Scalability of Shift-and-Invert Parallel Spectral Transformations for Quantum Chemistry Applications

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The problem

- Our goal is to discover new synthesis pathways through simulations involving tens of thousands of atoms for molecules and solids by developing scalable methods.
- Scaling bottleneck of many of the quantum chemistry methods is the diagonalization step.

$$\mathbf{Hx} = \lambda \mathbf{Sx}$$

- **H** and **S** are real and symmetric, and **S** is positive-definite.
- 40% to 60% of the eigensolutions are required.
- Matrices are sparse for large systems.

Strong scaling of SIPs