PHD PROJECT DESCRIPTION
(4000 characters max., including the aims and work plan to de published online)

Project title: Accelerating the pCCD-based methods in PyBEST with machine learning and modern GPUs.

1.1. Project goals

- Design optimized tensor contraction kernels leveraging modern GPU architectures and mixed-precision strategies.
- Integrate machine learning techniques to accelerate pCCD orbital optimization and electron correlation.
- Enable scalable multi-GPU execution with efficient CPU–GPU communication and distributed memory management.
- Establish a benchmarking suite to evaluate Python-based GPU frameworks on realistic quantum chemistry workloads.

1.1. Outline

- Challenges in quantum chemistry: High computational cost of tensor contractions, orbital optimization, and electron correlation calculations.
- Recent advances in machine learning techniques for quantum chemistry (wavefunction acceleration, optimization, and correlation methods).
- Background on PyBEST as a Pythonic platform for geminal-based and pCCD methods in electronic structure theory.
- Overview of Python-based GPU frameworks and their use in quantum chemistry workloads.
- Design optimized tensor contraction kernels leveraging modern GPU architectures and mixed-precision strategies.
- Integrate machine learning techniques to accelerate pCCD orbital optimization and electron correlation calculations.
- Significant performance gains in pCCD-based calculations and general tensor operations.
- New insights into the practical use of ML for accelerating orbital optimization and correlation methods.

1.2. Work plan

- Literature study of recent ML algorithms and their applicability to quantum chemistry-related problems.
- Survey over recent GPU architectures like NVIDIA Hopper, Grace Hopper, and Black Well architectures, including their multi-GPU capabilities.
- Benchmarking PyTorch, Cupy, Tensorflow, and other Python-based GPU accelerated libraries for the bottleneck contractions in PyBEST, including a mixed-precision capabilities.
- CPU-GPU communication optimization of the bottleneck mathematical operations in PyBEST
- Accelerating pCCD orbital optimization with ML in PyBEST (potential collaboration with NVIDIA).
- General tensor contraction optimization in PyBEST by combining GPU acceleration with ML to

enable large-scale quantum chemical modelling.

1.3. Literature (max. 7 listed as a suggestion for a PhD candidate preliminary study)

- P. Tecmer, K. Boguslawski "Geminal-based electronic structure methods in quantum chemistry. Toward a geminal model chemistry.", *Phys. Chem. Chem. Phys.* 24, 23026-23048 (2022)
- K. Boguslawski, A. Leszczyk, A. Nowak, F. Brzęk, P. Sz. Żuchowski, D. Kędziera, and P. Tecmer, *Comp. Phys. Comm.*, 264, 107933 (2021)
- M. H. Kriebel, P. Tecmer, M. Gałyńska, A. Lesczyk, and K. Boguslawski, "Accelerating Pythonic Coupled-Cluster Implementations: A Comparison Between CPUs and GPUs", *J. Chem. Theory Comput.* 20, 1130–1142 (2024).

1.4. Required initial knowledge and skills of the PhD candidate

The Ph.D. candidate should have experience in Python programming (including PyTorch), machine learning and artificial intelligence, Git, GitLab, and continuous integration. Ideally, the Ph.D. candidate should have basic knowledge of quantum mechanics, electronic structure theory, and GPU, and have some experience with modern Python-based quantum chemistry software packages. Moreover, the Ph.D. candidate should have solid knowledge of Linux/Unix and OSX operating systems, as well as computer clusters, and be fluent in English.

1.5. Expected development of the PhD candidate's knowledge and skills

- high-quality scientific papers where the Ph.D. student is the first/leading author.
- co-authorship in the PyBEST software package.
- proficiency in Latex, git, GitLab, Ruff, GitLab CI.
- high-performance computing skills, including GPU cards, and mixed precision arithmetic.
- big-data analysis, including data curation and preparation for ML, practical use of the newest ML techniques, and numerical algorithms.