Contribution ID: **1099** Type: **Invited Speaker / Conférencier invité**

Exploring conformational switching in proteins with coarse-grained molecular simulations

Monday 13 June 2016 16:30 (30 minutes)

The traditional view holds that proteins fold into essentially unique and stable 3-dimensional structures which, in turn, determine their biological functions. Evidence is mounting, however, for a pervasive role of large-scale conformational changes for how proteins carry out their functions. Examples include the ability of some proteins to switch between entirely different folded structures, and the disorder-order transitions exhibited by so-called intrinsically disordered proteins. I will introduce a coarse-grained approach that allows the physics of such conformational switching in proteins to be studied on the computer. The approach is characterized by an intermediate level of geometric detail and a procedure for determining effective model parameters based on the properties of proteins'global free energy landscapes. I will discuss the implications of our results for the mechanisms underlying molecular recognition and the evolution of new protein folds.

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Session Classification: M3-6 Computational Biophysics: Methods and Concepts (DPMB) / Biophysique numérique : méthodes et concepts (DPMB)

Track Classification: Physics in Medicine and Biology / Physique en médecine et en biologie (DPMB-DPMB)