# Visual Computing Forum

http://vis.UiB.no/vcf/

## VCF Seminar with two talks

**Friday, 19th of October, from 15:15**
Thormøhlens gate 55, Stort auditorium,
(Høyteknologisenteret, second floor, rom 209M3)

# Visualization of large molecular trajectories

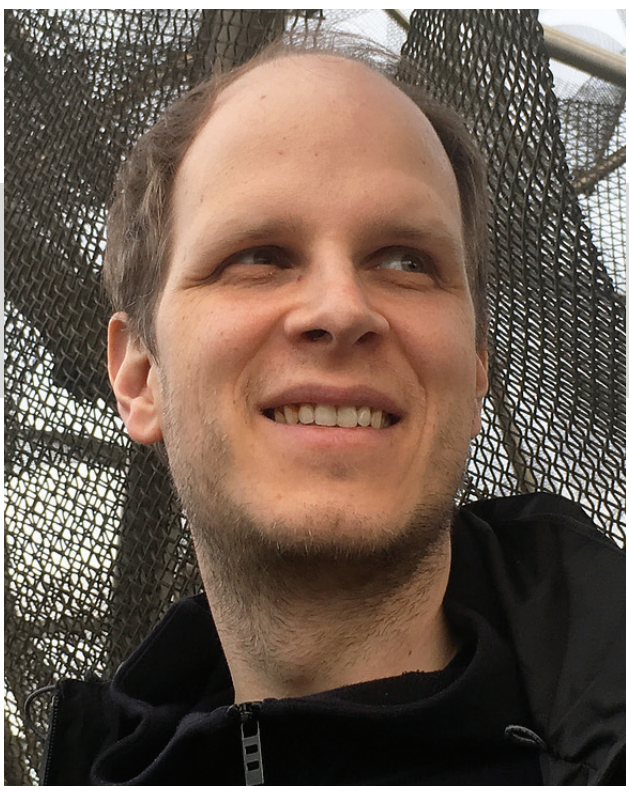

## Pere-Pau Vázquez

Associate Professor @ Universitat Politècnica de Catalunya in Barcelona



**Abstract**

The analysis of protein-ligand interactions is a time-intensive task. Researchers have to analyze multiple physico-chemical properties of the protein at once and combine them to derive conclusions about the protein-ligand interplay. Typically, several charts are inspected, and 3D animations can be played side-by-side to obtain a deeper understanding of the data. With the advances in simulation techniques, larger and larger datasets are available, with up to hundreds of thousands of steps. Unfortunately, such large trajectories are very difficult to investigate with traditional approaches. Therefore, the need for special tools that facilitate inspection of these large trajectories becomes substantial. In this paper, we present a novel system for visual exploration of very large trajectories in an interactive and user-friendly way. Several visualization motifs are automatically derived from the data to give the user the information about interactions between protein and ligand. Our system offers specialized widgets to ease and accelerate data inspection and navigation to interesting parts of the simulation. The system is suitable also for simulations where multiple ligands are involved. We have tested the usefulness of our tool on a set of datasets obtained from protein engineers, and we describe the expert feedback.

# Let's make computer graphics great again!


## Daniel Sýkora

Associate Professor
@ Czech Technical University in Prague



**Abstract**

Back in 1995, Ed Catmull and others launched a new era of computer-generated animated movies that quickly became mainstream and almost entirely replaced traditional hand-drawn animation. After more than two decades of constant development, algorithms and tools used in the creation process became mature and nowadays, the audience enjoys perfectly polished 3D visuals containing photo-realistic lighting effects and physically accurate simulations. One can assume this as a great success of computer graphics. However, the key users of CG, i.e., the artists, started to observe that the visual style they continue producing is becoming a bit predictable and that they foresee an issue in the future as the audience eagerly seeks for fresh new visual experiences. They noted that an essential feature which is missing in current computer-generated production is the uniqueness of visual style. Although creative freedom and expressiveness were typical for traditional animation, these desirable characteristics almost disappeared with the transition to 3D computer graphics. In theory, the artists still have full freedom and may create artwork without any limitations, however, in 3D this becomes hugely labor intensive and prohibitively expensive. This fact opens up a grand challenge for computer graphics researcher: is it possible to preserve unique artistic style while keeping the production time and cost-effective?