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Dynamic Models for Templated Viral Capsid Assembly

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The replication of many viruses with single-stranded genomes requires the simultaneous assembly of an ordered protein shell, or capsid, and encapsidation of the genome. In this talk, I will present coarse-grained computational and theoretical models that describe the assembly of viral capsid proteins around interior cores, such as polymers and rigid spheres. These models are motivated by two recently developed experimental model systems in which viral proteins dynamically encapsidate inorganic nanoparticles and polyelectrolytes. Model predictions suggest that some forms of cooperative interactions between subunits and cores can dramatically enhance rates and robustness of assembly, as compared to the spontaneous assembly of subunits into empty capsids. For large core-subunit interactions, subunits adsorb onto a core en masse in a disordered manner, and then undergo a cooperative rearrangement into an ordered capsid structure. These assembly pathways are unlike any seen for empty capsids formation. While model predictions suggest that cooperative interactions between disparate assembling components can overcome some limitations of spontaneous assembly, the complexity of multicomponent assembly introduces new forms of kinetic traps that can frustrate assembly, and hence introduces new limitations. These findings have implications for a mechanism in which viruses use interactions between proteins and genomic molecules to promote and control assembly, and thereby control the replication process.