APS March Meeting 2020

Volume 65, Number 1

Monday–Friday, March 2–6, 2020; Denver, Colorado

Session S45: Computational Methods for Statistical Mechanics: Advances and Applications II
11:15 AM–2:03 PM, Thursday, March 5, 2020
Room: 706

Sponsoring Units: DCOMP GSNP
Chair: Nathan Clisby, Swinburne Univ of Tech

Abstract: S45.00010 : Quantifying the disassembly of viral capsids from a multiscale molecular simulation approach*

← *Abstract* →

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Molecular simulation of large biological systems, such as viral capsids, remains a challenging task in soft matter research. On one hand, coarse-grained (CG) models attempt to make feasible the description of the entire viral capsids. On the other hand, novel development of molecular dynamics (MD) simulation approaches, like enhance sampling which attempt to overcome the time scales required in biophysics. Those methods have a potential for delivering molecular structures and properties of biological systems. Nonetheless, exploring the process on how a capsid disassembles by all-atom MD simulations has been rarely attempted. Here, we propose a methodology to analyze the disassembly process of viral capsids quantitatively. In particular, we look at the effect of *pH* and charge of the genetic material inside the capsid, and compute the free energy of a disassembly trajectory by combining CG simulatiosn to a Poisson-Boltzmann solver. We employ such multiscale approach on the triatoma virus as a test case, and find that even though an alkaline environment enhances the stability of the capsid, the resulting deprotonation of the internal solvent generates an electrostatic repulsion that triggers disassembly

*This research has been supported by the Slovenian Research Agency P1-0055

1:27PM S45.00010: Quantifying the disassembly of viral capsids from a multiscale molecular simulation approach* HORACIO ANDRES VARGAS GUZMAN (Presenter), Soft Matter Theory Department, Institute Josef Stefan, CHRISTOPHER COOPER, Department of Mechanical Engineering, Technical University Federico Santa Maria, ADOLFO POMA, Institute of Fundamental Technological Research, Polish Academy of Sciences — Molecular simulation of large biological systems, such as viral capsids, remains a challenging task in soft matter research. On one hand, coarse-grained (CG) models attempt to make feasible the description of the entire viral capsids. On the other hand, novel development of molecular dynamics (MD) simulation approaches, like enhance sampling which attempt to overcome the time scales required in biophysics. Those methods have a potential for delivering molecular structures and properties of biological systems. Nonetheless, exploring the process on how a capsid disassembles by all-atom MD simulations has been rarely attempted. Here, we propose a methodology to analyze the disassembly process of viral capsids quantitatively. In particular, we look at the effect of *pH* and charge of the genetic material inside the capsid, and compute the free energy of a disassembly trajectory by combining CG simulatiosn to a Poisson-Boltzmann solver. We employ such multiscale approach on the triatoma virus as a test case, and find that even though an alkaline environment enhances the stability of the capsid, the resulting deprotonation of the internal solvent generates an electrostatic repulsion that triggers disassembly

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1:39PM S45.00011: Exploring the Potential of Parallel-Biasing in Flat Histogram Methods* SHANGHUI HUANG (Presenter), JONATHAN K. WHITMER, University of Notre Dame — Metadynamics, a member fo the "flat histogram" class of advanced sampling algorithms, has been widely used in molecular simulations to drive exploration of states that are separated by high free energy barriers and promote the sampling of full free energy landscapes. A recently proposed variant, paralled bias metadynamics (PBMetaD) promises to aid in exploration of free energy landscape s along multiple important collective variables by exchanging the *n*-dimensional free energy landscape required by standard methods for *n* one-dimensional marginal free energy landscapes. In this study, we systematically examine how parallel biasing affects convergence of free energy landscapes along each variable relative to standard methods, and the effectiveness of the parallel biasing strategy for addressing common bottlenecks in the use of advanced sampling to calculate free energies.

*NSF DMR-1751988