**TASS**

Temperature Accelerated Sliced Sampling

Enhanced Sampling Method to Accelerate

Molecular Dynamics Simulation

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This manual is for Reweighting TASS

version 1.2

**Overview**

Biasing collective variables efficiently accelerates rare events in molecular simulations and explores free energy surfaces. Temperature Accelerated Sliced Sampling (TASS)1 method combines the temperature accelerated molecular dynamics (TAMD/d-AFED)2 with umbrella sampling3 and metadynamics (MTD)4 to sample the collective variable (CV) space efficiently.

This modular FORTRAN program is written to get the unbiased probability and Mean Force based free energy of TASS simulation generated from the CPMD5/PLUMED6 package. Probabilities can be then, used to computes 1D and 2D free energy via WHAM7. This code also calculates the 1-dimensional and 2-dimensional free energy using the Mean Force method (MF)8.

Basis Spline interpolation (1D & 2D) has also been implemented to get the intermediate points in free energy.

**Constants**

1 bohr = 0.529177 Å

1 au = 627.5094 kcal/mol = 2625.4996 kJ/mol

kB = 1.9872 ×10-3 kcal/mol

**Installation**

./configure #Choose compiler [gnu/intel]

A Makefile will be created:

…

# make install : create executable

# make bspline : compile B-spline modules for interpolation

# make wham : compile wham module (MPI needed)

# make clean : remove object and mod files

# make distclean : clean the directory (lib, bin)

**Running TASS-Reweighting**

Executable tass\_analysis.x will be created in the bin directory, which can be accessed via setting environment variables.

[export PATH=path\_to\_folder/bin:$PATH]

Running tass\_analysis.x requires the following files:

* **input.inp** file
* **INPUT** file
* input.inp

A dummy file is provided along with the code. There is a slight difference in this input file for PLUMED and CPMD because CPMD writes MTD cv position and bias information in two different files while PLUMED writes in the same file.

**IMPORTANT:** order of the files should be the same as below

2.0 1.0

! mean position of umbrella, kappa value during MD run

test/cv\_file/umb\_2.4/COLVAR

! location of cv file (COLVAR)

test/cv\_file/umb\_2.4/HILLS

! location of file in which bias is written (HILLS)

2.0 1.0

! mean position of umbrella, kappa value during MD run

test/cv\_file/umb\_2.4/cvmdck\_mtd

! location of cv file (cvmdck\_mtd)

test/cv\_file/umb\_2.4/parvar\_mtd

! location of file in which bias is written (parvar\_mtd)

test/cv\_file/umb\_2.4/colvar\_mtd

! location of file for MTD cv displacement (colvar\_mtd)

* **INPUT** file

A dummy bash script file is given with the code with the required input description to run the program.

$INPUT file.

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SYSTEM TEMP # Physical system Temperature (real)

300

CV TEMP # CV Temperature (real)

1000

CODE NAME # Name of MD package (CPMD/PLUMED) (character)

CPMD/PLUMED

MTD BIAS FACTOR # Metadynamics Bias Factor (real)

5.0

TMIN # Minimum MD steps to compute Probability (integer)

1000

TMAX # Maximum MD steps to compute Probability (integer)

10000

NUMBER OF CV # Total CV's in TASS Simulation (integer)

2

UCV COLUMN # Umbrella CV index (integer)

1

MTD ENABLED # y/n IF Metadynamics performed during simulation (character)

n

MTD CV COLUMN # IF MTD=y then Metadynamics CV index [else=0] (integer)

2

REWEIGHTING TOOL # pmf/prob [pmf-->mean force; ProbT => Probability]

pmf/prob (logical character)

B-SPLINE INTERPOLATION # Basis Spline 1D interpolation of free energy (logical)

NUMBER OF UMBRELLA # Number of replica (umbrella window) (integer)

14

PROBABILITY DIMENSION # Dimension of Probability to be generated [1/2] (integer)

1

PROBABILITY CV INDEX # Probability generated along CV indicis [1 => 1D, 1 2 =>

1 2 2D along CV1 and CV2 etc.] (integer, integer)

CV PRINT FREQUENCY # Frequency of printing cv’s during run (integer)

1

MTD PRINT FREQUENCY # Frequency of printing bias during Metadynamics (integer)

200

STATISTICAL ERROR BLOCK SIZE # Statistical error from MD run (logical)

5 optimal block size [4 - 6] (integer)

GRIDS

# gridmin, gridmax, griddif for every CV (real, real, real)

1.5 4.5 0.02

1.0 3.0 0.02

**IMPORTANT:** Input arguments in the file are case-sensitive.

**How to run**

tass\_analysis.x < INPUT

**Files:**

PROB.dat\_$i => 1D probability where $i is the umbrella index

PROB\_2D.dat\_$i => 2D probability where $i is the umbrella index

free\_energy.dat => 1D free energy generated from MF

free\_energy\_2d.dat => 2D free energy generated from MF

free\_energy\_wham => Free energy computed using WHAM module

interp\_free\_energy.dat => interpolated (1D) free energy

**B-Spline Interpolation:**

Basis spline interpolation scheme is implemented to get the intermediate points in the free energy computed from mean force method. 1D interpolation is the default with tass\_analysis.x executable. But, one can also compile the 1D and 2D interpolation executables separately (make bspline) which can later be used.

1d\_bspline.x => 1D interpolation

2d\_bspline.x => 2D interpolation

**Weighted Histogram Analysis Method (WHAM):**

WHAM (Weighted Histogram Analysis Method) is a standard technique for calculating potentials of mean forces (PMFs) from umbrella sampling/TASS simulations. Given several distributions collected from different windows, WHAM obtains the optimal estimate of the free energies of the states.

To enable the wham module, compile the code with make wham, it will create wham.x executable.

If prob is selected as REWEIGHTING TOOL, then the program will create a whaminput file on the fly with all the information needed for wham.x.

**References:**

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