**From Fundamentals, Innovations, to Challenges Ahead: An Overview of Enhanced Sampling Methods in Molecular Dynamics**

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With the fast advent and increasing availability of high-performance computing over the years, molecular dynamics (MD) simulations have become increasingly useful for elucidating the complex interactions and dynamics within a wide range of molecular systems, ranging from biomolecules to advanced materials. However, the usefulness of MD simulations hinges on sufficiently sampling all relevant metastable states of the system, a task that often poses significant challenges to conventional MD. Aiming the address these challenges, various enhanced sampling methods have been developed over the past decades and shown essential for studying molecular events with time scales beyond the reach of conventional methods. These methods enable much more efficient exploration of configurational space compared to direct sampling, facilitating the extraction of insights into the thermodynamic and structural properties of the system of interest, such as the solvation free energy of a molecule, or the binding ensemble of a binding complex. Starting with the introduction of the most popular enhanced sampling methods in molecular dynamics, such as umbrella sampling, metadynamics, and replica exchange, this presentation highlights the diverse strategies adopted by different methods for navigating the system between different metastable states in a simulation. Subsequently, the presentation delves into the latest innovations in enhanced sampling methods, especially in the wake of machine learning. Lastly, the presentation will conclude by discussing forthcoming challenges in the development and improvement of enhanced sampling methods.