Abstract Submitted
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**A theory for protein dynamics: Global anisotropy and a normal mode approach to local complexity**[1] JEREMY COPPERMAN, PABLO ROMANO, MARINA GUENZA, Univ of Oregon — We propose a novel Langevin equation description for the dynamics of biological macromolecules by projecting the solvent and all atomic degrees of freedom onto a set of coarse-grained sites at the single residue level. We utilize a multi-scale approach where molecular dynamic simulations are performed to obtain equilibrium structural correlations input to a modified Rouse-Zimm description which can be solved analytically. The normal mode solution provides a minimal basis set to account for important properties of biological polymers such as the anisotropic global structure, and internal motion on a complex free-energy surface. This multi-scale modeling method predicts the dynamics of both global rotational diffusion and constrained internal motion from the picosecond to the nanosecond regime, and is quantitative when compared to both simulation trajectory and NMR relaxation times. Utilizing non-equilibrium sampling techniques and an explicit treatment of the free-energy barriers in the mode coordinates, the model is extended to include biologically important fluctuations in the microsecond regime, such as bubble and fork formation in nucleic acids, and protein domain motion.

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