Visual Computing Forum

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

An update on seeing and touching molecules in motion through interactive molecular graphics

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Abstract

For several years now, our team pursues the goal to study complex molecular assemblies through interactive visualization, manipulation and analysis approaches to aid hypothesis generation and exploration of complex datasets. The UnityMol framework forms a central tool for these investigations and is based on the Unity3D game engine. A first line of research tries to help with the 3D context, for instance through content-guided navigation, exploded views and semantic links between molecular objects and their analysis data . Concerning the molecular representations, we extended the UnityMol repertoire to include specific visualizations for sugar molecules and are now including coarse-grained systems by default. These are particularly apt for interactive simulations, even in the classroom or via crowdsourcing. A particular focus lies on the integration of dedicated hardware such as large, high-resolution display walls, or more recently head-mounted virtual reality headsets or augmented reality setups.