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Entropy as a collective variable

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Sampling complex free energy surfaces that exhibit long lived metastable states separated by kinetic bottlenecks is one of the most pressing issues in the atomistic simulations of matter. Not surprisingly many solutions to this problem have been suggested. Many of them are based on the identification of appropriate collective variables that span the manifold of the slow varying modes of the system. While much effort has been put in devising and even constructing on the fly appropriate collective variables there is still a cogent need of introducing simple, generic, physically transparent, and yet effective collective variables. Motivated by the physical observation that in many case transitions between one metastable state and another result from a trade off between enthalpy and entropy we introduce appropriate collective variables that are able to represent in a simple way these two physical properties. We use these variables in the context of the recently introduced variationally enhanced sampling and apply it them with success to the simulation of crystallization from the liquid and to conformational transitions in protein.