Acceleration of Electron Repulsion integrals on Graphical Processing Units by using recurrence relations

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Abstract: Acceleration of quantum chemistry has been proved success by calculating time-deciding step, two-electron integral on Graphics Processing Units(GPUs). Ab initio Self-Consistence-Field calculation is implemented on GPUs using recurrence relation, one of the fastest electron repulsion integrals (ERI) algorithms. A scheme to assemble Fock matrix efficiently is presented, with which ERI is evaluated on-the-fly every iteration to avoid CPU-GPU data transfer, a bottleneck that slow down GPU architecture computation. Therefore it is especially suitable for direct SCF strategy. Speedup that GPU chips (single NVidia GTX 580 graphic card) achieved reaches as much as approximately 25 times faster compared with a traditional node as benchmark shown in context, and the accuracy is essentially zero with 64bit double-precision floating point supports from latest NVidia Tesla platform.