

Acceleration of Fragment MO method by GPU

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We accelerated the quantum chemistry computation using NVIDIA's graphics processing unit (GPU). The performance of commercially available low-cost GPU was superior to that of CPU by an order of magnitude. Based on the previous study [1,2] we developed the GPU computation module, XA-CUDA-QM, which replaces time-consuming procedures in quantum chemistry software. In this research the XA-CUDA-QM module was used together with GAMESS[3] to accelerate the fragment molecular orbital method (FMO) [4]. The most complicated step is the evaluation of Hartree-Fock exchange matrix (K-matrix). We developed a new K-matrix algorithm suitable for GPU, whose performance is shown in Table 1. As shown the algorithm performs very well even though it is not fully optimized.

Next the XA-CUDA-QM module was used to accelerate FMO. The test molecule, FK5, was spitted into 6 fragments. Table 2 compares the calculated energies of each fragment as well as the dipole moments.

Table 1 : K-matrix formation time (1CPU vs 1GPU)

Software Processor	GAMESS Core 2	GAMESS Xeon	GAMESS + XA-CUDA-QM GTX470 (Fermi)
Glycine	0.161	0.171	0.013
Glutamine	1.425	1.44	0.098
Tryptphan	4.415	4.393	0.275

Table 2 : FMO2 monomer property of each fragment of FK5 (RHF/6-31G)

	E (CPU)	E (GPU)	DX	DY	DZ
1 (FK5001 L1)	-402.317404135	-402.317404147	-0.20994	4.36026	1.16317
2 (FK5002 L1)	-459.054761634	-459.054761645	6.79290	0.29280	-3.10568
3 (FK5003 L1)	-466.843941102	-466.843941089	1.02059	-1.28229	-2.07834
4 (FK5004 L1)	-293.669434284	-293.669434291	-1.14973	-1.54089	1.95314
5 (FK5005 L1)	-407.321099998	-407.321099990	-2.14597	1.88929	-3.06977
6 (FK5006 L1)	-537.570750054	-537.570750051	-2.58186	2.29468	-1.05552

CPU : Core i7 860 @ 2.80GHz (4 core), GPU : Core i7 860 @ 2.80GHz (4 core) + one GTX 470

As shown the energies of each fragment calculated by CPU and GPU are almost the same and dipole moments (DX, DY, DZ) are exactly the same. The FMO total energies were -2657.853462811 by CPU and -2657.853429457 by GPU, and the error was just 3.3×10^{-5} a.u. The total computation time was 986.7 sec on CPU and 378.3 sec on GPU. In conclusion the newly developed GPU computation module (XA-CUDA-QM) can accelerate the FMO calculation considerably without any degradation of results.

References

- [1] Yasuda, K. *J. Comput. Chem.* **2008**, *29*, 334-342.
- [2] Yasuda, K. *J. Chem. Theory. Comput.* **2008**, *4*, 1230-1236.
- [3] M.W.Schmidt et al., *J. Comput. Chem.*, **14**, 1347-1363(1993)
- [4] D. G. Fedorov, K. Kitaura, in "Modern methods for theoretical physical chemistry of biopolymers", E. B. Starikov, J. P. Lewis, S. Tanaka, Eds., pp 3-38, Elsevier, Amsterdam, 2006.