PERFORMANCE EVALUATION OF NEW ALGEBRAIC ALGORITHMS AND LIBRARIES

Research Challenge
Design software and algorithms for applications running on Blue Waters addressing one of the biggest challenges facing parallel scalability of methods in computational science - the overhead of moving data between processors.
- Goal: Develop algorithms and libraries that minimize communication in the number of messages as well as in the amount of data moved.

Methods & Codes
- Various libraries available to application developers on BW.
- Focus Library: Cylops Tensor Framework (CTF) – provides distributed-memory support for sparse and dense tensors. Uses performance models to make runtime mapping decisions using autotuning to train the model parameters.

Results & Impact
- Impacts multiple domains from quantum chemistry to graph analysis
- Scalability of key kernels in quantum chemistry applications such as atomic-to-molecular orbital transformations
- Development of a new, scalable QR factorization

Why Blue Waters
Blue Waters is essential for testing and evaluation. While all of the codes developed are designed to be portable, demonstrating performance on Blue Waters helps foster local collaborations and deployment of parallel numerical library software.