Flow Annealed Importance Sampling Bootstrap meets Differentiable Particle Physics

NeurIPS Workshop ML4PS





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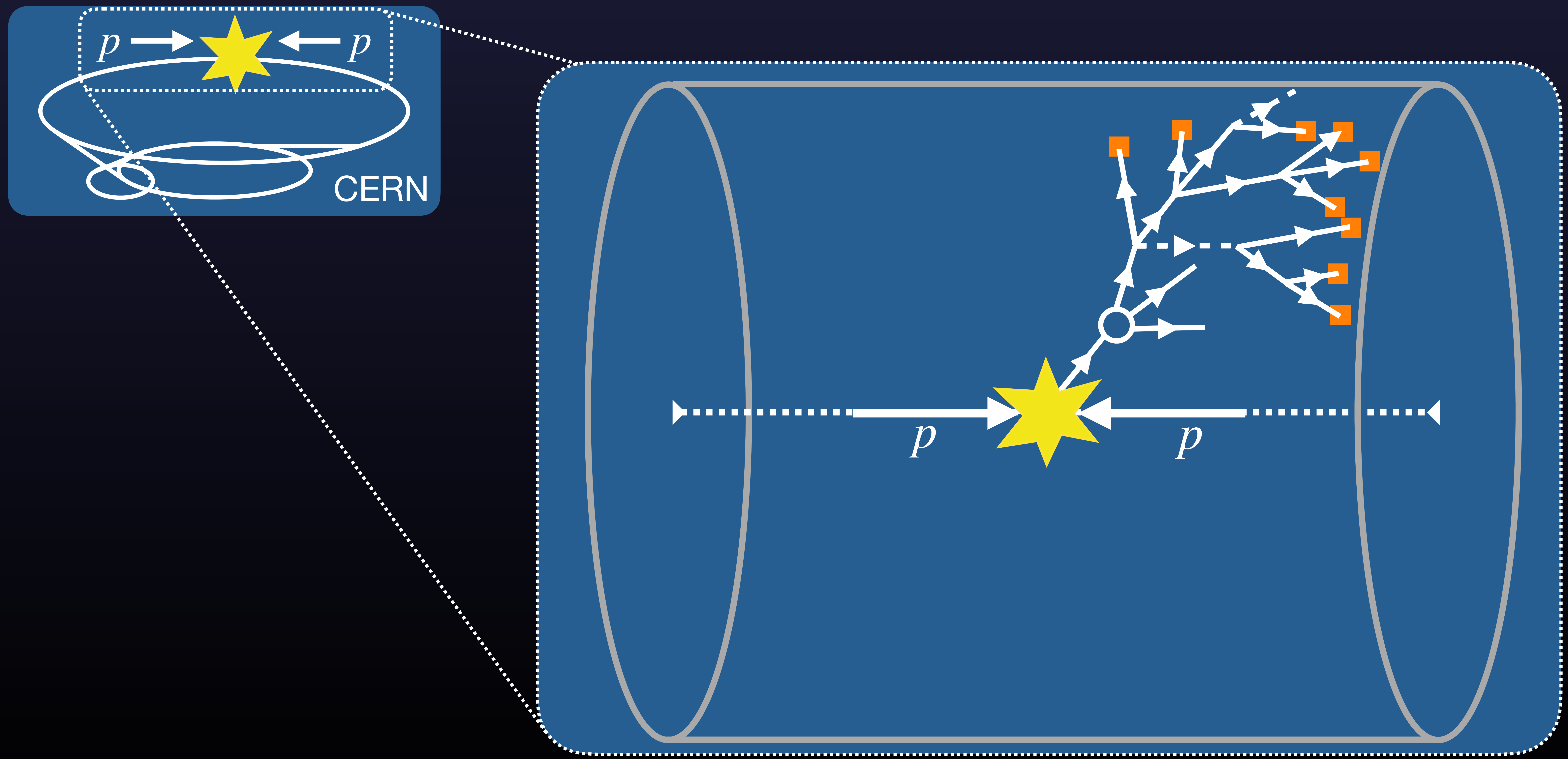
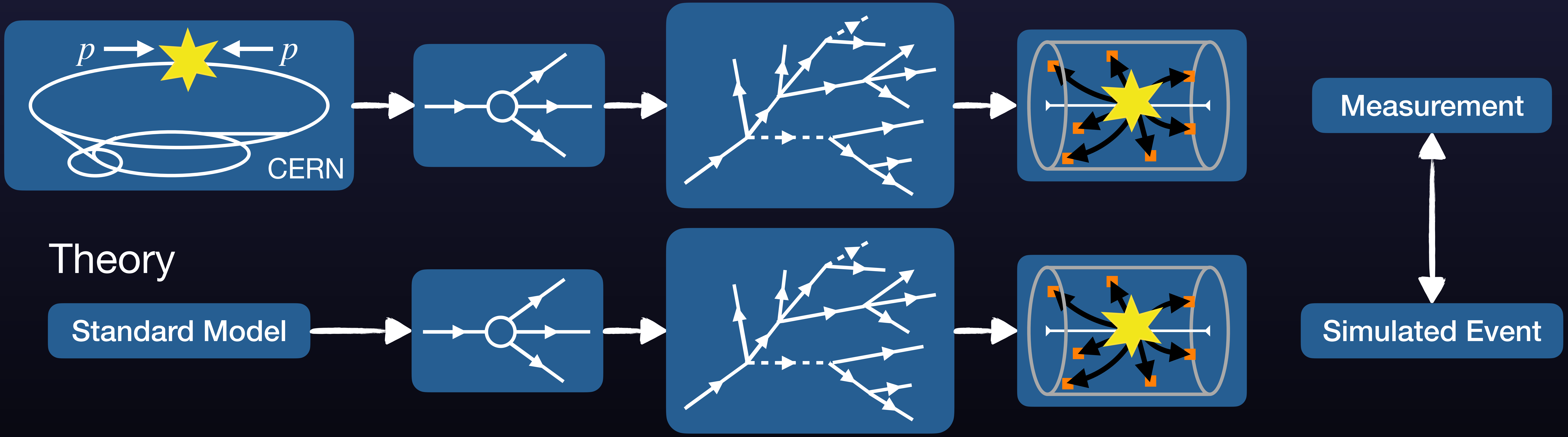
How can we learn more about particles?

Experiment



How can we analyze data?

Experiment



→ Find deviations from theory

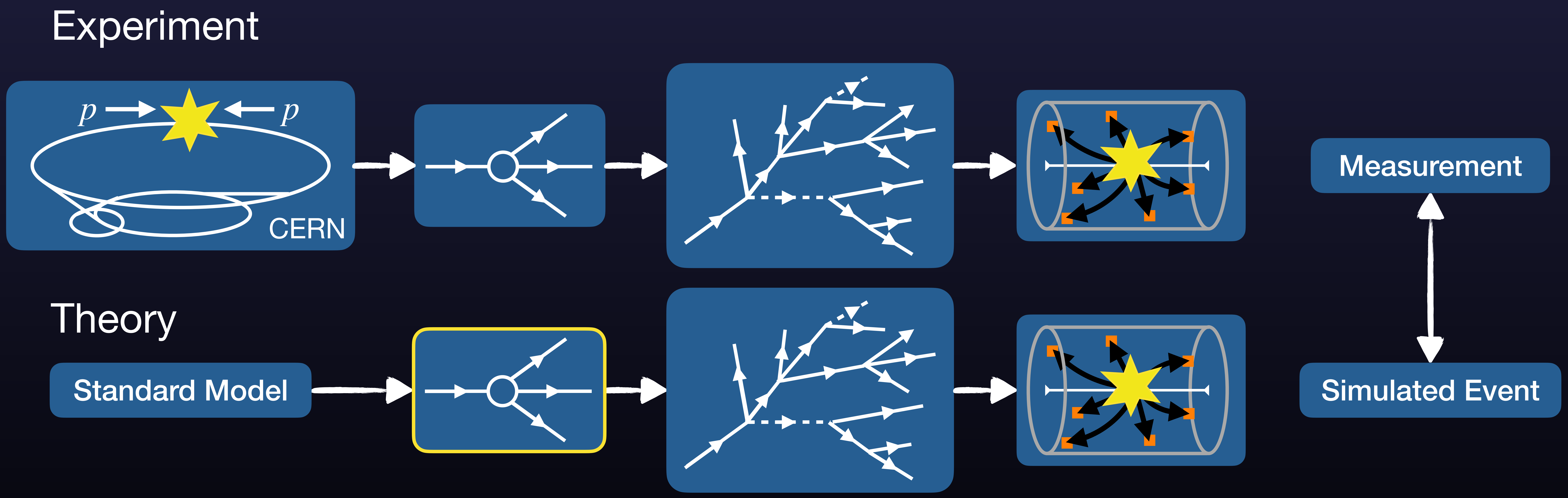
How to improve the precision of measurements?

→ Take more data!

Number of events until now

Number of events until 2030

What does this mean for the simulations?

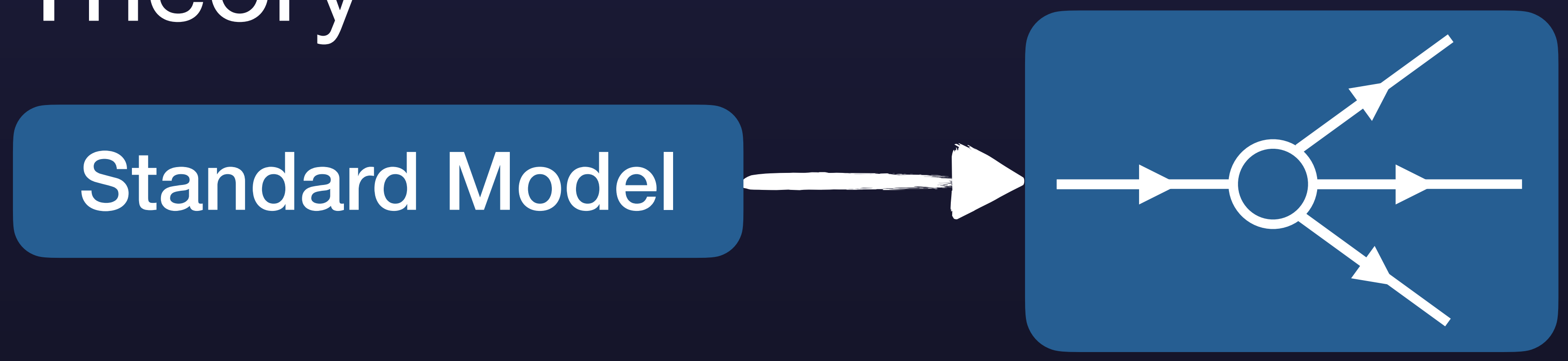


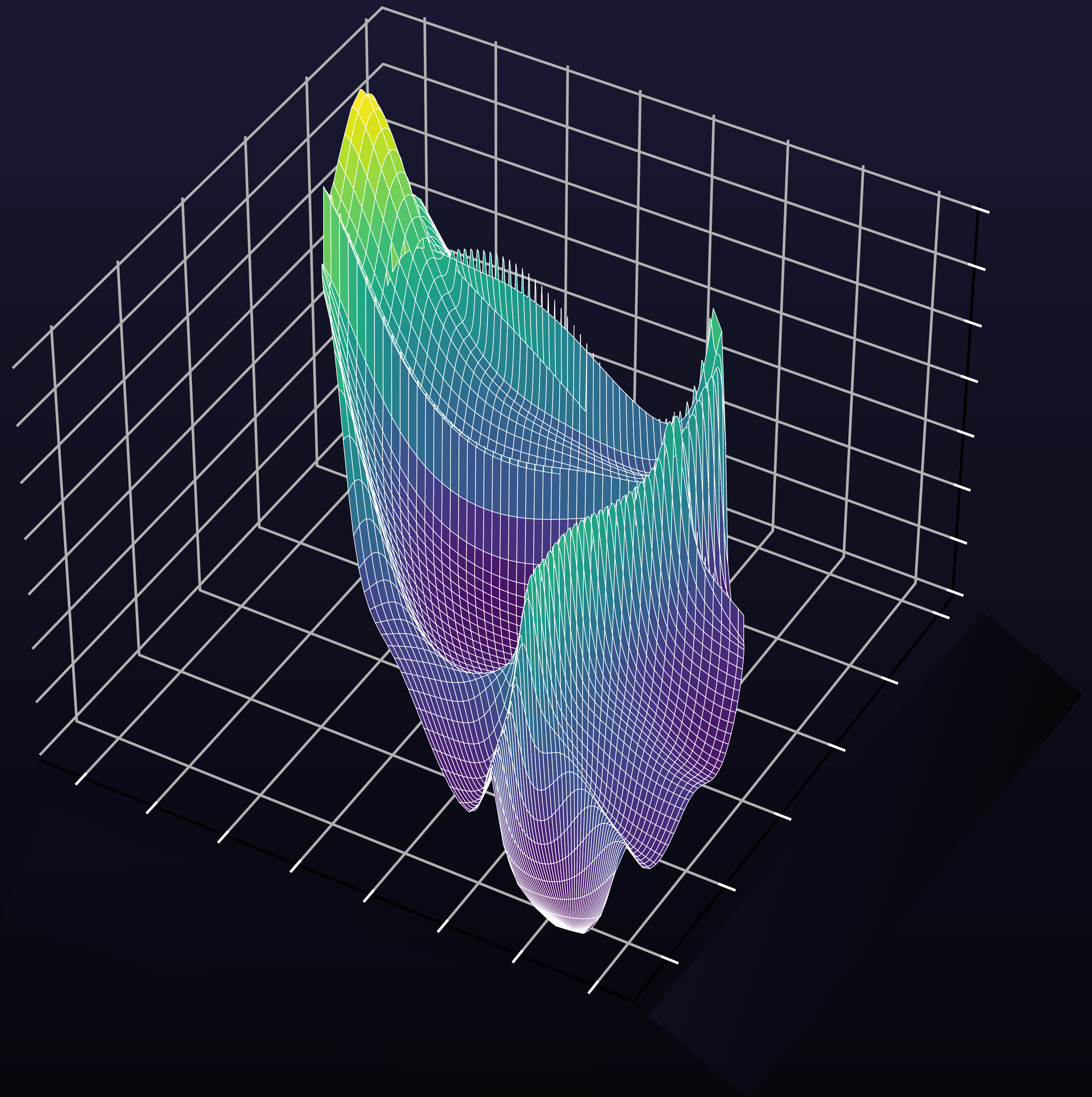
→ We need to speed up the simulation!

→ In this work: Event generation

What is event generation from a ML perspective?

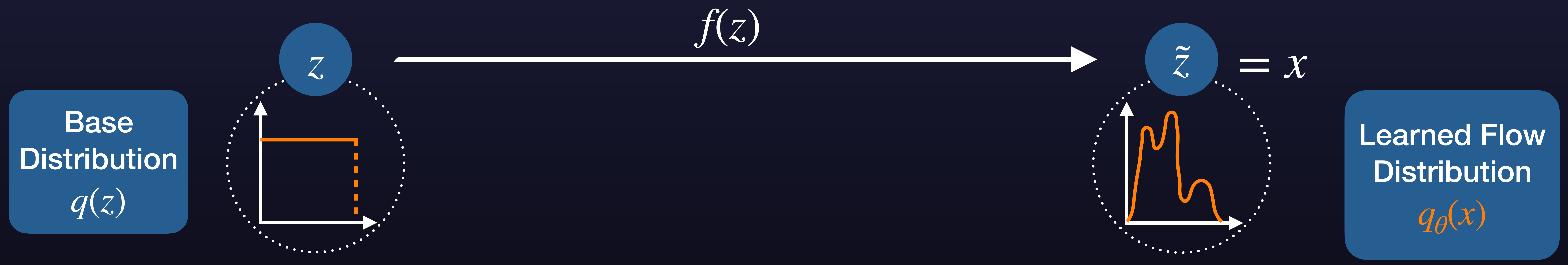
Theory





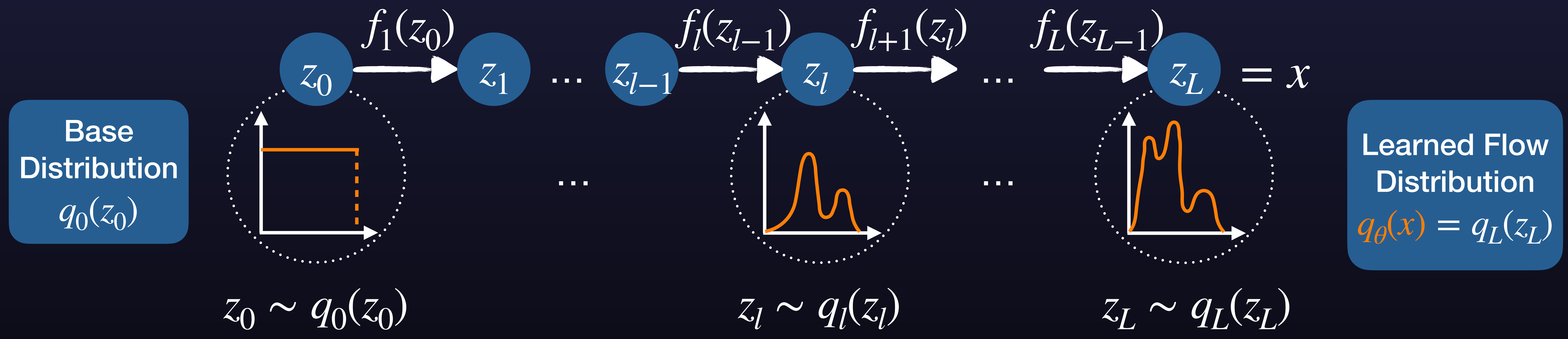
- Analytic formula for unnormalized distribution $p(x)$ ("matrix element")
- $p(x)$ describes the outgoing particles
- Sample from this distribution
- **Normalizing flow instead of standard methods**

What is a normalizing flow?



Rezende and Mohamed, “Variational Inference with Normalizing Flows.” ICML’15.
Durkan et al., “Neural Spline Flows.”, NeurIPS’19.

What is a normalizing flow?

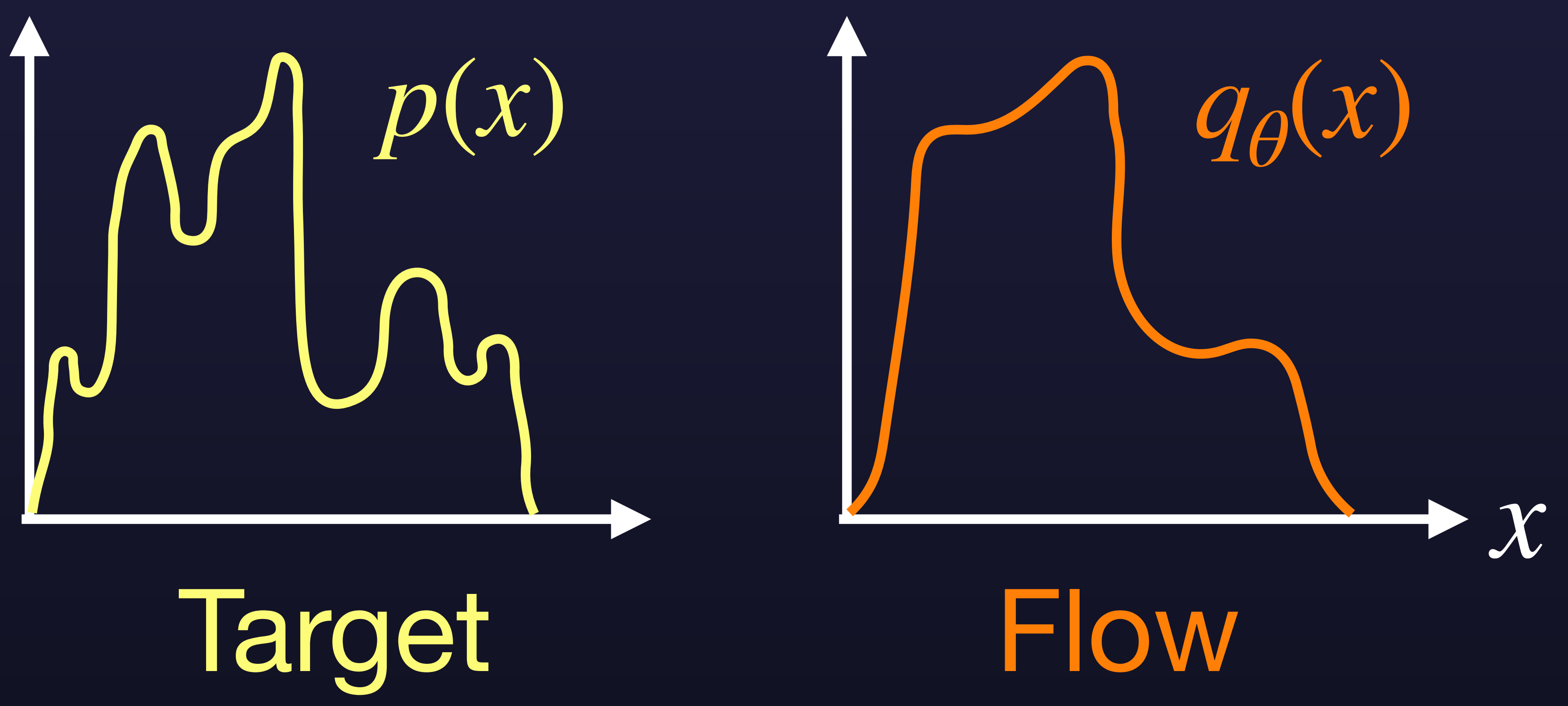


→ Generate samples x and evaluate density $q_\theta(x)$

Rezende and Mohamed, “Variational Inference with Normalizing Flows.” ICML’15.
Durkan et al., “Neural Spline Flows.”, NeurIPS’19.

How to train a normalizing flow?

3 Methods



Samples from target $x \sim p(x)$

(1) Forward KL Divergence (fKLD)

Samples from flow $x \sim q_\theta(x)$ and density evaluation of $p(x)$

(2) Reverse KL Divergence (rKLD)

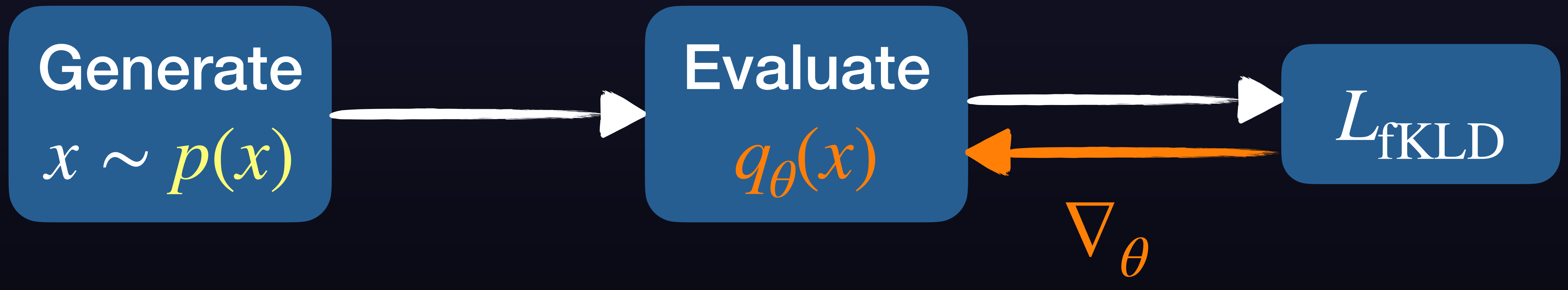
(3) Flow Annealed Importance Sampling Bootstrap (FAB)

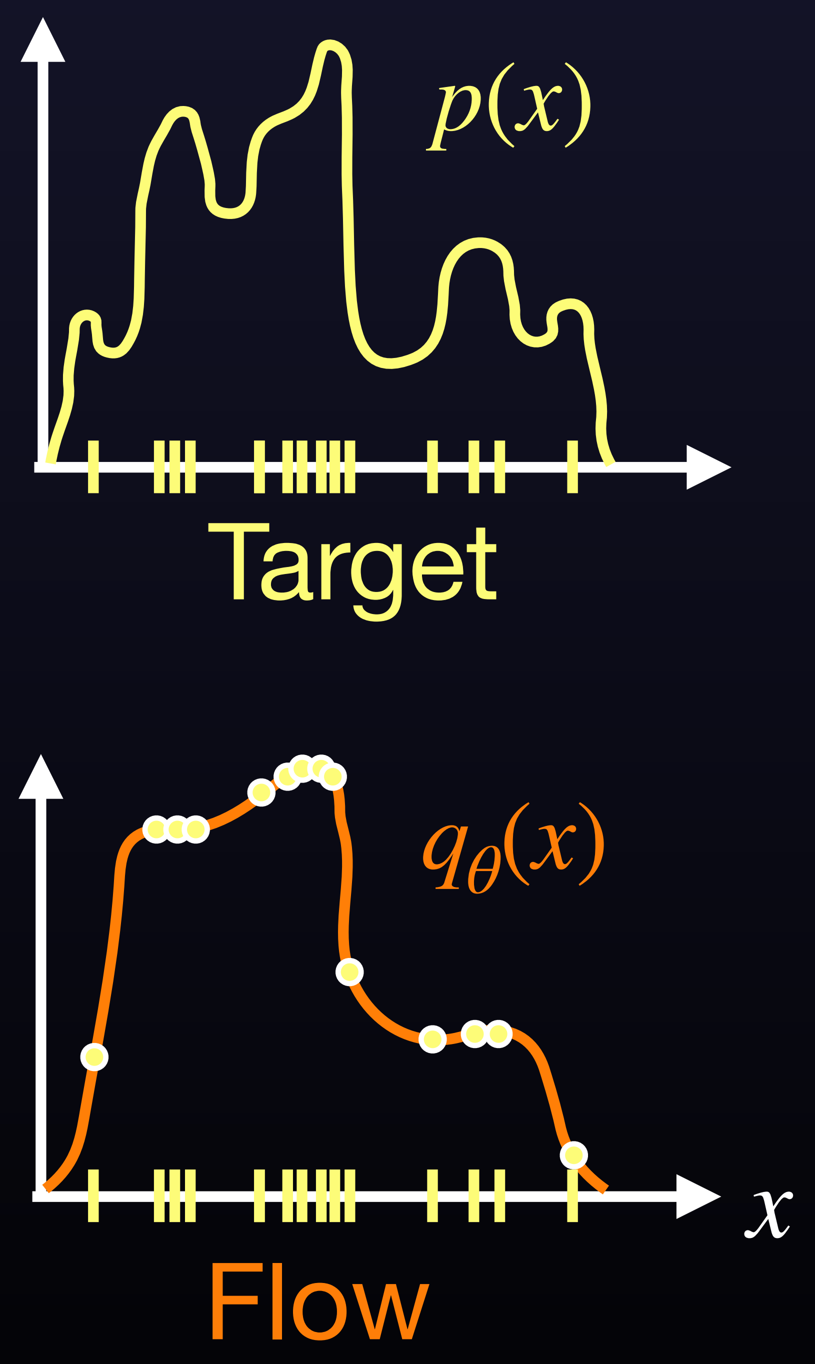
Midgley, Stimper, et al., “Flow Annealed Importance Sampling Bootstrap”, ICLR, 2023.

Training with Samples

Forward KL Divergence (fKLD)

$$L_{\mathrm{fKLD}} = D_{\mathrm{KL}}(p \,\|\, q_\theta) = \mathbb{E}_{x \sim p(x)}\left[\log \frac{p(x)}{q_\theta(x)}\right] = -\sum_{i=1}^{N} \log q_\theta(x_i) + \text{const.}$$



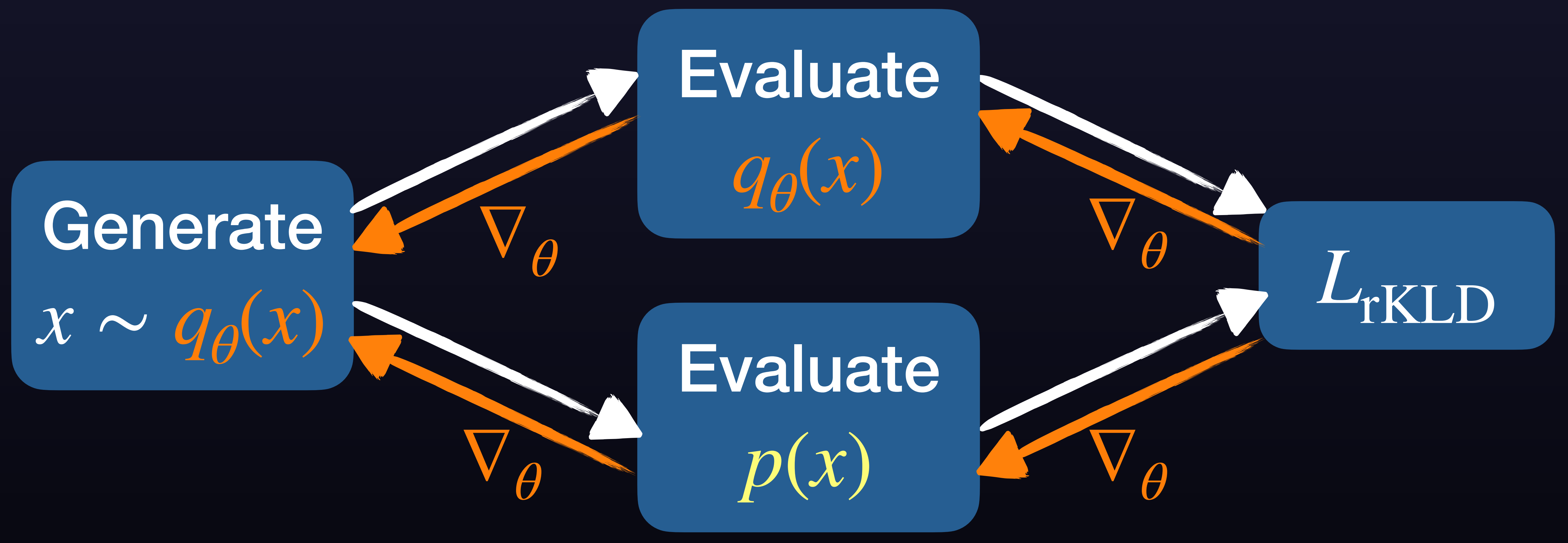


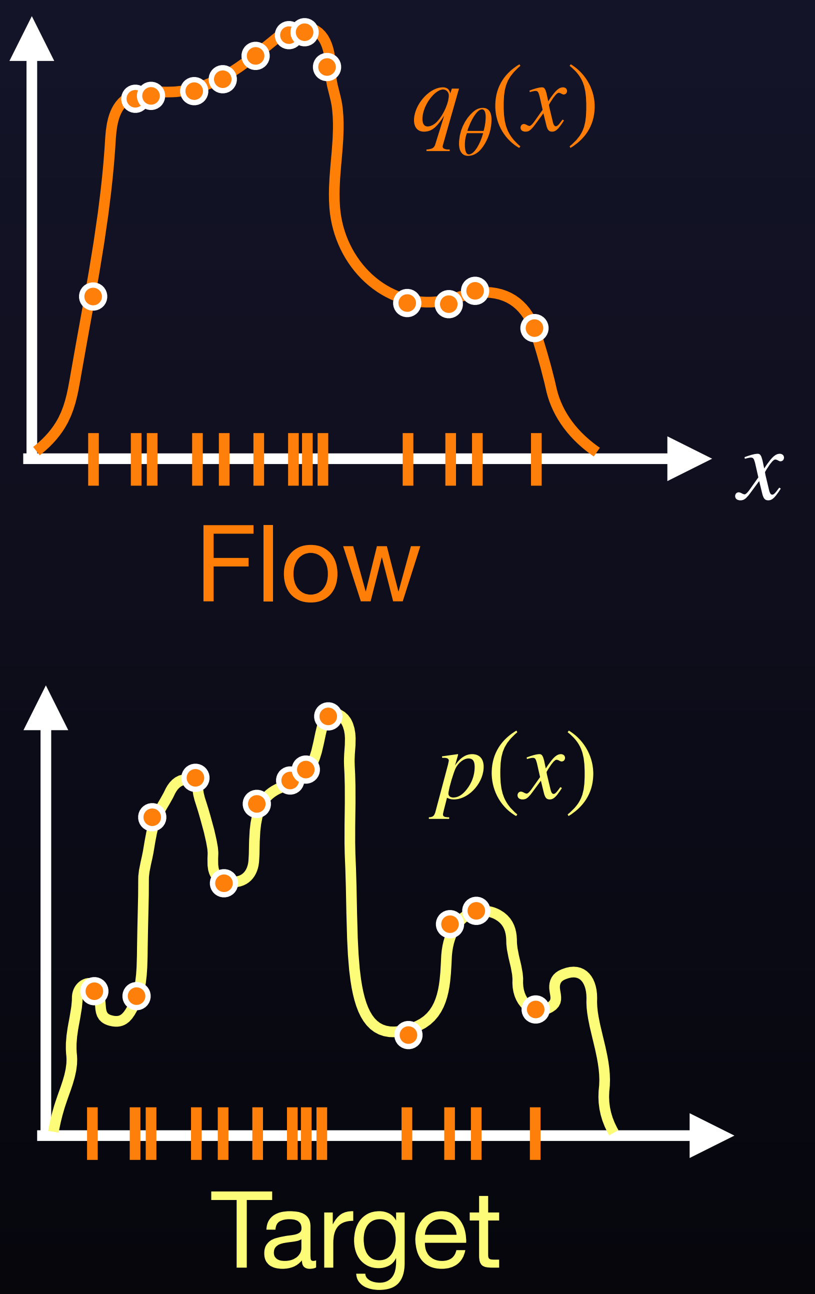
→ Expensive to generate training data

Training with Density Evaluation

Reverse KL Divergence (rKLD)

$$L_{\mathrm{rKLD}} = D_{\mathrm{KL}}(q_\theta \,\|\, p) = \mathbb{E}_{x \sim q_\theta(x)}\left[\log \frac{q_\theta(x)}{p(x)}\right]$$



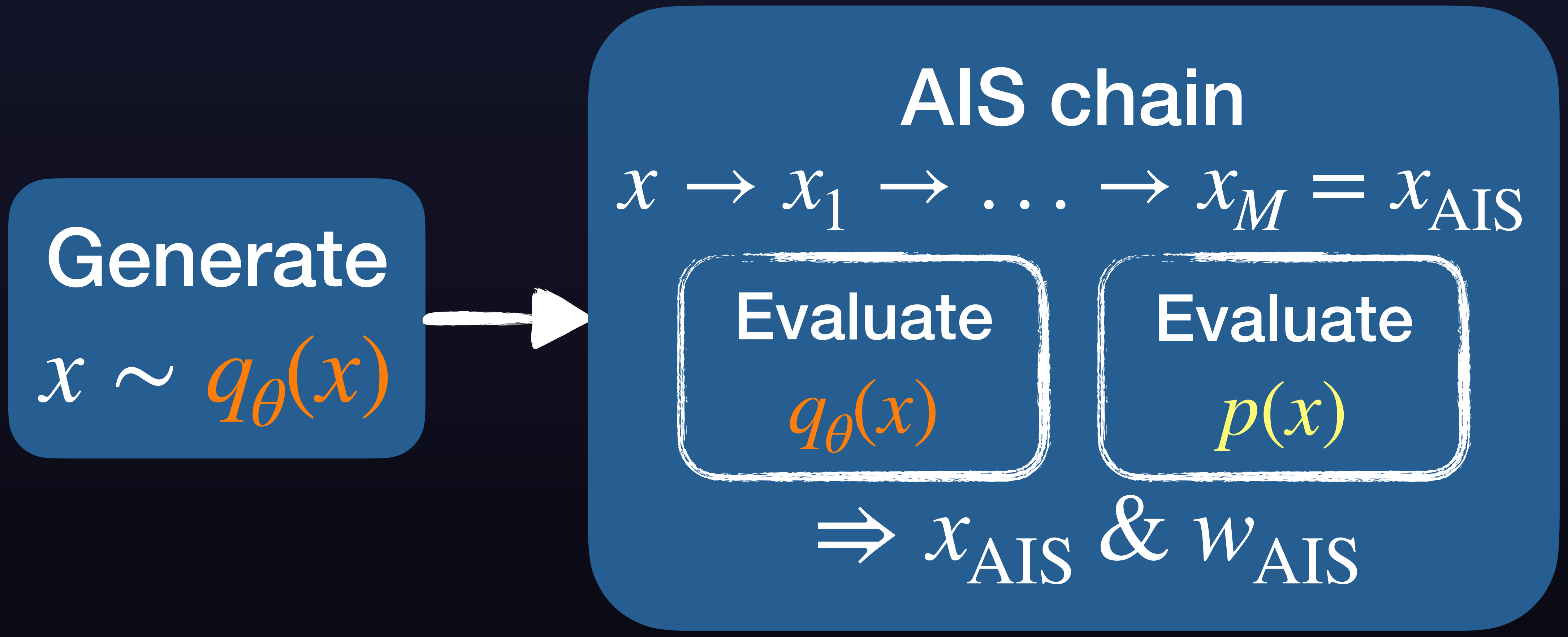


→ Requires differentiable target distribution $p(x)$

Training with Density Evaluation

Flow Annealed Importance Sampling Bootstrap (FAB)

Improve flow samples $x \sim q_\theta(x)$ with Annealed Importance Sampling (AIS)



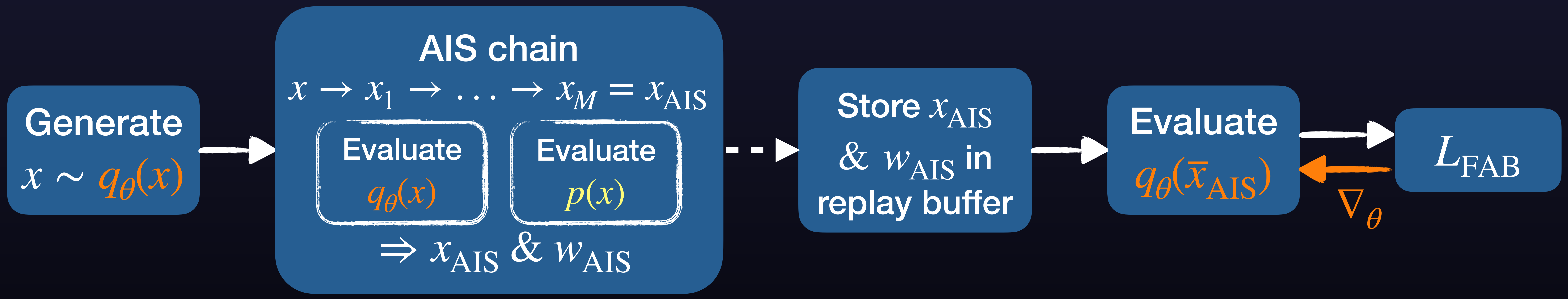
AIS chain implemented via Hamiltonian Monte Carlo (HMC)
$\to$ Requires differentiable target $p(x)$

Midgley, Stimper, et al., "Flow Annealed Importance Sampling Bootstrap", ICLR, 2023.

Training with Density Evaluation

Flow Annealed Importance Sampling Bootstrap (FAB)

Improve flow samples $x \sim q_\theta(x)$ with Annealed Importance Sampling (AIS)



$$L_{\text{FAB}} = -\sum_{i=1}^{N} \frac{\bar{w}_{\text{AIS}}^{(i)}}{\sum_j \bar{w}_{\text{AIS}}^{(j)}} \, q_\theta\left(\bar{x}_{\text{AIS}}^{(i)}\right)$$

→ minimizes variance of importance weights

Midgley, Stimper, et al., “Flow Annealed Importance Sampling Bootstrap”, ICLR, 2023.

Differentiable target distributions

Examples

Recent work in particle physics: differentiable implementations of $p(x)$

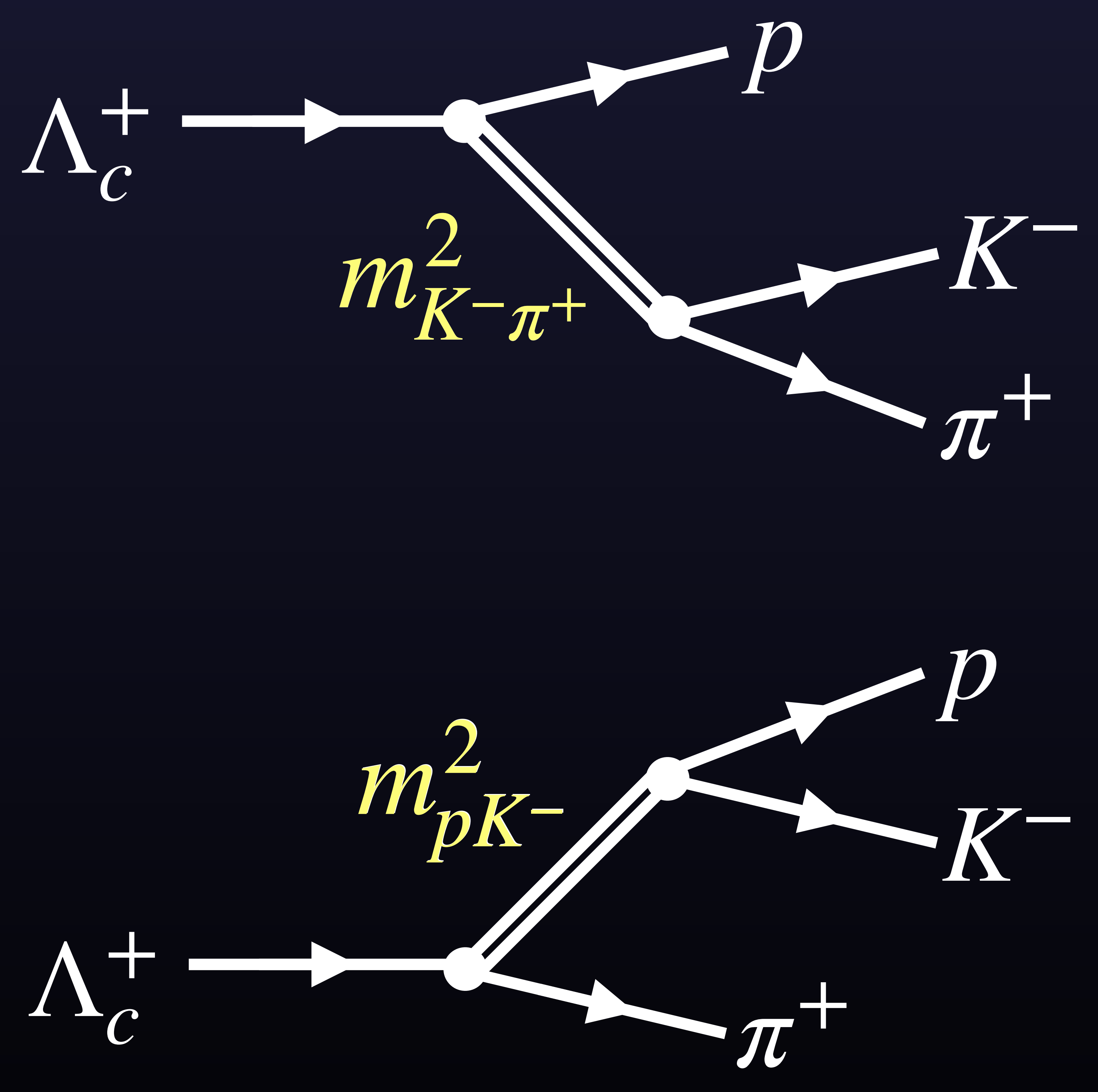
- **ComPWA:** $\Lambda_c^+ \to pK^-\pi^+$ (2D)
- **MadJAX:** $e^+e^- \to t\bar{t}, t\bar{t} \to W^+b, \bar{t} \to W^-\bar{b}$ (8D)

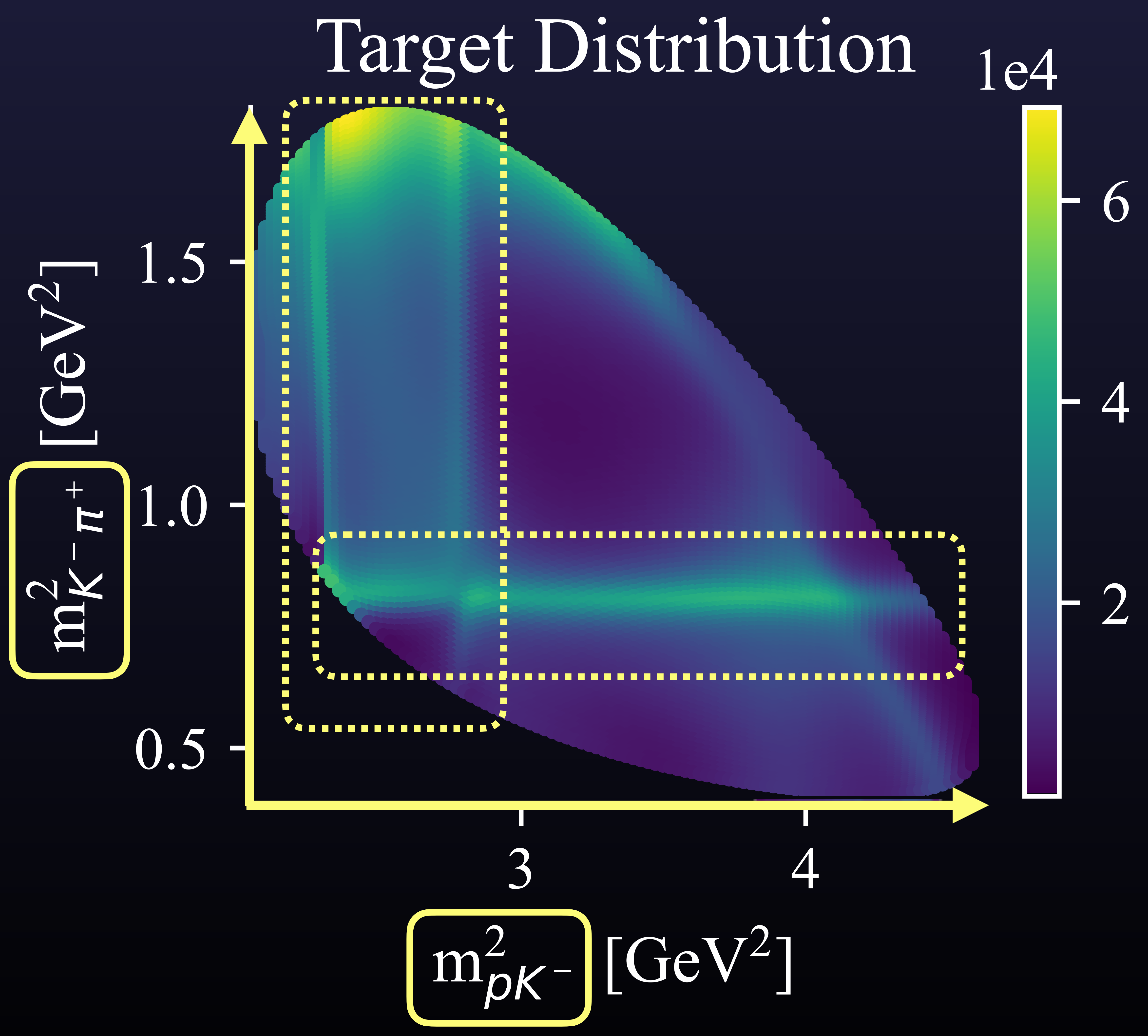
Common Partial Wave Analysis: A collaboration-independent organisation for amplitude analysis software, doi 10.5281/zenodo.6908150

Heinrich and Kagan, "Differentiable Matrix Elements with MadJax." J. Phys. Conf., 2023.

2D: $\Lambda_c^+ \to pK^-\pi^+$

What do we see?

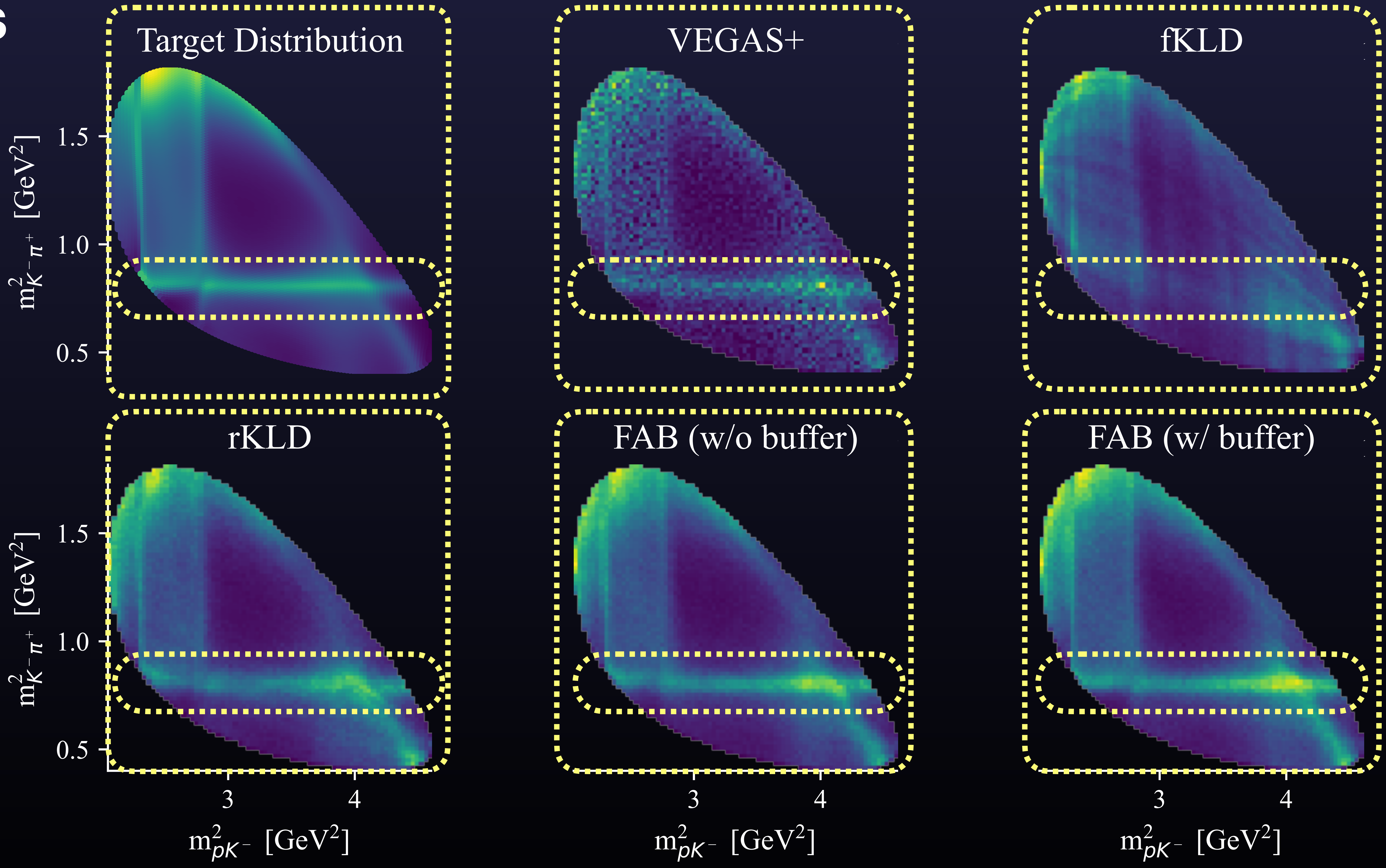




LHCb, "Amplitude analysis of the $\Lambda_c^+ \to pK^-\pi^+$ decay and Λ_c^+ baryon polarization measurement in semileptonic beauty hadron decays.", Phys. Rev. D 108, 2023.

2D: $\Lambda_c^+ \to pK^-\pi^+$

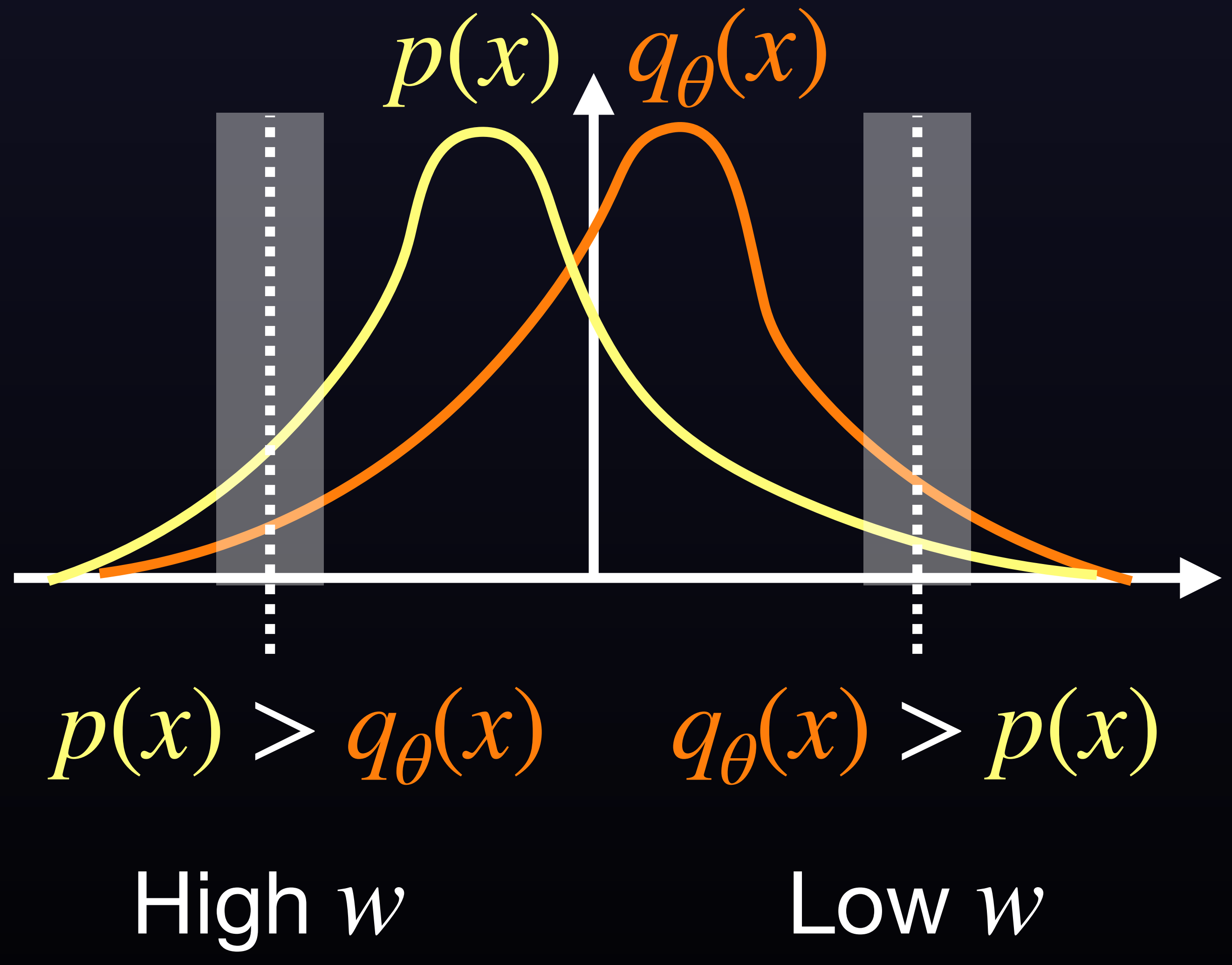
Histograms



How to compare?

- Efficiency ϵ

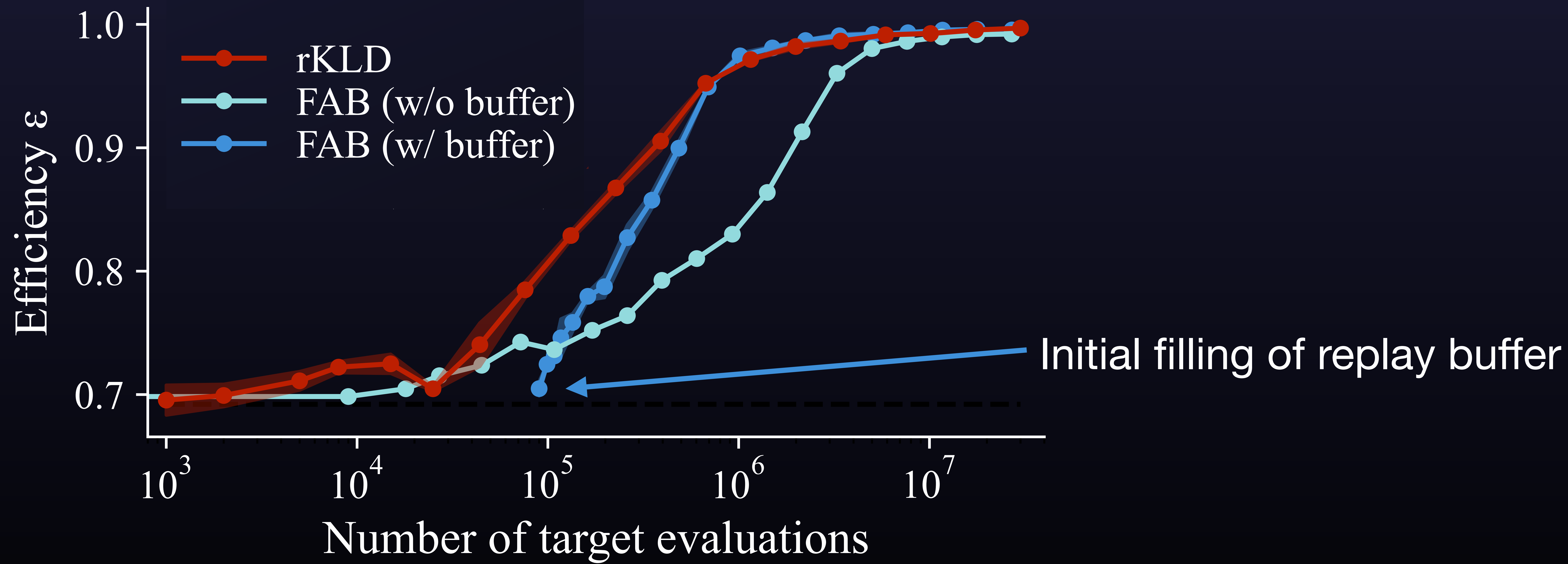
$$\epsilon = \frac{1}{N}\frac{\left(\sum_i w_i\right)^2}{\sum_i w_i^2} \in [0,1]$$ with importance weight $$w_i = \frac{p(x_i)}{q_\theta(x_i)}$$



$$p(x) \neq q_\theta(x) \rightarrow \epsilon \ll 1$$

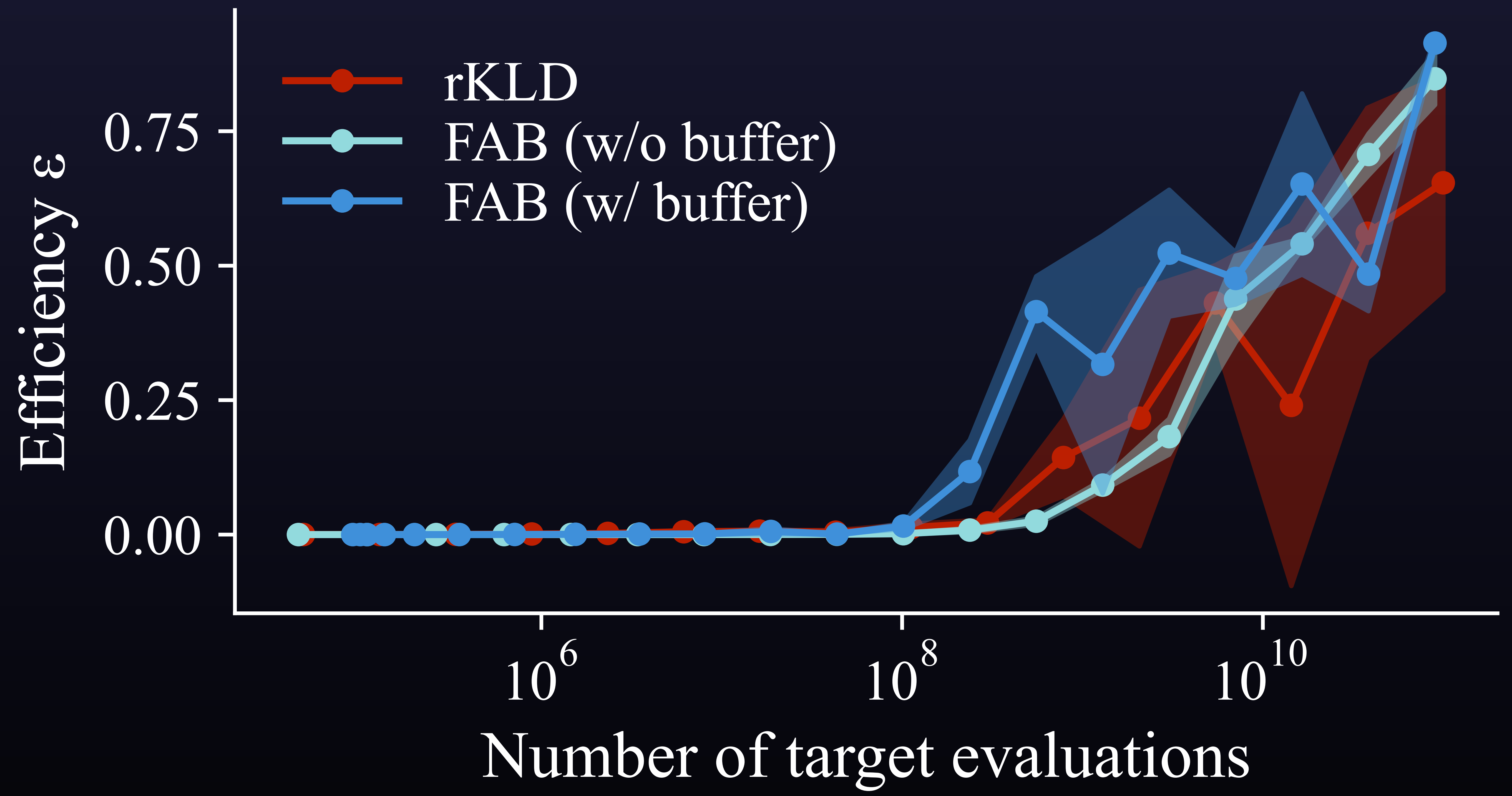
2D: $\Lambda_c^+ \to pK^-\pi^+$

Efficiency vs. Number of target evaluations

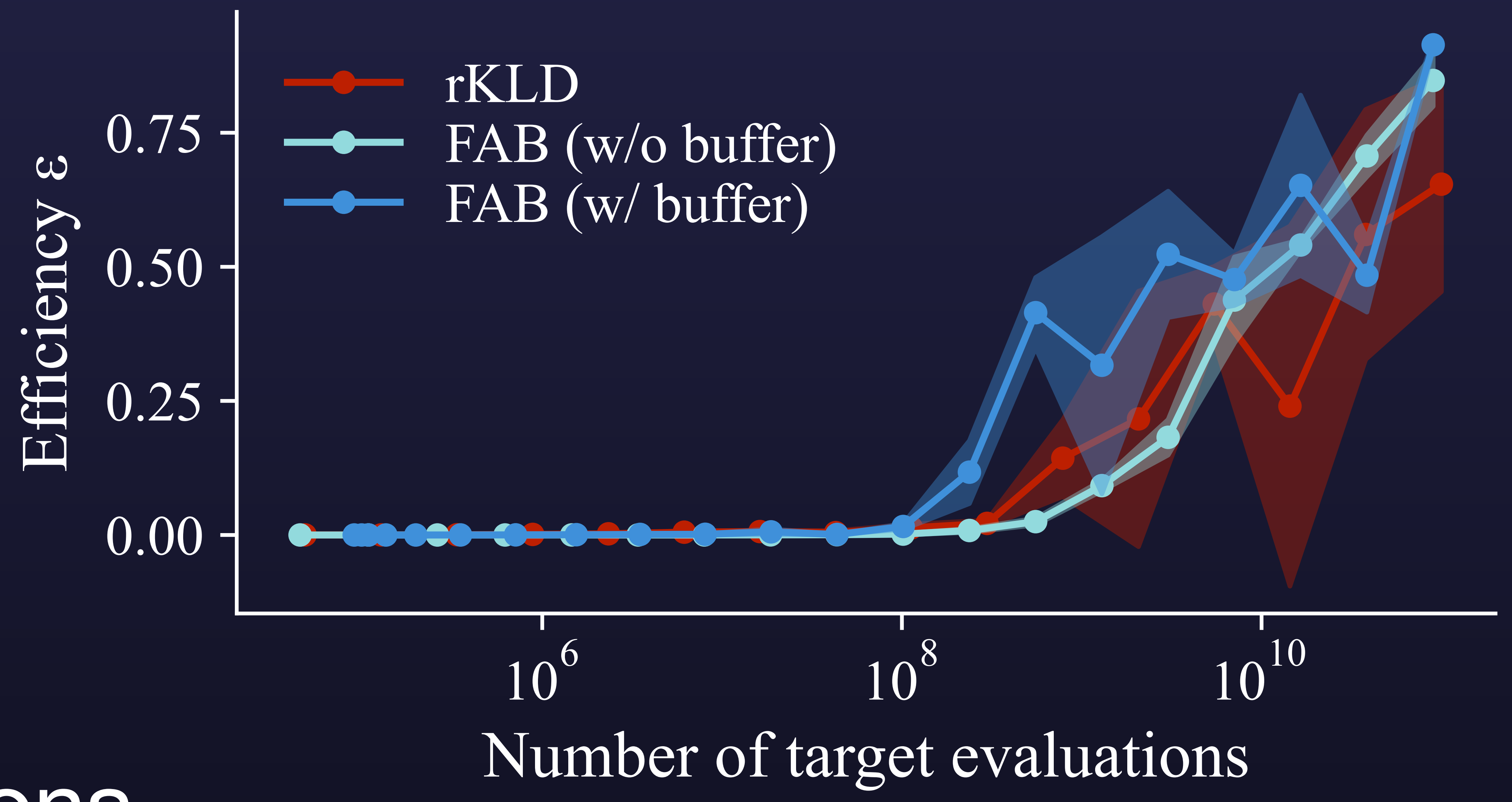


8D: $e^+e^- \to t\bar{t}, t\bar{t} \to W^+b, \bar{t} \to W^-\bar{b}$

Efficiency vs. Number of target evaluations



Take-Aways

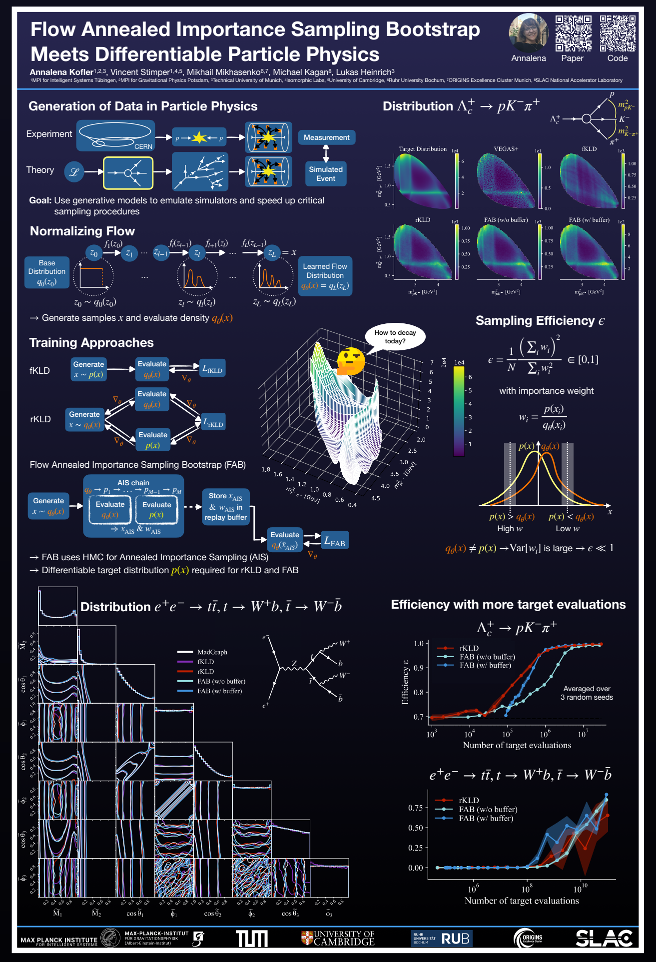


FAB (w/ buffer) …

… successfully adapted to particle physics

… outperforms other methods in high dimensions

… achieves higher sampling efficiency with fewer target evaluations



Visit my poster!
(16:15 - 17:25)

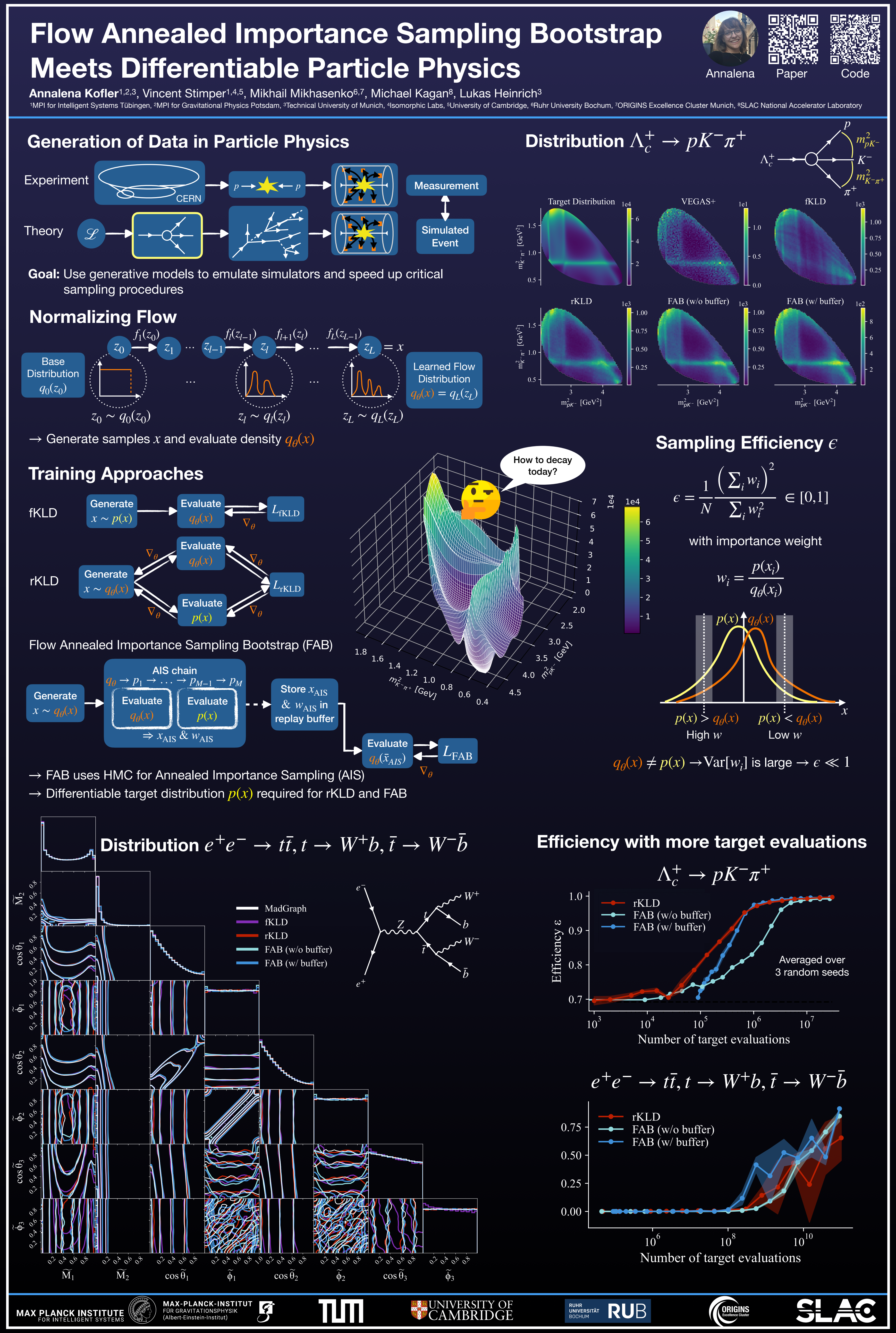
Paper

Code

Thanks to WiML for sponsoring my travel!

Do you have any questions?

You want to have an in-depth discussion?
→ Visit my poster (16:15 - 17:25)



Paper

Code

References

- ATLAS Software and Computing HL-LHC Roadmap, 2022.
- Rezende and Mohamed, “Variational Inference with Normalizing Flows.” ICML’15.
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