Collaborative Research: SI2-SSI: ELSI- Infrastructure for Scalable Electronic Structure Theory

PIs: V. Blum[1], L. Lin[2,3], J. Lu[1], Senior Personnel: C. Yang[2], Á. Vázquez-Mayagoitia[4], F. Corsetti[5]
Institutions: [1]Duke University, [2]Lawrence Berkeley National Laboratory, [3]University of California, Berkeley, [4]Argonne National Laboratory, [5]Synopsys QuantumWise

Awards #:
1450280, 1450372

ELSI [2,3] (https://elsi-interchange.org) provides an integrated software interface to state-of-the-art eigensolvers and density matrix solvers, facilitating large-scale electronic structure simulations

Example: Scaling of the distributed-parallel eigenvalue solver ELPA on ORNL's hybrid CPU-GPU supercomputer Summit

The efficient 2-stage algorithm ELPA2,begun by Peter Messmer (NVidia) in 2012, was completed, with enhanced robustness, efficiency, and scalability on distributed-memory (multi-nodes) hybrid CPU-GPU architectures.