Benchmark calculations of double ionization of Ne in Graphics Processing Units

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Synopsis In this work we present the analysis of the numerical performance and accuracy of the Monte Carlo Event Generator method applied to the double ionization of Neon by fast electrons. This implementation of the code runs in Graphics Processing Units, giving a clear advantage over other computational approaches. The code can provide five hundred cross sections per second with the optimal configuration, an order of magnitude faster than CPU counterparts.

Theoretical calculations of multiple ionization processes have become more and more feasible along with the advances in computer power. One of the most recent approaches is the Monte Carlo Event Generator (MCEG). It is a numerical technique that is able to compute differential cross sections for a variety of complex ionization processes and can simulate a given setup of a collision[1, 2]. The simulated events are convolved with experimental resolutions of the detectors, providing an accurate representation of many ionization processes[2]. The main shortcoming of this scheme is that it is usually necessary to compute billions of cross sections in order to get a physically meaningful statistics. Since each cross section can be computed independently, this calculation belongs to the so-called *embarrasingly parallel* numerical problems. Therefore, it perfectly suits the new computational features provided by latest generation of Graphical Processing Units (GPUs).

In this work we report benchmarks of the GPU implementation of the MCEG method, applied to the double ionization of Ne by high energy electron impact[3]. The collision is modeled as a two step process: the first collision induces the ionization of Ne, while the second one is the single ejection of one electron from the residual target Ne^+. Each step is computed with the First Born Approximation. The code procedes as follows: first, a large set of cross section is computed, and second, favourable events are selected from this set. These two computational steps can be repeated to obtain a given number of events. The code is written in C language using the Compute Unified Device Architecture (CUDA) extensions[4].

The running times for the calculation of 10^5 cross sections are depicted in Fig. 1, as a function of the number of threads and the total number of events per iteration. The performance exhibits a good scaling with the number of total events 2^J, and optimal times are achieved for 32 threads per calculation block.

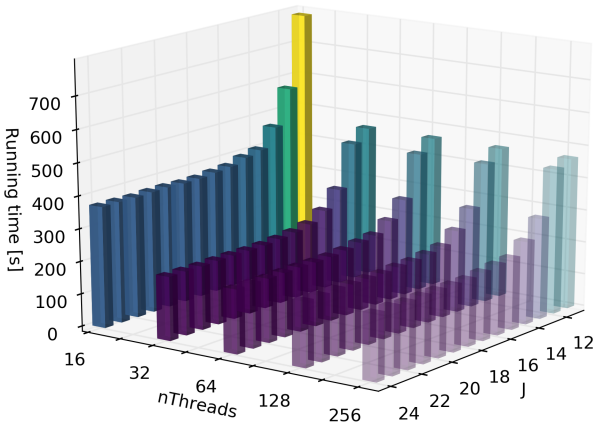

Figure 1. Running times of 2^J (e,3e) cross sections with different number of threads per computational block, to obtain 10^5 double ionization favourable events.

Our preliminary results show that the MCEG is accelerated in the GPU more than ten times, compared to the standard CPU code, providing the same accuracy.

References

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