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Acceleration of Electronic Structure Codes on Heterogeneous Hardware

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We describe the development of a new library, libGint, for the calculation of the four-centre, two electron integrals required by local basis set ab initio electronic structure codes such as CP2K and CRYSTAL. The focus of this new work is the acceleration of the calculation via Graphical Processing Units (GPUs), particularly for codes that employ periodic boundary conditions. The core kernels for general contracted gaussian basis set have been rewritten allowing efficient calculation on a GPU. Initial integration into CP2K has been completed and correctness demonstrated. The current challenges involve optimizing the existing code, particularly batching the integrals so they can be calculated effectively on one or more GPUs, and development of a flexible application programming interface.

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