Department of Mathematics

Colloquium

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Energetics and kinetic pathways of virus assembly

Abstract: Virus assembly is an intriguing biological process in which hundreds, or even thousands, of proteins come together simultaneously to create a highly symmetric nano-structure. It is particularly remarkable that the entire assembly can be completed within seconds to minutes. However, this rapidity also presents a challenge when it comes to understanding the underlying mechanisms of the capsid morphology and assembly pathways. In this talk, I employ continuum elasticity theory to show the role of capsid protein flexibility in the formation of structures with icosahedral symmetry. By solving the elasticity equations, our findings reveal that a nonspecific template, such as a non-native genome or scaffolding proteins, not only determines the capsid radius, but also leads to the error-free assembly of protein subunits, resulting in capsids with universal icosahedral order. Furthermore, using a coarse-grained model, we simulate the virus assembly pathways while taking into account the elastic energy involved in the growth of viral shells. We show that as a capsid grows, the structures of disordered intermediates in which the distribution of pentamers does not belong to the icosahedral subgroups become energetically unfavorable, leading to dissociation of the malformed shells and subsequent reassembly of perfect icosahedral shells, overcoming the involved energy barriers. The mechanism we study provide insight into the viral life cycle through the assembly of viral particles de novo and potentially identify therapeutic targets for future drug development.

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