



DFTB Performance Assessment Summary

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The POP Audit of DFTB identified an opportunity for improvement of its matrix multiplication kernel and this is being further investigated in a proof-of-concept study. It is hoped that this will lead to an increase in DFTB's scalability on distributed-memory HPC machines.

DFTB has very good computational load balance but relies on blocking MPI collective calls to communicate data between processes. A further study was recommended to investigate whether it might be possible to improve performance by using non-blocking collective operations to enable the overlap of communication and computation.

DFTB is an electronic structure code developed by the Amsterdam-based computational chemistry software company Software for Chemistry and Materials (SCM).

A full technical report can be found at https://pop-coe.eu/sites/default/files/pop_files/pop-ar-dftb.pdf

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