Accelerated Sampling of Rare Events using a Neural Network Bias Potential

Xinru Hua, Rasool Ahmad, Jose Blanchet, Wei Cai

NEURAL INFORMATION PROCESSING SYSTEMS

Stanford
ENGINEERING

Motivation

- In material science and bio-chemistry, we want to sample rare events that are associated with specific physical phenomena and estimate their probabilities.

- In this work, we focus on sampling the rare event that one molecule transits between two stationary metastable states in 2D.

- The molecule follows the over-damped Langevin Dynamics.

$$d\mathbf{x} = -\nabla U(\mathbf{x})/(m\gamma) \cdot dt + \sqrt{2k_B T/(m\gamma)} \cdot dB(t).$$

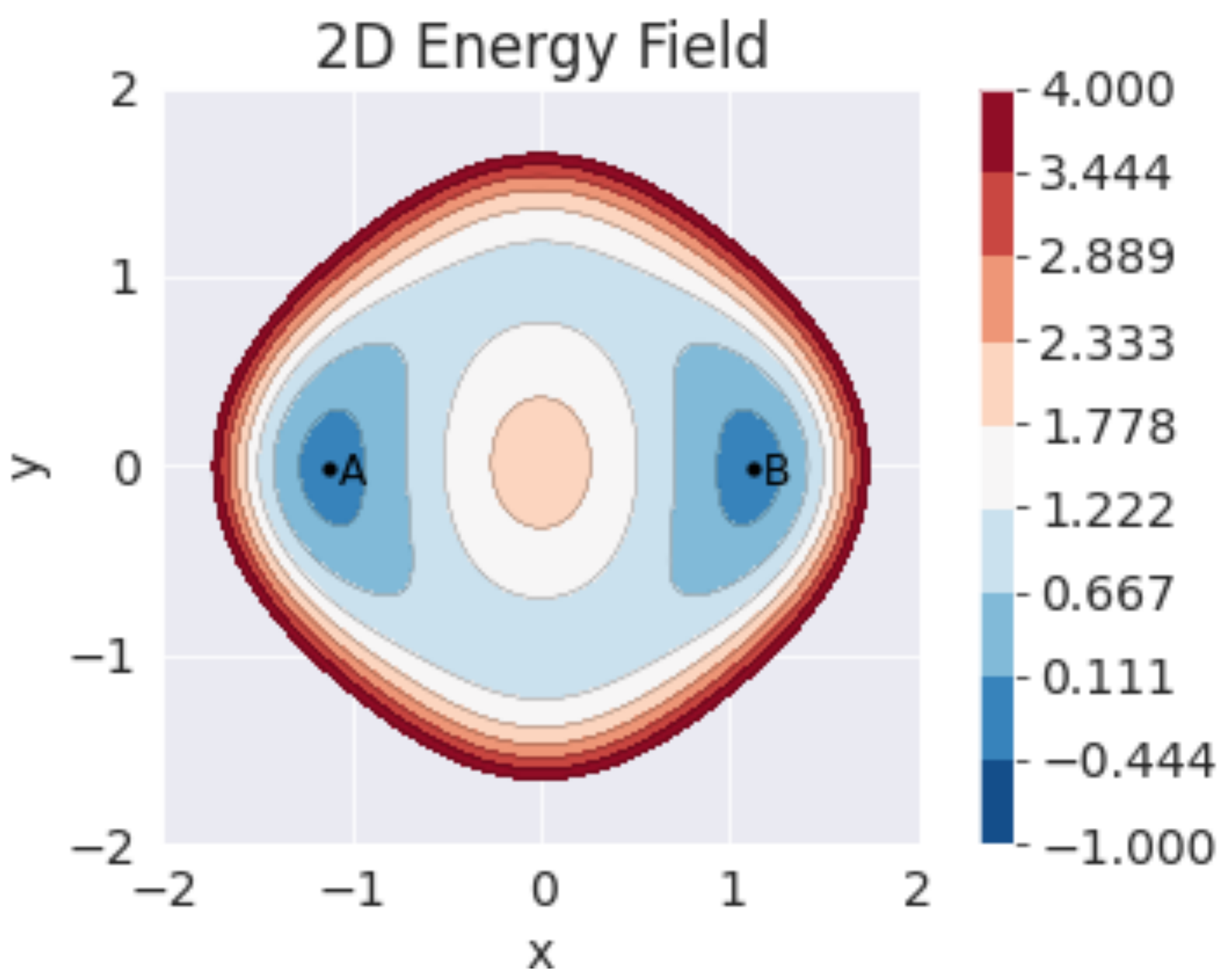
Energy function

Brownian motion

Problem

- The energy function is:

$$U(\mathbf{x}) = 0.05y + \frac{1}{6}\left(4(1-x^2-y^2)^2 + 2(x^2-2)^2 + [(x+y)^2-1]^2 + [(x-y)^2-1]^2 - 2\right). \tag{2}$$



- The two stationary metastable states are A and B, minima of the energy field.

- We are interested in the rate event that the molecule starts from A and eventually goes to B.

Optimization Problem

We represent the trajectories as $\nu = (x_0, x_1, \ldots, x_N)$ and our bias potential is parametrized by neural network θ.

Our objectives are:

1. Ensure all the trajectories reach B

2. The distribution of successful trajectories is similar to the distribution of unbiased successful trajectories

Optimization Problem

We represent the trajectories as $\nu = (x_0, x_1, \ldots, x_N)$ and our bias potential is parametrized by neural network θ.

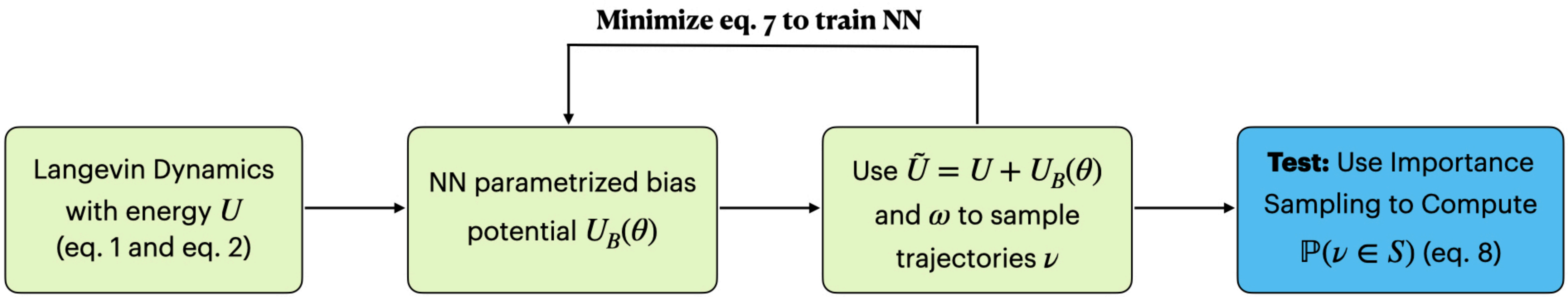
Our objectives are:

1. Ensure all the trajectories reach B

2. The distribution of successful trajectories is similar to the distribution of unbiased successful trajectories

$$\inf_{\theta} \mathbb{E}_Q \left[\underbrace{\boxed{\log\left(\frac{dQ(\nu_\theta(\omega))}{dP(\nu_\theta(\omega))}\right)}}_{2} + \underbrace{\boxed{F_{\text{smooth}}\left(\nu_\theta(\omega)\right)}}_{1} \right] \qquad \text{(eq.7 in the paper)}$$

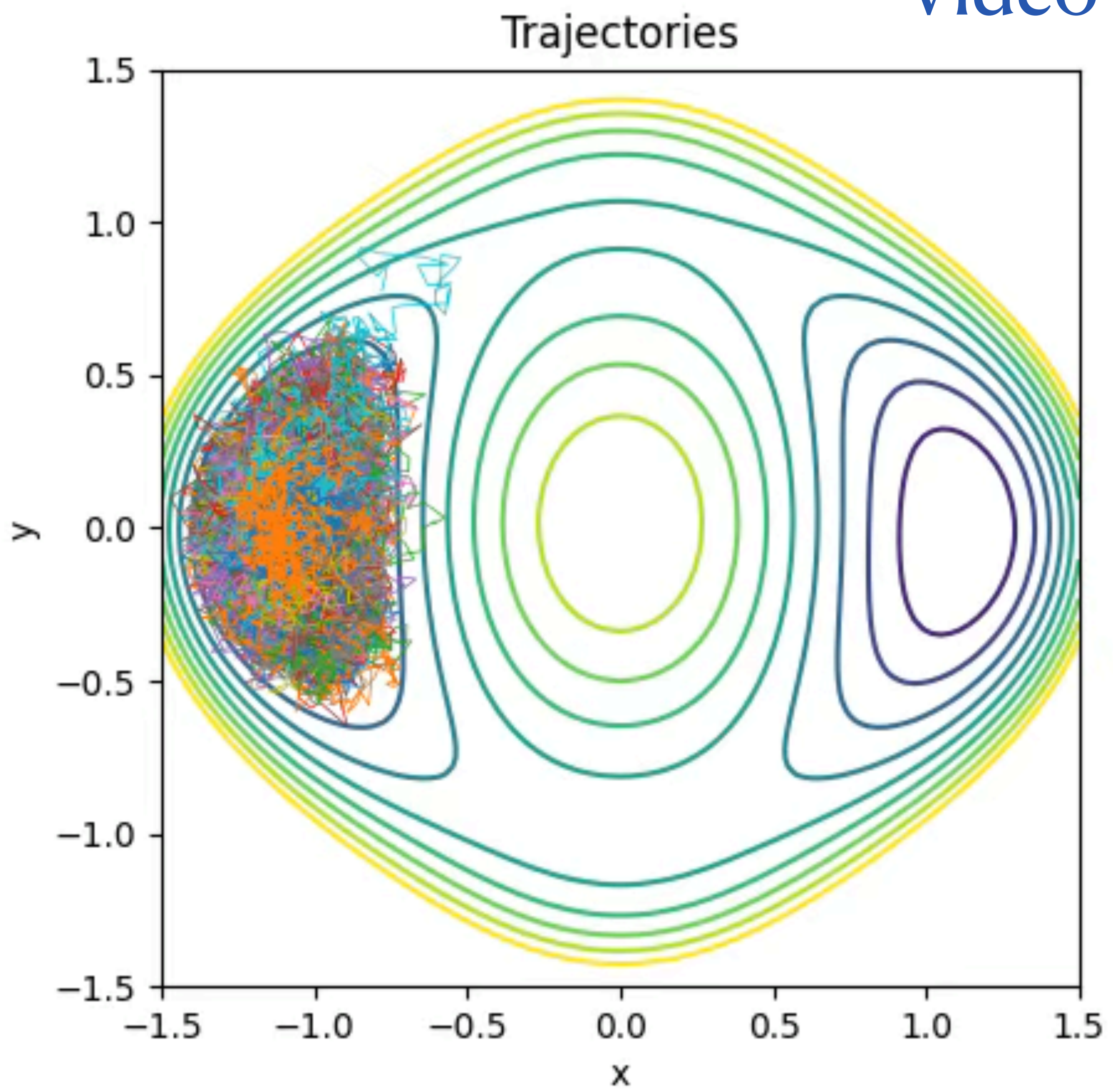
Method


Minimize eq. 7 to train NN
Langevin Dynamics with energy U (eq. 1 and eq. 2)
NN parametrized bias potential $U_B(\theta)$
Use $\tilde{U} = U + U_B(\theta)$ and ω to sample trajectories ν
Test: Use Importance Sampling to Compute $\mathbb{P}(\nu \in S)$ (eq. 8)

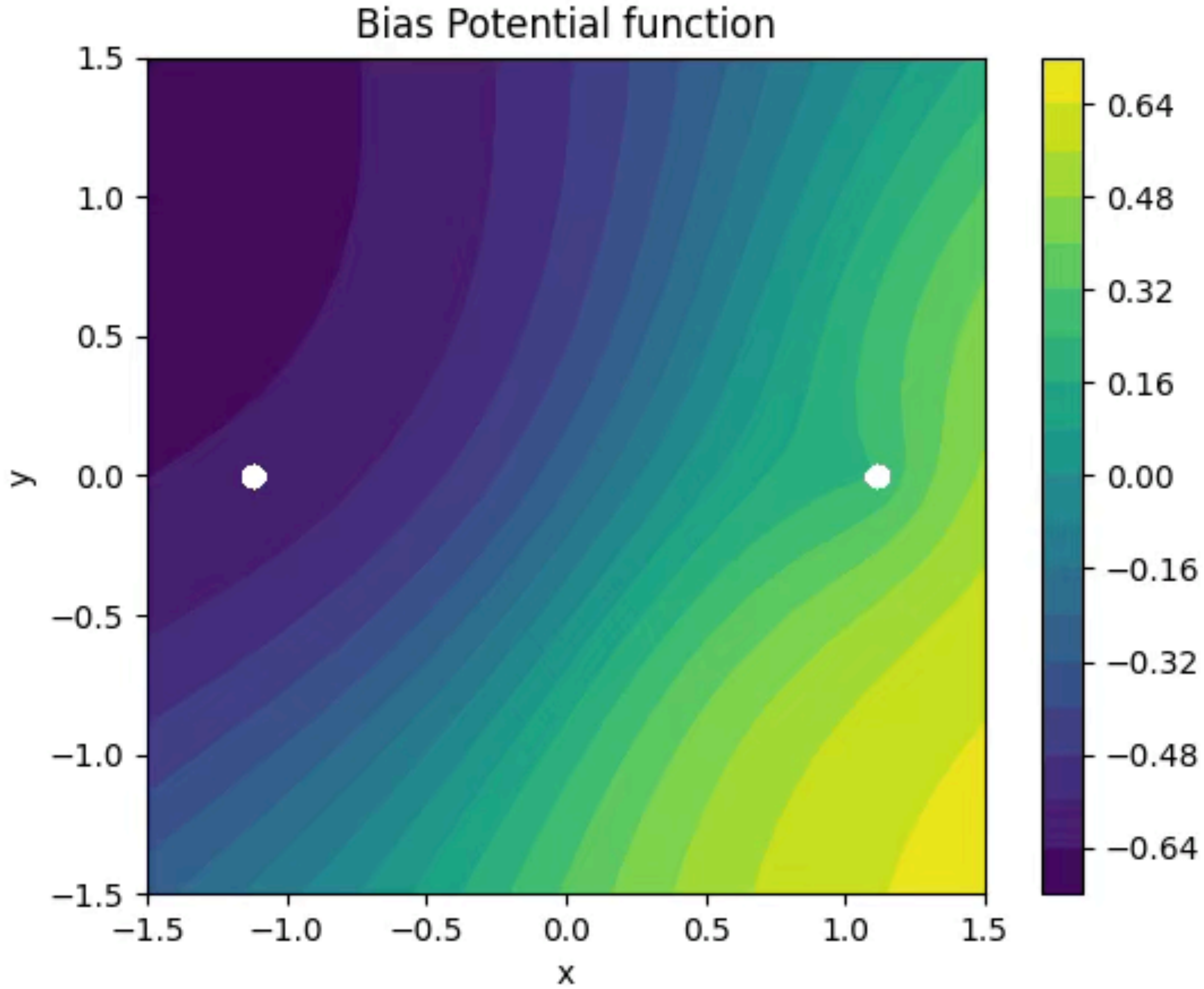
Training Process

The DNN-based bias potential eventually make a large portion of the trajectories to move from A to B.

Video Link

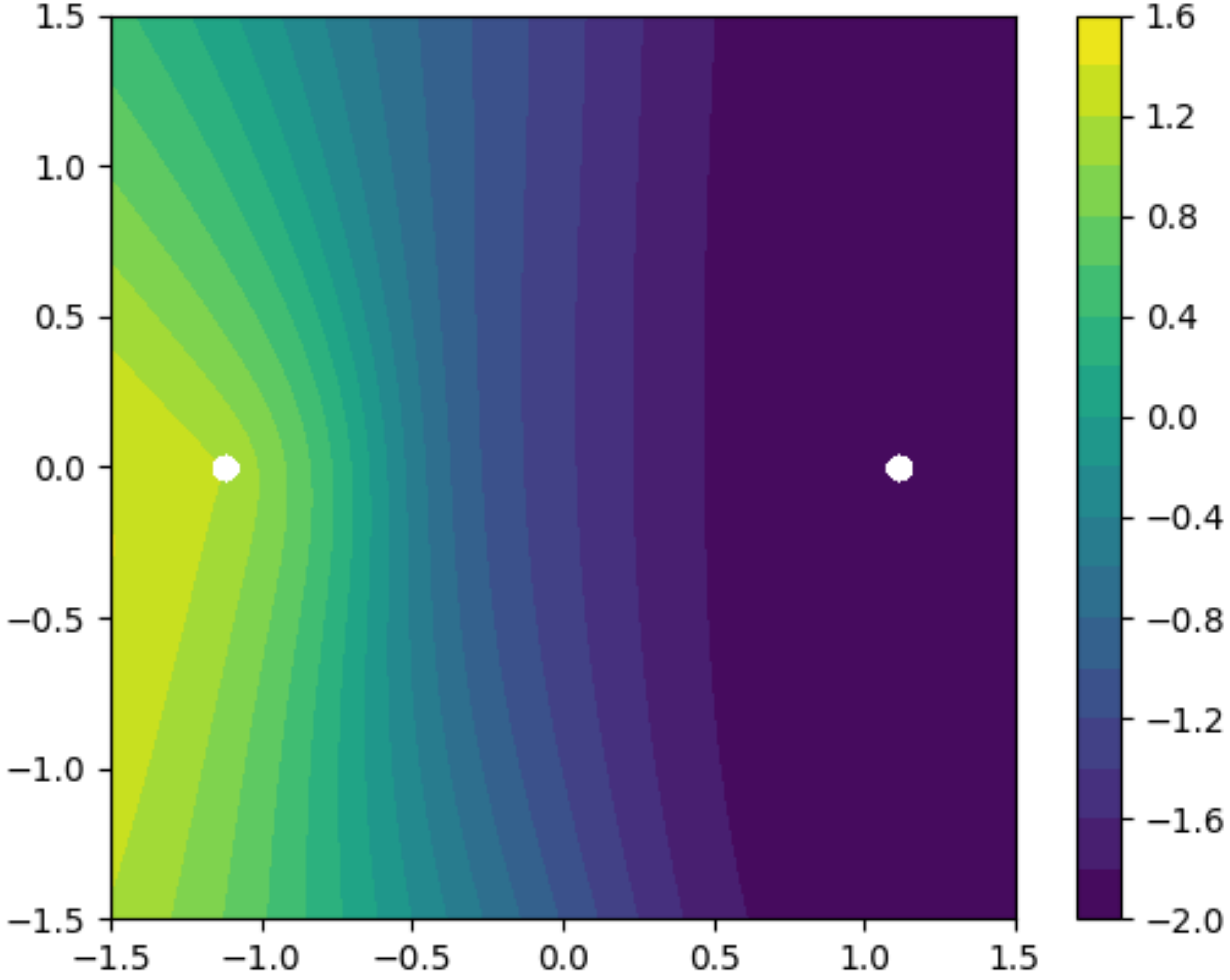


Video Link

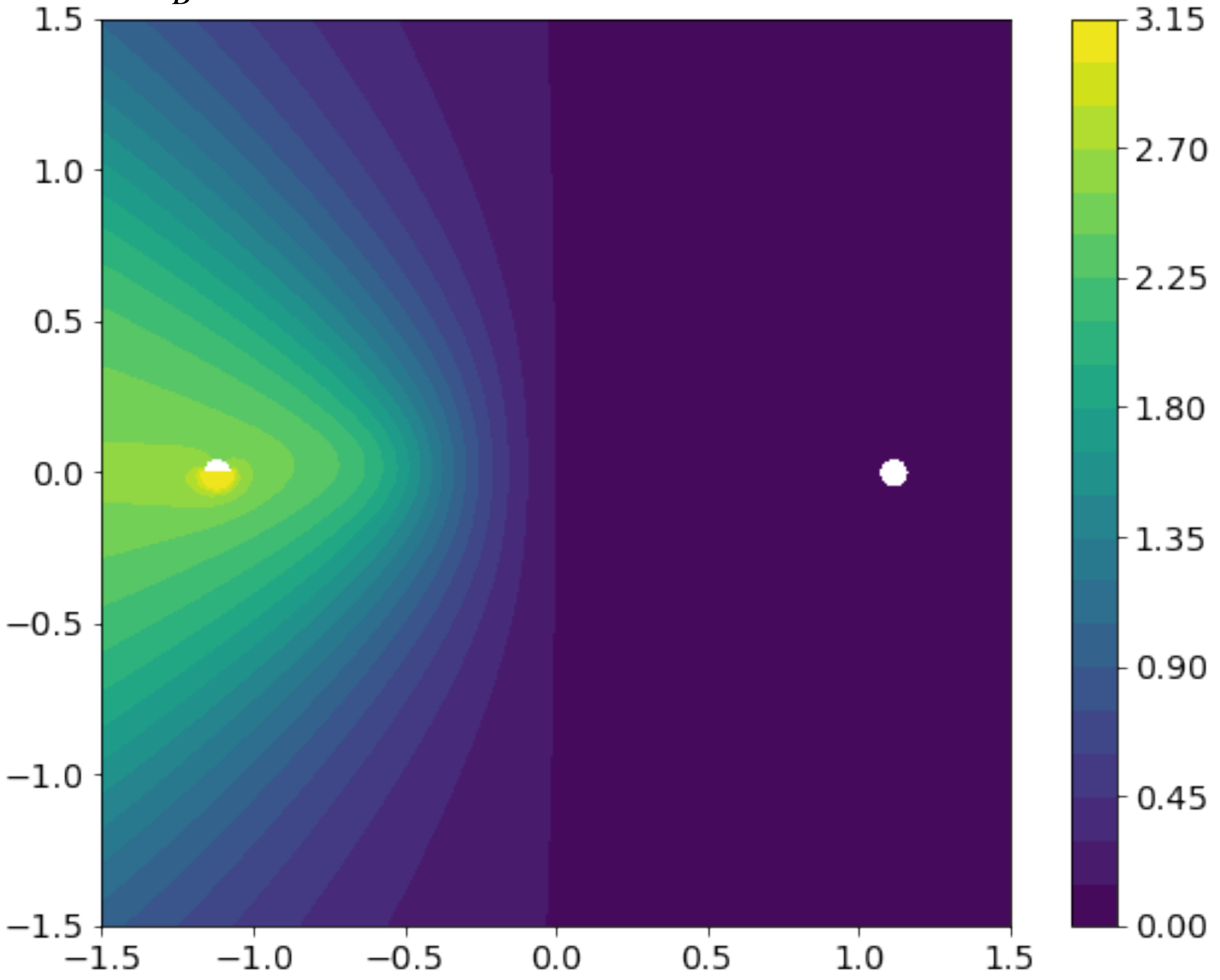


Training Results

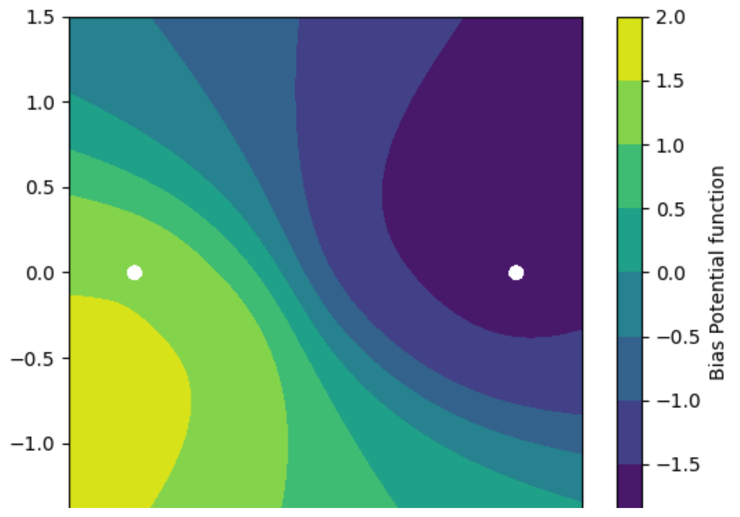
$U_B(x)$, our method solved bias potential at 1200K



$U_B^{gt}(x)$, the ground-truth bias potential at 1200K

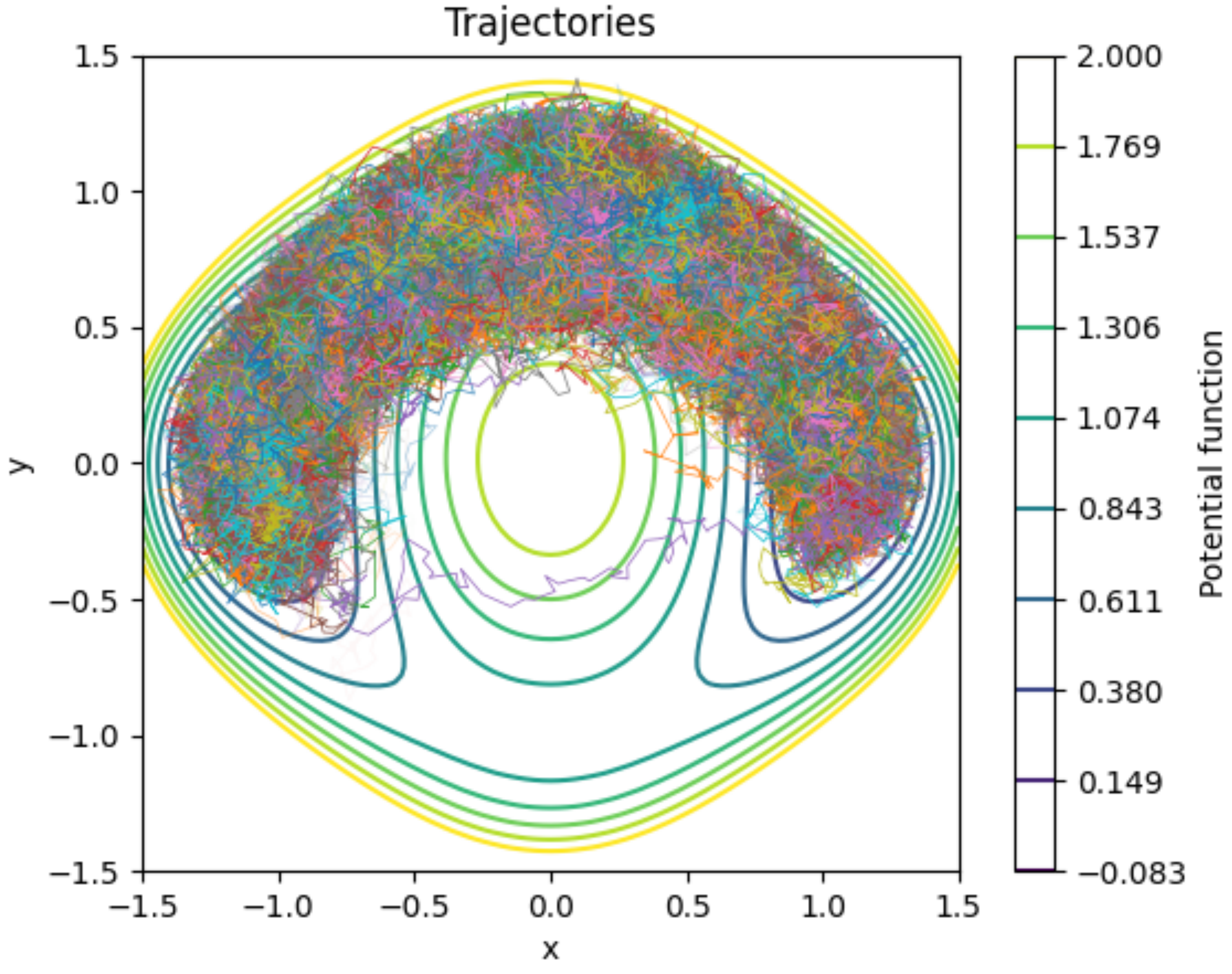


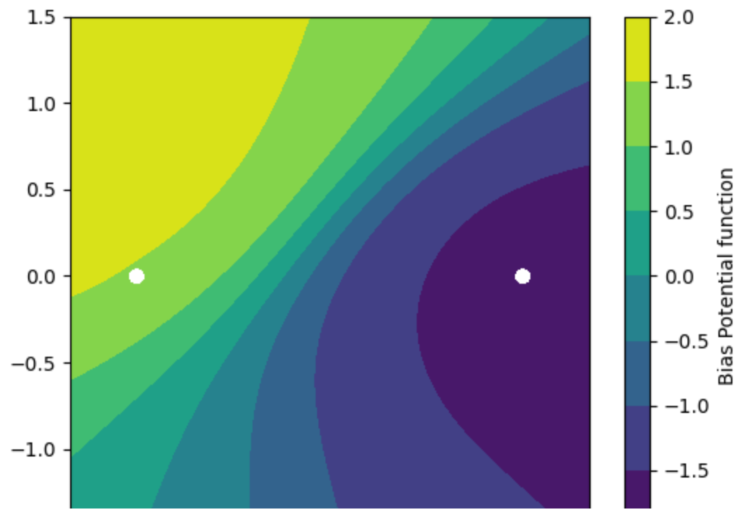
Combine Past Knowledge



Training result 1:

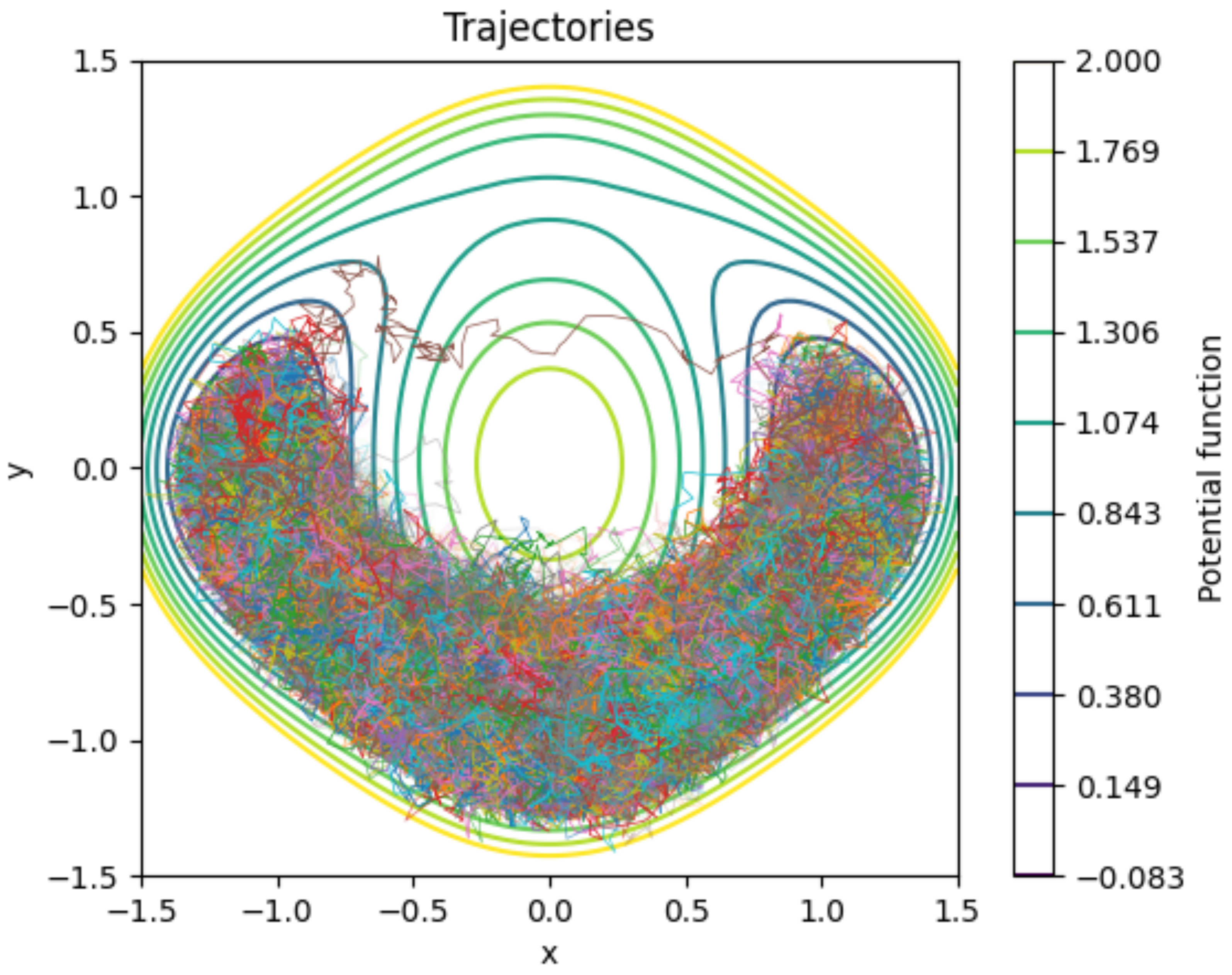
A list of trajectories





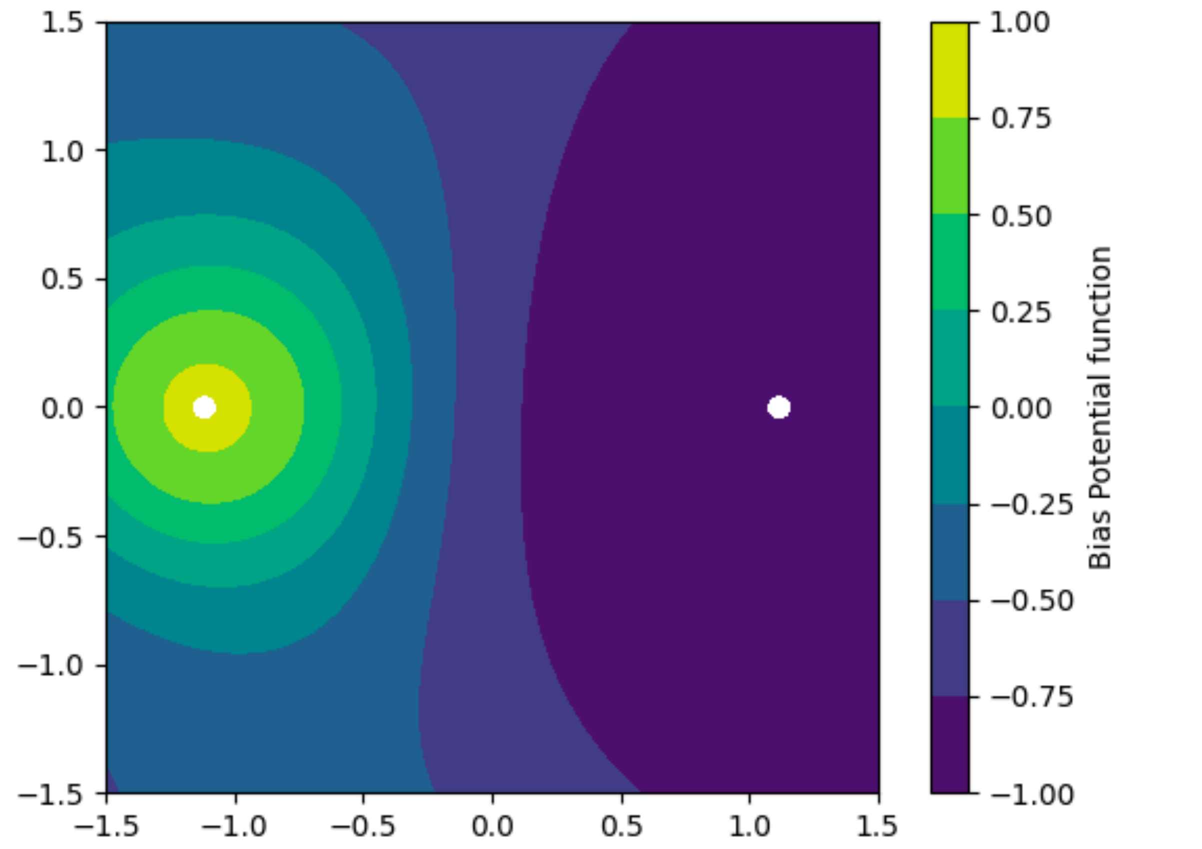
Training result 2:

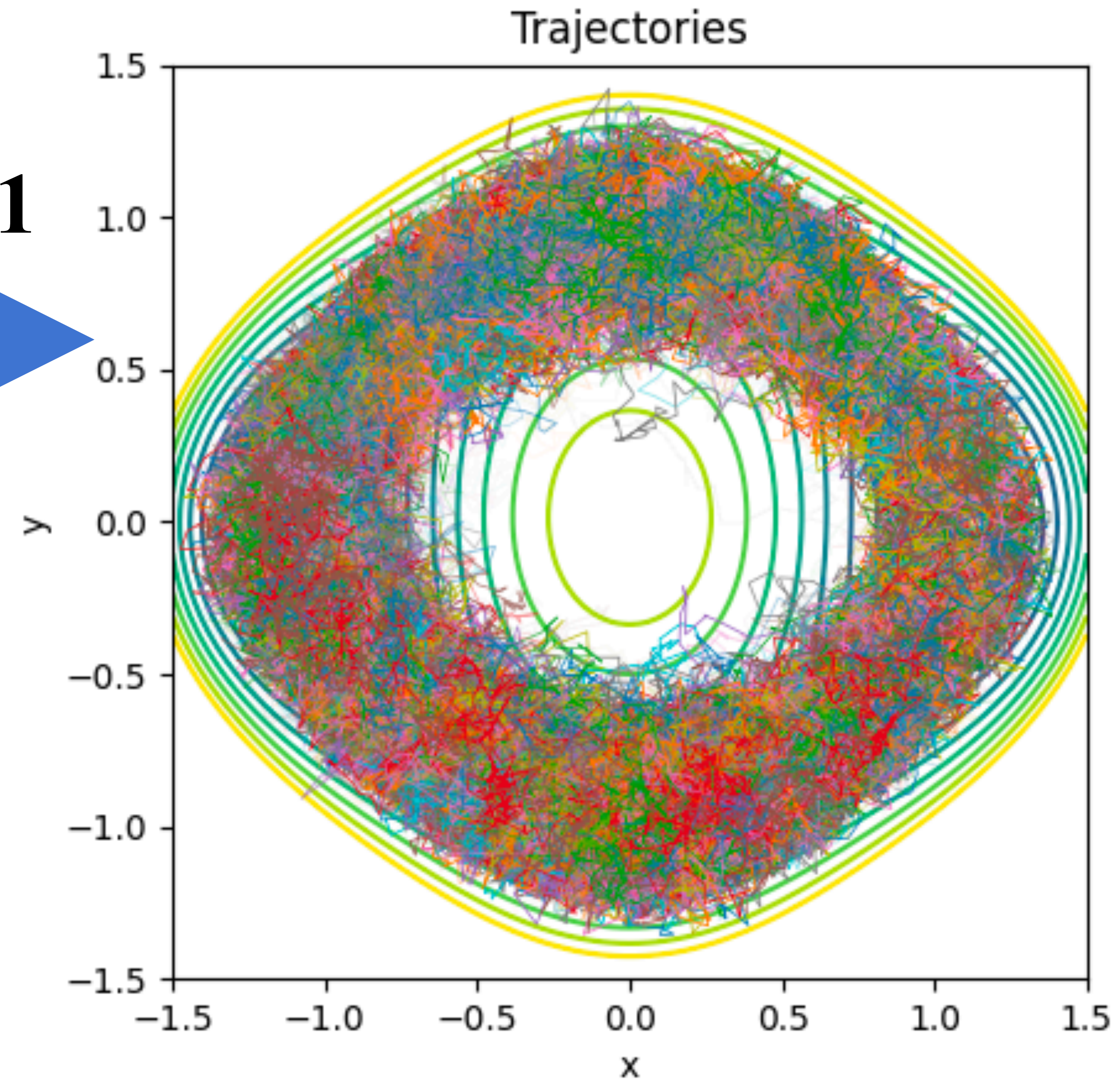
A list of trajectories



Sec 4.1

Combined Model

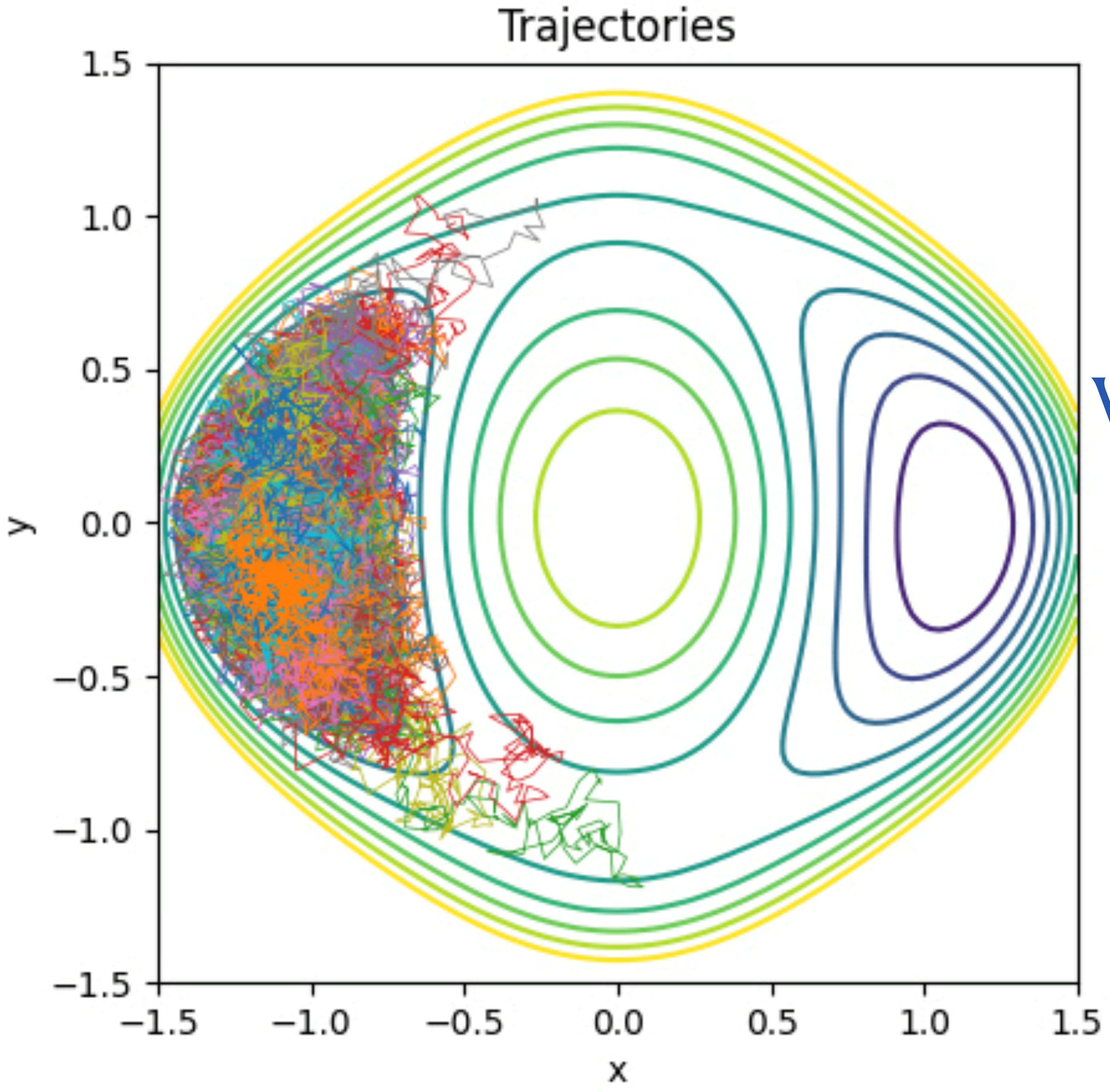




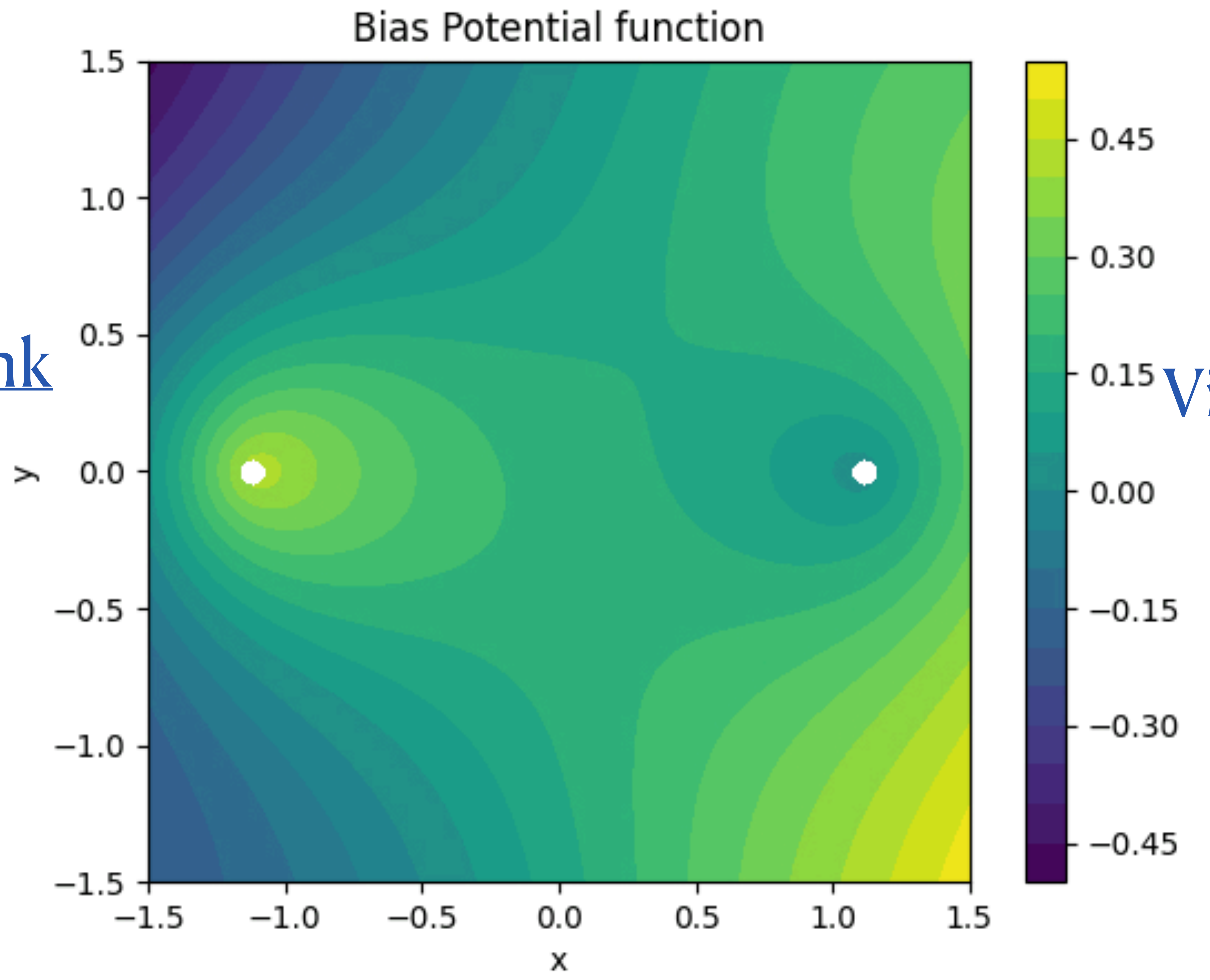
Combine Training Process

The input is all the training trajectories (positions of the molecule only).

The training result is one bias potential that can generate trajectories in both channels.



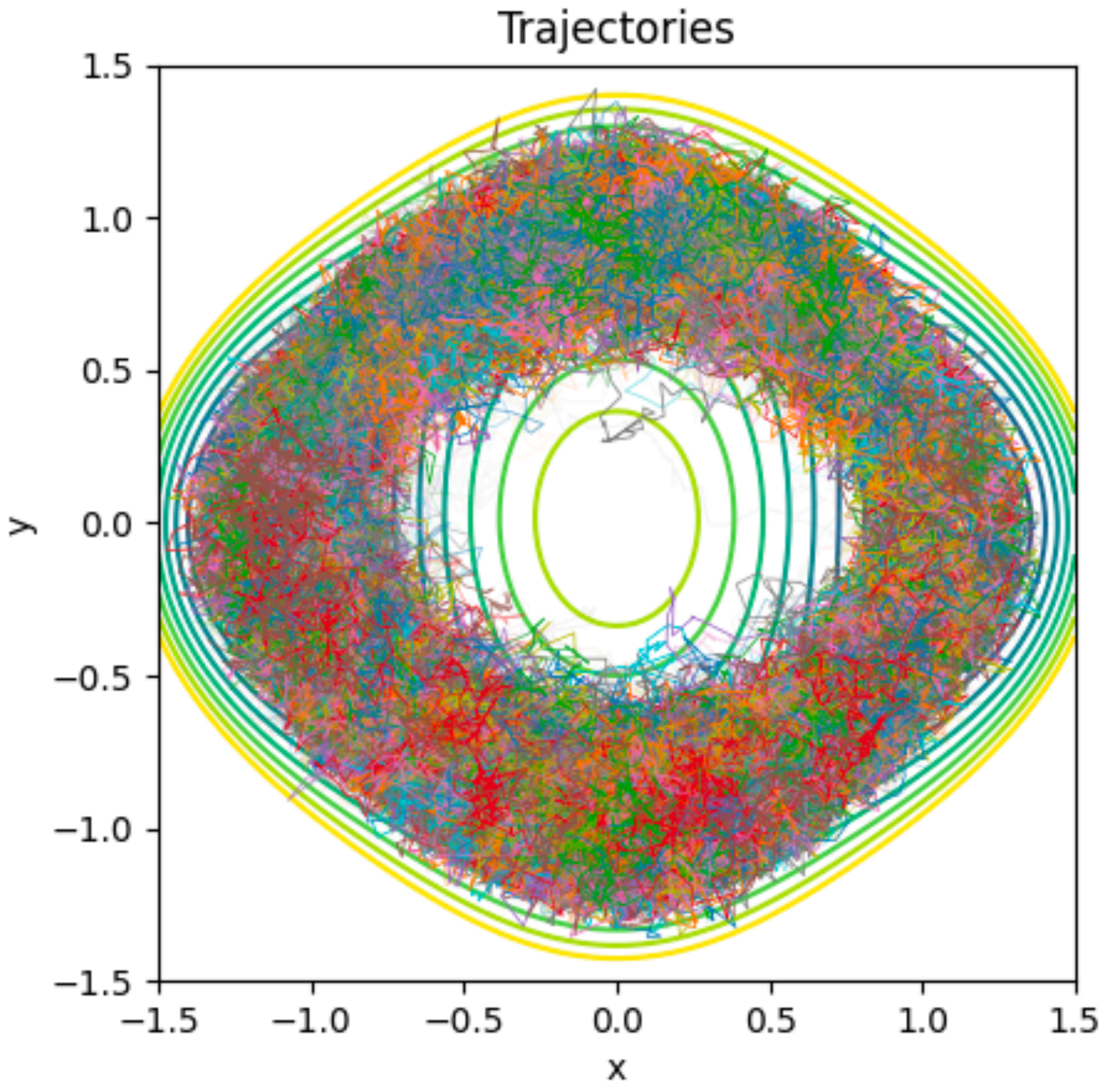
Video Link

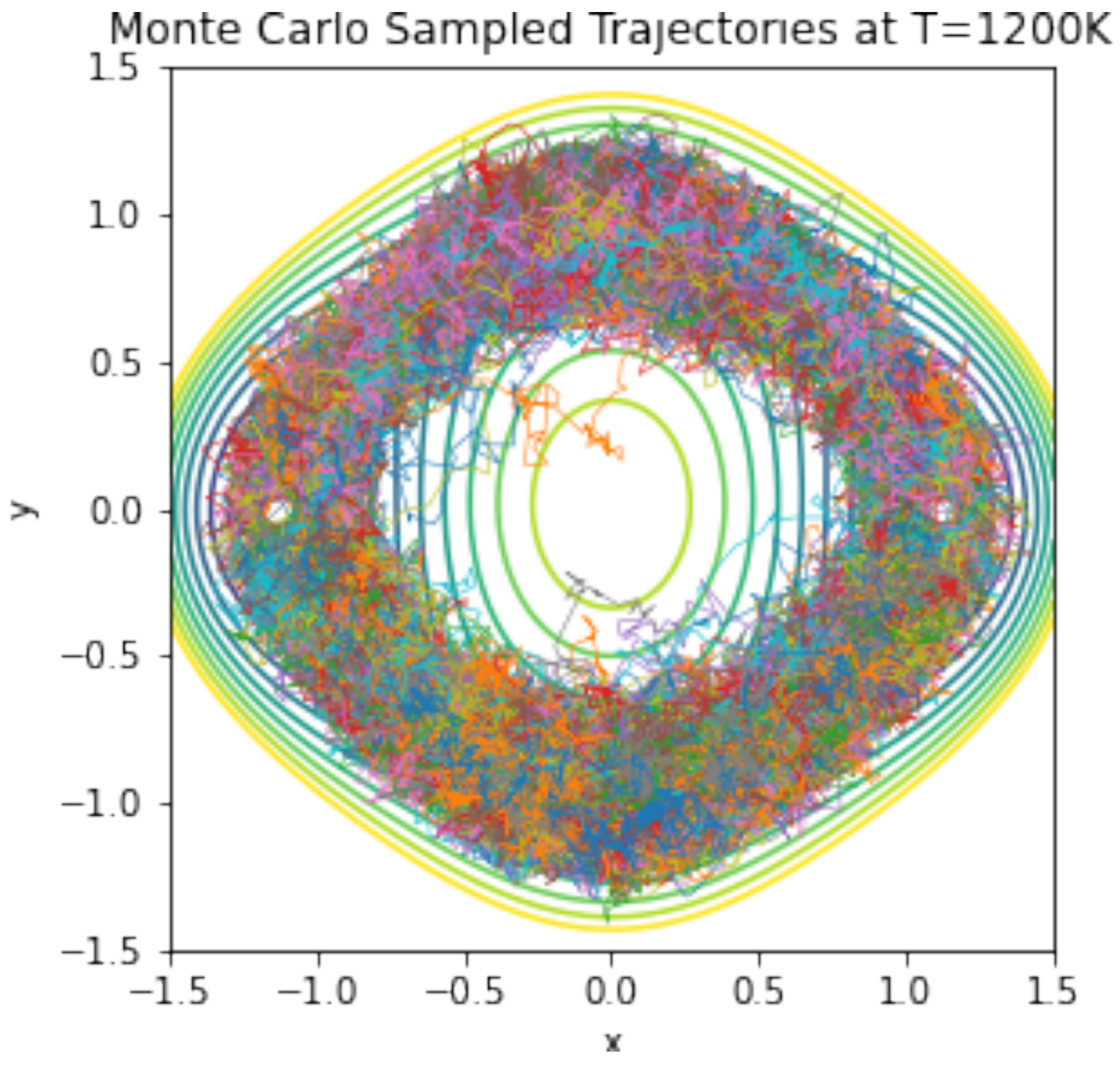


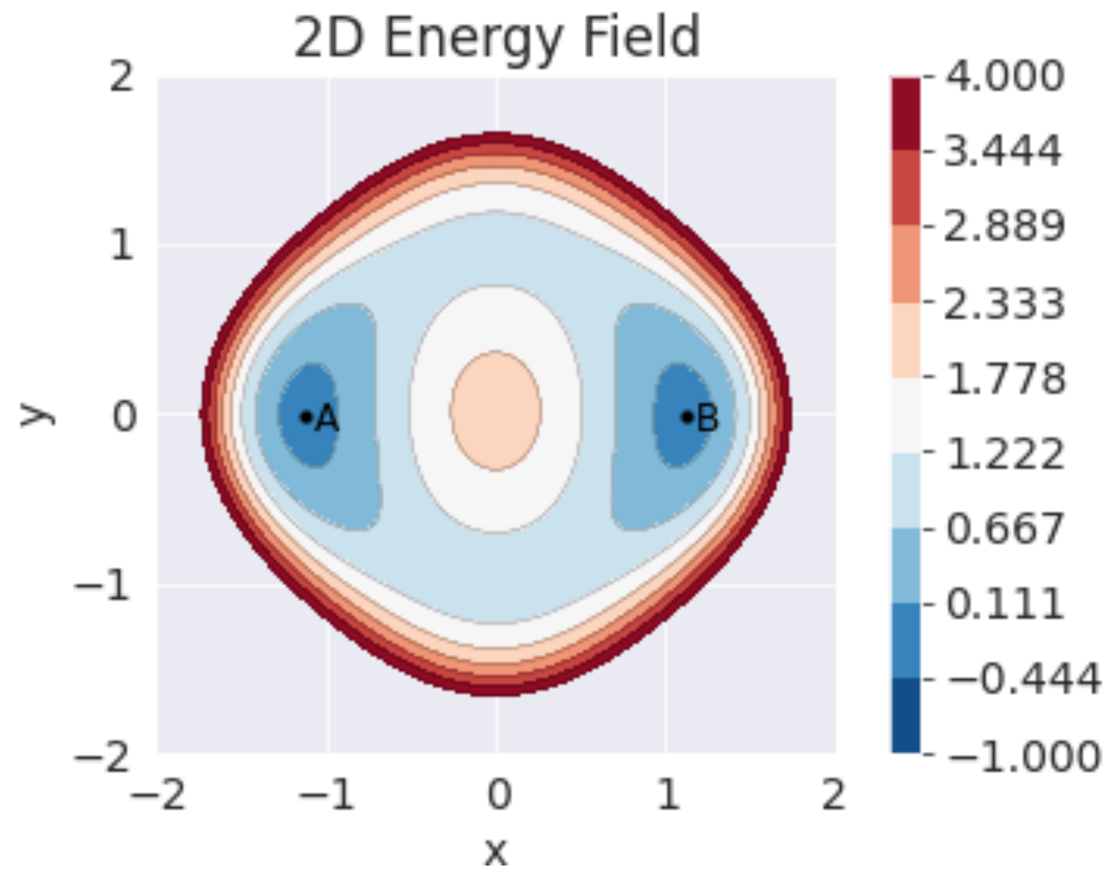
Video Link

Results

Results at 1200 Kelvin. The successful trajectories look similar to the Monte Carlo sampled trajectories.







Numerical Comparison

Efficient Sample Size (ESS) measures the ratio of samples are effective in importance sampling.

$$\mathrm{ESS} = \frac{(\sum_{i:\nu_i \in S} W_i)^2}{\sum_{i:\nu_i \in S} W_i^2}.$$

Coefficient of Variation (CV) is the ratio between std. and the mean.

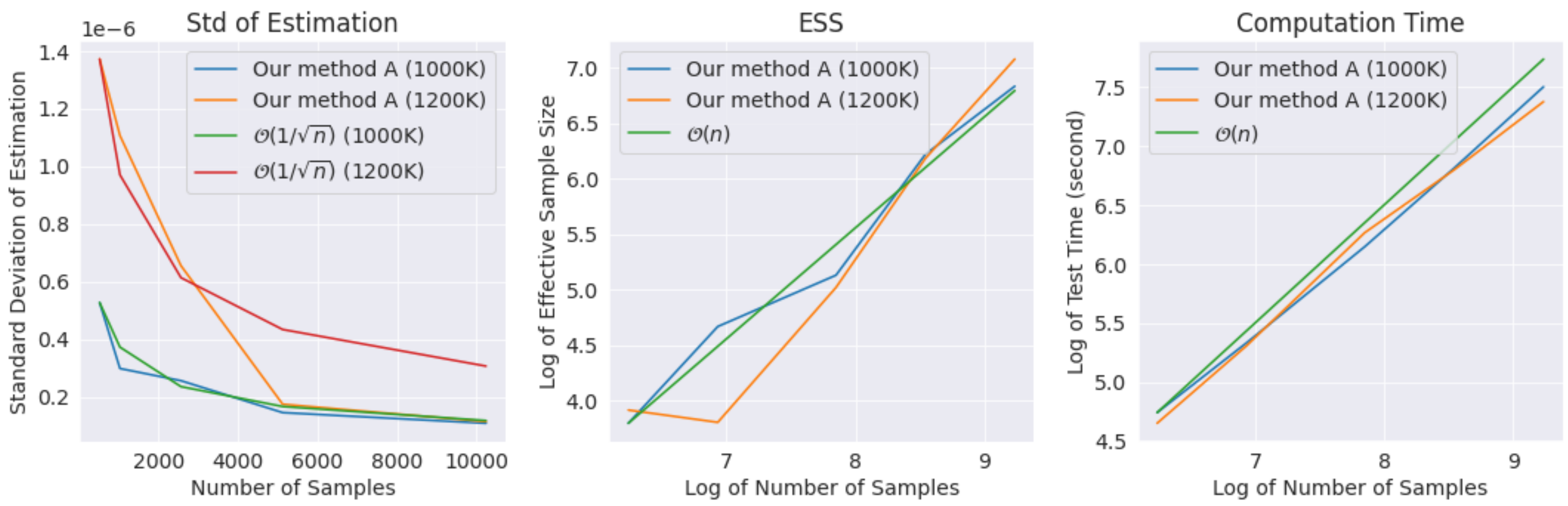
Temperature 1200K	Confidence Interval	CV	Success Rate	ESS ratio	t_{train}	t_{test}
Our method A	$4.037 \pm 0.342\text{e}{-6}$	3.0933	0.770	0.095	122	16
Our method B	$3.232 \pm 0.743\text{e}{-5}$	8.402	0.396	0.014	14	16
Monte Carlo	$4.410 \pm 0.412\text{e}{-6}$	1505.846	$4.410\text{e}{-6}$	-	-	708

Robustness

Our method is robust in scaling up:

★The standard deviation of the estimator decreases as $\mathcal{O}\left(1/\sqrt{n}\right)$.

★The ESS and computation time grows linearly.



Thank you!

Xinru Hua: huaxinru@stanford.edu