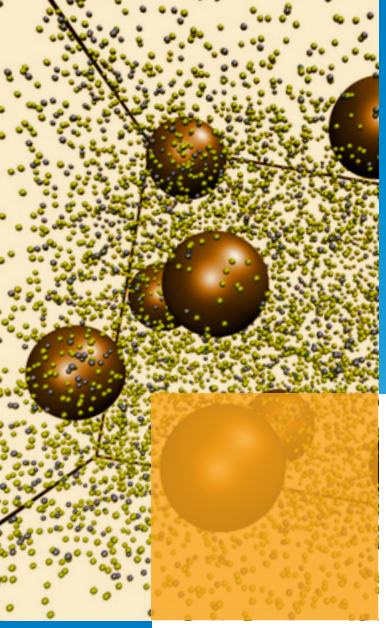


University of Stuttgart
SFB 716

Colloquium of the SFB 716

October 26th, 2017 | 4 pm

University of Stuttgart
Campus Vaihingen
Allmandring 3
Room 1.079

The Collaborative Research Center (SFB) 716 invites colleagues and interested persons to the upcoming colloquium. In this lecture series renowned researchers and members of our subprojects talk about their research findings regarding dynamic simulation of systems with large particle numbers.

www.sfb716.uni-stuttgart.de

TALK

Daniel Baum

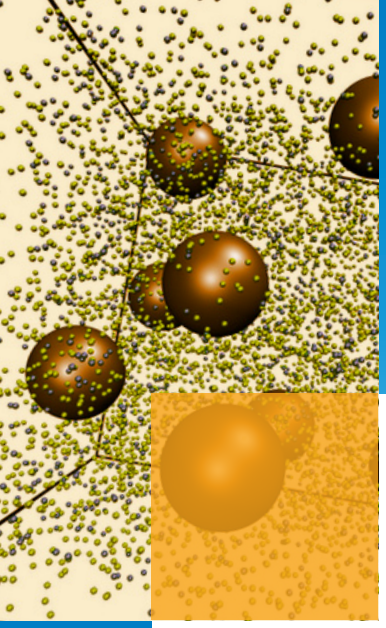
Zuse Institute
Berlin (ZIB)

Visualization and Analysis of Atomic Structures based on the Hard Sphere Model

Atoms and molecules are the constituents of matter, be it inorganic or organic, non-biological or biological. Thus, all physical properties of matter can in principle be understood by analyzing these fundamental constituents and their mutual interactions. Even though the hard sphere model of atoms is a great simplification of physics, it is often used to visualize and analyze molecular structures as well as fluids and solids. In this talk I will present methods that we contributed to the field of molecular visualization and analysis, based on the hard sphere model, over the last few years. Most of these methods are applicable to large atomic systems both in terms of visualization and analysis due to the exploitation of GPU-based rendering and computation.

The major part of the talk concerns molecule-molecule interactions, the transport of small molecules into cavities of large molecules, and the dynamic behavior of cavities in molecular trajectories. To analyze the potential interaction surface of macromolecules with other molecules like ligands, the solvent excluded surface (SES) is most often used. Methods for real-time rendering of the SES suitable for molecular trajectories of even large proteins will be presented along with the definition and computation of the generalization of the SES, called the ligand excluded surface (LES). For the computation of cavities, we utilize the concept of the Voronoi diagram of spheres. We show that it can be efficiently used to compute both static and dynamic molecular paths. Furthermore, I will present visualizations that we developed based on this concept to allow the interactive analysis of the computed cavities, which often is required to incorporate the knowledge of expert users.

In the rest of the talk I will show that by exploiting the fact that very large macromolecular systems often consist of many recurring structures, we can greatly speed up the rendering and achieve interactive frame rates for molecular structures with



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more than a billion atoms. By using deferred shading, we can obtain a smooth transition between the atomic details for close-ups and surface-like structures for objects far away from the observer without changing the underlying representation.

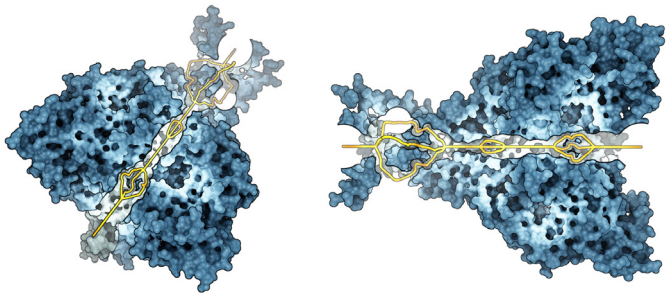

Fig.: Molecular path visualization of a sodium ion channel (PDB: 3HGC). The channel is important for epidermal ion transport into the cell.

TALK

Daniel Weiskopf & Stefan Reinhardt

Visualization Research Centre, Subproject D.5

Multivariate Data Visualization and SPH Simulation

In this talk, we will present recent results from project D.5. We focus on two specific topics: (1) improved multivariate data visualization with parallel coordinates and (2) asynchronous simulation to speed up SPH (smoothed particle hydrodynamics).

In the first part, we address the problem of visualizing multivariate correlations in parallel coordinates. We focus on multivariate correlation in the form of linear relationships between multiple variables. Traditional parallel coordinates are well prepared to show negative correlations between two attributes by distinct visual patterns. However, it is difficult to recognize positive correlations in parallel coordinates. Furthermore, there is no support to highlight multivariate correlations in parallel coordinates. We exploit the indexed point representation of p-flats (planes in multidimensional data) to visualize local multivariate correlations in parallel coordinates. Our method yields clear visual signatures for negative and positive correlations alike, and it supports large datasets. All information is shown in a unified parallel coordinates framework, which leads to easy and familiar user interactions for analysts who have experience with traditional parallel coordinates.

With our asynchronous SPH simulation presented in the second part of the talk, we allow a dedicated time step for each particle. Therefore, we are able to increase the efficiency of SPH simulations. Previous approaches of locally adaptive time steps have shown promising results in the form of increased time steps, however, they need to synchronize time steps in recurring intervals, which involves either interpolation operations or matching time steps. With our method, time steps are asynchronous through the whole simulation and no global time barriers are needed. In addition, we present an efficient method for parallelization of our novel asynchronous time integration.