Usage Report for Fiscal Year 2020

Project Title: R4QMC/NECI - A Quantum Monte Carlo Toolchain

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1. Background and purpose of the project, relationship of the project with other projects

The project is part of an effort to set up a hybrid Quantum Monte Carlo (QMC) scheme to combine the accuracy of Full Configuration Interaction QMC (FCIQMC) methods with the scalability of Variational & Diffusion Monte Carlo (VMC & DMC) methods. By these means, a highly parallelizable, high-accuracy scalable QMC scheme can be implemented.

2. Specific usage status of the system and calculation method

Since the start of the project end of November, only a few profiling calculations have been run on Hokusai, mainly to probe and optimize the DMC implementation of the NTChem quantum chemistry suite. Thus, the Diffusion Monte Carlo method has been the utilized method for the analysis on Hokusai so far. Further methods, namely the FCIQMC method as well as the calculation of effective Hamiltonian matrix elements by numerical integration, are expected to be of relevance in the future.

3. Result

By addition of a load balancing step, the parallel performance of the NTChem DMC implementation was greatly improved, while a hybrid MPI+OpenMP parallelization was found unfit to reduce dynamic load imbalance.

4. Conclusion

The NTChem VMC and DMC implementations are suitable for treating extended systems.

5. Schedule and prospect for the future

A numerical integration library is currently under development in collaboration with Researchers from the Max-Planck Institute for Solid State Research, which is expected to reach production stage in April. This library will be of great usefulness to the project, such that a powerful combined QMC scheme can then be applied to the paradigmatic system of solid Hydrogen as well as potentially for studying surface absorption processes as first applications. Depending on the nature of the problem, further optimizations to the implementations are likely to be required, especially regarding trial wave function compression in NTChem.