GPU-Accelerated Math Libraries for Quantum Many-Body Theory

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As heterogeneous computer node architectures are becoming progressively more widespread, the challenge of porting scientific codes to such architectures, while keeping the performance at a high level, is growing alike. A robust solution to this challenge is delivered by hardware-optimized math libraries which provide a set of math primitives the domain-specific algorithms are composed of. In particular, the *ab initio* (correlated) quantum many-body theory, used by quantum chemists and quantum physicists, heavily relies on numeric tensor algebra operations. In preparation to the upcoming NVIDIA GPU accelerated Summit supercomputer to be deployed by the Oak Ridge Leadership Computing Facility (OLCF) in 2018, we have developed a GPU-accelerated library of basic tensor algebra primitives, called TAL-SH, to be used by scientific codes for offloading numerical tensor computations to one or more GPU devices available on a node:
https://github.com/DmitryLyakh/TAL_SH.git
The library is being deployed by a number of quantum chemistry codes which will become available for computational chemistry applications on Summit, including DIRAC (relativistic coupled-cluster theory), LS-DALTON (linear-scaling non-relativistic coupled-cluster theory), and NWChem (non-relativistic coupled-cluster theory). Since the TAL-SH library is open sourced, it can also be used by any other open-source quantum chemistry code that could benefit from GPU acceleration of basic tensor operations. The TAL-SH library also serves as the CPU/GPU single-node backend for the distributed tensor algebra library ExaTENSOR being developed at OLCF for Summit (to be released in 2018).

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