Motivation and Problem Definition:
Through the constantly improving hardware and ever-increasing computing power, molecular dynamics (MD-)simulations are more easily available, they consist of thousands of individual simulation frames, and are getting much more detailed. The calculation of such simulations is no longer limited by algorithms or hardware, nevertheless it is still not possible to efficiently explore this huge amount of simulation data, as animated 3D visualization, with ordinary visualization tools.

Contribution:
The aim of this thesis is a novel CAVER Analyst [1] extension for exploring MD-simulations in real-time. We designed a focus & context approach that guides the user to the most relevant temporal and spatial events. Since the very beginning, this work was developed in close collaboration with international universities, such as Masaryk University, Czech Republic, and the University of Bergen, Norway, together with biochemists from the Loschmidt Laboratories in Brno, Czech Republic.