XXIX International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC2015) IOP Publishing
Journal of Physics: Conference Series **635** (2015) 022070 doi:10.1088/1742-6596/635/2/022070

Fast calculation of cross sections using graphics processing units

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Synopsis Continuum Distorted Wave methods are adapted to new heterogeneous computing architectures, exhibiting excellent speed ups in performance.

The theory of collisions of photons, leptons, ions or other species with atomic targets is devoted to compute a key observable of physics: the cross sections. Much of the work in this area in the last decades has been oriented to establish the formal mathematical foundations of different models and theories to represent the complex quantum-mechanical dynamics of the few particle problem. Besides, the calculation of cross sections involves the use of innovative numerical methods and becomes more and more intensive in the use of computational resources.

The first step in the computation of cross sections is the evaluation of the transition matrix element T_{if} between the initial and final states of the collision. The second step involves the (usually multidimensional) integration of the probabilities of transition to match the specific cross sections obtained in the experimental realization of the collision under scrutiny. While the details of the model determine the first step, this crude two-stages description is quite independent of the theory selected.

Theoretical models have become more and more advanced as the computational infraestructure evolved. Nowadays, there are several methods that solve three-body Schrdinger equation from first princiles, without approximations, but require the intensive use of clusters of computing machines[1, 2, 3]. However, the rise of heterogeneous computer architectures in the last years requires the development of new numerical methods and different approaches to the calculations: the computational capability of each piece of hardware as well as the vastly different bandwidths among them have to be carefully considered to port codes to contemporary computers. The ability to use graphics processing units (GPUs) as massivelly parallel processors with standard programming languages leads to big speed ups in optimized codes[4].

In this work the performance of the well-known Continuum Distorded Wave – Eikonal Initial State (CDW–EIS) method for the ionization of atoms by charged particles at intermediate to high energies[5] is explored. The code is completely rewritten to take advantage of heterogeneous hardware architectures with GPUs. Two main optimization points were developed: the calculation of partial waves (or hypergeometric functions for pure Coulomb potentials), and the multidimensional integration to compute total cross sections. Special purpose libraries are used to compute on the GPU[6, 7]. Workload balancing between CPU cores and GPU is an important factor affecting performance. Preliminary calculations show that the code runs at least ten times faster than the CPU only counterpart.

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