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Mechanisms of viral capsid assembly around a polymer ALEKSANDR KIVENSON, MICHAEL HAGAN, Brandeis University — We present a coarse-grained computational model inspired by the assembly of viral capsid proteins around nucleic acids or other polymers. Specifically, we simulate on a lattice the dynamical assembly of closed, hollow shells composed of several hundred to 1000 subunits, around a flexible polymer. As a function of capsid size, we determine the maximum polymer length that can be dynamically encapsidated and the polymer length around which assembly is most effective. The assembly process can often be described by three phases: nucleation, growth, and a completion phase in which any remaining polymer segments are captured. We find that the polymer can increase the rate of capsid growth by stabilizing the addition of new subunits and by enhancing the incoming flux of subunits. We determine the relative importance of these mechanisms as a function of parameter values, and make predictions for the dependencies of assembly rates and effectiveness on polymer length. These predictions can be tested with bulk experiments in which capsid proteins assemble around nucleic acids or other polymers; in addition, we will discuss how predictions for the polymer-length dependence of assembly rates during the growth phase can be tested with single molecule experiments.

Aleksandr Kivenson
Brandeis University

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