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Protein slaving to the solvent and the relation to hydrodynamics P. W. FENIMORE, GUO CHEN, B. H. MCMAHON, Los Alamos National Lab — Protein motions can be categorized by the nature of their coupling to solvent dynamics. Some protein motions, including the final ligand binding process in myoglobin (Mb), are largely independent of solvent fluctuations. Others, such as entry and exit of ligands from Mb require Debye-like α fluctuations in the solvent to proceed. A third class of motions, including the r. m. s. displacments of atoms are controlled by solvent β fluctuations. We show that a slaving picture of protein dynamics, $k_{\rm protein} = k_\alpha/n$, where n is a nearly T-independent factor, known to be as large as 10^5, is consistent with an essentially hydrodynamic picture of α-slaved protein motions. Consistency with hydrodynamics (i. e. the Stokes-Einstein equation) can be demonstrated by considering changes to protein stability caused by ordinary experimental protocols for measuring viscosity- and T-dependent protein dynamics data. The decomposition of protein dynamics into several discrete classes suggests modelling techniques to simplify the simulation of protein dynamics.

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