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Invited Speaker

Visual Interactive Analysis of Molecular Dynamics

Mathieu Linares

Abstract

Today, classical force field Molecular Dynamics (MD) simulations are routinely carried out in full atomistic detail for systems involving several million atoms over time scales ranging into the microsecond region and it has become an indispensable tool in the field of materials and life sciences. Those simulations are generating a wealth of data that has to be analyzed, which is currently done with a multitude of decoupled tools for visualizing trajectories and extracting statistical data making an interactive exploration infeasible. Events of interest however are hidden in long time series and complex geometric structures. Therefore an interactive exploration is fundamental for exploring the data and understanding the key geometrical parameters at play. For the last two years we have developed a visual environment for exploration of the simulated molecules and their descriptive properties. The environment is built on tight integration of statistics, plots and visualization of the molecules. This enables global overview as well as in-detail inspection of selected events and features. The environment includes spatial, temporal and property-distribution windows, which are linked together to facilitate effective data filtering. The software developed also includes a multi-selection scheme for complex molecular structures and a tool for spatio-temporal aggregation of distribution for selected structures. In this talk, I will illustrate how this tool has been used to explore interactively dataset connected to both material and life sciences, as for instance with the case of a biomarker used to detect amyloid fibril misfold related to Alzheimer's disease.

Short Biography

Mathieu Linares obtained his PhD in Theoretical Chemistry at the Paul Cézanne University (Marseilles, France) in 2005, where he developed a valence bond method under the supervision of Prof. S. Humbel. In 2006, he joined the Laboratory for Chemistry of Novel Materials in Mons (Belgium) for a post-doctoral stay where he worked on the modeling of self-assembly in solution and at surfaces. He then worked as postdoctoral researcher in the Computational Physics group at Linköping University (Linköping, Sweden) with Prof. S. Stafström (2008-2009) and in the group of Theoretical Chemistry at the Royal Institute of Technology (Stockholm, Sweden) with Prof. Hans Ågren (2010). He currently hold an associate Professor position shared between the laboratory of organic electronics and the group of scientific visualization at Linköping University (Linköping, Sweden). His main research interests are chirality, self-assembly in solution and on surface, charge transport in organic materials, and molecular visualization.

Invited Speaker

Molecular Visualization in Virtual Reality: Challenges and Opportunities

Pere-Pau Vázquez

Abstract

Molecular visualization is a mature field that has seen continuous growth in the last years. As technology improves, we are able to visually inspect larger and more complex systems. However, there is still a limitation on how much information we can display in a single desktop screen, or the interaction that can be achieved with mouse and keyboard. As a result, in many laboratories, researchers are experimenting with large resolution screens and Virtual Reality setups. In this talk, some of those developments will be analyzed, and point to some of the challenges that are still to be solved, such as data visualization, accurate selection and interaction, or collaboration. Since immersive analytics is becoming a reality, molecular visualization researchers are in a sweet spot to lead the transition of scientific visualization into 3D environments and tools.

Short Biography

Pere-Pau Vázquez is an associate Professor of Computer Science at ViRVIG group, Universitat Politècnica de Catalunya (UPC). Before joining the UPC in 2002, he had been working for four years at Universitat de Girona, where he completed his Ph.D. His interests are the application of Information Theory tools to computer graphics and visualization, and the wide variety of GPU-based techniques for scientific visualization as well as mobile rendering. He also has an interest in virtual reality and 3D interaction.