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Variational Molecular Dynamics

Wednesday, 11 February 2015 16:30 (20 minutes)

The Variational Molecular Dynamics (VMD) approach is a framework aimed at the efficient computation of the most probable folding pathways connecting denatured protein configurations with the native state. Its high computational efficiency enables the simulation of very slow (up to hours) transitions on large systems (hundreds of residues), with realistic atomistic force fields. The VMD approach can also be used to predict the most probable pathways for a conformational transition between given states of macromolecules. In my talk I will outline the main features of DRP and give an account of our latest results. I will first discuss the folding of a natively knotted protein. I will then talk about the conformational transition of a serpin comprised of 373 residues between its active (metastable) state and its latent state. I will also show how our method allowed us to give some explanation for the working of a pharmaceutical used in connection with the PAI-1 serpin.

Presenter: BECCARA, Silvio