Insights: Publications

A partitioned shift-without-invert algorithm to improve parallel eigensolution efficiency in real-space electronic transport

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"A partitioned shift-without-invert algorithm to improve parallel eigensolution efficiency in real-space electronic transport," Co-Author, *Comp. Phys. Communic. 207, 105*

Abstract

We present an eigenspectrum partitioning scheme without inversion for the recently described real-space electronic transport code, TRANSEC. The primary advantage of TRANSEC is its highly parallel algorithm, which enables studying conductance in large systems. The present scheme adds a new source of parallelization, significantly enhancing TRANSEC's parallel scalability, especially for systems with many electrons. In principle, partitioning could enable super-linear parallel speedup, as we demonstrate in calculations within TRANSEC. In practical cases, we report better than five-fold improvement in CPU time and similar improvements in wall time, compared to previously-published large calculations. Importantly, the suggested scheme is relatively simple to implement. It can be useful for general large Hermitian or weakly non-Hermitian eigenvalue problems, whenever relatively accurate inversion via direct or iterative linear solvers is impractical.