TECHNISCHE UNIVERSITÄT WIEN
Institut für Computergraphik und Algorithmen
Arbeitsbereich für Computergraphik

zentrum für virtual reality und visualisierung forschungs-gmbh

OESTERREICHISCHE COMPUTER GESELLSCHAFT
AUSTRIAN COMPUTER SOCIETY

laden gemeinsam zum

GASTVORTRAG

Timo Ropinski
Ulm University, Institute for Media Informatics
Visual Computing Research Group

“Interactive Visualization Techniques for Molecular Structures”

Abstract:

TWithin this talk I will cover our recent work in the area of molecular visualization. Two techniques will be presented, which have been developed with the goal to improve the spatial comprehension of complex molecular structures. First, coverage-based opacity estimation is discussed as a technique to achieve Depth of Field (DoF) effects when visualizing molecular structures. The proposed algorithm is an object-based approach which eliminates many of the shortcomings of state-of-the-art image-based DoF algorithms. Based on observations derived from a physically-correct reference renderer, coverage-based opacity estimation exploits semi-transparency to simulate the blur inherent to DoF effects. It achieves high quality DoF effects, by augmenting each atom with a semi-transparent shell, which has a radius proportional to the distance from the focal plane of the camera. Thus, each shell represents an additional coverage area whose opacity varies radially, based on our observations derived from the results of multi-sampling DoF algorithms. Second, I will discuss the integration of diffuse illumination effects into molecular visualization. While current molecular visualization techniques utilize ambient occlusion as a global illumination approximation in order to improve spatial comprehension, interreflections are also known to improve the spatial comprehension of complex geometric structures. To realize these interreflections in real-time, an analytic approach is exploited for capturing interreflections of molecular structures. By exploiting the knowledge of the underlying space filling representations, the required parameters can be reduced and symbolic regression can be applied to obtain an analytical expression for interreflections. I will discuss how to obtain the data required for the symbolic regression analysis, and how to exploit the analytic solution to enhance interactive molecular visualizations. For both presented techniques, high quality results will be shown, which a re visually comparable to those of state-of-the-art offline renderers.

Biography:

Prof. Ropinski heads the Opens internal link in current windowVisual Computing Research Group at Opens external link in new windowUlm University. Before moving to Ulm he was Professor in Interactive Visualization at Opens external link in new windowLinköping University in Sweden, where he was heading the Opens external link in new windowScientific Visualization Group. Prof. Ropinski has received his Ph.D. in computer science in 2004 from the Opens external link in new windowUniversity of Münster, where he has also completed his Habilitation in 2009.

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