TASS

Temperature Accelerated Sliced Sampling

Enhanced Sampling Method to Accelerate
Molecular Dynamics Simulation

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This manual is for Reweighting TASS
version 1.1

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 sampling[3] and metadynamics (MTD)[4] to sample the collective variable (CV) space efficiently.

This modular FORTRAN program is written to get the unbiased probability of TASS simulation generated from the trajectory of CPMD[5]/PLUMED[6]. These probabilities then can be used to computes 1D and 2D free energy via WHAM[7]. This code also calculates the 1dimensional 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 = 2525.4996 kJ/mol

k_B = 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
# make clean         : remove object and mod files
# make distclean     : clean the directory
```

Running TASS-Reweighting

Executable Probability_analysis.x will be created in the bin directory, which can be accessed.

Running Probability_analysis.x requires the following files:

- **input.inp** file
- **run_tass.sh** file

➢ input.inp

A dummy file is provided with the code. There is a slight difference in the 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 not be changed

```
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 where 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 where bias is written (parvar_mtd)
test/cv_file/umb_2.4/colvar_mtd
! location of file for MTD cv displacement (colvar_mtd)
```

- run_tass.sh
  A dummy file is given with the code with the required arguments to run the program.

```
Probability_analysis.x
# Executable with path
-T0 300
# Physical system Temperature (real)
-T 1000
# CV Temperature (real)
-prog_name CPMD/PLUMED
# Name of MD package (CPMD/PLUMED) (character)
-bias_fact 5.0
# Metadynamics Bias Factor (real)
-tmin 5000
# Minimum MD steps to compute Probability (integer)
-tmax 10000
# Maximum MD steps to compute Probability (integer)
-ncv 2
# Total CV's in TASS Simulation (integer)
-UCV 1
# Umbrella CV index (integer)
-MTD n
# y/n IF Metadynamics performed during simulation (character)
-MCV 0
# IF MTD=y then Metadynamics CV index [else=0] (integer)
-tool pmf
# pmf/probT [pmf-->mean force; ProbT => Probability] (logical character)
-interpolate
# Basis Spline 1D interpolation of free energy (logical)
-nr 14
# Number of replica (umbrella window) (integer)
-Prob_nD 1
# Dimension of Probabilty to be generated [1/2] (integer)
-CV_num 1 2
# Probabilty generated along CV indicis [1 => 1D, 1 2 => 2D along CV1 and CV2 etc.]
(integer, integer)
-pfrqMD 1
# Frequency of printing cv's during run (integer)
-dtMTD 200
# Frequency of printing bias during Metadynamics (integer)
-grid 1.5 4.5 0.02 1.0 10.0 0.02
# gridmin, gridmax, griddif for every CV (real, real, real)
```

IMPORTANT: All the arguments are case-sensitive.

Files

PROB.dat_$i => 1dimensional probability where $i is the umbrella number

PROB_2D.dat_$i => 2dimensional probability where $i is the umbrella number

free_energy.dat => free energy generated from pmf

interp_free_energy.dat => interpolated free energy

References

1) S. Awasthi, N. N. Nair, *J. Chem. Phys.* 146, 094108, **2017**. https://doi.org/10.1063/1.4977704

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