

493b Modeling Virus Capsid Assembly Dynamics

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The assembly of protein subunits into a virus capsid is remarkable. In many different organisms and environments, capsids avoid kinetic and thermodynamic traps to assemble rapidly and with high fidelity. Identifying the properties of capsid components that enable such robust assembly could play a critical role in the development of anti-viral strategies and drug delivery vehicles. In this work we develop a class of models with which we study the assembly of capsid-like objects without pre-assumed paths or nucleation steps. Using Brownian dynamics, we generate an ensemble of paths with which we characterize features essential for successful assembly and we also identify two forms of kinetic traps. By comparing these results to the dynamics of a Master-equation description of assembly, we shed light on some approximations that are commonly used to develop coarse-grained models of capsid assembly.