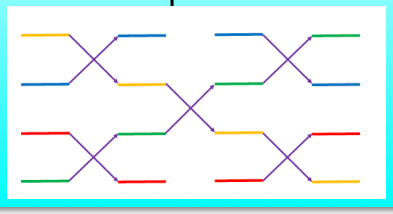
A Quick Summary of Enhanced Sampling and Analysis Methods

Enhanced Sampling Methods

Replica Exchange (REMD)

T-REMD: multiple temperatures

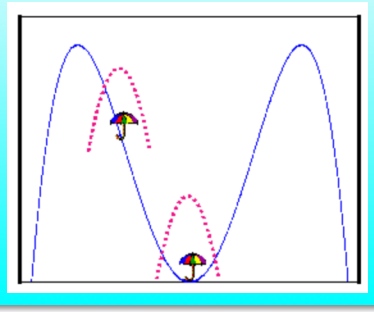
H-REMD: multiple Hamiltonians



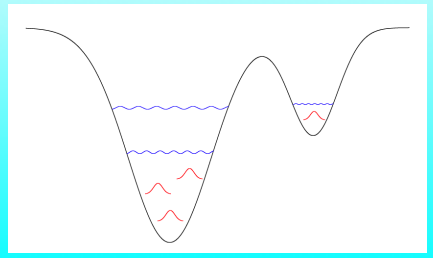
λ-Dynamics

$\lambda \in [0,1]$, added as an extra DOF

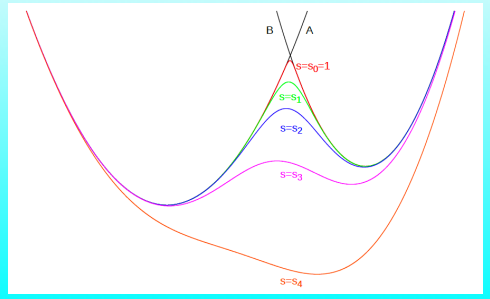
Umbrella Sampling



Metadynamics



Enveloping Distribution Sampling (EDS)



Orthogonal Space Random Walk (OSRW)

Post-Processing Methods

Thermodynamic Perturbation (TP)
= Free Energy Perturbation
= Exponential Average
= Zwanzig Equation

$$\Delta A_{0\to 1} = -\frac{1}{\beta}\ln\left\langle \exp(-\beta(U_1 - U_0))\right\rangle_0$$

Thermodynamic Integration (TI)

$$\Delta A_{0\to 1} = \int_0^1 \left\langle \frac{\partial H(\lambda)}{\partial \lambda}\right\rangle_\lambda d\lambda$$
$$= \sum_i \left\langle \frac{\partial H(\lambda)}{\partial \lambda}\right\rangle_{\lambda_i} \Delta\lambda_i$$

Bennett Acceptance Ratio (BAR)

Weighted Histogram Analysis Method (WHAM)

Non-Boltzmann Bennett (NBB)

Molecular Mechanics/Poisson Boltzmann Surface Area (MM/PBSA)