Real-Time Ray Tracing in Molecular Visualization

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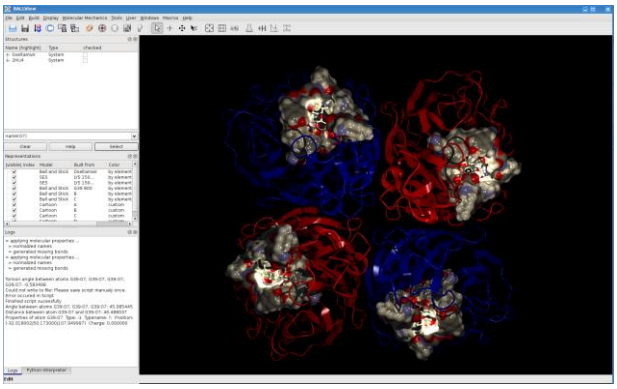

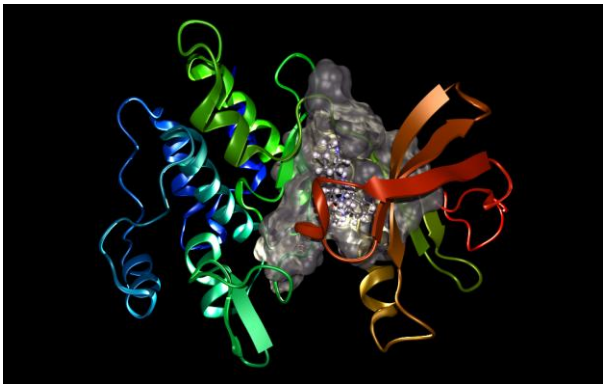

Molecular viewing and editing tools are an important part of many applications and processes in structural bioinformatics, computational chemistry, and pharmacy. Consequently, molecular graphics has historically been very fast to adopt the most recent graphics technologies available. Particularly important is providing the user with an accurate (3d) spatial representation of molecular structural arrangements. Another important goal of molecular graphics is to create publication quality images.

To this end, ray tracers are usually the method of choice; although these traditionally take minutes to hours to produce high quality results. However, recent developments in computer graphics have made real-time ray tracing of complex scenes with high visual quality a reality. Indeed, ray tracing has now been widely recognized as the upcoming graphics standard, and will receive particular attention by hardware vendors. We present a full integration of a general purpose real-time ray tracing architecture into a molecular viewing and modelling tool by integrating the RTfact library [3] into BALLView [2, 3, 4]. This allows the user to add advanced visualizations, such as realistic shadows and reflections, to existing techniques and representations. The ability to combine real-time ray tracing with 3d stereo visualization, as it is offered by BALLView, can maximize the structural perception of a molecular scene even more. This opens up completely new avenues of perception and interaction. Furthermore, ray tracing not only serves as a method for high quality rendering, it can also be used as a fast sampling method for the extraction of relevant information from volumetric data arising from X-Ray crystallography or electron microscopy. The use of ray tracing technology allows the fast and accurate detection of molecular geometric properties such as volume, exposed surface area, and the occurrence of internal cavities [4].

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