WESTPA

Purpose: Molecular Dynamics
Latest version: 1.0 beta
License: Free of use
GNU GPL _ext-link
Website: *https://westpa.github.io/ _ext-link*

The **Weighted Ensemble Simulation Toolkit with Parallelization and Analysis (WESTPA)** is a high-performance framework for carrying out extended-timescale simulations of rare events with rigorous kinetics using the weighted ensemble algorithm of ***Huber and Kim (1996)***.

The software works with any dynamics engine and has already been used with a variety of molecular dynamics (e.g. GROMACS, NAMD, AMBER) and cell-modeling packages (e.g. BioNetGen, MCell).

SLURM Submit script example

For more information use the ***Job Script Generator***.

Sbatch options:

The options shown in the example are detailed below. For more information and a more comprehensive list of available options, see the ***sbatch command page***.

- **-J**: Name for the job's allocation.
- **-e**: Name of the stderr redirection filename.
- **-o**: Name of the stdout redirection filename.
- **-p**: Name of the partition (queue) where the job will be submitted.

starccm_example.slm

```
#!/bin/bash
#SBATCH -J westpa_example
#SBATCH -e westpa_example.%j.err
#SBATCH -o westpa_example.%j.out
#SBATCH -p std
#SBATCH -n 1
#SBATCH -t 0-02:00

module load apps/westpa/2017.10
module load apps/gromacs/2018.1

##
#  Modify the input and output files!
cp -r ${SLURM_SUBMIT_DIR}/{init.sh,run.sh}
${SCRATCH}
cd ${SCRATCH}

srun init.sh >& init.out
srun run.sh >& run.out

cp ./{init.out,run.out} ${SLURM_SUBMIT_DIR}
```

- **-n**: Number of tasks.
- **-c**: Number of cores per task.
- **-t**: Set the job's time limit. If the job don't finish before the time runs out, it will be killed.