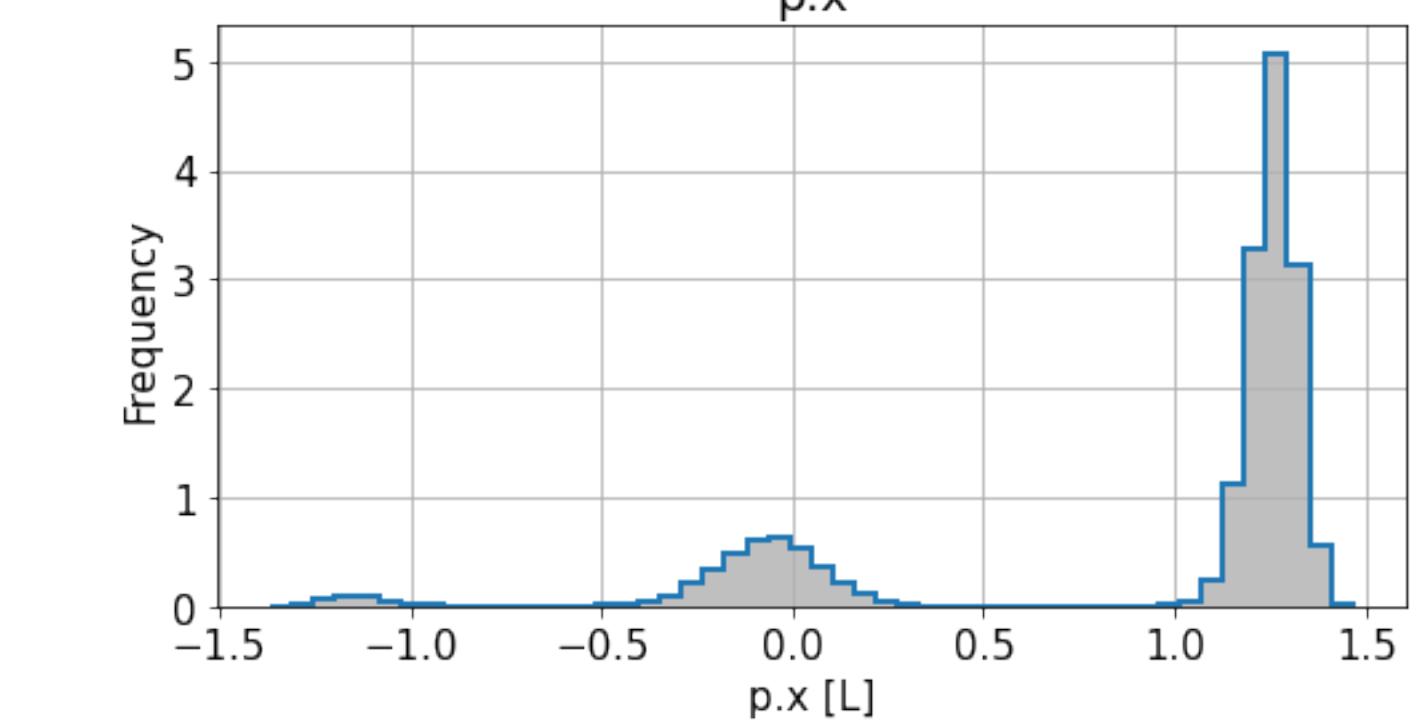
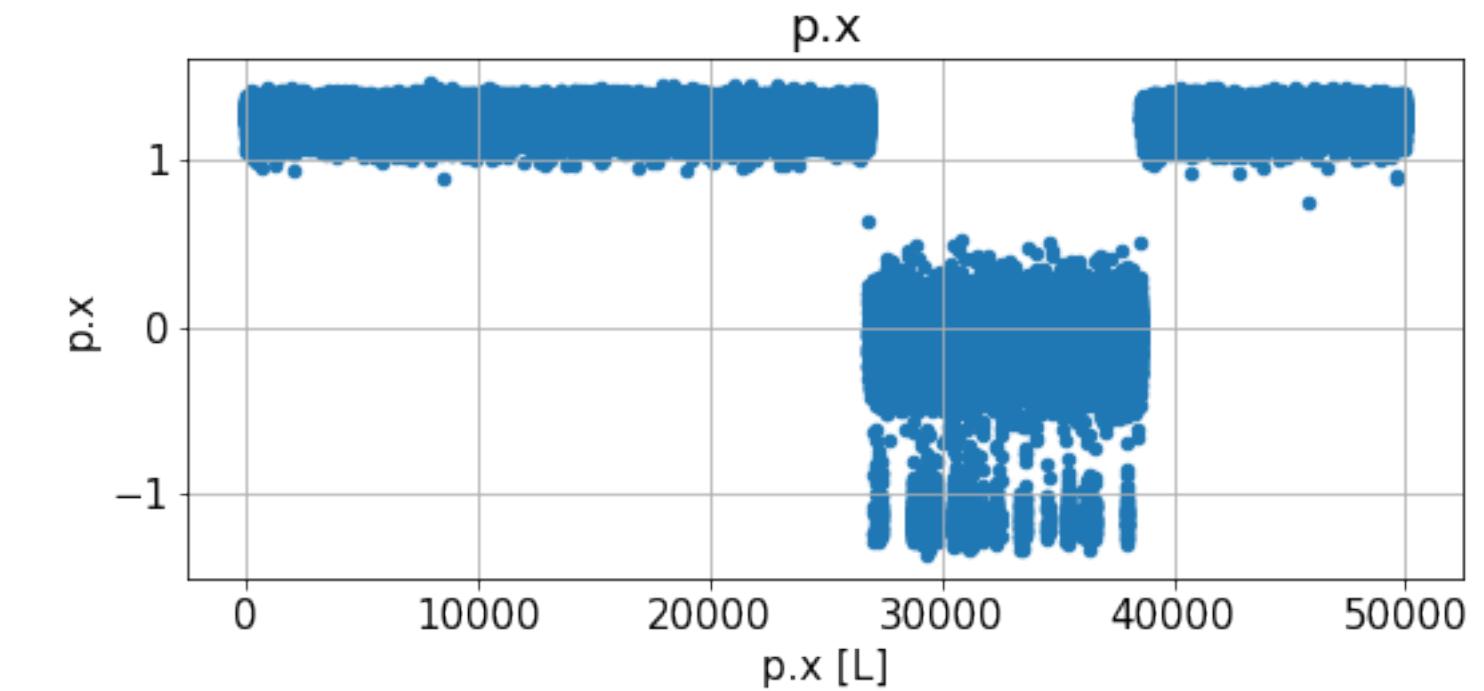
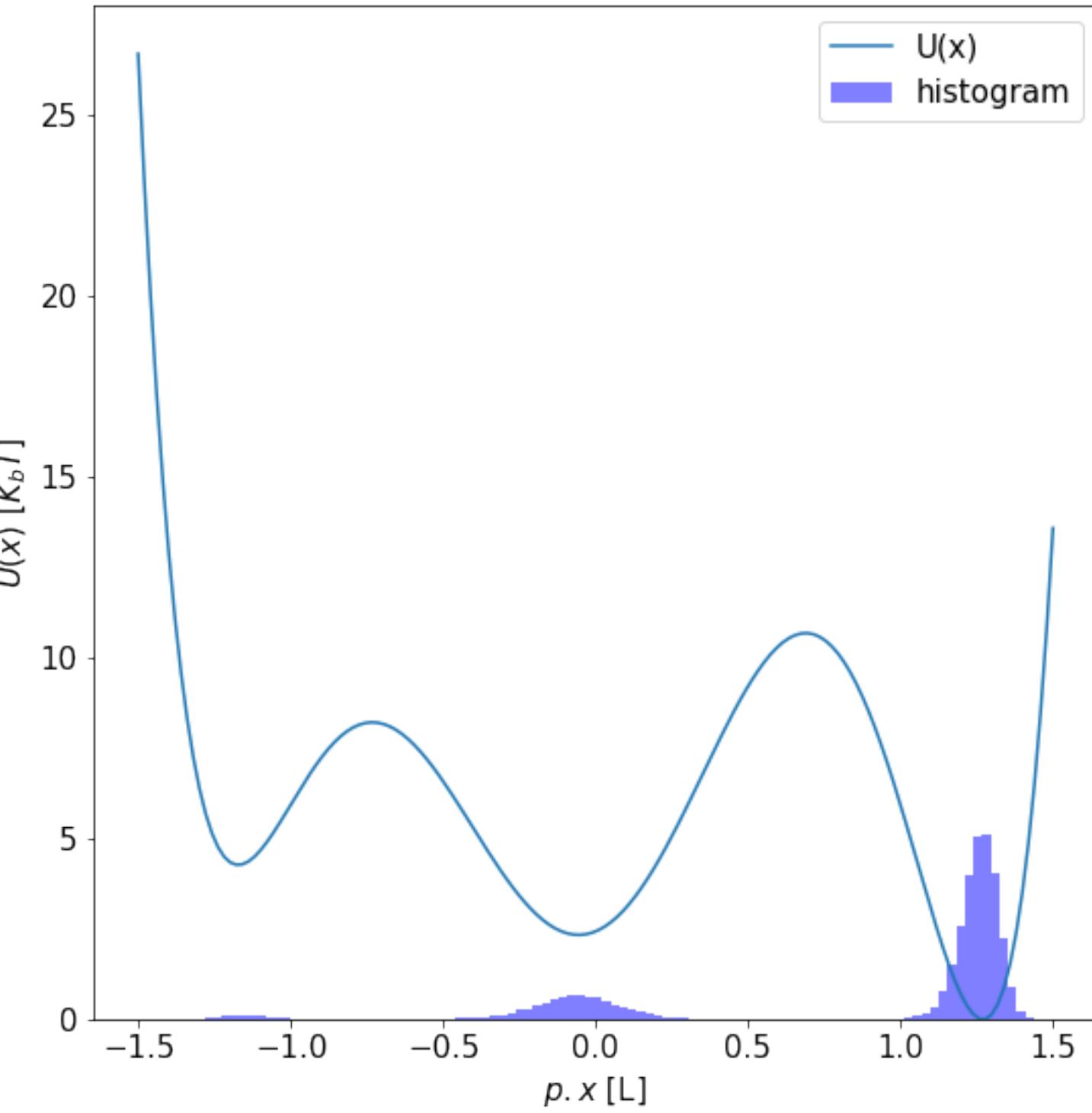
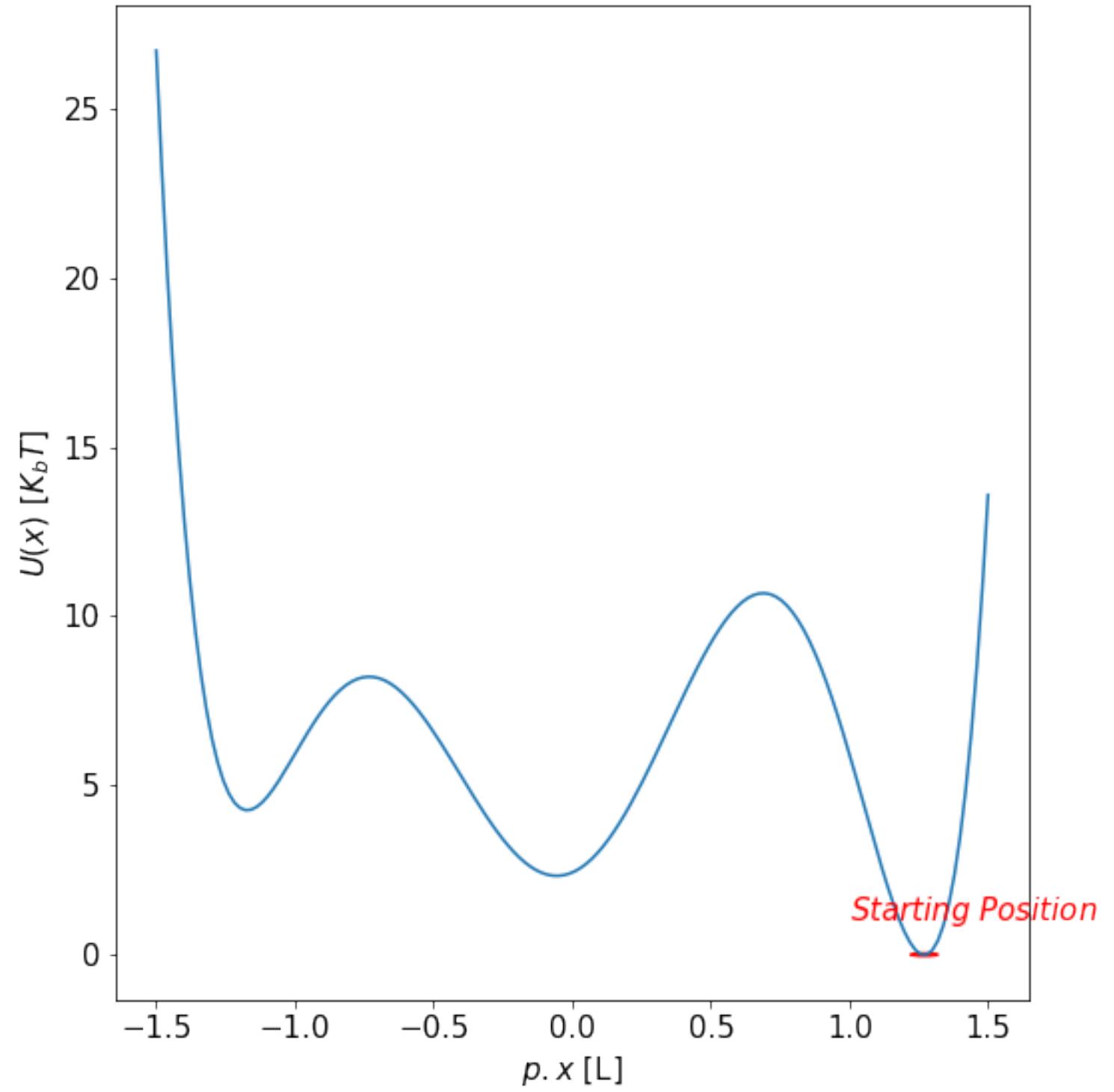


# **Hyper TICA**

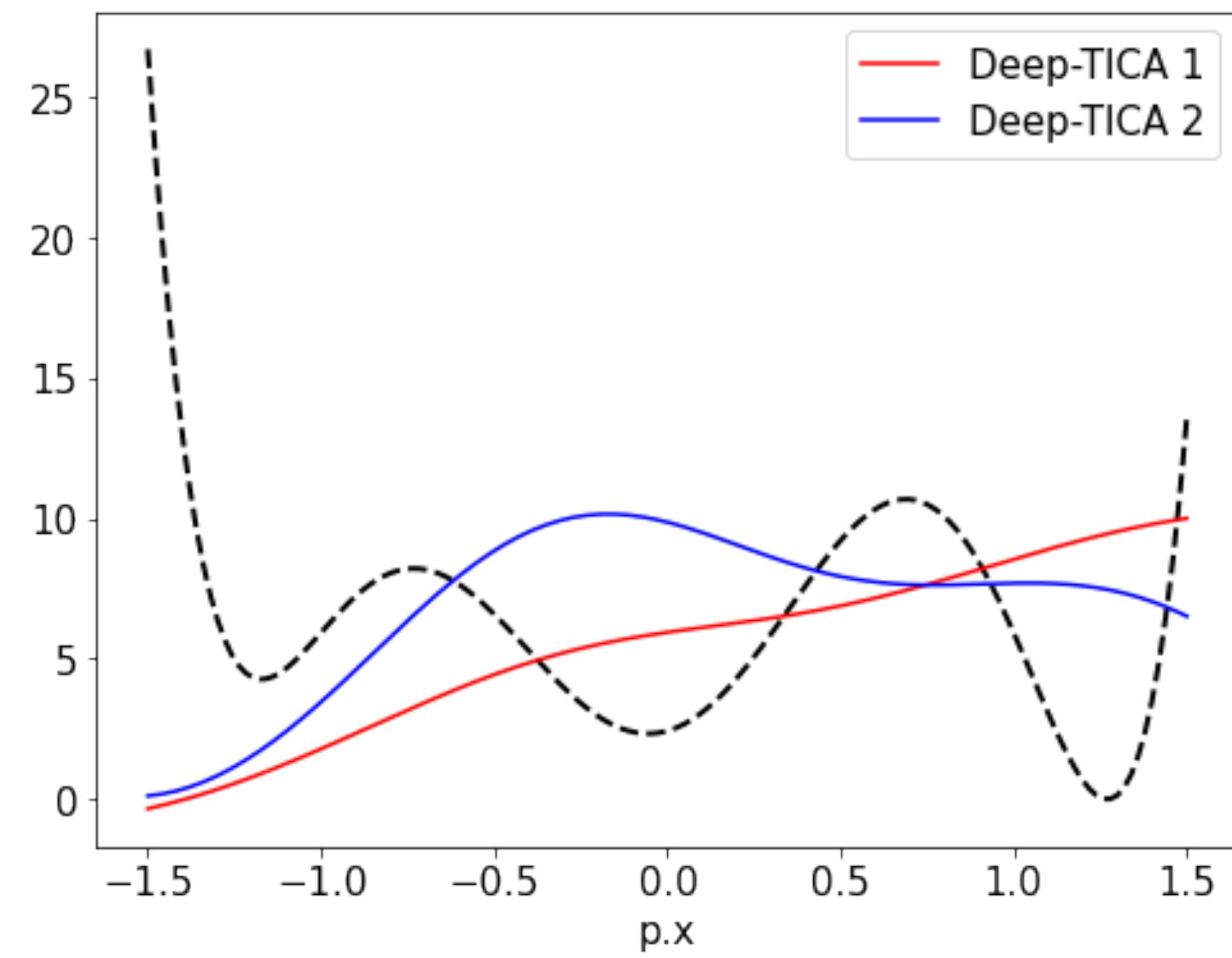
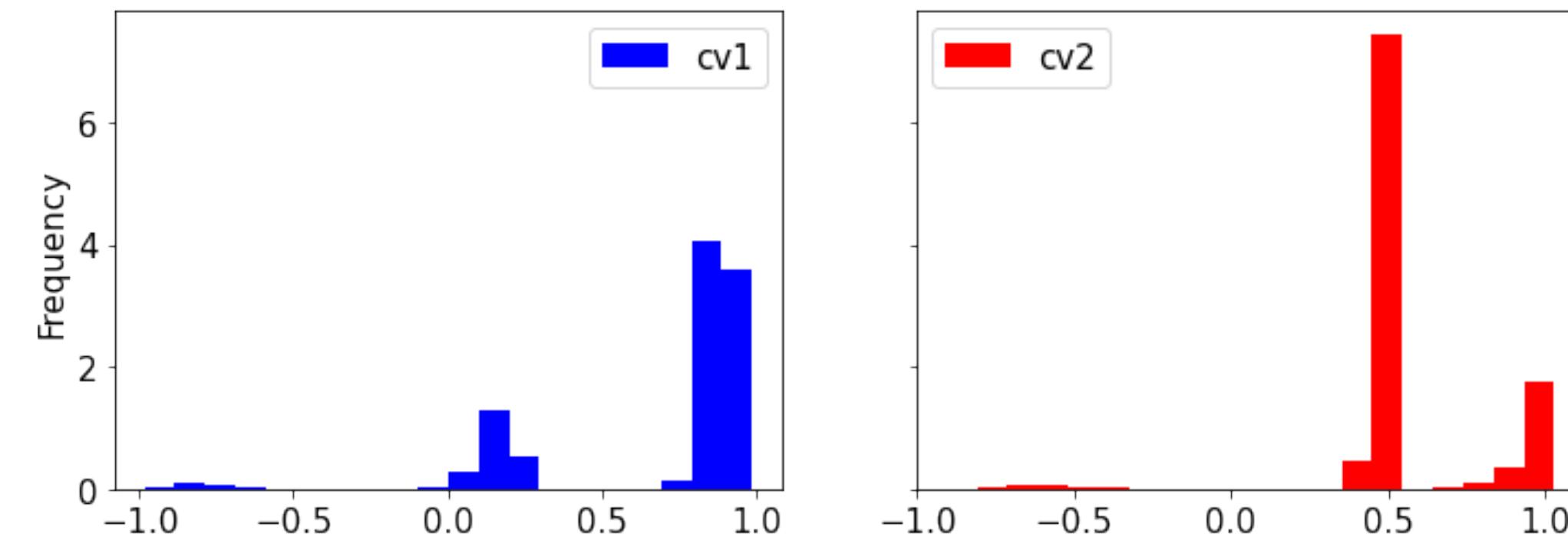
## **Phd Project**

**Nicolo' Pedrani**

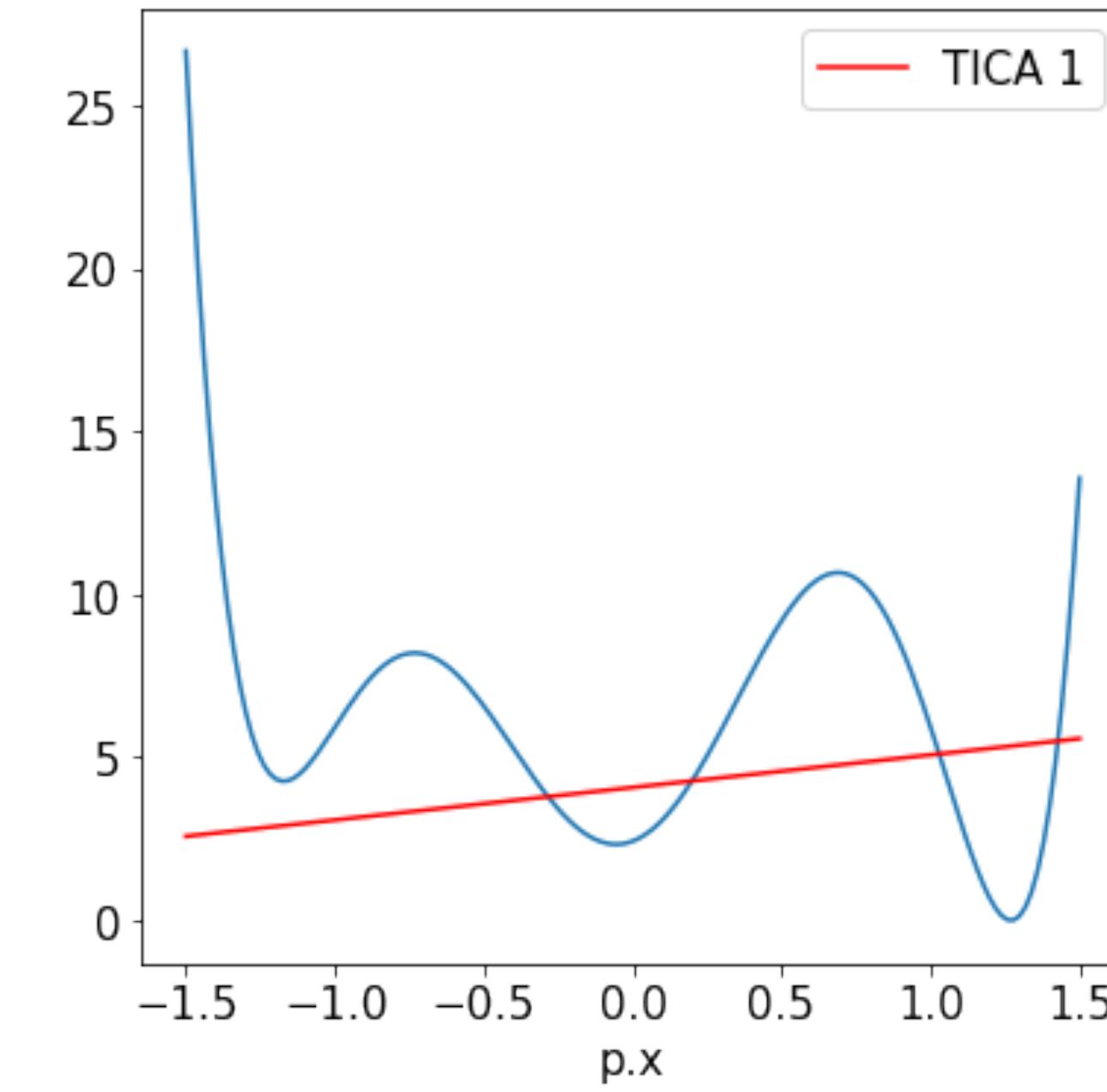
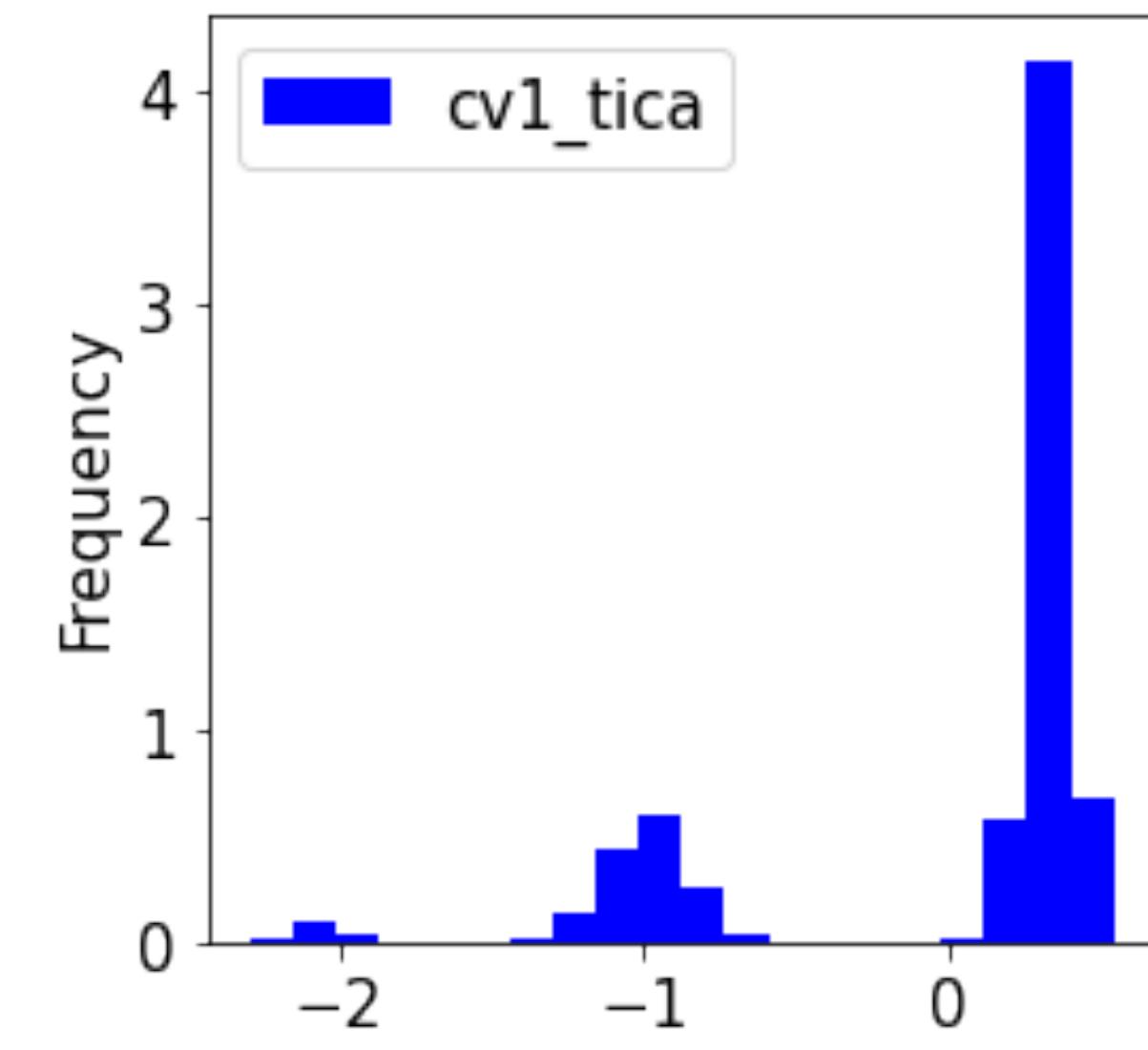
# 1D System



# Deep-TICA Analysis

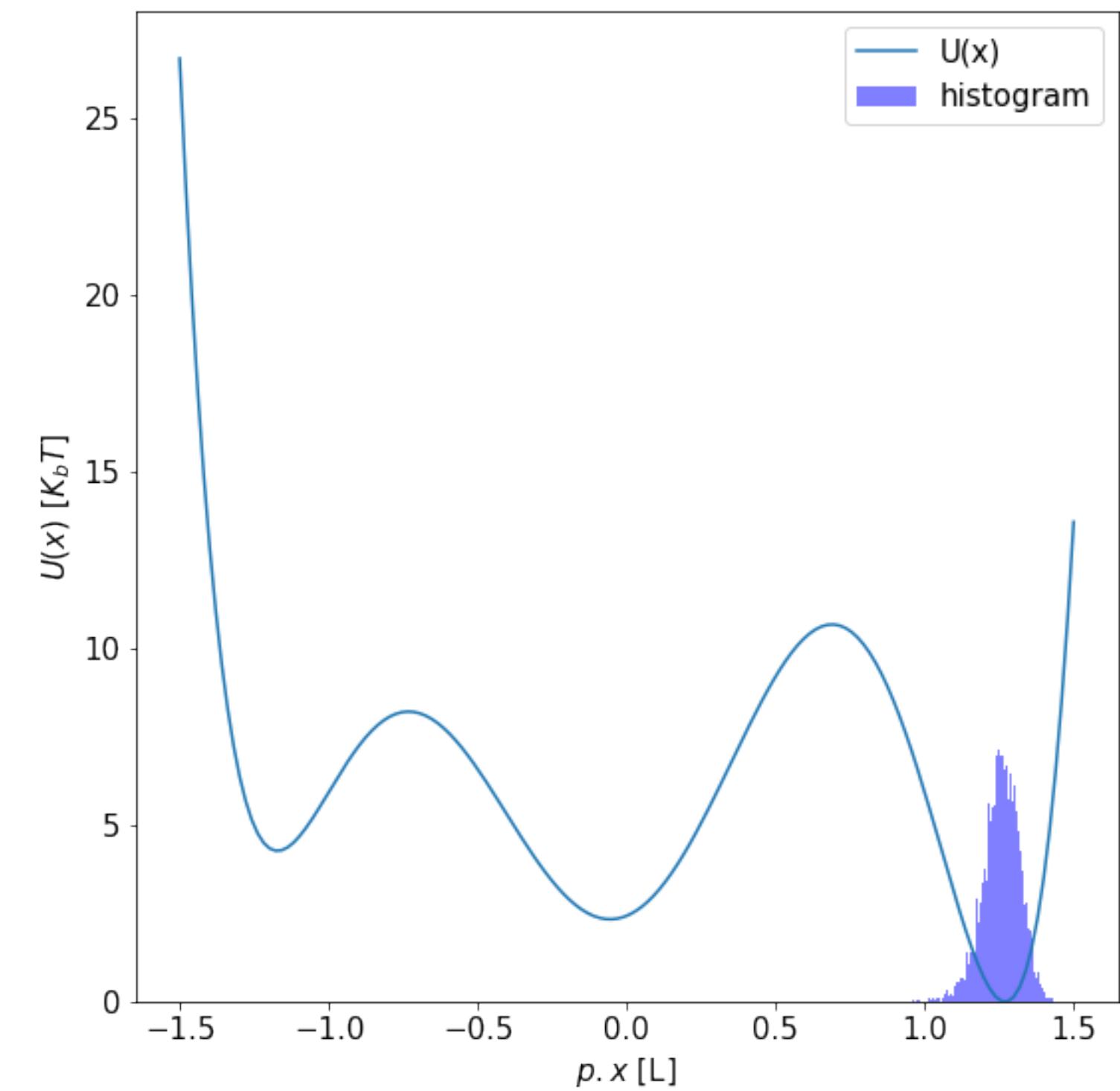


# TICA Analysis

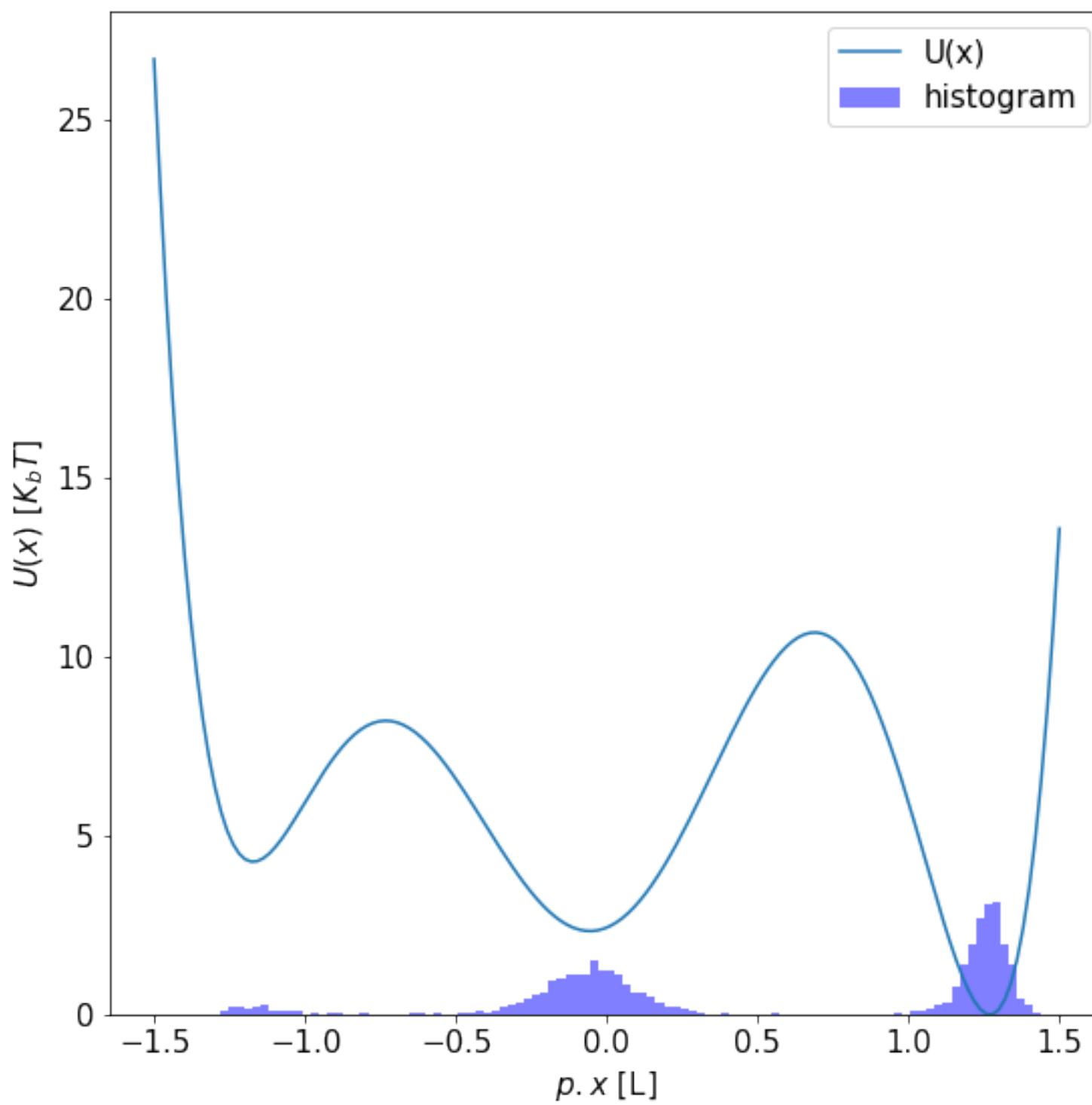


# Short Simulation

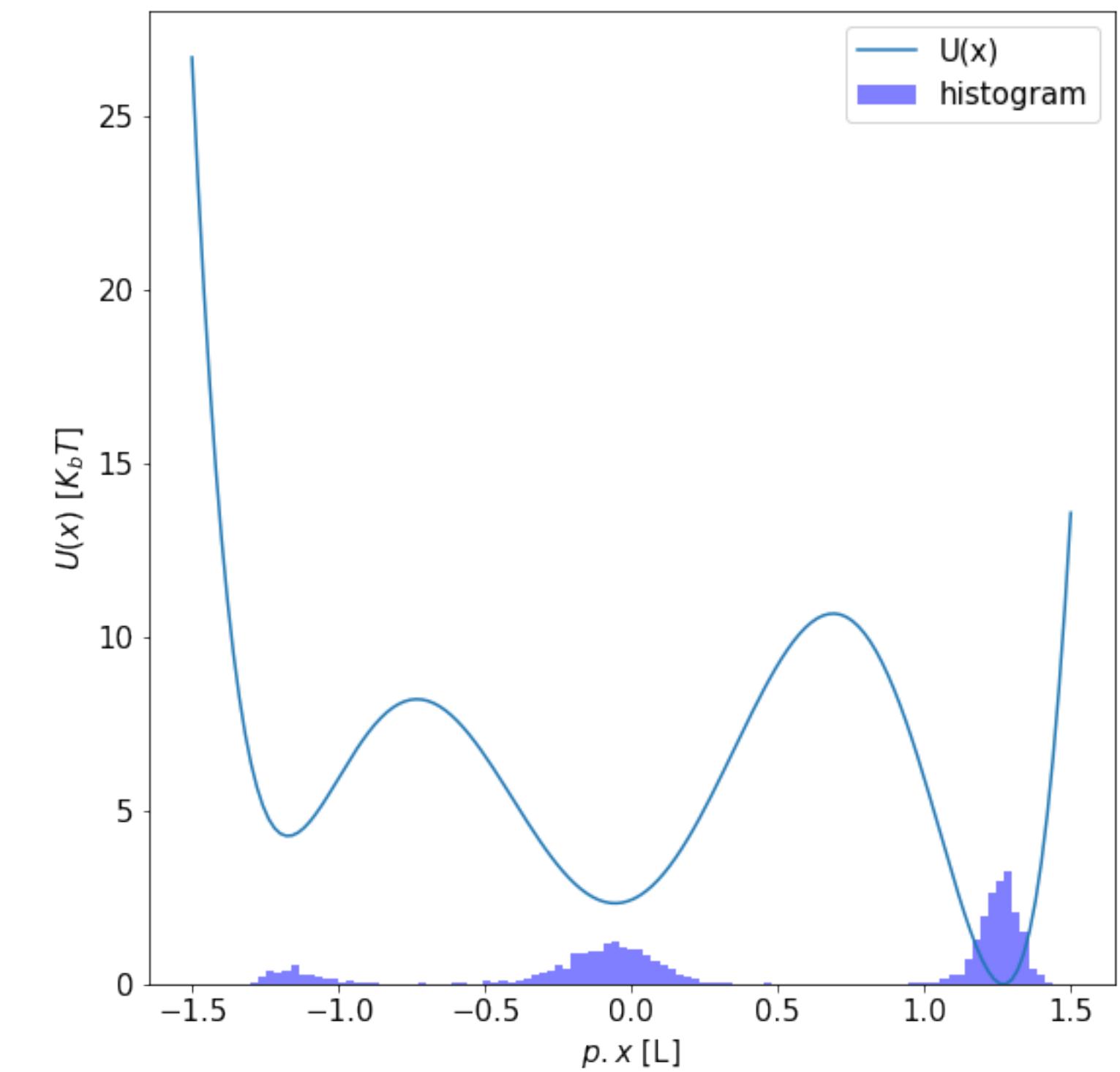
Short unbiased trajectory



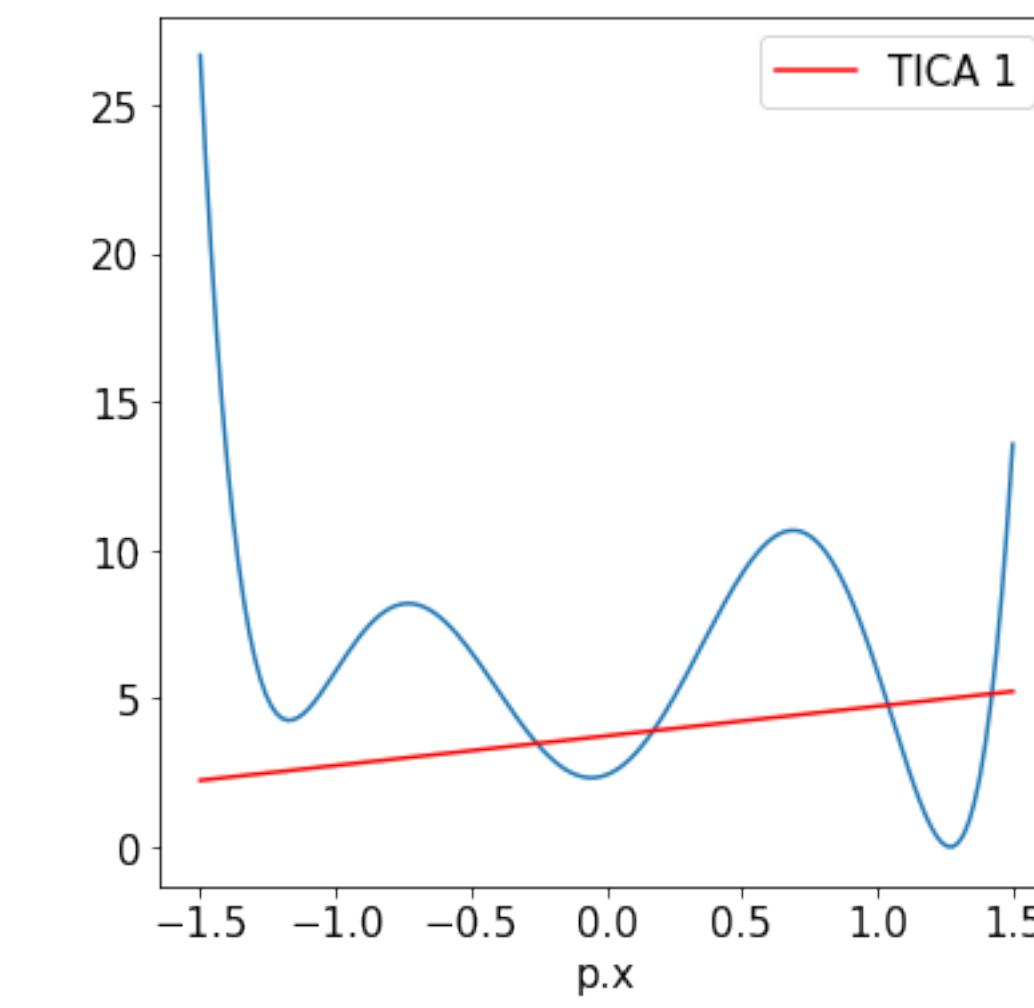
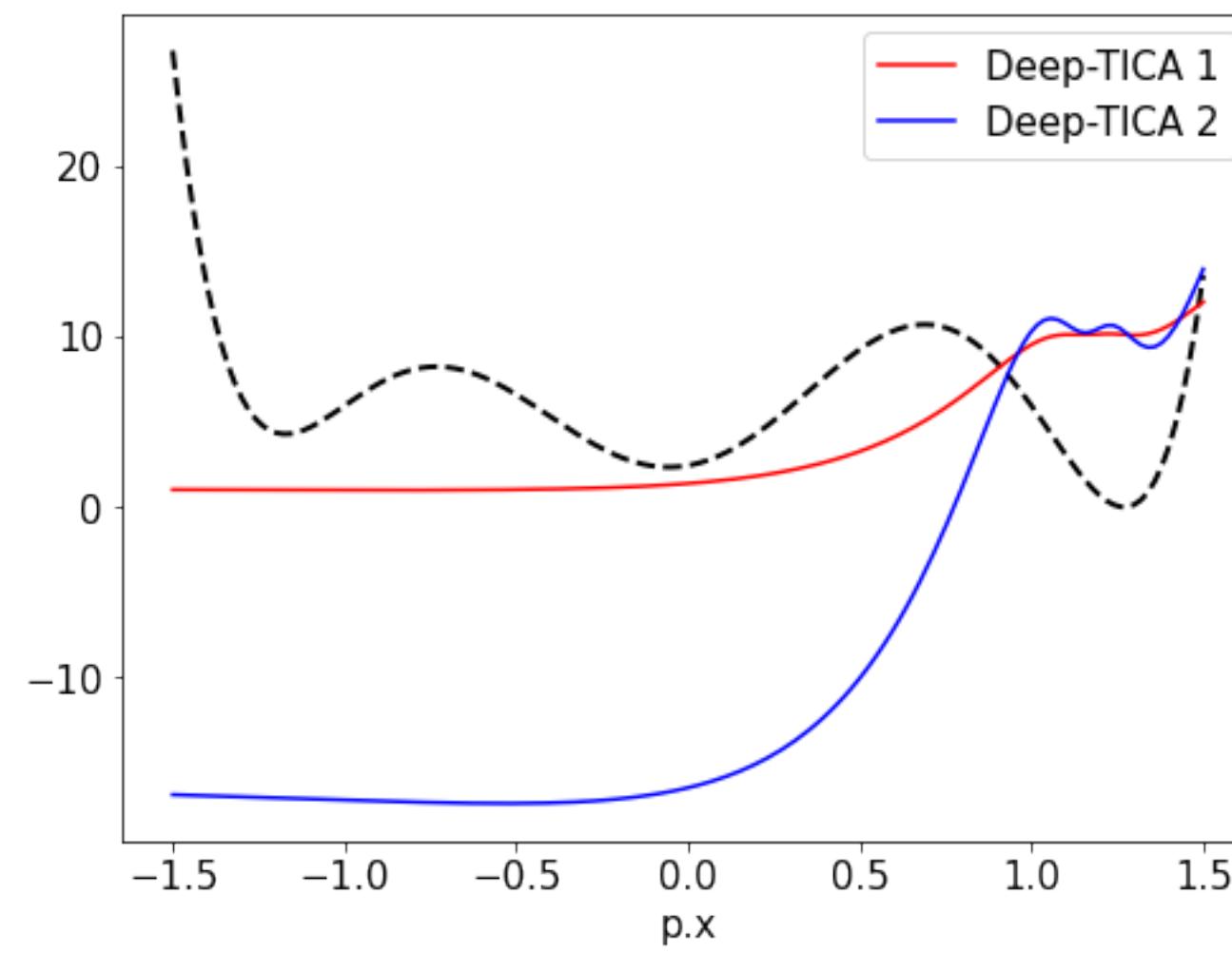
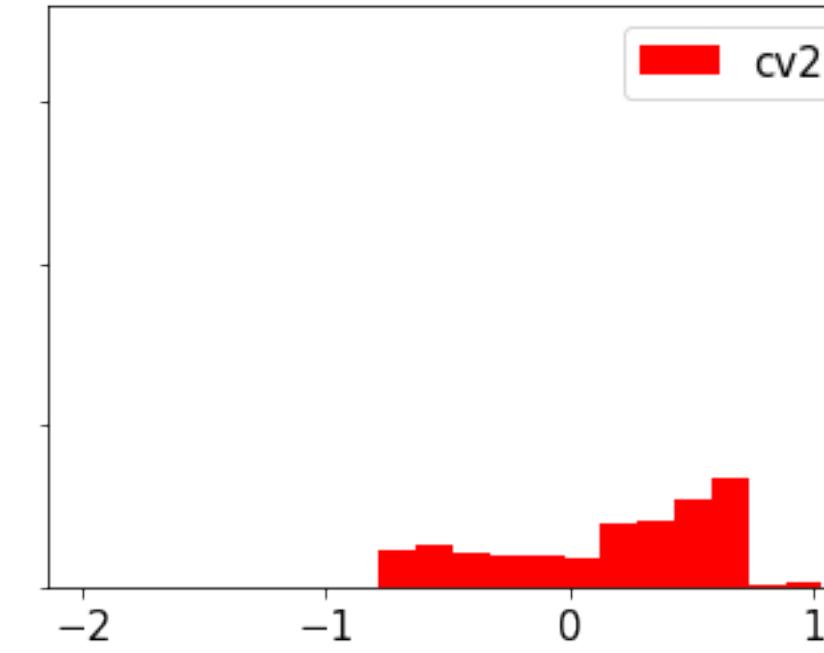
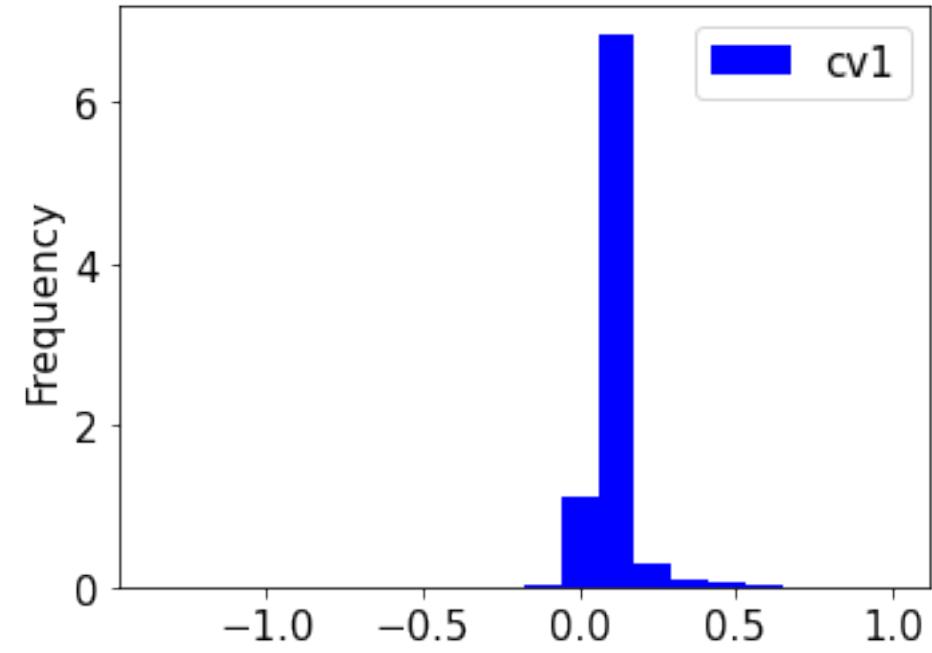
Short TICA biased trajectory



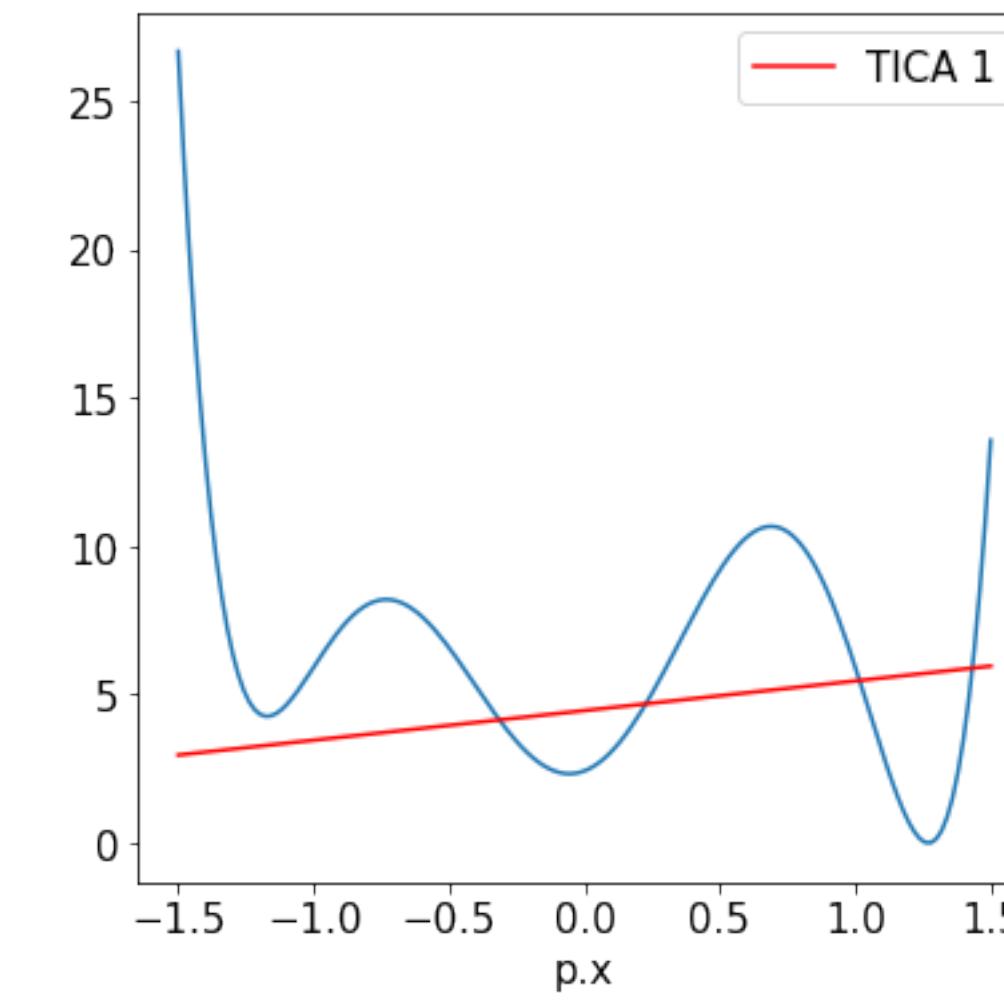
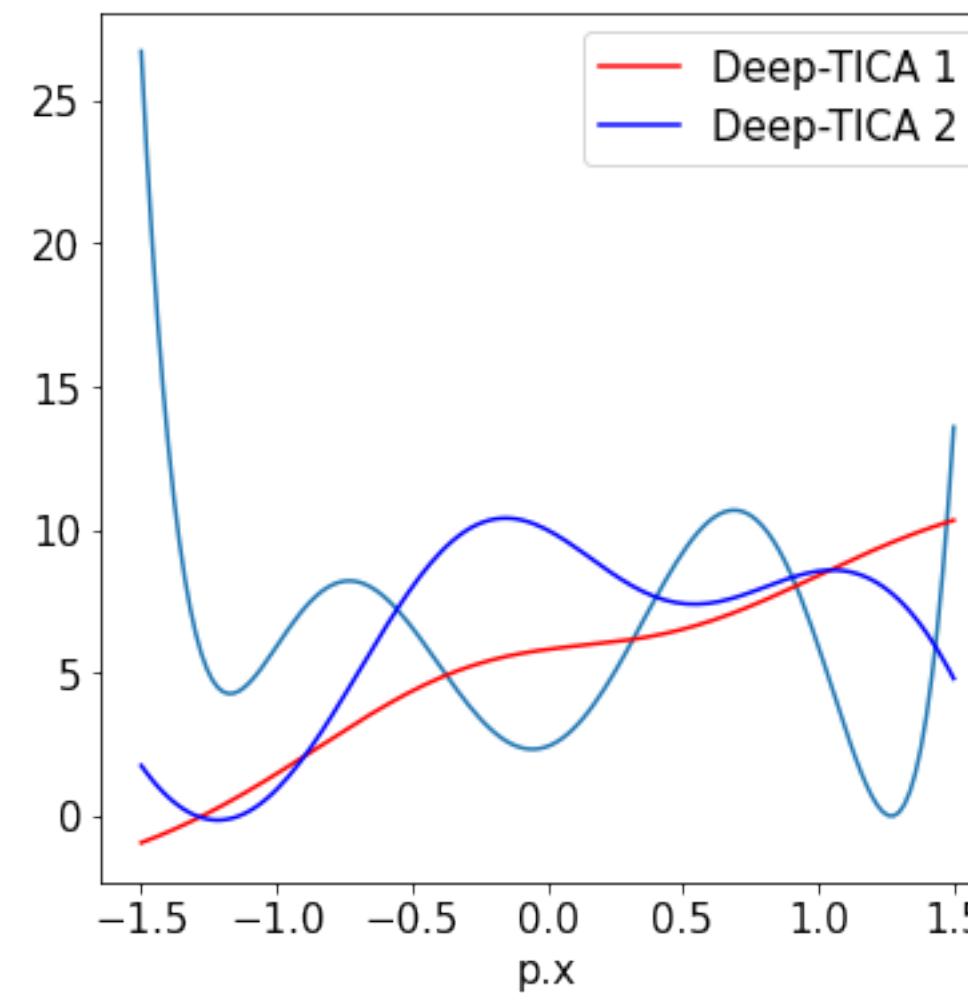
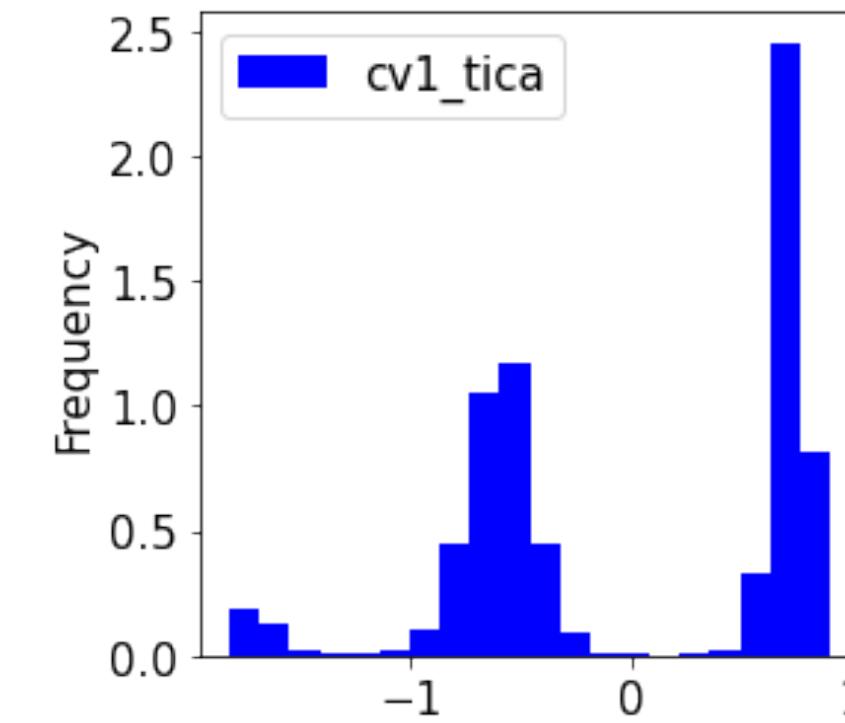
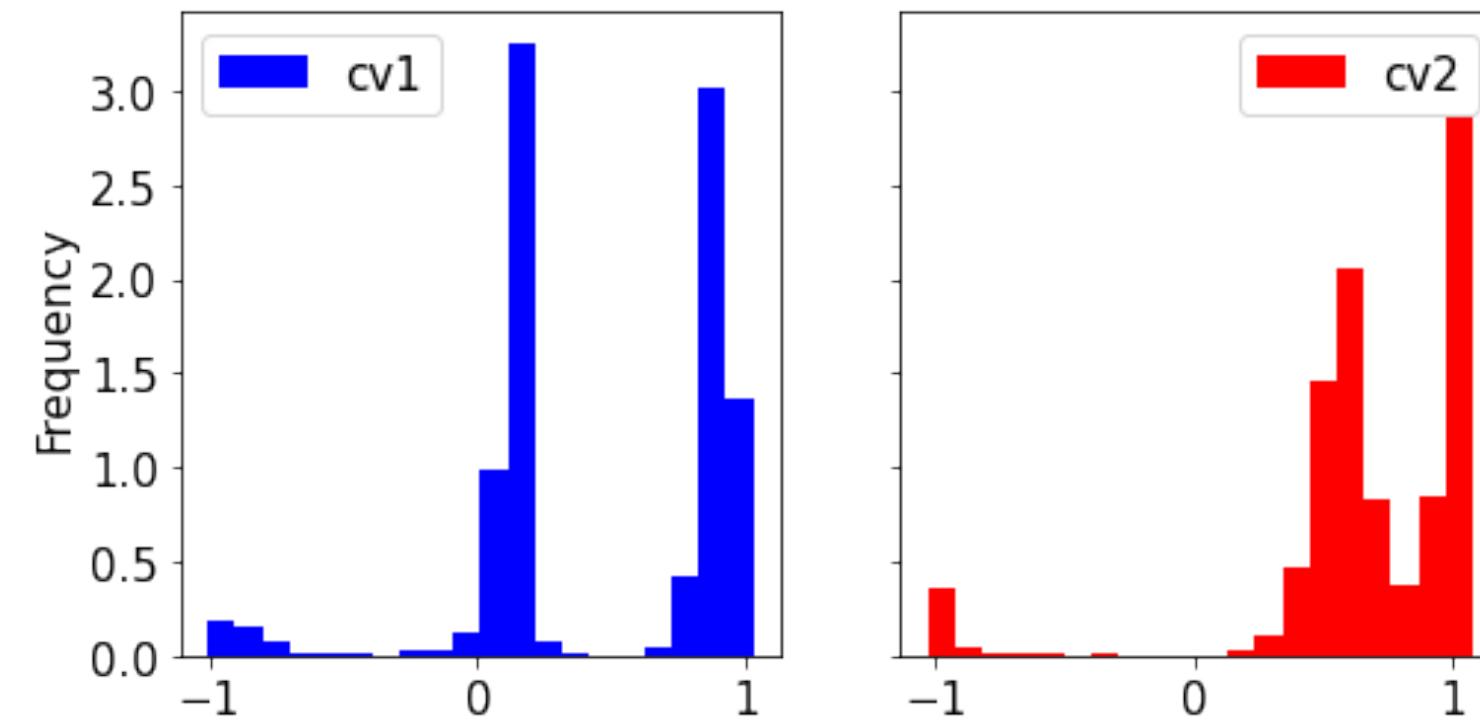
Short Deep-TICA biased trajectory



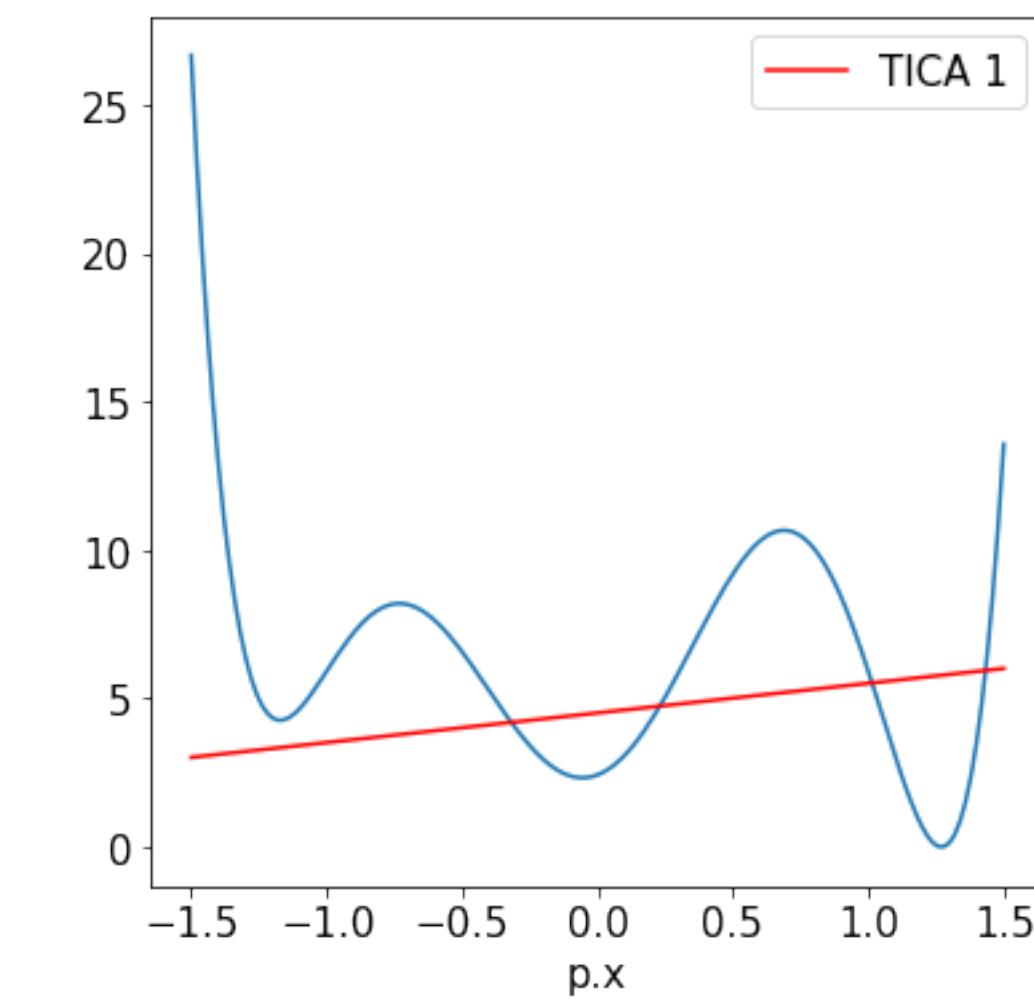
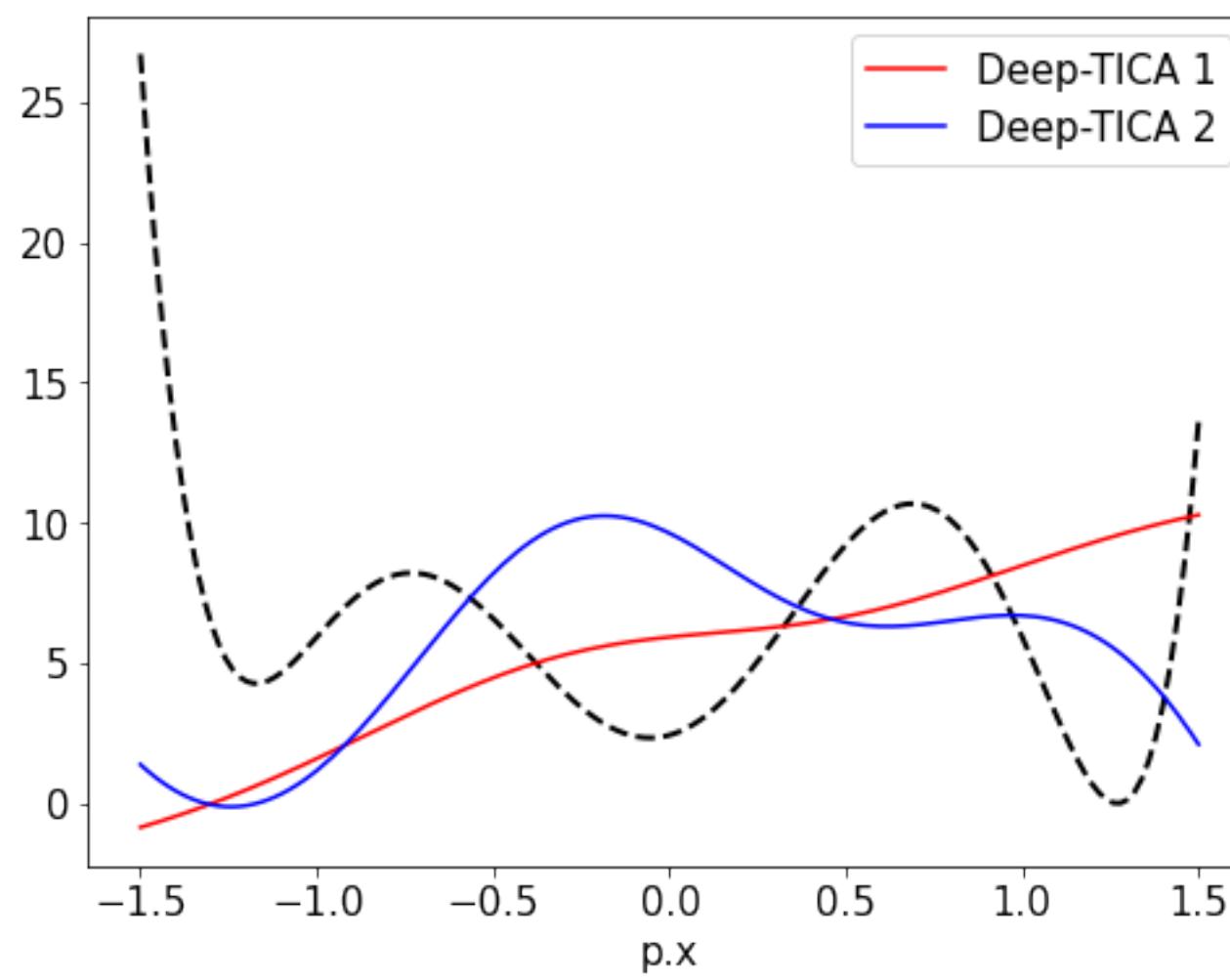
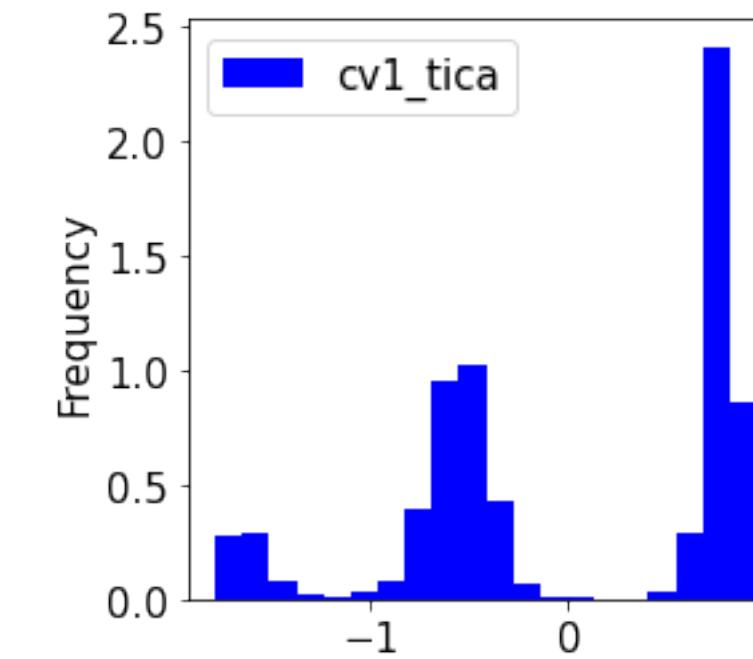
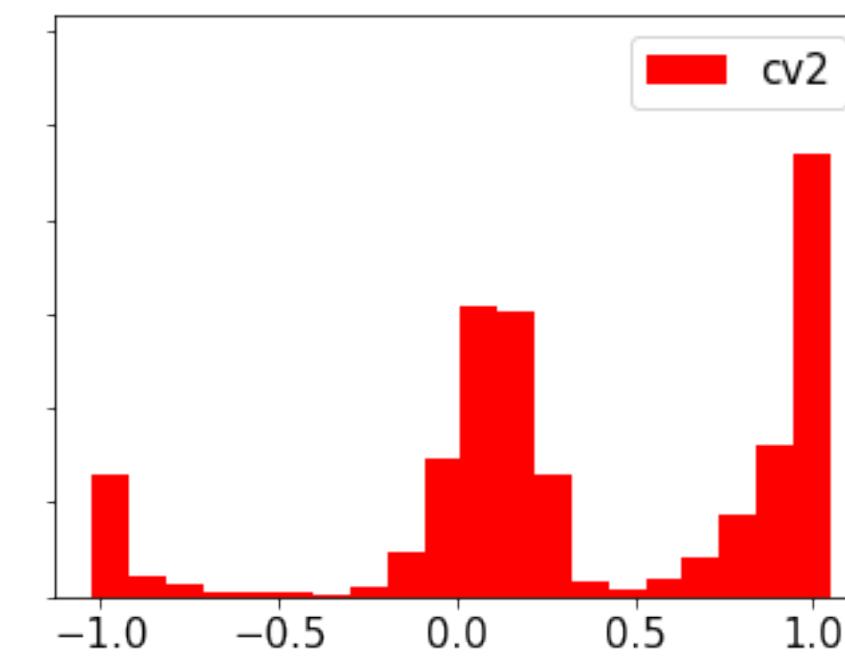
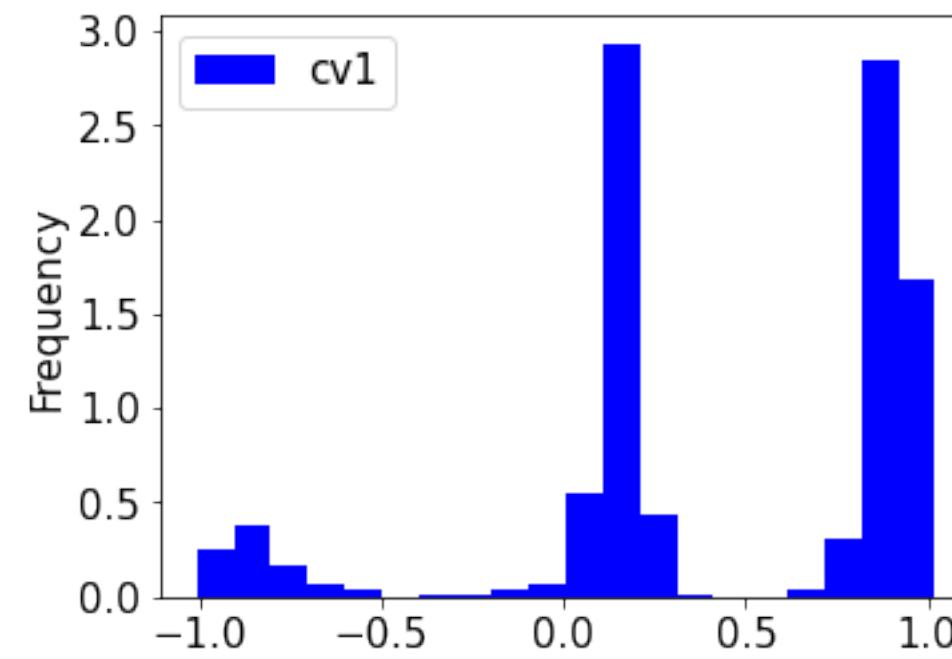
# Deep-TICA & TICA Analysis of short trajectory



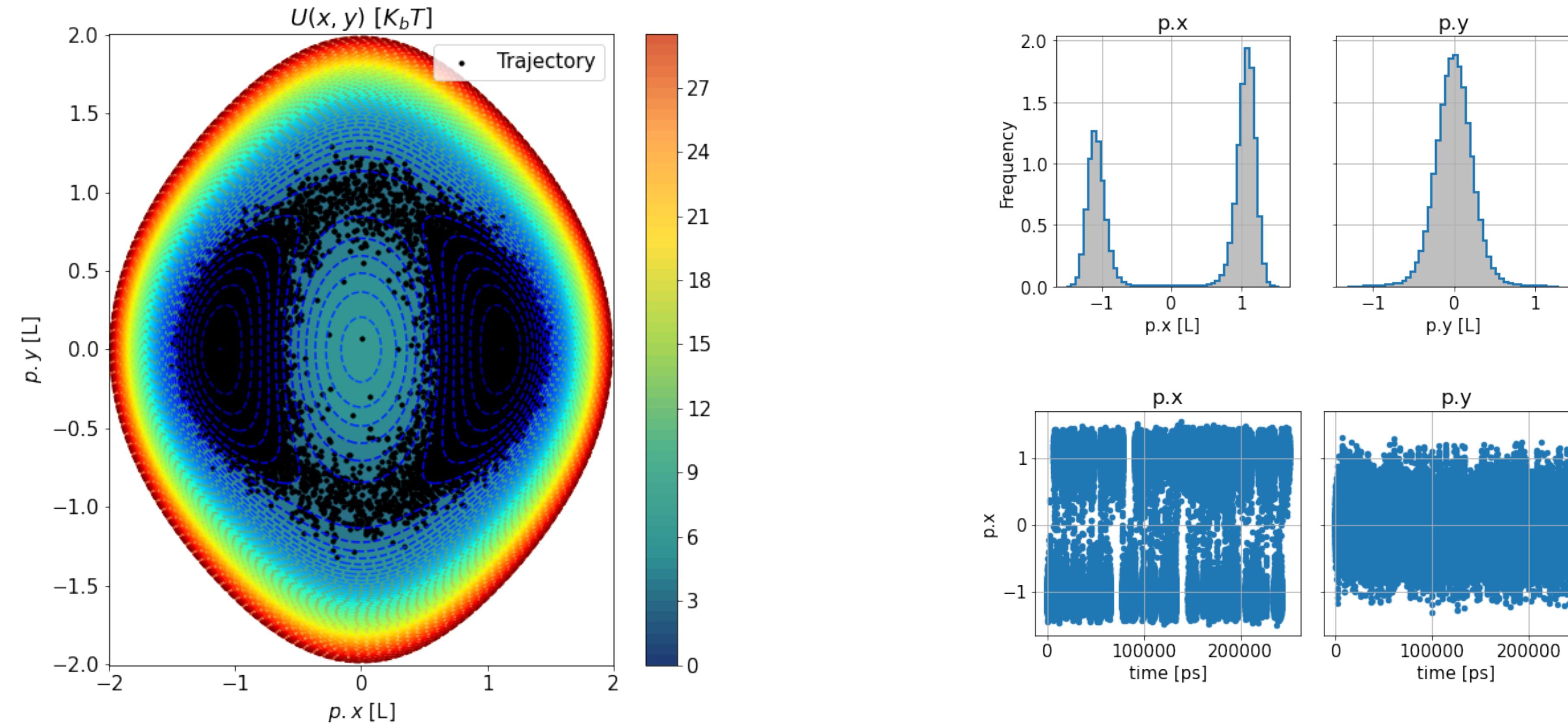
# Deep-TICA & TICA Analysis of TICA biased trajectories



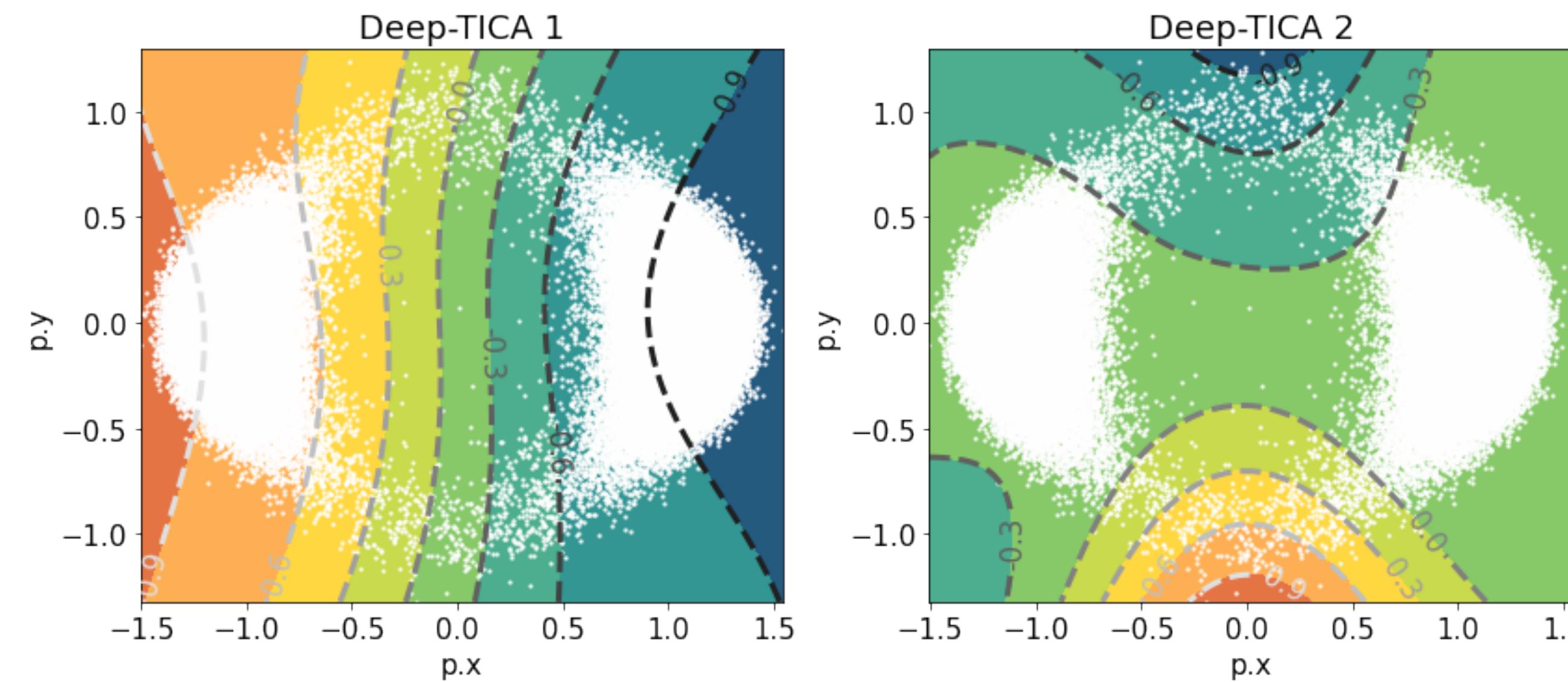
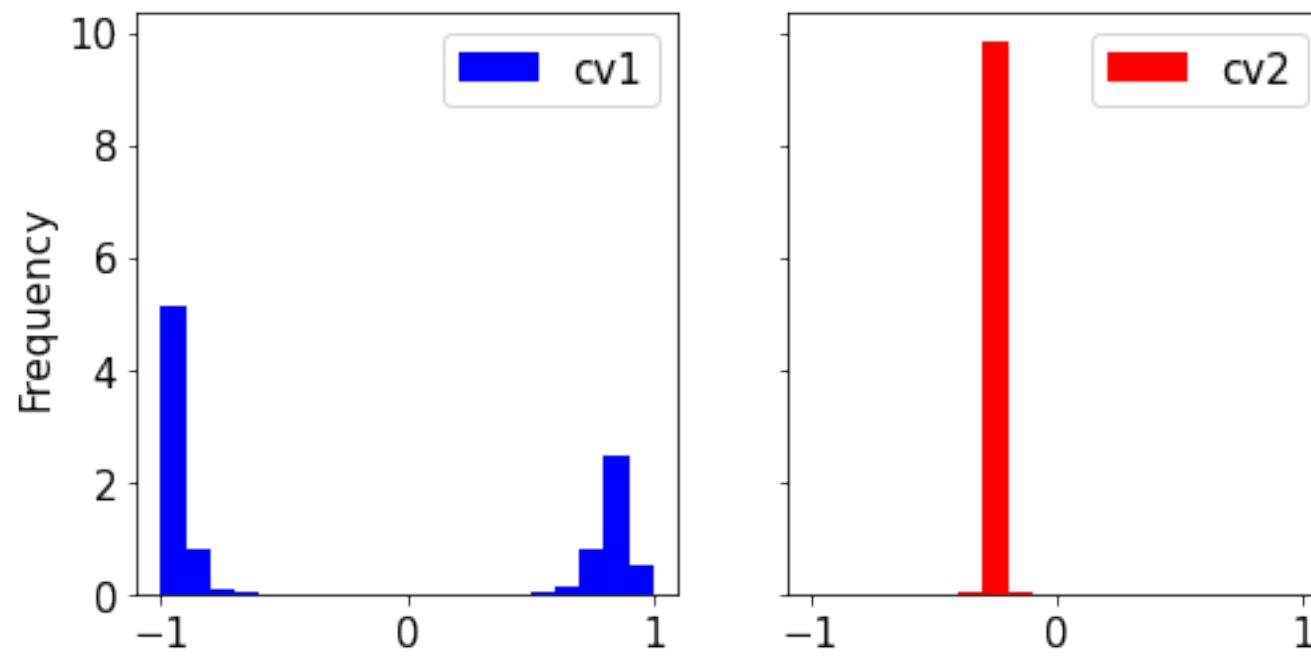
# Deep-TICA & TICA Analysis of Deep-TICA biased trajectories



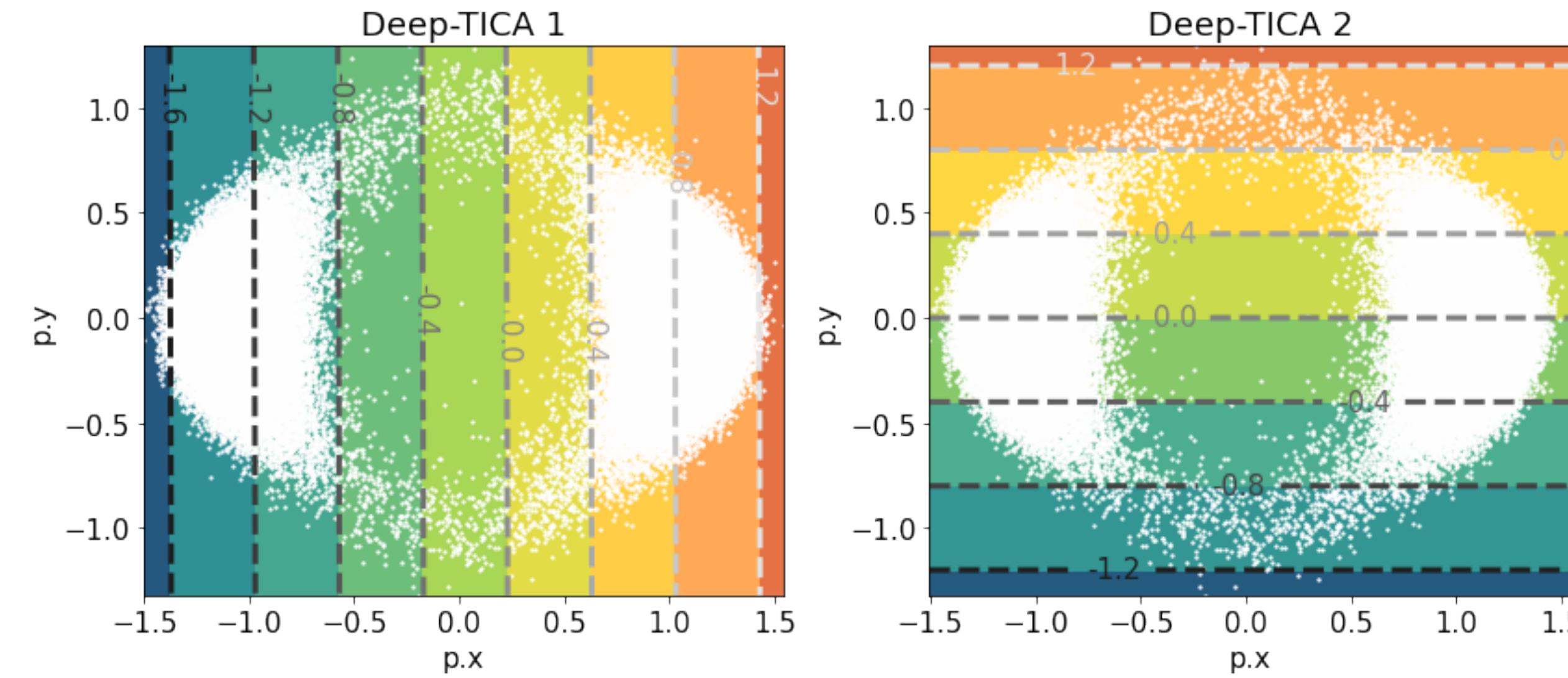
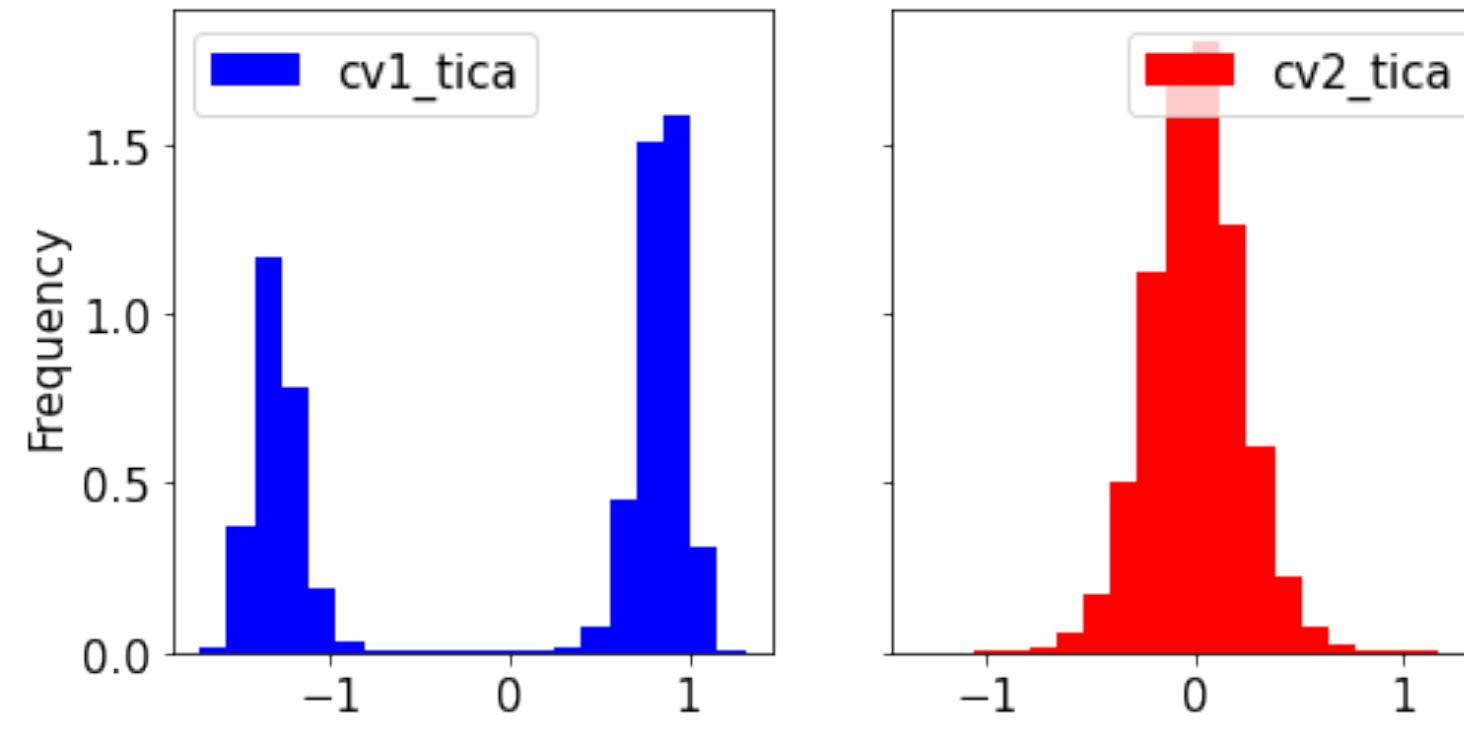
# 2D System



# Deep-TICA Analysis

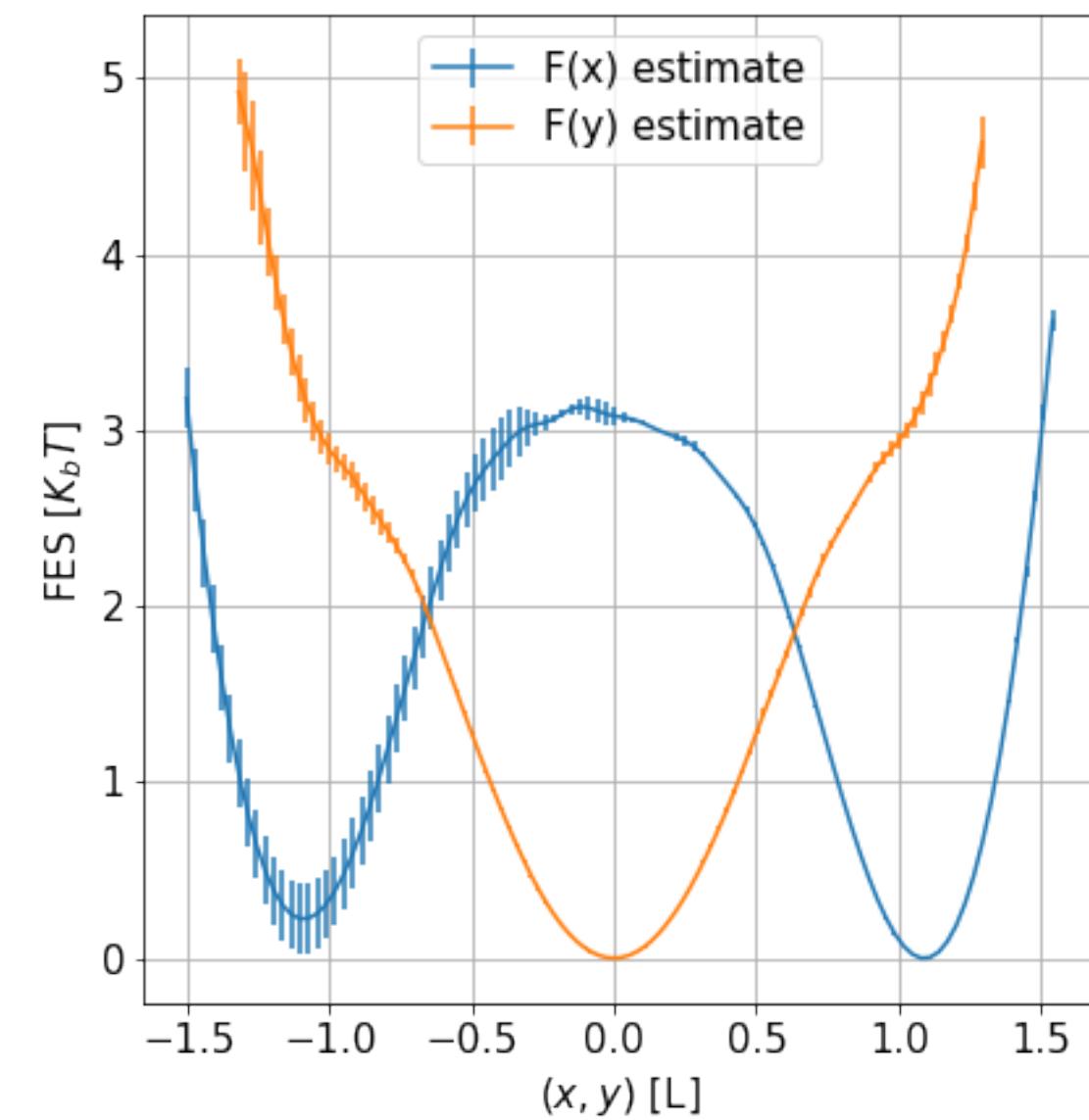


# TICA Analysis

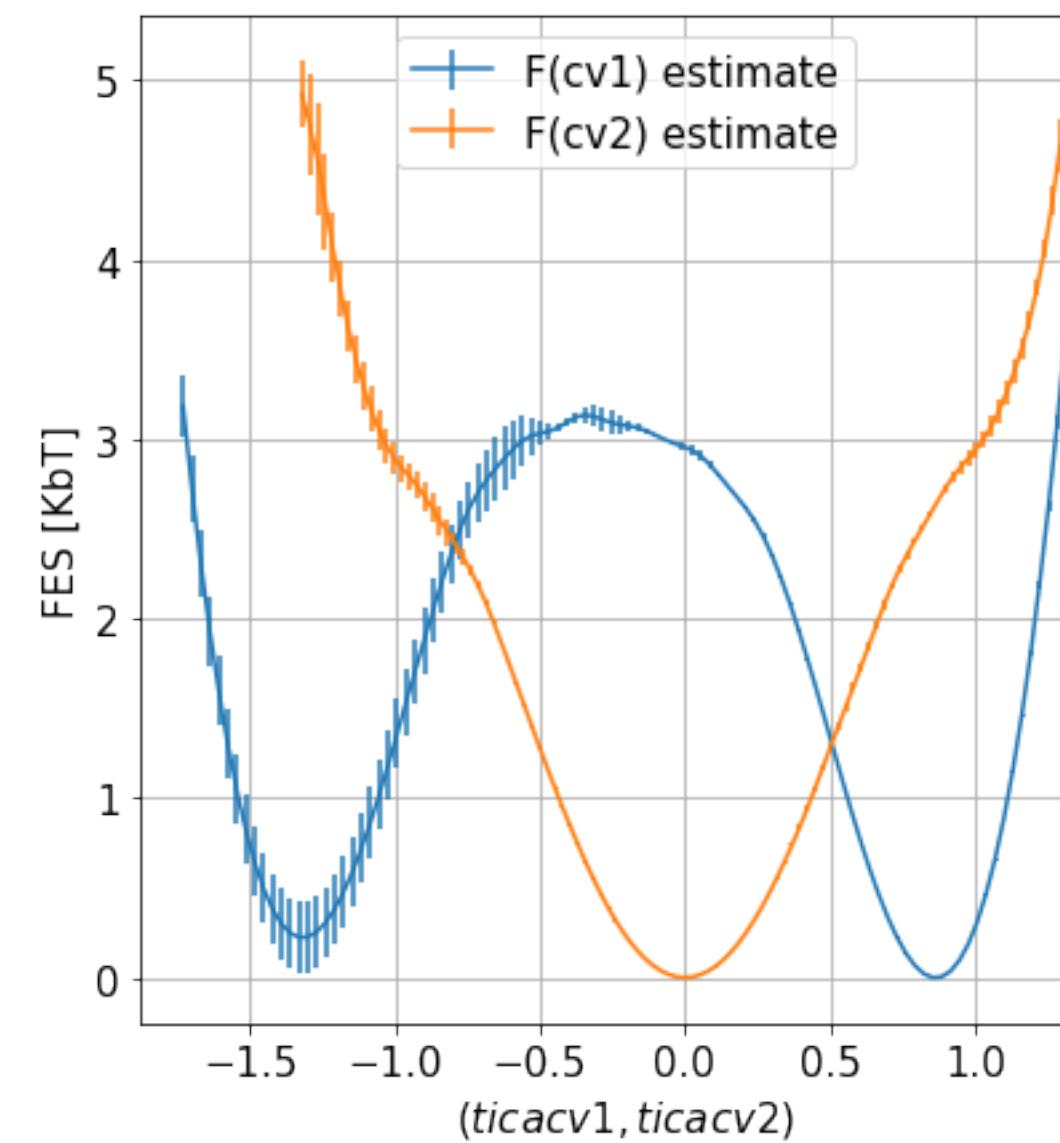


# Free Energies Surface (FES)

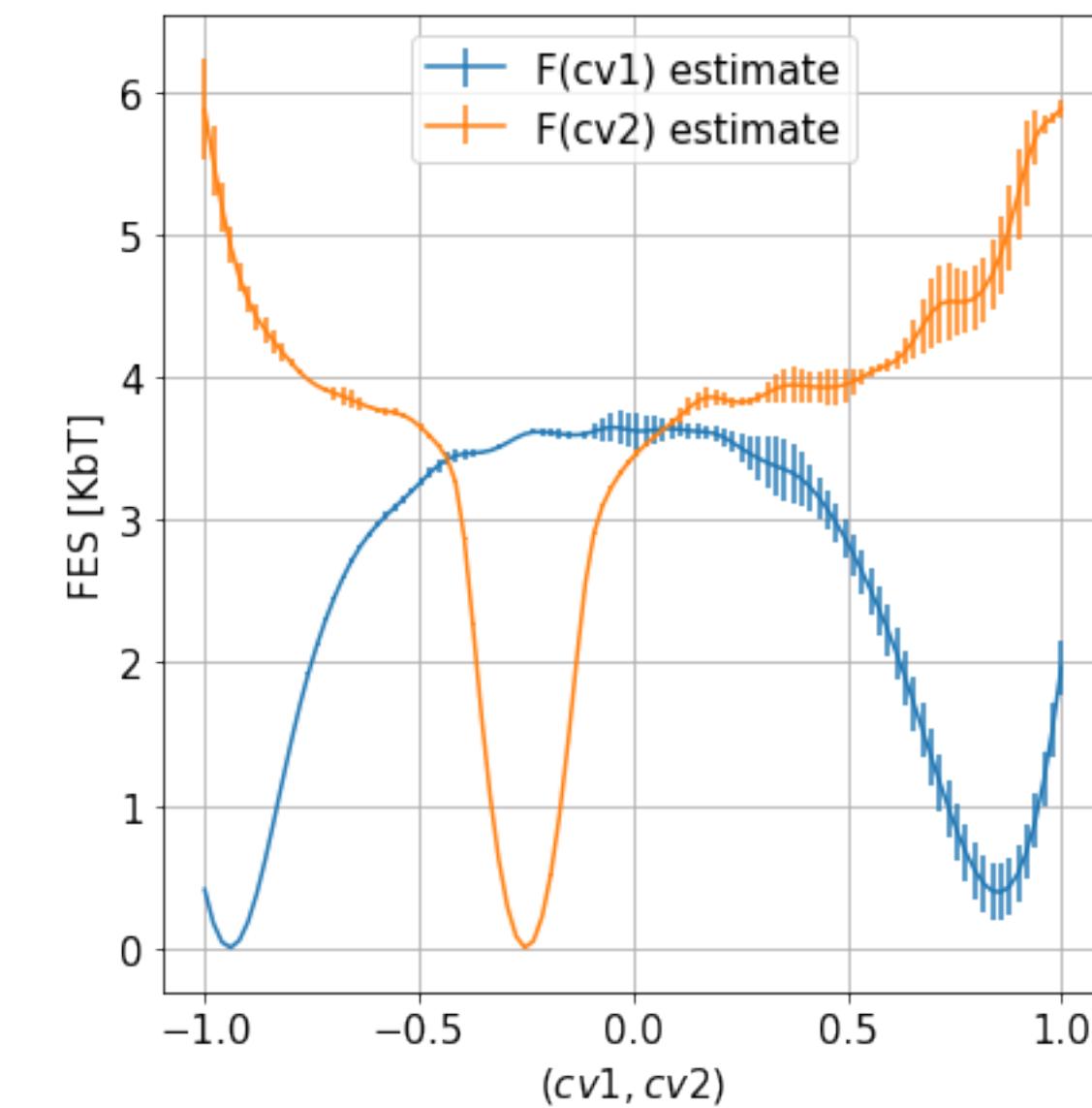
unbiased



TICA biased

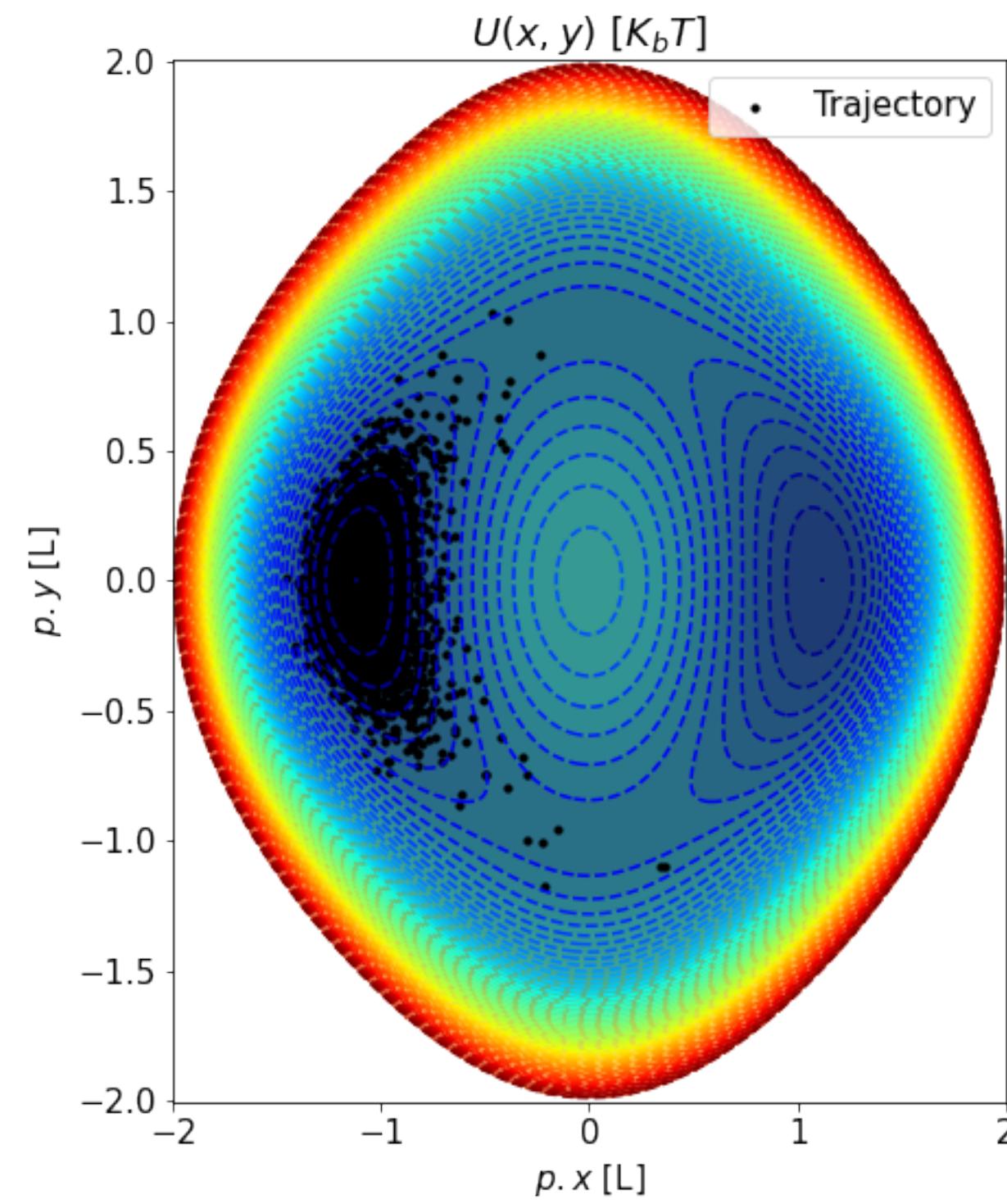


Deep-TICA biased

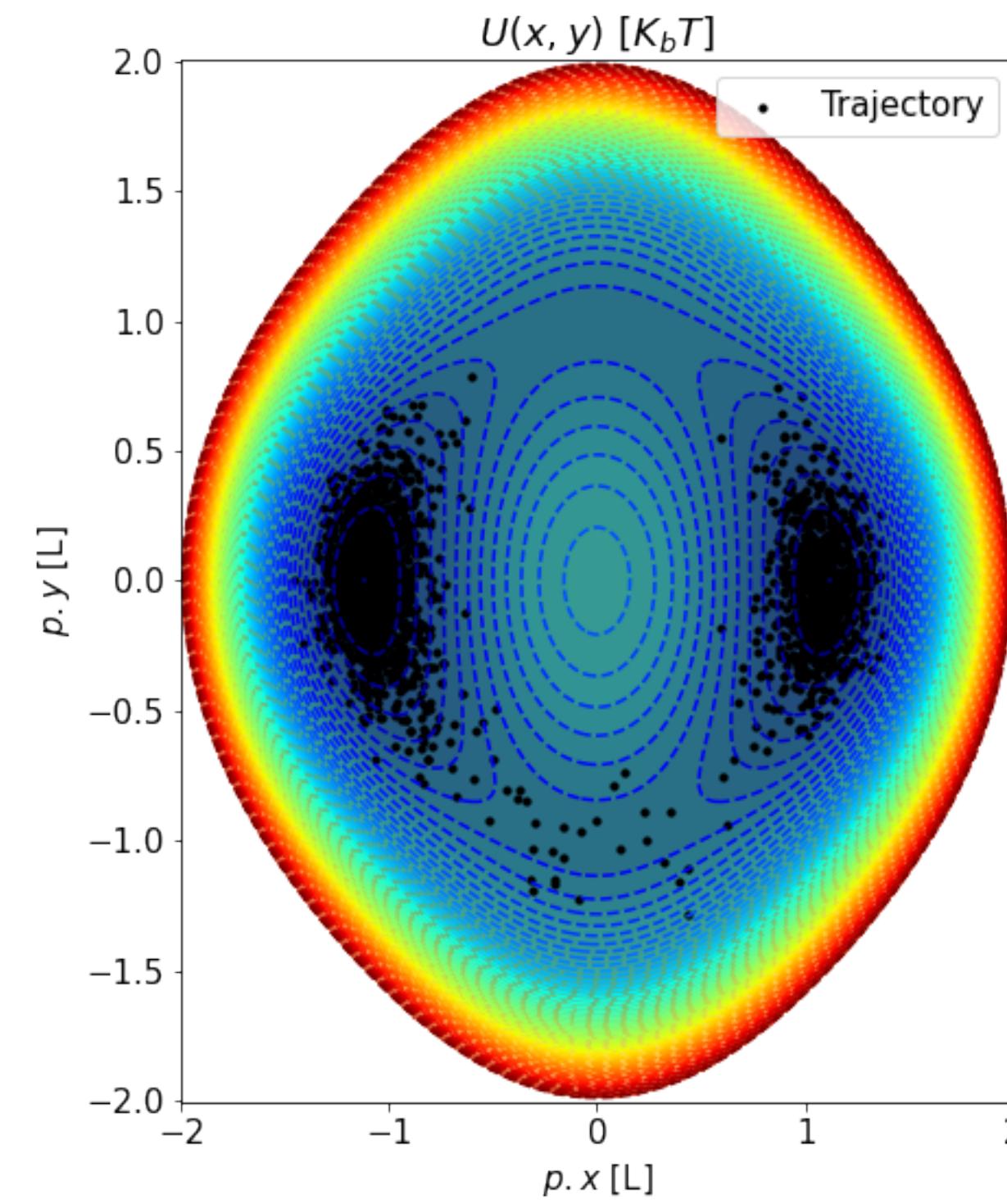


# Short Simulation

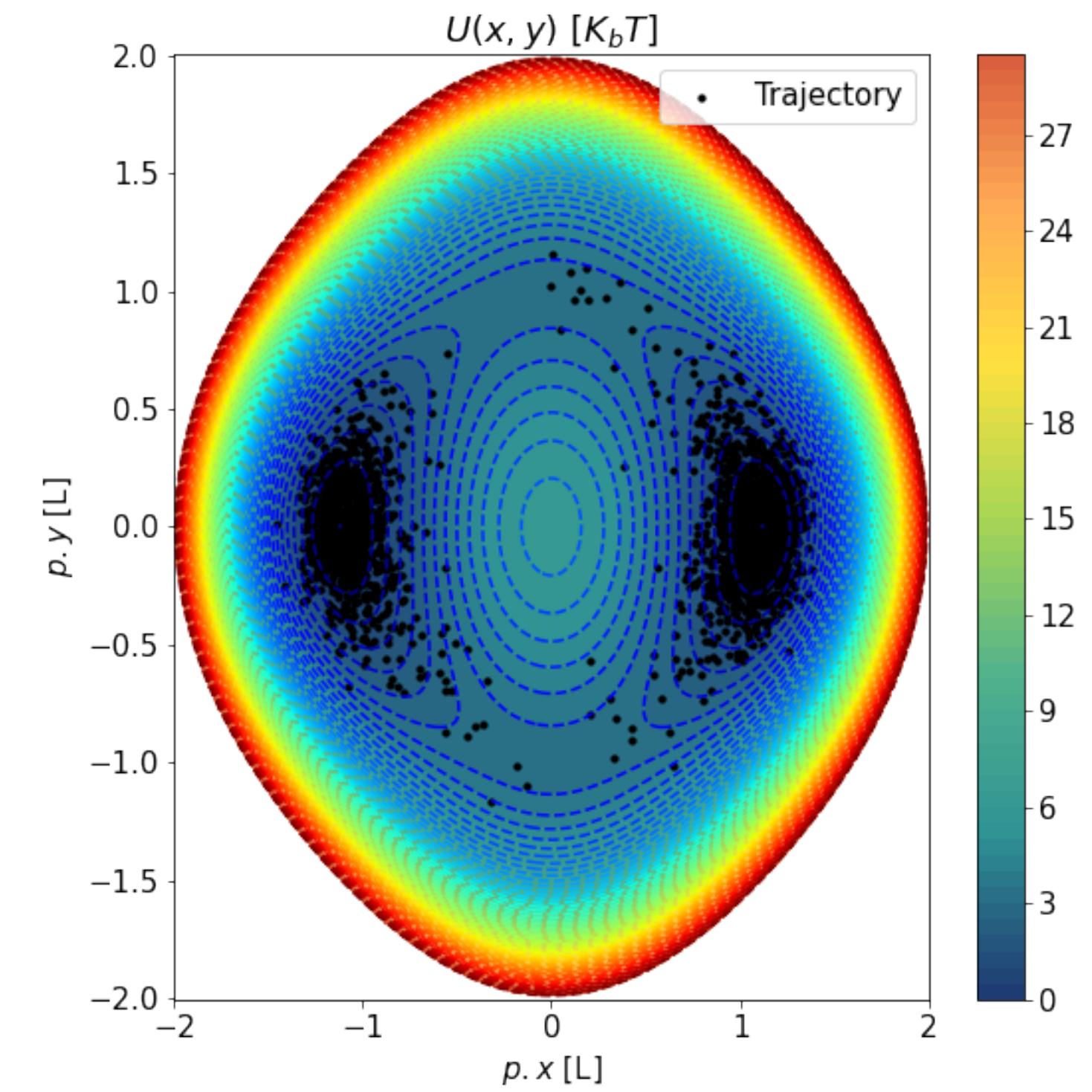
Short unbiased trajectory



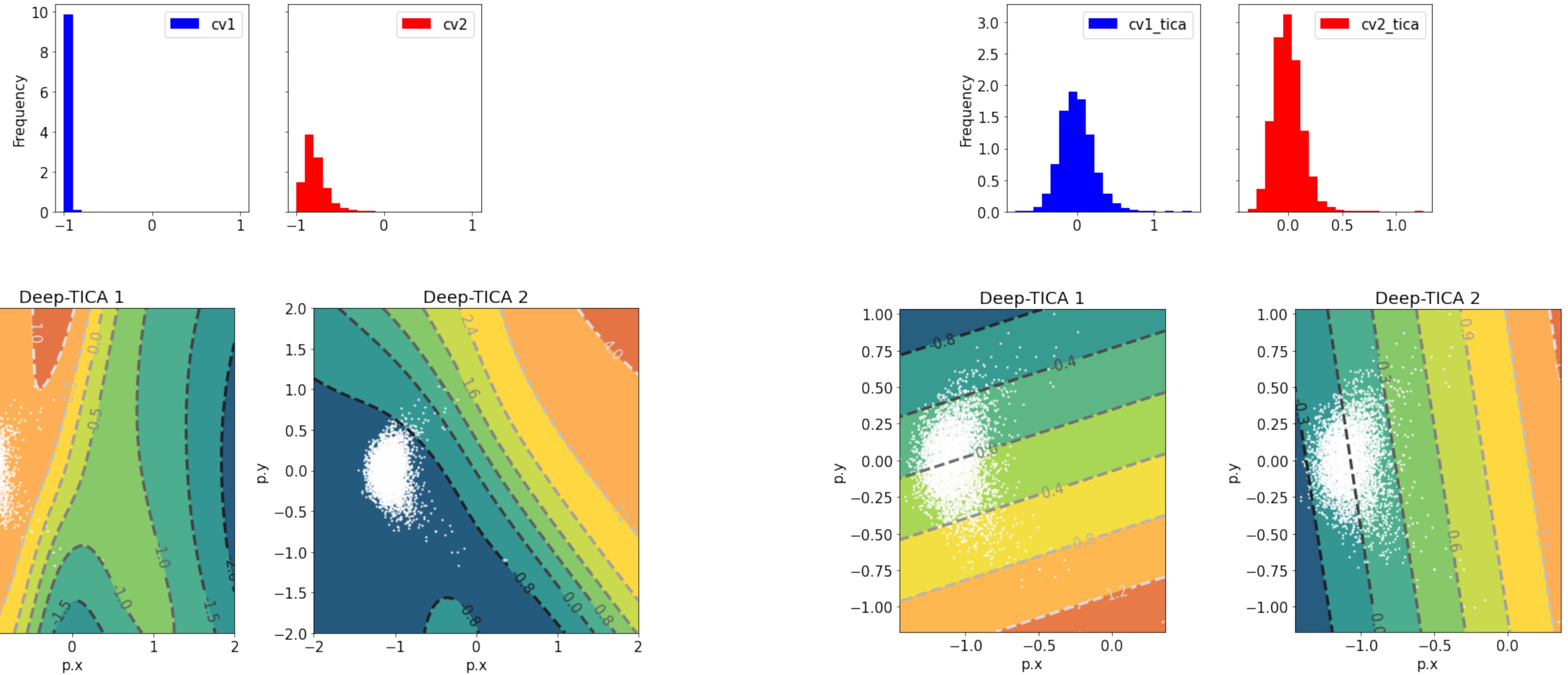
Short TICA biased trajectory



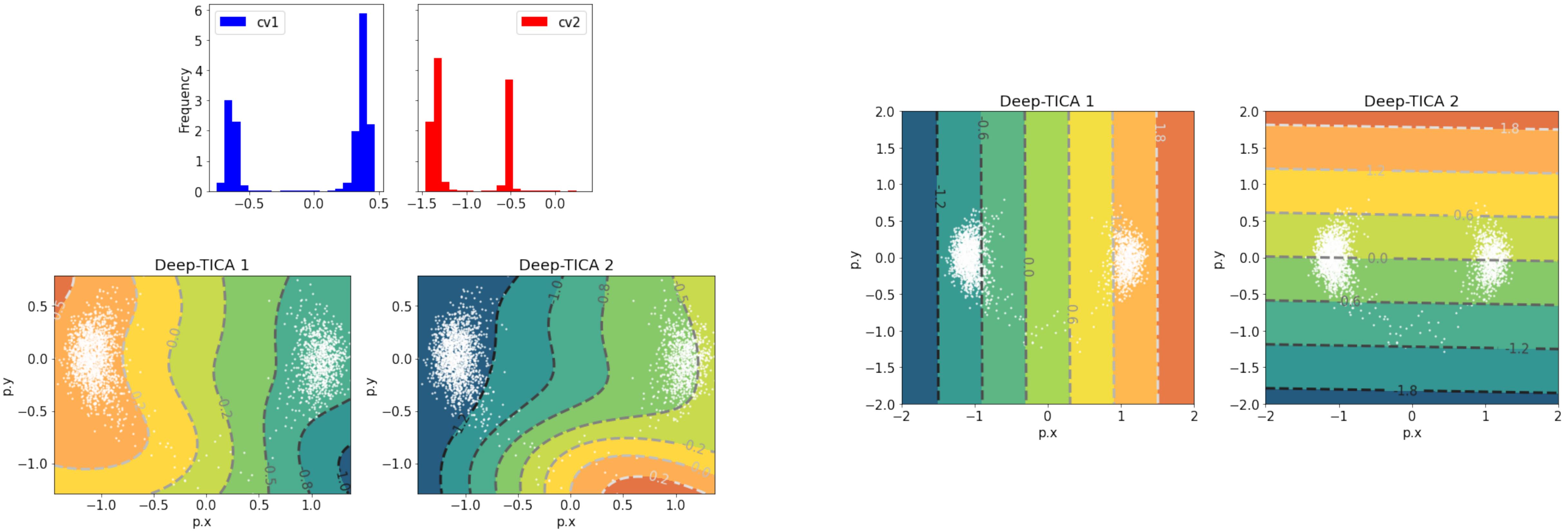
Short Deep-TICA biased trajectory



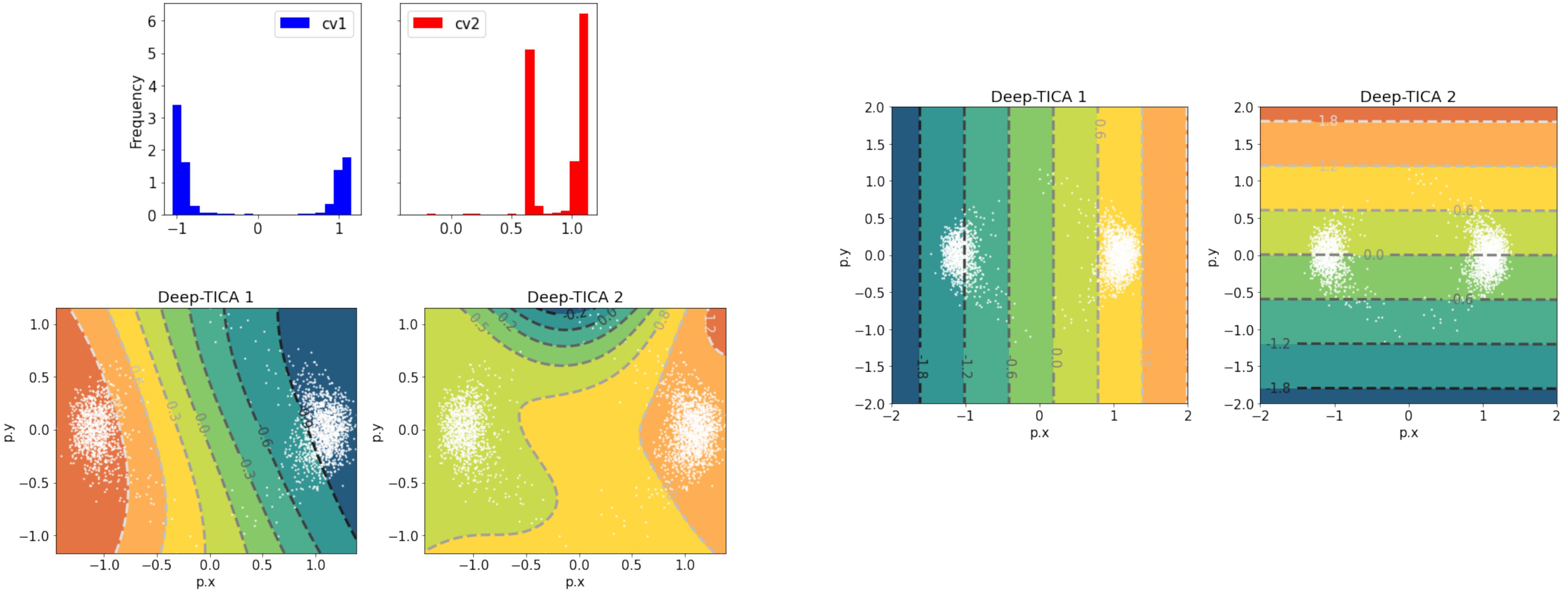
# Deep-TICA & TICA Analysis short trajectory



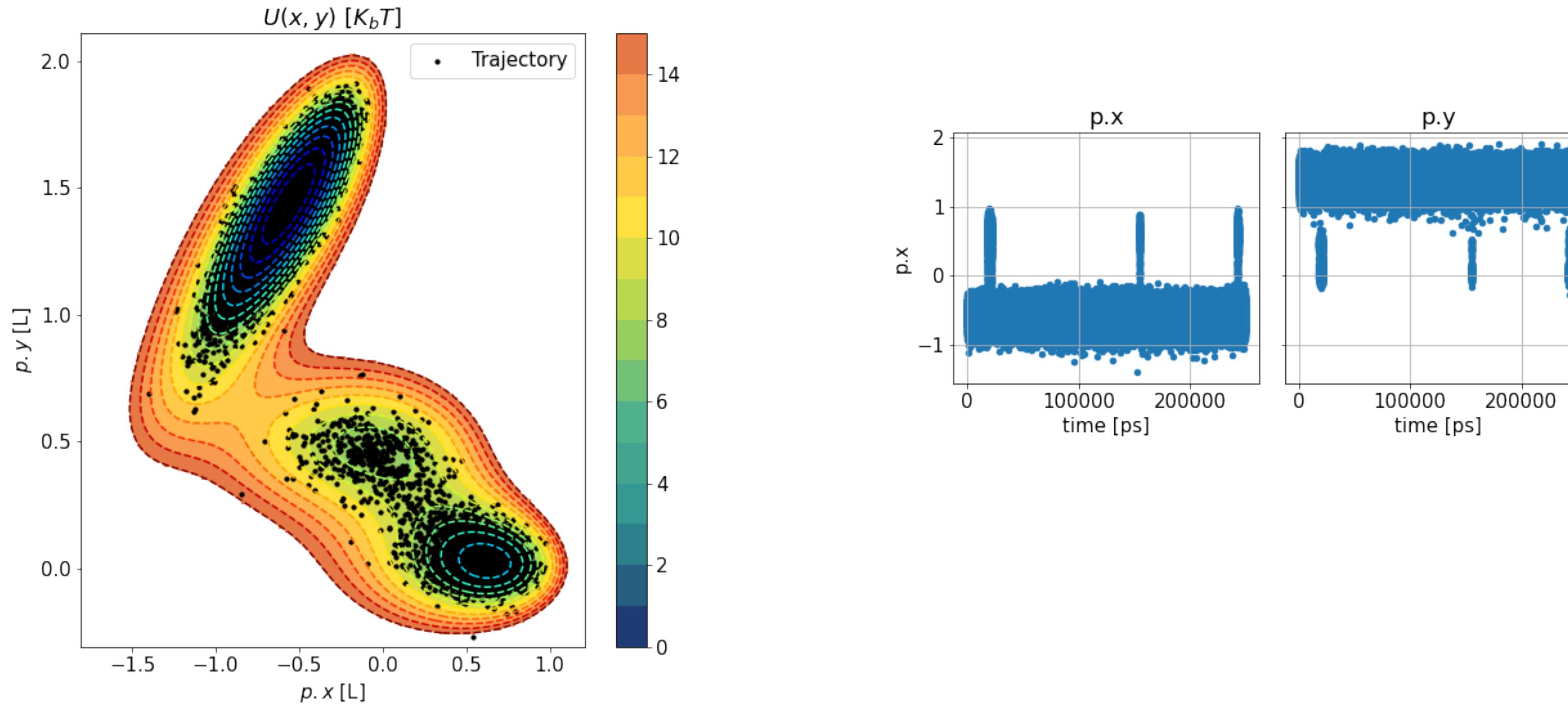
# Deep-TICA & TICA Analysis of TICA biased trajectories



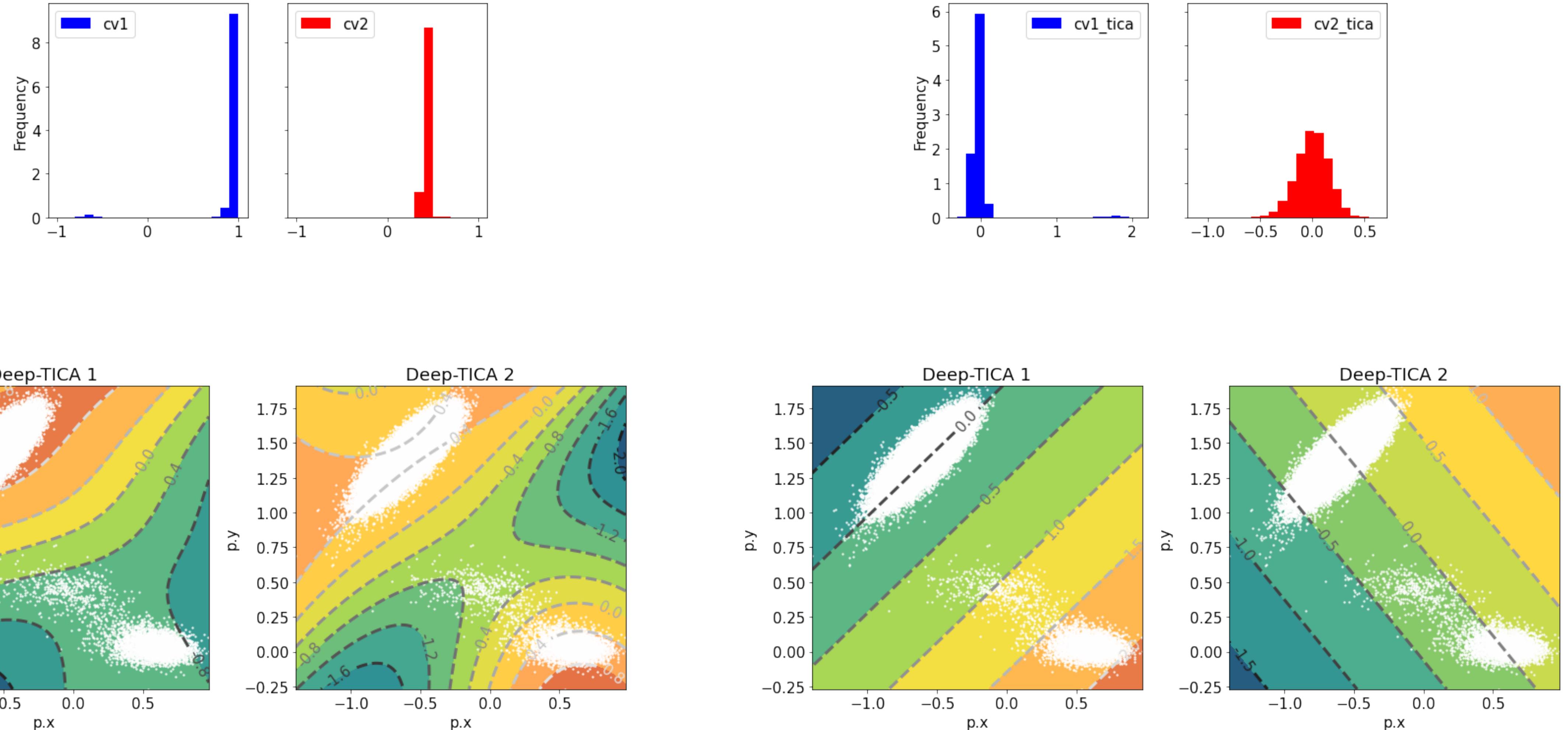
# Deep-TICA & TICA Analysis of Deep-TICA biased trajectories



# Muller Potential

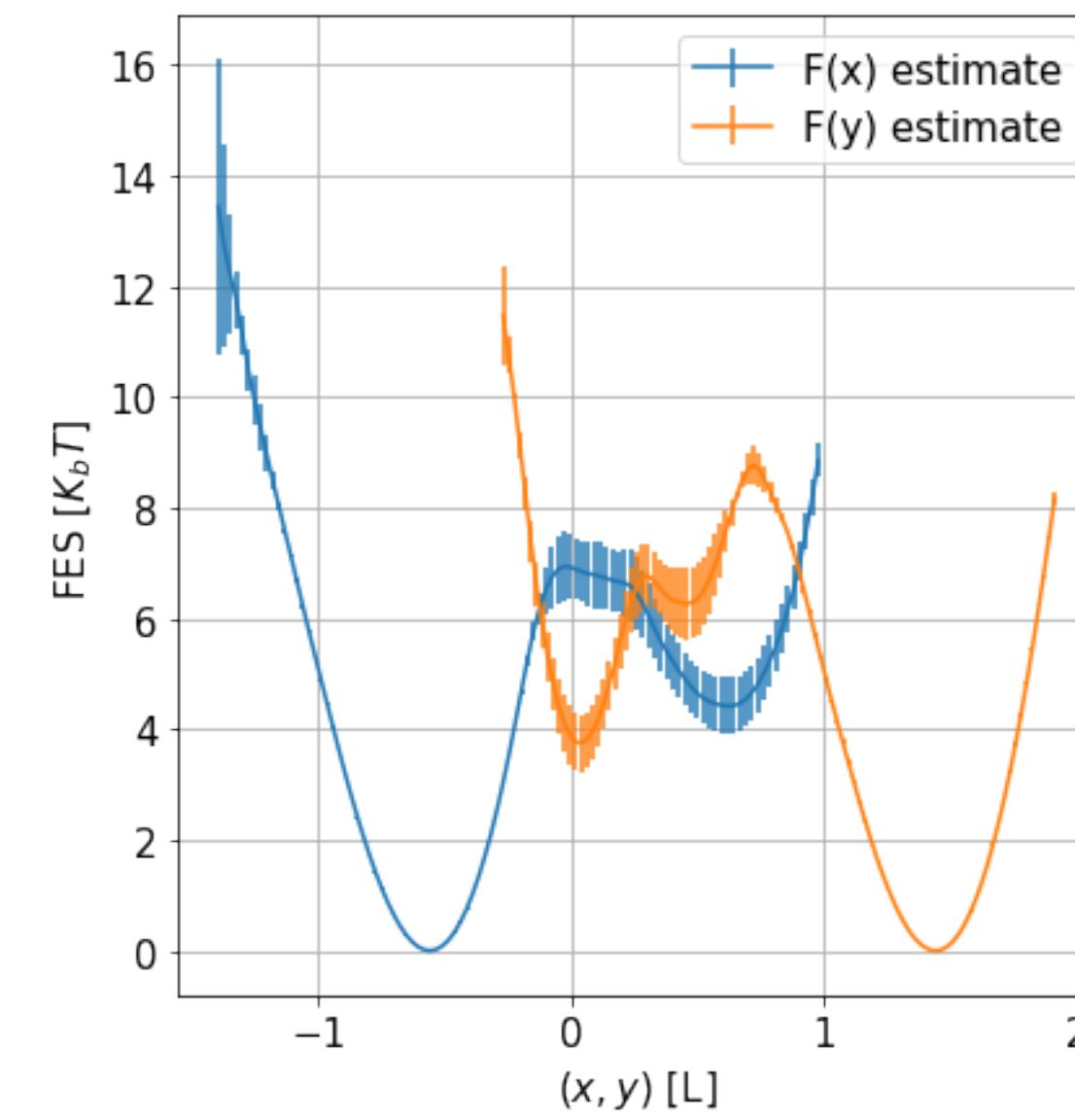


# Deep-TICA & TICA Analysis

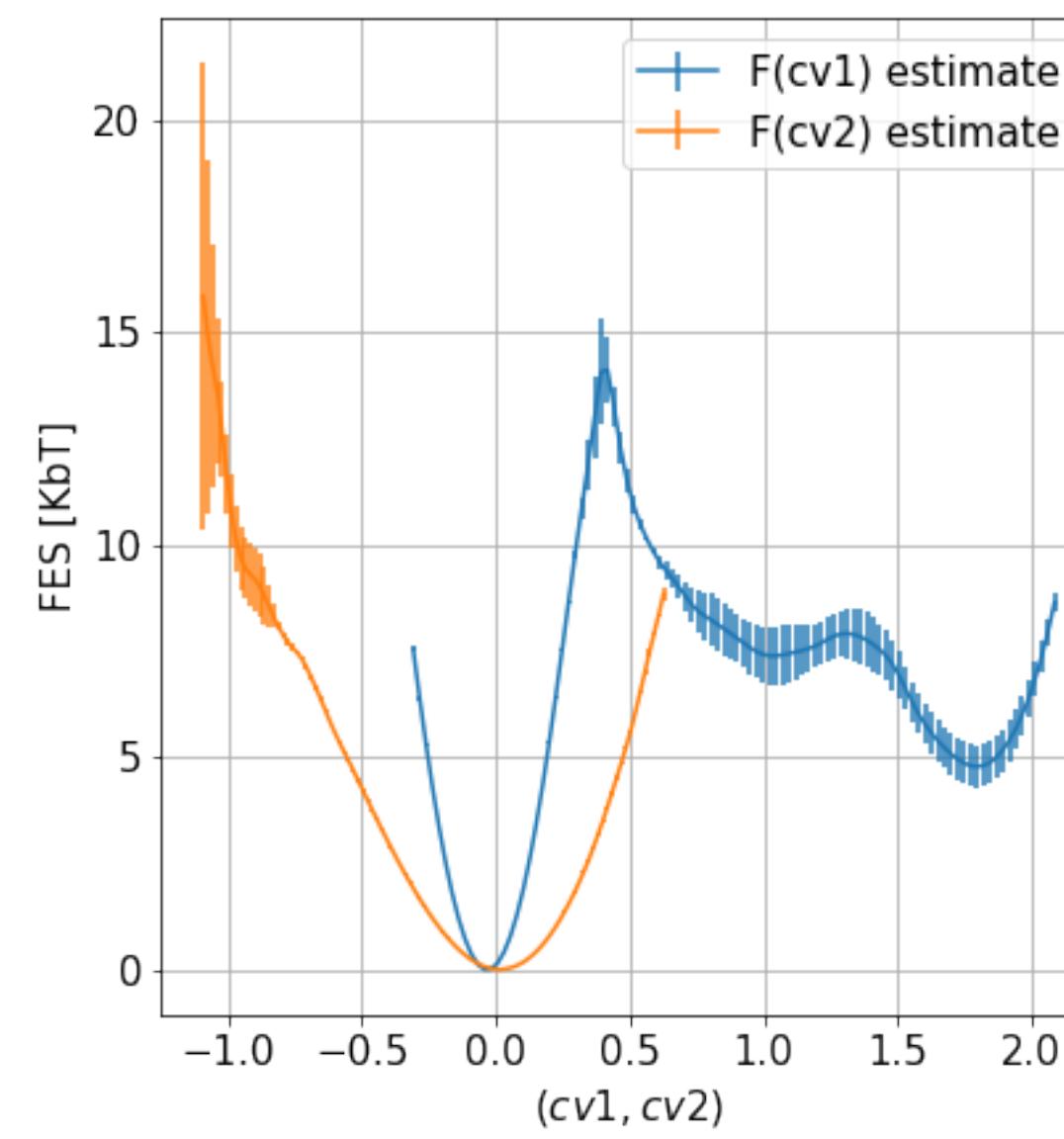


# Deep-TICA & TICA FES

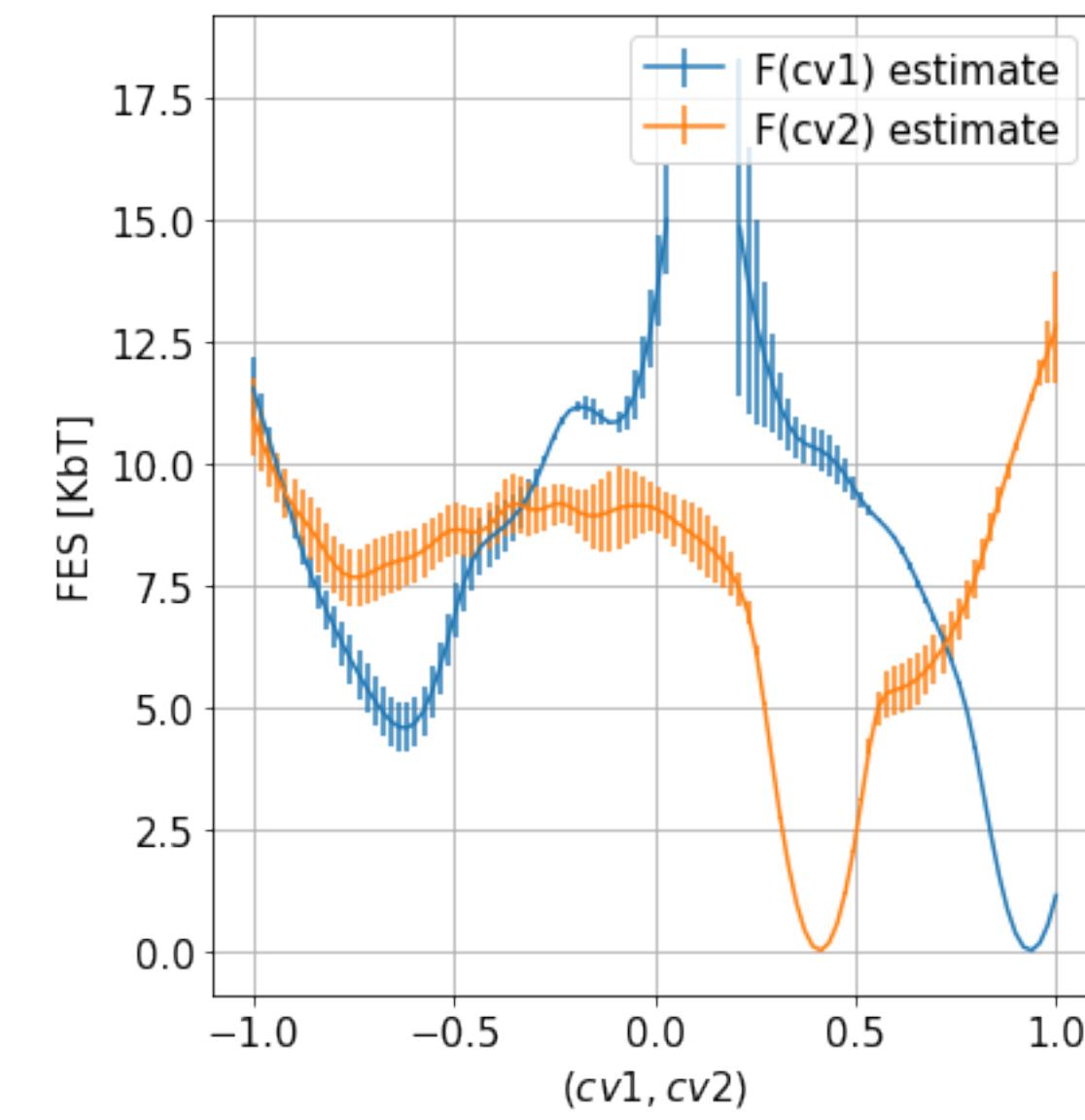
unbiased



TICA biased

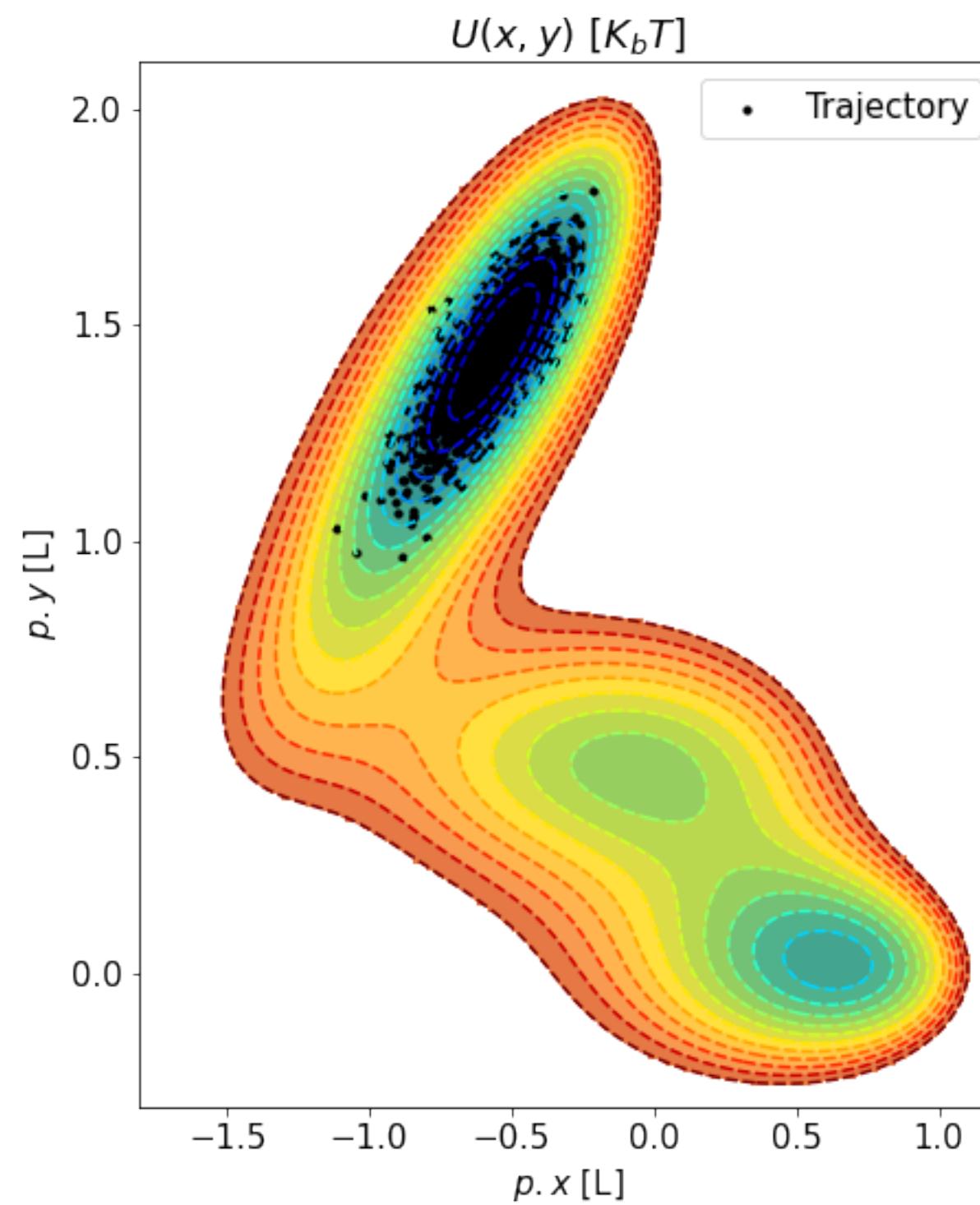


Deep-TICA biased

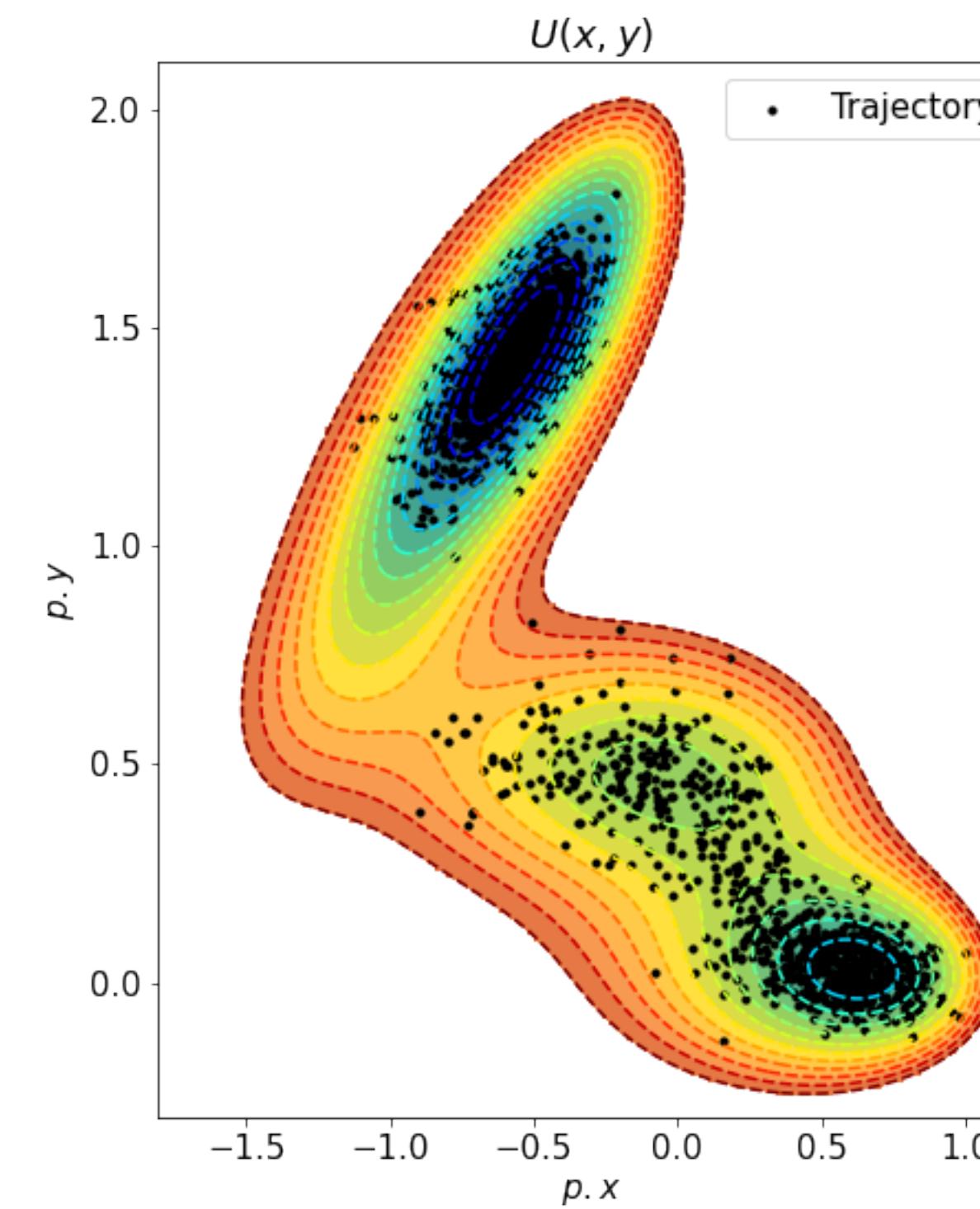


# Short Simulation

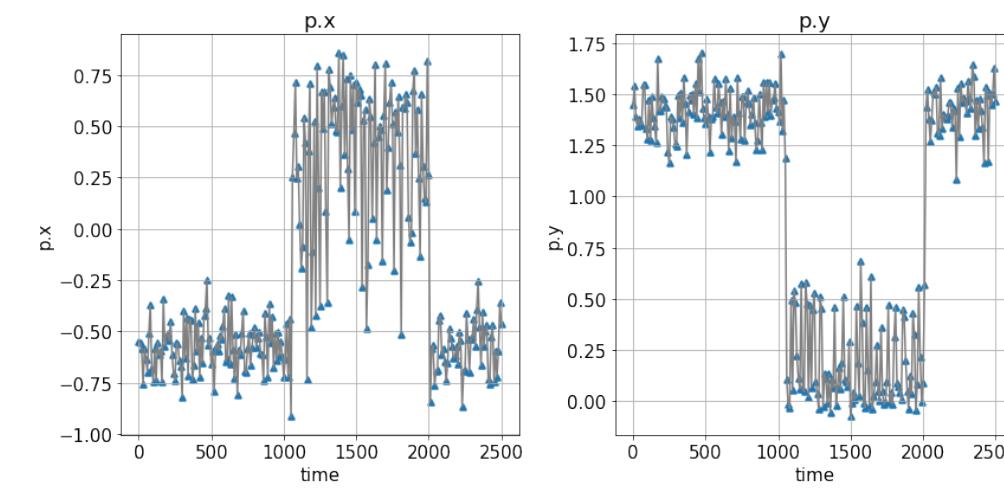
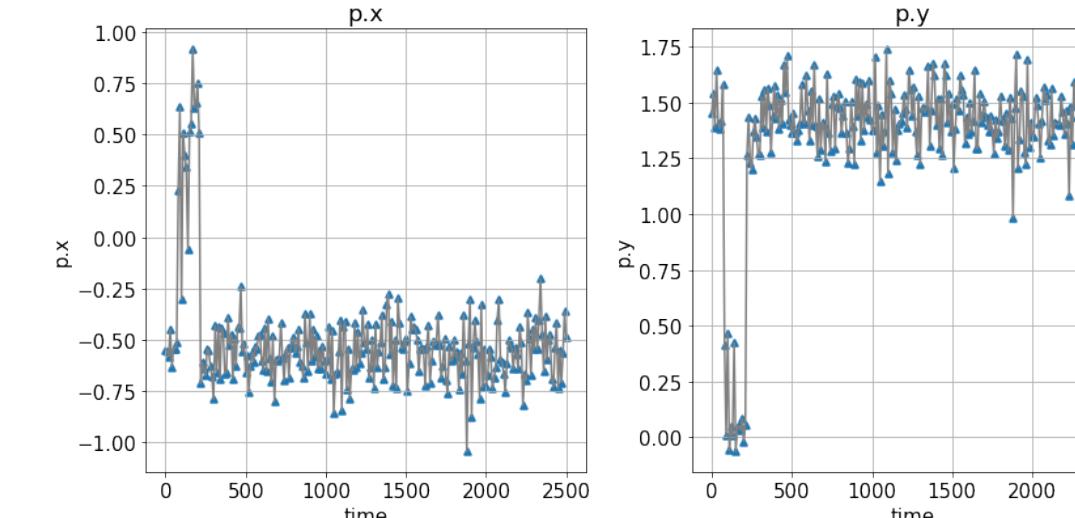
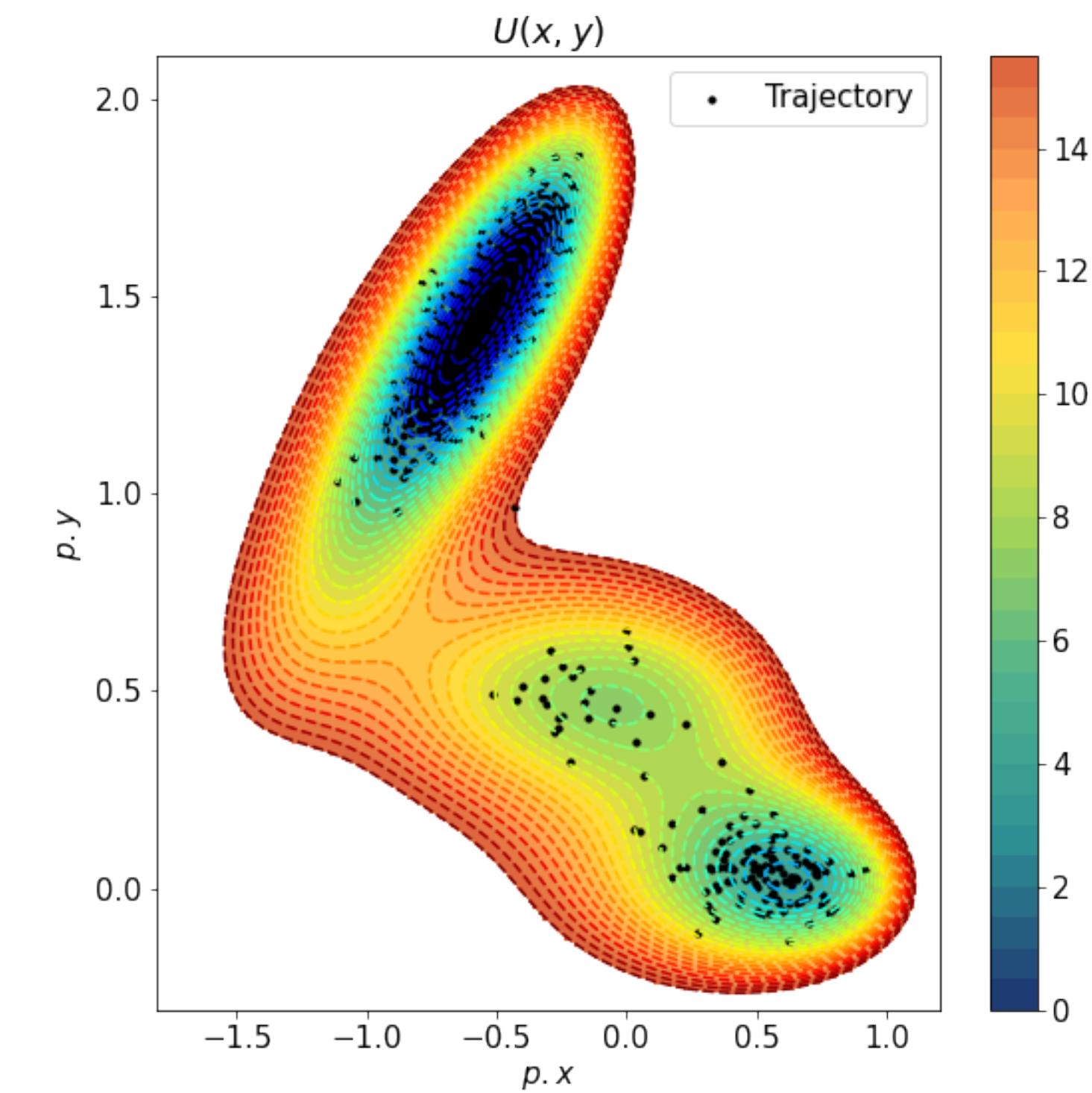
Short unbiased trajectory



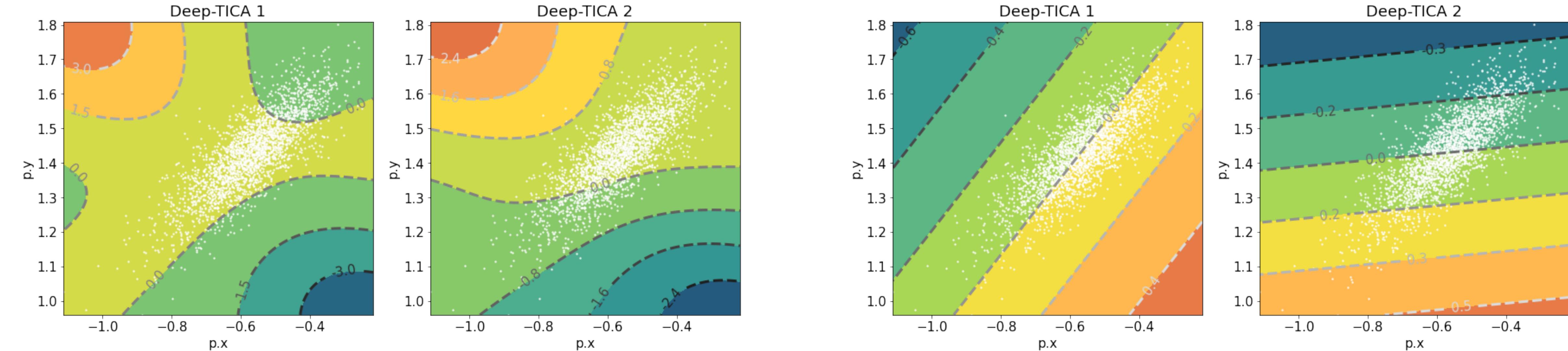
Short TICA biased trajectory



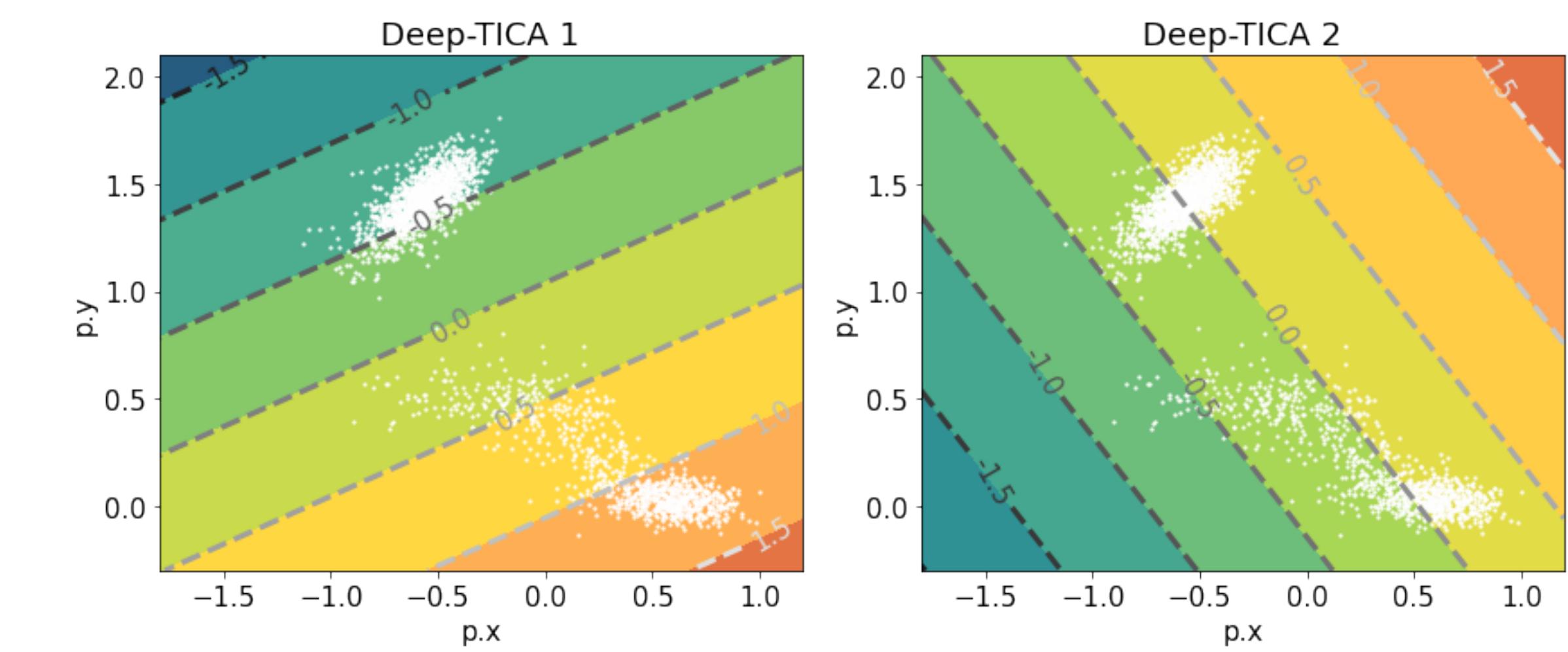
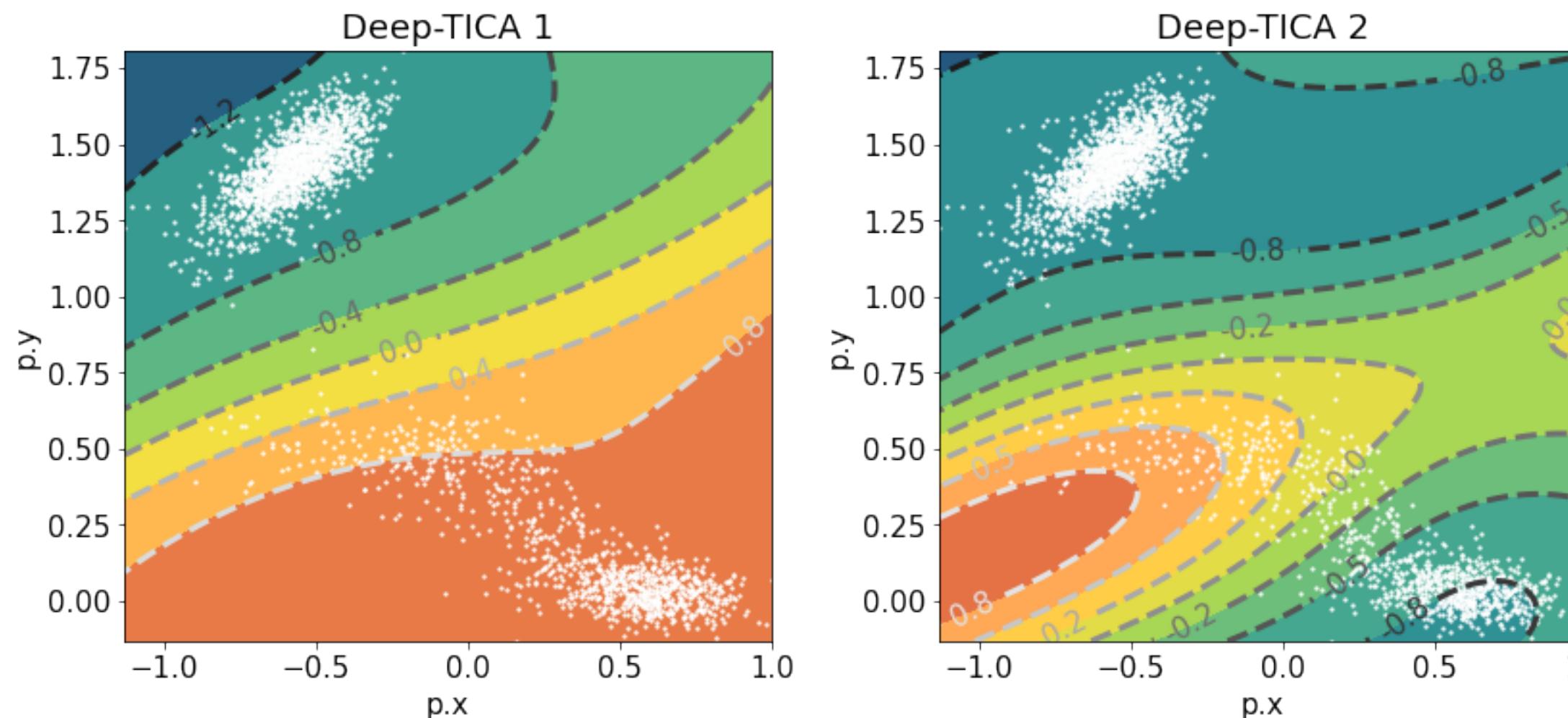
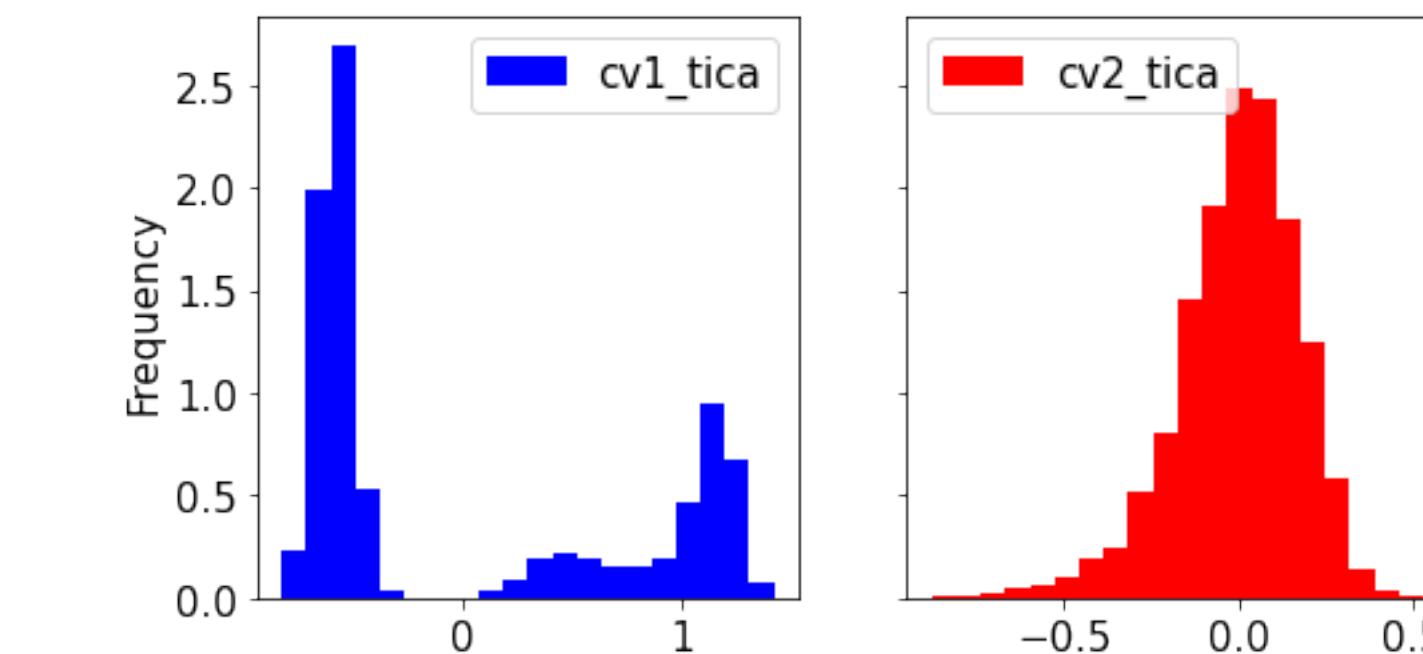
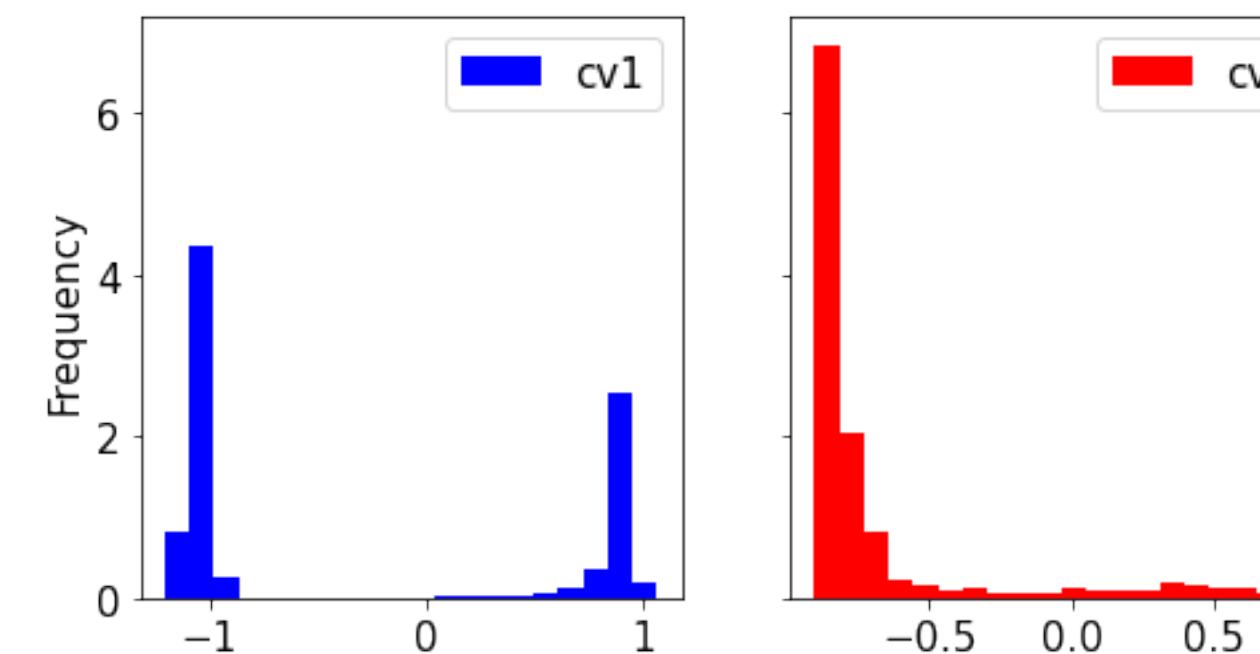
Short Deep-TICA biased trajectory



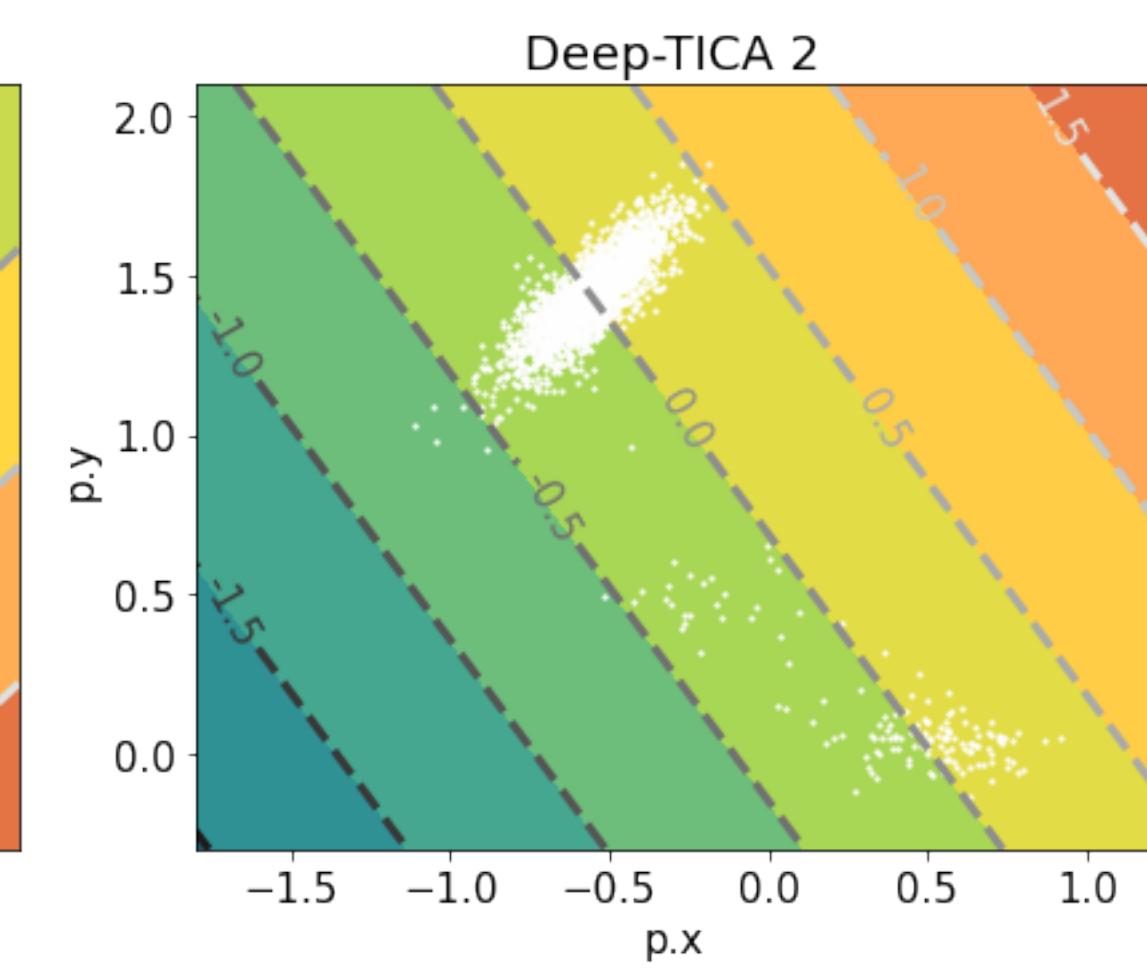
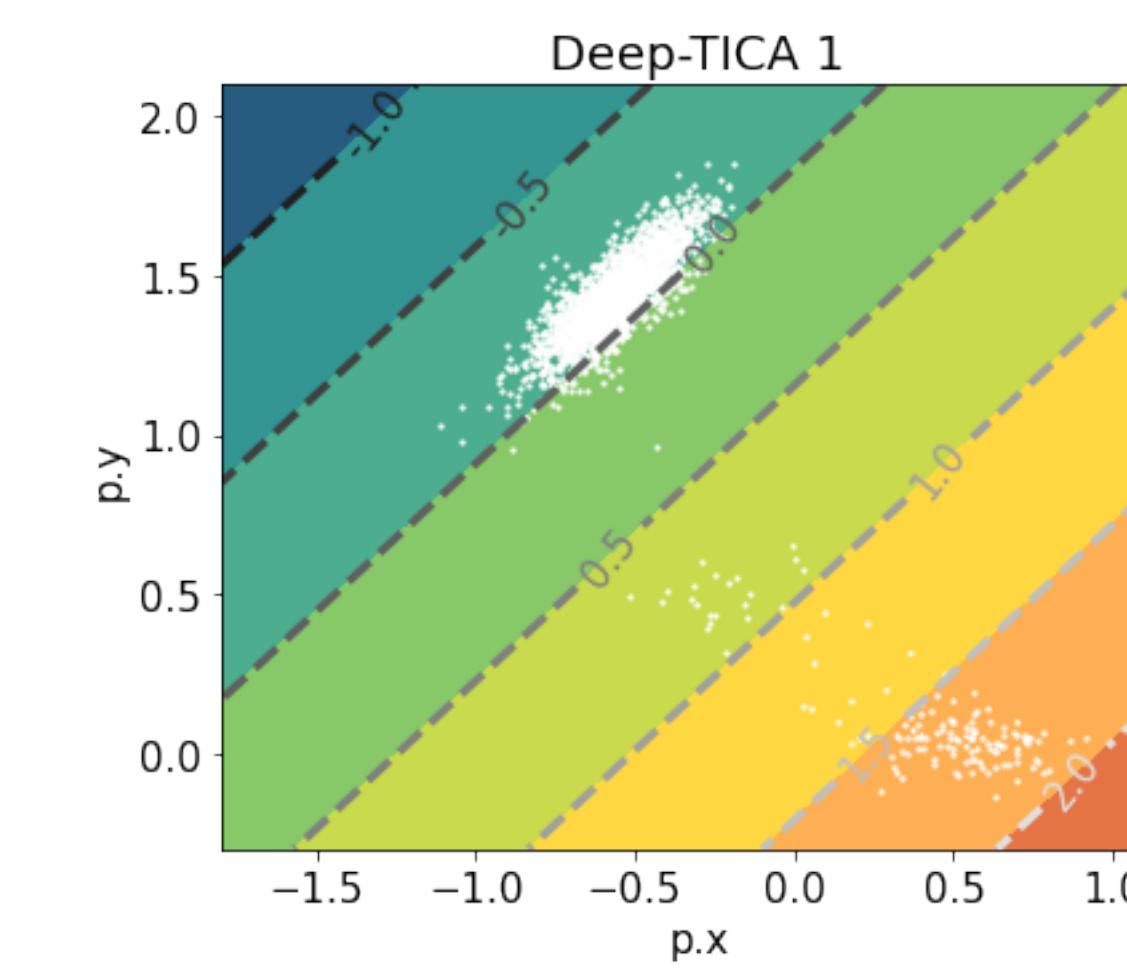
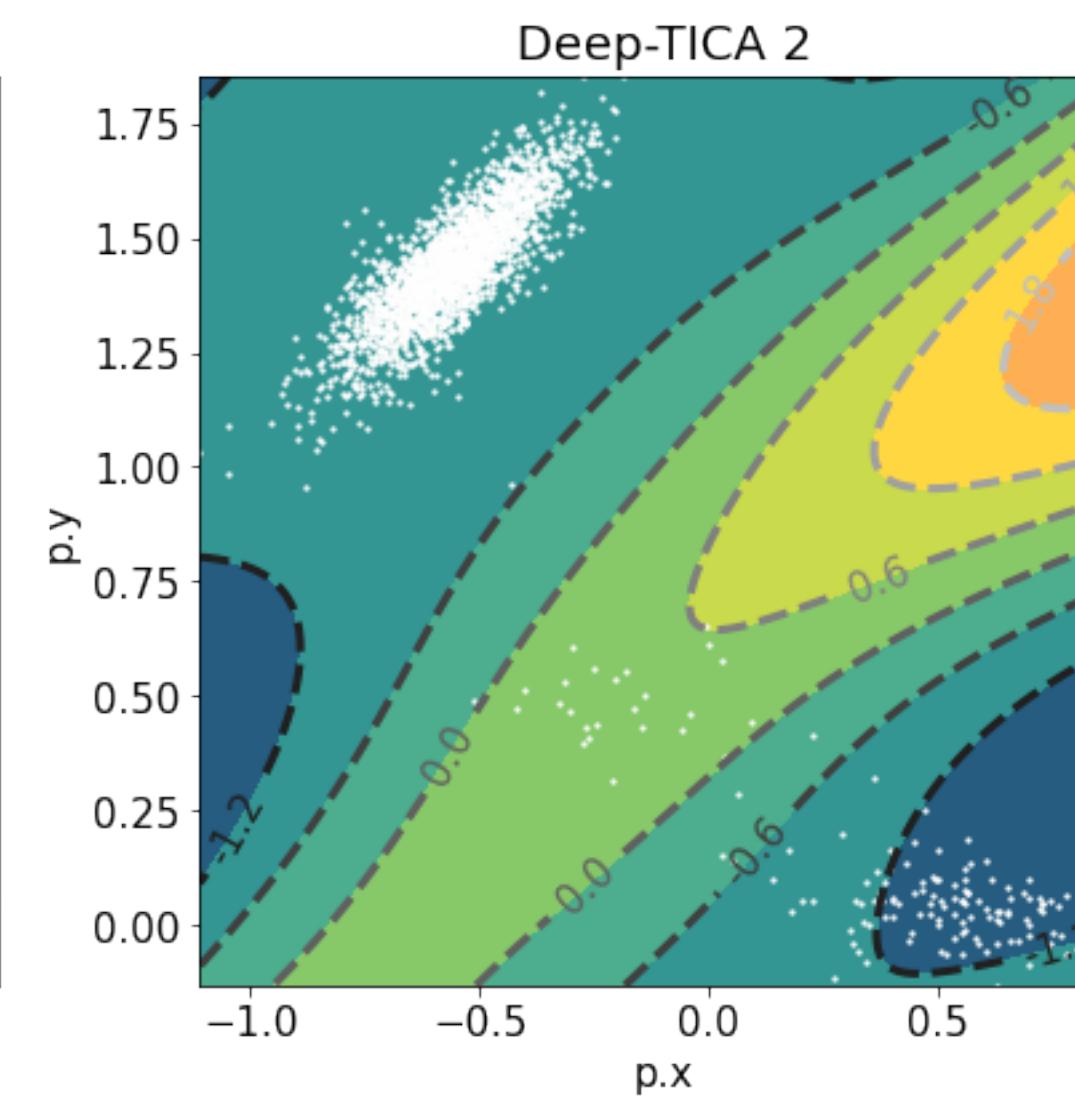
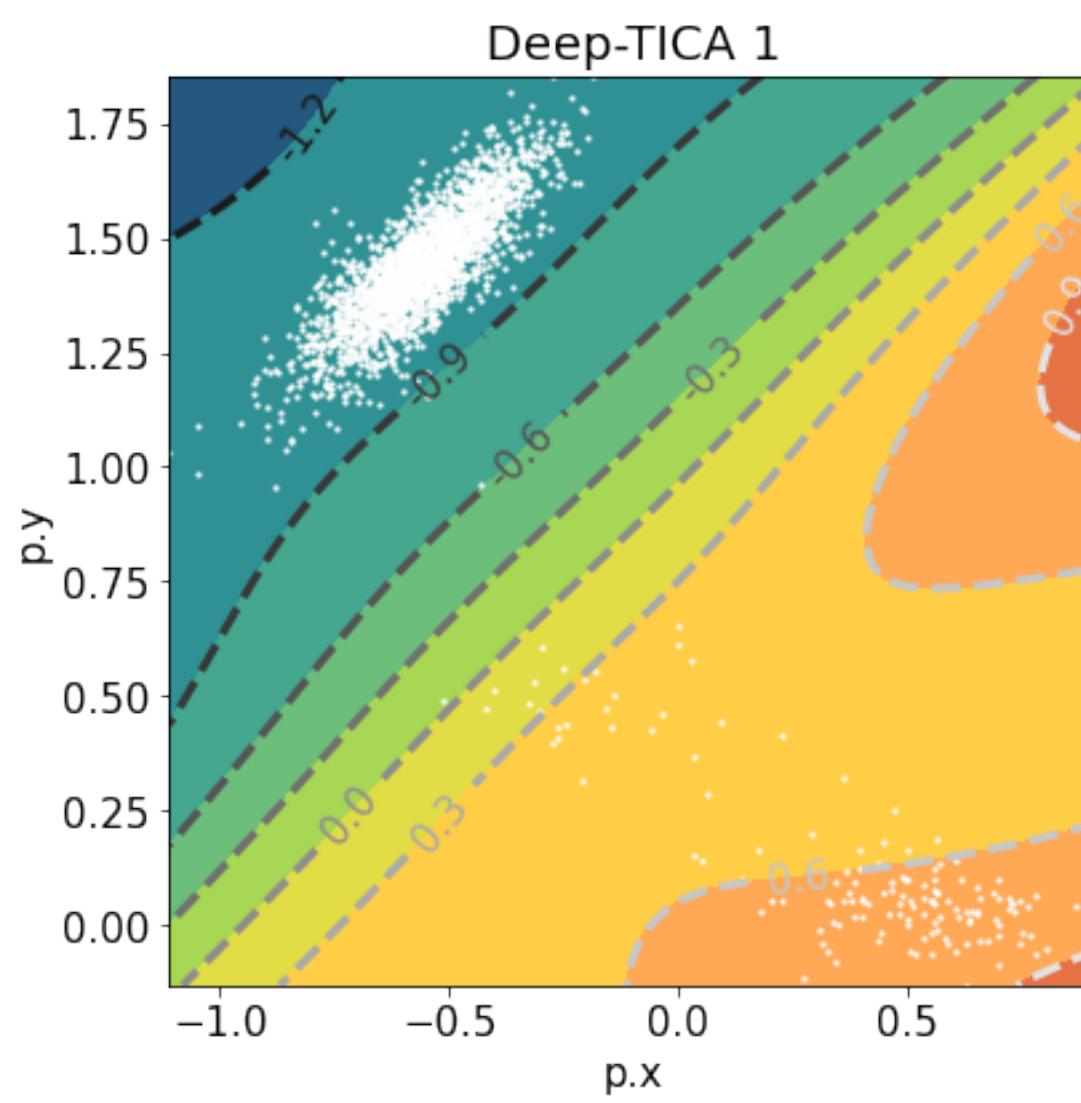
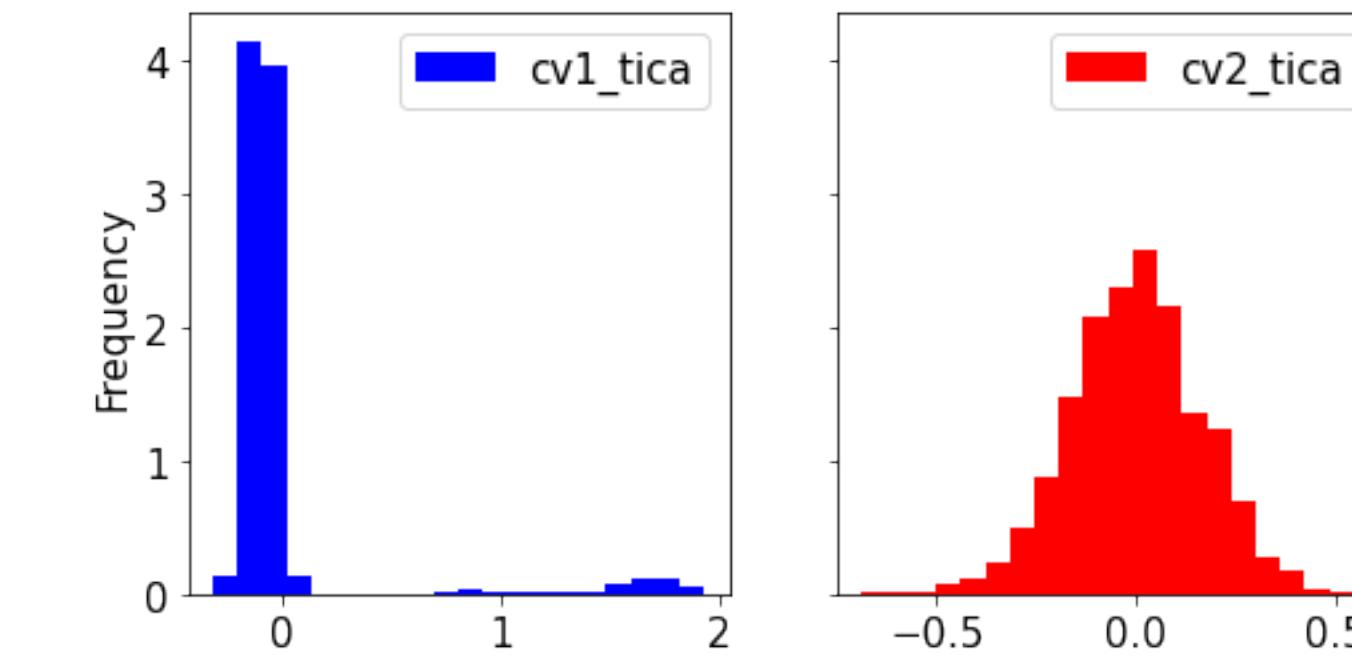
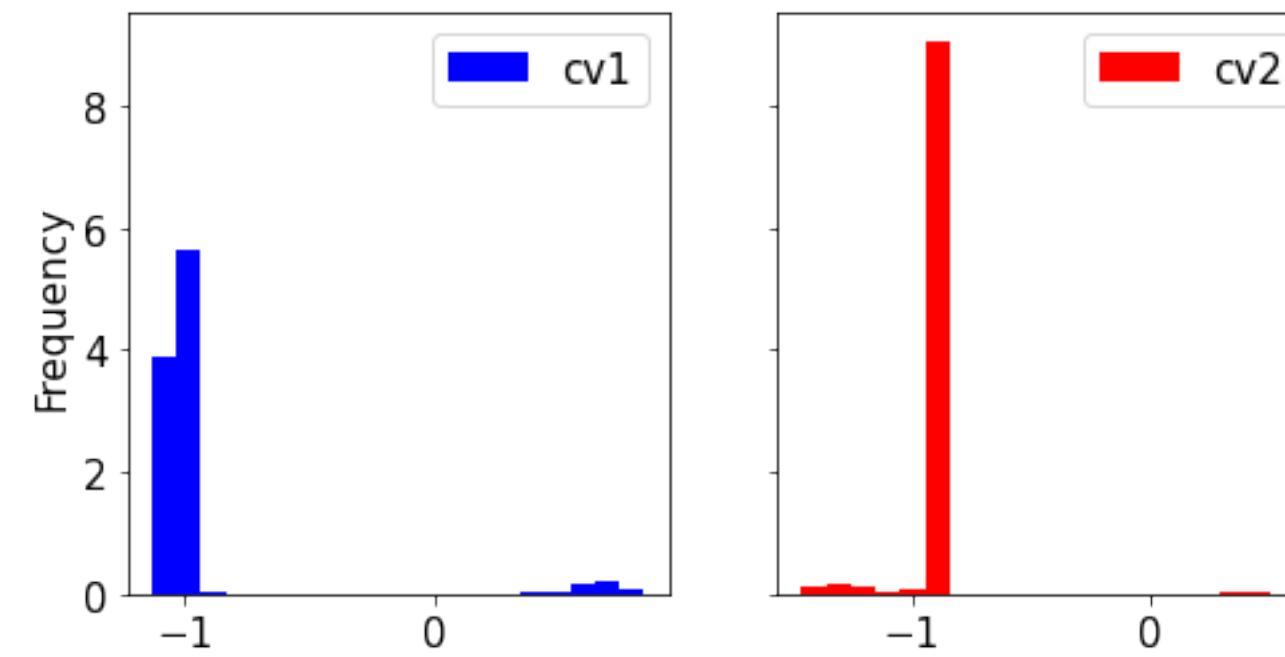
# Deep-TICA & TICA Analysis short trajectory



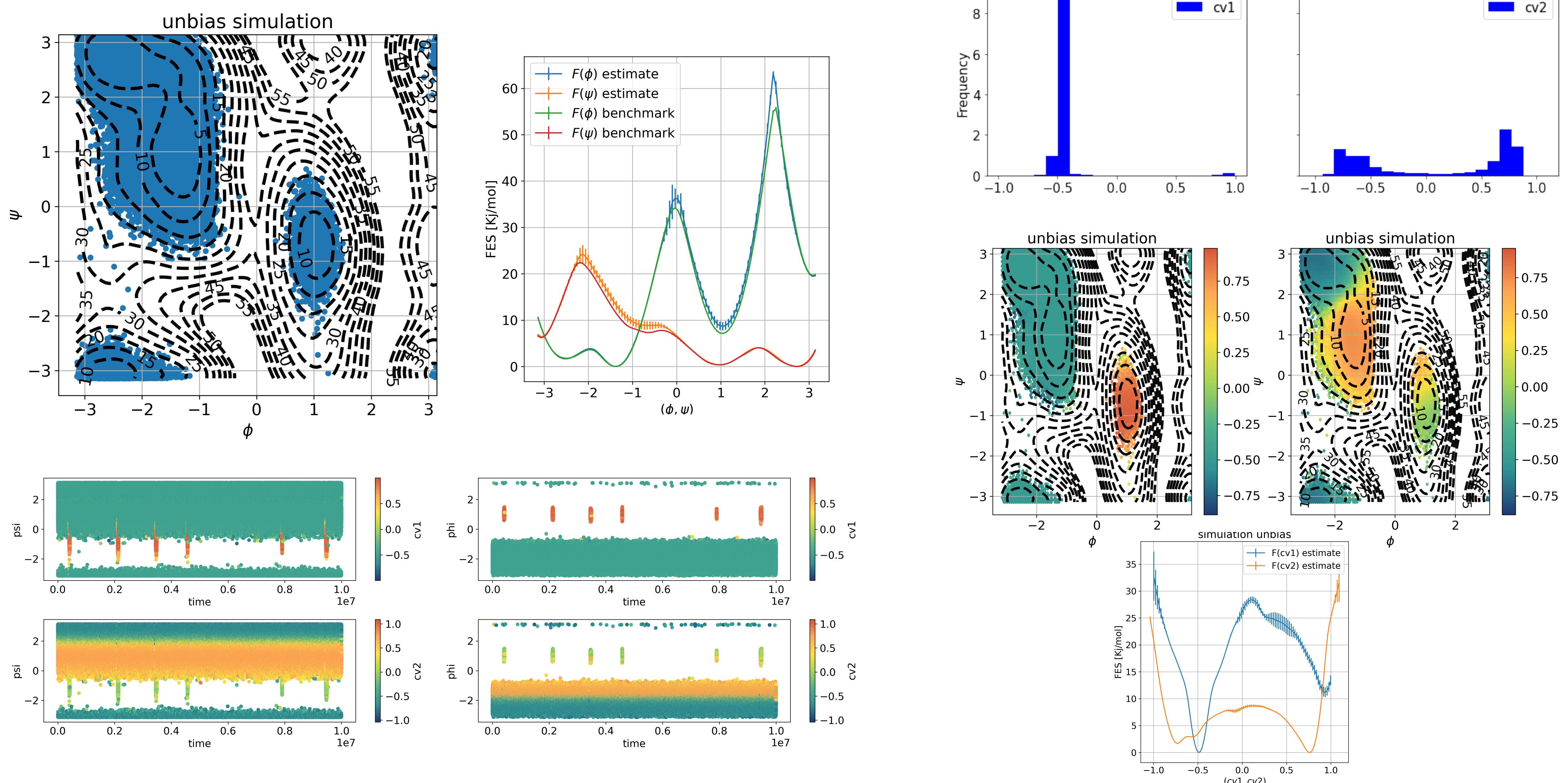
# Deep-TICA & TICA Analysis of TICA biased trajectories



# Deep-TICA & TICA Analysis of Deep-TICA biased trajectories

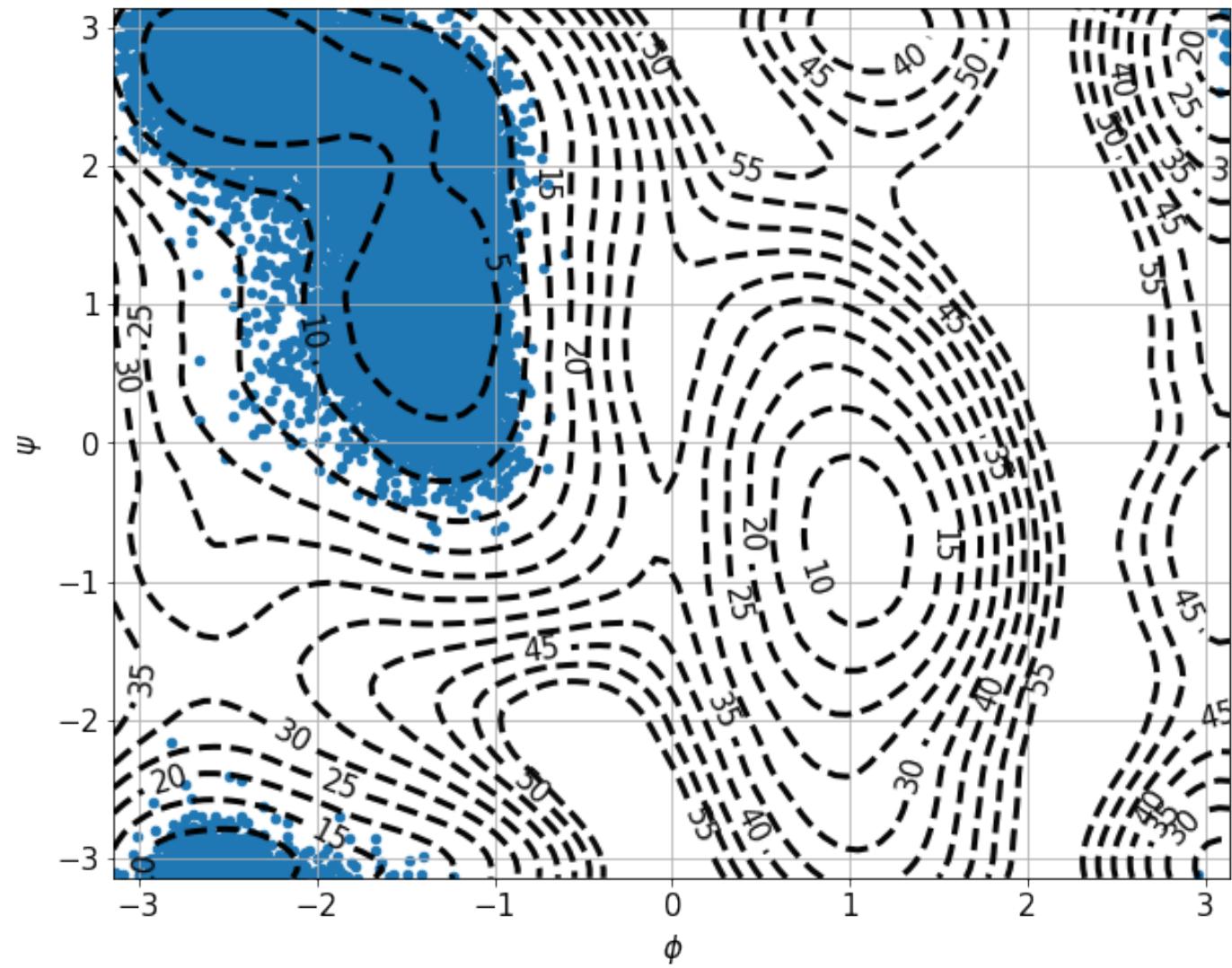


# Alanine Dipeptide

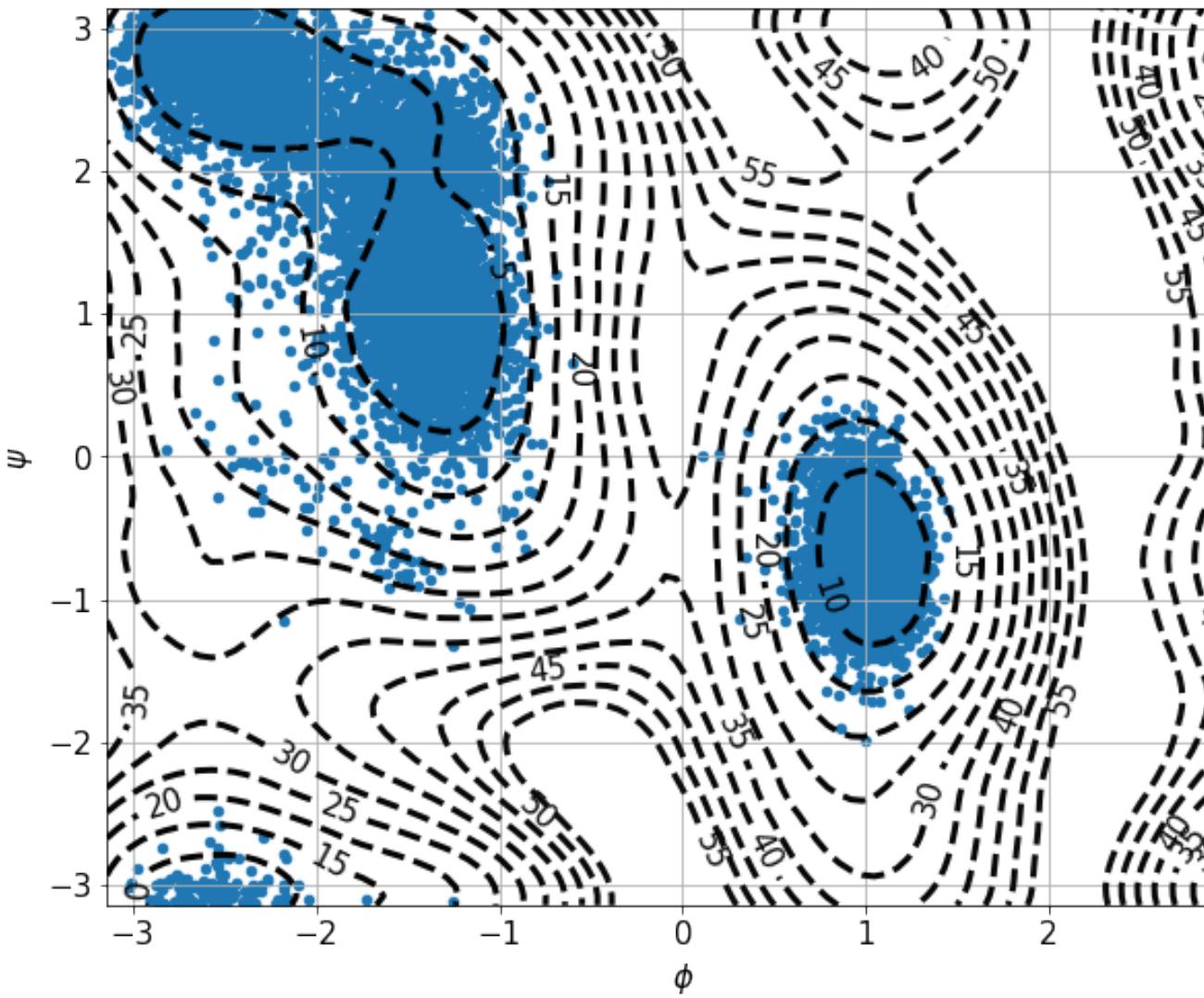


# Short Simulation, state A

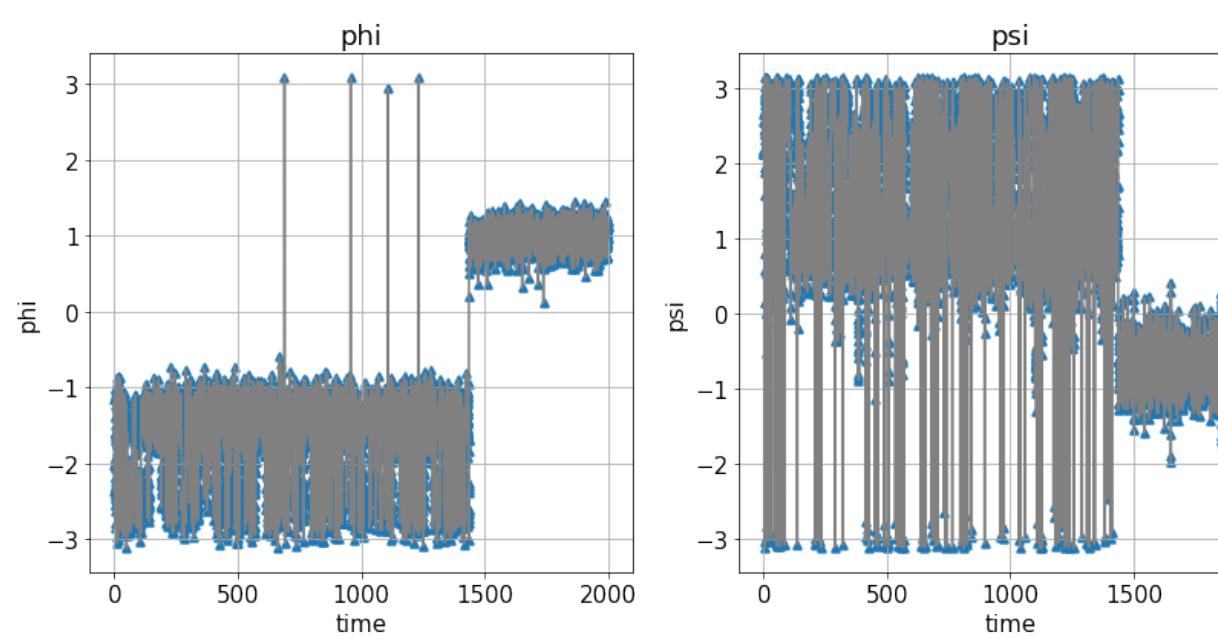
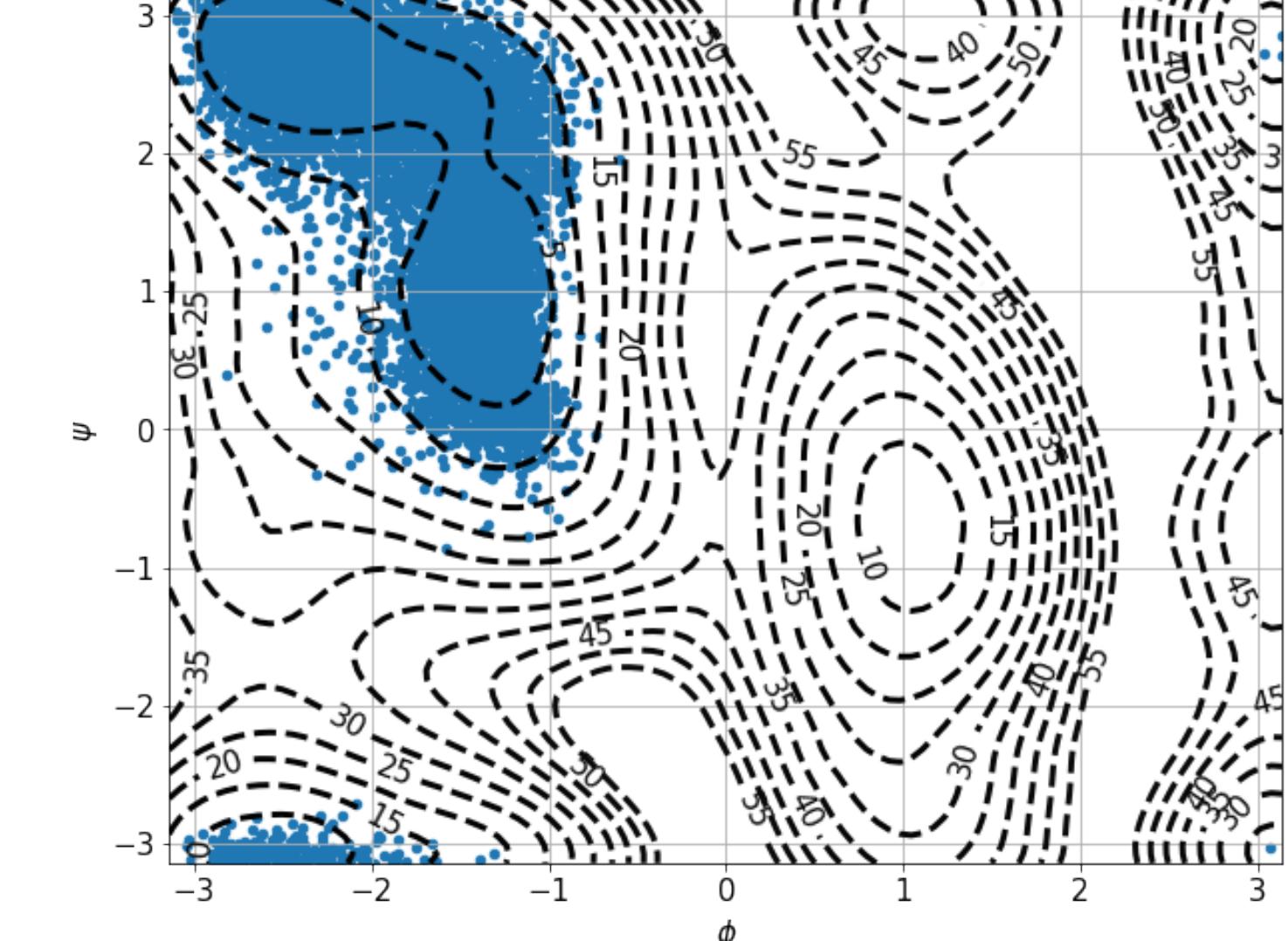
Short unbiased trajectory



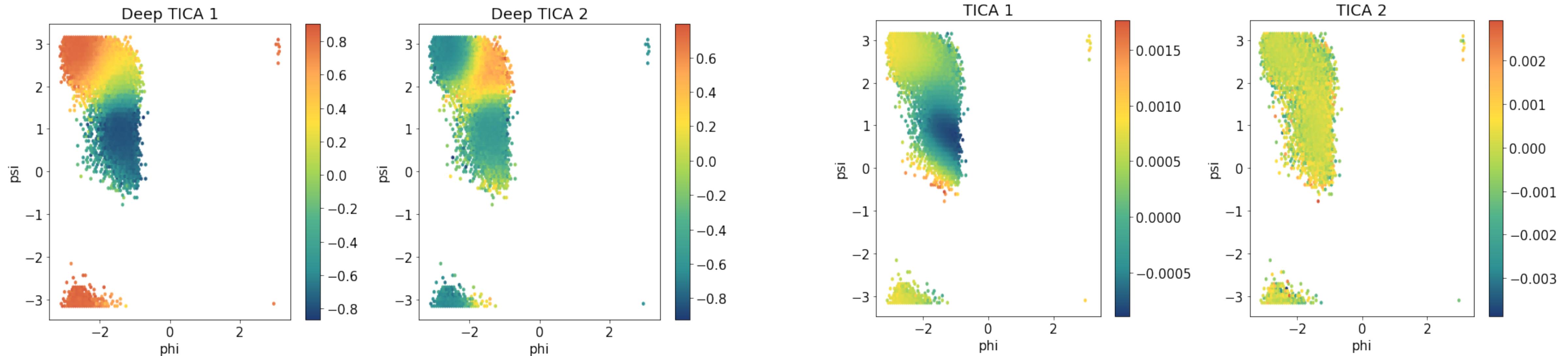
Short TICA biased trajectory



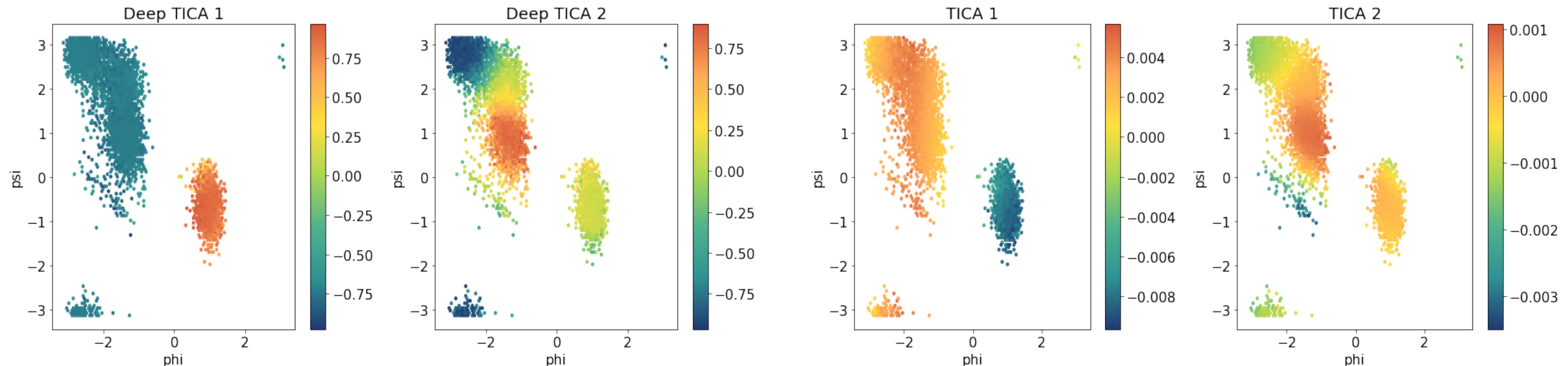
Short Deep-TICA biased trajectory



# Deep-TICA & TICA Analysis short trajectory

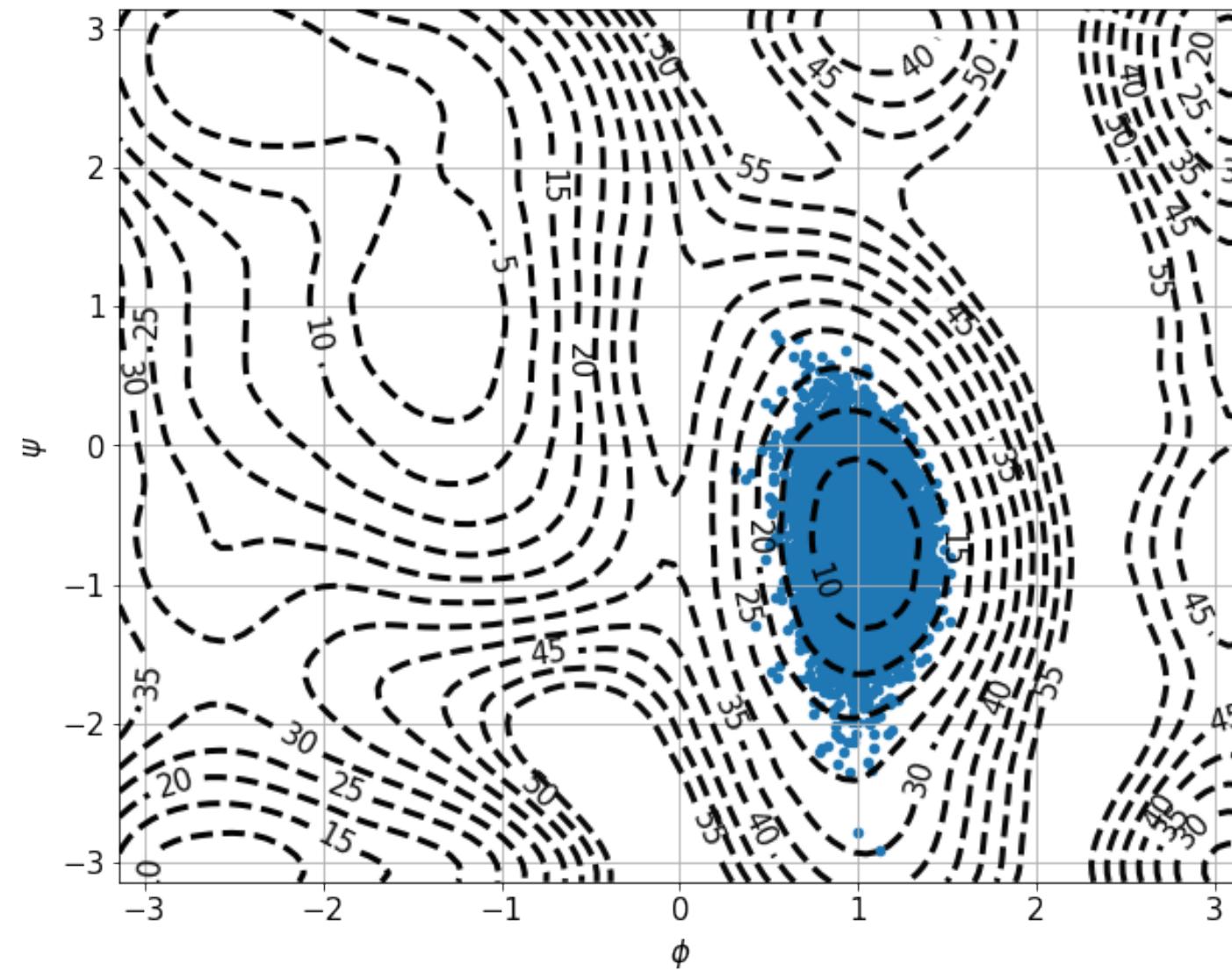


# Deep-TICA & TICA Analysis of TICA biased trajectories

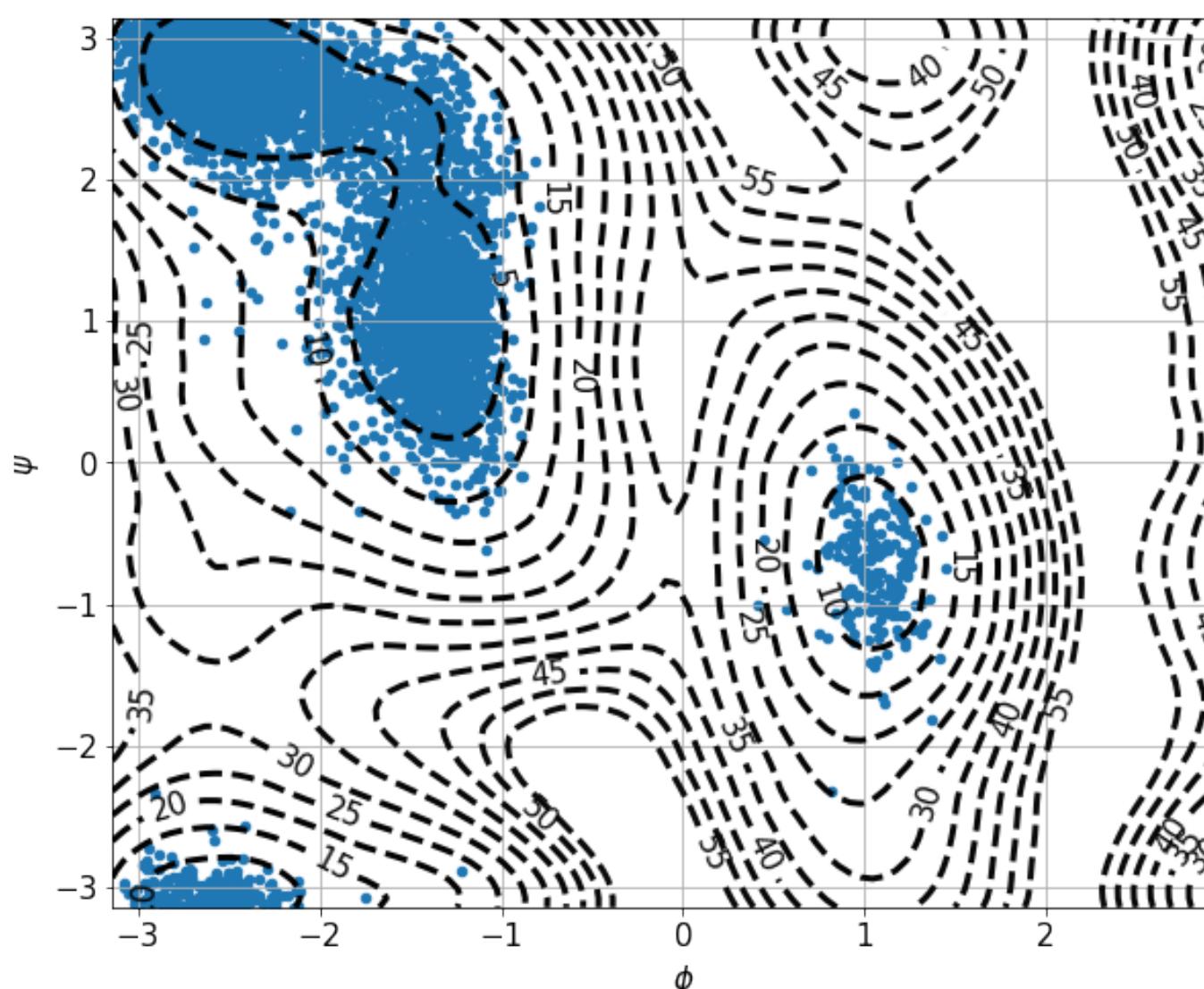


# Short Simulation, state B

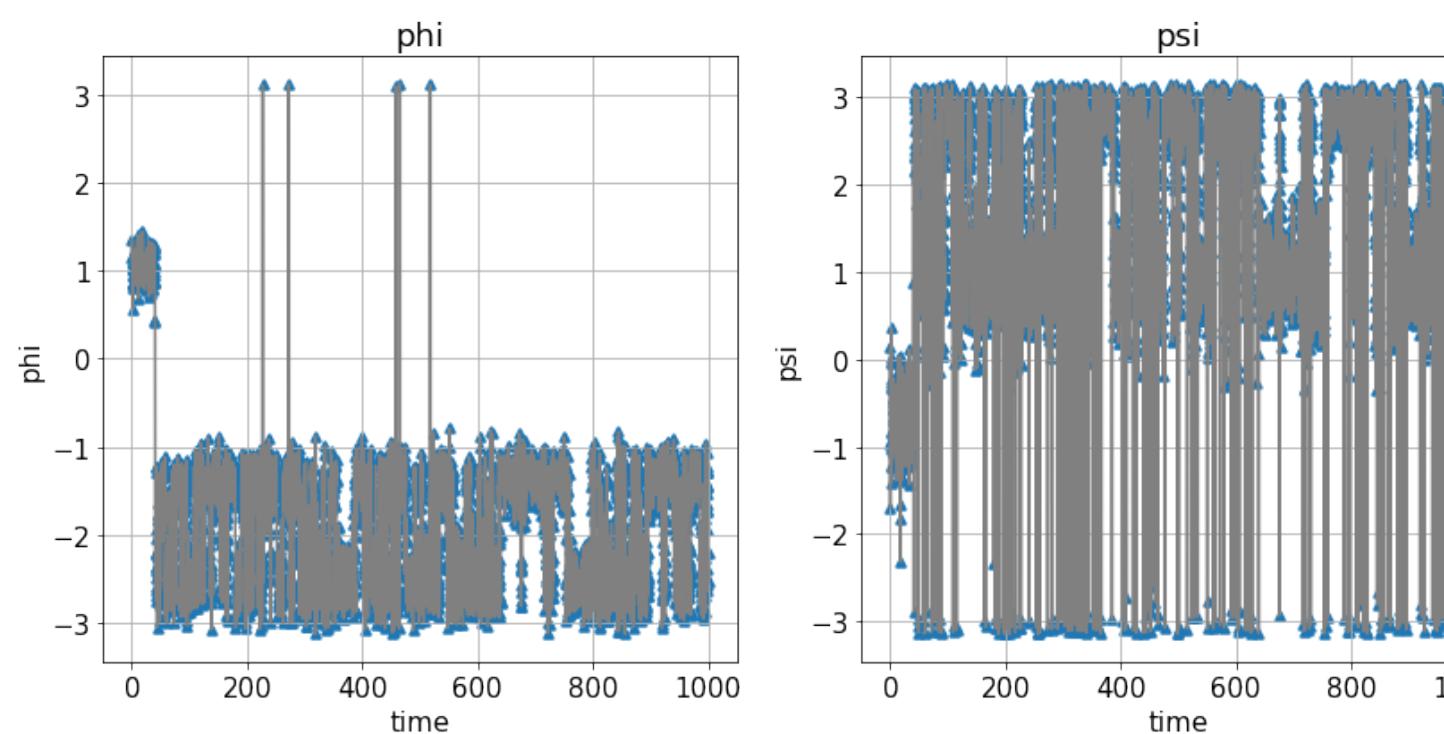
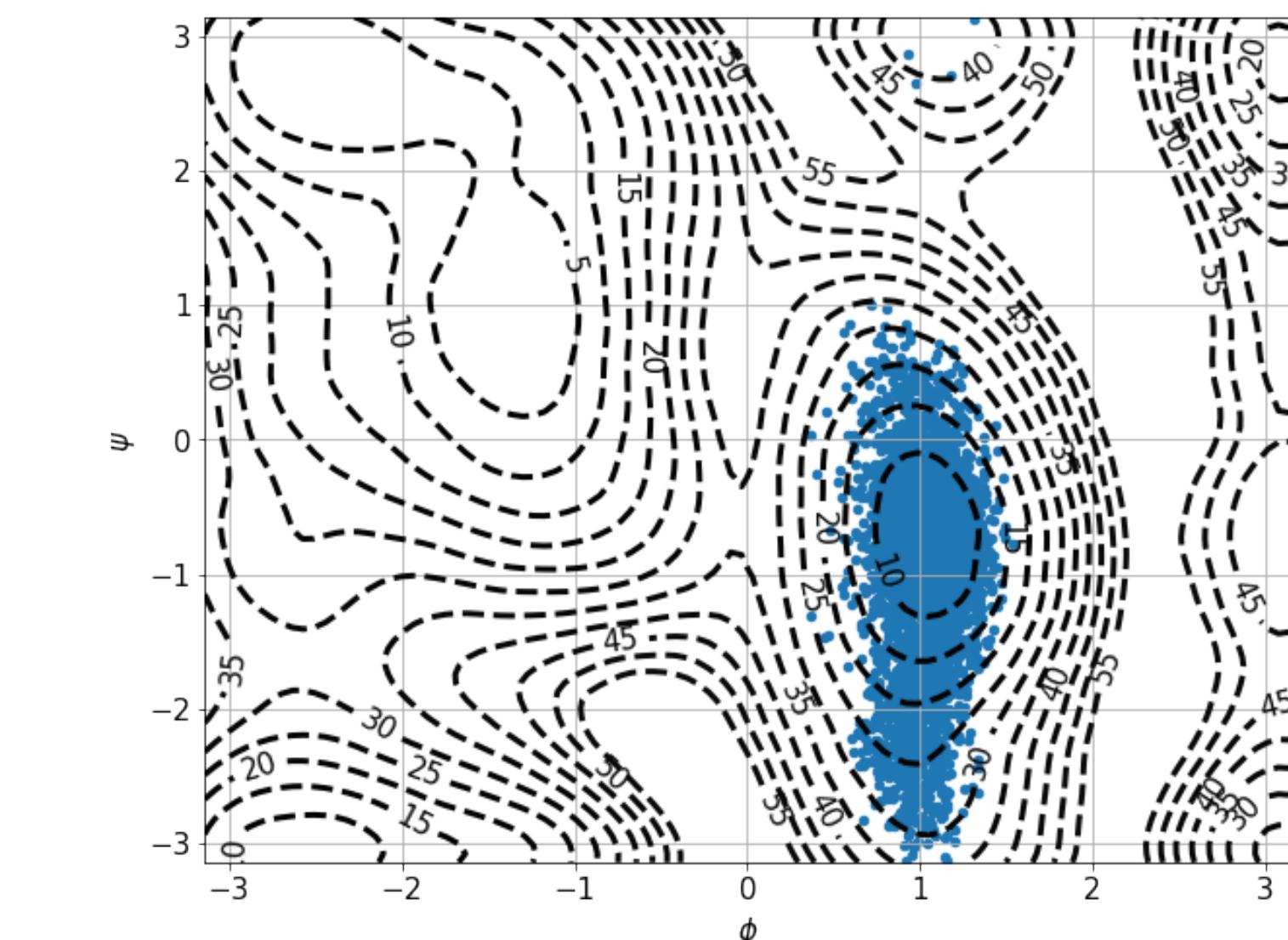
Short unbiased trajectory



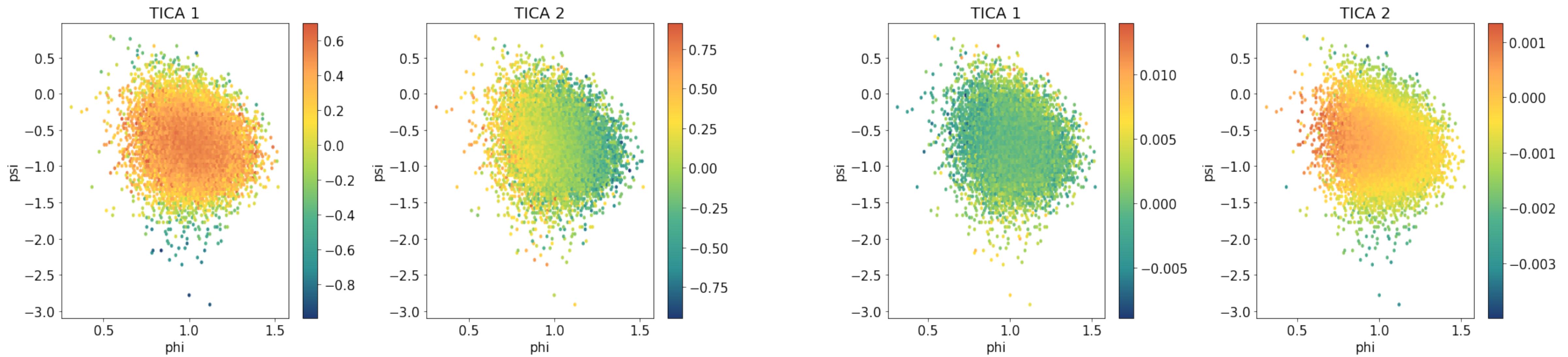
Short TICA biased trajectory



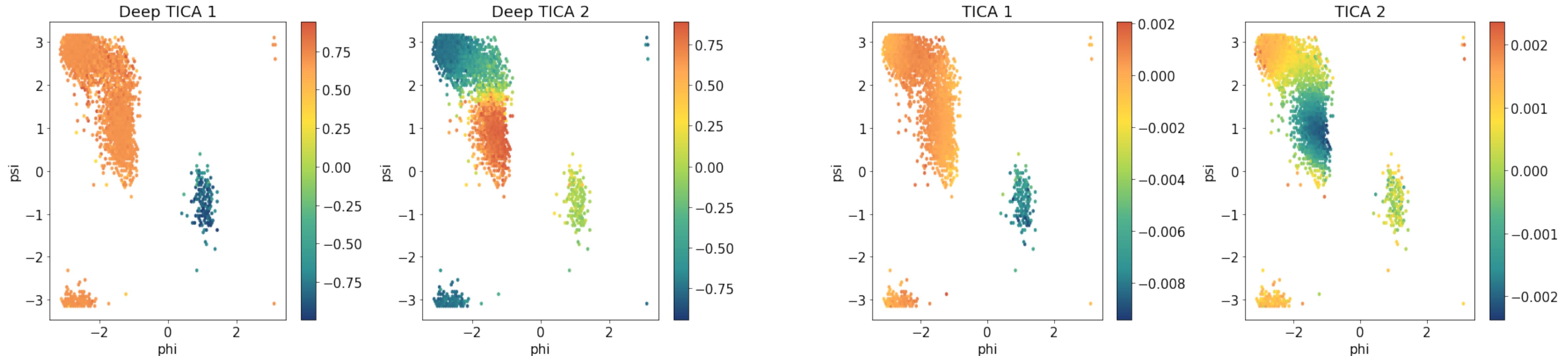
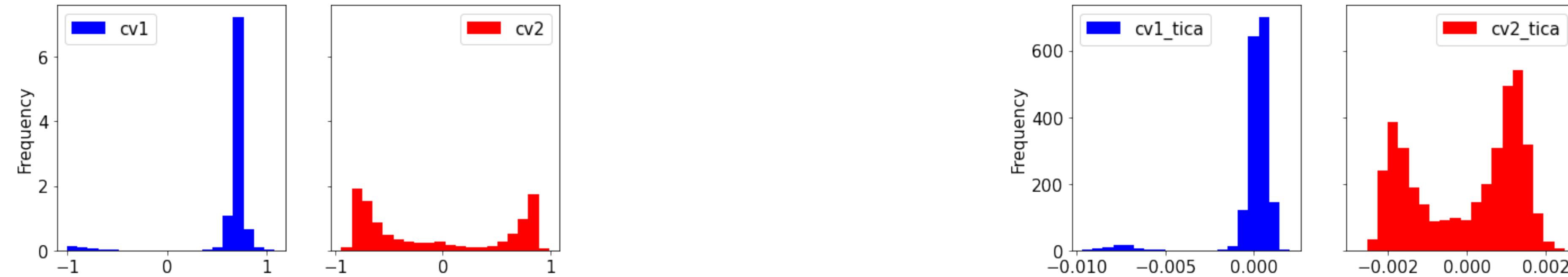
Short Deep-TICA biased trajectory



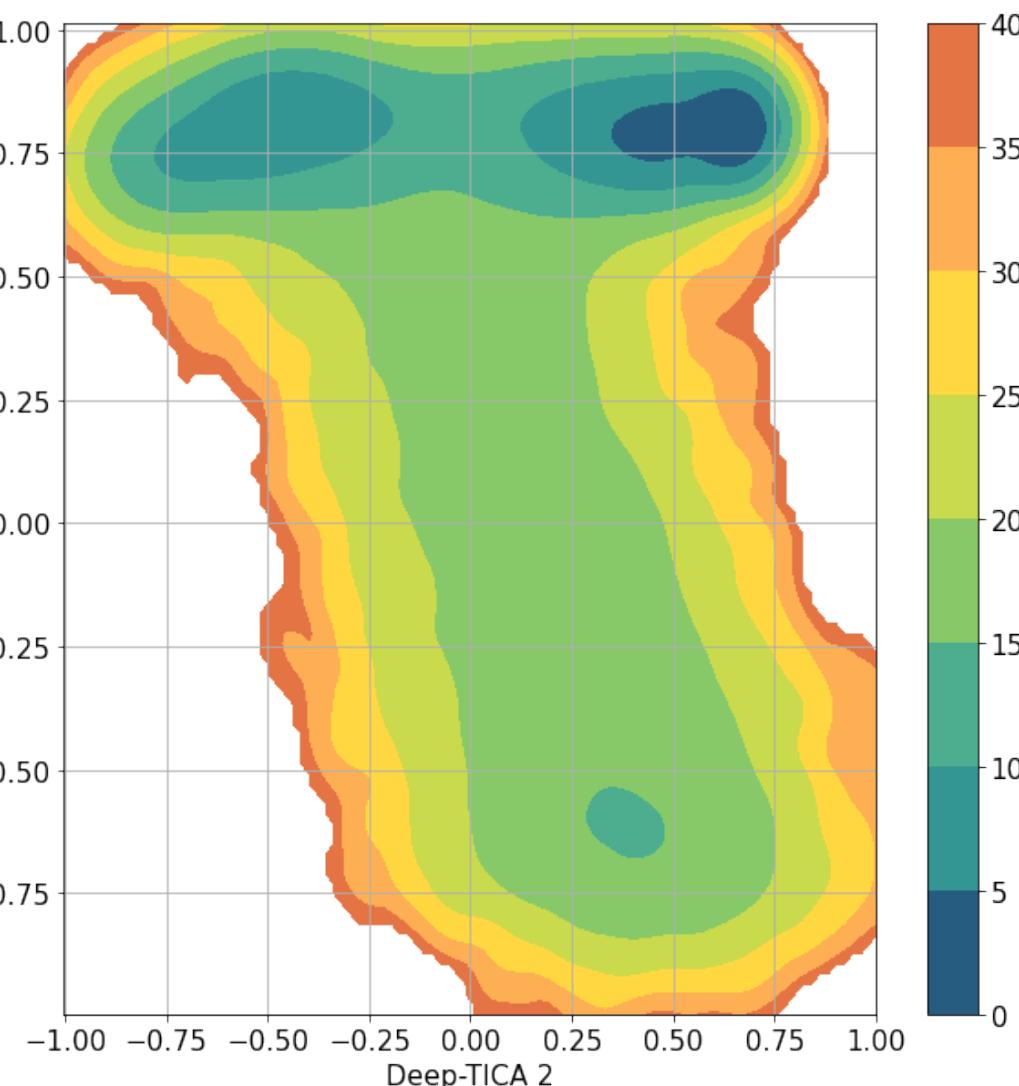
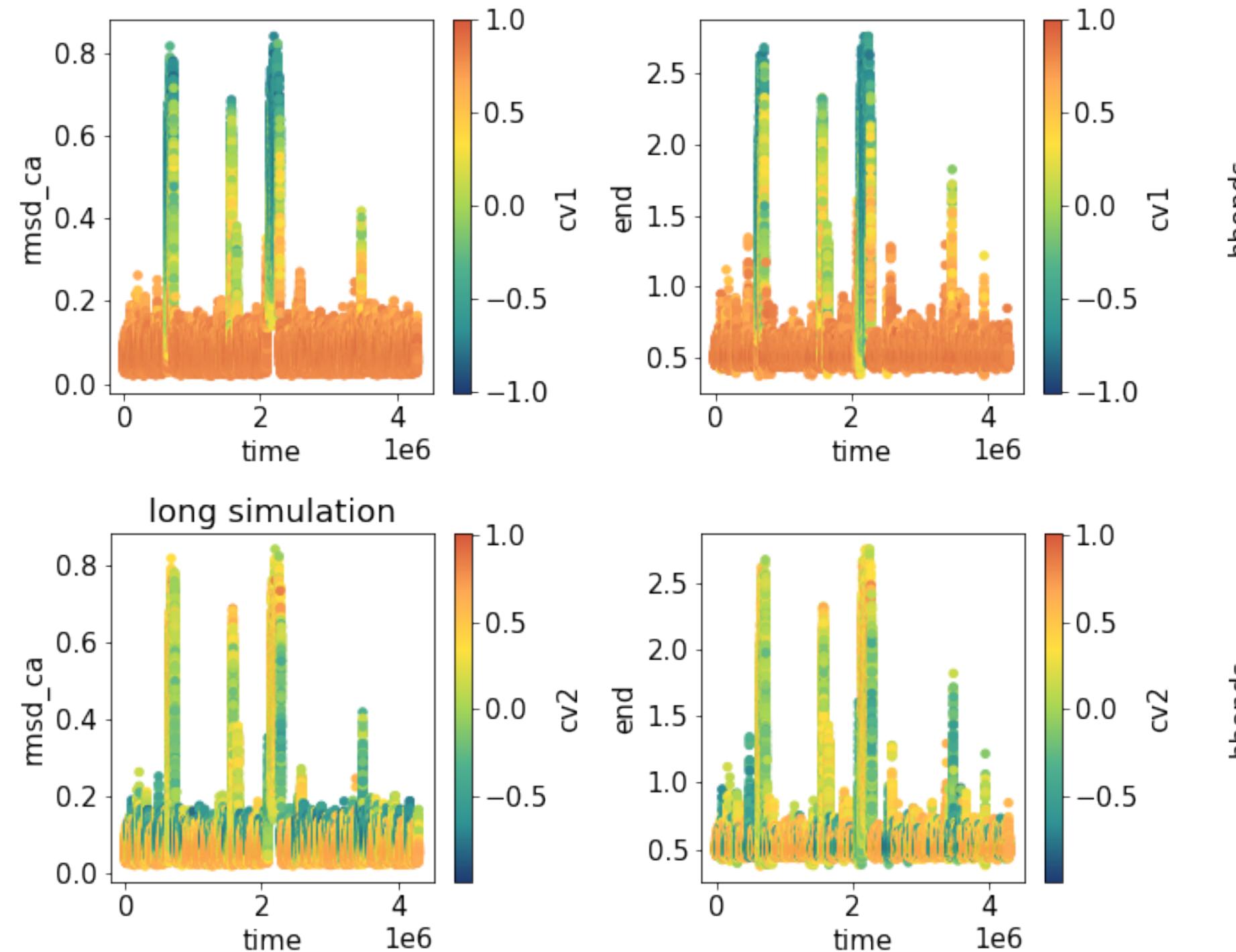
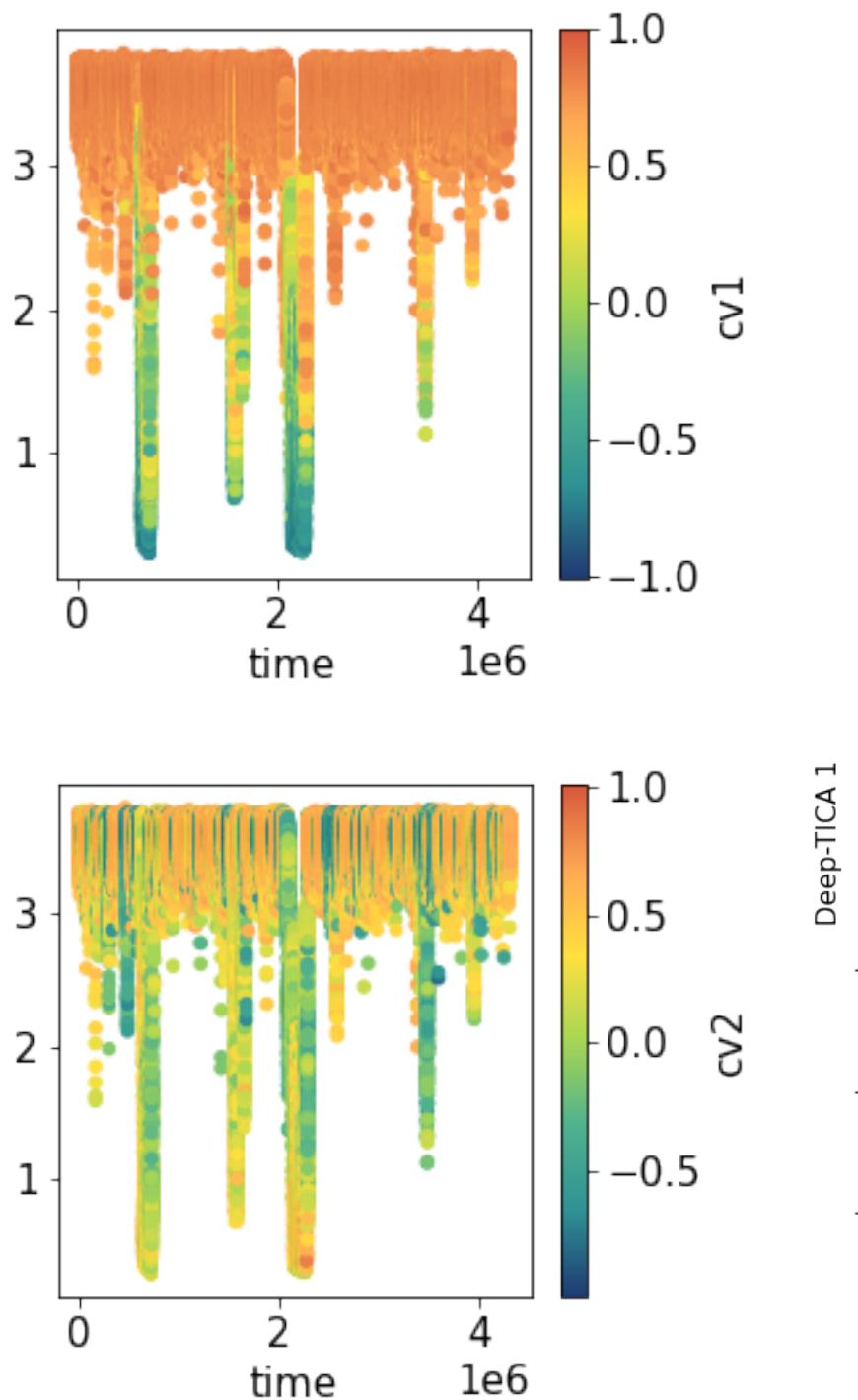
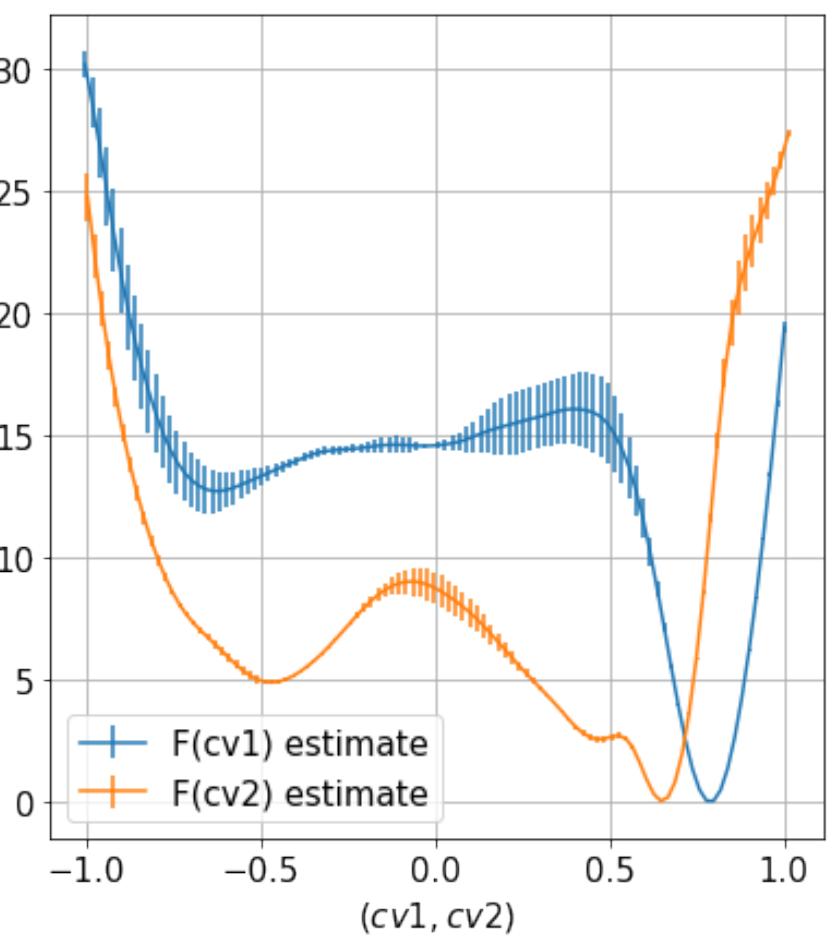
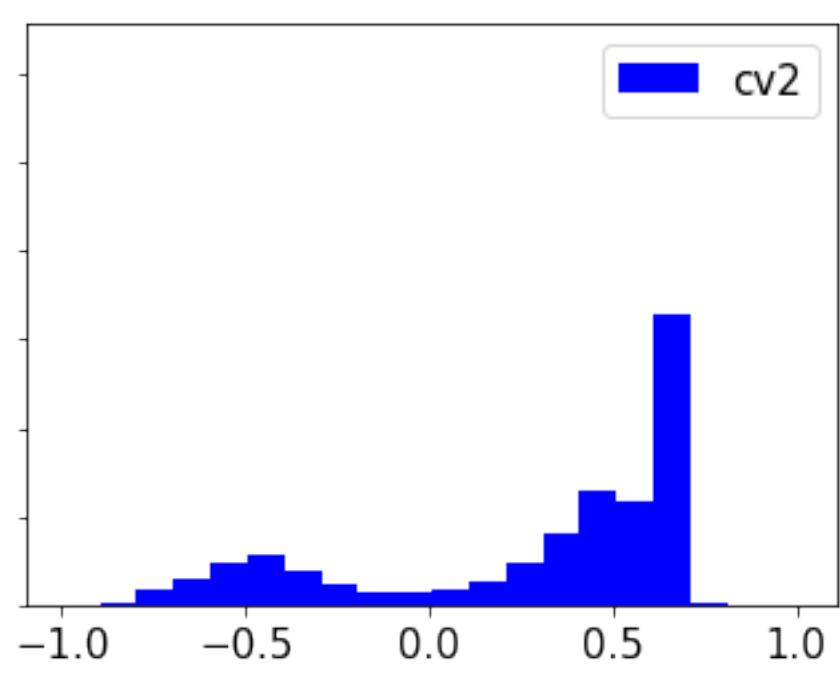
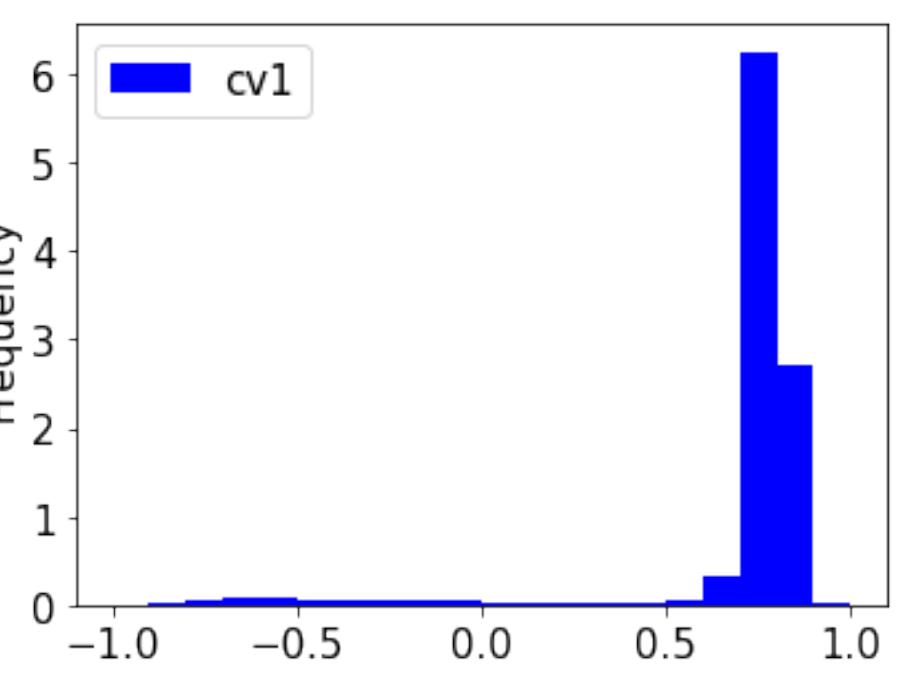
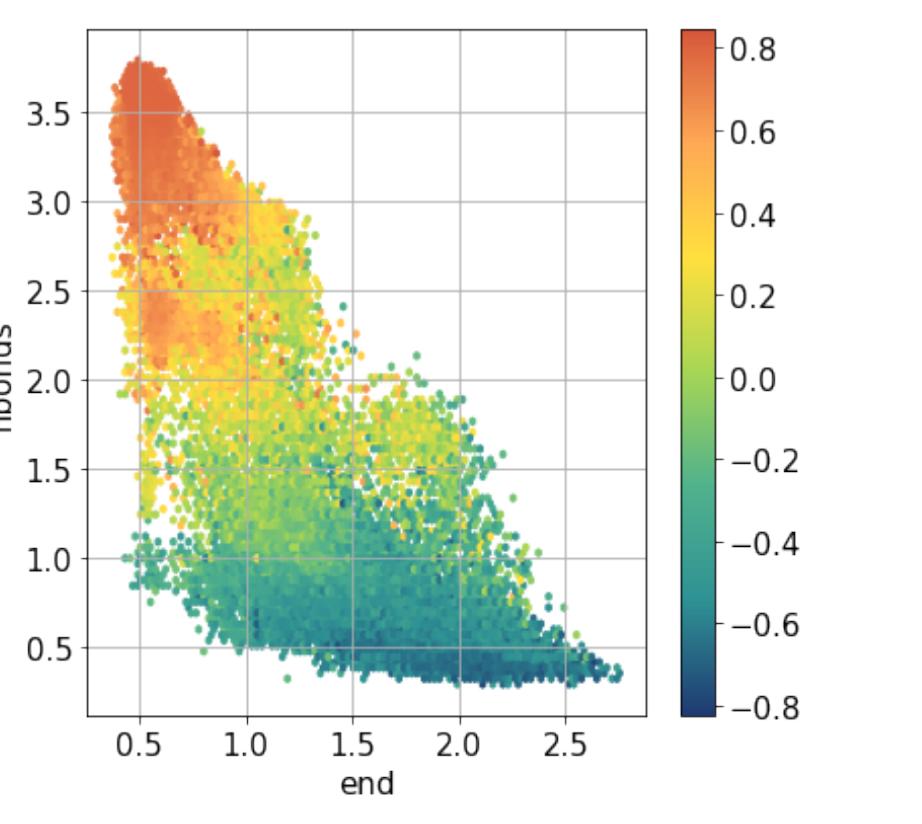
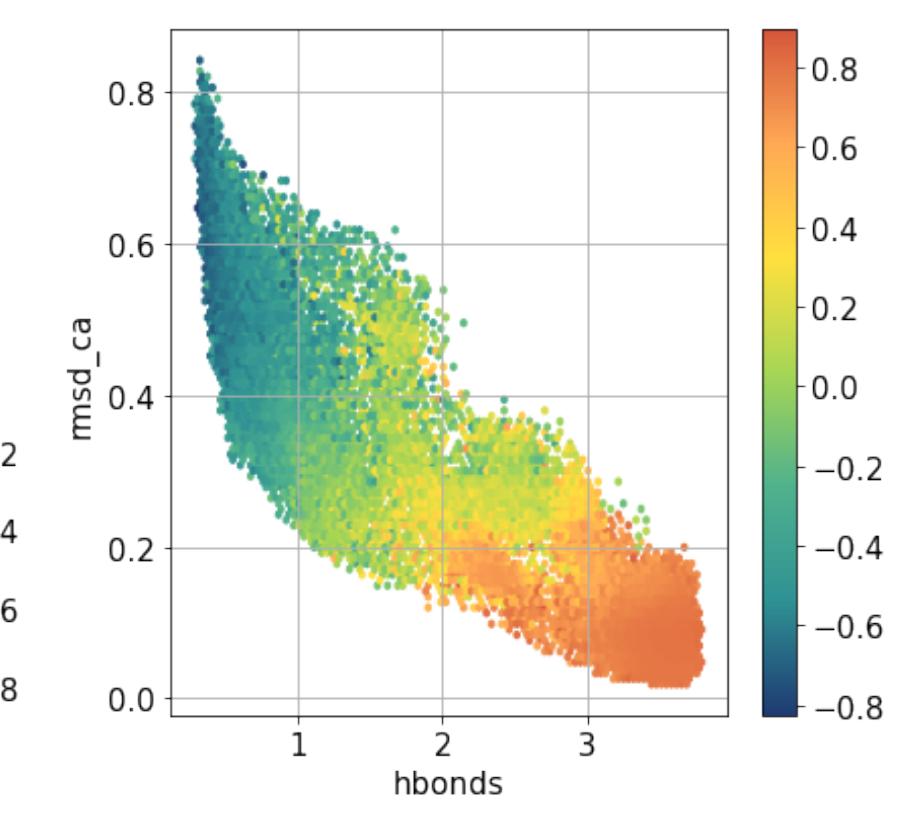
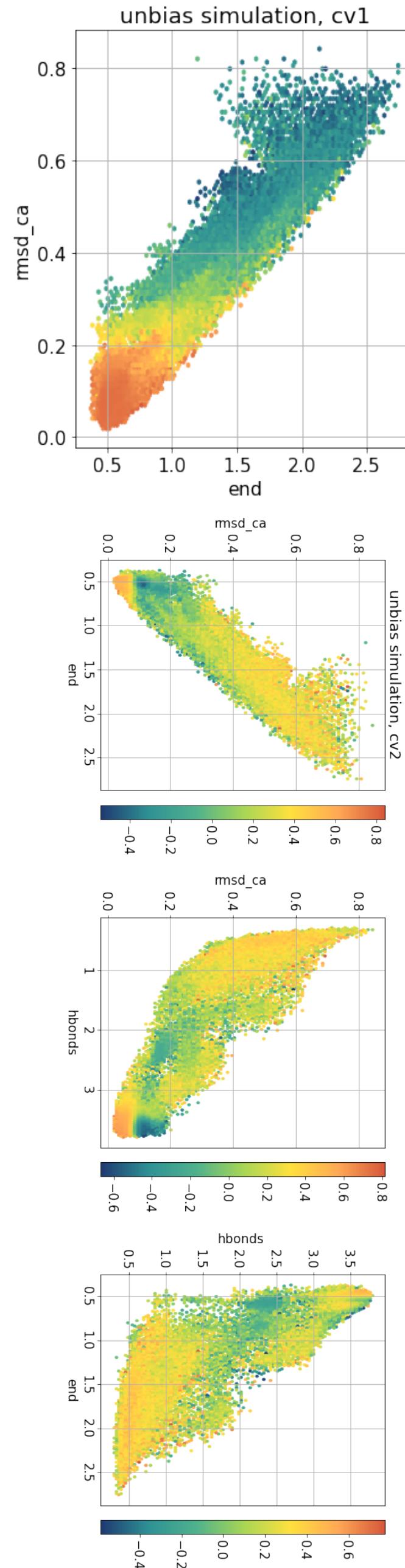
# Deep-TICA & TICA Analysis short trajectory



# Deep-TICA & TICA Analysis of TICA biased trajectories

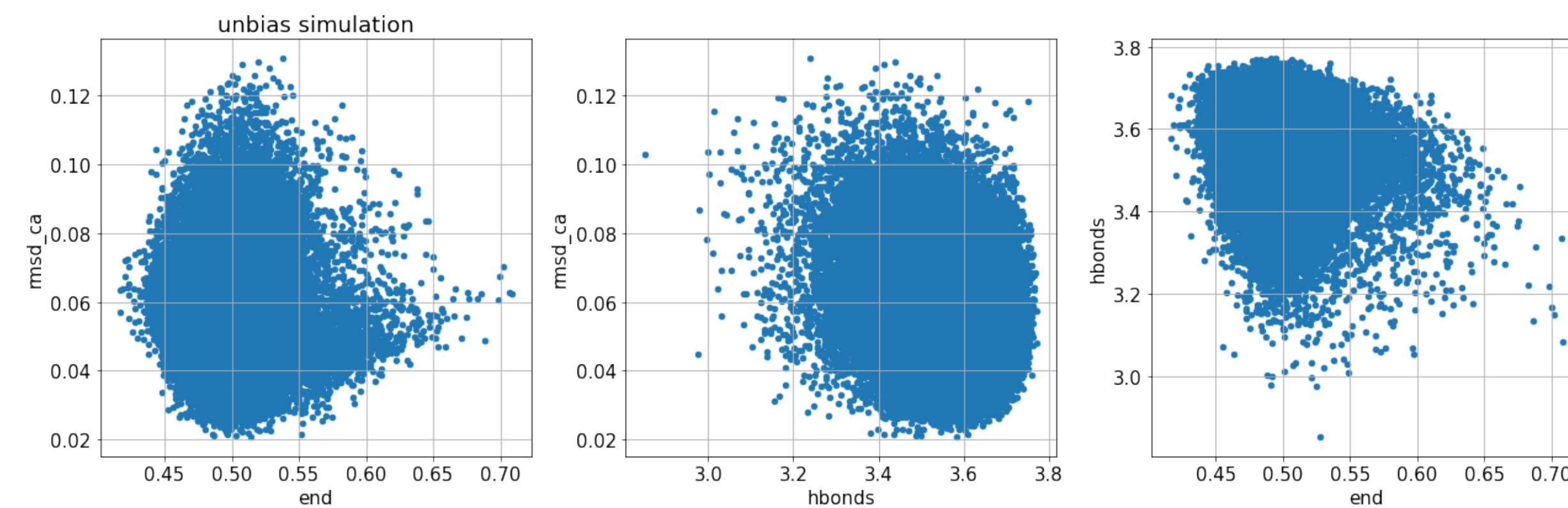


# Chignolin

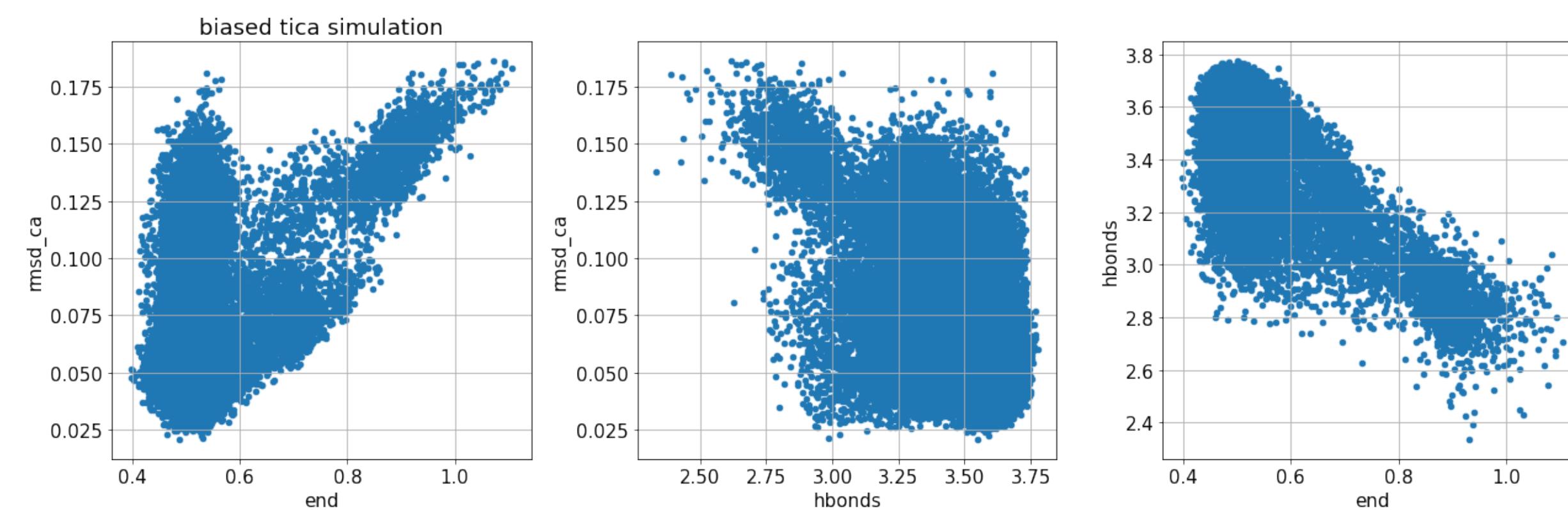


# Short Simulation, folded state

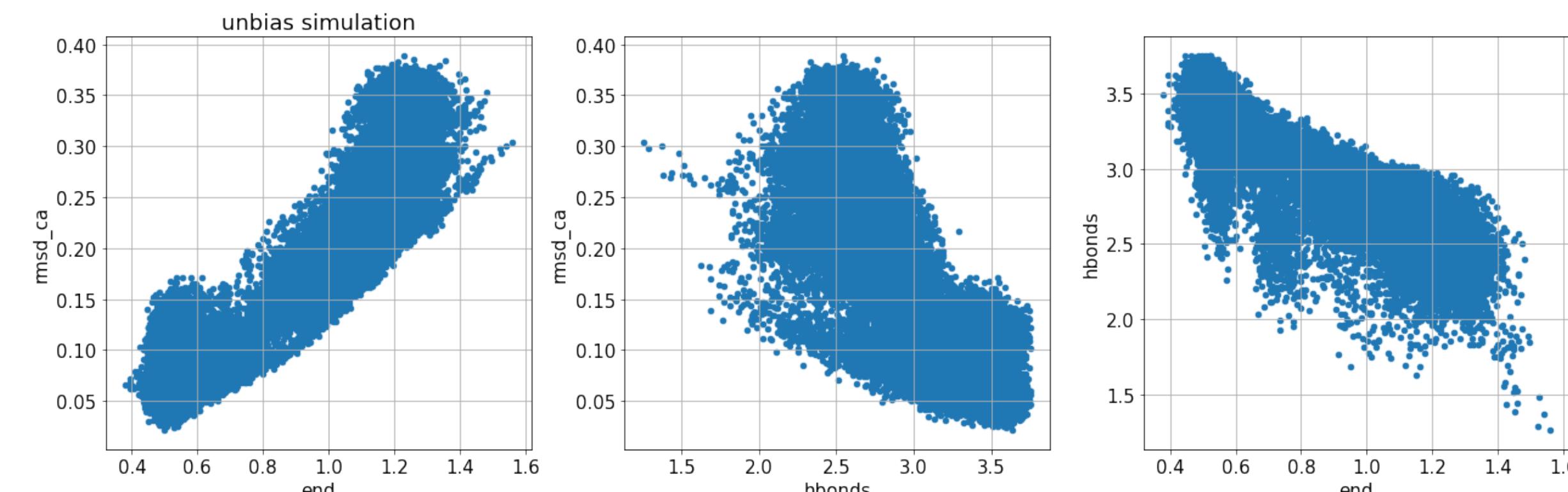
Short unbiased trajectory



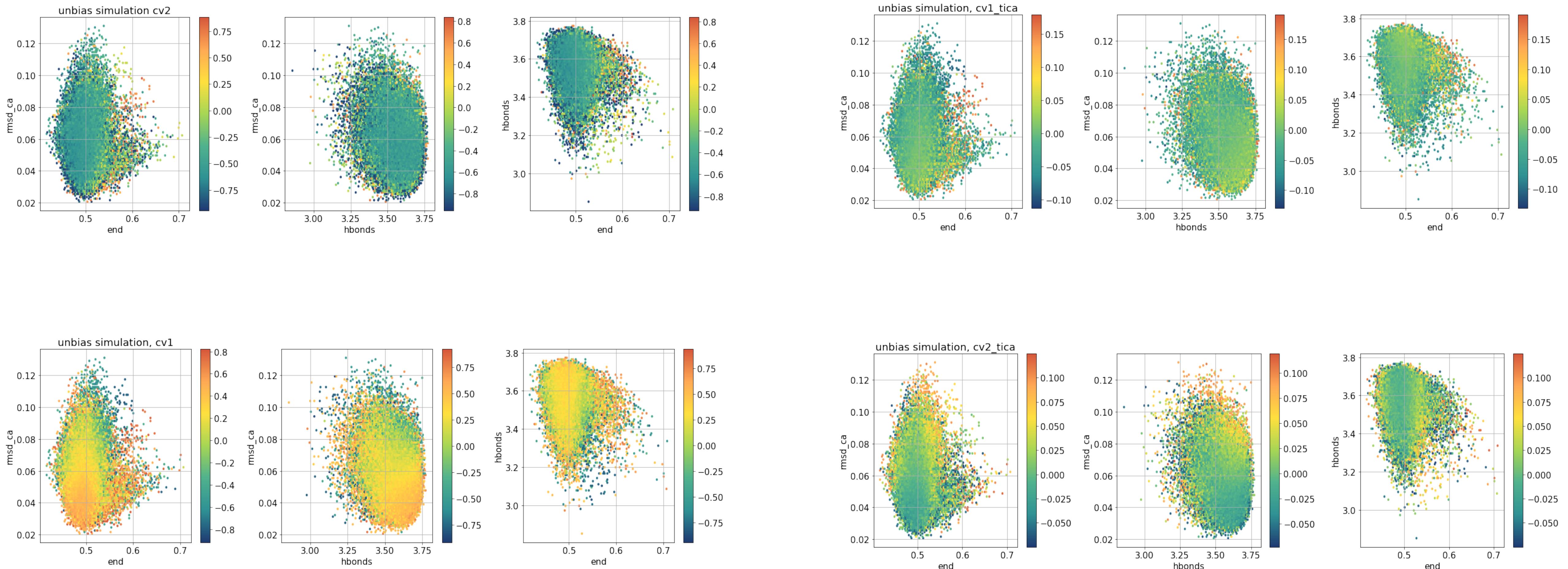
Short TICA biased trajectory



Short Deep-TICA biased trajectory



# Deep-TICA & TICA Analysis short trajectory



# Iterative procedure

## A. Explorative iterations with TICA:

- The TICA algorithm is computationally more efficient
- A linear approximation can be more efficient to escape from a basin rather than the Deep-TICA cvs
- Stop when a transition occurs

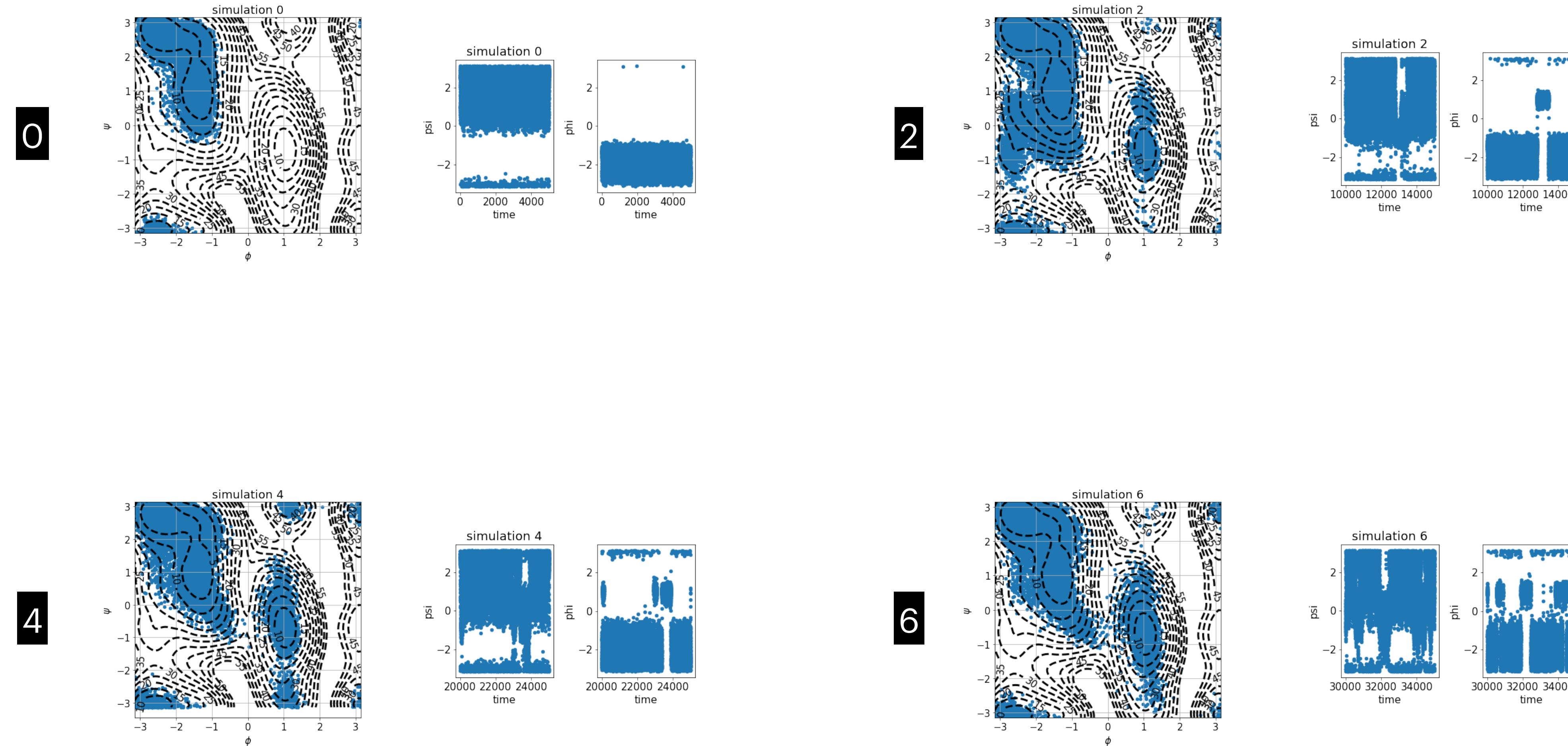
## B. Final iterations with Deep-TICA :

- When a transition occurs the Deep-TICA algorithm is more efficient in detect the associated slow mode
- The first transition can be not efficient. The final ones are.

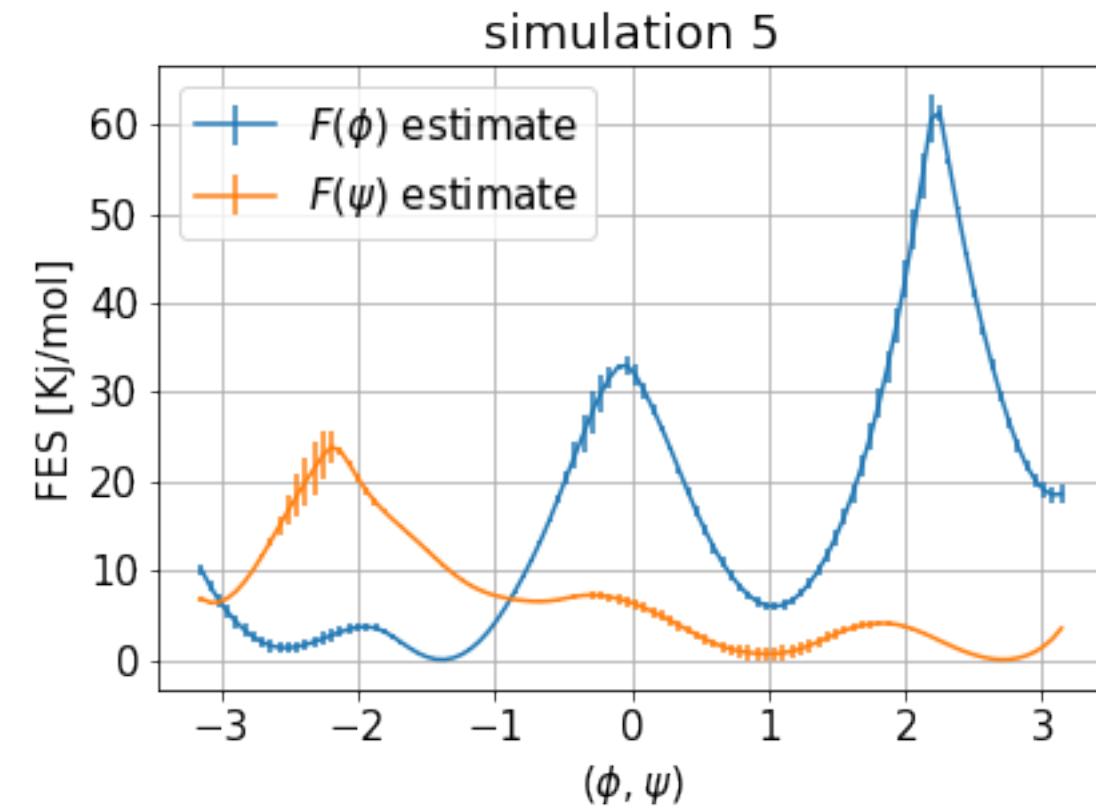
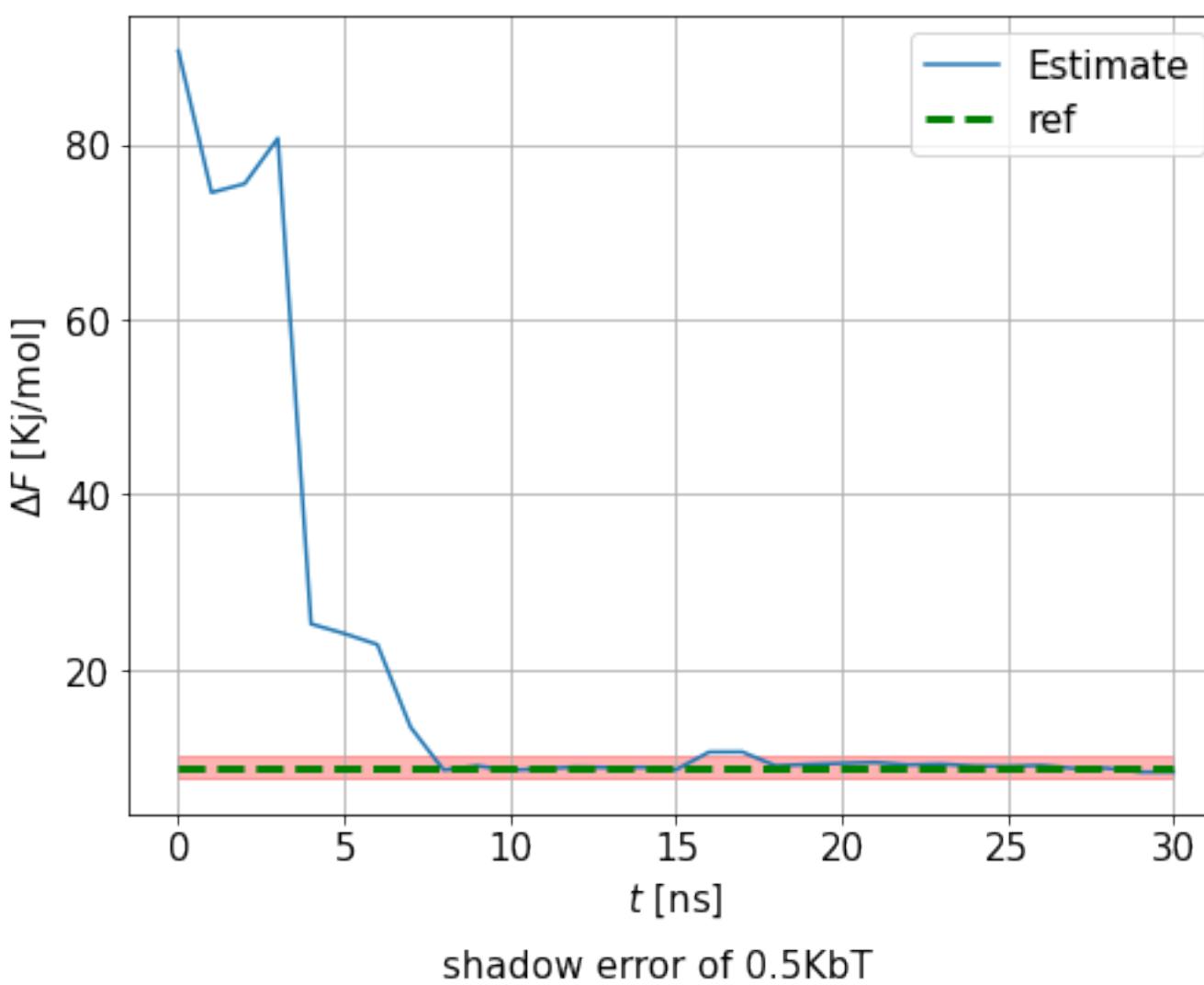
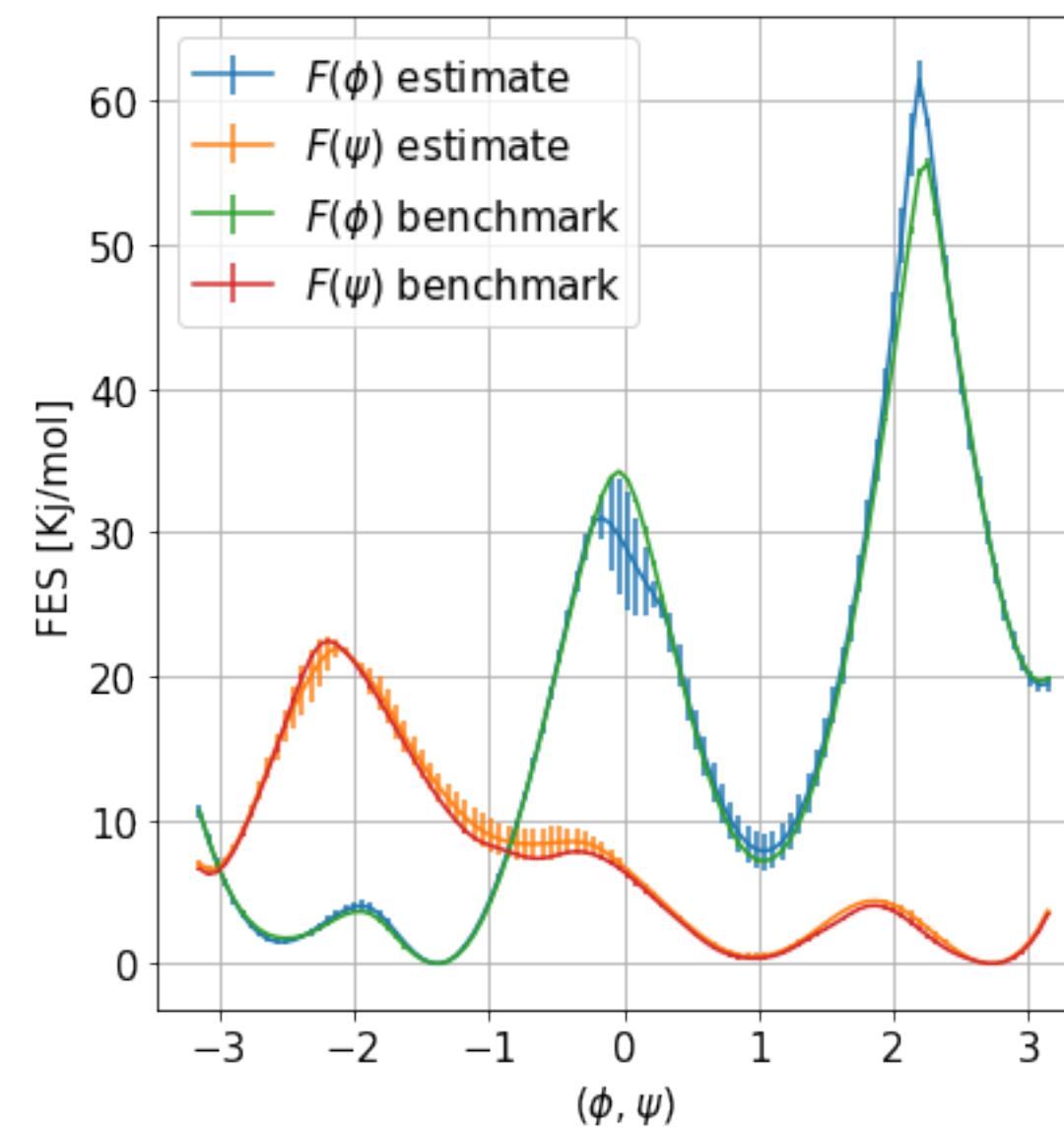
Problem: when to stop the iteration?

This procedure does not work with Alanine. I'll show that one with only TICA or only Deep-TICA

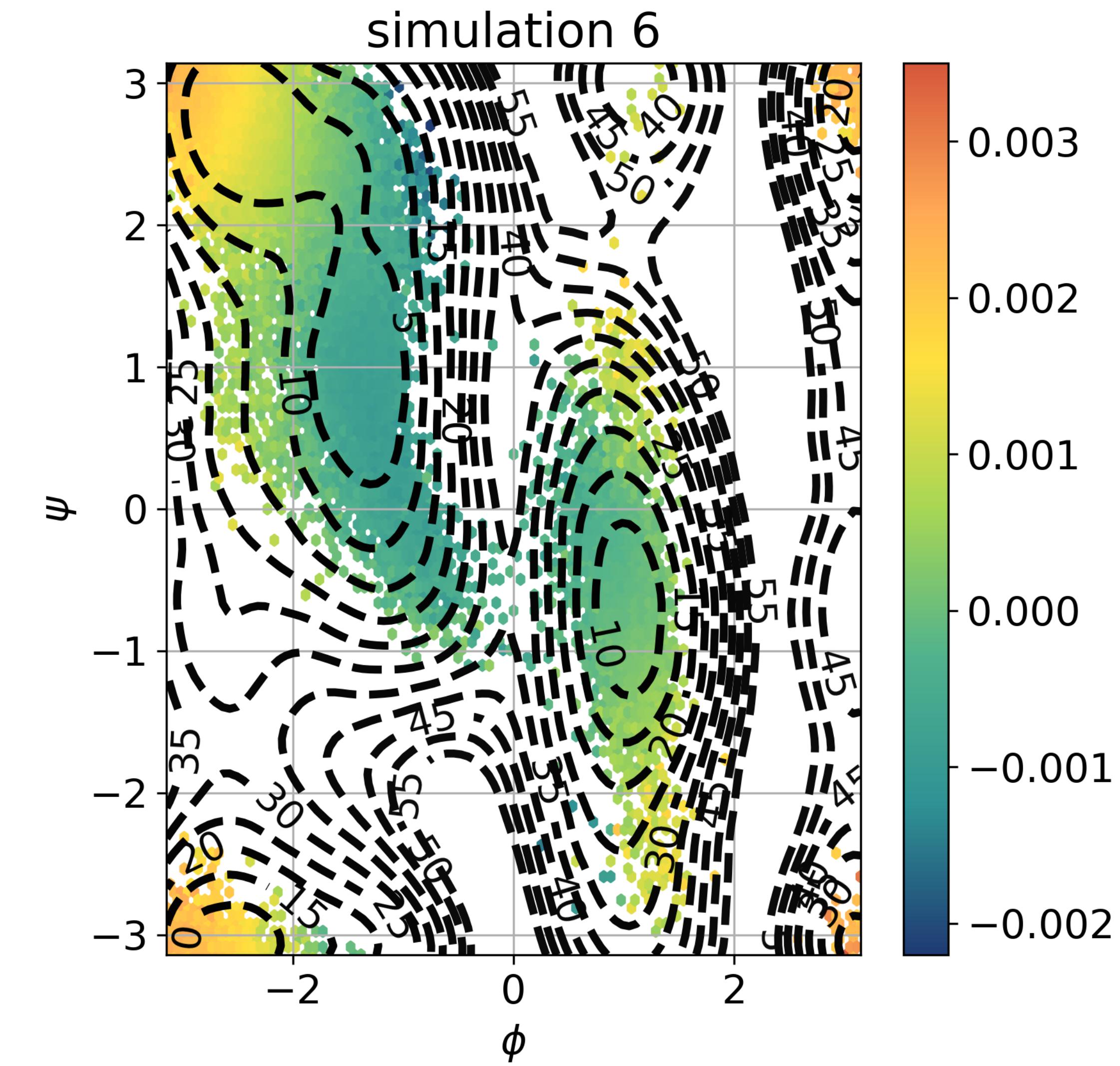
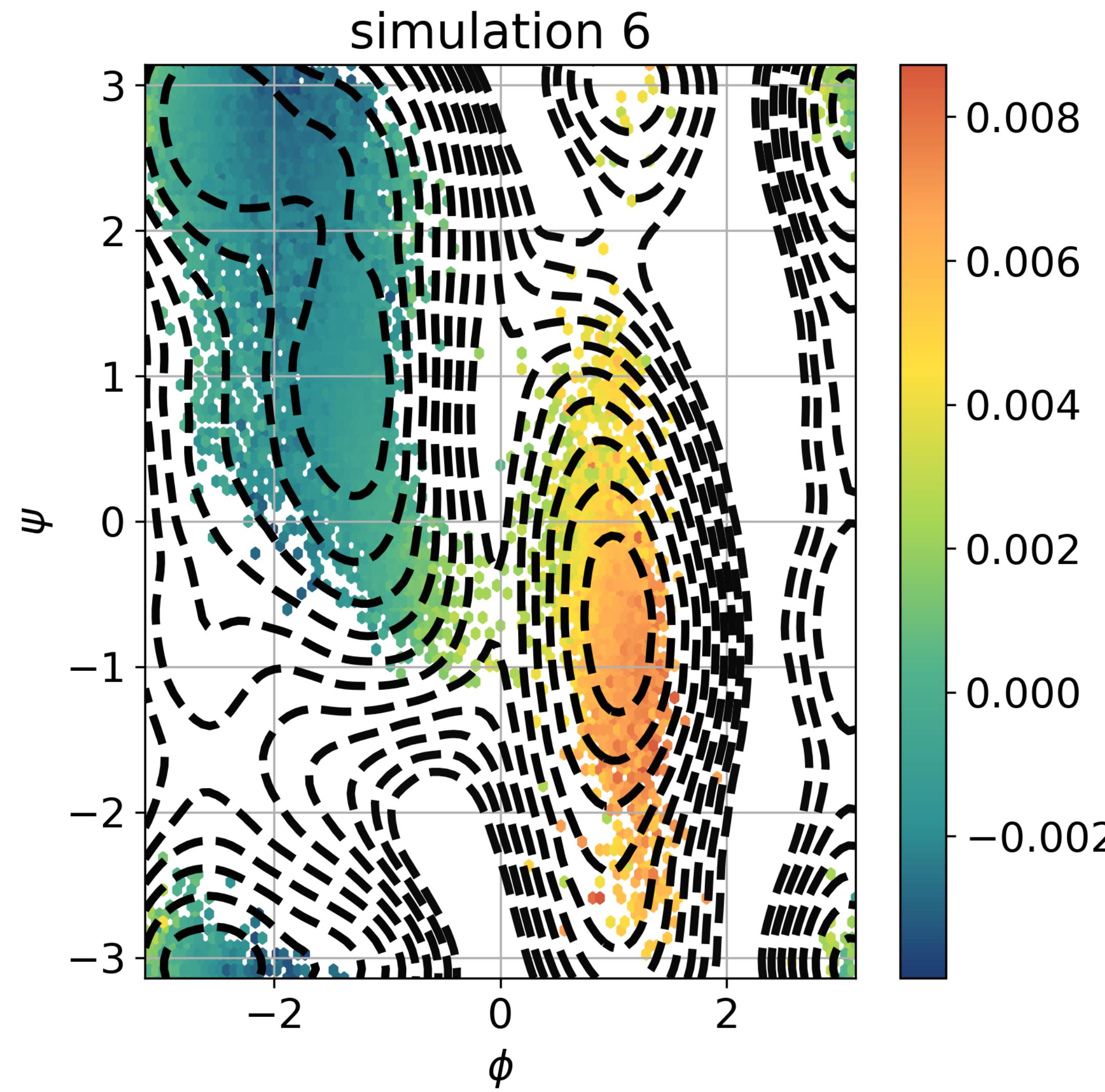
# Alanine Dipeptide, TICA



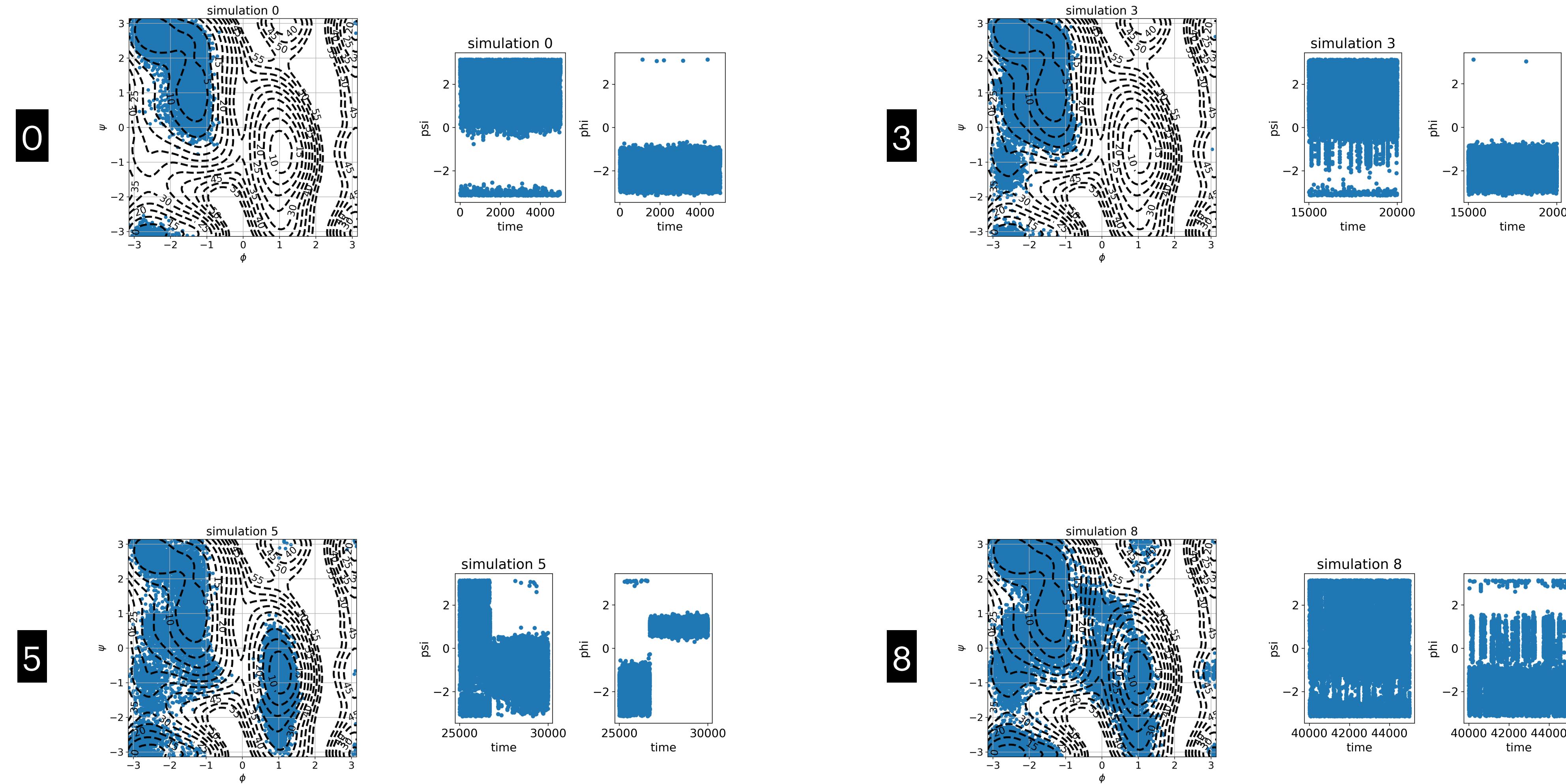
# FES Estimate



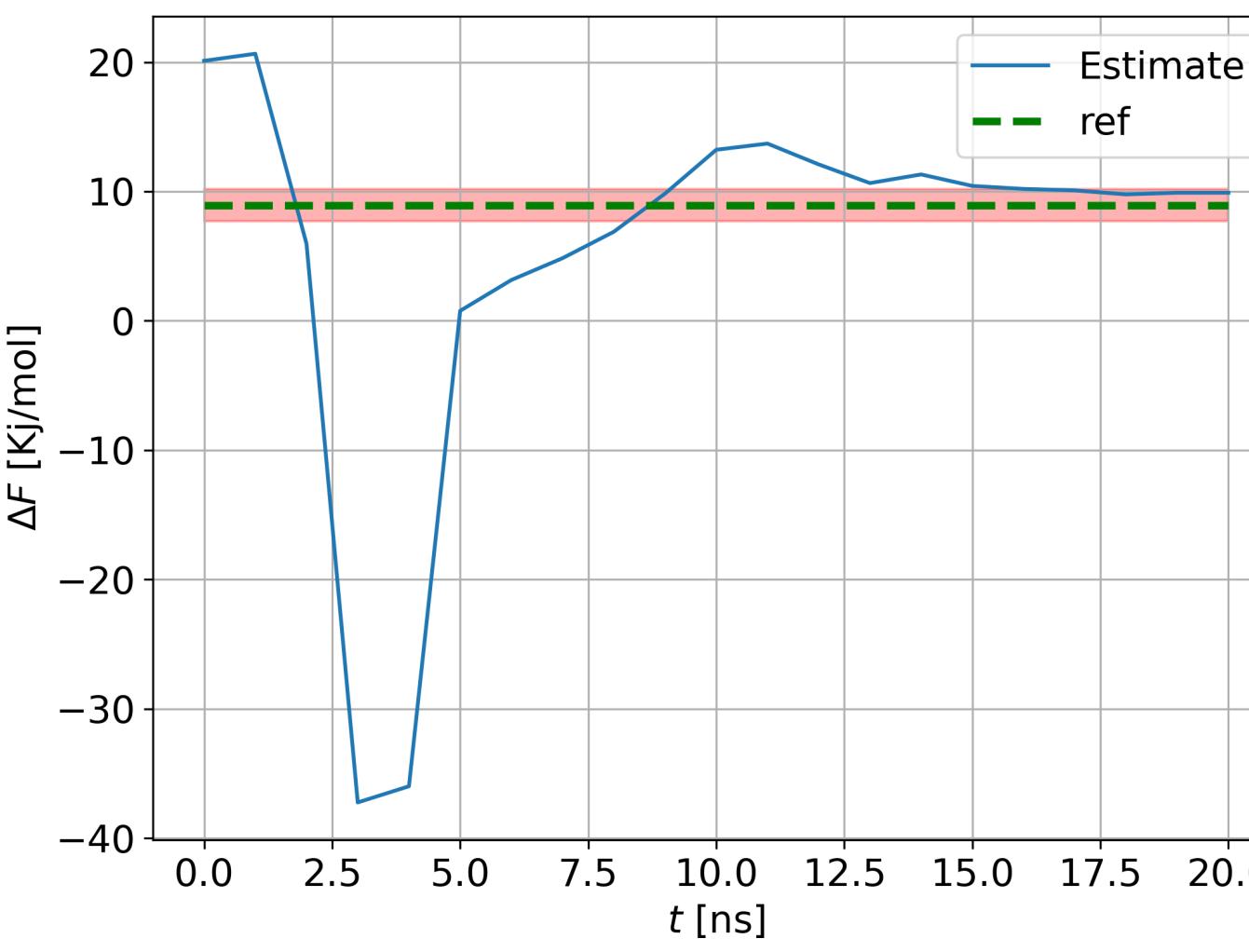
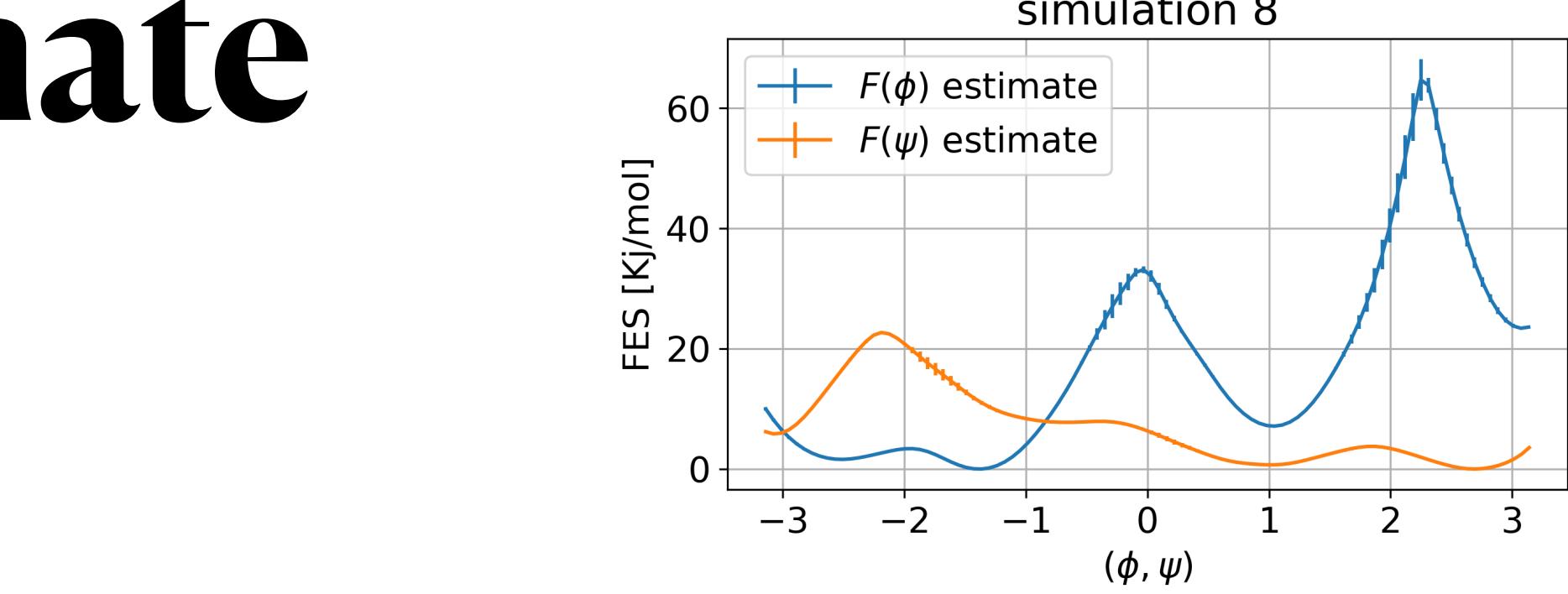
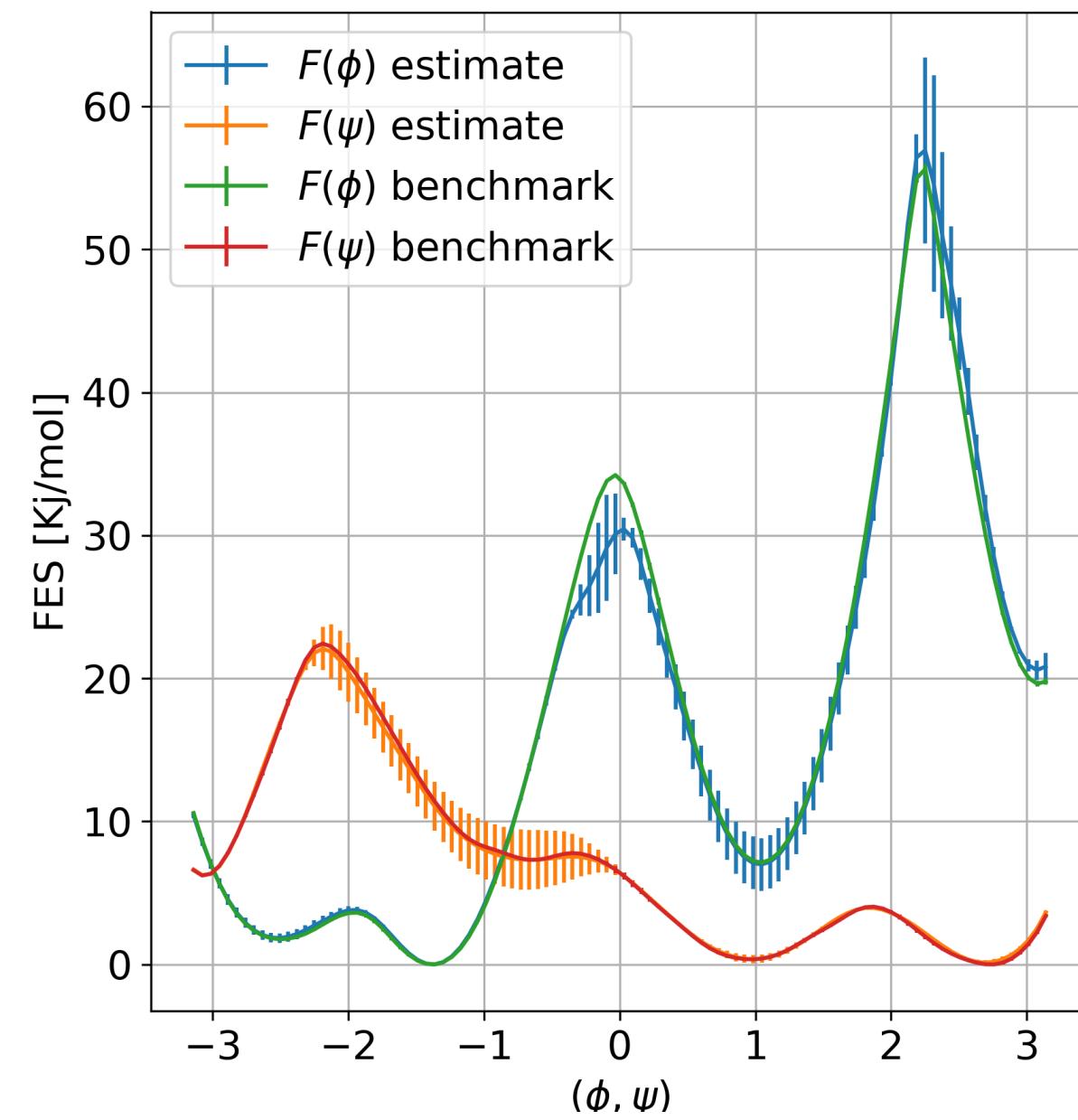
# Last CVs



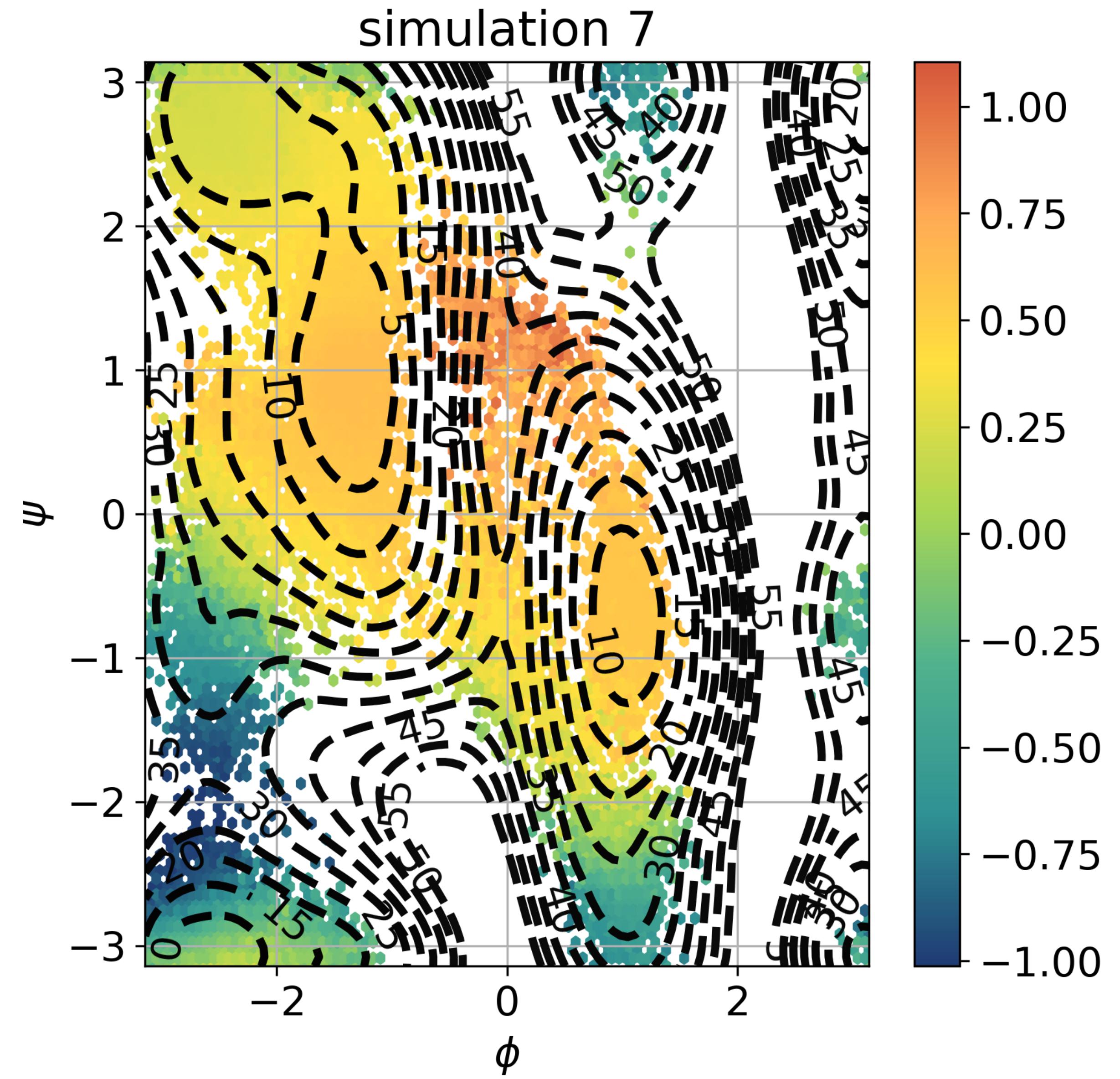
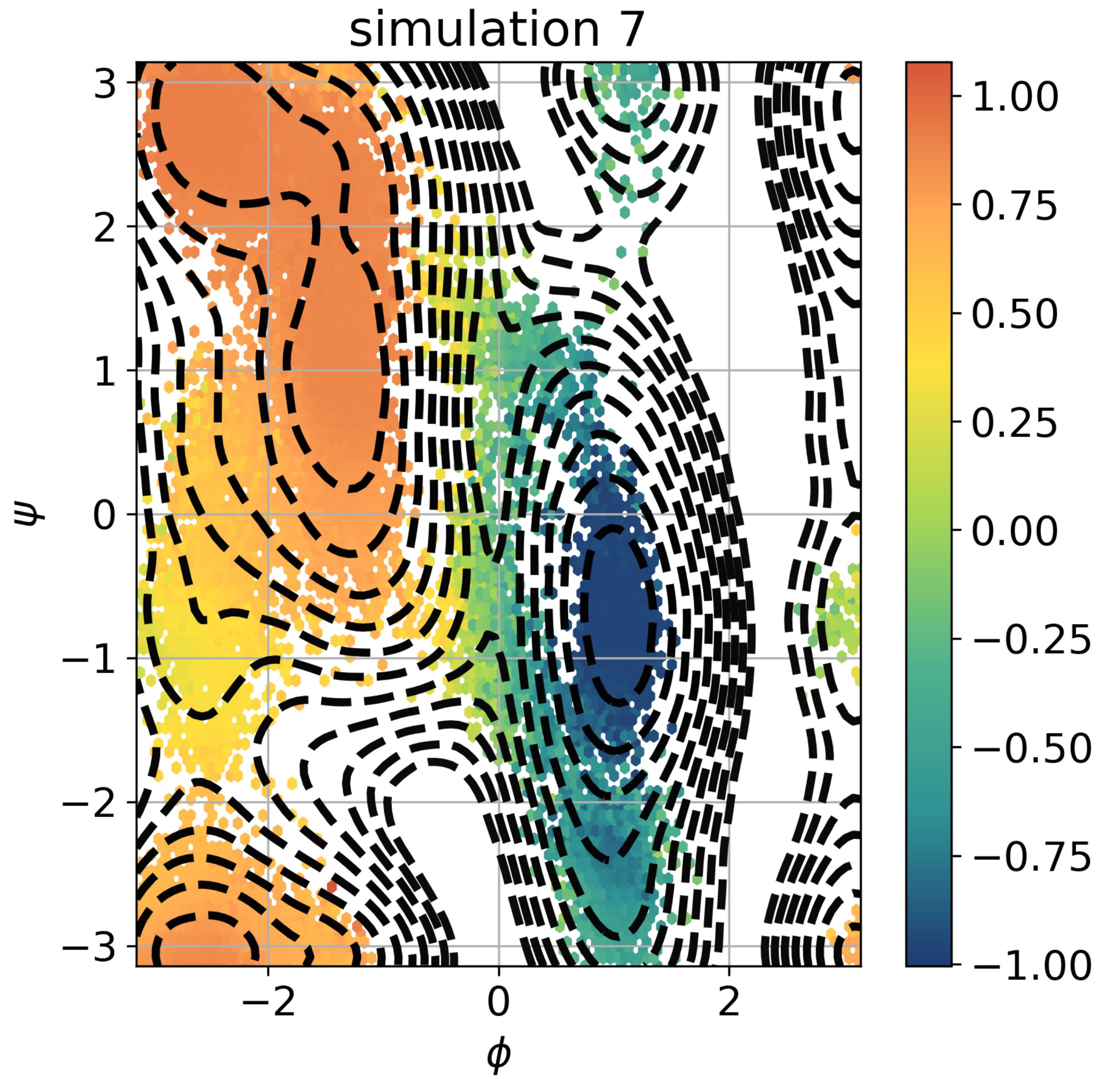
# Alanine Dipeptide, Deep-TICA



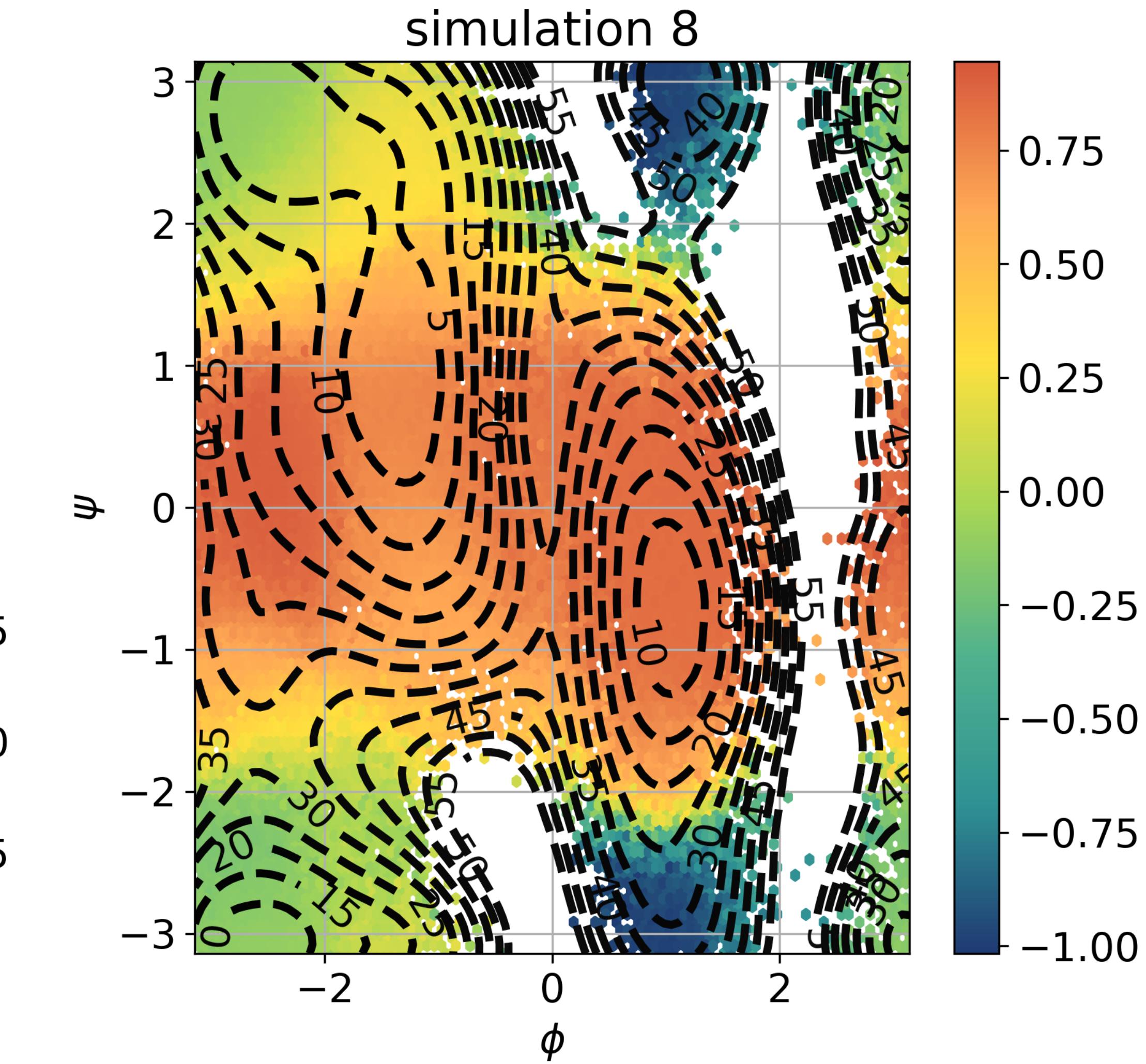
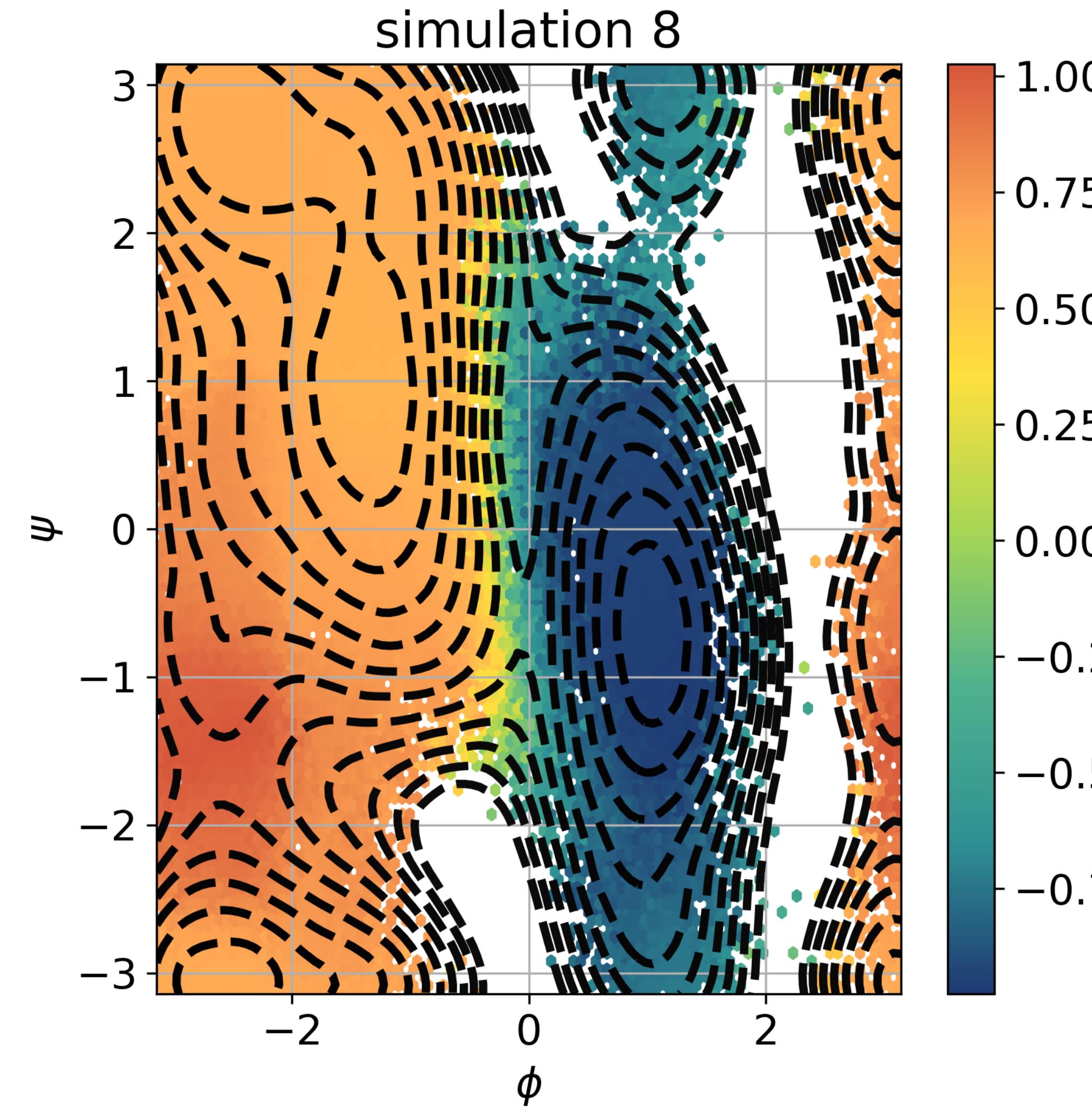
# FES Estimate



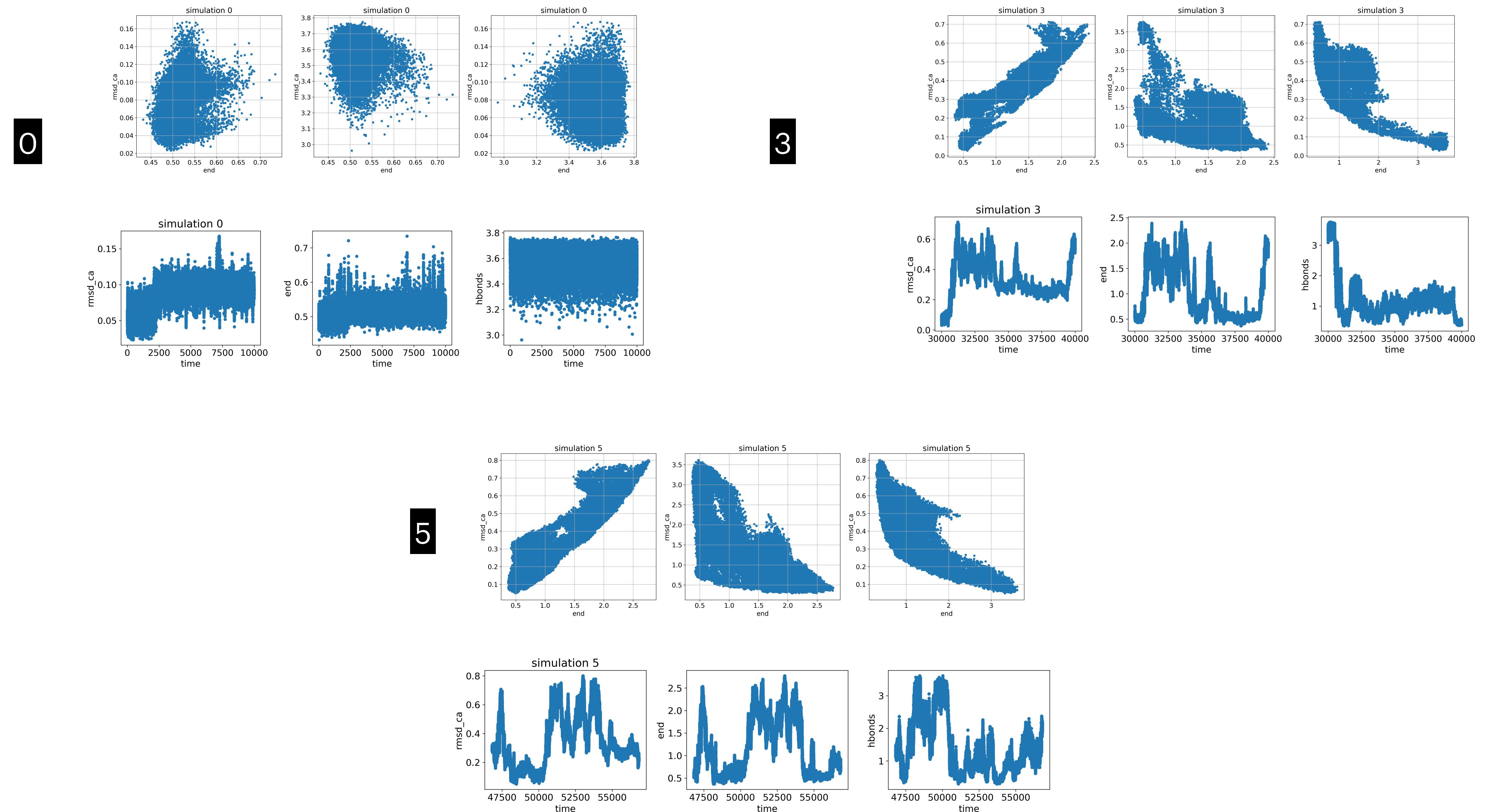
# Last CVs



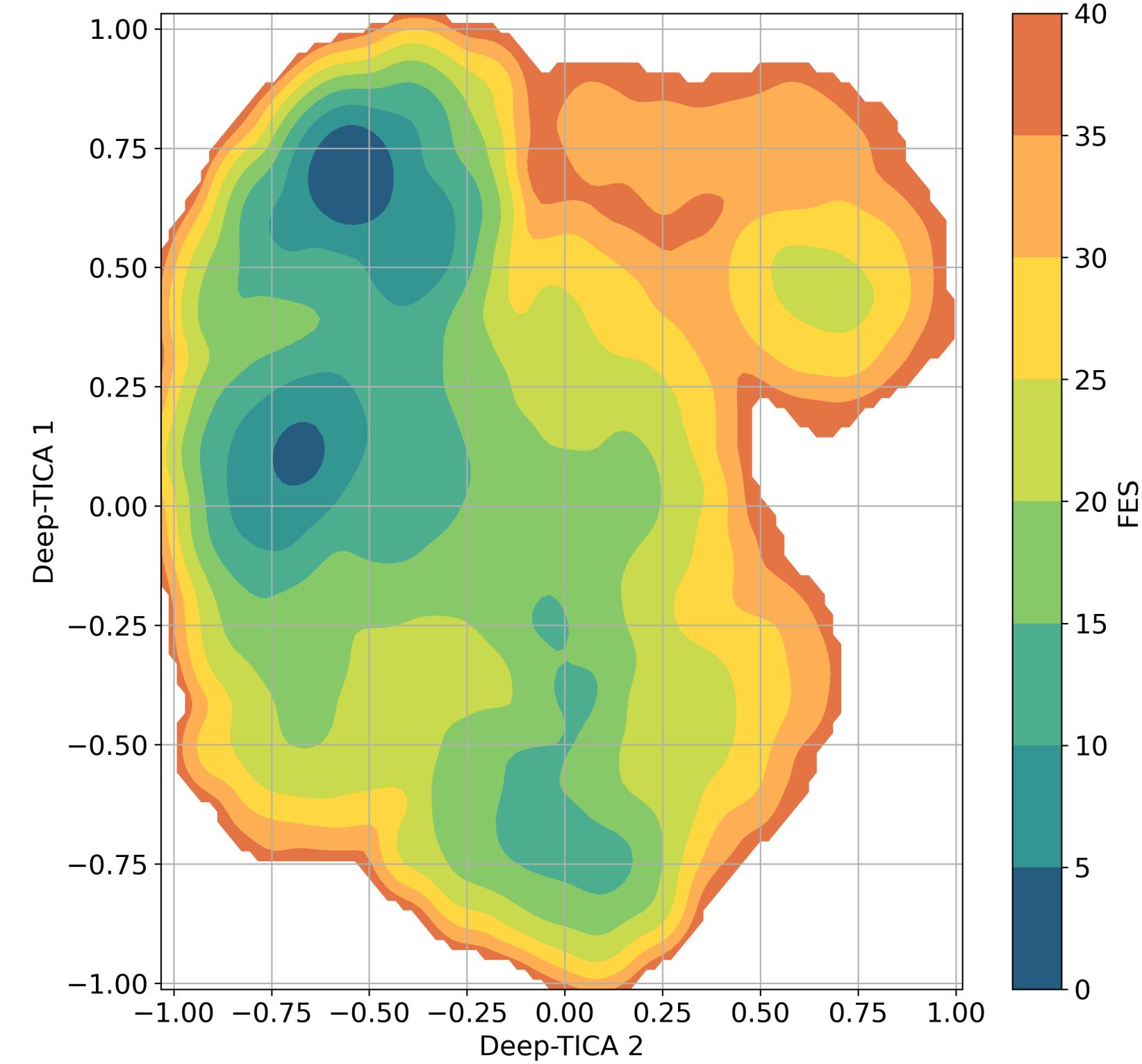
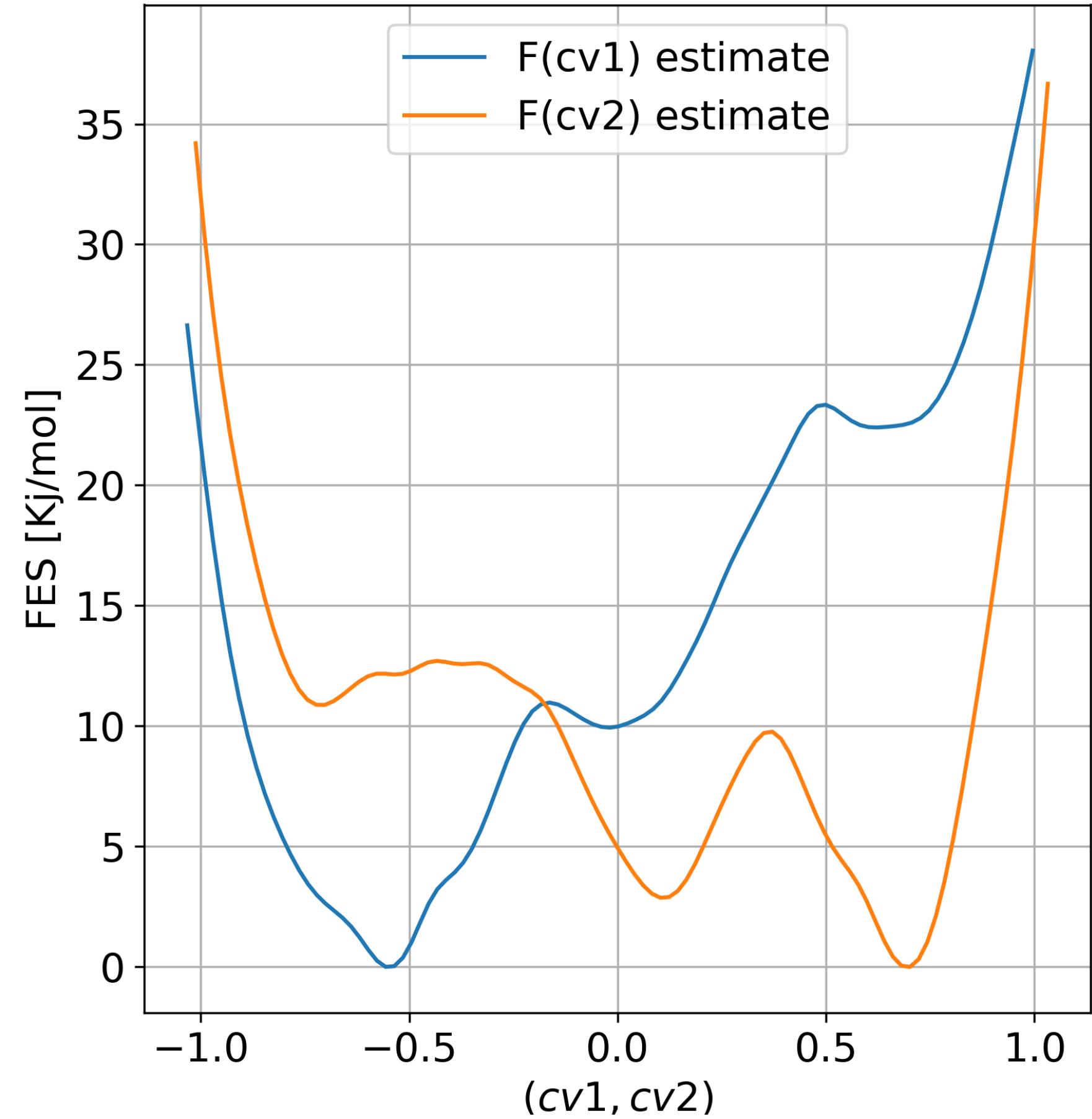
# New CVs from last trajectory



# Chignolin, TICA

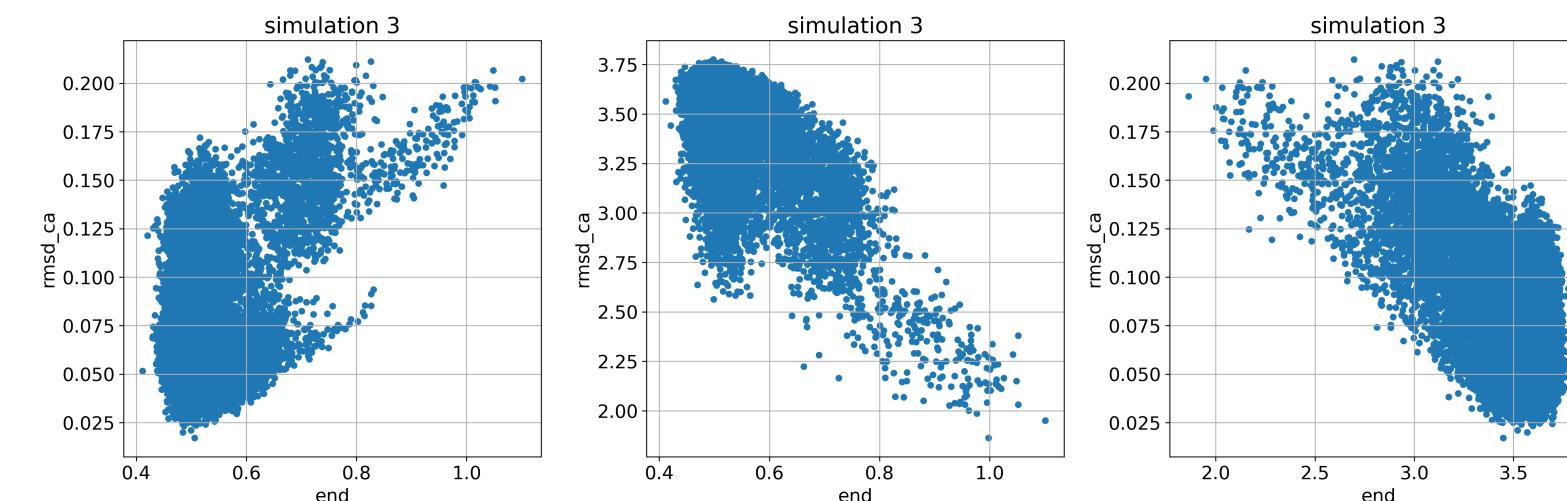


# FES

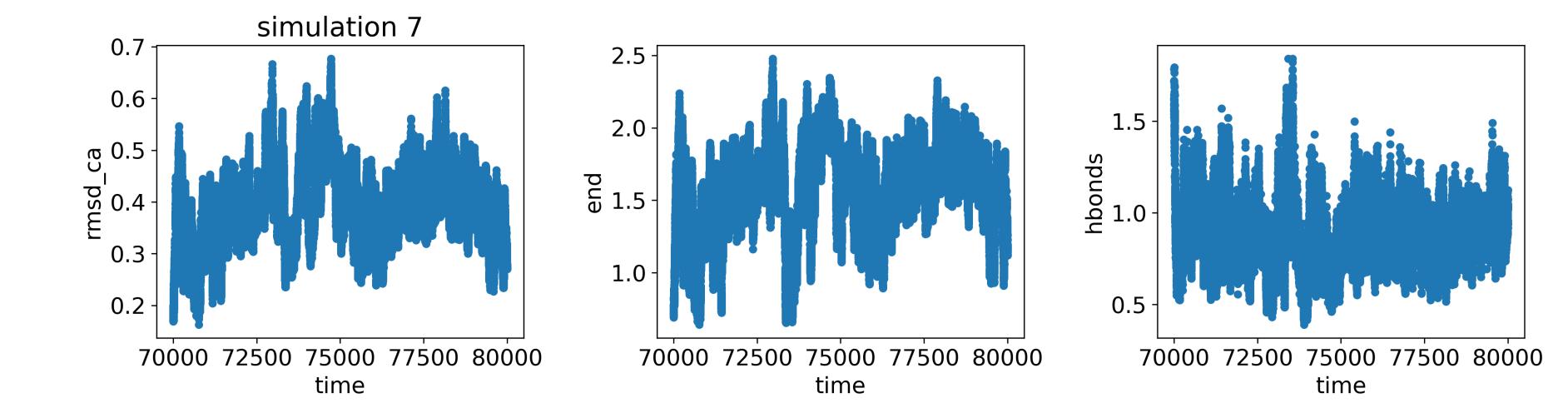
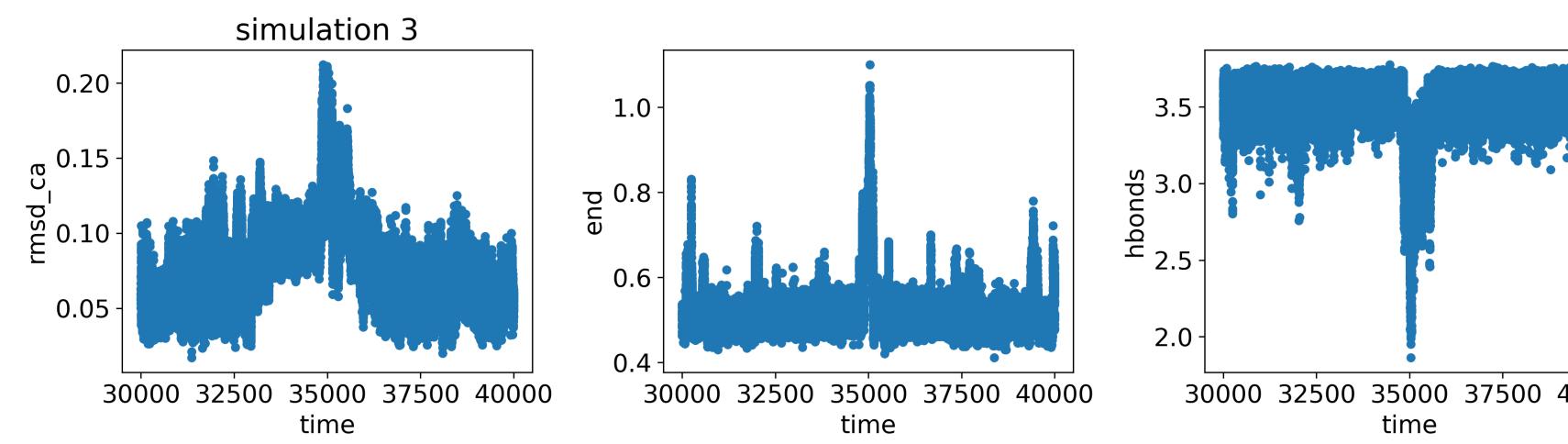
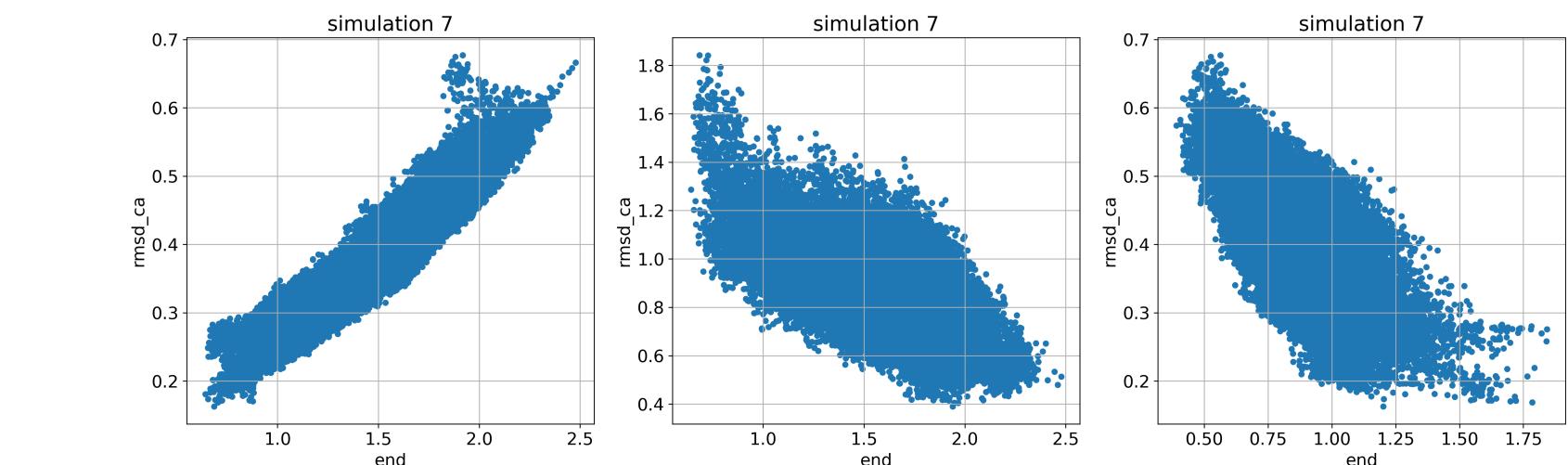


# Chignolin, Deep-TICA

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7



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