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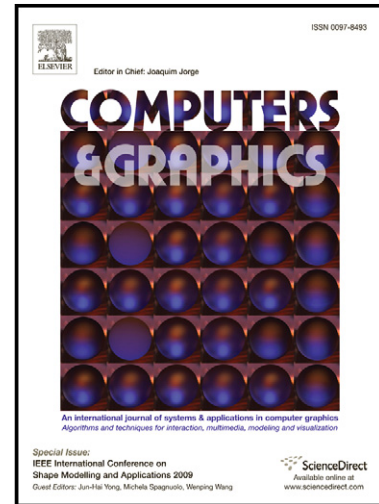
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High quality illustrative effects for molecular rendering

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Abstract

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.

Keywords: Molecular Visualization, Ambient Occlusion, Halos

1. Introduction

Molecular Visualization is of key importance in elucidating the atomic mechanism for protein-ligand recognition, a crucial process in pharmacology drug design and enzymatic catalysis. The specificity and potency of a drug, for example, will depend on its molecular interactions at the bound complex. Moreover, drug efficacy might also depend on its delivery to the target active site —i.e. fluctuations in the entrance pathway/channel (for instance from mutations, etc.) can decrease or abolish its action. These aspects can be clearly understood when visualizing the continuous dynamical protein-ligand recognition, typically a microsecond timescale process. Recent developments in software and hardware, such as the special purpose Anton machine [1], allow today biophysical simulations at such timescales if large dedicated computational time is available. Moreover, breakthrough technological advances have reduced this computation time from weeks/days to hours/minutes [2], introducing processes that can be interactively inspected and directed. In this interactive new scenario, enhanced molecular visualization is essential. Inspection may be used both to understand the recognition process and, more importantly, to change parameters of the simulation process in an interactive and iterative manner. These changes might improve the exploration (sampling) process but also, for example, introduce modifications *on the fly* to drug candidates to better design more effective inhibitors. These substantial advances in the speed of simulation will continue to evolve. We are working thus, on the next generation of simulation software that will bring a tight control of the process to the desktops of the researchers (see Figure 1). In this paper we concentrate on the visualization cues that facilitate the comprehension of the simulation.

Illustrative visualization techniques help researchers gain insights about the structure of large proteins [3]. Some of these techniques include abstraction [4] salient region enhancement [5], halos or ambient occlusion [6, 7]. Popular molecular visualization packages such as Avogadro [8] or VMD [9] include some of these techniques in different ways. However, most previous approaches do not support illustrative effects in real-time for molecules in constant motion. This makes our scenario different from other approaches in that we need to recompute the illustrative visualization motifs for each frame. Thus, our requirements are:

- Facilitate molecule understanding: We achieve this with high quality ambient occlusion both for far views and closeups.

- Illustration of the ligand position and trajectory: This provides better comprehension of the current