BRIDGING JARZYNSKI'S EQUALITY AND THE RENORMALIZATION GROUP

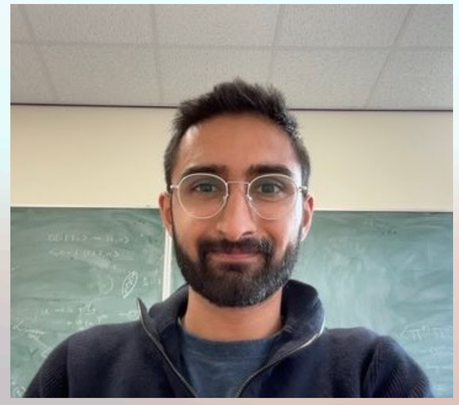
ELIA CELLINI

8/09/2026

Bridging Machine Learning and Statistical Field Theory through generative and diffusion processes

ECT* Trento

In collaboration with:



Gurtej Kanwar

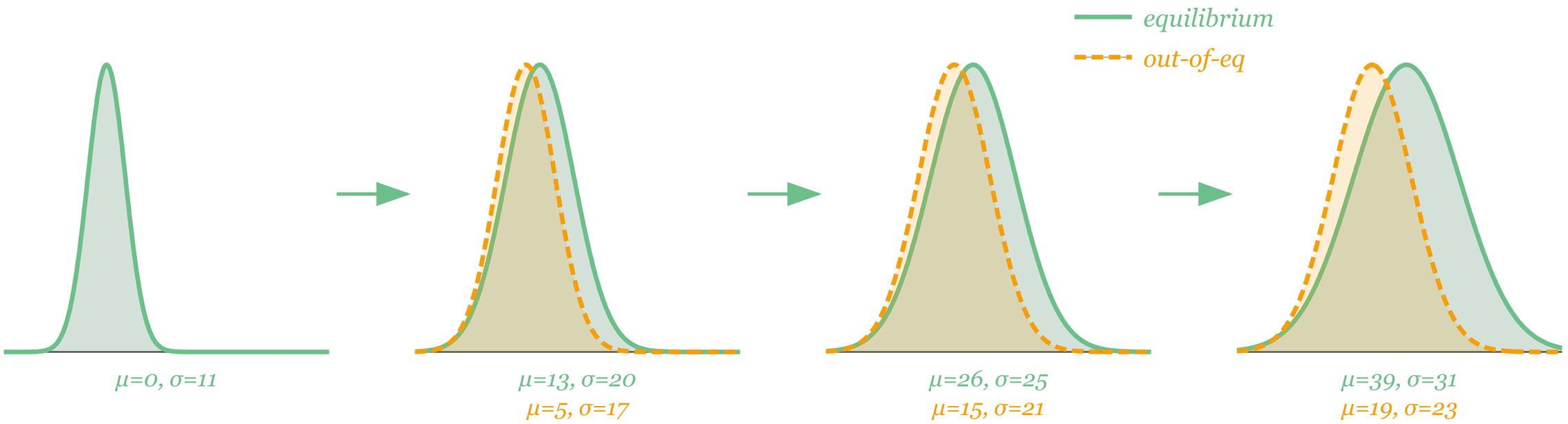


Satria Widyanto

THE UNIVERSITY of EDINBURGH

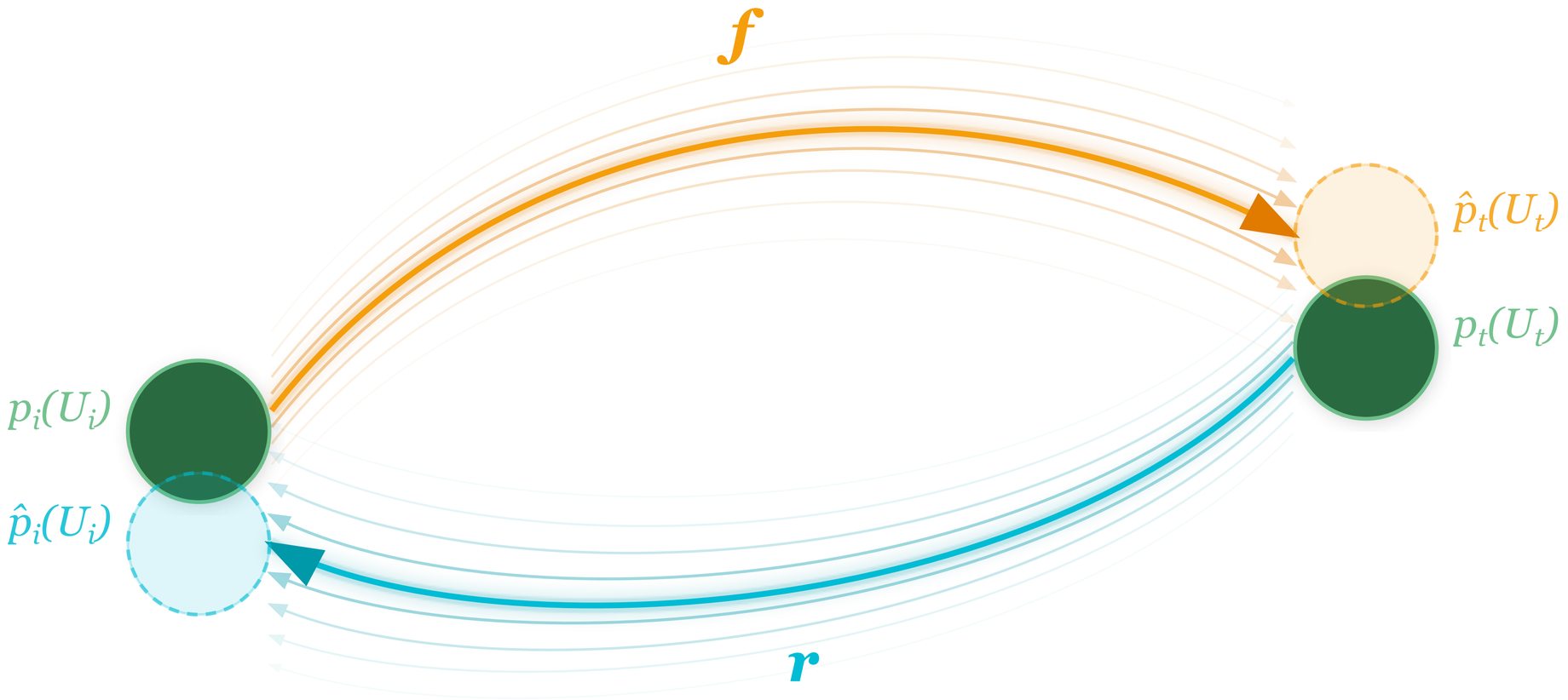
OUT-OF-EQUILIBRIUM TRANSFORMATIONS

A system is driven out of equilibrium when it is **perturbed faster than its relaxation timescale**, so it never settles into the stationary distribution of the current conditions.



TRANSIENT ENSEMBLE

Given an initial distribution p_i and final distributions p_t, driving the system out of equilibrium generates a **transient ensemble of stochastic trajectories**, a biased transport between the two distributions.



For each trajectory, we can compute the **thermodynamic work** done on the system: $W(U) = \int_0^T dt \, \frac{\partial S(U(t), \lambda(t))}{\partial \lambda} \dot{\lambda}(t)$

JARZYNSKI'S EQUALITY

The Crooks' theorem states that the ratio of **forward and reverse work distributions** gives direct access to the **dissipated work** W_d along each trajectory.

[Crooks; cond-mat/9901352]

$$\frac{P_f(+W)}{P_r(-W)} = e^{W-\Delta F} \qquad W_d = W - \Delta F$$

Using Crooks' theorem it is possible to prove **Jarzynski's Equality (JE),** that provides a powerful reweighting to **compute the free-energy difference at the equilibrium** between p_i and p_t

$$\langle e^{-W} \rangle_f = e^{-\Delta F}$$

General identity, widely used for **computing free energies and sampling**, also in LFT.

[Neal; physics/9803008],[Caselle et al.; 1604.05544]

DRAWBACKS

The identities derived before are exact, however, the **exponential average:**

$$\langle e^{-W_d} \rangle_f$$

can be highly inefficient when W_d **is large** and **statistics are limited**.

In order to fight this problem, we want W_d to be "small"

Solution 1) **quasi-static transformations** → "small" W_d systematic but expensive scaling

Solution 2) use Machine Learning to minimize W_d → **Neural-Enhanced Out-of-Equilibrium (NEO)** sampling

STOCHASTIC NORMALIZING FLOWS

Stochastic Normalizing Flows (SNFs) combine **Non-Equilibrium Monte Carlo updates** and **Normalizing Flows blocks**:

$$x_0 \longrightarrow g_\theta^1(x_0) \xrightarrow{P_1} x_1 \longrightarrow g_\theta^2(x_1) \xrightarrow{P_2} \dots \xrightarrow{P_N} x_N \equiv x$$

Where g_θ^i are NF layers and P_i are MCMC updates interpolating between prior and target

$$W_d^\theta = S_N(x_N) - S_0(x_0) - Q_\theta - \Delta F$$

$$Q_\theta = \sum_{n=0}^{N-1} \left(S_{n+1}(x_{n+1}) - S_{n+1}(x_n) + \ln |\det J_{g_\theta^n}| \right)$$

- **Power law scaling** with **N**
- **Linear scaling** with the **volume**
- **Improvement of the prefactor** with g_θ

[Wu et al; 2002.06707],[Caselle, EC, Nada, Panero; 2201.08862],[Bulgarelli, EC, Nada.; 2412.00200], [Bonanno, Bulgarelli, EC et al.: 2510.25704]

LOSS FUNCTION

NEO samplers can be optimized by minimizing:

$$\mathscr{L}(\theta) = \langle W_d^\theta \rangle_f = D_{KL}(P_f || P_r) \geq 0$$

$$\langle W \rangle_f \geq \Delta F$$

Second Law!

More reversible trajectories → smaller work → **better error!**

From the D_{KL} it is possible to derive other losses, e.g. PINN, Path Gradient, etc.

[Vaitl et al.; 2206.09016],[Albergo et al.; 2410.02711],[Abbott et al.; 2603.02984]

See **G. Kanwar M10:15**

NON-EQUILIBRIUM SAMPLERS FOR LFT

JE-based samplers have been **widely investigated in lattice field theory:**

- **Free energy calculations** e.g. pressure, entropies, etc.

  [Caselle et al.; 1604.05544],[Caselle et al.; 1801.03110], [Francesconi et al.; 2003.13734],[Bulgarelli and Panero; 2304.03311, 2404.01987]
  [Bulgarelli et al.; 2505.20403],[Bulgarelli, EC et al.; 2410.14466]

- **Transport between distributions** e.g. Open-Periodic boundary conditions, couplings, etc.

  [Bonanno et al.; 2402.06561, 2411.00620],[Caselle, EC, Nada, Panero; 2201.08862],[Caselle, EC, Nada; 2409.15937],
  [Bulgarelli, EC, Nada.; 2412.00200], [Bonanno, Bulgarelli, EC et al.: 2510.25704]

  See **L. Verzichelli Tu11:55**

- **Alternative NEO samplers** e.g. NETS, SPS, etc.

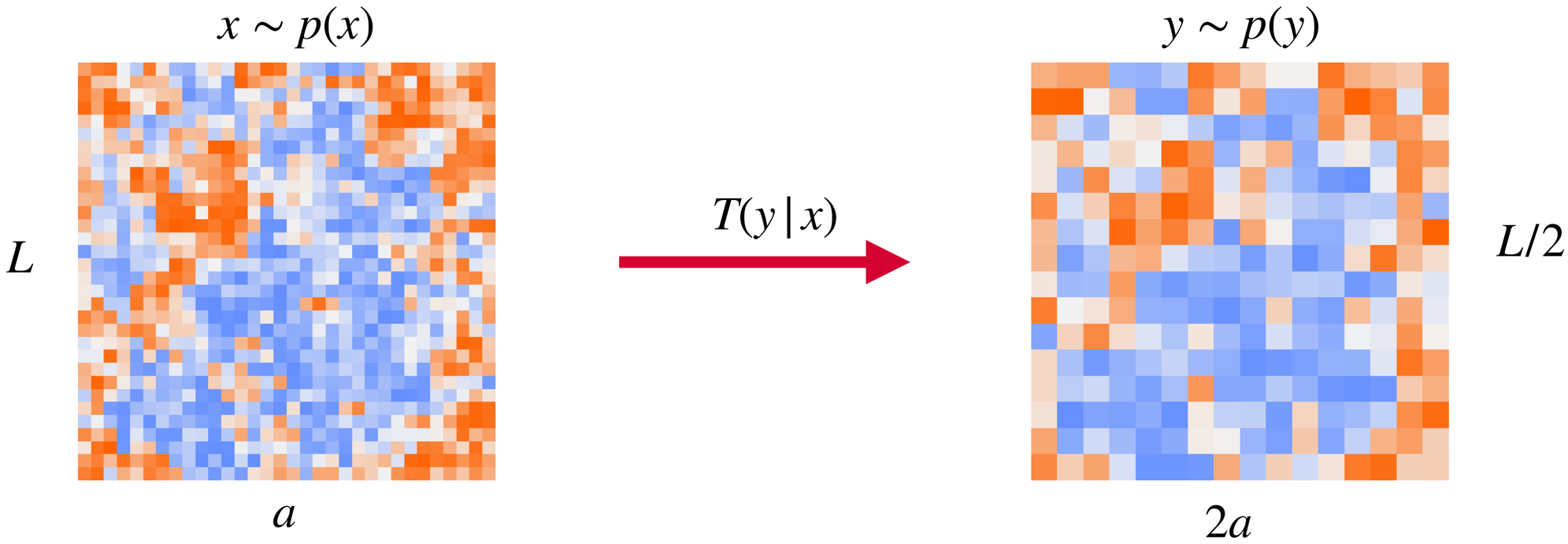
  [Albergo et al.; 2410.02711],[Chen et al.; 2606.13790]

  See
  - **G. Kanwar M10:15,**
  - **B. Lucini M15:45**

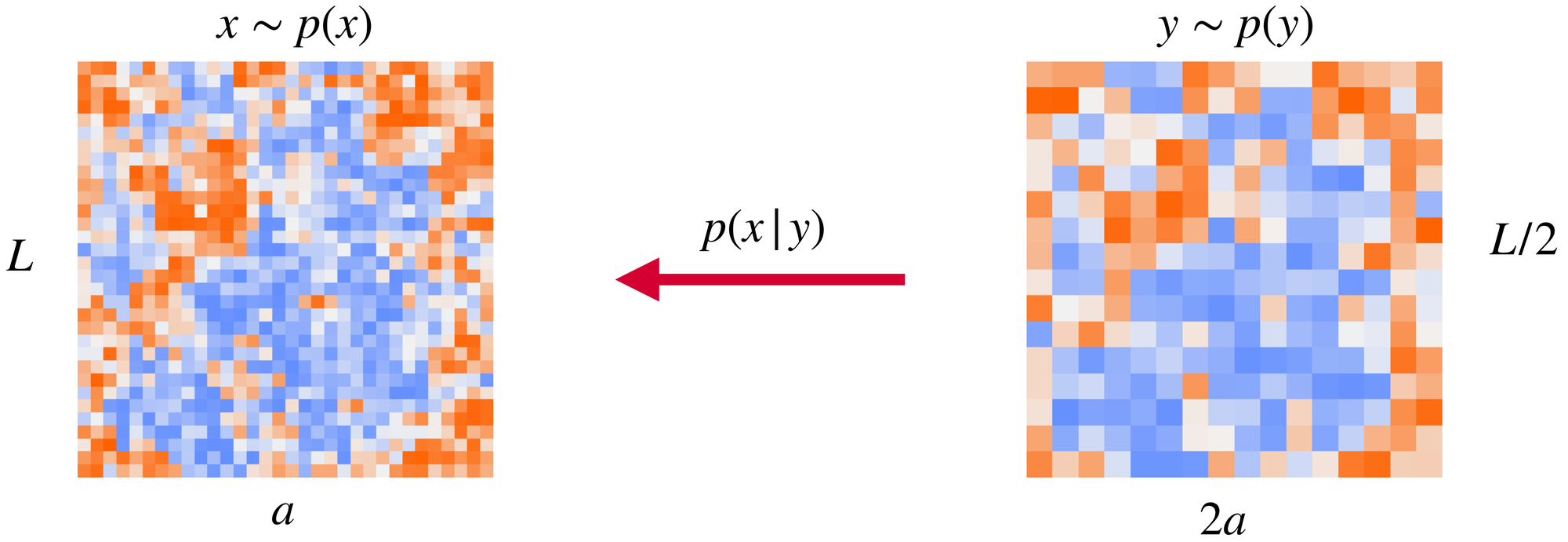
Are there **new contexts** in which Jarzynski's equality and Crooks' theorem can be used?

RENORMALIZATION GROUP

Consider a **target distribution** $p(x)$ and a **stochastic blocking** $T(y|x)$



INVERSE RG SAMPLING



Thanks to **Bayes' theorem:**

$$p(x\,|\,y) = \frac{p(x)T(y\,|\,x)}{\int dx' p(x')T(y\,|\,x')} = \frac{p(x,y)}{p(y)}$$

Why? <u>Slow modes become fast on coarser scales</u> → milder Critical Slowing Down

IRG AND ML BASED SAMPLERS

Sampling by “inverting” RG, and more broadly, leveraging different scales, is an **old idea** that goes back to the ’80s.

[Schmidt; PRL 51, 2175 (1983)][Goodman and Sokal; PRL 56, 1015 (1986)], and many others

However,

- $p(y)$ **is generally unaccessible**
- **Upscaling transformations can be hard to design**

ML and deep learning have opened new routes to hierarchical sampling in LFT!

[Bachtis et al; 2107.00466][Bauer et al.; 2412.12842],[Singha, EC et al.; 2503.08918],[Singha, Kauffmann, EC et al.; 2604.10209]

[Hasenfratz et al.; 2608.28580, 2608.28581]

See:

- **A. Singha M16:10: Black-box NN** $q(y)$
- **A. Hasenfratz Tu09:30: Perfect -blocking** $q(y) \simeq p(x)$
- **Y. Ashida Th09:30: Diffusion and RG**

BRIDGING RG AND STOCHASTIC THERMODYNAMICS

Building **a non-equilibrium transport** on the joint distribution, **at fixed y**:

$$p(x,y)^t = p(x)^t T(y\,|\,x)^t; \quad t:0\to 1$$

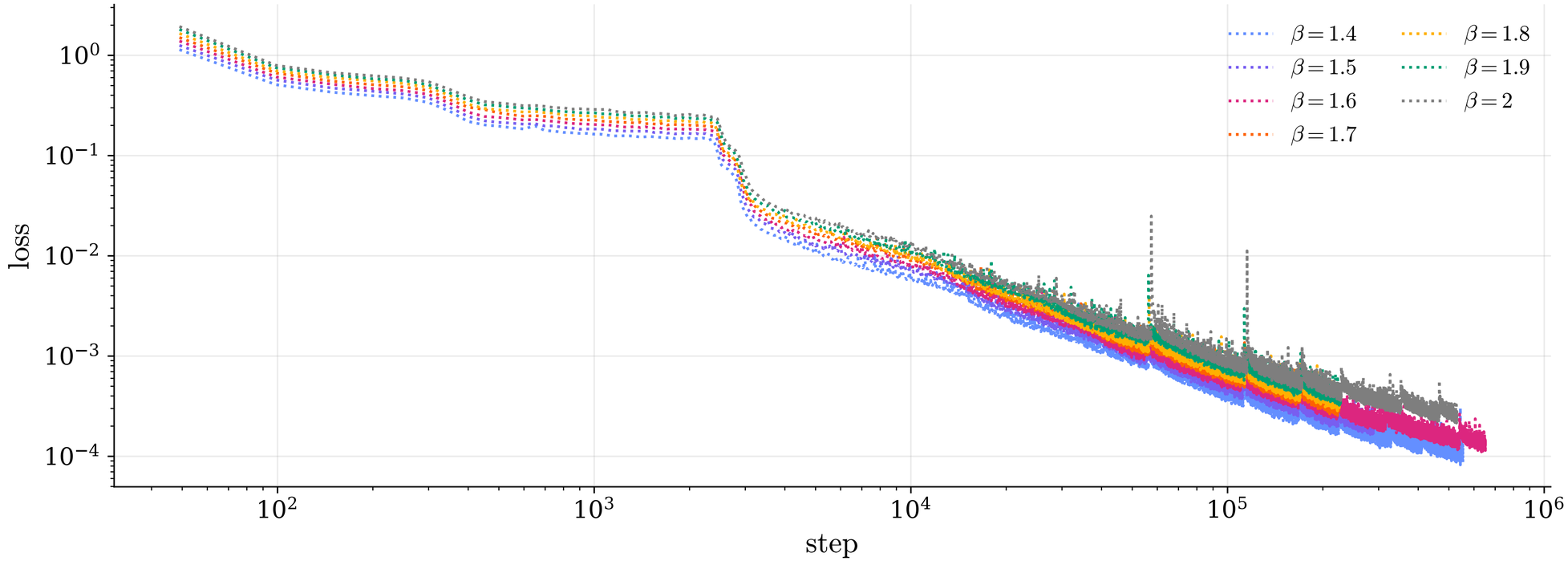
Allows to **compute the exact normalization of** $p(x\,|\,y)$ **i.e** $p(y)$ **using the Jarzynksi's equality:**

$$\left\langle e^{-W_{0\to 1}(x,y)} \right\rangle_{f_x}(y) = \frac{p(y)}{C}$$

JE gives the exact $p(y)$, enabling **hierarchical inverse-RG sampling** → the method **can be iterated also over many scales**

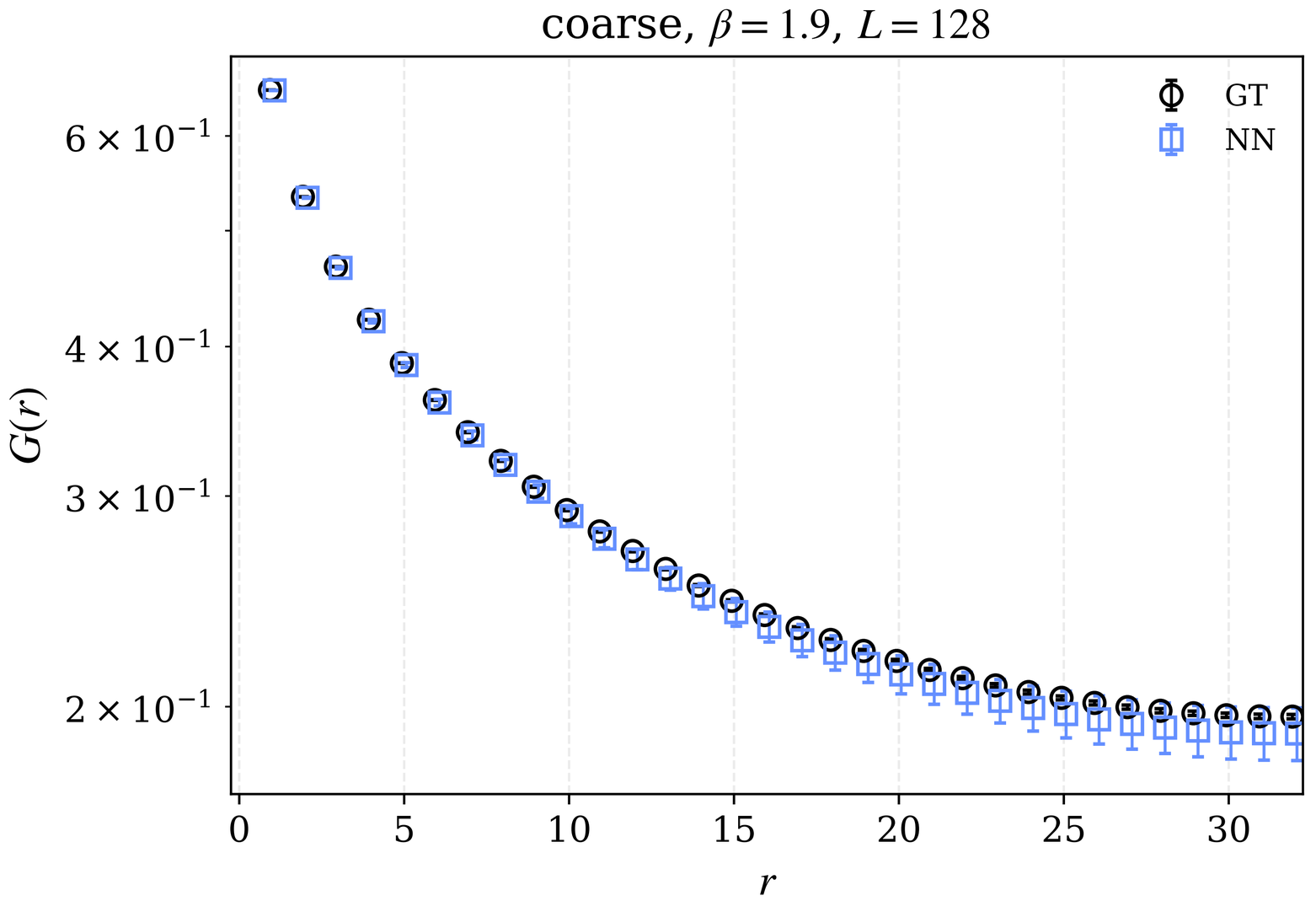
LEARNING SNF FOR $p(x, y)^t$

- **O(3)-non linear sigma model**, simple but non trivial (compact, topology, asymptotic freedom)
- We used an **SNF** interleaving **HMC** and physics-informed **continuous NF**.
- Training done on 32×32 **lattices on thermalised synthetic** y **configurations** obtained with **Parallel Tempering → no target samples for training**



LEARNING $p(y)$

- **Physics-informed U-Net** for $-\log q_\theta(y)$
- **Score matching** training:
  $\mathscr{L}(\theta) = \left(\nabla_y \log \hat{p}(y) - \nabla_y \log q_\theta(y)\right)^2$
- Training done on **synthetic coarse** y 16×16 **lattices**
- **Evaluated on coarse** 64×64 **lattices**
- Ground Truth (GT) computed with (almost) uncorrelated configurations



[Favoni et al.; 2012.12901][Backfried; Master Thesis]

BIASED SAMPLING $p(x)$

Sample a set of $y \sim q_\theta(y) \simeq p(y)$ and then run MCMC on:

$$p(x \mid y) = \frac{p(x, y)}{p(y)}, \qquad y \sim q_\theta(y)$$

Biased but cheap

x can be used as starting noise for a Markov chain on $p(x)$

[Hasenfratz et al.; 2608.28580, 2608.28581]

See: A. Hasenfratz Tu09:30

UNBIASED SAMPLING $p(x)$

Sample a set of $y \sim q_\theta(y) \simeq p(y)$, then run the SNFs on:

$$p(x,y)^t = p(x)^t T(y\,|\,x)^t; \quad t: 0 \to 1$$

Then reweight:

$$\langle \mathcal{O} \rangle_{p(x)} = \frac{\langle \mathcal{O} w \rangle_{f_x,y}}{\langle w \rangle_{f_x,y}} \qquad w = \frac{e^{-W(x,y)}}{q_\theta(y)}$$

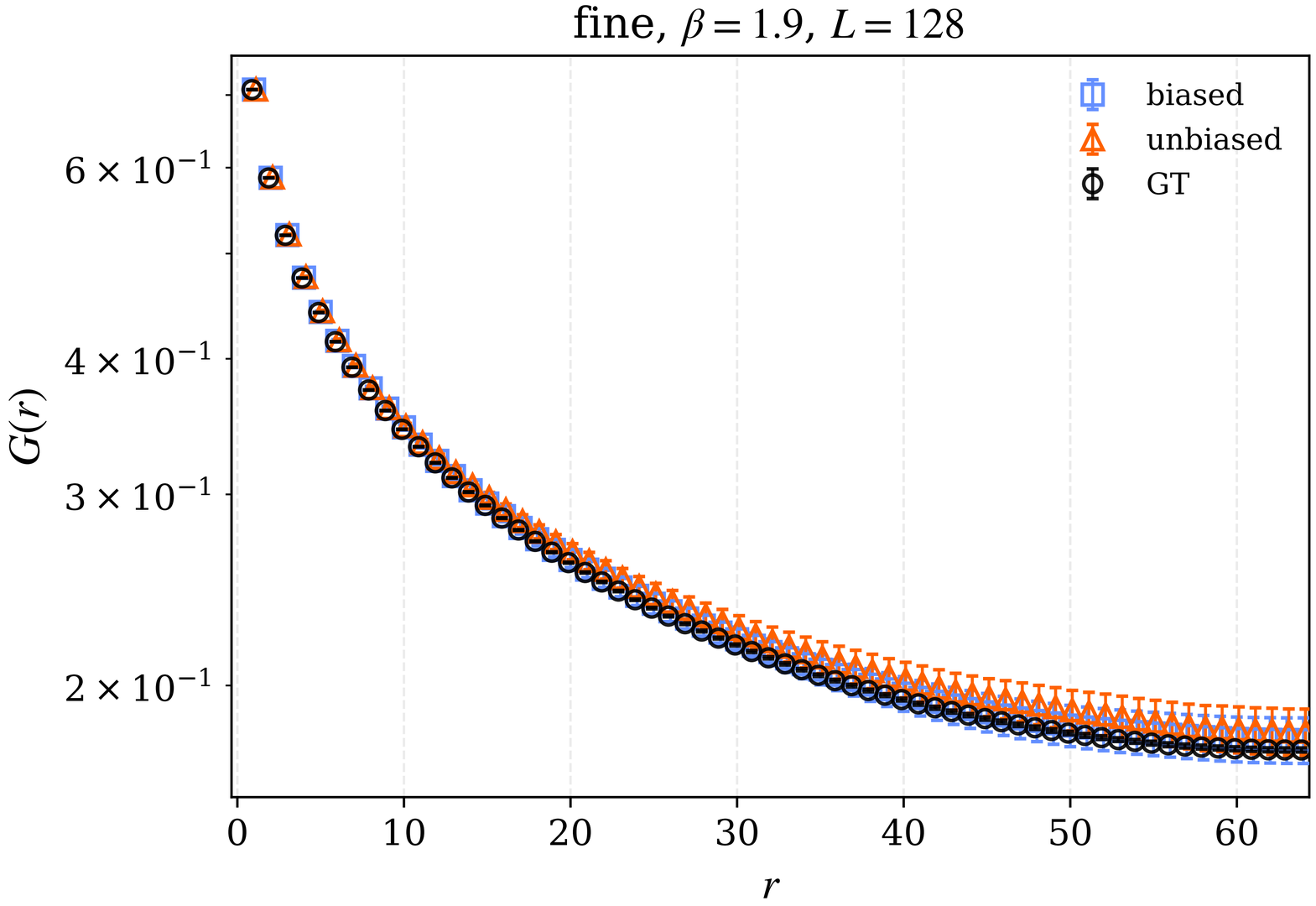
Many n_{anneal} may be required for reliable calculations, but w can be used as a diagnostic:

$$\left\langle \frac{e^{-W(x,y)}}{q_\theta(y)} \right\rangle_x \propto \frac{p(y)}{q_\theta(y)}$$

Short flow can be used for biased sampling termalization

SAMPLING $p(x)$

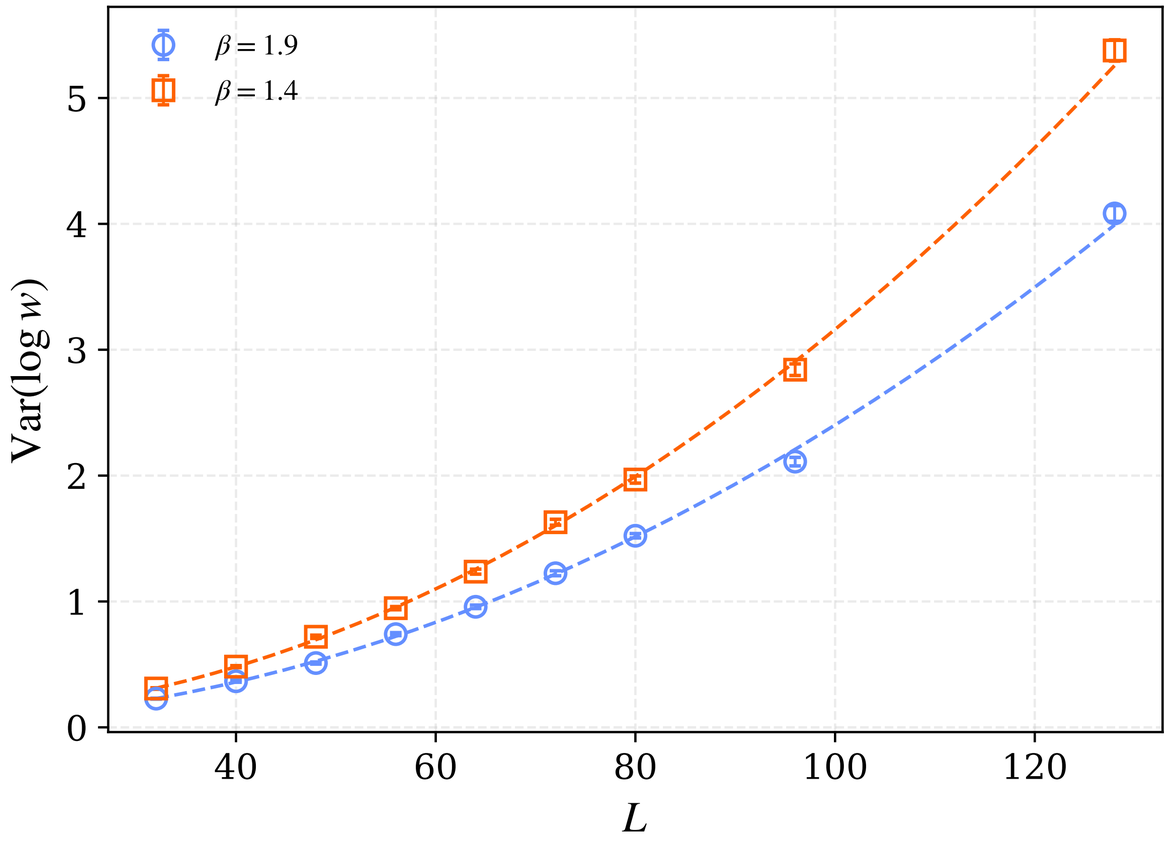
- **Sample** 128×128 **fine lattices from coarser machine-learned** 64×64
- **Remark: Models have been trained on synthetic fine** 32×32 **lattices**
- $n_{\text{anneal}} = 20$
- **Upscaling works because** $q_\theta(y)$ **is volume independent, and SNFs work only on UV fluctuations**

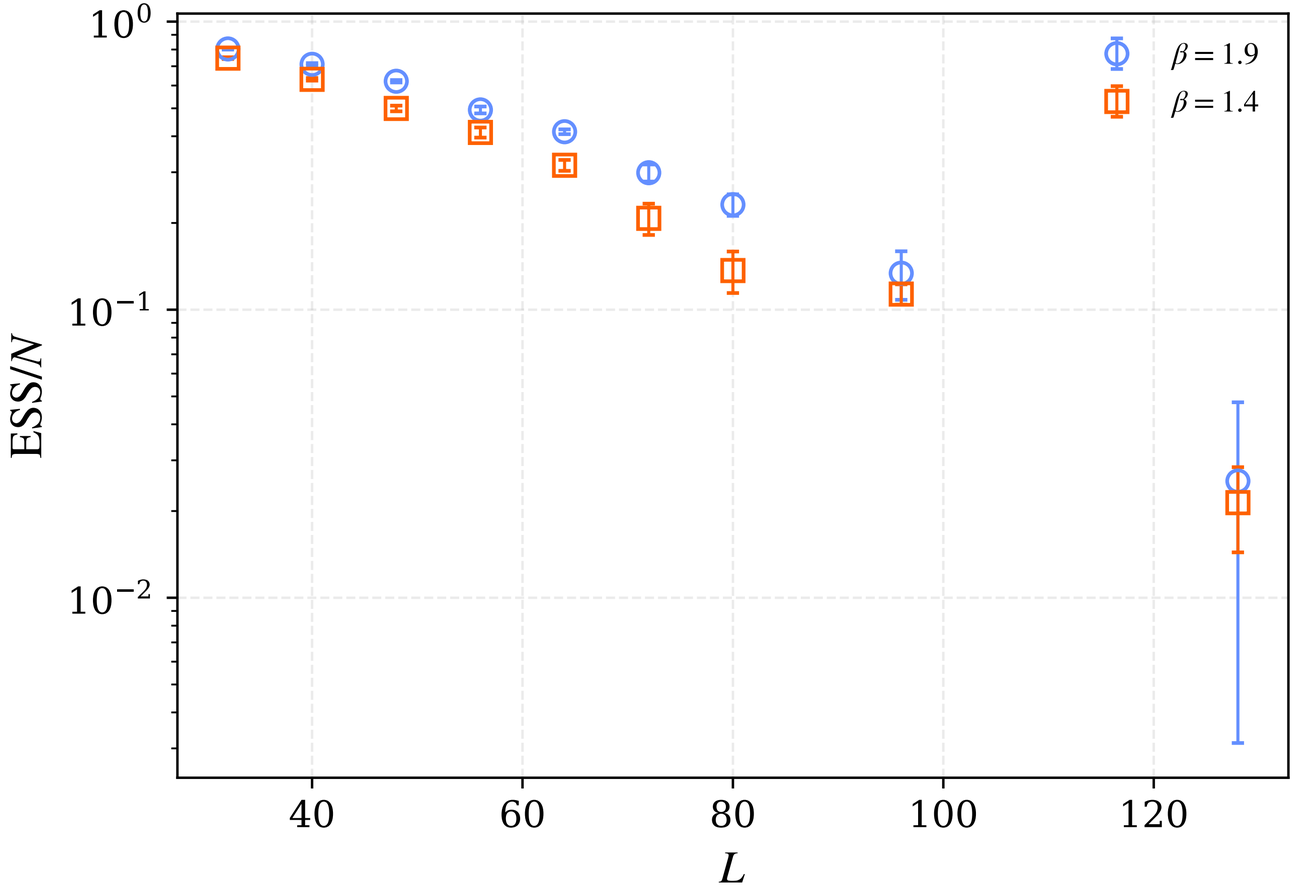


O(3) non-linear sigma model $\beta = 1.9$, preliminary

SCALING WITH THE VOLUME

The variance of $\log w$ scales linearly with the volume at fixed n_{anneal}

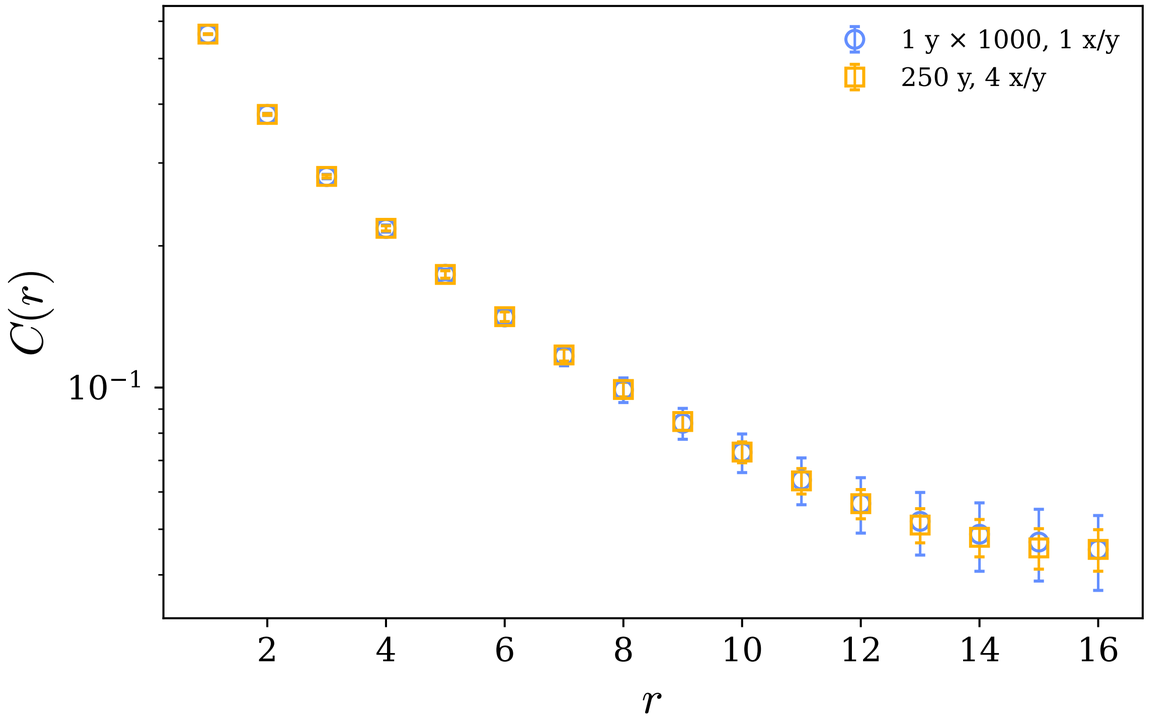


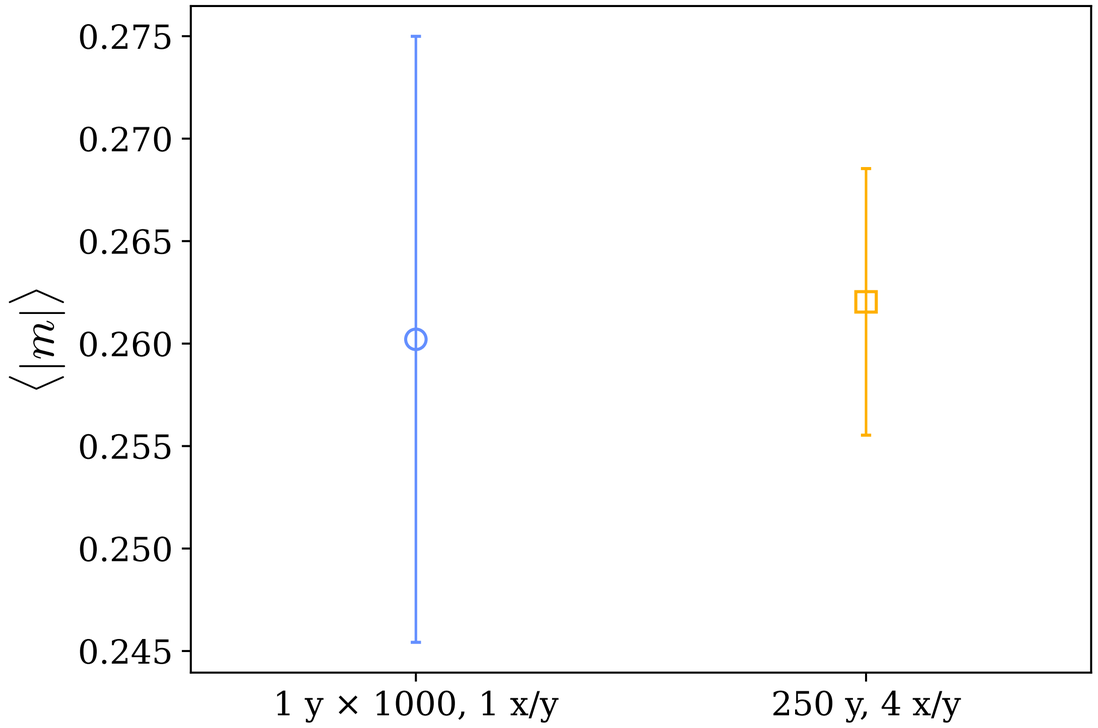


MULTI-HIT VARIANCE REDUCTION

Sampling **many fine configurations for a fixed coarse sample** can be used as a **multi-hit** implementation

[Parisi, Petronzio, Rapuano; Phys. Lett. B 128 (1983)]

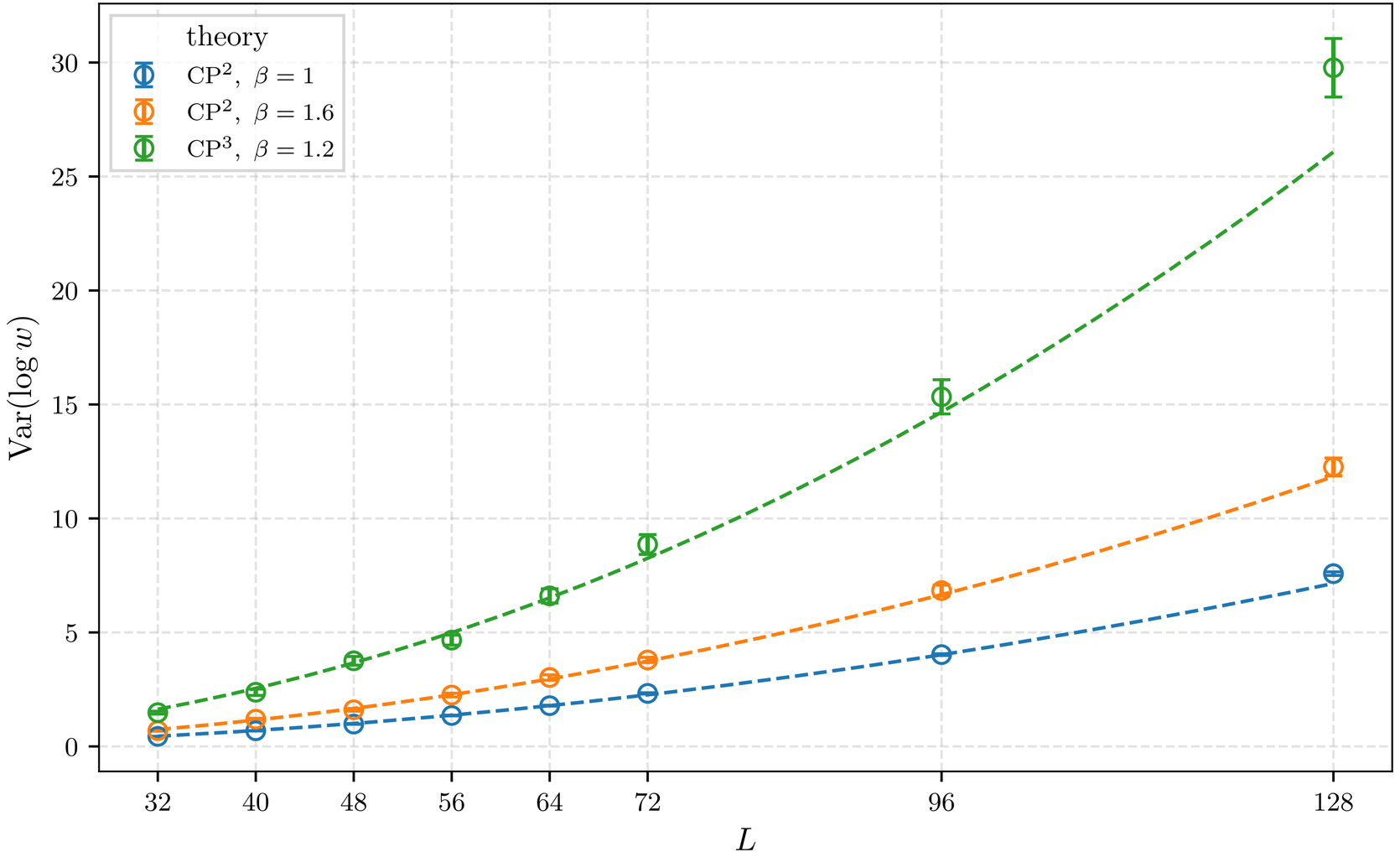




Averaging over fine configurations at fixed coarse background s**uppresses UV noise while preserving the long-distance signal.**

$\mathbf{CP}^{n-1}$

Some results for the $\mathbf{CP}^{n-1}$ model (preliminary):



CONCLUSIONS AND OUTLOOKS

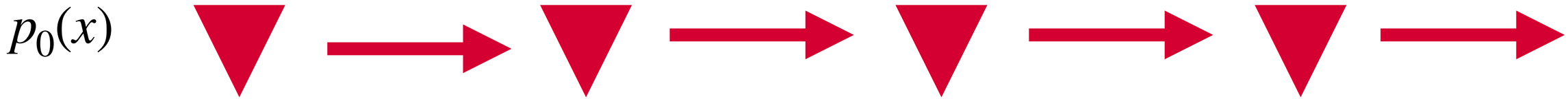
- We introduced **Crooks' theorem and Jarzynski's equality** and outlined **SNFs**, a class of NEO samplers that display **great scalability with the capacity and the volume**
- We introduced a new way of using Jarzynski's equality, **bridging Renormalization Group with Stochastic Thermodynamics through Bayes's theorem**
- We introduced a single-scale **"inverse" RG sampler**
- The fitting of coarse action **can be iterated over many scales**
- **Multi-hit approaches** leveraging different scales

- **Multi-scale** samplers for $\mathbf{CP}^{n-1}$ and $\mathbf{O}(3)$ nonlinear sigma models
- **Single-scale** sampler for $\mathbf{SU}(3)$

THANK YOU

BACKUP

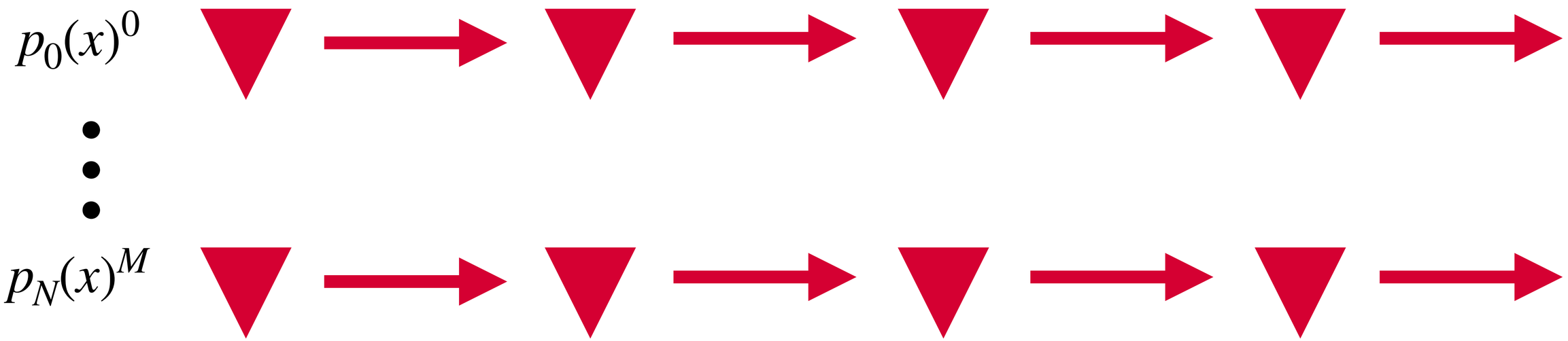
VANILLA TRAINING



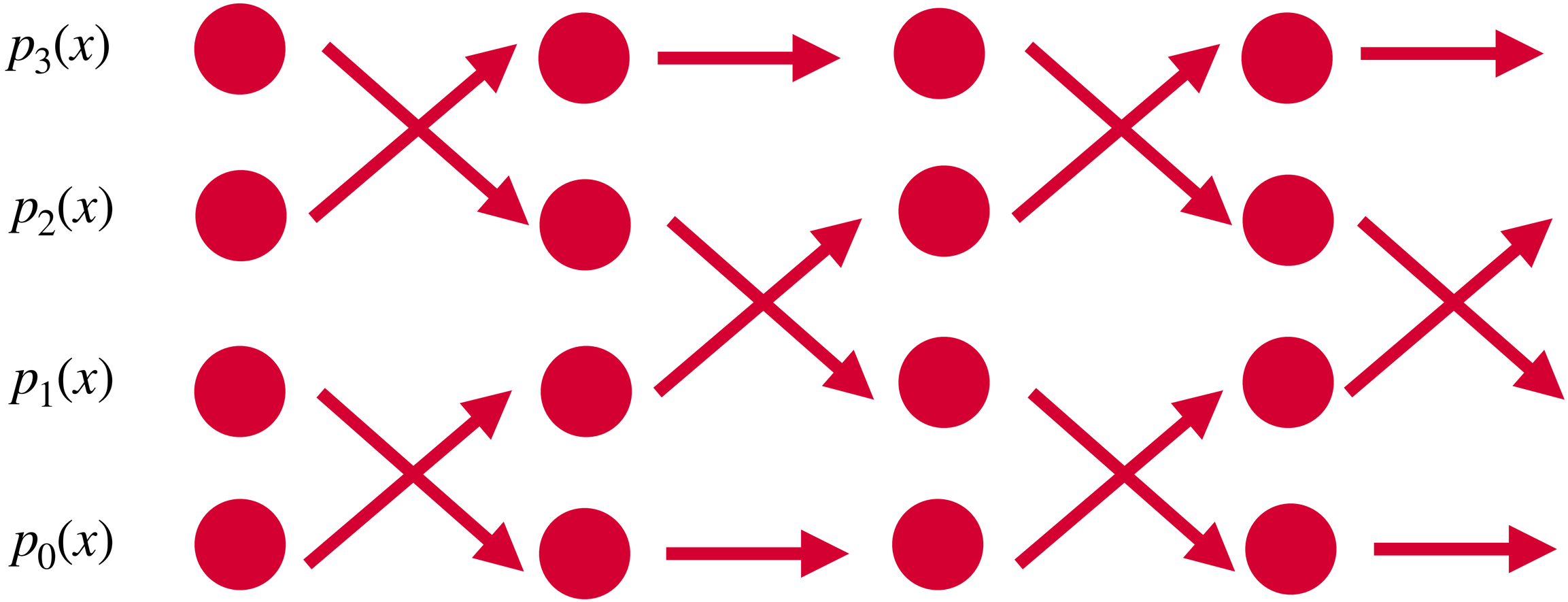
: Compute the full SNF forward → gradient optimized locally for NF layers

: MCMC kernel

Usually batched/parallelized over M independent replicas:



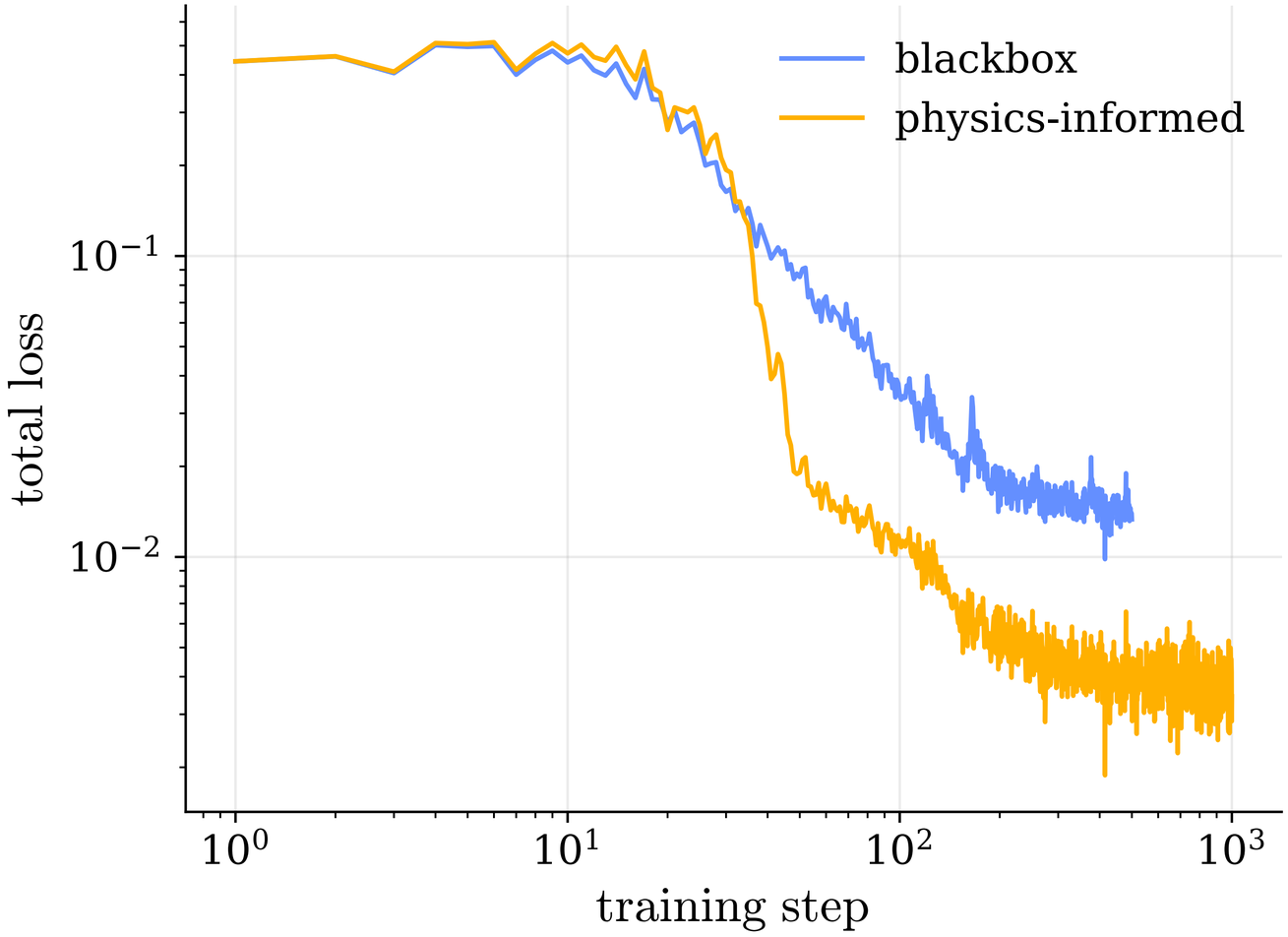
PARALLEL TEMPERING TRAINING



Compute the local loss and update the gradients, with some losses, no explicit forward pass is required

Can be batched!

LEARNING $p(y)$



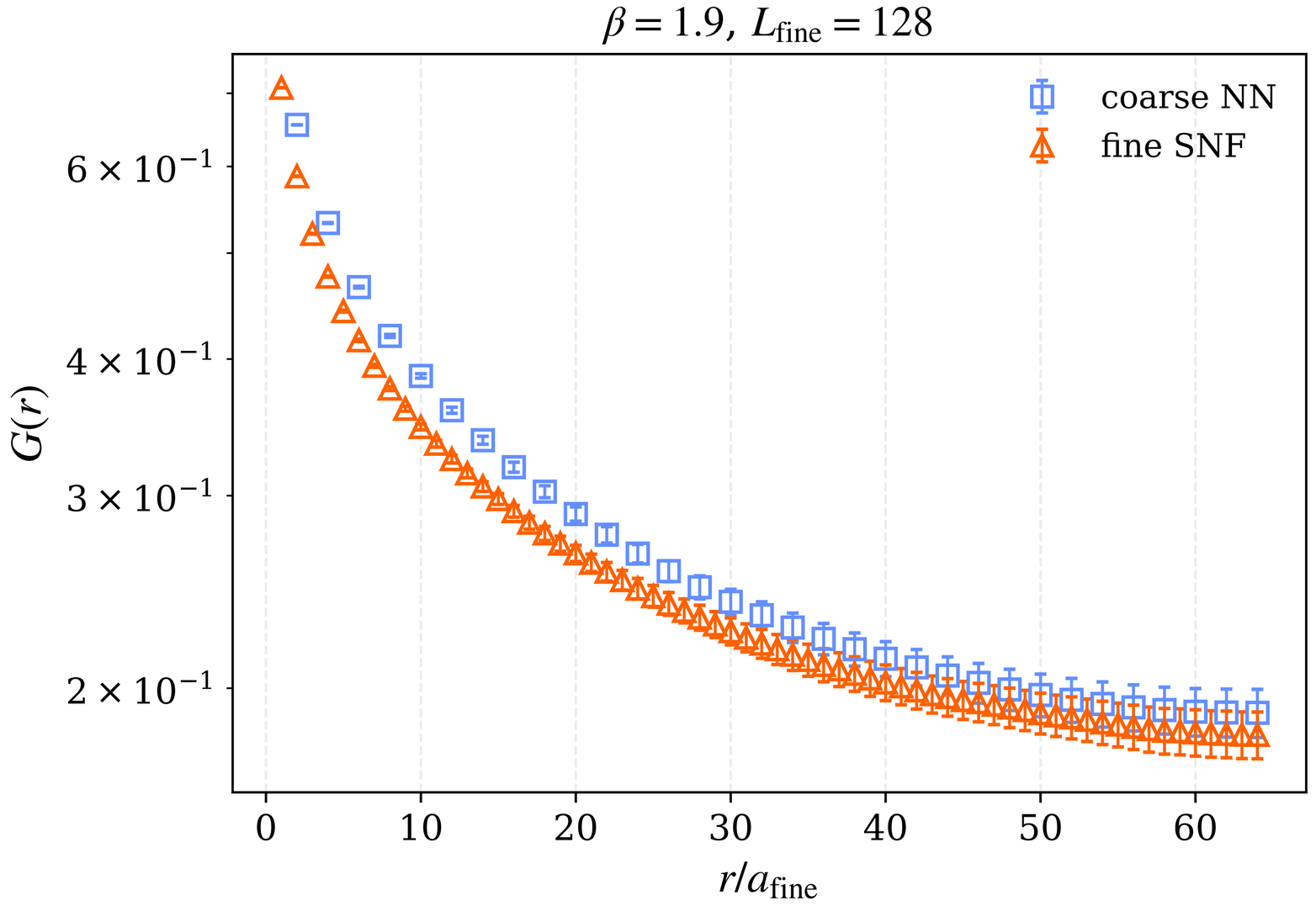
[Favoni et al.; 2012.12901][Backfried; Master Thesis]

FINE VS COARSE PHYSICS

- ML-generated coarse and fine ensembles have **compatible physical correlation lengths.**

$\xi_{\text{coarse}} = 62(4)/a_{\text{fine}}$

$\xi_{\text{fine}} = 63(5)/a_{\text{fine}}$



O(3)-non linear sigma model $\beta = 1.9$, preliminary

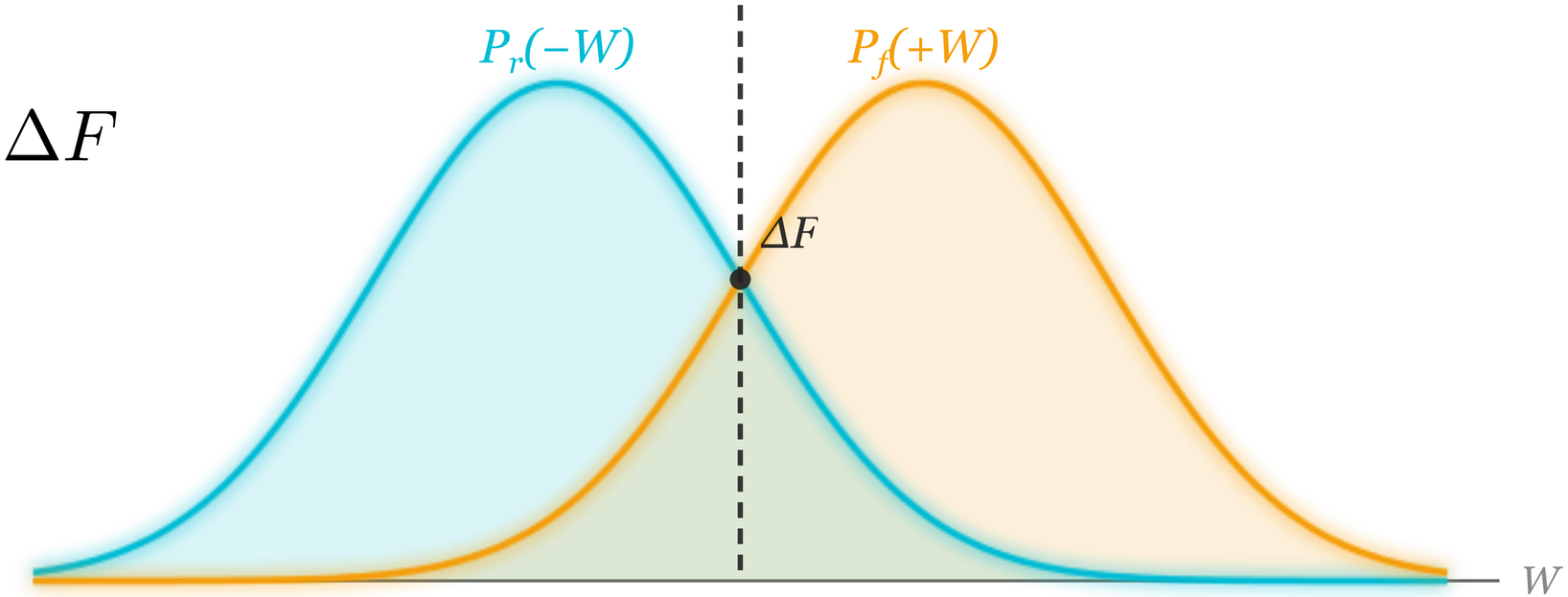
CROOKS' FLUCTUATION THEOREM

The ratio of **forward and reverse work distributions** gives direct access to the **dissipated work** W_d along each trajectory.

[Crooks; cond-mat/9901352]

$$W_d = W - \Delta F$$

$$\frac{P_f(+W)}{P_r(-W)} = e^{W-\Delta F}$$



JARZYNSKI'S EQUALITY

Jarzynski's Equality (JE) provides a powerful reweighting to **compute the free energy** and **correct the bias** of the non-equilibrium transport

[Jarzynski; cond-mat/9610209]

$$1 = \int dW\, P_f(W) \left(\frac{P_r(-W)}{P_f(W)} \right) = \int dW\, P_f(W)\, e^{-(W-\Delta F)} = e^{\Delta F} \langle e^{-W} \rangle_f$$

$$\langle e^{-W} \rangle_f = e^{-\Delta F} \qquad \langle \mathcal{O}\, e^{-W_d} \rangle_f = \langle \mathcal{O} \rangle_{p_t}$$

General identity, widely used for **computing free energies and sampling**, also in LFT.

[Neal; physics/9803008],[Caselle et al.; 1604.05544]