Biomolecular Modeling across Spatial & Temporal Scales

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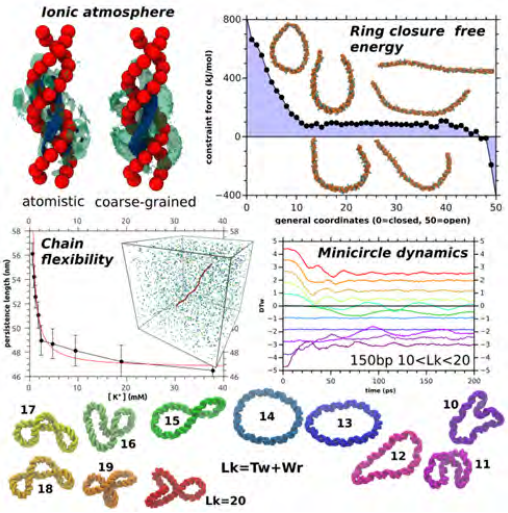
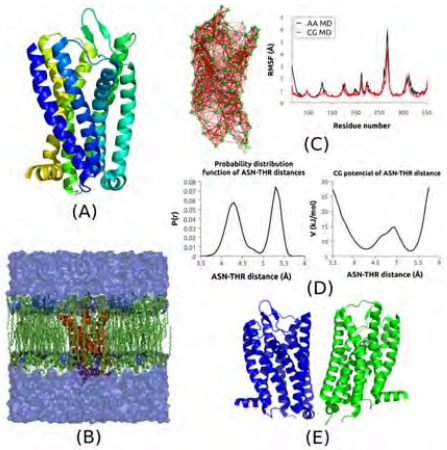
In this talk a hierarchical methodology is outlined to bridge temporal and spatial scales in computer simulations over several physical descriptions of matter: quantum mechanical, molecular mechanical and mesoscopic. It based on construction of effective pair-potentials from pair correlation functions using a technique called the Inverse Monte Carlo (IMC). Using this technique it is possible to start from first-principles simulations and compute a force field to be used in atomistic classical simulations and enlarge the system 1-2 orders of magnitude. In classical simulations it is possible to construct coarse-grained force-field using the same inverse scheme and simulate a system of soft particles beyond the atomistic resolution. In this way the whole methodology becomes a hierarchical multi-scale modeling method where information is taken from *ab initio* simulations with electrons and nuclei, carried out at desired physical conditions, to atomistic molecular mechanical level after reducing those degrees of freedom not needed in classical simulations. In doing coarse-graining from





atomistic simulations it is possible to construct solvent-mediated interaction potentials in addition to having a model for mesoscopic particles. The methodology can be used to obtain very accurate force fields not bound to any mathematical functions like what is used virtually in all common force fields today. The disadvantage is that the obtained force fields are temperature dependent, meaning they are applicable within a certain interval of temperatures and pressures. This disadvantage is less important for biological simulations which are normally carried out at physiological conditions. Several examples of applying the IMC scheme are given using different simulation methods such as MD, MC, BD and DPD.