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 · LaTeX(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 2021 to present — Advanced Micro Devices

AMD

Part of the Deep Learning Frameworks team. Worked on improving novel AI models with end-to-end specifications for AMD hardware.

- Collaborated with several large clients on various tasks.
- Major contributor to an internal project that provides dashboards and metrics on the performance of novel AI models using AMD hardware.
- Directed projects that significantly influenced the company's AI strategy.
  - **Clusters:** Leveraged my experience at NERSC to ensure the hardware setup and software stack followed best practices for AI scaling.
  - **Knowledge:** Equipped the team with essential frameworks for analyzing multi-node performance, including strong and weak scaling, and using roofline analysis for targeted optimizations.

- Some contributions to frameworks (not including creating/maintaining ROCm ports):
  - **PyTorch:** Led ROCm compatibility with Inductor/triton for the day one release of 2.0 functionality.
  - **Triton:** Managed compatibility on our Navi lineup, overseeing the development of triton implementation to leverage WMMA instructions.
  - **TensorFlow:** Led compatibility and performance enhancements on our Navi lineup.
  - **XLA:** Helped team understand cost model and developed the AMD port of the Profile Guided Latency Estimator targeting multi-GPU collectives.
  - **Jax:** Led Navi compatibility efforts.
  - **TinyGrad:** Developed a fuzzer (fuzzyHSA) that exposes a Python API for the Kernel Fusion driver, facilitating quicker investigation of the attack surface of AMD GPUs.
- Used profilers like OmniPerf and OmniTrace to identify bottlenecks and optimize kernels.
- Advanced understanding of AI research directions and advised on how AMD can leverage new neural-network architectures.
- Regarded as "Professor-in-house" and led a paper series to enhance understanding of novel techniques as the AI industry evolves.
- Mentor summer interns so they have an enjoyable and educational experience at AMD!

Manager: Peng Sun · Peng.Sun@amd.com

Internships and Research Positions

Summer 2016 to August 2021 — Lawrence Berkeley National Laboratory

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 programing using PETSC, MPI, CUDA, and OpenMP.
Reference: Clyde W. McCurdy +1 (510) 486 4283 · cwmccurdy@lbl.gov

Spring 2015 — 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

Summer 2014 — 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

2012–2013 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

Spring 2021 fuzzyHSA

Author and Maintainer fuzzyHSA is a python API designed to interact with the Kernel Fusion Driver (KFD) on AMD GPUs, serving as a tool for fuzz testing the lower-level software stack. Fuzz testing involves sending unexpected or random inputs to the hardware to uncover vulnerabilities and ensure robustness. The main features of fuzzyHSA include:

- Simplified API for interacting with KFD.
- Enhanced debugging capabilities for kernel fusion operations.
- Fuzz testing to assess the robustness of AMD hardware by provoking unintended behavior and observing how gracefully the system handles these scenarios.

fuzzyHSA aims to provide a clear insight into the hardware's robustness by identifying how the firmware or other managing programs respond to atypical inputs. This project is currently in active development, continuously evolving to meet the needs of GPU programming and kernel fusion optimization, ensuring AMD hardware can handle unexpected inputs without compromising stability.

Spring 2020 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

2015-August 2021 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. Lucchese (LBNL)

Fall 2019 The University of California, Berkeley

Notable Course
CS294 – 73 *Software Engineering for Scientific Computing*
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

Spring 2020 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 programing. 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.edu
Professor: James Demmel · demmel@cs.berkeley.edu
Professor: Aydin Buluç · aydin@eecs.berkeley.edu

2007–2009, 2011–2015 The University of Louisiana, Monroe

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 2020 University of California, Davis

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 2020 — University of California, Davis

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 2015 — Queens College

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 Confrences

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 CH_3I perturbed by diatomic molecules: electron scattering in H_2, HD, D_2, O_2 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 CH_3I Perturbed by Diatomic Molecules: Electron Scattering in H_2, D_2, O_2, and CO,*" 45^{th} 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 H_2, D_2, and O_2,*" 45^{th} 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 H_2, D_2, and O_2: 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 H_2O," 48^{th} 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,*" 225^{th} ACS National Meeting and Exposition, New Orleans, LA, March $18 - -22$, 2018.

2019 DAMOP Z. L. Streeter, and C. W. McCurdy, "*Sequential dissociation of H_2O^{++} following double photoionization*" 50^{th} 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 H_2, D_2 and O_2: 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, Demitri Call, Robert Moshammer, 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, Demitri Call, Robert Moshammer, 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 NH3 at 61.5eV*"Journal of Physics B., **53**, 24 (2020).

Published Chuan Cheng, Zachary L. Streeter, Andrew J. Howard Michael Spanner, Robert R. Lucchese, C. William McCurdy, Thomas Weinacht, Phillip H. Buchsbaum, Ruaridh Forbes, "*Strong-field ionization of water. II. Electronic and nuclear dynamics en route to double ionization*" Physical Review A, **104**, 02 (2021).

Published Travis Severt, Zachary L. Streeter, Wael Iskandar, Kirk A. Larsen, Avverell Gatton, Daniel Trabert, Bethany Jochim, Brandon Griffin Elio G. Champenois, Matthew M. Brister, Dylan Reedy, Demitri

Call, Richard Strom, Allen L. Landers, Reinhard Dorner, Joshua B. Williams, Daniel S. Slaughter, Robert R. Lucchese, Thorsten Weber, C. William McCurdy, Itzik Ben-Itzhak, "*Step-bystep state-selective tracking of fragmentation dynamics of water dications by momentum imaging*" Nature Communications, **13**, 51 (2022).

Published Andrew J. Howard, Mathew Britton, Zachary L. Streeter, Chuan CHeng, Ruaridh Forbes, Joshua L. Reynolds, Felix Allum, Gregory A. McCracken, Ian Gabalski, Robert R. Lucchese, C. William McCurdy, Thomas Weinacht, Phillip H. Bucksbaum, "*Filming enhanced ionizatin in an ultrafast triatomic slingshot*" Nature Communications Chemistry, **6**, 81 (2023).

Published Roger Y. Bello, Frank L. Yip, Zachary Streeter, Robert Lucchese, C. William McCurdy, "*An orbital Basis Set for Double Photioionization of Atoms and Molecules*" Journal of Chemical Theory and Computation, **20**, 20 (2024).

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