Real-Time Ray Tracing and Volume Rendering In Molecular Visualization

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PRINCIPLES OF RAY-TRACING

Introduction

A particularly important task in structural bioinformatics is to provide:

- Accurate and informative (3D) spatial representation of molecular arrangements.
 Quantitative and topological measurements like molecular volumes, surface areas, or cavities.
- Effective extraction of relevant information from volumetric data arising in X-Ray

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crystallography or electron tomography.
Fast and simple creation of publication-quality images.

Recent developments in real-time ray tracing have enabled fast and high-quality visualization of complex 3D scenes and also forged its perception as a general sampling metod reaching well beyond rendering only.

We demonstrate this flexibility, intuitiveness and practical usability on the following examples:

Volume Rendering
Ray tracing employed for effective extraction of information from volumetric data.

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Quantitative

Measurements

Ray tracing as a technique for volume

Versatile High-Quality Rendering Ray tracing of arbitrary

representations with

enhanced spatial

realistic light

simulation.

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ZN ... Residur

perception through



BALLView & RTfact

The ray tracing techniques are delivered by **RTfact**, a C++ real-time ray tracing library that utilizes generic programming concepts to deliver both performance and flexibility. We have integrated it into **BALL**-View, the GUI of the Biochemical Algorithms Library (BALL), a comprehensive and extensive rapid C++ application development framework for structural bioinformatics and molecular modelling, creating a single versatile piece of software. ctinger domain bound (1TF6.pdb, Asymmeti

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.

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