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ELSI: A unified software interface for Kohn-Sham electronic structure solvers

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Solving the electronic structure from a generalized or standard eigenproblem is often the bottleneck in large-scale molecular and materials simulations based on Kohn-Sham density-functional theory. This problem must be addressed by essentially all current electronic structure codes, based on similar matrix expressions, and by high-performance computation. We present a unified software interface, ELSI (elsi-interchange.org), that simplifies the implementation and optimal use of multiple Kohn-Sham electronic structure solvers. ELSI offers reasonable default parameters for the solvers; dynamic switch between solvers within a single calculation; and automatic conversion between input and internal working matrix formats. Comparative benchmarks performed with multiple solvers on distributed memory supercomputing architectures are shown for system sizes up to tens of thousands of atoms.

HPC content

Large-scale molecular and materials simulations require high-performance computation. The Kohn-Sham electronic structure solvers supported in ELSI are highly scalable. As an example, the ELPA solver can scale to ∼100k CPU cores given a sufficiently large problem to solve; and the PEXSI solver, with its multi-level parallelization, easily scales to ∼500k CPU cores. Results presented in this work were performed on the Cray XC30 supercomputer Edison at National Energy Research Scientific Computing Center (NERSC).

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