The value is square brackets at the end of every parameter is the current default value. Change the following parameters to suit your needs.

==================================================================

FILE FORMATS:

1. ENERGY Input Files:

1st Line MUST be replica number

2nd Line MUST be a header line

3rd line onwards, the energy values must be printed line by line

2. temps:

temperatures [tab/space separated]

3. CV files:

separate files for each CV

line by line cv value

DO NOT INCLUDE HEADER

note the column number of desired value

==================================================================

FILE NAMING RULES:

1. ENERGY Input Files:

MUST have unique extension i.e. if I have a energy file etot1.en then the only files that have .en extension should be the desired energy input files

2. temps:

No rules. Don't forget to update the TEMPFILENAME variable in required program files.

3. CV Files:

PREFIX [part of file name preceeding replica number] not compulsory, but recommended to help distinguish between CV1 and CV2 files.

Replica number for every cv file COMPULSORY [MUST be an integer]

MUST have an extension. Extensions for CV1 and CV2 MUST be same.

==================================================================

=>input\_gen.py

INPUTFOLDERNAME = change this to locate your input files' folder

TEMPFILENAME = change this to locate your temp file

ENERCOL = Column number of your energy in the input files

INPUTEXT = Extension of your energy input files. [Change it to "rmsd" if your file is 'xyz\_1.rmsd']

REPSHIFT = the amount by which you have to shift to get to 0. [Ex. Your Files start from 'abcde5.out' to 'abcde28.out', then REPSHIFT = 5] [1]

==================================================================

=>histo\_gen.py

M = change the number of bins that you want to make [500]

==================================================================

=>free\_gen.py

MAXITS = Max Number of Iterations for free-energy:Density of States Loop. [1000]

k\_boltz = Boltzmann constant in kcal/mol/K [1.3806503 \* 6.0221415 / 4184.0]

\*\*Make sure to change this value in wt.py too\*\*

TOLERANCE = Tolerance [1.0e-5]

==================================================================

=>wt\_gen.py

k\_boltz = Boltzmann constant in kcal/mol/K [1.3806503 \* 6.0221415 / 4184.0]

==================================================================

=>1dpmf\_gen.py

M = Number of bins for observable [CV] [20]

STARTIDX = Start Index of temp number/Replica Number of OBSERVABLE Files. [Ex. STARTIDX = 5 if your filename is 'abcde3.hbond'][3]

OBSCOL = Column number of observable in observable input files [1]

TEMPFILENAME = change this to locate your temp file

FOLDERPATH = Change this to locate your observable files' folder. PLEASE REMEMBER TO ADD A ‘/’AT THE END

EXT = Extension of your observable files. [Ex. EXT = "hbond" if your filename is 'abcde3.hbond']["obs"]

TEMPNOSHIFT = If your files have numbering from 1 suppose, then TEMPNOSHIFT is the amount by which you have to shift to get to 0. [Ex. Your Files start from 'abcde5.hbond' to 'abcde28.hbond', then TEMPNOSHIFT = 5] [1]

PMFTEMP = Temperature at which you want to find your PMF [307]

==================================================================

=>2dpmf.py

M = Number of bins for one CV. [NOTE: nstates = M\*\*2] [20]

TLOW = Lower Range of temperature [286]

TUP = Upper range of temperature [373]

Tdel = Temperature delta [3.0]

REPS = Replicas [30]

OBSCOL = Column number of CV in their respective files [1]

PMFTEMP = Temperature at which you want to find your PMF [307]

STARTIDX1 = Start Index of temp number/Replica Number of CV1 Files. [Ex. STARTIDX = 5 if your filename is 'abcde3.hbond'][54]

STARTIDX2 = Start Index of temp number/Replica Number of CV2 Files. [Ex. STARTIDX = 5 if your filename is 'abcde3.hbond'][56]

CVPREFIX1 = Prefix of cv1 files [CVPREFIX1 = ‘Helix1rms18mic.out.’, if filename is ‘Helix1rms18mic.out.15.rms’]

CVPREFIX2 = Prefix of cv2 files [CVPREFIX2 = ‘Helix2\_3rms18mic.out.’, if filename is ‘Helix2\_3rms18mic.out.15.rms’]

CVFOLDER = Folder path where the CV files are located. [Ex. "/home/krb/New CDAC/remd/shruti\_inp/"]

CVEXT = Extension of CV files [Ex. "rms"]

TEMPFILENAME = Temperature file location along with name [Ex. "/home/krb/New CDAC/remd/shruti\_inp/temps"]

TEMPNOSHIFT = the amount by which you have to shift to get to 0. [Ex. Your Files start from 'abcde5.hbond' to 'abcde28.hbond', then TEMPNOSHIFT = 5] [1]