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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. 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

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. 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. Hoefler., "High-Performance and Programmable Attentional Graph Neural Networks with Global Tensor Formulations", *Supercomputing* 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

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.

Technical Skills

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