

A photograph of a large server rack, the Anton 2, with a grid of blue lights. The rack is composed of several vertical panels. The text 'Anton 2' and 'Enhanced Sampling' is overlaid in white. The name 'ANTON2' is visible in green on the server panels.

Anton 2

Enhanced Sampling

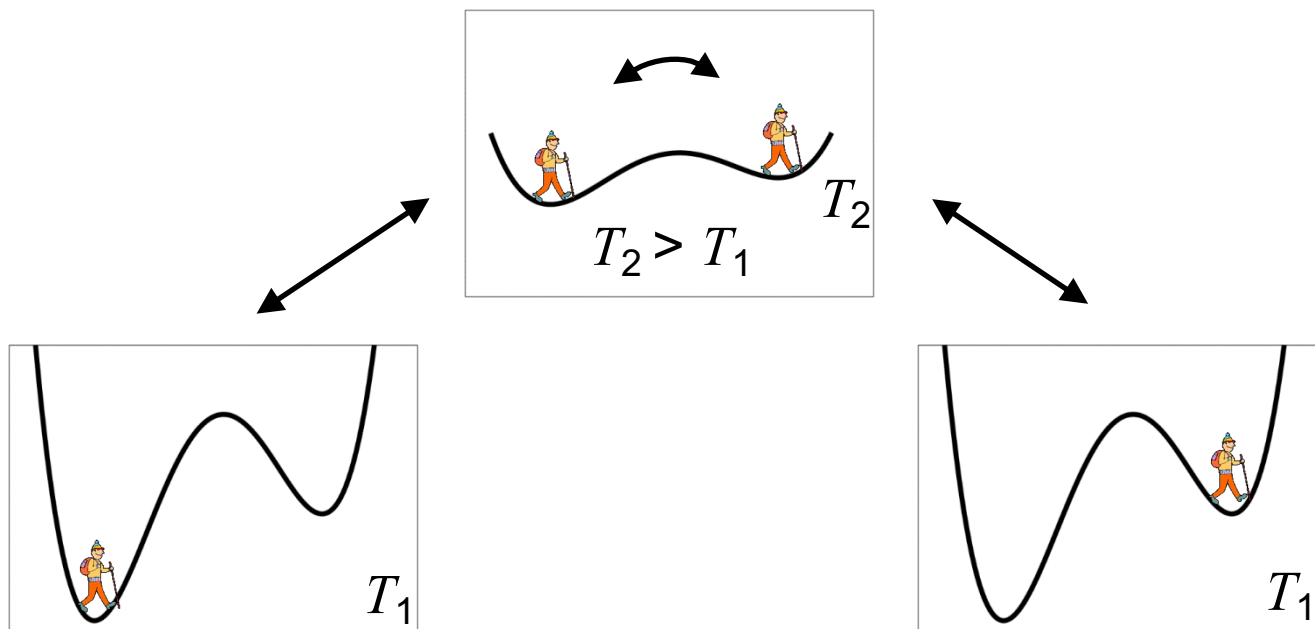
Avi Robinson-Mosher
Michael LeVine

D E Shaw Research

June 9, 2022

Enhanced sampling with TSS

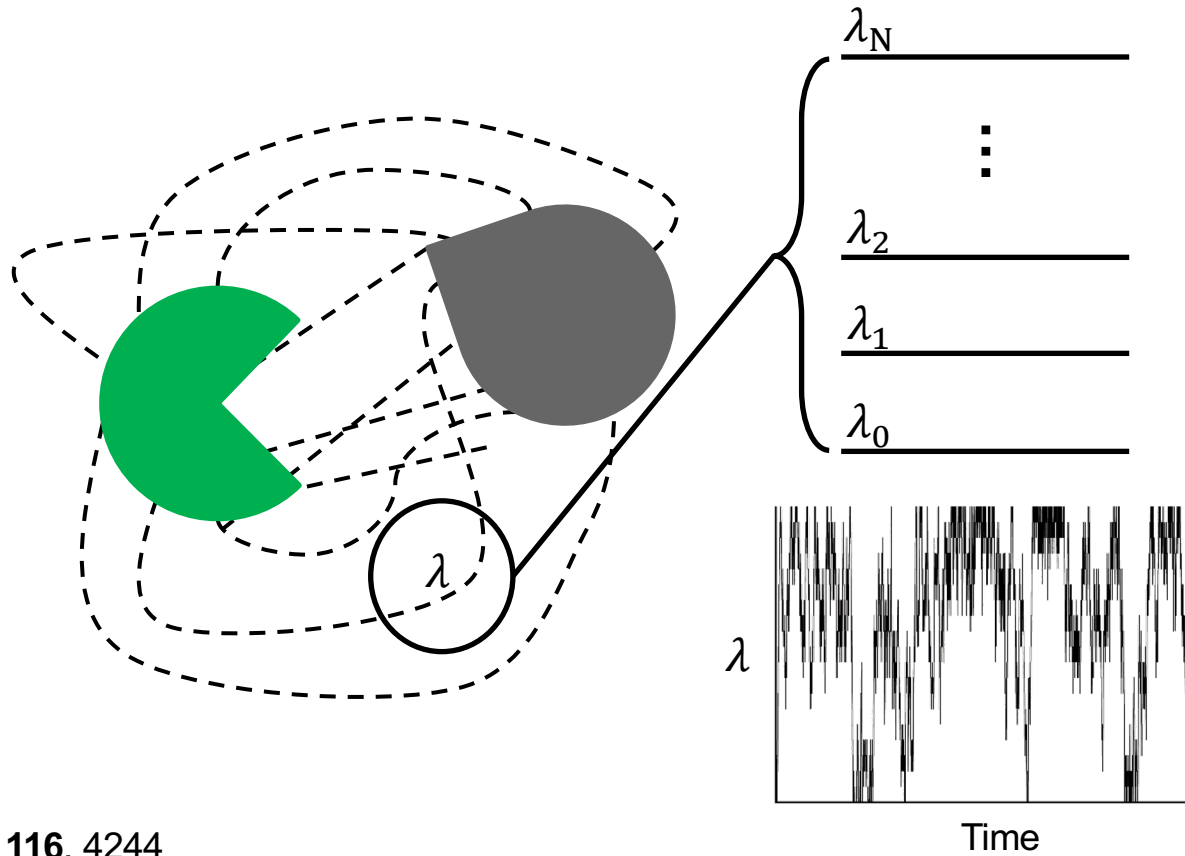
- Times Square Sampling (TSS) is an enhanced sampling approach related to simulated (Hamiltonian) tempering
- TSS has built-in online free energy estimators



[arXiv:2112.05109](https://arxiv.org/abs/2112.05109)

<https://github.com/DEShawResearch/tss>

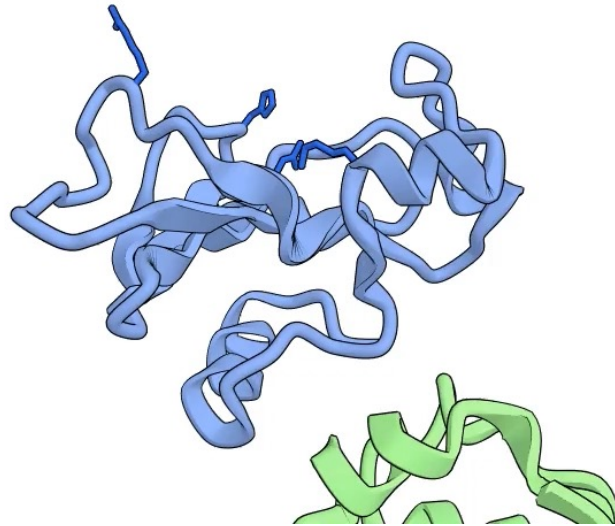
Tempered binding



PNAS (2019), **116**, 4244

Tempered binding speeds up escape from metastable traps

0.0 μ s



Available forms of enhanced sampling

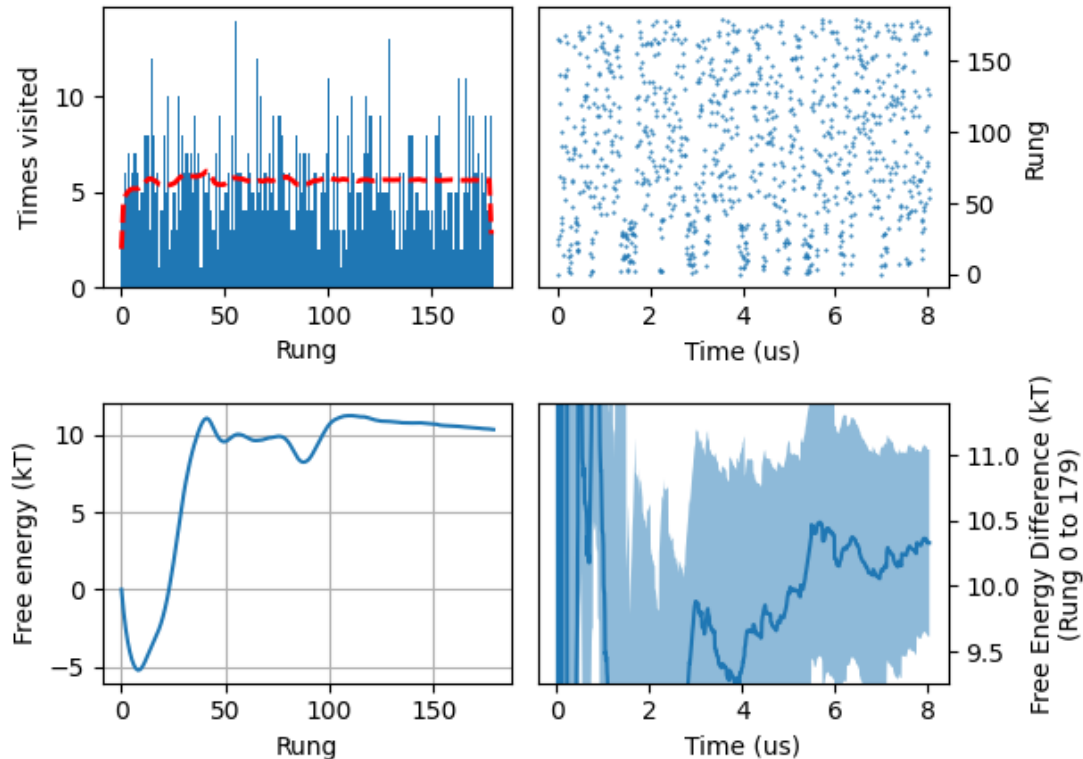
1. Simulated tempering (temperature tempering with adaptive weighting)
2. Tempered binding
3. Restraints between centers of mass of groups of atoms
4. Conformational restraints based on the calculation of the RMSD (root mean squared deviation) of a group of atoms with respect to the positions of a given reference structure

For restraints in (3) and (4), equilibria and spring constants can be varied during a simulation either according to a schedule or controlled adaptively by TSS to implement a form of umbrella sampling

Analyzing enhanced sampling runs

```
$ pytss_psc plot_basic /path/to/workdir
```

13220586



https://wiki.psc.edu/twiki/view/Anton/a2docs/proj/desres/doc/build/html/adaptive_enhanced_sampling.html

Survey

<https://forms.gle/18NimygFsJACXsj5>