High Quality Illustrative Effects for Molecular Rendering

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All-atom simulations are crucial in biotechnology. In Pharmacology, for example, molecular knowledge of protein-drug interactions is essential in the understanding of certain pathologies and in the development of improved drugs. To achieve this detailed information, fast and enhanced molecular visualization is critical. Moreover, hardware and software developments quickly deliver extensive data, providing intermediate results that can be analyzed by scientists in order to interact with the simulation process and direct it to a more promising configuration. In this paper we present a GPU-friendly data structure for real-time illustrative visualization of all-atom simulations. Our system generates both ambient occlusion and halos using an occupancy pyramid that needs no precalculation and that is updated on the fly during simulation, allowing the real time rendering of simulation results at sustained high framerates.

http://dx.doi.org/10.1016/j.cag.2015.07.017