

An Innovative Approach for Watching Dynamic Conformational Changes in Proteins at Ultrafast and Atomistic Levels

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Addressing the temporal and spatial resolution discrepancies between experimental high-speed atomic force microscopy (HS-AFM) data and simulation data necessitates a comprehensive strategy. This strategy employs advanced computational methods such as novel molecular dynamics (MD) and coarse-grained (CG) models, as well as artificial intelligence (AI) techniques. The primary challenge in studying "Protein Dynamics" in real time is bridging the time scale gap: HS-AFM captures dynamics in the millisecond to second range, while simulations typically operate from femtoseconds to microseconds. Additionally, simulations face spatial modeling constraints, limiting the study of large, complex biological systems. HS-AFM, however, allows for the construction of detailed protein models, enabling high temporal imaging of their structures and dynamics during functional activity.

We are developing an innovative method called Simulation Artificial Intelligence-Atomic Force Microscopy (SAI-AFM) to visualize dynamic structural changes in proteins at ultrafast and atomistic levels. This novel workflow integrates multiscale computational models (MDs and CGs) with AI-driven analysis and HS-AFM data across multiple timescales and spaces. The advanced SAI-AFM technology allows for concurrent observation of protein structures, dynamics, and functions at the ultrafast and atomistic levels, surpassing individual methods.

Our goals include:

1. Creating a library of experimental PDBs, including saiPDBs, that accurately reflect the atomic structures of protein dynamics in real time, bridging the time and space gaps between individual methods.
2. Applying SAI-AFM to uncover dynamic conformational changes in alpha actinin at super-high spatiotemporal resolutions.

Keywords: High speed atomic force microscopy, SAI-AFM, alpha actinin, actin