Visualization of Large Molecular Trajectories

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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.

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