



Large-scale particle-based simulation of human cytomegalovirus and its interaction with host cells

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Short abstract

Computational modeling enhances our understanding of biological systems by providing a bottom-up, mechanistic perspective. This approach necessitates physics-based modeling to interpret the motion, deformation, and interaction of a biological system's constituents, proving indispensable for complex systems whose emergent behaviors defy straightforward derivation from first principles. This project concentrates on the particle-based modeling of an entire virion and its interactions with living cells, specifically focusing on the Human cytomegalovirus from the herpes family. This virus assembles into an intricately complex virion particle, comprising tens of thousands of biomolecules arranged in a structured system. Deciphering the physical principles underlying this organization and its dynamic transformation during infection can inform the development of more effective antiviral drugs or vaccines. Preliminary work on constructing a particle-based virion model, built upon quantitative biological data procured collaboratively, has been completed. By leveraging high-performance computing, we aim to simulate biologically-relevant timescales of the virion's behavior and gain insights into its large-scale dynamics.