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The ugly truth of enzyme dynamics: coupled chaos and biological function

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One of the most remarkable findings in the field of protein dynamics has been the discovery that functionally important regions of proteins have evolved to be flexible, yet how such dynamics relate to function still remains obscure at best. Specifically, dynamic movements on the micro-millisecond timescale, otherwise referred to as conformational exchange, are thought to be especially important for enzymes that rely on conformational changes for catalysis. The widely accepted paradigm is that an inherent conformational exchange comprises a highly concerted process that is “fine-tuned” to match the catalytic function. However, our studies on multiple enzymes as well as multiple members within an enzyme family suggest that dynamics may instead be a collection of partially coupled dynamic segments tied to the active site. Our lab has even altered dynamic segments distal to an enzyme active site leading to modulated function, providing a proof-of-principle that dynamic segments may be engineered to modify protein function.