1 Introduction

This document outlines the error in merging more than one replica after FEP calculations using Q and a trial method to reduce noise.

2 Method 1

1. Run qdyn on all the 10 replicas and obtain the .en files in each (these contain the energy files for all 51 windows considered).
2. Copy all .en files from all replicas into one `qfep.inp`.
3. The `qfep.inp` file contains lines where the number of energy files, states, gap bins, H_{ij}, and α can be defined.
4. Change the number of files to 510 instead of 51 (since we want all 51 windows in 10 replicas).
5. Run `qfep` on `qfep.inp` to generate a `qfep.out` file. This file contains the change calculated relative to the previous and following perturbation steps (dGf and dGr for forward and reverse, respectively). It also provides the accumulated sum of energy changes between ϵ_1 and ϵ_2 (sum(dGf) and sum(dGr)), as well as the average accumulated change calculated from the forward and reverse directions (dG).
6. Run `analysefeps` on `qfep.out` to generate a JSON file and plot the data.
7. The resulting plot has a lot of noise (see Figure).

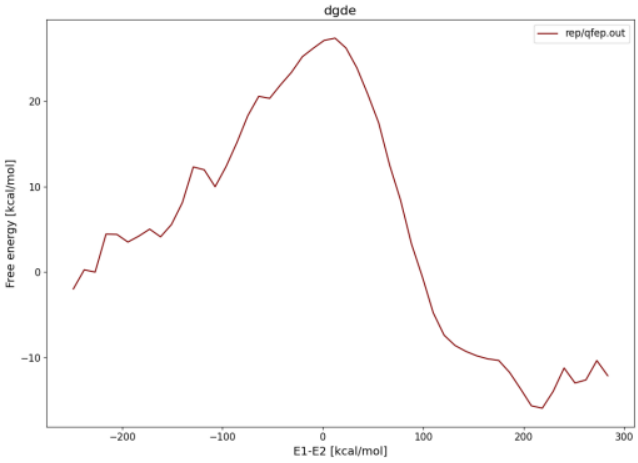

Figure 1: The resulting plot with a lot of noise.

3 Noise Reduction

To reduce the noise:

3.1 Method 2

1. Run qdyn on all the 10 replicas and obtain the .en files in each (these contain the energy files for all 51 windows considered).
2. Create a `qfep.inp` in all replicas.
3. The `qfep.inp` file contains lines where the number of energy files, states, gap bins, H_{ij}, and α can be defined.
4. Run `qfep` to seperately generate `qfep.out` and generate a JSON file for each replica. This file contains the change calculated relative to the previous and following perturbation steps (dGf and dGr for forward and reverse, respectively). It also provides the accumulated sum of energy changes between ϵ_1 and ϵ_2 (sum(dGf) and sum(dGr)), as well as the average accumulated change calculated from the forward and reverse directions (dG).
5. Run `analysefeps` on `qfep.out` to generate a JSON file and plot the data.
6. Plot the data separately for each JSON in the replicas and combine the free energy plots in one file using the script.
7. The resulting plot has lesser deviation (see Figure)

Figure 2: The resulting plot with lesser deviation.