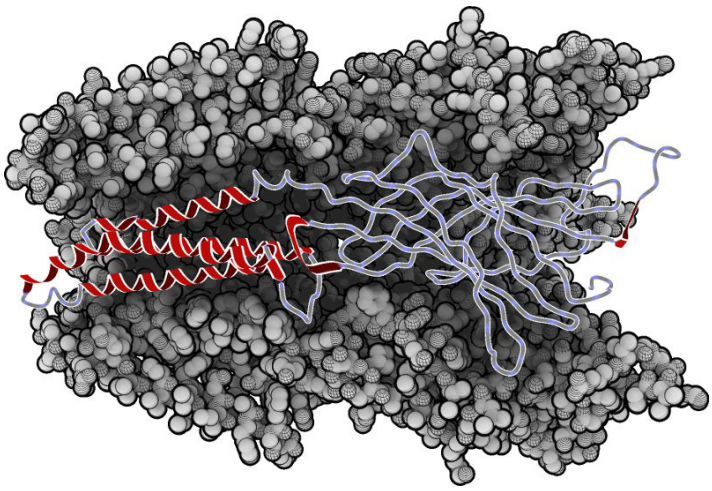
PhD Project Proposal:

Illustrative Molecular Abstraction & Visualization



The comprehension of structural properties of complex molecules is of utmost importance in many scientific areas including (bio-)chemistry, genetics, pharmaceutics, or material science. For the development of drugs against AIDS or cancer, for example, it is essential to understand how molecules in the human body interact with externally introduced chemicals. An understanding of these complex interactions is no longer possible through the analysis of statistical molecular properties alone; instead it is essential to ***visualize*** molecular data so that the depicted structure and non-spatial parameters reveal the interactions' functional nature.

Past research on molecular visualization has produced specialized tools to depict the 3D nature of molecular structures which have been proven beneficial to researchers. Yet, novel approaches for integrating a ***variety of representations and data types*** are urgently required as the scientific data collection process in the affected sciences progresses. To make a significant progress in the field the grand challenge is, however, to find approaches for ***visualizing large-scale molecular structures at different abstraction levels*** and ***depicting complex molecular interactions*** to allow the scientific process in the affected sciences to progress.

This PhD project will significantly advance the state-of-the-art in molecular visualization to offer sophisticated visualization algorithms and models. Specifically, the PhD student will focus on developing novel structural abstraction algorithms, embedded parameter visualization, and depictions of molecule interactions. ***Visual abstraction algorithms*** allow individual and integrated depiction of 3D molecular structures on different levels of scale. Molecular visualization has a number of domain-specific abstraction prerequisites, preventing typical focus+context or zoomable-user-interface techniques from being applied and requiring the development of dedicated structural and visual abstraction algorithms. ***Embedded parameter visualization*** methods support the depiction of physical properties of molecular information within different levels of structural abstraction. Finally, the ***depiction of molecular interactions*** such as those of proteins with water is essential to comprehend molecular behavior.

Specifically, the PhD student will investigate structural abstraction algorithms within the context of ***illustrative visualization***, a newly emerging domain within scientific visualization that takes inspiration from traditional illustration. The development of dedicated illustrative visualization techniques for molecular data is particularly appropriate because no `photorealistic' way exists to depict molecules due to their physical size. Consequently, illustrators have developed several---now

traditional---forms of illustration for molecular data. For instance, illustrators often employ several levels of straightforward abstraction such as space-filling, balls-and-sticks, licorice, and backbone models. Further ***structural abstraction*** leads to the molecule being represented as ribbons, sheets, helices, and cylinders. The project aims to develop illustrative techniques for higher-level abstractions such as coarse-grained simulations to visualize very large molecular systems. Moreover, the goal is to develop methods that permit the visualization of interactions between large molecules and between molecules and solvents. Finally, the PhD student will study the depiction of physical properties such as force fields and/or electrostatics to facilitate the understanding of strong contextual and functional relationships.

The PhD research will be conducted under the supervision of Tobias Isenberg and within the AVIZ research team at INRIA Saclay—Île-de-France which concentrates on the visualization of complex data. AVIZ is one of the most respected research labs in information visualization and visual analytics worldwide. The PhD student will closely collaborate, in particular, with Julie Bernauer from the AMIB research team, also at INRIA Saclay—Île-de-France, as the domain expert with expertise n coarse-grained models for 3D interaction prediction and especially macromolecule docking.

In summary, with the development of dedicated abstraction models/algorithms in combination with embedded contextual parameter visualization and the depiction of molecular interactions this PhD project will advance the state-of-the-art in molecular visualization and offer powerful instruments for the scientific molecular data analysis process.

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