EPW Performance Assessment Summary

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Analysis of EPW identified two distinct phases with significant computation imbalances. Follow-on work improved both balance and performance, but at larger scale revealed a critical bottleneck writing the final simulation state to file. This was subsequently remedied for a 10-fold scalability improvement with 85% parallel efficiency to 960 processes.

A variety of load balance issues were identified in an initial audit, as well as excessive time in the simulation phase. The latter became the focus of a subsequent performance plan, where specialised routines avoided unnecessary calculation and optimised vector summations. When used for larger execution configurations, this 60% faster version was then found to be dominated by writing the final simulation results. A proof-of-concept investigation replaced concurrent file writing by all processes with serial writing only by rank zero, which reduced writing time from over seven hours to under one minute. The code now scales well efficiently supporting larger simulations with 960 MPI processes.

EPW (Electron-Phonon using Wannier interpolation) is a material science DFT code distributed in the Quantum ESPRESSO suite. It is developed by the University of Oxford and written using Fortran parallelised with MPI.

Performance Audit report: https://pop-coe.eu/sites/default/files/pop_files/pop-ar-epw.pdf
Performance Plan report: https://pop-coe.eu/sites/default/files/pop_files/pop-pp-epw.pdf
Proof-of-Concept report: https://pop-coe.eu/sites/default/files/pop_files/pop-poc-epw.pdf
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