshua B. Williams, C. William McCurdy, Robert R. Lucchese, Itzik Ben-Itzhak, Daniel S. Slaughter, Thorsten Weber, “Photoelectron and fragmentation dynamics of the $H^+ + H^+$ dissociative channel in NH_3 following direct single-photon double ionization,” *Phys. Rev. Res.*, **2**, 043056 (2020).

Published

Kirk A. Larsen, Thomas N. Rescigno, Zachary L. Streeter, Wael Iskandar, Saijoscha Heck, Averell Gatton, Elio G. Champenois, Travis Severt, Richard Strom, Bethany Jochim, Dylan Reedy, Dimitri Call, Robert Moshhammer, Reinhard Dörner, Allen L. Landers, Joshua B. Williams, C. William McCurdy, Robert R. Lucchese, Itzik Ben-Itzhak, Daniel S. Slaughter, Thorsten Weber, “Photoionization and dissociation dynamics of the $NH_2^+ + H^+$ and $NH^+ + H^+ + H$ fragmentation channels upon single-photon double ionization of NH_3 at 61.5 eV” *Journal of Physics B*, **53**, 24 (2020).

August 7, 2022