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Accuracy and Precision in Atomistic Molecular Dynamics Simulations

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Abstract

Proteins are dynamic entities that can undergo large conformational changes critical to their biological function. While existing experimental methods can capture snapshots of a protein structure with atomic resolution, the detailed characterization of protein dynamics with full atomic resolution remains a difficult task. Atomistic molecular dynamics simulations are ideally suited for these types of studies; however, as is the case for experimental techniques, limitations in accuracy and precision can restrict their range of applicability. Here I will describe how accuracy and precision can be defined in the context of atomistic simulations, and I will discuss some of the ways in which these quantities are impacted by the use of approximate physical models and limited sampling.