Wavelet-Based DFT calculations on Massively Parallel Hybrid Architectures

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In this contribution, we present an implementation of a full DFT code that can run on massively parallel hybrid CPU-GPU clusters. Our implementation is based on modern GPU architectures which support double-precision floating-point numbers. This DFT code, named BigDFT, is delivered within the GNU-GPL license either in a stand-alone version or integrated in the ABINIT software package. Hybrid BigDFT routines were initially ported with NVidia’s CUDA language, and recently more functionalities have been added with new routines written within Kronos’ OpenCL standard. The formalism of this code is based on Daubechies wavelets, which is a systematic real-space based basis set. As we will see in the presentation, the properties of this basis set are well suited for an extension on a GPU-accelerated environment. In addition to focusing on the implementation of the operators of the BigDFT code, this presentation also relies on the usage of the GPU resources in a complex code with different kinds of operations. A discussion on the interest of present and expected performances of Hybrid architectures computation in the framework of electronic structure calculations is also addressed.