# An implementation of Full/Single Batch Scoring Function Replica Positioning Optimizers Version 1.0

## Command line arguments for Full and Single Batch Scoring Functions

* **-il** input list, it contains a list of pre-simulated files + their bias centers(more on this in the next part)
* **-o** output file
* **-col** column number which contains dumped US values (default is 2, which is compatible with amber format)

* **-sc** spring\_constant/2 (i.e. )

Note: In amber bias potential is of the format , where is half of the regular spring constant. Here we follow the same format.

* **-cc** conversion constant (e.g. degree 🡪 radian)

Note: unit of dumped values should be compatible with spring constant. For example if the unit of spring constant is and the unit of dumped values isthen conversion constant will be .

* **-wmin** position of center of bias in lowest windows on reaction coordinate
* **-wmax** position of center of bias in highest windows on reaction coordinate
* **-nr** number of replicas (FBSF method only)
* -**ea** exchange acceptance (SBSF method only)
* **-pr** convergence criteria (default is 0.001)

## Input list format

Input list file contains two columns . In each row consists of dumped value file name the of center of bias in that window.

## Example (Butane Dihedral)

In the “example” folder, there are 12 dumped values of equi-distance replicas, which belong to a butane dihedral. Those are simulated in implicit solvent by Amber’s umbrella sampling replica exchange algorithm. In order to optimize the positions of replicas, follow this instruction:

Change the directory to “example” by

***> cd example***

If you open the list.in file, there are 12 lines in this file and each line contain dumped file name and center of bias for that windows.

For running FSBF type:

***> python ../SBSF\_us\_exchange\_overlap\_optimizer\_V1.0.py -il list.in.2 -o Butane\_FBSF.out -sc 30 -cc 0.0174 -wmax 67.0 -wmin -65 -nr 12 -col 2***

After it finishied open “Butane\_FBSF.out”, the final EAR between every neighbor windows should be around 0.14.

In order to reproduce the same result using the SBSF optimization method, set the exchange acceptance equal 0.14, type:

***> python ../SBSF\_us\_exchange\_overlap\_optimizer\_V1.0.py -il list.in.2 -o Butane\_SBSF.out -sc 30 -cc 0.0174 -wmax 67.0 -wmin -65 -ea 0.14 -col 2***

## Citation

If you use this code as part of an original piece of research, we’d appreciate a reference or acknowledgment. The publication is still pending, but you can use the following:

Sabri Dashti, D.; Roitberg, A. E. Optimization of Umbrella Sampling Replica Exchange Molecular Dynamics by Replica Positioning. *(submitted)*