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Immersive Analytics for Molecular Dynamics Simulations

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Abstract

*In order to gain insights into structural and dynamic properties of biomolecules, molecular dynamics (MD) simulations are commonly employed [AM06, HOvG02, KM02]. To reach biologically relevant timescales, a tremendous amount of data can be generated due to computational and methodological developments.These MD simulation data are hard to interpret and analyse [DP14]. Analysis routines include clustering of structures, identification of interesting events, data aggregation, comparison of simulation runs and much more. Thus, a typical workflow is rather complex and a lot of different tools were developed to analyse MD simulation data, for example, analysis tools in GROMACS [AMS*15], with Python packages [MADWB11, MBH*15] or VMD plugins [HDS96]. These different tools enable the user to perform specific steps in the analysis, but support of a full analysis workflow is still difficult. An important step in MD simulation analysis is 3D visualisation, as spatial information of biomolecular structures is important [KSES12] and the representation of biomolecules in 3D virtual reality environments facilitates understanding of molecular structures and their interaction [dCN17]. In addition, visualising complex data in an immersive environment with head mounted displays helps users to perform tasks faster and less error-prone. Virtual reality and augmented reality environments, sensor devices or large touch surfaces are used as technologies in the field of immersive analytics (IA). The main research focus of IA is to investigate how new multi-sensory interfaces, interaction and display technologies can be used to facilitate analytical reasoning and decision making. IA aims to aid the user in workflows for detailed data analysis of big and complex data sets by not only supporting visualisation, but also integrating automated analysis with immersive environments to support a full analysis workflow [MSD*18, DMI*18]. Even though first attempts to build up an immersive environment for MD simulation data analysis were made [SKVS10, LTDS*13, BDF*14], various research challenges are still left. Some of these challenges include: 1) Integration of existing interfaces and tools, 2) Aggregation of temporal and structural data, 3) Intuitive and natural interaction with MD simulation data, 4) Development of novel visualisations and metaphors to benefit from three dimension. This poster summarises related challenges and presents a metaphor on MD simulation data visualisation (see Fig. 1) as a first step towards an immersive environment with the support of a full analysis workflow to enable fast and efficient data analysis.*

CCS Concepts

• ***Human-centered computing*** → ***Visualization design and evaluation methods; Visualization design and evaluation methods;*** • ***Applied computing*** → ***Bioinformatics;***

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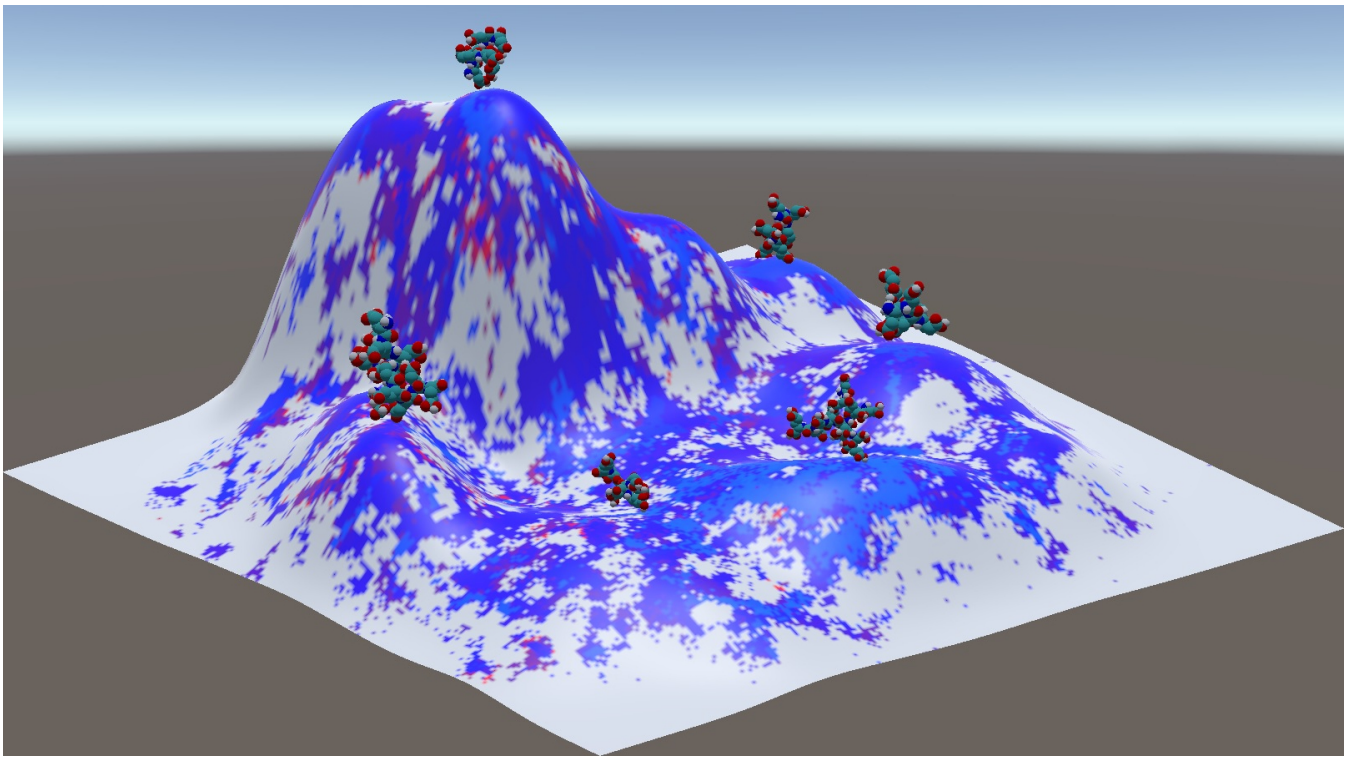

Figure 1: *Multi-dimensional scaling of a MD Simulation represented as landscape in virtual reality.*

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