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Variationally optimal selection of slow coordinates and reaction coordinates in macromolecular systems[1]

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To efficiently simulate and generate understanding from simulations of complex macromolecular systems, the concept of slow collective coordinates or reaction coordinates is of fundamental importance. Here we will introduce variational approaches to approximate the slow coordinates and the reaction coordinates between selected end-states given MD simulations of the macromolecular system and a (possibly large) basis set of candidate coordinates. We will then discuss how to select physically intuitive order paremeters that are good surrogates of this variationally optimal result. These result can be used in order to construct Markov state models or other models of the stationary and kinetics properties, in order to parametrize low-dimensional / coarse-grained model of the dynamics.

[1]Deutsche Forschungsgemeinschaft, European Research Council