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Using stochastic dynamics to validate runtimes of protein simulations[1] STEPHEN D. HICKS, CHRISTOPHER L. HENLEY, Cornell University — We use short molecular dynamics simulations (∼200 cpu-hr, using NAMD) of individual bonds between capsid proteins to microscopically determine coarse-grained elastic parameters of entire virus capsids. In particular, we treat each protein (or for larger proteins, each domain) as a rigid body described by a 6-vector of translational and orientational degrees of freedom, $x_i(t)$. We then model the evolution of the relative positions as an overdamped random walk, $\dot{x}_i(t) = -\Gamma_{ij}K_{jk}(x_k(t) - \bar{x}_k) + \zeta_i(t)$, where $\zeta_i(t)$ are random variables satisfying $\langle\zeta_i(t)\zeta_j(t')\rangle = 2\Gamma_{ij}T\delta(t-t')$. Our goal is to determine the stiffness matrix K_{ij}, but this requires long-time data to measure accurately. We therefore measure the noise matrix $2\Gamma_{ij}T$, which depends on much shorter timescales, and compute the relaxation times by diagonalizing $\Gamma^{\frac{1}{2}}K\Gamma^{\frac{1}{2}}$. Although we use biologically relevant configurations in each simulation, we have taken the domains out of their full context by simulating one pair at a time, and therefore external stresses are missing, which we measure from the drift and compensate for in subsequent simulations. Finally, we apply this technique to the HIV capsid protein.

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Stephen Hicks
Cornell University

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