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Fluctuation-allosteric regulation of protein function: Continuum elastic model and its geometrical implications MICHAEL S. DIMITRIYEV, PAUL M. GOLDBART, Georgia Institute of Technology, T.C.B. MCLEISH, Durham University — In many proteins, function is strongly modified by the binding of some small ligand to the protein surface. We address the issue of *fluctuation* allostery, in which thermal motion of the protein medium far from the binding site is a key factor in determining the activity of the protein (i.e., the strength with which it functions). We develop a simple, coarse-grained model in which the protein is viewed as a homogeneous, isotropic, elastic continuum of specified shape, and the binding of the ligand is regarded as a small alteration of this shape. We construct a perturbative approach to the response of the thermal fluctuations to a shape-alteration as a diagnostic of the impact on protein activity that ligand binding causes. At leading order in the size of the ligand, we show how this response is determined via familiar geometrical properties of the ligand shape. Thus, we find that there are "sweet spots" for ligand binding—determined by the overall shape of the protein and location of its active site—for which the effects of ligand binding are qualitatively enhanced. To simplify the analysis whilst retaining the essential geometrical ideas, we present results for the case of a scalar field rather than the true vector displacement field of elasticity.

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