Interactive Real-Time Ray Tracing

In Molecular Visualization

Anna Katharina Dehof[1], Lukas Marsalek[2], Iliyan Georgiev[2], Daniel Stöckel[1], Stefan Nickels[1], Hans-Peter Lenhof[1], Philipp Slusallek[2,3], Andreas Hildebrandt[1]

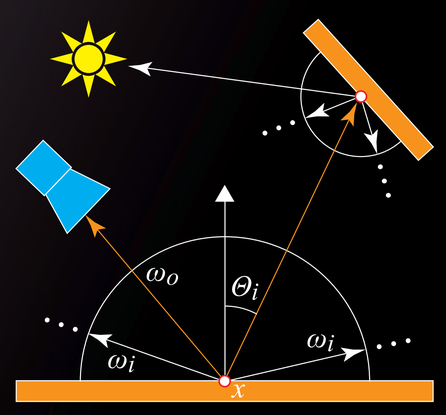
UNIVERSITY OF SAARLAND

[1] Center for Bioinformatics
[2] Computer Graphics
[3] DFKI Saarbrücken

Introduction

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

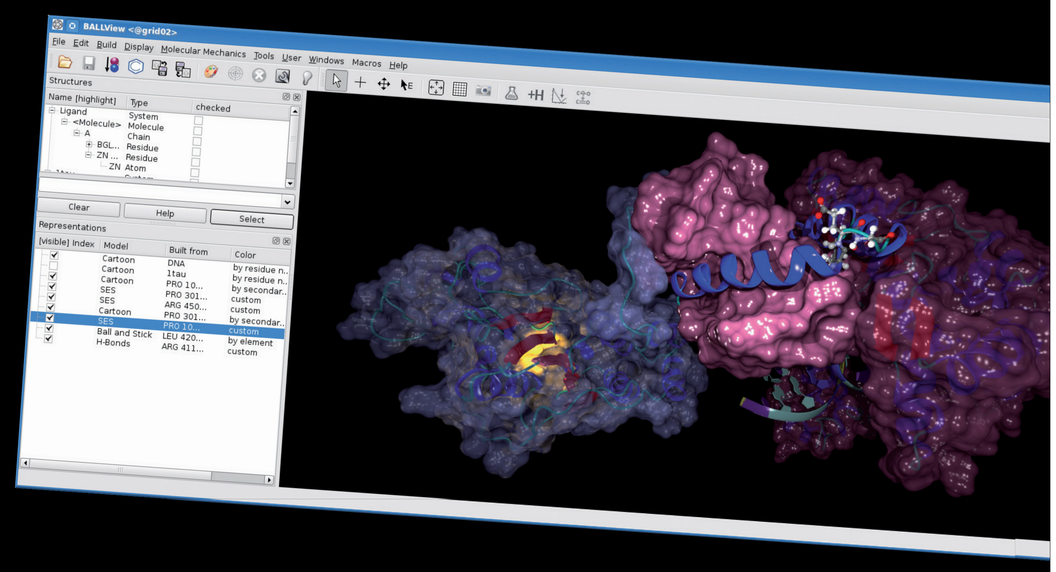
A particularly important factor is to provide the user with an accurate and informative **(3D) spatial representation** of molecular structural arrangements, the effective extraction of relevant information from volume data, and the fast and simple creation of publication-quality images.



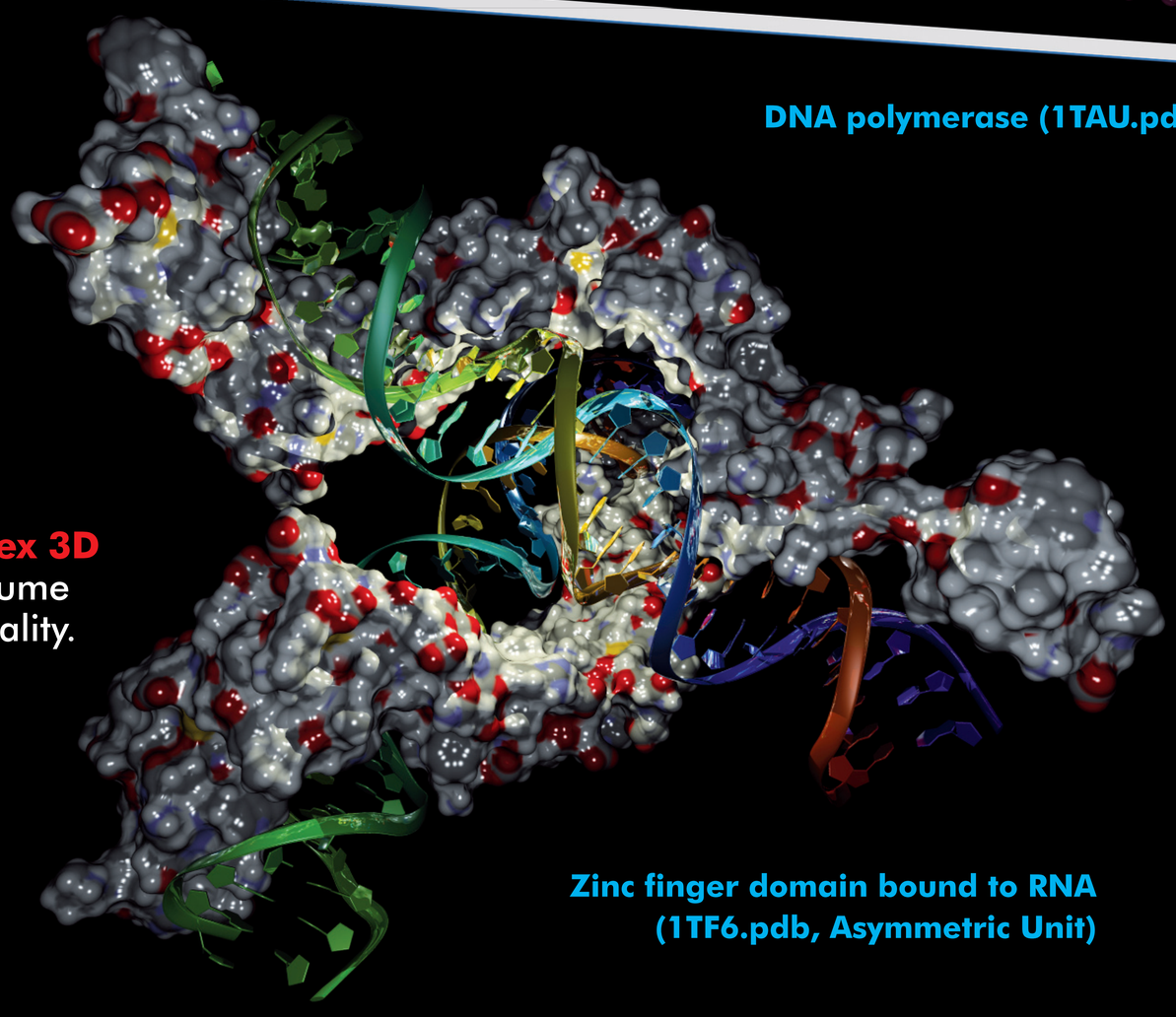
PRINCIPLES OF RAY TRACING

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.



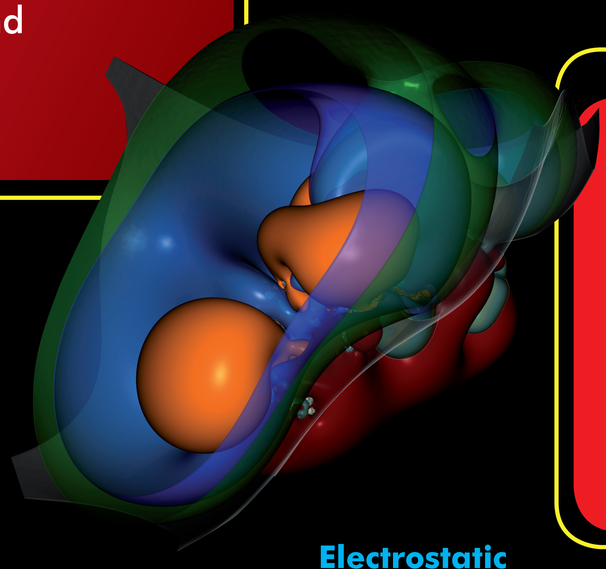
DNA polymerase (1TAU.pdb)



Zinc finger domain bound to RNA (1TF6.pdb, Asymmetric Unit)

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.

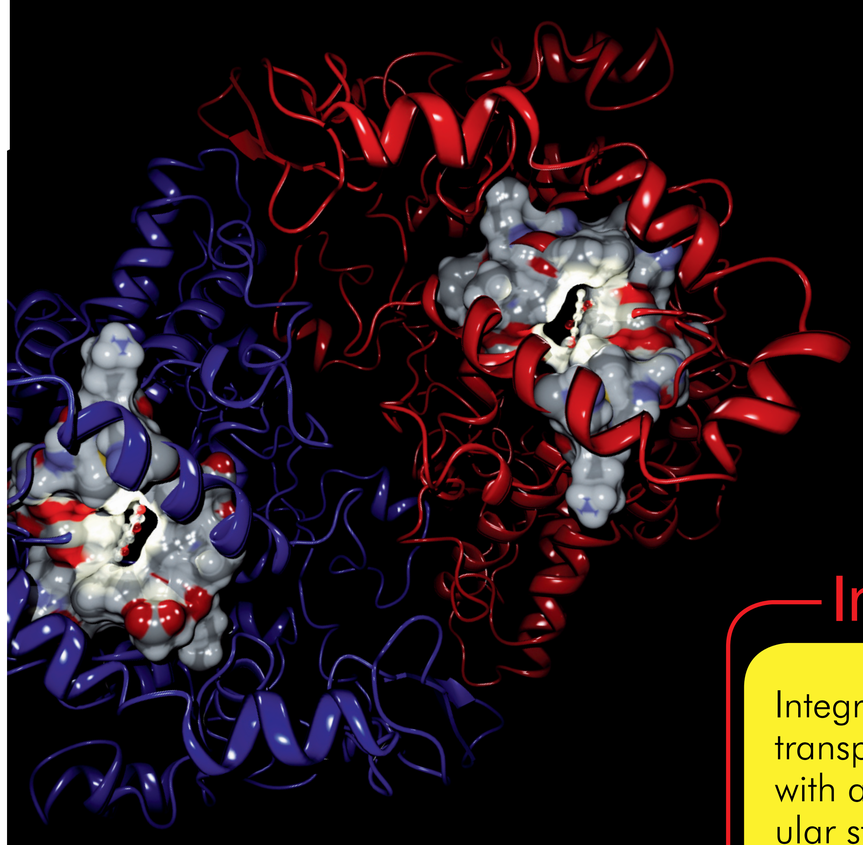


Electrostatic potential of a multidomain protein (3go5.pdb)

BALLView

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

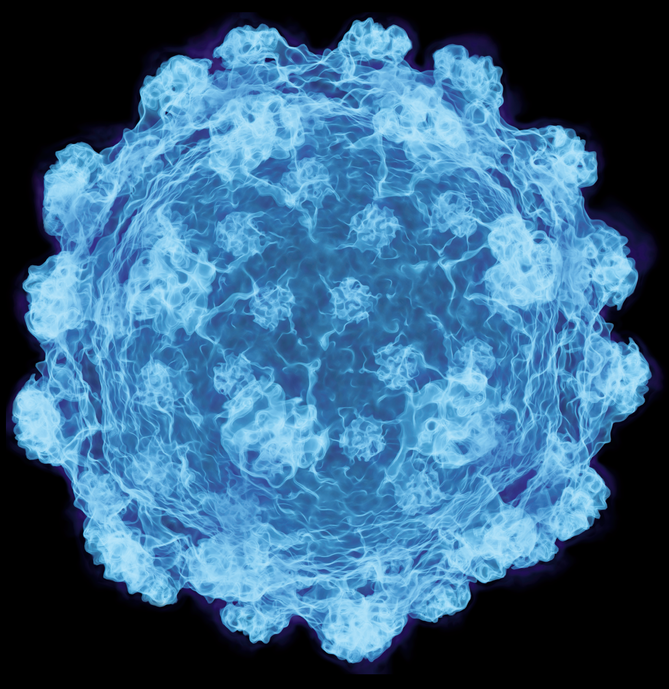
It is available free of charge under the LGPL and GPL for all major operating systems. Both source code and binary packages can be found at the project web site: **http://www.ball-project.org**.



Aspirin in complex with COX 2 (1PTH.pdb)

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.



Φ 29 dsDNA bacteriophage

L. Marsalek, A. Hauber, and P. Slusallek: High-speed volume ray casting with CUDA, Poster on Symposium on Interactive Ray Tracing 2008, Los Angeles, CA.
S. Stegmaier, M. Strenger, T. Klein, and T. Ertl: A simple and Flexible Volume Rendering Framework for Graphics-Hardware-based Raycasting, Volume Graphics, 2005
A. Moll, A. Hildebrandt, H.-P. Lenhof, and O. Kohlbacher. BALLView: an object oriented molecular visualization and modeling framework. J Comput Aided Mol Des,19(11):791-800, Nov 2005.
A. Moll, A. Hildebrandt, H.-P. Lenhof, and O. Kohlbacher. BALLView: a tool for research and education in molecular modeling. Bioinformatics, 22(3):365-366, 2006.

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