

# Infrastructure Developments for Electronic Structure Codes in ELSI

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This talk describes the open-source infrastructure “ELSI” (<https://wordpress.elsi-interchange.org/> and Ref. [1]), which provides simple access to state-of-the art solutions to the Kohn-Sham eigenvalue problem for different codes and solvers using a single uniform interface. ELSI provides a uniform solutions ranging from simple serial to large-scale massively parallel solutions, with efficient matrix conversion between dense and sparse matrix formats. Supported solvers include ELPA (massively parallel  $O(N^3)$  eigenproblem solutions), PEXSI ( $O(N^2)$  density-matrix based solutions including for metallic systems), NTPoly ( $O(N)$  density matrix purification), and several further, specialized solvers. ELSI is a cross-code development, now used in production versions of FHI-aims, Siesta, DFTB+, and DGDFT; additionally, ELSI is part of the broader “Electronic Structure Library” Bundle of open-source libraries for electronic structure theory. Different solvers have different use scenarios in terms of system size, system type and parallelism, assessed in a comprehensive set of benchmarks in this talk. Finally, we outline a new reverse communication interface (RCI) enabling the facile, efficient implementation of different iterative solver strategies aimed at plane wave basis sets, led by ELSI developers Yingzhou Li and Jianfeng Lu (Duke University).

## References

- [1] V. Yu *et al.*, Comput. Phys. Commun. **222**, 267 (2018).