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Workshop on Molecular Graphics and Visual Analysis of Molecular Data

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Keynote

Playing the Molecular Graphics Game – Visual Analysis of Molecular Data in a Game Engine

Marc Baaden

Abstract

Molecular graphics is essential for the visual analysis of molecular data, ranging from depictions of experimental measurements such as deposited in the PDB or similar databases to the scrutiny of results from computational investigations, for instance molecular dynamics trajectories. In the past, visualization software tools were mostly "magic" black boxes, even if the source code was available, because their understanding by the scientists that wanted to use such tools in their research required an excessive level of technical expertise. With UnityMol, we explore the possibilities offered by using a game engine as a development platform for a scientific tool, where the learning curve can be significantly lowered compared to traditional approaches. This strategy enables scientists to actually and more easily modify, extend and adapt the software to their particular needs. Running the "application" in the Unity editor, while being able to adjust parameters and test the effect of modifications significantly speeds up the trial-and-error development cycle. UnityMol is intended both as a ready-to-use tool and a development platform for easy customization. It currently provides an optimized VR implementation, interactive simulation facilities and an early prototype of web integration among its original features.

Short Biography

Marc Baaden is a computational chemist who works on modeling biological systems and processes at the molecular and atomic level. Work includes both application of existing packages like Amber, Gromacs, Yasara and NAMD but also development of novel software and exploration of innovative methods (like for example virtual reality and haptics). A broad range of methods is used from simple minimization via coarse grained modeling up to molecular dynamics and docking approaches. In addition, he develops molecular visualization applications such as HyperBalls and UnityMol. He is actively collaborating with experimental groups, linking and validating computational observations with data from crystallography, NMR spectroscopy and electrophysiology. Marc is Directeur de Recherche de 1ère classe and Director of the CNRS UPR 9080 laboratory, Paris. He is member of a number of national and internationally renowned committees and got a number of fellowships, such as the prestigious EU Marie Curie fellowship.

Keynote

Building on UnityMol to develop a VR solution fit for the BioPharma drug discovery needs of tomorrow through an industrial-academic collaboration

Zara Sands

Short Biography

After gaining her Ph.D. in computational chemistry at the University of Nottingham, in 2003 she took a Wellcome Trust Fellowship position at the University of Oxford, and under the direction of Professor Mark Sansom developed an expertise in membrane protein (MP) structural biology & biophysics. She joined AstraZeneca in 2009, where she developed and applied cutting edge in silico technologies for studying complex MP CNS targets. In 2009, she was recruited by UCB BioPharma to support and strengthen their CNS drug discovery programmes. She has been instrumental in developing UCB's drug discovery capabilities and through the judicious application of computational approaches has successfully driven their GPCR drug discovery projects towards clinical candidates. She currently serves on the Scientific Advisory Board of BioExcel, a European Centre of Excellence for Computational Biomolecular Research.

Keynote

About the Future of Molecular Visualization – from Quantum Chemistry to Molecular Microscopy

Hans-Christian Hege

Abstract

Molecular visualization is one of the most successful areas of data visualization in terms of actual use by experts. This applies both to its use in communication and teaching, as well as to its use in molecular research and molecular design. In this talk we focus on the latter: molecular research and molecular design. Many new techniques have been developed in recent decades, in particular for the interactive, visually supported analysis of biomolecules. This includes, for example, the computation and graphical representation of molecular surfaces, the identification of cavities and tunnels, or the interactive analysis of large MD trajectories. The vast majority of these tools is based on an extremely simplified physical model in which atoms are represented as (almost) hard spheres that move in classical force fields according to Newtonian mechanics – although we are well aware that atoms and molecules are objects whose correct physical description is quantum mechanical. Furthermore, most of the existing molecular visualization tools focus on a certain spatiotemporal scale: that of a few molecules, possibly surrounded by many small solvent molecules. We will discuss which new problems arise for molecular visualization if one leaves this frame — for example, because the classical model produces inconsistent results, or because one looks at molecules in detail and can no longer neglect quantum mechanical effects, or because one goes to a completely different length scale, for example to study cellular phenomena while also considering effects on the molecular level.

Short Biography

Hans-Christian Hege is head of the Visual Data Analysis Department at Zuse Institute Berlin (ZIB). After studying physics and mathematics, he performed research in computational physics and quantum field theory at Freie Universität Berlin (1984-1989). Then, he joined ZIB, initially as a scientific consultant for high-performance computing, and then as head of the Department Scientific Visualization (now: Visual Data Analysis), which he started in 1991. His group performs research in visual data analysis and develops visualization software such as Amira/Avizo. He is also the co-founder of Mental Images (1986) – now NVIDIA Advanced Rendering Center –, Indeed-Visual Concepts (1999) – now Visage Imaging –, and Lenné3D (2005). He has taught as guest professor at Universitat Pompeu Fabra (Barcelona), and as honorary professor at the German Film School (University for Digital Media Production) /Film School Babelsberg. His research interests include visual computing and applications in life sciences, natural sciences and digital humanities. He is a member of ACM, IEEE, Eurographics (since 2016 elected fellow), GI, DPG and CURAC.