Abstract Submitted for the MAR14 Meeting of The American Physical Society

Continuum model of non-conformational allosteric regulation MICHAEL S. DIMITRIYEV, PAUL M. GOLDBART, Georgia Institute of Technology, T.C.B. MCLEISH, Durham University — Allosteric regulation of proteins, in which the activity of one binding site on a protein is modified by the binding of a small ligand elsewhere on the protein, is traditionally understood as the result of conformational changes. It is now known that allostery is not always conformational: it may be attributed to an alteration of the thermal motion of the protein about an unchanged mean shape. We present a simple model in which the addition of a small ligand alters the thermal fluctuations about the equilibrium configuration of a continuum linear elastic caricature of a protein, and the attached ligand is treated as a small, localized shape perturbation. To determine the change in fluctuations, we develop a perturbation expansion for the change in the elastic fluctuation correlator due to the shape perturbation. We apply this scheme to a simple binding model, and calculate the change in binding energy due to the presence of a ligand.

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Date submitted: 15 Nov 2013

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