Interactive Real-Time Ray Tracing

In Molecular Visualization

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Introduction

Molecular viewing and editing tools are an important part of many applications and processes in structural bioinformatics, computational chemistry, and pharmacy.

A particularly important factor is to provide the user with an accurate and informative (3D) spatial representation of molecular structural arrangements, the effective extraction of relevant information from volume data, and the fast and simple creation of publication-quality images.

To this end, ray tracing is usually the method of choice; although it traditionally takes minutes to hours to produce high-quality results.

However, recent developments in computer graphics have made real-time ray tracing of complex 3D scenes (polygonal based and volume data) with high visual quality a reality.

RTfact

RTfact is a C++ real-time ray tracing library that utilizes generic programming concepts to deliver both performance and flexibility. The generic design allows to combine the most suitable algorithms and data structures both in polygonal and volumetric rendering in order to achieve optimal performance.

BALLView

The Biochemical Algorithms Library (BALL) is a comprehensive and extensive rapid C++ application development framework for structural bioinformatics and molecular modelling.

It is available free of charge under the LGPL and GPL for all major operating systems. Both source code and binary packages can be found at the project web site: http://www.ball-project.org.

Integration

Integration of the ray tracer in BALLView is done tightly and transparently, allowing advanced effects to work seamlessly with any combination of available representations - molecular structure representations as well as three-dimensional scalar quantities like cryo-em data or electrostatic potentials - in interactive speed.