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

Michael Krone
VISUS, University of Stuttgart

“Interactive Visual Analysis of Biomolecular Simulations”

Abstract:

Molecular dynamics simulations allow scientists to run virtual experiments that can even reproduce the interactions in molecular systems with previously unknown behavior. That is, these simulations provide us with a “Computational Microscope” that enables studying the dynamic behavior of proteins and other biomolecules down to individual atoms. Interactive visualization is an essential part of this Computational Microscope, since it allows domain experts to explore the results of their simulations. Direct visualizations of the data using established molecular models show the dynamics of the simulated molecules. While such direct visualizations can already reveal many interesting processes, interactive analysis can further enhance the exploratory data analysis with the results of feature extractions. In my talk, I will discuss algorithms for direct molecular visualization as well as several examples of interactive visual analysis methods for biomolecular simulation data, including real-time cavity detection algorithms and comparative visualizations. I will also present actual use cases where interactive visual analysis led to the discovery of unexpected phenomena in the simulated molecular systems.

Biography:

Michael Krone successfully defended his PhD thesis at the Visualization Research Center (VISUS), University of Stuttgart, Germany in 2015, where he also currently works as a researcher. He received his diploma in computer science from the University of Stuttgart. His main research interests lie the fields of in molecular visualization, particle rendering, and GPU-accelerated computing. In particular, this includes interactive molecular graphics and visual analysis methods for structural biology.

Datum: 15. Jänner 2016, 10:30 Uhr s.t.
Ort: TU Wien, Favoritenstr. 9, Stiege 1, 5. Stock, Seminarraum E186