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Molecular Visualization Mini-Symposium

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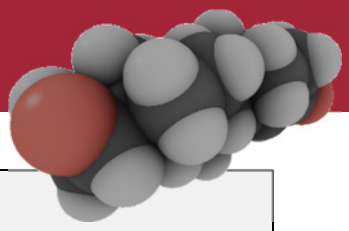
Building O27, Room 3211



09:00 **Timo Ropinski (Ulm University, Germany)**
Opening Remarks

09:05 **Ivan Viola (TU Wien, Austria)**
Bridging Spatial and Temporal Scales in Biological Data Visualization

09:35 **Victor Guallar (Barcelona Supercomputer Center, Spain)**
On the Fly Molecular Simulations for a Visual Interactive Use

10:05 **Michael Krone (University of Stuttgart, Germany)**
Enhancing the Computational Microscope - Interactive Visual Analysis of Biomolecular Simulations

10:35 Coffee Break

11:00 **Robin Skånberg (Ulm University, Germany)**
Real-Time Molecular Visualization Supporting Diffuse Interreflections and Ambient Occlusion

11:30 **Pere-Pau Vázquez (UPC Barcelona, Spain)**
High Quality Illustrative Visualization of Secondary Structures

12:30 Lunch

13:30 **Martin Falk (Linköping University, Sweden)**
Interactive Molecular Visualization with Large-scale Instancing and Depth of Field

14:00 **Barbora Kozlíková (Masaryk University, Czech Republic)**
Visualization Techniques for Exploration of Tunnels in Proteins and their Molecular Dynamics of Field

14:30 **Timo Ropinski (Ulm University, Germany)**
Closing Remarks

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Abstracts

Ivan Viola (TU Vienna, Austria)
Bridging Spatial and Temporal Scales in Biological Data Visualization

The study of biological processes carried out in living organisms is among the central foci of modern science. The field is nowadays by large extent computational, there are many kinds of digital models that characterize particular aspects of life. To provide a comprehensive view on biological phenomena, visualization offers itself for integrating multiple models into one visual environment. One of the interesting challenges, associated with such a visual integration, is to communicate phenomena that are simultaneously described on several spatial and temporal scales.

In my talk I will discuss visualization techniques that bridge five orders of magnitude of spatial scale by interactively displaying structural information from a single atom level up to entire bacteria cell size with complete molecular machinery. When dealing with simulation of molecular interactions in living organisms, agent-based models are used to model long sequences of Brownian motion that randomly carry out several physiologically relevant events. One such event occurs on average every thousandth simulation iteration in the agent based simulation. In order to perceive random motion but also to see relevant events simultaneously, we bridge two temporal scales that are three orders of magnitude apart from each other. The approach is based on a special timelapse approach inspired from scientific animation techniques. In the last part of my talk I will present a technique for interactive 3D visualization of molecular reaction pathways that is controlled in a top-down manner by quantitative simulation and is simultaneously co-visualized. In such visual environment the viewer can interactively control the visualization as well as simulation parameters.

Victor Guallar (Barcelona Supercomputer Center, Spain)
On the Fly Molecular Simulations for a Visual Interactive Use

In this talk we will describe our recent efforts in speeding up molecular simulations to achieve real interactive usage. We will introduce our Monte Carlo code, PELE (Protein Energy Landscape Exploration), and its current developments to use modern hardware architectures, such as mobile processors with embedded accelerators. In this context, visualization is a crucial aspect, responsible of transmitting the information in a fast and intuitive way. We envision a future where, combining these elements, experts in biomolecule engineering (such as drug design, enzyme engineering...) will improve their design experience and performance.

Michael Krone (University of Stuttgart, Germany)
Enhancing the Computational Microscope - Interactive Visual Analysis of Biomolecular Simulations

Interactive visualization is a powerful tool to analyze biomolecular simulations. It allows domain experts to explore the results of their simulations. This not only helps to validate existing hypotheses but also to spot new, unexpected phenomena that may lead to new insights into the behavior of the simulated molecular systems. While a direct visualization of the data can already reveal many interesting processes, interactive analysis can further enhance the exploratory data analysis. In this talk, several interactive visual analysis methods for biomolecular simulation data are discussed, for

example real-time cavity detection algorithms for binding site analysis, and comparative visualizations. Furthermore, actual use cases where interactive visual analysis helped domain scientists to discover unanticipated phenomena are presented.

Robin Skånberg (Ulm University, Germany)
Real-Time Molecular Visualization Supporting Diffuse Interreflections and Ambient Occlusion

Today molecular simulations produce complex data sets capturing the interactions of molecules in detail. Due to the complexity of this time-varying data, advanced visualization techniques are required to support its visual analysis. Current molecular visualization techniques utilize ambient occlusion as a global illumination approximation to improve spatial comprehension. Besides these shadow-like effects, interreflections are also known to improve the spatial comprehension of complex geometric structures. Unfortunately, the inherent computational complexity of interreflections would forbid interactive exploration, which is mandatory in many scenarios dealing with static and time-varying data. In this paper, we introduce a novel analytic approach for capturing interreflections of molecular structures in real-time. By exploiting the knowledge of the underlying space filling representations, we are able to reduce the required parameters and can thus apply symbolic regression to obtain an analytic expression for interreflections. We show how to obtain the data required for the symbolic regression analysis, and how to exploit our analytic solution to enhance interactive molecular visualizations.

Pere-Pau Vázquez (UPC Barcelona, Spain)
High Quality Illustrative Visualization of Secondary Structures

All-atom simulations are crucial in biotechnology. In Pharmacology, for example, molecular knowledge of protein drug interactions is essential in the understanding of certain pathologies and in the development of improved drugs. To achieve this detailed information, fast and enhanced molecular visualization is critical. Moreover, hardware and software developments quickly deliver extensive data, providing intermediate results that can be analyzed by scientists in order to interact with the simulation process and direct it to a more promising configuration. In this paper we present a GPU-friendly data structure for real-time illustrative visualization of all-atom simulations. Our system generates both ambient occlusion and halos using an occupancy pyramid that needs no precalculation and that is updated on the fly during simulation, allowing the real time rendering of simulation results at sustained high framerates.

Molecular Dynamics simulations are of key importance in the drug design field. Among all possible representations commonly used to inspect these simulations, Ribbons has the advantage of giving the expert a good overview of the conformation of the molecule. Although several techniques have been previously proposed to render ribbons, all of them have limitations in terms of space or calculation time, making them not suitable for real-time interaction with simulation software. In this paper we present a novel adaptive method that generates ribbons in real-time, taking advantage of the tessellation shader. The result is a fast method that requires no precomputation, and that generates high quality shapes and shading.

Martin Falk (Linköping University, Sweden)
Interactive Molecular Visualization with Large-scale Instancing and Depth of Field

Visualizing cellular systems at an atomistic level of detail is quite demanding with respect to the total number of atoms. Typically, data sets obtained from in vivo or in silico experiments already comprise several billions of atoms when including only parts of a single cell. However, many instances of only a few different proteins occur in the intracellular environment, a fact which can be exploited to fit the data into the graphics memory. For each protein species, one model is stored and rendered once per instance. The presented method exploits recent algorithmic advances for particle rendering and the repetitive nature of intracellular proteins to visualize dynamic results from mesoscopic simulations of cellular transport processes at interactive frame rates.

The second part of my talk will cover our depth of field approach tailored to molecular visualization. This object-space method eliminates many shortcomings of image-based algorithms, e.g. occlusion-based artifacts. Based on observations derived from physically-correct renderings, we formulate an analytical opacity estimation which can be used instead of blurring the atoms. This opacity estimation combined with the spherical shape of atoms allows us to approximate the depth-of-field effect with one sample per pixel instead of computing multiple samples as required by physically-based approaches. The proposed technique is interactive and its results are comparable to images produced by existing ray tracing engines.

Barbora Kozlíková (Masaryk University, Czech Republic)
Visualization Techniques for Exploration of Tunnels in Proteins and their Molecular Dynamics of Field

Visualization techniques for exploration of tunnels in proteins and their molecular dynamics Studying the dynamic behavior of protein inner pathways, called tunnels, has a deep impact on the understanding of protein reactivity with other small molecules. However, the increasing length of molecular dynamics simulations makes the detailed exploration of tunnel movements almost impossible. In this talk we will present our novel and highly abstracted visualization techniques for conveying biochemical properties across and along protein tunnels. These techniques aim to aggregate the most important information about the tunnel and its surrounding amino acids and to present it to the biochemists in a simple and comprehensible manner. Moreover, these representations can help the domain experts in targeted mutagenesis around the tunnel which leads to desired changes of protein function or its properties.