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Kalman Szenes

Curriculum Vitae

Education

04/2023 - Present **PhD Student in Quantum 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. Hoefler

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

09/2025 - 01/2026 **Software Engineer Intern**, *Algorithmiq*, Helsinki, Finland
- Performance analysis and optimization of multi-GPU tensor network software for quantum error mitigation.

03/2022 - 07/2022 **Software Engineer 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**, R. Kayal, K. Sivalingam, R. Feldmann, F. Neese and M. Reiher, "Efficient Implementation of the Spin-Free Renormalized Internally-Contracted Multireference Coupled Cluster Theory", *arXiv*, 2511.03567

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*, 129, 7549-7574

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, 359-381

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. Hoefler., "High-Performance and Programmable Attentional Graph Neural Networks with Global Tensor Formulations" *Proceedings of Supercomputing '23*, 1–16

Conferences and Workshops

09/2025 **Workshop on Tensor Contraction Library Standardization**, Toulouse, France
- Talk "The Density Matrix Renormalization Group in Quantum Chemistry"

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
- 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*

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 periodically 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 and contributor to the ORCA quantum chemistry software.

Python Advanced: Contributed to the platform portable GPU-enabled stencil kernel DSL GT4Py.

Julia Intermediate: Developed a GPU-accelerated porous convection PDE solver PorousConvection.jl.

Fortran Basic Syntax: Contributed to the OpenMolcas quantum chemistry package.

Parallelization Paradigms

OpenMP Advanced

MPI Advanced

CUDA Intermediate: Developed native CUDA tensor contraction routines and currently working on tensor network techniques in `CuPy`.

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)