BIOMATERIALS

Forces in Biomolecular Systems SFB 863

Protein folding and conformational dynamics by molecular simulations

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Abstract:

All-atom molecular dynamics simulations provide a vehicle for capturing the structures, motions, and interactions of biological macromolecules in full atomic detail. Such simulations have, however, been limited both in the timescales they could access and in the accuracy of computational models used in the simulations. I will begin by presenting briefly how progress has been made in both of these areas so that it is now possible to access the millisecond timescale, and how we have been able to parameterize relatively accurate energy functions. I will then present results that highlight how such long-timescale simulations have been used to provide insight in to the process of protein folding.

Once folded, proteins display dynamical motions and their ability to adopt alternative conformations is often central to their biological function. I will present work on several proteins showing how simulations, either based purely on force fields or by integrating simulations with NMR data, can be used to provide detailed information on the conformational dynamics in folded proteins. In particular, our results show that modern simulation methods may be able to provide detailed, accurate models of slow conformational changes that underlie protein functions such as ligand binding on enzyme turnover.

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