

Workflow "Reweighting Dynamics in Non-Equilibrium Steady States"

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1 Structure of Thesis

- Background
 - Molecular Dynamics Simulation
 - Off-Equilibrium Dynamics
 - * Stochastic Thermodynamics
 - * Non-Equilibrium Steady States
 - Minimal Model for Non-Equilibrium Steady States
Needs introduction here for showing steps on MSM. Fig: Potential surface
 - * Entropy Production
 - Markov State Modelling
 - * Transfer Operators
 - * Markov Property
Fig: lagtime Analysis , relaxation analysis (CK test) ,
 - * Clustering
Fig: Apply PCCA on system, for now and later Mostly PCCA+, because it is used later.
 - * First-Passage-Time Distribution
Fig: FPTs of states, plot moments vs lagtime
This chapter contains first result about MFPT non-markovian.
- Jaynes Maximum Caliber
 - Equilibrium Constraints
Theory and Application on statics. Fig: Show on ISAW Model
 - Non-Equilibrium Steady State Constraints
General discussion of changes in Caliber (trajectories, Markov,...)
 - * Theory of Constraints
Discussion of local/global, symmetric/asymmetric constraints, general

- * Application of Constraints

Explicitly chosen constraints. Minimisation will be performed for different set of constraints (with/without global/+ balance, global/local constraints). Conclude with final set that will be used in next chapter. Test consistency by reweighting test. Include subsection about resulting Invariant and meaning of it

Fig: Single dynamics and statics global entropy productions, repeat for local entropy production, then with global balance (show for all 6 processes), show exactness of enforced entropy production, Invariant of system

- Numerical Minimisation

Discuss numerical algorithm, including all the failed attempts to include the full Caliber.

Fig: Do this later, show non convergence of algorithms (2nd order, full set, basin hopping algorithm, thermodynamic integration, increase order of expansion). What happens to small system sizes? Result for $m_s = 30$?

- Reweighting Dynamics on Potential Surface

Full discussion of the final choice of constraints from previous chapter. The discussion starts here with theoretical value of ΔS_{ij} and $\Delta\Delta S_{ij}$ for each system.

I am not happy with the repetitive mentioning of 'single particle'

- Single Particle in 1D Potential Well
- Single Particle under Global Driving
- Single Particle under Local Driving
- Single Particle in 2D Potential Well

Fig: Obvious here, most from publication. Indicate core states

- Reweighting Dynamics on Free Energy Surface

- Single Particle under Global Driving
- Alanine-4-Peptide

Fig: stick to style here. Indicate core states, entropy productions in next chapter!

- Extensions to Reweighting Scheme

- Local Entropy Production Histograms

Compare the entropy production from trajectory analysis, MSM and theory for each model here. Fig: Histograms of entropy production with indicator for all systems. 1D representation of Ala4 difference

- Constructing MSM in Non-Equilibrium Steady States

Self Reweighting and discussion of convergence speed for all systems. Fig: speed of convergence of MFPT/lagtime in equilibrium, MFPT out of equilibrium

- Conclusion

2 Timeline

Suggested Timeline. Many Figures and almost all data exist. Most of Jaynes and part of Background is written. Numerical Minimisation is poorly documented and the extensions have to be expanded to all systems.

07. April - 12. April	Finish Jaynes chapter
13. April - 19. April	Finish Background
20. April - 26. April	Reweight on U-Surface
27. April - 03. Mai	Include suggested Changes
04. Mai - 10. Mai	Reweight on F-Surface
11. Mai - 17. Mai	Extension and Conclusion
18. Mai - 21. Mai	Numerical Minimisation
22. Mai - 31. Mai	Include suggested Changes