Quantum Chemistry on Graphical Processing Units. 2. Direct Self-Consistent-Field (SCF) Implementation. [*J. Chem. Theory Comput. 5,* 1004–1015 (2009)]. By Ivan S. Ufimtsev and Todd J. Martinez*.

In our recent manuscript,[1] we compared timings for Coulomb matrix formation on graphical processing units (GPUs) with a previous implementation reported by Yasuda.[2] Our intention was to compare the performance that could be obtained from porting CPU code to the GPU as compared to completely redesigning the algorithms for stream processors. It has come to our attention that Yasuda's implementation was in fact not ported from CPU code but rather from code developed for the GRAPE-DR (a custom accelerator that has many features in common with stream processors). Had this been clear to us from ref 2, there would have been no reason to compare timings of the two implementations. A further issue is that the timings presented in Table 4 of ref 2 were misinterpreted. Although the caption states "Computational Time in Seconds of the Coulomb Potential Evaluation During *the* SCF Iteration" (emphasis added), these timings in fact refer to the entire SCF procedure, that is, *all* SCF iterations. Prof. Yasuda has kindly informed us how many iterations were required in each case. Thus, we present a revised table that is a fair comparison and should replace Table 2 in ref 1. The timings for the "present work" correspond to Coulomb matrix formation in the first 13/11 iterations for taxol/valinomycin, respectively. The difference in timings observed reflects different compilers and CPU hardware as well as coding strategies and algorithms. For example, accumulation of the two-electron integrals in ref 1 was performed with single precision accuracy (in the code version designed for the G80 architecture), while emulation of double precision accuracy was used in ref 2. Nevertheless, one can conclude that both implementations perform similarly. This is not surprising since both reflect redesign of the fundamental algorithms for the stream processor.

Table 2. *J*-Matrix Formation Time (in Seconds) for Taxol and Valinomycin Molecules Using 3-21G and 6-31G Basis Sets[a]

	J-matrix formation time (seconds)			
	Gaussian on GPU[7]		present work	
molecule	3-21G	6-31G	3-21G	6-31G
Taxol (13 iterations)	16.8	31.9	5.1	13.4
Valinomycin (11 iterations)	23.8	57.4	8.3	22.6

[a] Previously reported GPU-accelerated timings are compared to timings from our code. Timings for the present work include construction and sorting of pair quantities, data transfer to/from the GPU, construction of *J* on the GPU, and post-processing of the intermediate *J*-matrix on the CPU. All timings were obtained on one GeForce 8800GTX card. The GPU code was compiled with Nvidia CUDA Compiler ver. 2.0.

References

(1) Ufimtsev, I. S.; Martinez, T. J. *J. Chem. Theory Comput.* **2009**, *5*, 1004.

(2) Yasuda, K. *J. Comput. Chem.* **2008**, *29*, 334.

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