

Abstract Submitted
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Calibrating elastic parameters from molecular dynamics simulations of capsid proteins¹ STEPHEN HICKS, CHRISTOPHER HENLEY, Cornell University — Virus capsids are modeled with elastic network models in which a handful of parameters determine transitions in assembly [1] and morphology [2]. We introduce an approach to compute these parameters from the microscopic structure of the proteins involved. We consider each protein as one or a few rigid bodies with very general interactions, which we parameterize by fitting the simulated equilibrium fluctuations (relative translations and rotations) of a pair of proteins (or fragments) to a 6-dimensional Gaussian. We can then compose these generalized springs into the global capsid structure to determine the continuum elastic parameters. We demonstrate our approach on HIV capsid protein and compare our results with the observed lattice structure (from cryo-EM [3] and AFM indentation studies).

[1] R. Zandi et al, PNAS 101 (2004) 15556.

[2] J. Lidmar, L. Mirny, and D. R. Nelson, PRE 68 (2003) 051910.

[3] B. K. Ganser-Pornillos et al, Cell 131 (2007) 70.

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Stephen Hicks
Cornell University

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