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Simulation of signal transduction in model multiprotein systems

JULIUS SU, Caltech — To simulate the dynamics of multiprotein machines, I have developed a method called multiconformer Brownian dynamics (mcBD). In this method, proteins rotate and translate via Brownian motion while their conformations are varied among a prestored set of structures on a simplified energy landscape, taking into account inter-protein interactions. As an example, I build a simple model of a G-protein coupled receptor/G-protein complex, and show that ligand binding causes conformational shifts, which induce GDP to leave, GTP to bind, and the complex to dissociate. The two proteins couple their fast fluctuations together into large-scale coordinated functional motions, resulting in signal transduction. I vary the shapes, electrostatics, and energy landscapes of the proteins independently and examine the impact this has on the system's function. In one result, increasing the binding between proteins improves the fidelity of communication, but at the expense of overall switching frequency.

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