Modelling DNA Radiation Damage on many-core architectures: current GP-GPU implementation and a perspective view

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There is a variety of processes initiated by the primary radiation impinging on DNA which can induce serious genetic effects, such as mutation [1]. At energies below the DNA ionization threshold the main mechanism responsible for single- and double-strand-breaks (SSBs and DSBs) has been linked to the action of low energy electrons (LEEs) [2-4] which have been proven to be the most abundant among the secondary species produced by the primary radiation[5]. The essential intermediates between the initial electron collision and the final molecular break-up have been identified as the Transient Negative Ions (TNIs), i.e. metastable states occurring in the scattering process which originate from the temporary trapping of the incident electron in the molecular potential field. The TNIs show a strong `local' character in the sense that they can essentially be associated to quantum resonances of the single DNA basic constituents [6, 7]. The characterization of these anionic intermediates is crucial in order to gather critical data for the analysis of the biological consequences of the electron interaction with the complex structures of the living tissues.
The approach we follow to model the electron-molecule interaction is based on a Single-Centre Expansion (SCE) of the molecular and incident electron wavefunctions about the centre of mass of the molecule and by solving the resulting scattering Volterra equations we calculate electron-molecule resonance positions and widths (further details on our theoretical procedure when applied to biological systems can be found in Ref. [8]). In our studies [9,10], these observables have been correlated with viable breaking pathways of various biosystems such as the DNA molecular components (i.e., bases and (deoxy)-riboses) whose TNIs are possible precursors of SSBs and DSBs. The encouraging fairly good results we obtained in modelling some recent experimental data [11,12] suggest the extension of the method to larger molecular sections of the DNA, but this application is currently limited by computational bottlenecks. In fact, although the whole set of codes we developed for electron-molecule scattering [13,14] has been implemented to efficiently run in parallel on most of the high performance computing architectures, the extremely large dimension of the molecular target to take into account require, with respect to present, resources with one (or more) order(s) of magnitude in computing power. In line with recent applications [15-16], a possible approach to have some of the most time-consuming parts of our codes running faster, could be the use of accelerating coprocessors. To this end, we tested the NVIDIA GP-GPUs and we will present at the conference some preliminary results on the performance evaluation of the GTX and Tesla GPUs when applied in a mixed many-core computing system. The resulting benchmarks of the ported codes with respect to the size of the molecular systems taken into account will be assessed, and a perspective view to future application of these and similar computing architecture (FPGA) will be discussed in detail.

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