Contribution ID: **109** Type: **Talk**

Developing a Sustainable and Performant GPU Implementation of Plane-Wave DFT

Wednesday, 4 December 2024 14:30 (20 minutes)

We present the GPU port of CASTEP (www.castep.org), which is scheduled for a full public release in early 2025 and developed as part of the PAX-HPC project under the UK's ExCALIBUR exascale-readiness programme. CASTEP is a well-established density functional material modelling software suite, consisting of 750k lines of modern Fortran with extensive support for distributed memory parallelism via MPI. The application profile is relatively flat, meaning that the run-time is not always dominated by a specific set of computational operations, and workloads per kernel are often insufficient to achieve device saturation easily.

We describe how we meet the challenges of porting the code while adhering to our development principles of portability, sustainabilty, and efficiency. We discuss the benefits and limitations of using OpenACC/MP for device offloading, how we integrate these approaches with MPI, and illustrate performance on UK HPC.

Student or Postdoc?

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Co-Authors

CHPC User

No

CHPC Research Programme

Workshop Duration

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