WHAM Documentation v1.0

WHAM Input Format

In the following examples, we assume that:

S = 10 windows

N = 1000 data points per window

Umbrella Sampling

Metadatafile



Where the v.i files contain



and the rc.i files contain



WHAM Extrapolation

Metadatafile



Where the v.i files contain



and the rc.i files contain





Temperature Replica Exchange

Umbrella Sampling & WHAM Extrapolation

Metadatafile



Where the v.i files contain



and the rc.i files contain



Umbrella Sampling & Temperature Replica Exchange