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A Study of Internal Friction in Proteins Using a Diffusive, Langevin Formalism[1] ERIC BEYERLE, MARINA GUENZA, University of Oregon — Although internal friction in polymers has been studied since the 1940s, a molecular-level explanation of the phenomenon remains elusive. Proteins, biological heteropolymers, are important testing grounds for theories describing internal friction due to its relevance in biologically significant events such as protein folding. We are studying internal friction using a diffusive, Langevin formalism developed in the Guenza lab, the Langevin Equation for Protein Dynamics (LE4PD), which includes site-specific friction coefficients and hydrodynamic interactions between amino acid residues in its description of protein dynamics. Using the protein ubiquitin as a model system, we have performed molecular dynamics simulations in explicit water to test our theoretical predictions. Preliminary results of our study show an internal viscosity with a contribution dependent on the solvent viscosity and a contribution independent of the solvent viscosity.

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