Real-time ray tracing of complex molecular scenes with BALLView and RTfact

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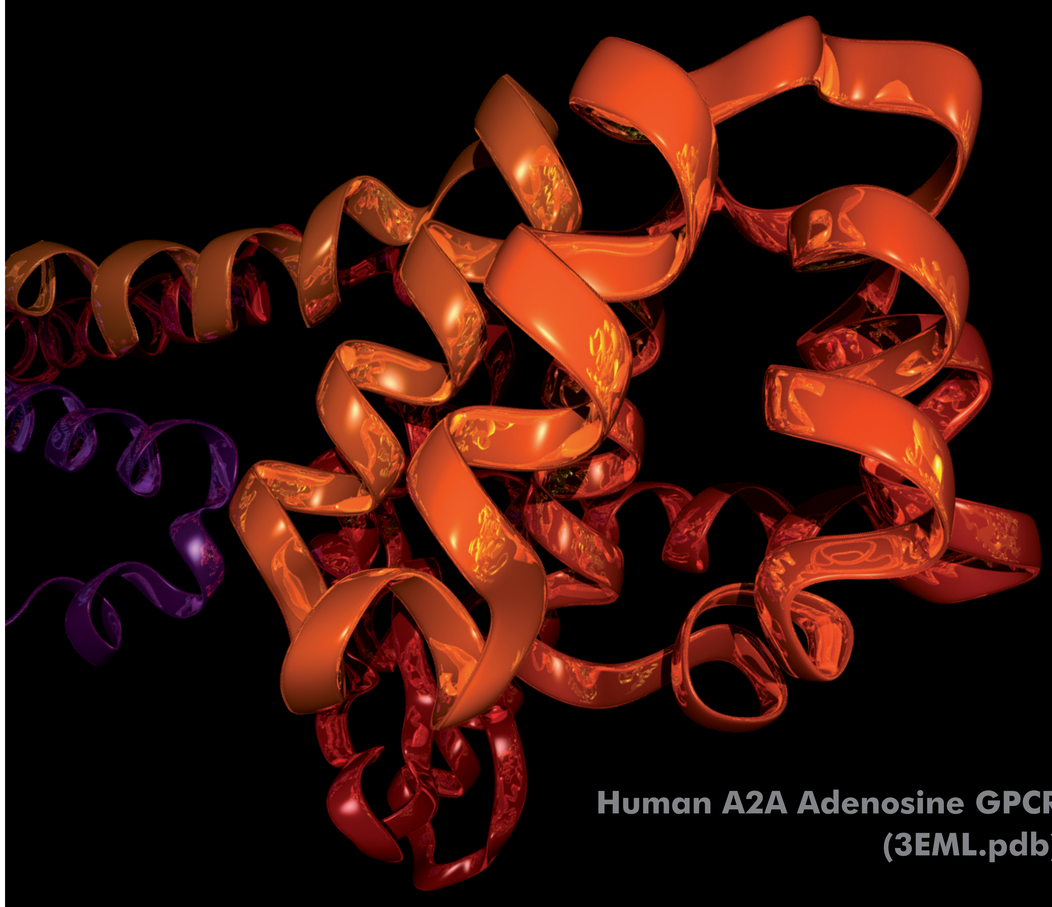


Human A2A Adenosine GPCR (3EML.pdb)

Introduction

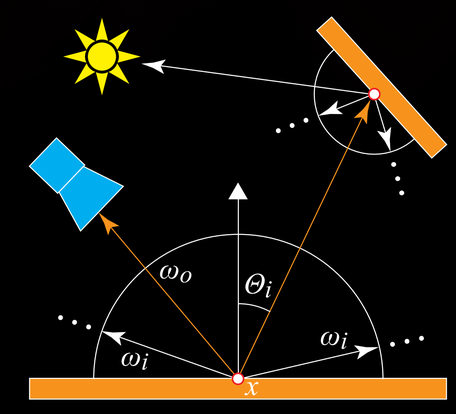
Molecular viewing and editing tools are an important part of many applications and processes in structural bioinformatics, computational chemistry, and pharmacy.

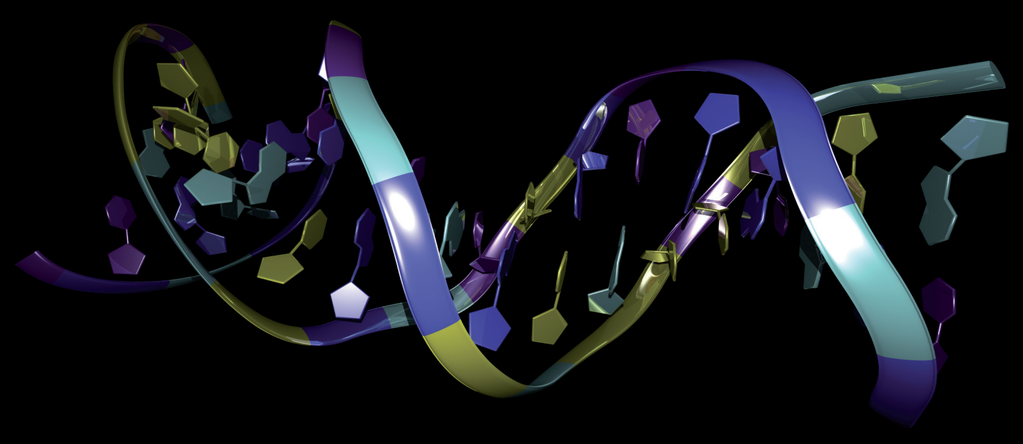
A particularly important factor is to provide the user with an accurate and informative (3D) spatial representation of molecular structural arrangements. Another important goal of molecular graphics is to create publication-quality images.

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 scenes with high visual quality become a reality.

PRINCIPLES OF RAY-TRACING



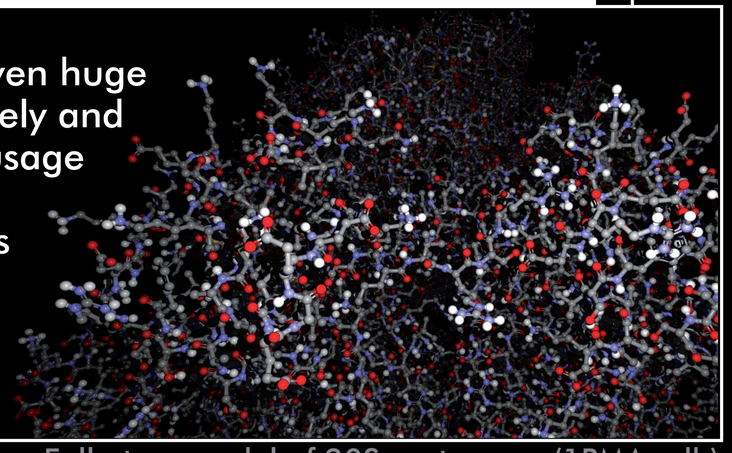


19 residue DNA segment (1GLU.pdb, chain C,D)

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** for a specific application in order to achieve optimal performance.

RTfact handles even huge models interactively and through correct usage of shadows and lighting enhances the structural perception significantly.



Full atom model of 20S proteasom (1PMA.pdb)

Integration

We present the first integration of a general purpose real-time ray tracing architecture into a molecular viewing and modelling tool by integrating the RTfact library into BALLView.

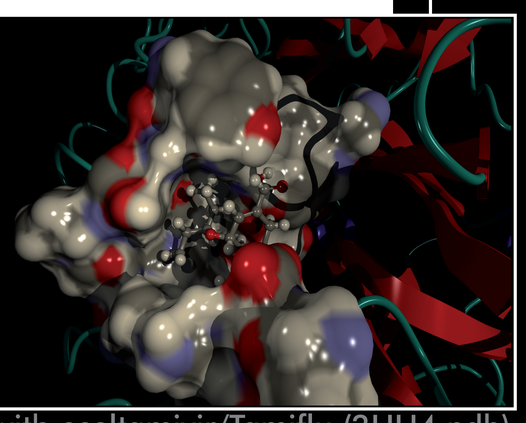
Integration of the ray tracer is done tightly and transparently, allowing advanced effects to work seamlessly with any combination of available representations in interactive speed.

BALLView

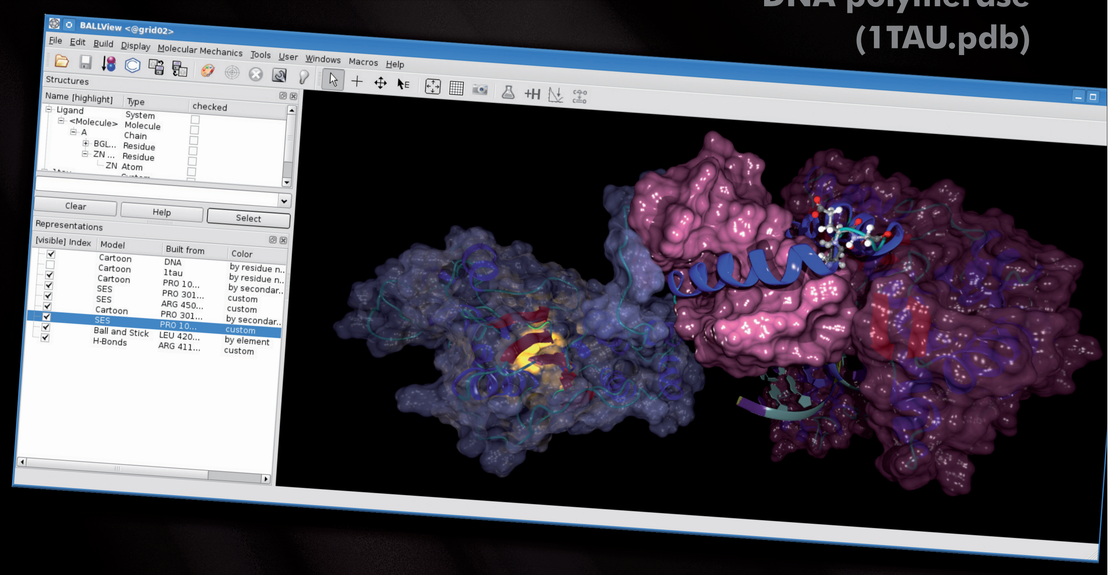
The Biochemical Algorithms Library (BALL) is a comprehensive and extensive rapid C++ application development framework for **structural bioinformatics and molecular modelling**.

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**.

Albeit in a naive fashion, we can handle unstructured movement, as it occurs, e.g., in molecular dynamics simulation, interactively.



N1 Neuraminidase with oseltamivir/Tamiflu (2HU4.pdb)



DNA polymerase (1TAU.pdb)

A. Moll, A. Hildebrandt, H.-P. Lenhof, and O. Kohlbacher. BALLView: an object-oriented molecular visualization and modeling framework. J. Comp. Aided Mol. Des., 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), 2006.
O. Kohlbacher and H. P. Lenhof. BALL–rapid software prototyping in computational molecular biology, Bioinformatics 16(9), 2000
I. Georgiev and P. Slusallek. RTfact: Generic Concepts for Flexible and High Performance Ray Tracing, IRT 2008

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