Parallel Evaluation of Two-Electron Integrals using a Wavelet Approach on the Graphics Processor Unit

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In high precision electron structure calculations of chemical and solid-state physics, traditionally atom-specific basis functions are used to compute one- and two-electron integrals of the Coulomb interaction potential. In the present study we show, that using a wavelet approach, the evaluation of such integrals can lead to a much more economical scheme compared to the atomic basis function (LCAO) based calculations. Using the wavelet (scaling function) basis set gives a general, system independent, therefore more efficient solution.

However, the calculation of such integrals is a highly time-consuming and CPU-intensive task. Therefore, we propose a method to reduce significantly the evaluation time by introducing parallel processing techniques.

Recently, the graphics processor unit (GPU) has become a powerful platform for parallel computing and a new approach was offered to evaluate specific tasks in computational chemistry. In this study, we describe the implementation of calculating two-electron integrals using a GPU to improve the computation time. The algorithm was developed on an Nvidia Tesla M2070 GPU using the compute unified device architecture (CUDA).