

## **ADVANCED** THEORY AND SIMULATIONS

Progress Report | 🙃 Open Access | 💿 📵 😂

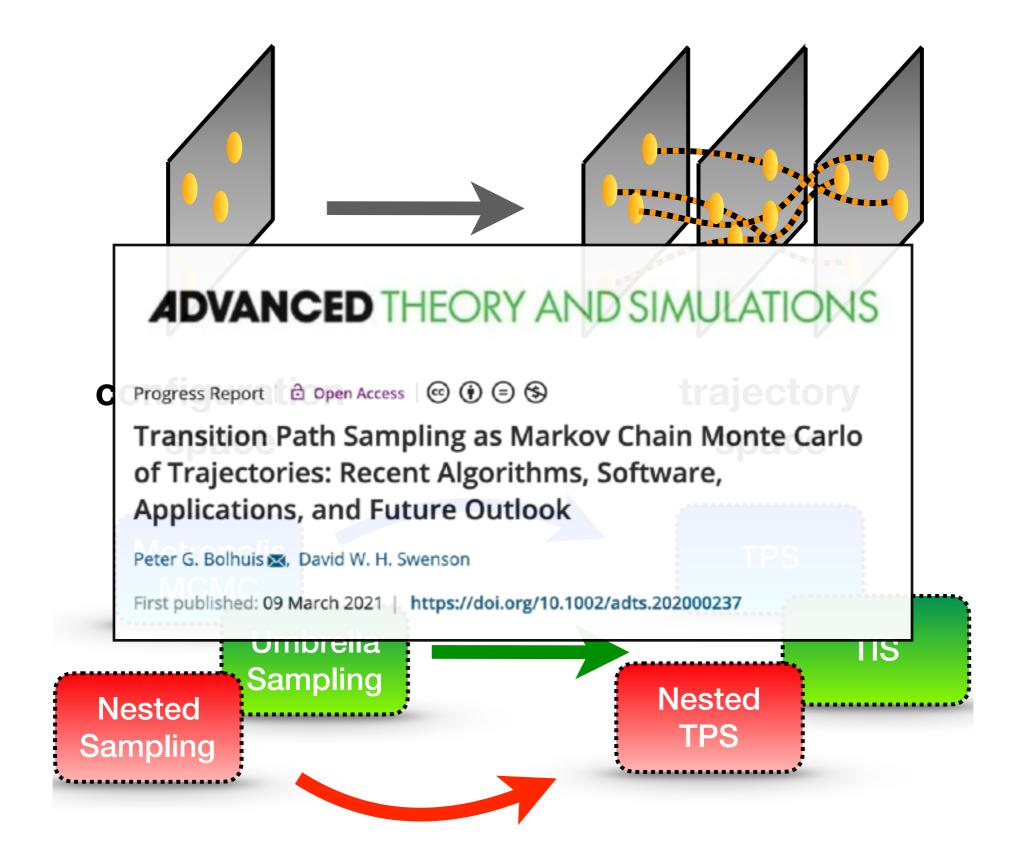
Transition Path Sampling as Markov Chain Monte Carlo of Trajectories: Recent Algorithms, Software, Applications, and Future Outlook

Peter G. Bolhuis , David W. H. Swenson

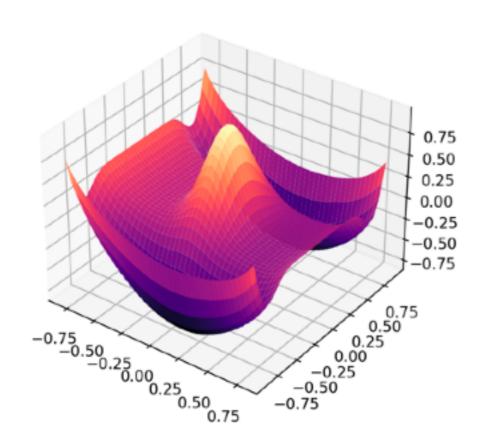
First published: 09 March 2021 | https://doi.org/10.1002/adts.202000237

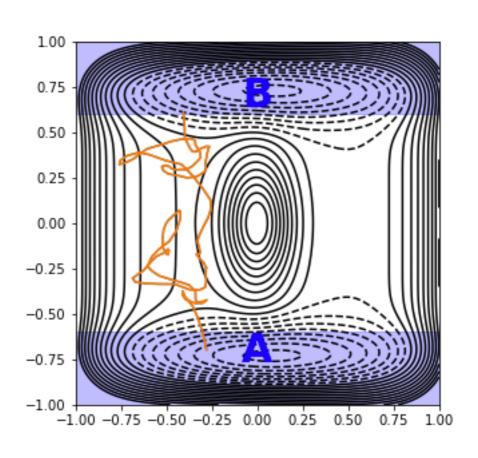
## TPS: Generalize MC to Trajectories

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## Rare events within rare events?





- Experimental connection: relative probability of channels
- Rate of switching: kinetics of kinetics! Metakinetics!