FAKULTÄT FÜR !NFORMATIK
Faculty of Informatics

Diplomarbeitspräsentation

Importance-Driven Exploration of Molecular Dynamics Simulations

Masterstudium:
Visual Computing

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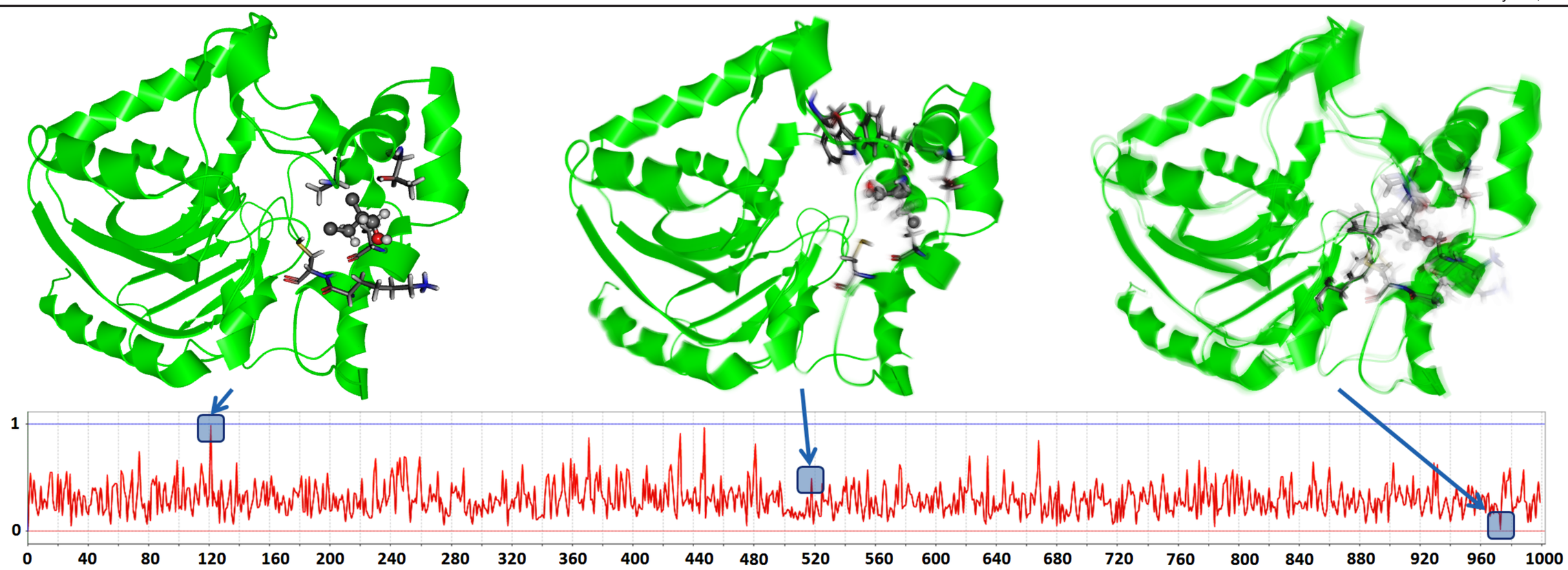


Motivation and Problem Definition:

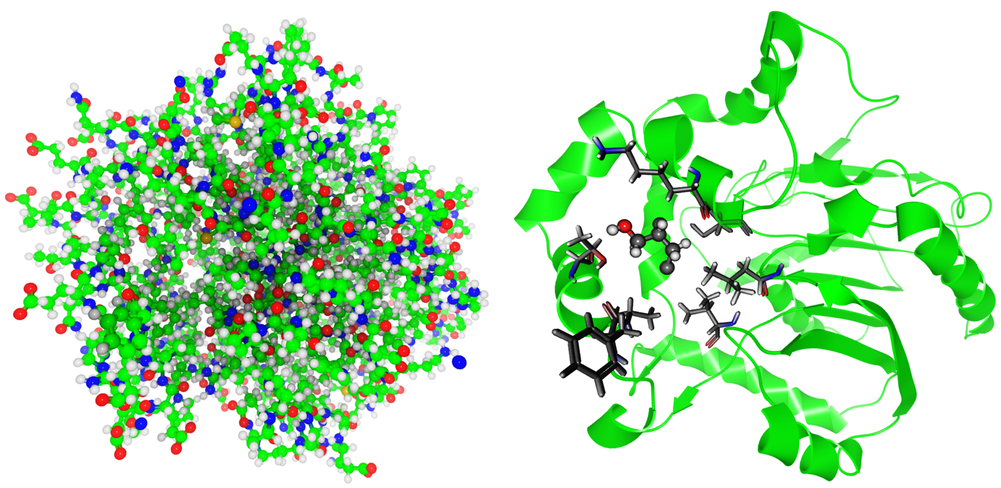
Through the constantly improving hardware and ever-increasing computing power, **molecular dynamics (MD-)simulations** are more easily available, they consist of thousands of individual simulation frames, and are getting much more detailed. The calculation of such simulations is no longer limited by 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:

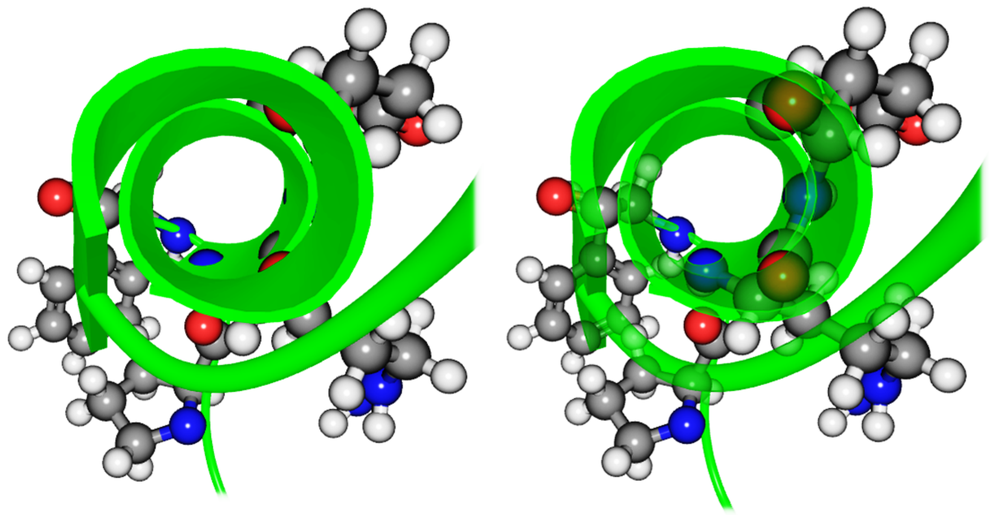
The aim of this thesis is a novel **CAVER Analyst** [1] extension for exploring MD-simulations in real-time. We designed a **focus & context approach** that guides the user to the most relevant **temporal** and **spatial events**. Since the very beginning, this work was developed in close collaboration 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.

Spatial Importance

Spatial importance through different **levels of detail** for both, focus and context elements depending on the research task.

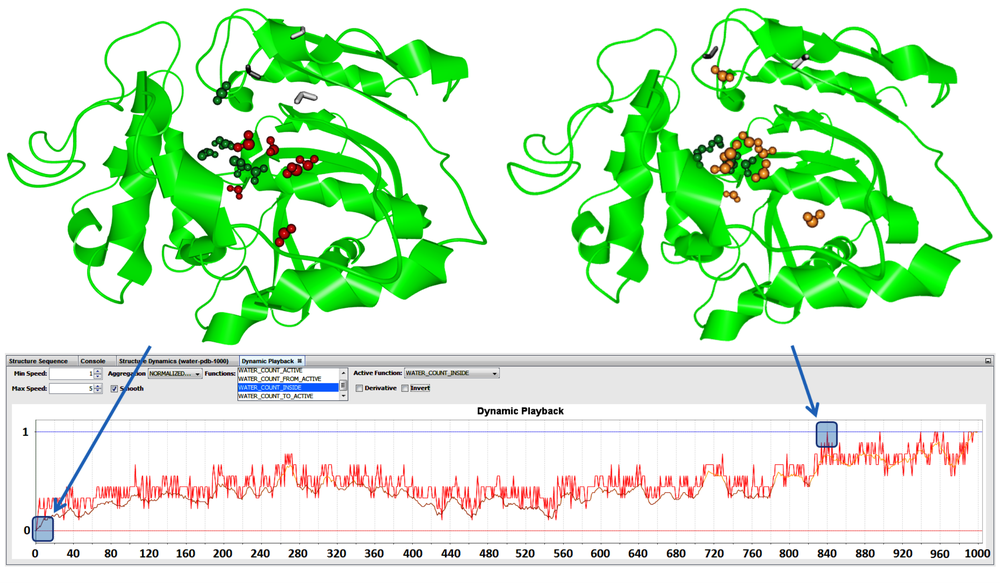


Importance driven visibility management using a **ghosting procedure**, to prevent occlusions from focus elements.

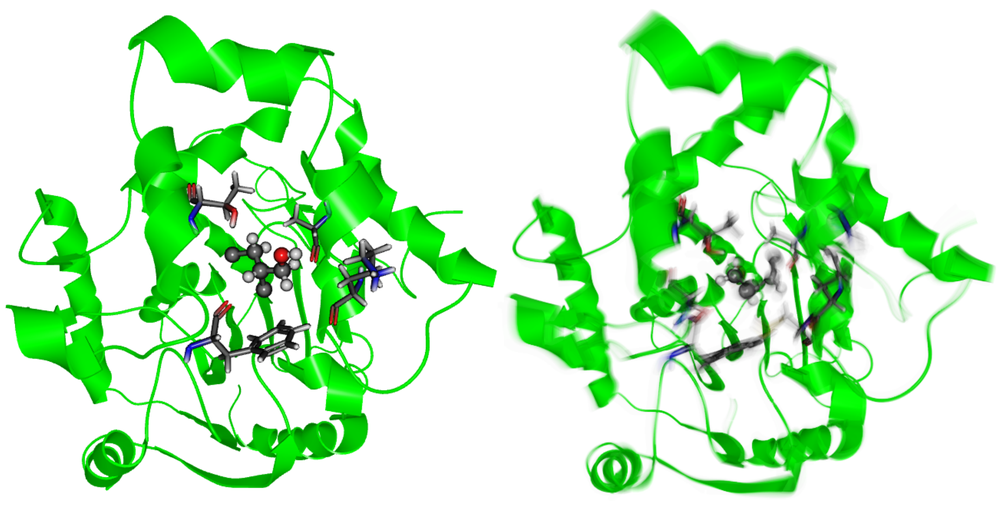


Temporal Importance

Temporal importance through **adaptive fast-forward** depending on single or a combination of multiple 2D importance functions.



Visual declutter of accumulated frames through **motion blur**, which additionally illustrates the playback speed-up.



[1] Kozlíková, B., Šebestová, E., Šustr, V., Brezovský, J., Strnad, O., Daniel, L., Bednář, D., Pavelka, A., Maňák, M., Bezděka, M., Beneš, P., Kotry, M., Gora, A. W., Damborský, J., and Sochor, J.: **CAVER Analyst 1.0: Graphic tool for interactive visualization and analysis of tunnels and channels in protein structures**, Bioinformatics, 30(18), 2014.

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