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Kalman Szenes

Curriculum Vitae

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. Hoeffler
- 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

- 2025 **K. Szenes**, N. Glaser, M. Erakovic, V. Barandun, M. Mörchen, R. Feldmann, S. Battaglia, A. Baiardi, M. Reiher, "QCMAquis 4.0: Multi-Purpose Electronic, Vibrational, and Vibronic Structure and Dynamics Calculations with the Density Matrix Renormalization Group", *J. Phys. Chem. A*, 5c02970
- 2024 **K. Szenes**, M. Mörchen, 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. Hoeffler., "High-Performance and Programmable Attentional Graph Neural Networks with Global Tensor Formulations" *Proceedings of Supercomputing '23*, 1–16

Conferences and Workshops

- 06/2025 **World Association of Theoretical and Computational Chemists**, Oslo, Norway
- Poster: "Multi-State CASPT2 with a DMRG Reference Wavefunction"
- 06/2025 **OpenMolcas Developers' Workshop**, Munich, Germany
- Talk: "QCMAquis 4.0: Multi-Purpose Electronic, Vibrational, and Vibronic Structure and Dynamics Calculations with the Density Matrix Renormalization Group"
- 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
o 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
o 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
o 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
o 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

Side Projects

- MementoChem** A convenient web interface for generating input files for common quantum chemistry calculations.
- 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 PDF outlines based on parsing the Table of Contents of the PDFs.

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.

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.

Languages

English (Fluent), French (Fluent), Hungarian (Fluent), Russian (Fluent), German (B2)