

Kalman Szenes

Curriculum Vitae

ETH Zürich
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Citizenship: USA and Hungarian



Education

- 04/2023 - Present **PhD Student in Theoretical Chemistry, ETH Zurich, Zurich, Switzerland**
- Development of tensor network algorithms for applications in quantum chemistry.
 - Advisor: Prof. M. Reiher
- 09/2020 - 03/2023 **MSc Computational Science and Engineering, ETH Zurich, Zurich, Switzerland**
- Specialization in computational physics with a focus on partial differential equations and HPC.
 - MSc Thesis: "Tensor Computations on GPUs: From Dense Contractions to Sparse Decompositions"
 - Advisors: Dr. A. Ziogas, Dr. T. Ben-Nun, Prof. T. Hoefer
- 09/2019 - 05/2020 **Exchange Year, Imperial College London, London, UK**
- Advanced topics in physical chemistry.
- 09/2017 - 05/2020 **BSc Chemistry and Chemical Engineering, EPFL, Lausanne, Switzerland**
- Fundamental chemistry and engineering with a focus on physical chemistry.

Professional Experience

- 03/2022 - 07/2022 **Scientific Software Intern, CSCS (Swiss National Supercomputing Centre), Zurich, Switzerland**
- Implementation of Discontinuous Galerkin schemes for weather and climate simulations using the GPU-enabled DSL [GT4Py](#). Resulted in publication in *Comput. Phys. Commun.*

List of Publications

- 2024 **K. Szenes**, M. Mörchén, P. Fischill and M. Reiher, "Striking the right balance of encoding electron correlation in the Hamiltonian and the wavefunction ansatz", *Faraday Discuss.* 254, 359
- 2024 **K. Szenes**, N. Discacciati, L. Bonaventura, and W. Sawyer, "Domain-specific implementation of high-order Discontinuous Galerkin methods in spherical geometry" *Comput. Phys. Commun.* 295, 108993
- 2023 M. Besta, P. Renc, R. Gerstenberger, P. Sylos Labini, A. Ziogas, T. Chen, L. Gianinazzi, F. Scheidl, **K. Szenes**, A. Carigiet, P. Iff, G. Kwasniewski, R. Kanakagiri, C. Ge, S. Jaeger, J. Was, F. Vella, and T. Hoefer., "High-Performance and Programmable Attentional Graph Neural Networks with Global Tensor Formulations" *Proceedings of Supercomputing '23*, 1–16

Conferences and Workshops

- 09/2024 **Swiss Chemical Society Fall Meeting**, Fribourg, Switzerland
- Poster: "Striking the right balance of encoding electron correlation in the Hamiltonian and the wavefunction ansatz"
- 09/2024 **Workshop on Tensor Contraction Library Standardization, CECAM**, Toulouse, France
- Poster: "Implementation Considerations for the Second-Generation Density Matrix Renormalization Group"
- 06/2024 **Faraday Discussion on Correlated Electronic Structure**, Royal Society of Chemistry, London, UK
- Paper: "Striking the right balance of encoding electron correlation in the Hamiltonian and the wavefunction ansatz"
- 01/2024 **The Path of Quantum Chemistry into the 21st Century, ETH Zurich**, Zurich, Switzerland
- Poster: "Implementation Considerations for the Second-Generation Density Matrix Renormalization Group Algorithm"
- 09/2023 **Symposium of Theoretical Chemistry**, Zurich, Switzerland

06/2023 **17th International Congress of Quantum Chemistry Satellite Meeting on Strong Correlation in Molecules**, Znojmo, Czech Republic

06/2022 **Platform for Advanced Scientific Computing**, Basel, Switzerland

Summer Schools

08/2023 **Modern Wavefunction Methods**, Pisa, Italy

◦ Poster: "Tensor Computations on GPUs: From Dense Contractions to Sparse Decompositions"

06/2023 **International Summer School on High Performance Computing**, PRACE, XSEDE, RIKEN, SciNet, EPCC and Pawsey, Atlanta, USA

◦ Poster: "Tensor Computations on GPUs From Dense Contractions to Sparse Decompositions"

08/2021 **Summer School in Effective HPC and Data Analytics with GPUs**, CSCS (Swiss National Supercomputing Center), (Virtual) Switzerland

Teaching Experience

Spring 2025	Quantum Chemistry Practical Course , Teaching Assistant	ETH Zurich
Fall 2024	Advanced Quantum Chemistry , Teaching Assistant	ETH Zurich
Spring 2024	Quantum Chemistry Practical Course , Teaching Assistant	ETH Zurich
Fall 2023	Advanced Statistical Physics , Teaching Assistant	ETH Zurich
Fall 2022	Programming Techniques for Scientific Simulations , Teaching Assistant	ETH Zurich

Volunteer

07/2021 **Tech Support at PASC Conference**, (Virtual) Switzerland

◦ Aided the logistics of the Platform for Advanced Scientific Computing (PASC) 2021 conference by providing tech support to the online Zoom sessions.

Side Projects

h5tui A terminal user interface (TUI) application for quickly navigating HDF5 files and plotting datasets straight in the terminal.

tocPDF A CLI tool for automatically generating the PDF outline based on parsing the Table of Contents from the PDF.

Technical Skills

Outreach

Blog I write a technical [blog](#) on various lesser-known workflow and development tips.

Programming Languages

C++ Advanced: One of the lead developers of the [QCMaquis](#) DMRG program.

Python Advanced: Contributed to the platform portable GPU-enabled stencil kernel DSL [GT4Py](#).

Julia Advanced: Developed a GPU-accelerated porous convection PDE solver [PorousConvection.jl](#).

Fortran Basic Syntax: Contributed to the [OpenMolcas](#) quantum chemistry package.

Parallelization Paradigms

OpenMP Advanced: Participated in multiple HPC courses and summer schools.

MPI Advanced: Participated in multiple HPC courses and summer schools.

CUDA Intermediate: Developed native CUDA tensor contraction routines during my Master's Thesis.

AVX Intrinsics Intermediate: Took a dedicated Master's level course on single-threaded CPU optimizations.

Languages

English	Fluent
Hungarian	Fluent
Russian	Fluent
French	Fluent
German	Conversational: B2