Hydrodynamic effects in proteins

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Water constitutes a natural environment for the protein molecules: it stabilizes their native structures, influences their enzymatic activity and is critical in phenomena such as molecular recognition and protein-protein interactions. However, the impact of larger-scale, hydrodynamic processes on protein dynamics is considered less frequently, even though strong fluid flows may unfold the protein molecule as effectively as the mechanical force in the AFM experiment.

Here we report the results of a numerical study of flow-induced effects in proteins using a coarse-grained model of a protein, constructed based on the knowledge of its native state. As it turns out, the proteins in the flow show a surprisingly rich dynamical behavior, as a result of an interplay between the hydrodynamic forces and direct molecular forces. Unfolding of proteins induced by a flow usually involves a larger number of intermediate states than the force-induced unfolding (as in the AFM force clamp), since flow induces highly non-uniform tension along the protein, probing different bond groups with different intensities. These features offer potentially wider diagnostic tools to investigate structure of proteins compared to experiments based on the atomic force microscopy. Understanding of the behavior of proteins in the flow is crucial not only for the development of new tools for probing the conformational landscape of proteins, but also for understanding of many *in vivo* processes, such as hemostasis or ion channel activation. The presence of the solvent must also be taken into account to correctly predict the force and time scales of conformational changes of protein structure: we show that the hydrodynamic interactions between different segments of a protein reduce the peak force when stretching the protein at constant speed, especially at larger speeds. Hydrodynamic interactions are also shown to facilitate unfolding at a constant force and inhibit stretching by fluid flows.

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