



TASS Reweighting Code

Structure of the Code

PROGRAM TASS_Reweight

USE Prepare_Inputs

USE welcome

USE Check_File

USE Plumed_Read

USE GetSteps

USE ReadFiles

USE Reweight_MTD

USE Probability

USE Print_Data

Call welcome()

Call Set_Defaults()

Call Check_Files()

Call Read_Plumed()

Call Get_Inputs()

Call Print_Data()

Call Read_Cvfile()

If(metad) **then**

Call Reweight_MTD(**rbias**, **mtd_dimension**)

Endif

Call Calculate_Probability(**rbias**, **prob_dimension**, **metad**)

ENDPROGRAM TASS_Reweight

Modules

- Sets Imp variables to default values
(system temp, cv temp, t_min,, t_max,
Mtd = ON, prob_dimension =1, etc)
- Reads plumed.dat file & user input for input data.
- Reads Cvfile and does periodicity for given CV number.
- If metad ON, Reweights Metad Bias
- Calculates Probability in any dimension
1D, 2D, 3D, 4D and 1D & 2D , 2D & 4D etc.
- Parallel Calculation of ct, vbias calculations with openmpi.
- Reweights 1D, 2D & 3D MTD Bias

Work In Progress:

Extend this code to CPMD input as well

Include a KEYWORD = Method , (MTD, TASS, PBTASS..etc)

To include WHAM

Input Parameters

CVFILE	:	COLVAR
HILLSFILE	:	HILLS
METAD	:	ON/OFF
NCV	:	No. of CVs
NMETAD	:	No. of MTD CVs (1)
PACE	:	Frequency of Gaussians
STRIDE	:	Freq. of CV printing
BIASFACTOR	:	--NA--
SYSTEM_TEMP	:	300.d0
CV_TEMP	:	Extended_Lagrangian Temp (300.d0)
KAPPA	:	US KAPPA

PERIODICITY	:	ON/OFF
PERIODIC_CV	:	NONE/ALL/CV1/CV2/CV1.and.CV2/..etc
PROB_DIMENSION	:	1 or 2 or 3 or 4 or 12 or 13 or 14 or 24
MTD_DIMENSION	:	1 or 2 or 3
T_MIN	:	(1) Start time
T_MAX	:	(mdsteps) End time
GRID_INFORMATION	:	Grid min, grid max for NCV
NBIN	:	No. of Bins. (101)
MDSTEPS	:	Total MD steps
MTDSTEPS	:	Total MTD steps

* Red color indicates the default values

Sample Input file

input.inp

```
CVFILE      = COLVAR
HILLSFILE   = HILLS
METAD        = ON
NCV          = 4
NMETAD       = 1
PACE         = 500
STRIDE       = 10
BIASFACTOR  = 4.0
SYSTEM_TEMP = 300.d0
CV_TEMP      = 900.0
KAPPA        = 500
PERIODICITY  =. ON
PERIODIC_CV =  ALL
PROB_DIMENSION = 2
MTD_DIMENSION = 1
T_MIN        = 100001
T_MAX        = 300000
GRID_INFORMATION
GRID1: -3.14.  3.14
GRID2: -3.14.  3.14
GRID3: -3.14.  3.14
GRID4: -3.14.  3.14
NBIN         =. 101
```

./reweighting_tass.x