Estimation and Optimization of the Exchange Acceptance in Umbrella Sampling Replica Exchange Molecular Dynamics

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We developed, validated and tested a method for estimating the probability of exchange between neighboring replicas in Umbrella Sampling Replica Exchange MD. We use information from very short umbrella runs, needing only a handful of windows.
We designed a multi dimensional scoring function to optimize the set of replicas (windows). By maximizing the scoring function, we make the exchange acceptance the same for all neighbor replica pairs.
We tested our algorithm by simulating butane in implicit solvent and a salt bridge in explicit solvent. We find that setting the replicas to equal exchange acceptance between pairs increases the number of round trips and improves efficiency of sampling.