Title: Algorithms to accelerate sampling in atomistic simulations of membrane proteins

Abstract:
A current limit of the computational strategies usually adopted to estimate the energy profiles for permeation events, is that the number of permeating ions has to be defined in advance. As consequence, it is difficult to compare energetically conduction mechanisms characterized by different number of ions. In order to overcome this limit, we developed a novel approach for the analysis of ion conduction based on bias-exchange metadynamics simulations. In bias-exchange, several replicas of the system are simulated in parallel. A metadynamics simulation is performed for each replica, along one or a few collective variable, and at fixed time intervals swaps of configurations between replicas are attempted. Using this approach it is possible to analyze by a single set of simulations the free energy for permeation events with different number of ions.