(R)evolution(s) in Molecular Modeling: What Lies Ahead?

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Molecular modeling and simulations are currently undergoing a remarkable transformation, driven by groundbreaking advances in computing power, data sharing, artificial intelligence (AI), and advanced visualization and data analytics techniques. The advent of GPU computing and the arrival of exascale machines have dramatically expanded the realm of feasible simulations, shattering previously insurmountable barriers. In biological applications, tools such as AlphaFold have revolutionized this domain, enabling significant leaps forward. However, our discipline has yet to fully embrace and integrate such emerging technologies, presenting both challenges and opportunities for growth.

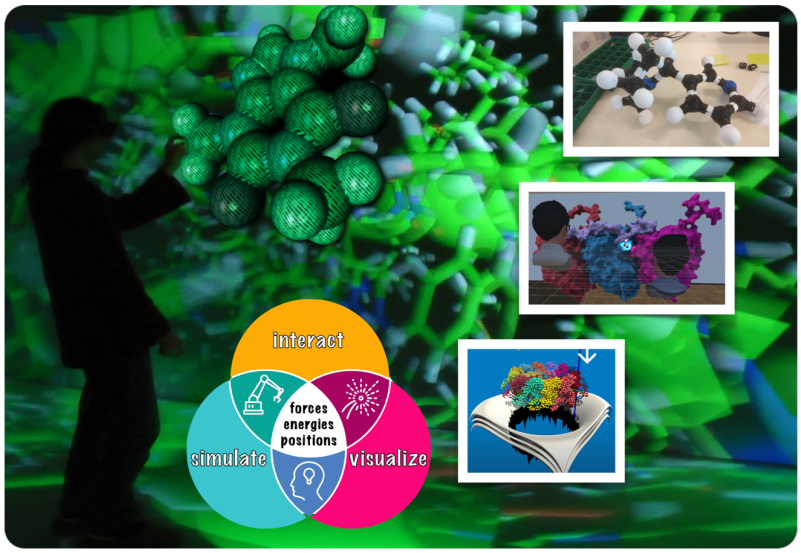

Figure 1. Emerging technologies for molecular modeling: advanced immersive visualization techniques for enhanced spatial perception of molecular structures; interactive simulations that enable real-time exploration and manipulation of molecular dynamics; collaborative virtual environments that facilitate seamless remote scientific collaboration; tangible smart molecular objects that combine 3D-printed physical models with digital data and interactive features.

This contribution will explore selected topics, including the transition to exascale simulations, the data-driven era in science, the ubiquitous integration of AI into our workflows, and the potential for adopting and leveraging new technologies within our field. Novel opportunities for global scientific collaboration, interactive simulations, virtual reality, visual analytics, and the incorporation of 3D-printed objects for molecular modeling and analysis tasks will be discussed.

Through this exploration, I aim to shed light on the transformative developments reshaping molecular modeling and simulation, offering insights into the exciting possibilities that lie ahead as we harness the power of cutting-edge technologies and collaborative efforts.

Keywords: exascale, artificial intelligence, virtual reality, interactive simulations, data.