MAR17-2016-020191

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Adaptive sampling strategies with high-throughput molecular dynamics[1]

CECILIA CLEMENTI, Rice University

Despite recent significant hardware and software developments, the complete thermodynamic and kinetic characterization of large macromolecular complexes by molecular simulations still presents significant challenges. The high dimensionality of these systems and the complexity of the associated potential energy surfaces (creating multiple metastable regions connected by high free energy barriers) does not usually allow to adequately sample the relevant regions of their configurational space by means of a single, long Molecular Dynamics (MD) trajectory. Several different approaches have been proposed to tackle this sampling problem. We focus on the development of ensemble simulation strategies, where data from a large number of weakly coupled simulations are integrated to explore the configurational landscape of a complex system more efficiently. Ensemble methods are of increasing interest as the hardware roadmap is now mostly based on increasing core counts, rather than clock speeds. The main challenge in the development of an ensemble approach for efficient sampling is in the design of strategies to adaptively distribute the trajectories over the relevant regions of the systems' configurational space, without using any a priori information on the system global properties. We will discuss the definition of smart adaptive sampling approaches that can redirect computational resources towards unexplored yet relevant regions. Our approaches are based on new developments in dimensionality reduction for high dimensional dynamical systems, and optimal redistribution of resources.

[1]NSF CHE-1152344, NSF CHE-1265929, Welch Foundation C-1570