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Stochastic modeling of virus capsid assembly pathways[1]

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Virus capsids have become a key model system for understanding self-assembly due to their high complexity, robust and efficient assembly processes, and experimental tractability. Our ability to directly examine and manipulate capsid assembly kinetics in detail nonetheless remains limited, creating a need for computer models that can infer experimentally inaccessible features of the assembly process and explore the effects of hypothetical manipulations on assembly trajectories. We have developed novel algorithms for stochastic simulation of capsid assembly [1,2] that allow us to model capsid assembly over broad parameter spaces [3]. We apply these methods to study the nature of assembly pathway control in virus capsids as well as their sensitivity to assembly conditions and possible experimental interventions.

[1] F. Jamalyaria, R. Rohlfs, and R. Schwartz. J Comp Phys 204, 100 (2005).
[2] N. Misra and R. Schwartz. J Chem Phys 129, in press (2008).
[3] B. Sweeney, T. Zhang, and R. Schwartz. Biophys J 94, 772 (2008).

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