

# Learning Particle Physics - From Simulation to Inference with uncertainty aware Neural Networks

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# Why use machine learning in particle physics?

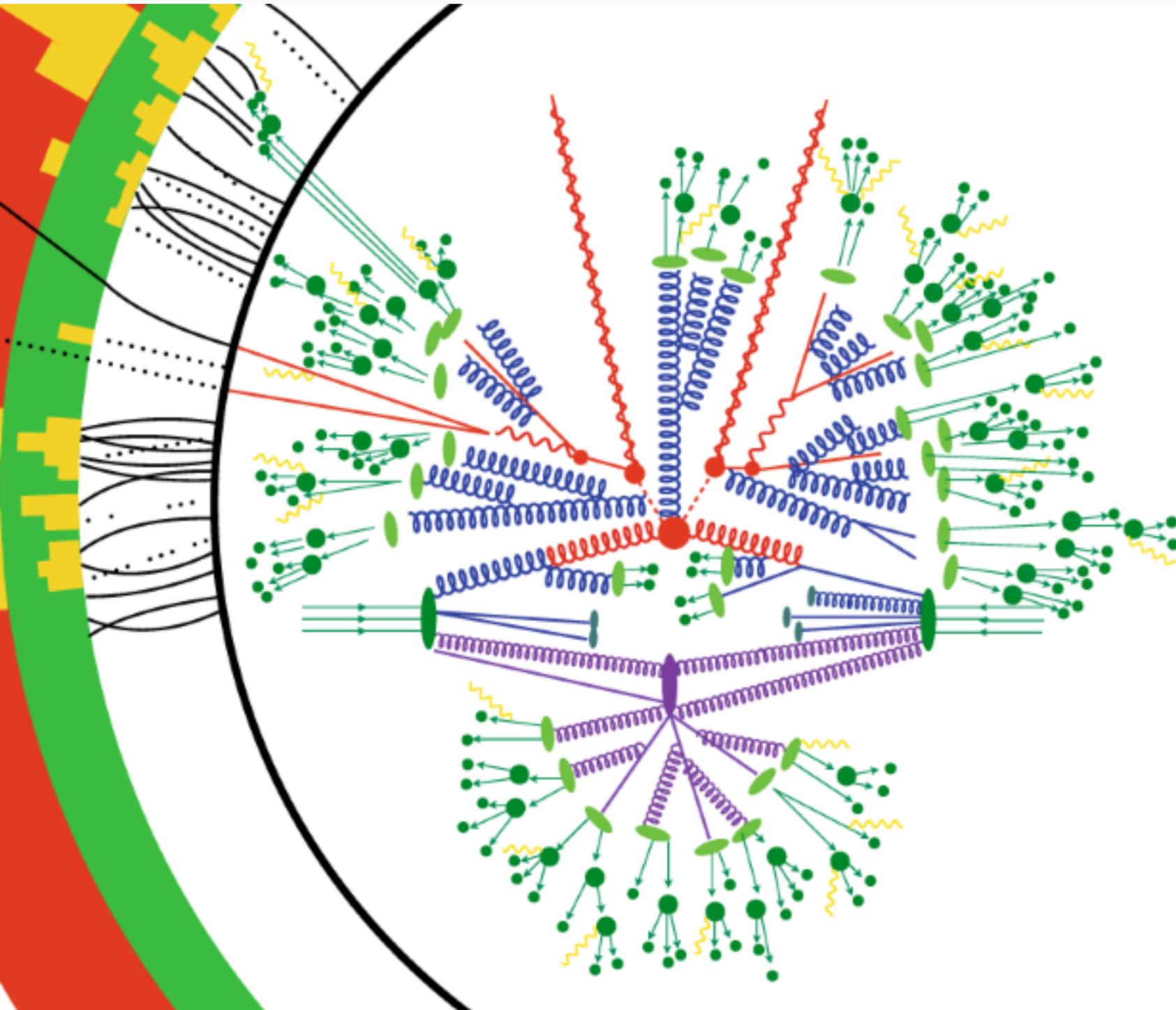
**Why use machine learning in particle physics?**

**Curiosity**

# Pile up event in ATLAS



# Control from theory & phenomenology



LHC analyses require for each analysis:

- \* High statistics - millions of events
- \* High precision -  $N^x$ LO process, off-shell,...

State of the art runtime for individual diagrams

Integrator \ Accuracy		$10^{-2}$	$10^{-3}$	$10^{-4}$	$10^{-5}$	$10^{-6}$	$10^{-7}$	$10^{-8}$
banana_3mass	DISTEVAL	2.1 s	2.1 s	2.4 s	2.6 s	2.6 s	2.9 s	3.6 s
	INTLIB	5.0 s	4.9 s	6.4 s	7.2 s	8.5 s	8.5 s	13.8 s
	Ratio	2.3	2.3	2.7	2.7	3.2	3.0	3.9
bubble6L	DISTEVAL	1.8 m	1.8 m	1.8 m	2.1 m	3.8 m	10.2 m	1.2 h
	INTLIB	39.5 m	38.8 m	39.6 m	43.8 m	85.1 m	170.7 m	11.6 h
	Ratio	22	22	22	21	22	17	10
formfactor4L	DISTEVAL	4.1 m	4.1 m	4.1 m	4.4 m	7.7 m	14.6 m	0.96 h
	INTLIB	74 m	73 m	73 m	74 m	136 m	246 m	10.9 h
	Ratio	18	18	18	17	18	17	11
elliptic2L_physical	DISTEVAL	1.6 s	1.5 s	1.7 s	1.9 s	4.0 s	19 s	7.6 m
	INTLIB	3.1 s	4.8 s	4.9 s	7.3 s	13.8 s	53 s	4.3 m
	Ratio	1.9	3.1	2.8	3.9	3.4	2.9	0.6
hz2L_nonplanar	DISTEVAL	2.1 s	2.6 s	4.6 s	30.4 s	2.2 m	5.1 m	27.1 m
	INTLIB	9 s	17 s	41 s	163 s	9.6 m	16.0 m	27.3 m
	Ratio	1.8	3.4	4.6	4.4	4.2	3.0	1.0
Nbox2L_split_b	DISTEVAL	2.7 s	9.8 s	16.8 s	0.58 m	2.4 m	9.1 m	20 m
	INTLIB	24 s	73 s	223 s	6.6 m	26 m	43 m	93 m
	Ratio	3.0	4.6	9.7	9.9	10.5	4.8	4.7
pentabox_fin	DISTEVAL	5 s	8 s	11 s	0.71 m	3.7 m	18.5 m	1.1 h
	INTLIB	45 s	65 s	88 s	3.2 m	11.3 m	74.8 m	4.6 h
	Ratio	8.6	7.9	7.7	4.5	3.1	4.0	4.2

Table 4: Integration timings on a GPU for different examples using the INTLIB qmc integrator and the new DISTEVAL integrator. All timings are using the CBC generating vectors from the previous release, meaning the ratios between INTLIB and DISTEVAL are purely due to the improvements described in Section 2.1. The significantly improved timings achieved by using the new median generating vectors are shown in Table 1.

# Why use machine learning in particle physics?

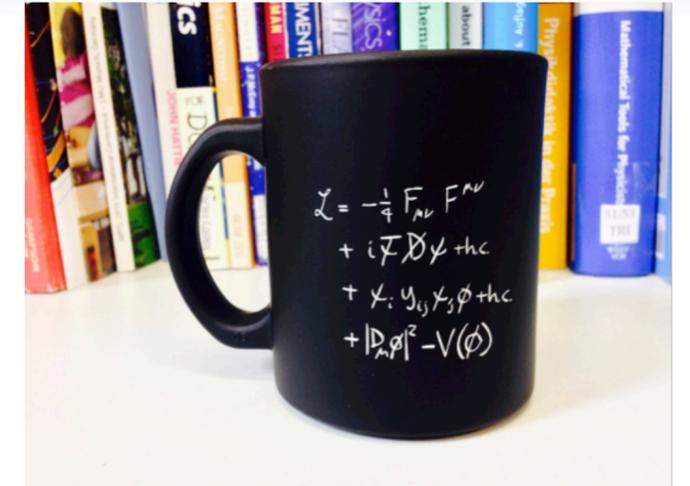
## 1. Curiosity

## 2. Perfect conditions

- Big data
- Full control through simulations
- Interesting Problem

## 3. Large gain

- Improve efficiency & precision -> better reach of analyses
- Free capacity through agentification
- New ideas (anomaly detection, unbinned unfolding, ...)
- New dynamic from fast moving developments in ML



# Why use machine learning in particle physics?

## 1. Curiosity

## 2. Perfect conditions

- Big data
- Full control through
- Interesting Problem

## 3. Large gain

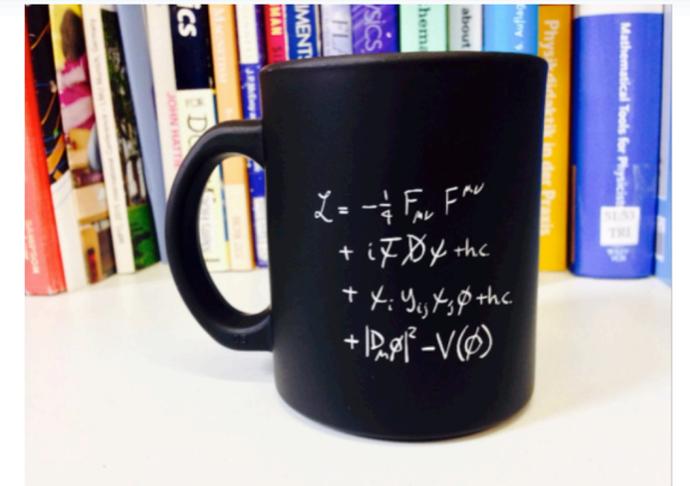
- Improve efficiency &
- Free capacity through
- New ideas (anomaly)
- New dynamic from fast moving developments in ML

**Develop & adapt ML techniques**  
→ **right balance between ML & theory**

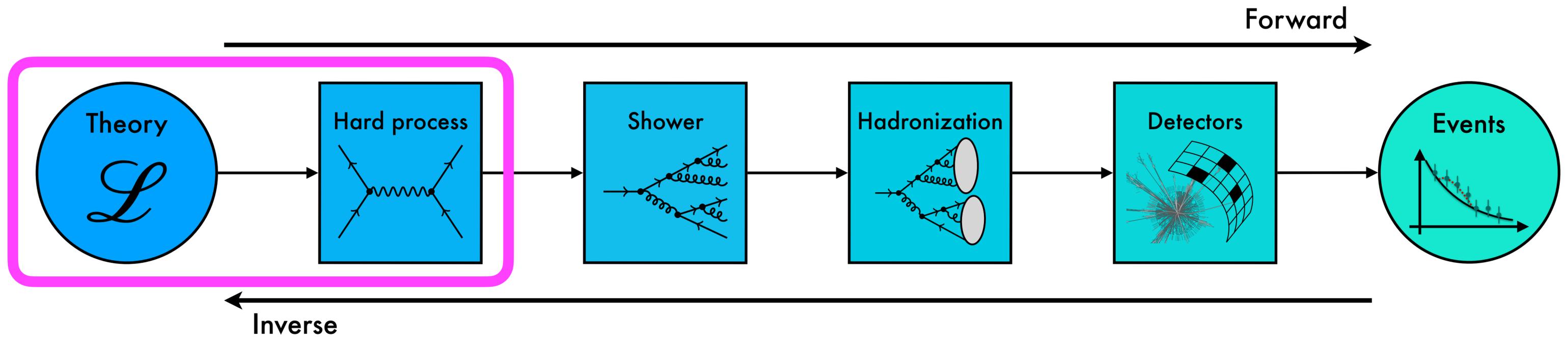
- *Fast precision calculations & simulations* -

- *Optimized data analysis* -

- *Calibrated uncertainties* -

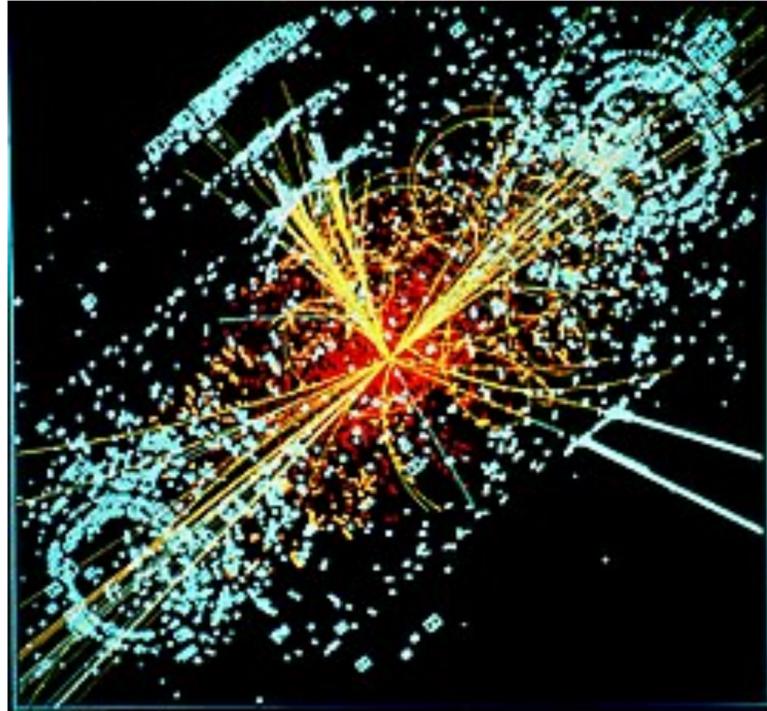


# Monte Carlo event generation

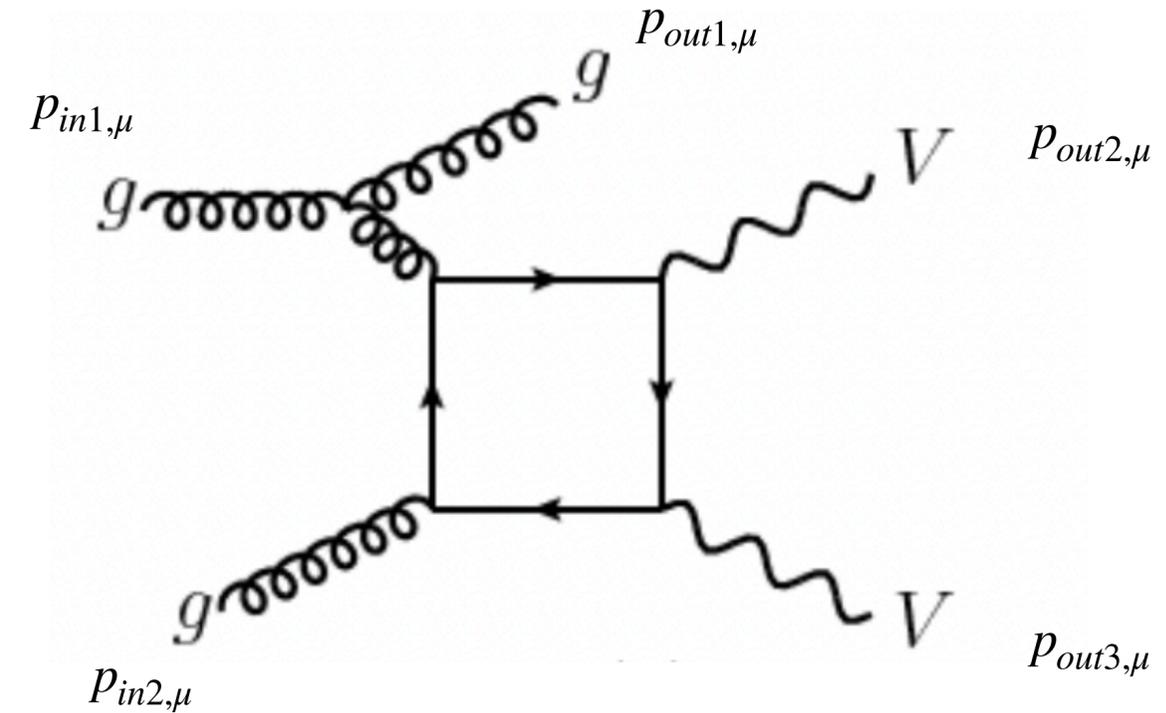


**1. Precision amplitudes**  
or  
**Quantifying uncertainties in regression problems**

# Learning Amplitudes - A Regression Problem



Experimentalist's view



Theorist's view

- Amplitudes are @ the heart of LHC physics - probability of particle interactions
- Compute  $A(\{p_{i,\mu}\} | i = 1, \dots, N_{particles})$  as function of particle momenta  $p_\mu$
- Spans multiple orders of magnitude
- Very expensive for higher order processes and large  $N_{particles}$

→ **Use NN to interpolate between known amplitudes**

# Machine Learning for theorists

## Machine Learning

## Physics

### Problem setting

Loss function  $\mathcal{L}$

Likelihood  $\mathcal{L}$

### Learnable function

Neural network  $f_\theta$

Physics knowledge  $f_{physics}$

### Data

Sampling  $\frac{1}{N} \sum_{i=1}^N \mathcal{L}(f_\theta(x_i); x_i)$

Phase space integration  $\int dx p(x) \dots$

### Solving the problem

Gradient descent  $\theta^i \rightarrow \theta^{i+1} = \theta^i - \nabla_{\theta_i} \mathcal{L}$

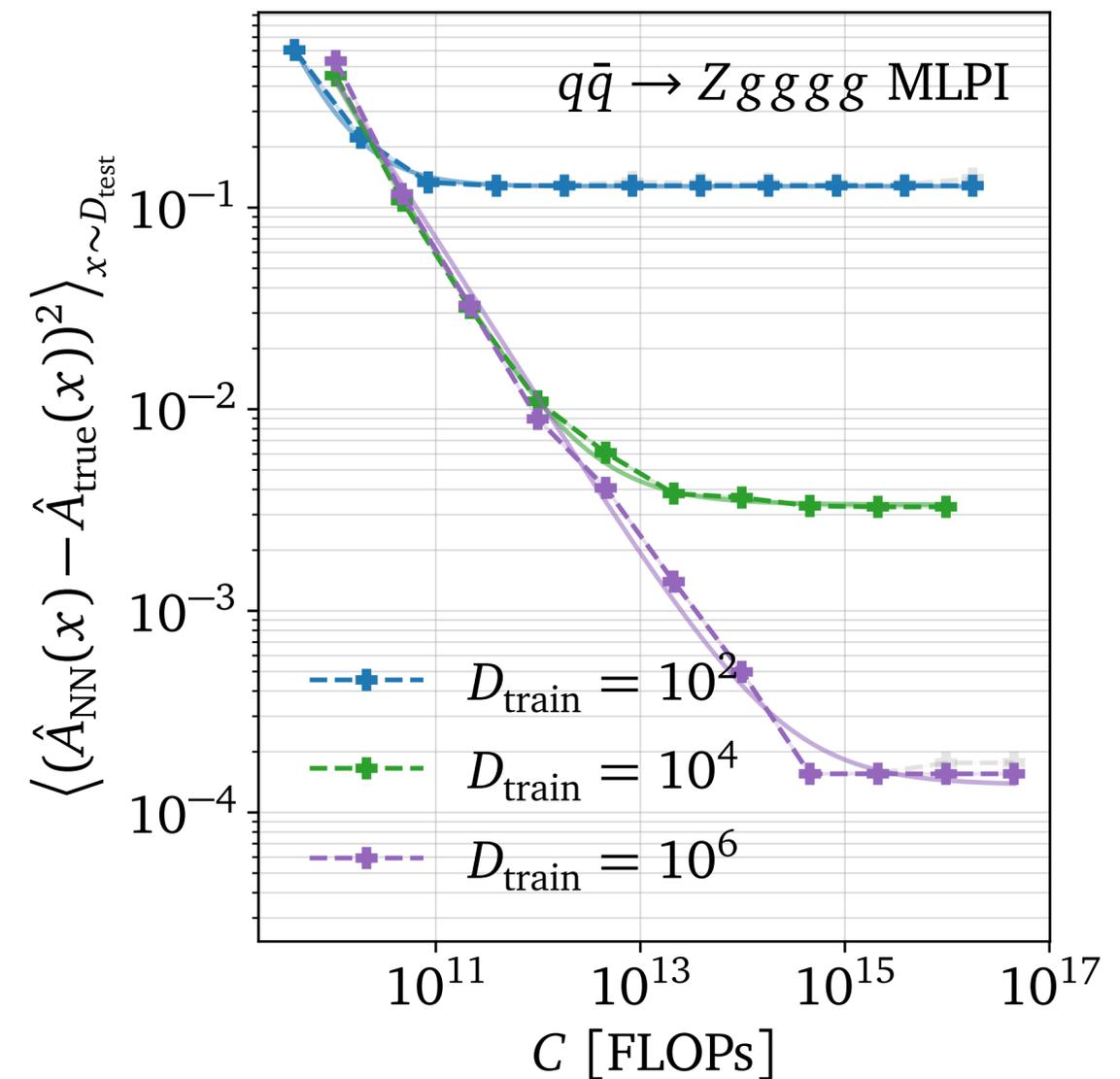
Functional derivative  $\frac{\delta \mathcal{L}}{\delta f} \stackrel{!}{=} 0$

# How to achieve high accuracy amplitudes?

[2601.13308] H. Bahl, V. Brésó, AB, J. Ramirez

## Example $q\bar{q} \rightarrow Zgggg$

- Reminder:
  - Amplitudes are known exactly
  - Numerical noise negligible
- Setup:
  - Standard NN (MLP)
  - Use invariants  $(s, t, u)$  as input
  - Evaluate MSE over test data set



# How to achieve high accuracy amplitudes?

[2601.13308] H. Bahl, V. Brésó, AB, J. Ramirez

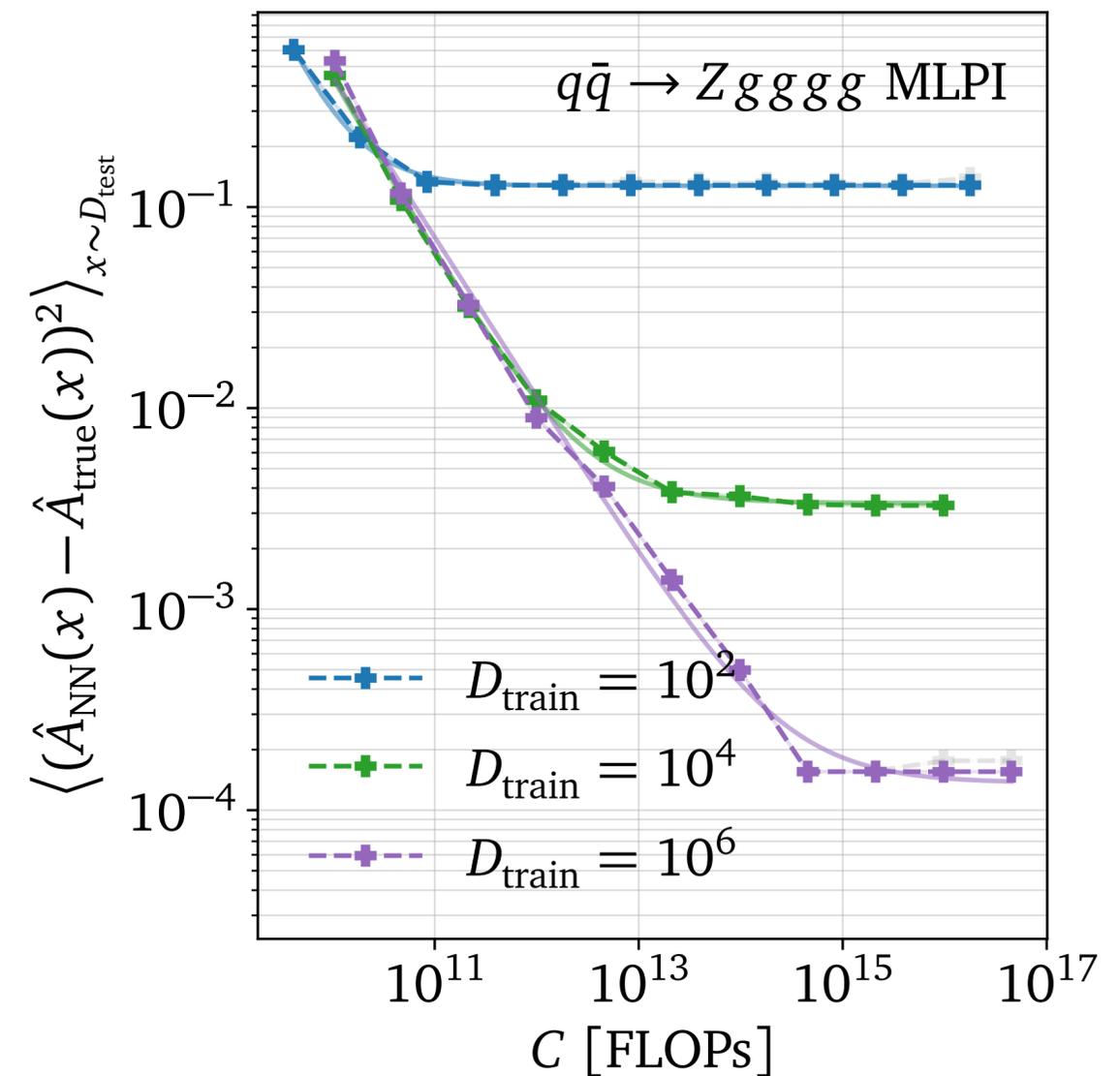
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**Power law scaling**

$$L(X, Y, Z) = (X_c/X)^{\alpha_x} + K(Y, Z)$$

for  
*Model size*  
*Dataset size*  
*Compute*

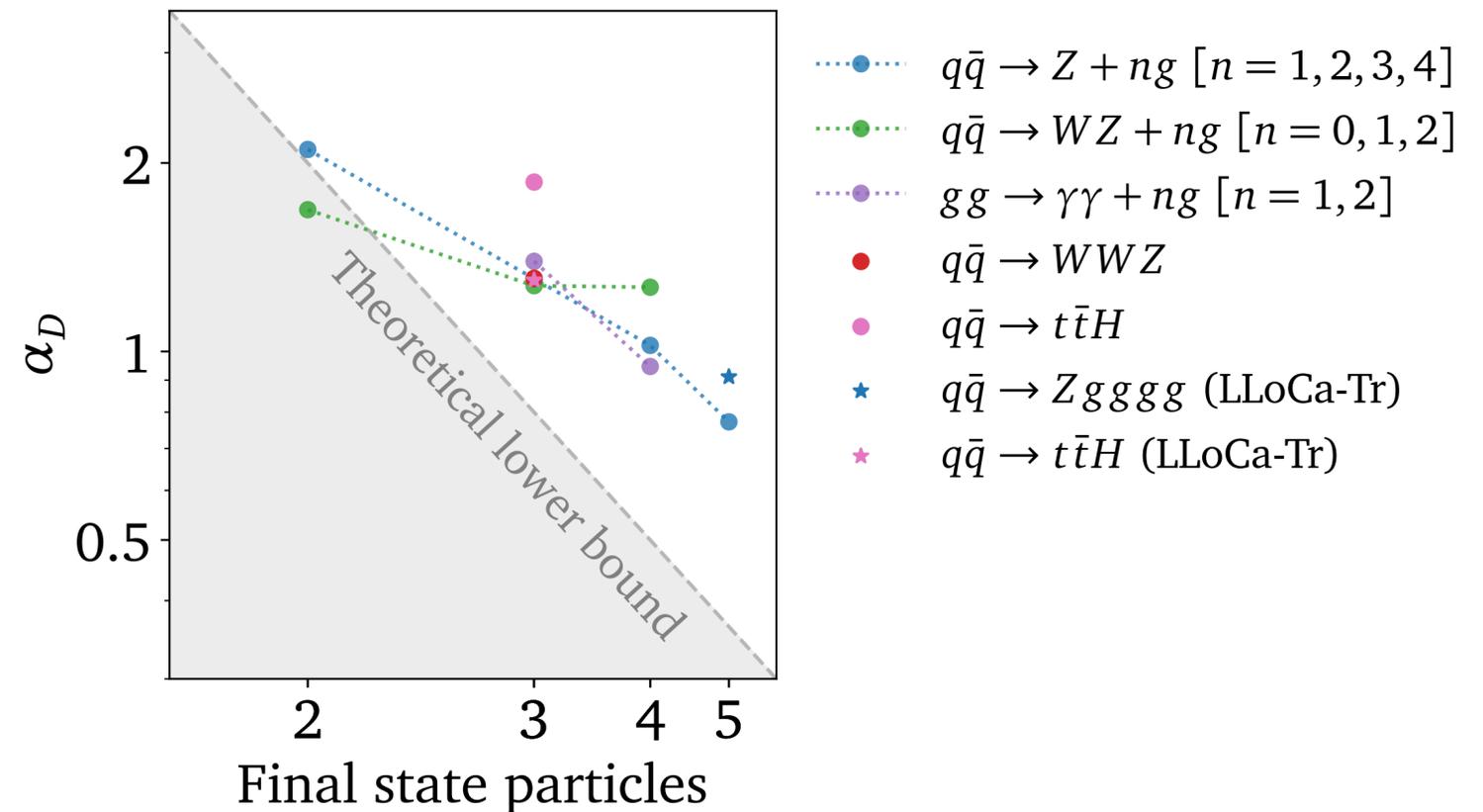
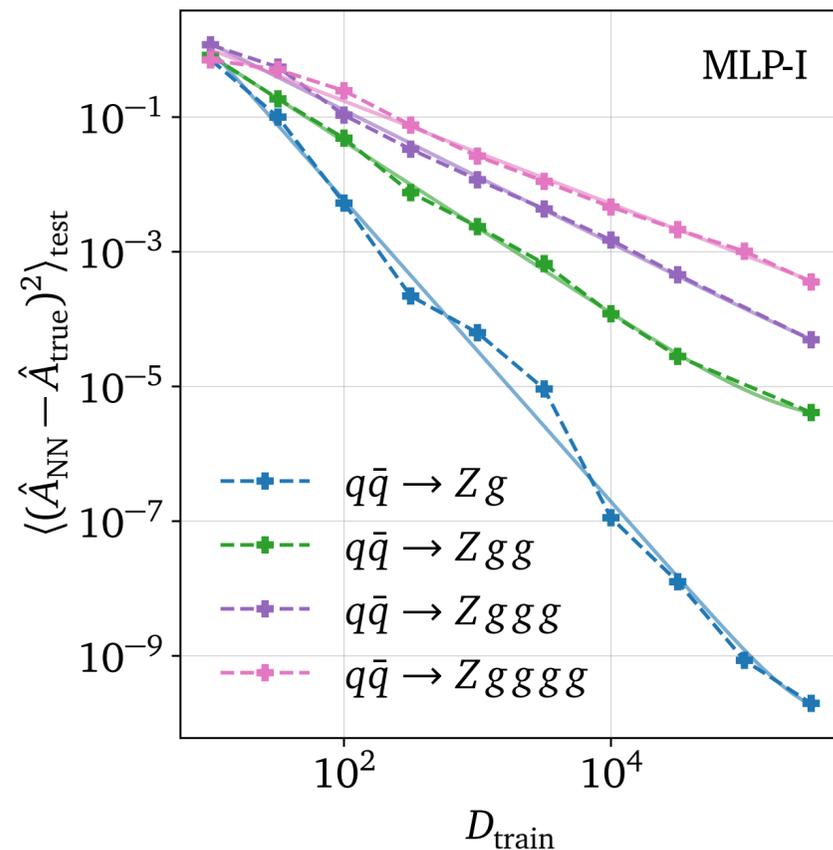


# Can we predict the scaling?

[2601.13308] H. Bahl, V. Bréso, AB, J. Ramirez

**Example**  $q\bar{q} \rightarrow Z + ng$

- Scaling depends on degrees of freedom



# Including symmetries

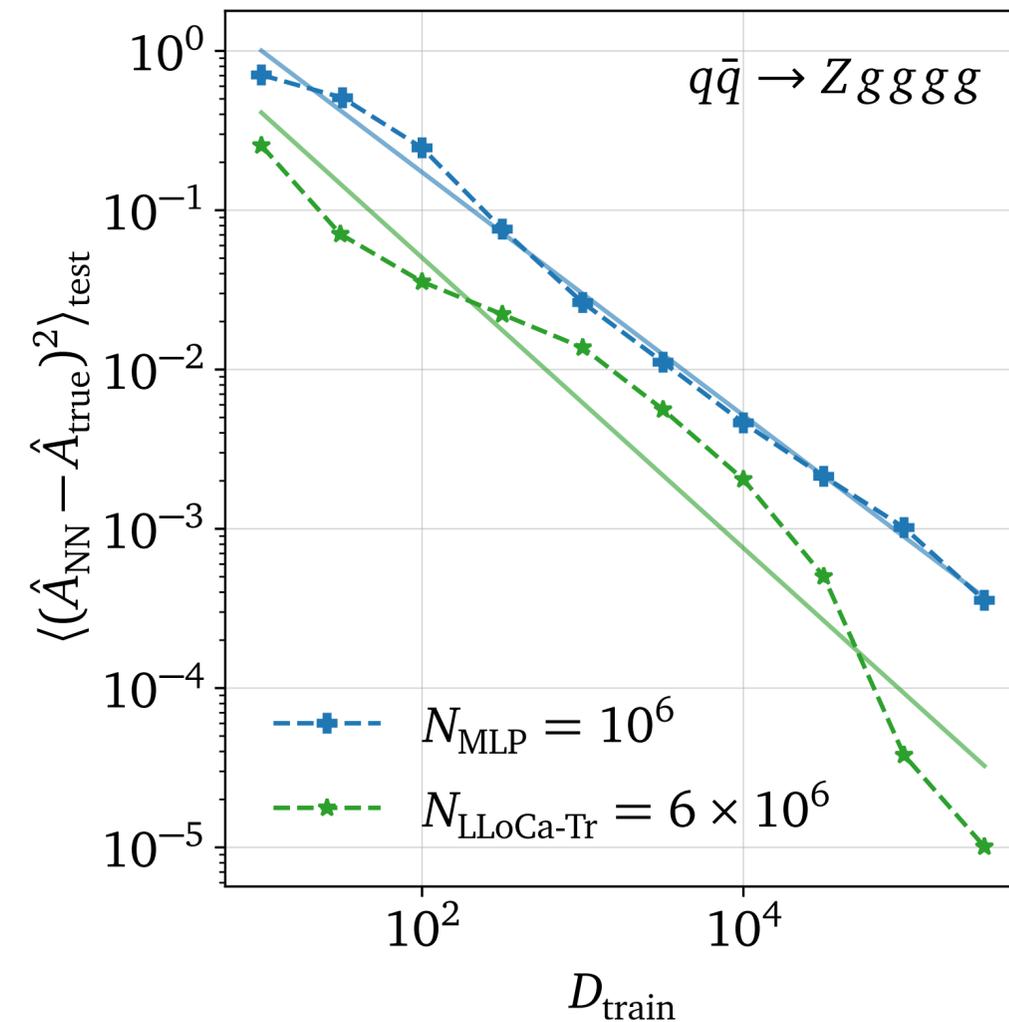
[2601.13308] H. Bahl, V. Bréso, AB, J. Ramirez

## LLoCa network

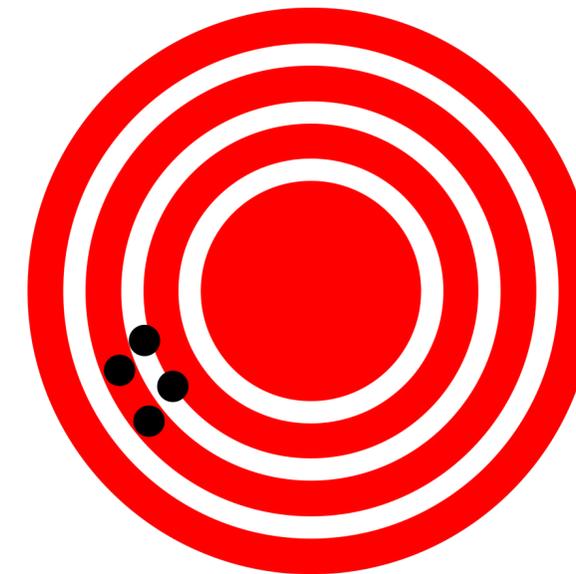
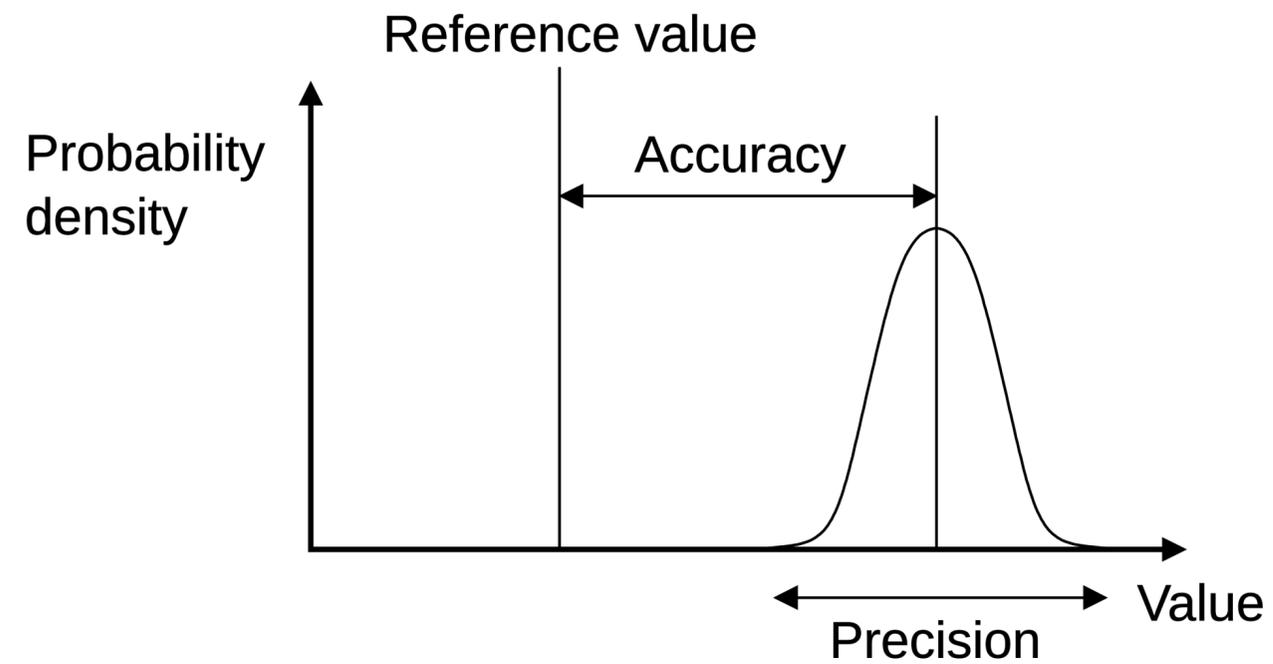
Lorentz Local Canonicalization [2505.20280]

J. Spinner, L. Favaro, P. Lippmann, S. Pitz,  
G. Gerhartz, T. Plehn, F. A. Hamprecht

- Equivariance wrt. Lorentz transformations
  1. Transforms each particle into local reference frame
  2. Apply arbitrary backbone architecture
  3. Transform back to initial frame work



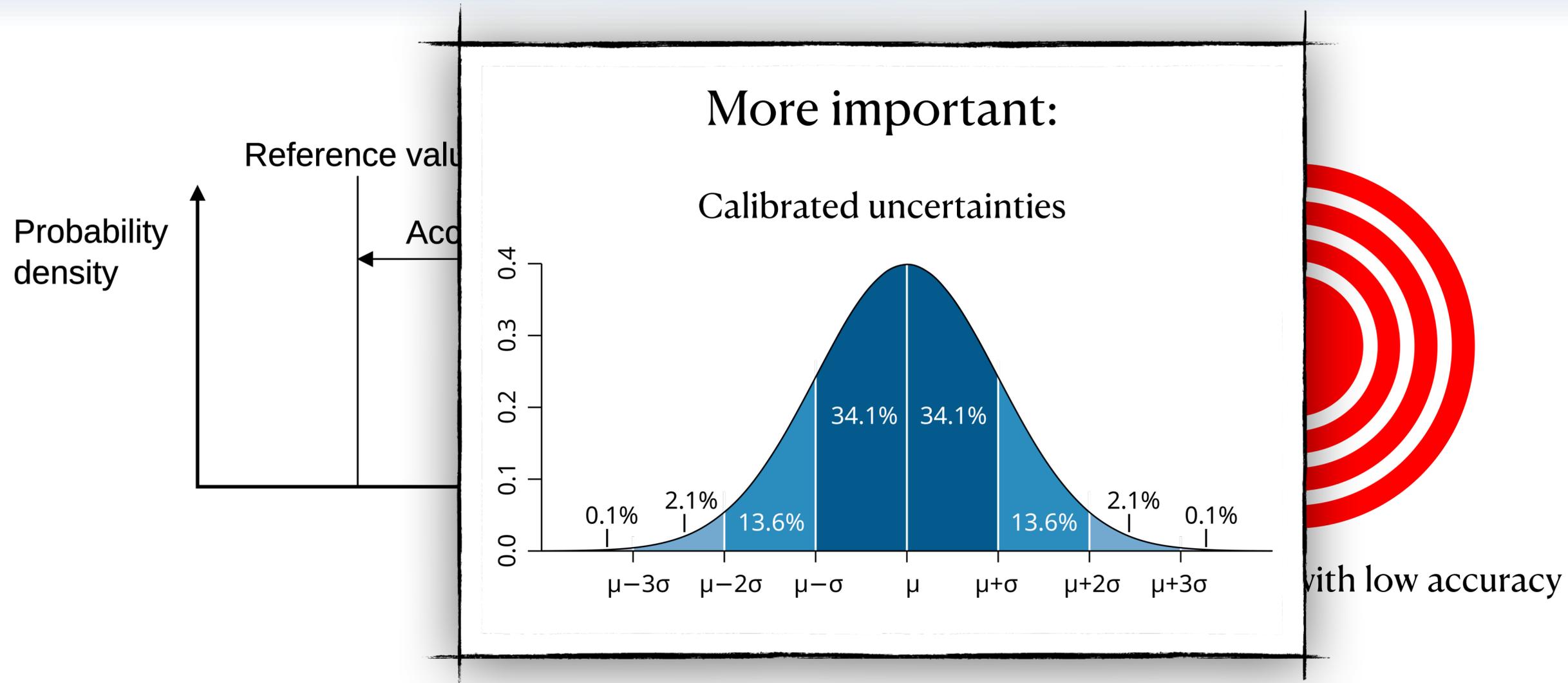
# Accuracy vs precision



High precision with low accuracy

Best of all worlds: high accuracy & high precision

# Accuracy vs precision



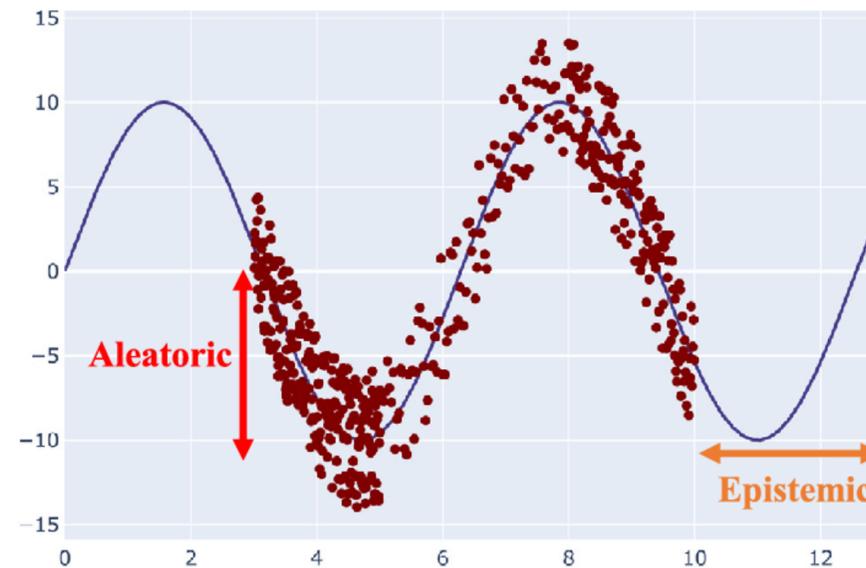
Best of all worlds: high accuracy & high precision

# Who is talking about uncertainties?

Physicist	Why?	How?	ML researcher	Meaning
Statistical	Limited data	Poisson	Aleatoric /Stochastic	Intrinsic noise, irreducible with more data
Systematic	Jet energy resolution	Gaussian		
Theorie	Higher order calculation	Flat?		



... what you say vs what they hear ...



# Heteroscedastic loss

**Heteroscedastic = variance depends on input parameter**

**Traditional** approach:

Fit with **known** uncertainties

**New:**

Learn **unknown** uncertainties

Direct consequence of likelihood approach

Maximize:

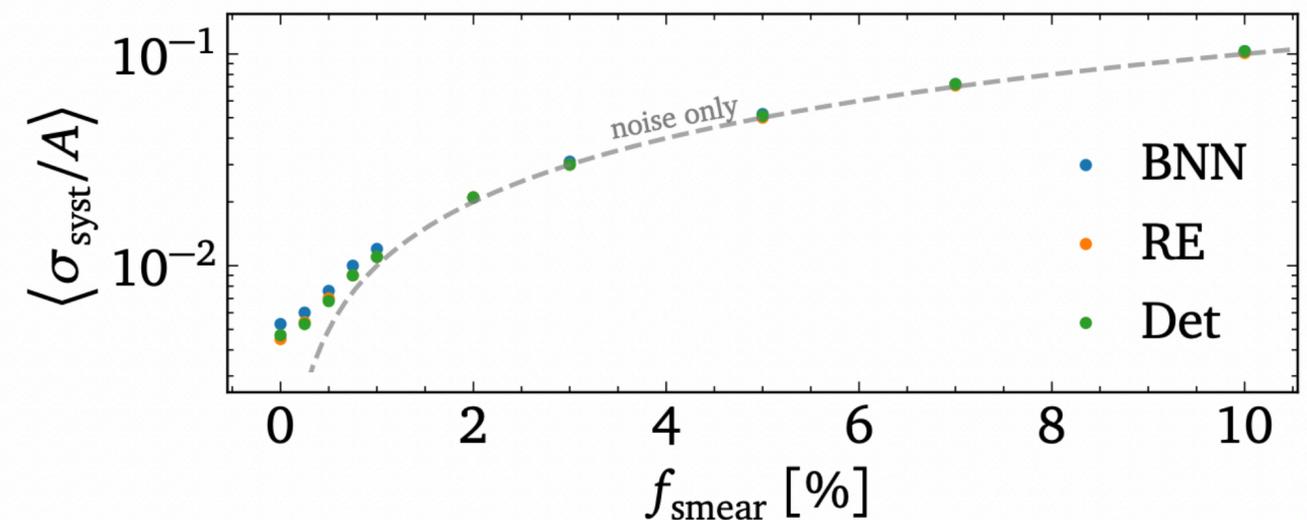
$$p(\theta | x_{\text{train}}) = p(x_{\text{train}} | \theta) \cdot p(\theta) \cdot \text{const}$$

Assume Gaussian likelihood

$$p(x_{\text{train}} | \theta) = \mathcal{N}(y_{\text{true}} | y_{\theta}, \sigma_{\theta})$$

$$-\log p(x_{\text{train}} | \theta) = \frac{|y_j - y_{\theta}(x_j)|^2}{2\sigma_{\theta}^2} + \log \sigma_{\theta}(x_j) + \text{const}$$

**Add artificial noise to check calibration**

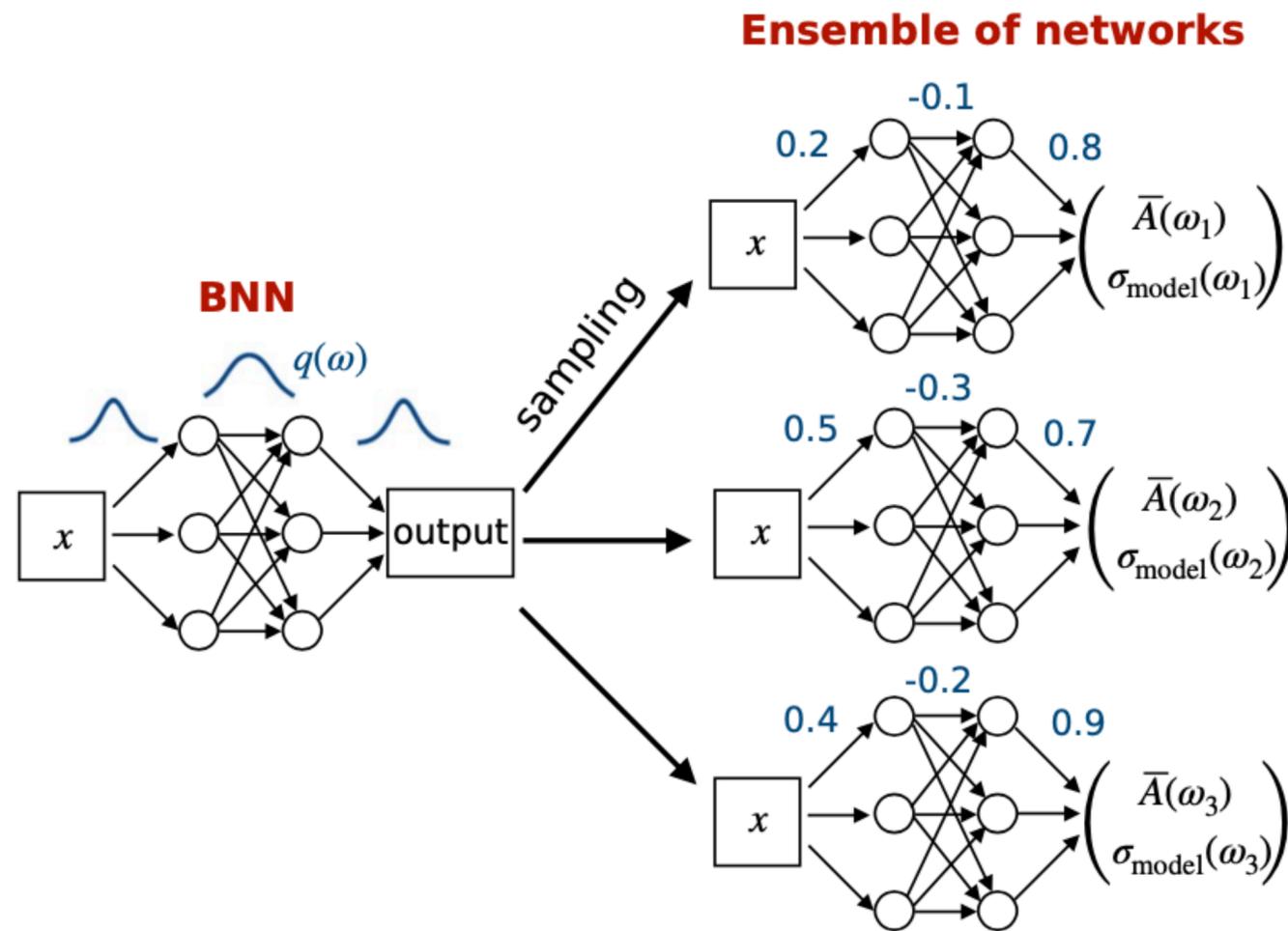


[2412.12069](#) H. Bahl, N. Elmer, L. Favaro, et al.

**Det:** correctly calibrated as long as noise dominates  
Can not cover uncertainty on network parameters

# Separating uncertainties with Bayesian networks

$$p(A) = \int d\omega p(A | \omega) p(\omega | T) \approx \int d\omega p(A | \omega) q(\omega)$$



$$\langle A \rangle(x) = \int d\theta q(\theta) A(x, \theta)$$

$$\begin{aligned} \sigma_{\text{sys}}^2 &= \int d\theta q(\theta) [\bar{A}^2(x, \theta) - \bar{A}(x, \theta)^2] \\ &= \int d\theta q(\theta) \sigma_{\text{model}}(\theta)^2 \end{aligned}$$

→ Captures noise, etc.

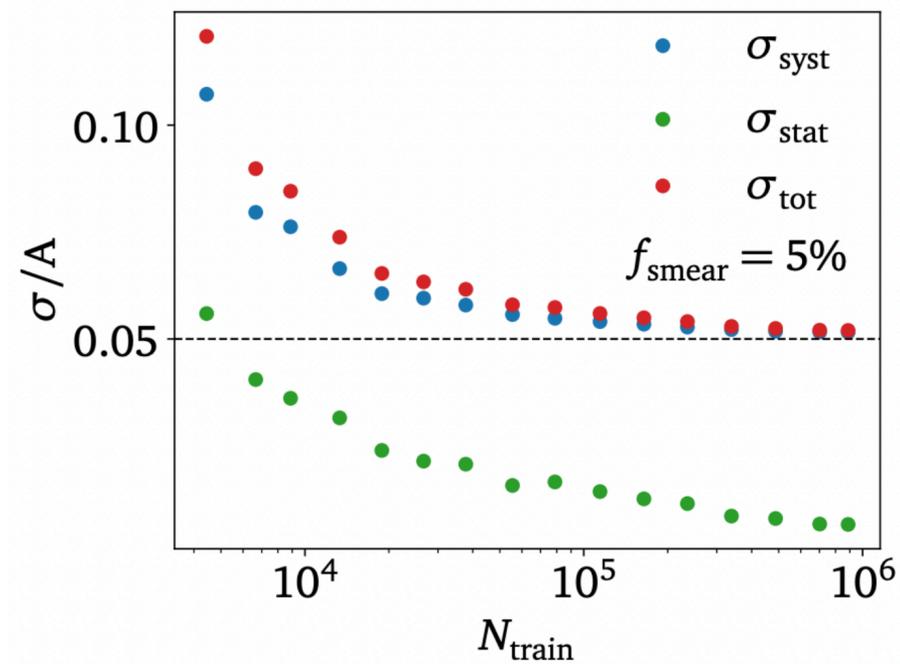
→ Plateaus for large training data

$$\sigma_{\text{stat}}^2 = \int d\theta q(\theta) [\bar{A}(x, \theta) - \langle A \rangle(x, \theta)]^2$$

→ Vanishes for identical weights  
[= in the limit of infinite data]

# Uncertainties from limited training data

[2412.12069](#) H. Bahl, N. Elmer, L. Favaro, et al.



$$\langle A \rangle(x) = \int d\theta q(\theta) A(x, \theta)$$

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→ Captures noise, etc.

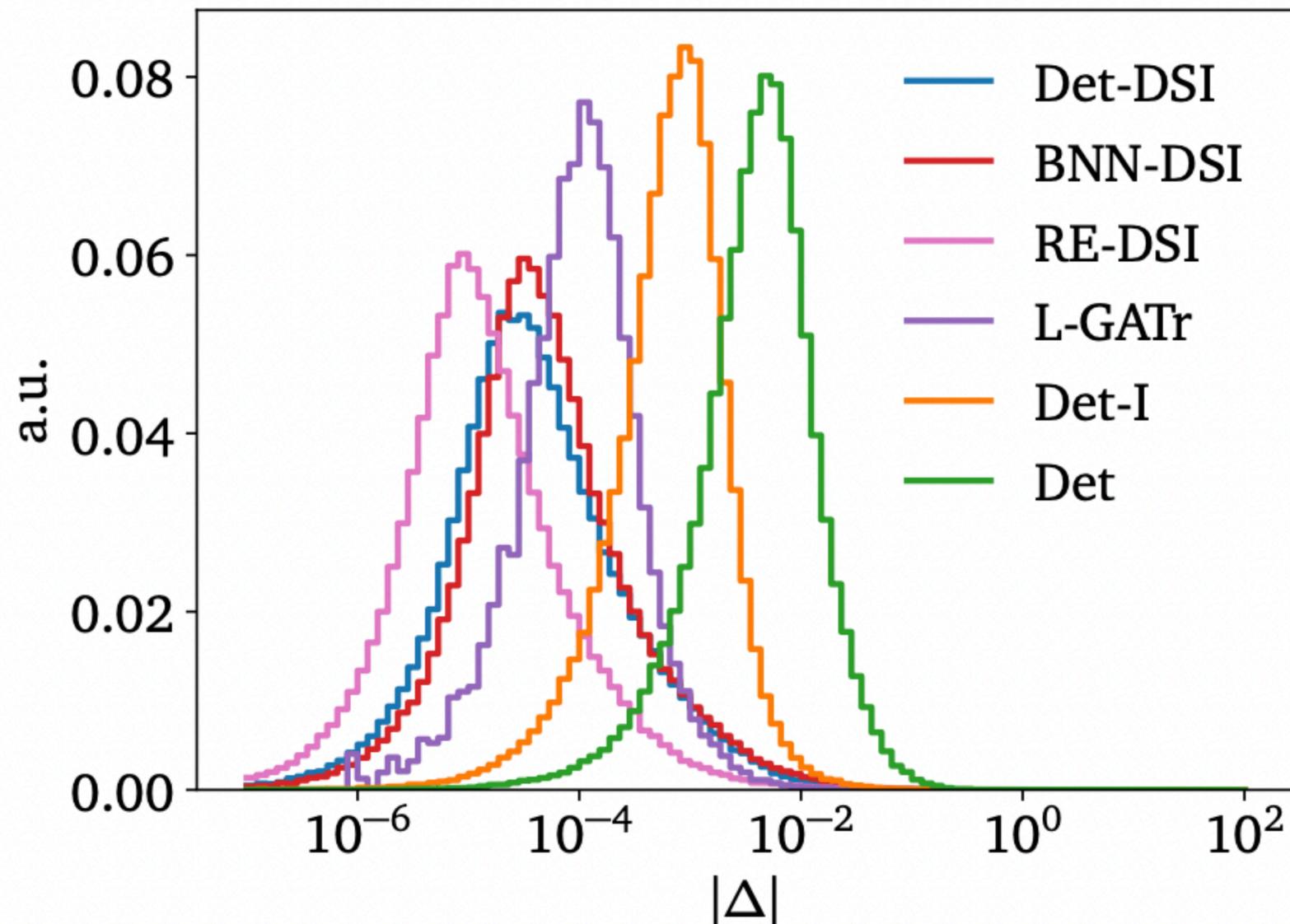
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# What remains? Network size & symmetries (again)

[2412.12069](#) H. Bahl, N. Elmer, L. Favaro, et al.



Optimisation of network architecture

No noise

+ Large dataset

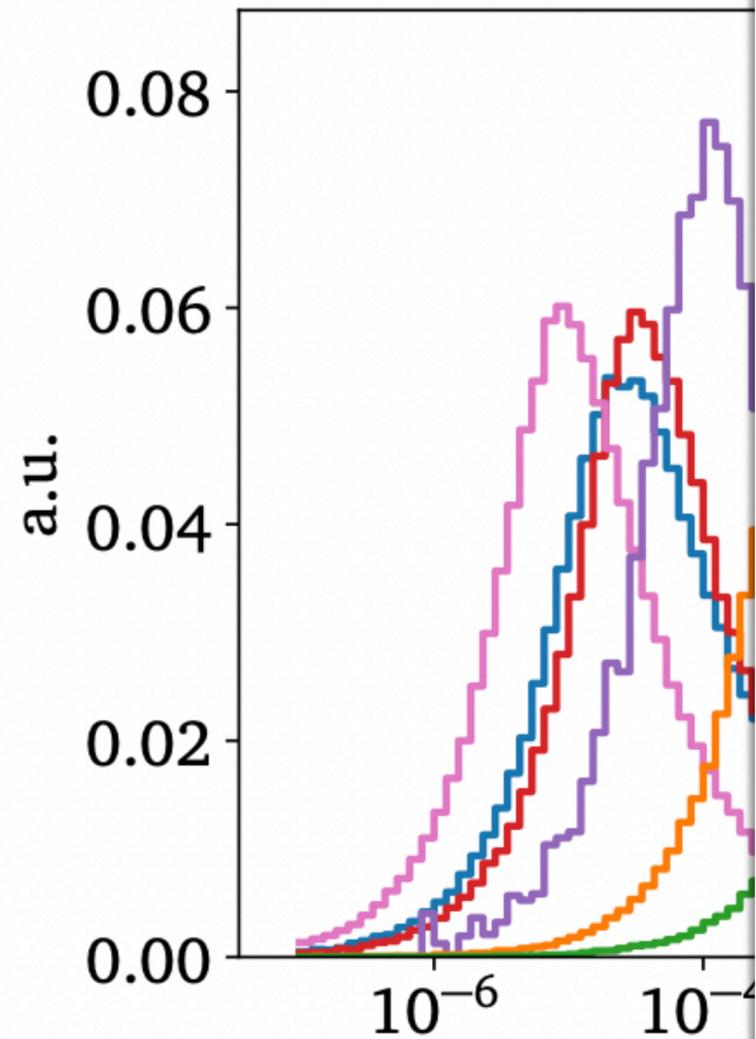
+ Include invariants

+ Deep sets architecture

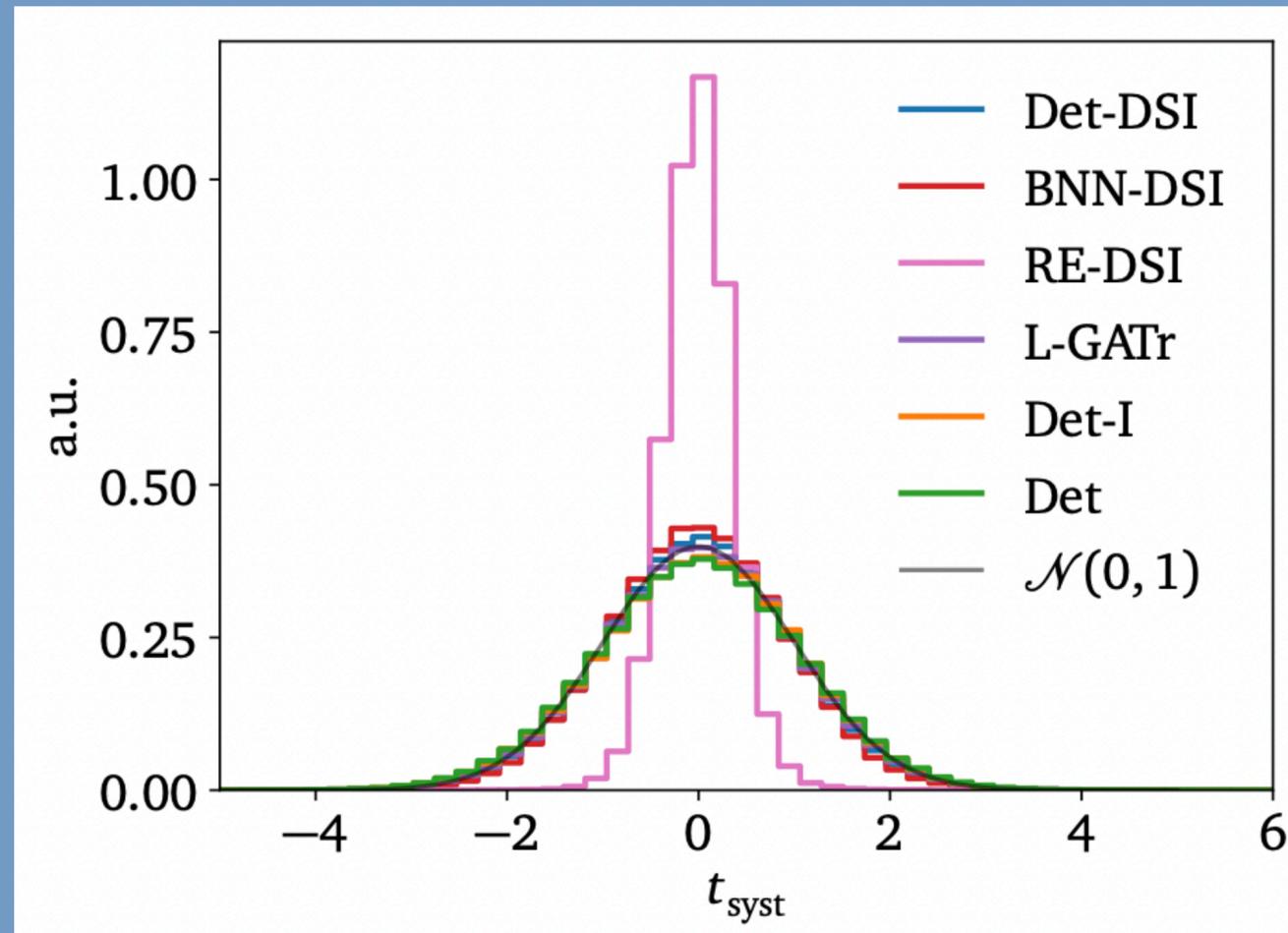
Reaching Precision of  $10^{-5}$  !

# What remains? Network size & symmetries (again)

[2412.12069](#) H. Bahl,



## Calibrated!



network architecture

noise

dataset

invariants

architecture

precision of  $10^{-5}$  !

1. Precision amplitudes

or

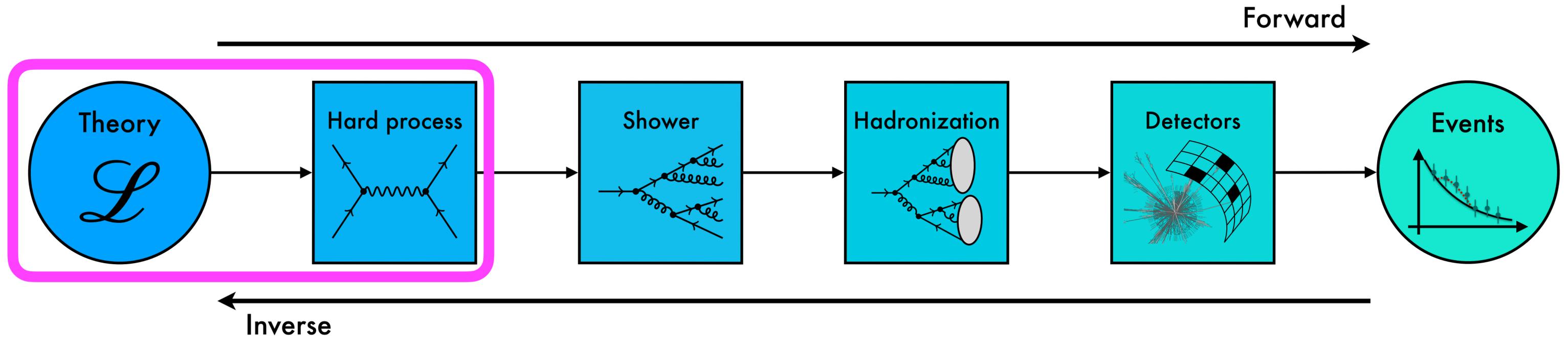
Quantifying uncertainties in regression problems

**2. Event generation**

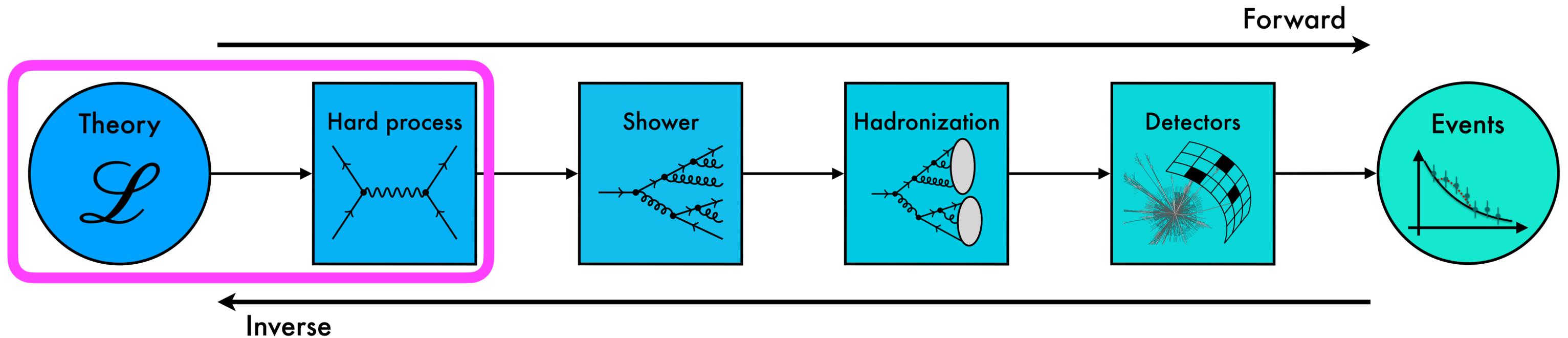
or

**Controlling generative networks**

# Monte Carlo event generation



# Monte Carlo event generation



## 1. Generate

**phase space points**

→ set of four-momenta  $p_i$

## 2. Calculate event weight

$$w_{\text{event}} = f(x_1, Q^2) f(x_2, Q^2) \times |\mathcal{M}(x_1, x_2, p_1, \dots, p_n)|^2 \times J(p_i(r))$$

PDF

Matrix element

Phase space

## 3. Unweighting

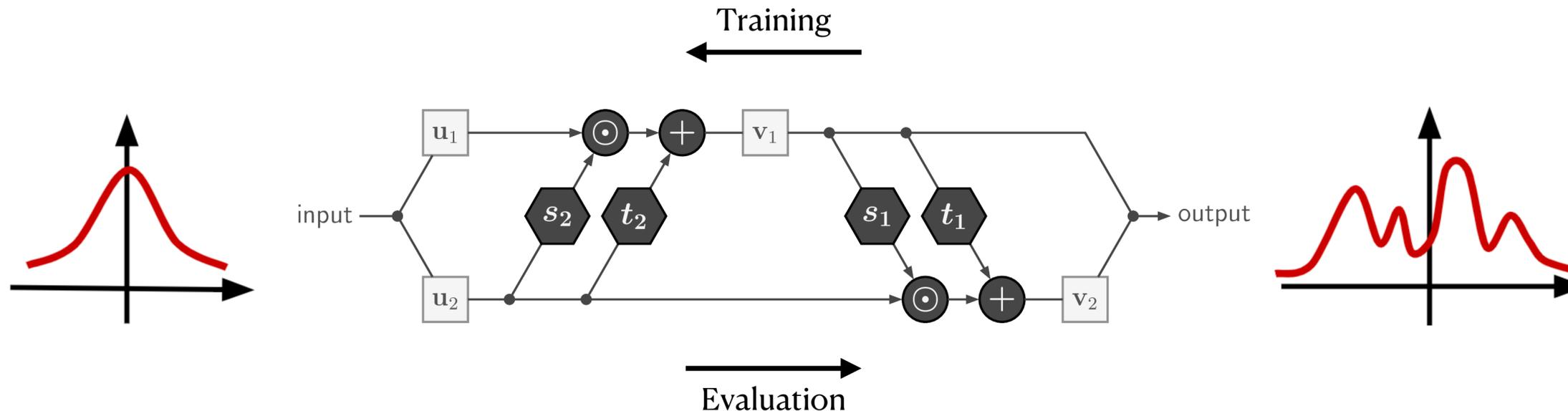
keep events with

$$\frac{w_i}{w_{\text{max}}} > r \in [0,1]$$

# Normalizing flows

## Invertible networks for complex transformations

- + Bijective mapping
- + Tractable Jacobian  $\rightarrow p_x(x) = p_z(z) \cdot J_{NN}$
- + INN  $\rightarrow$  flow with fast evaluation in both direction



Training on density  $t(x)$   
 $\rightarrow$  Minimize difference

$$\begin{aligned}\mathcal{L} &= \log p_x(x)/t(x) \\ &= \log p_z(z(x)) J_{NN} / t(x)\end{aligned}$$

Requires evaluation of  $t(x)$

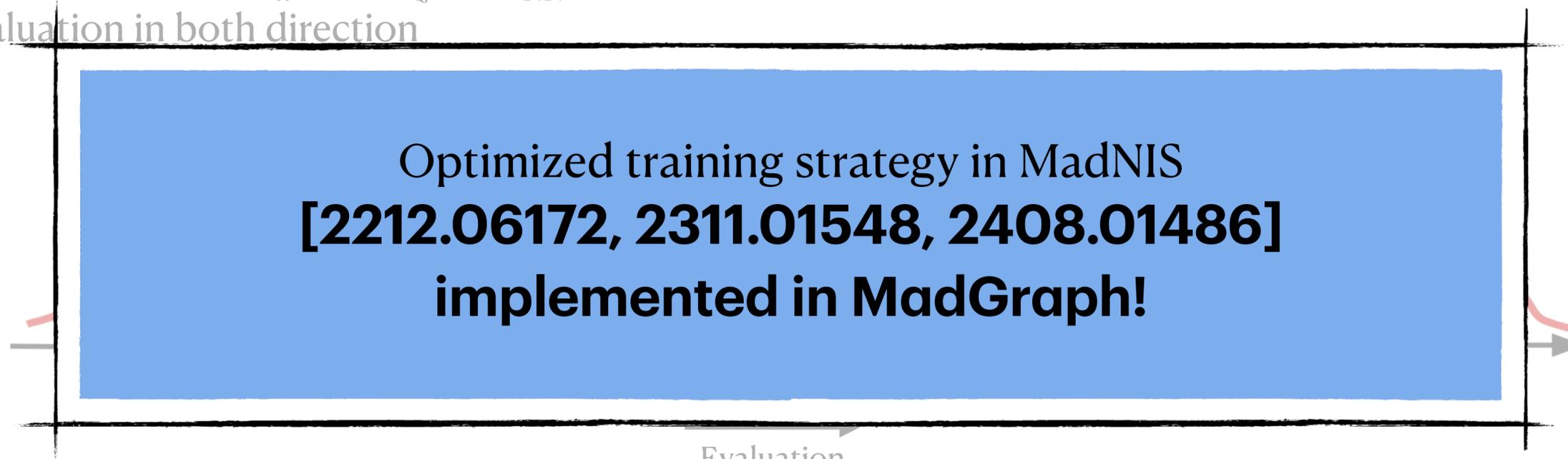
Training on samples  $x$   
 $\rightarrow$  Maximize the log-likelihood

$$\begin{aligned}\mathcal{L} &= \log p(\theta | x) \\ &= \log p(z | \theta) + \log J_{NN} + p(\theta) + \text{const}\end{aligned}$$

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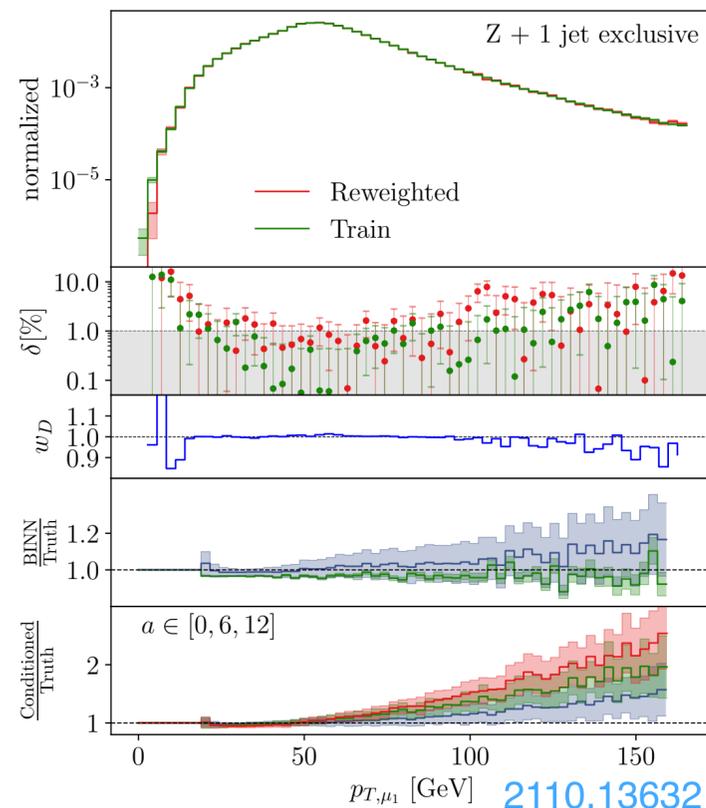
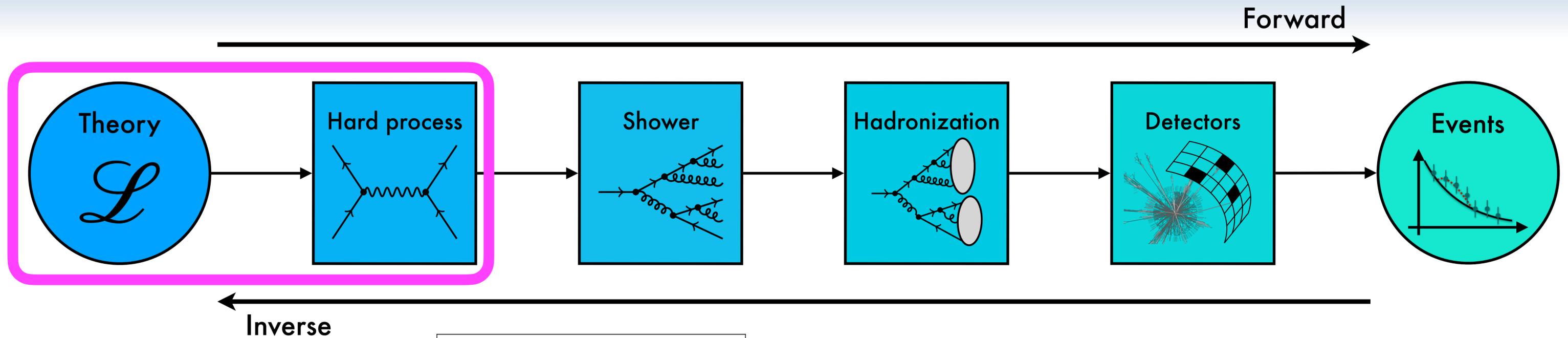
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# Monte Carlo event generation



- Basis: INN, diffusion networks
  - Phase space symmetries in architecture

- Control via classifier  $D$

$$\frac{p_{\text{truth}}(x)}{p_{\text{INN}}(x)} = \frac{D(x)}{1 - D(x)}$$

← ACCURACY

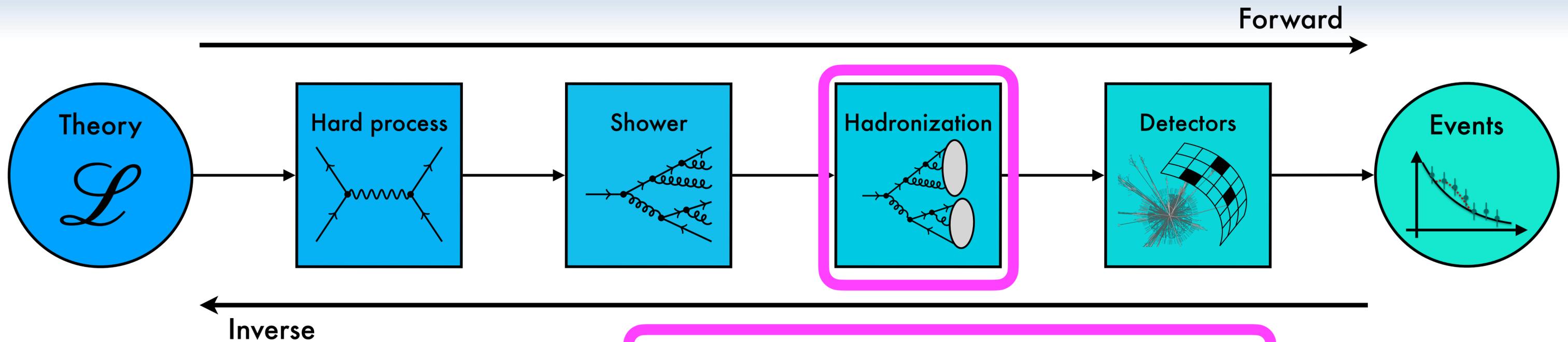
- Accuracy via reweighting

- ➔ Uncertainty estimation via Bayesian NN

← PRECISION

- ➔ Uncertainty propagation via conditioning

# Monte Carlo event generation

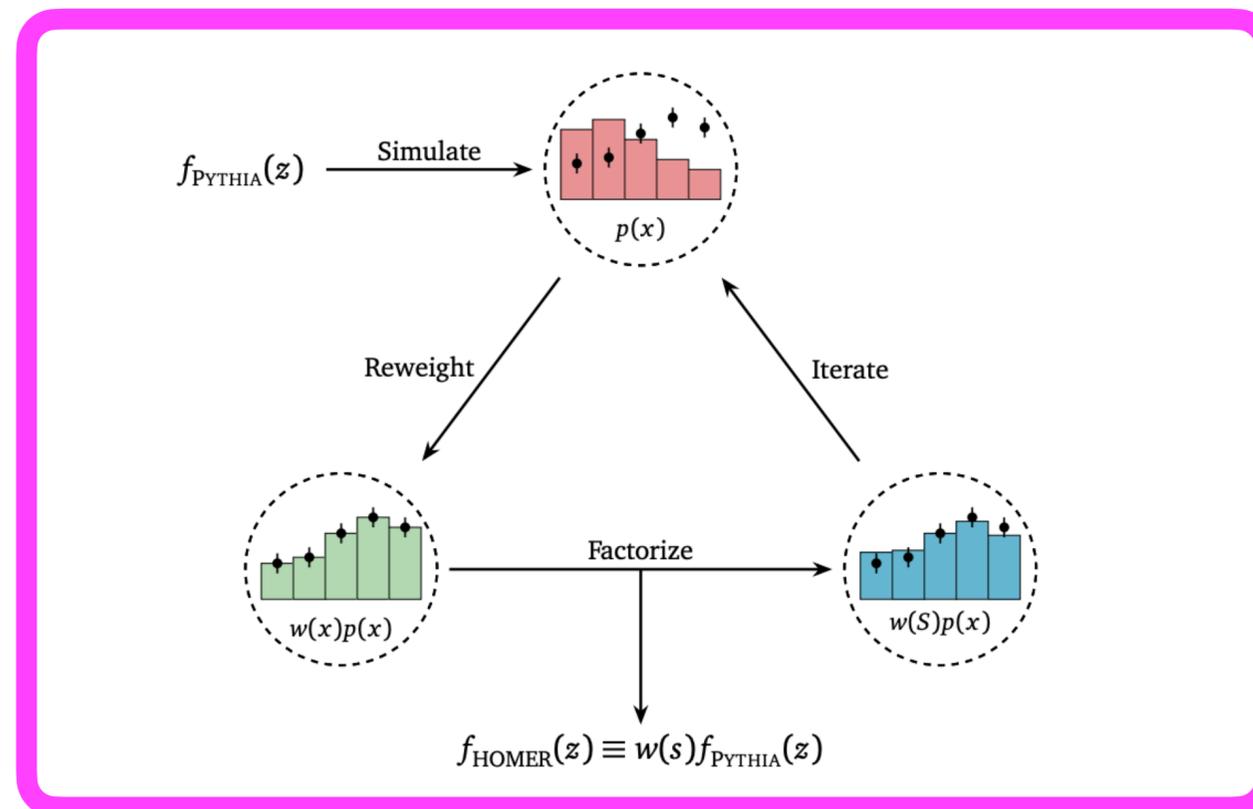


Optimal fragmentation function:

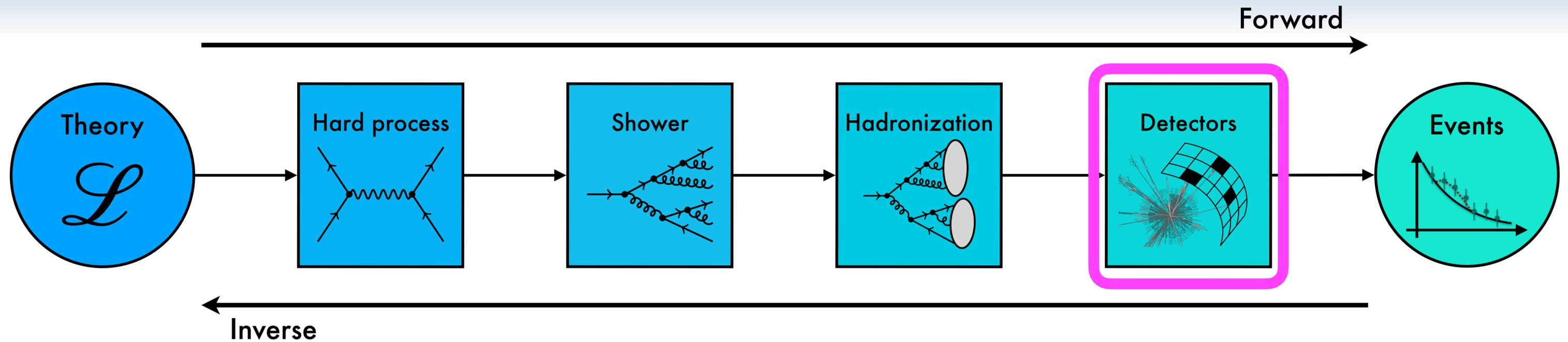
Reweighting PYTHIA to match data

[2509.03592] AB, A. Ore, S. Palacios

Schweitzer, et al.



# Monte Carlo event generation



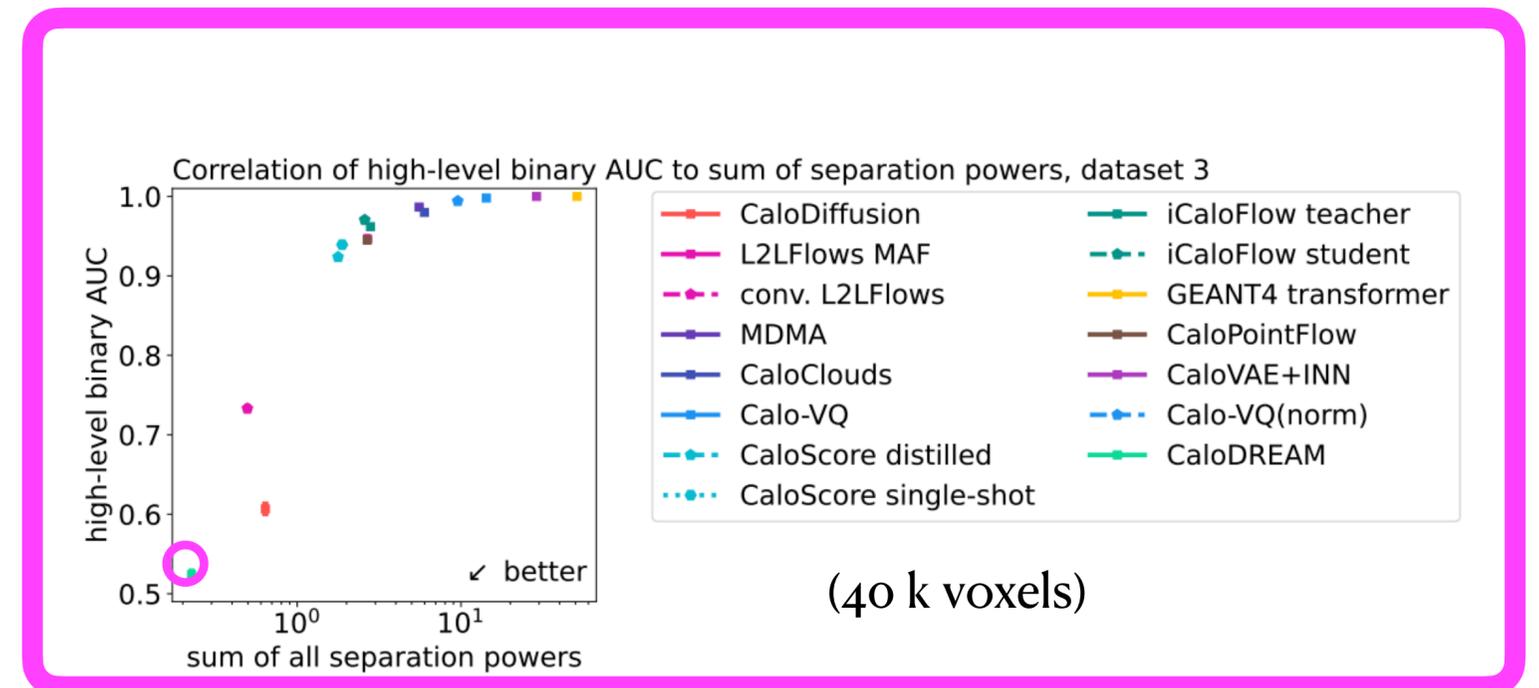
## Efficient detector simulations:

- Transfer concept from phase space generation
- Same networks (diffusion + transformers)
- Challenge: high dimensional

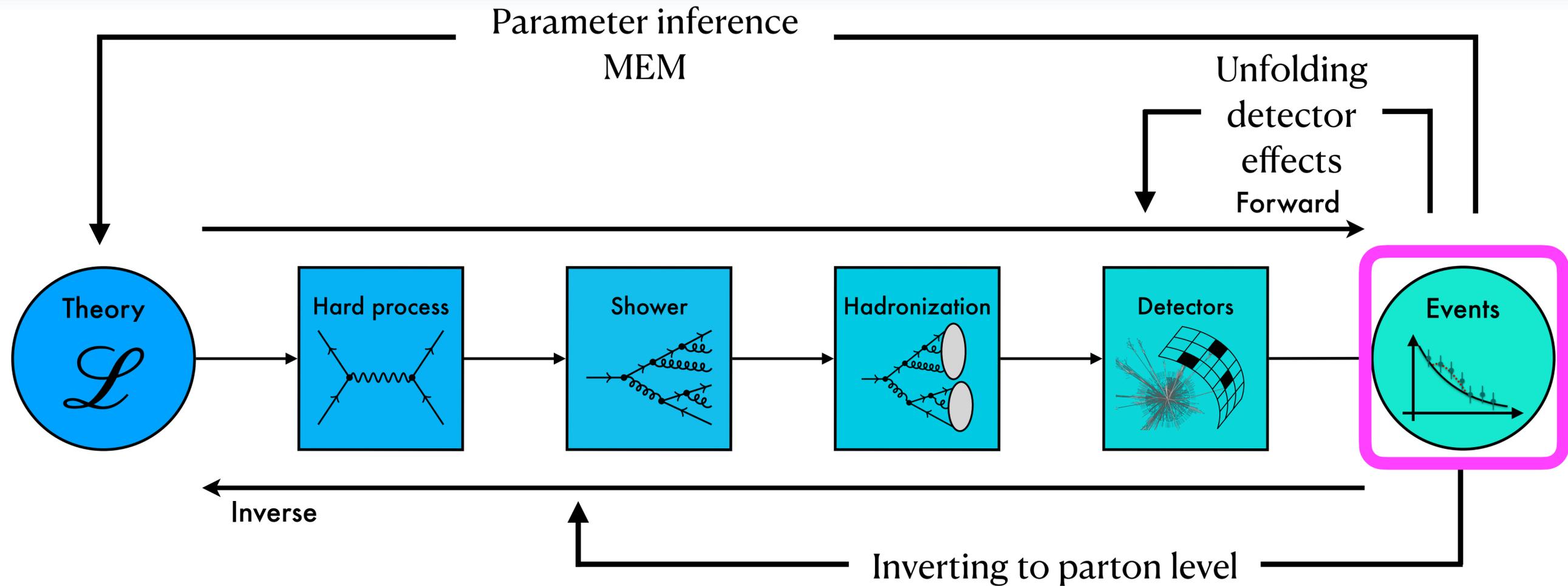
**CaloChallenge 2022** [2410.21611]

CaloDREAM [2405.09629]

L. Favaro, A. Ore, S. Palacios Schweitzer, T. Plehn



# Inverting the simulation chain



- Requirements
- High - dimensional
  - Bin - independent
  - Statistically well defined

1. Precision amplitudes

or

Quantifying uncertainties in regression problems

2. Event generation

or

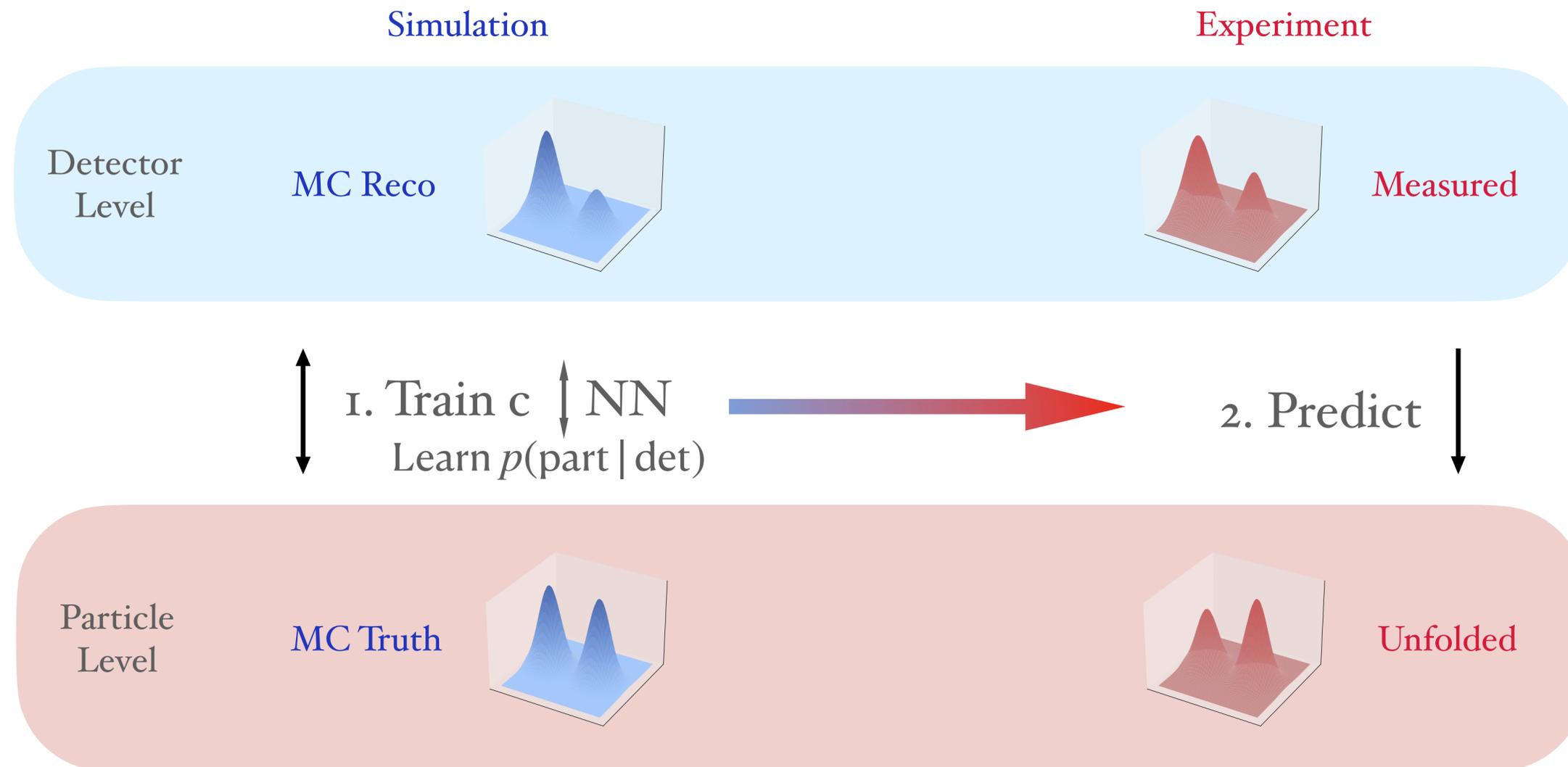
Controlling generative networks

**3. Unfolding new physics**

or

**Overcoming bias in inverse problems**

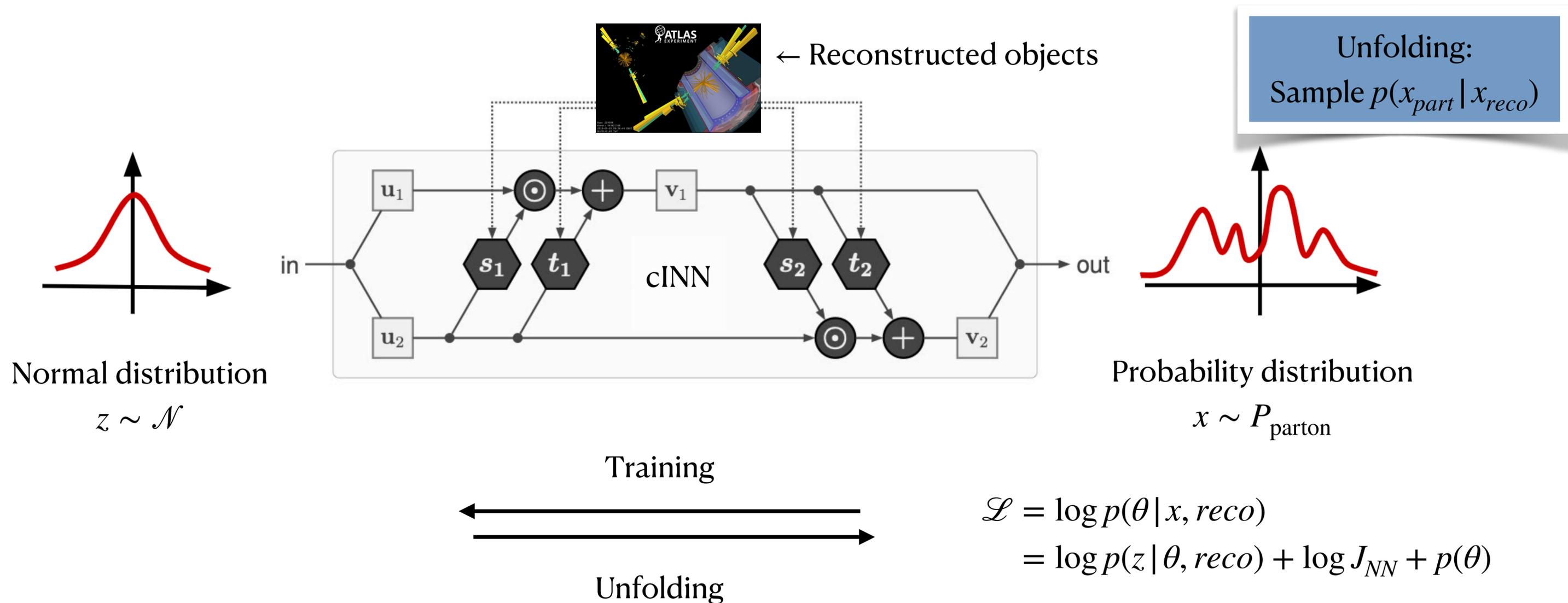
# Generative unfolding methods



# Generative unfolding

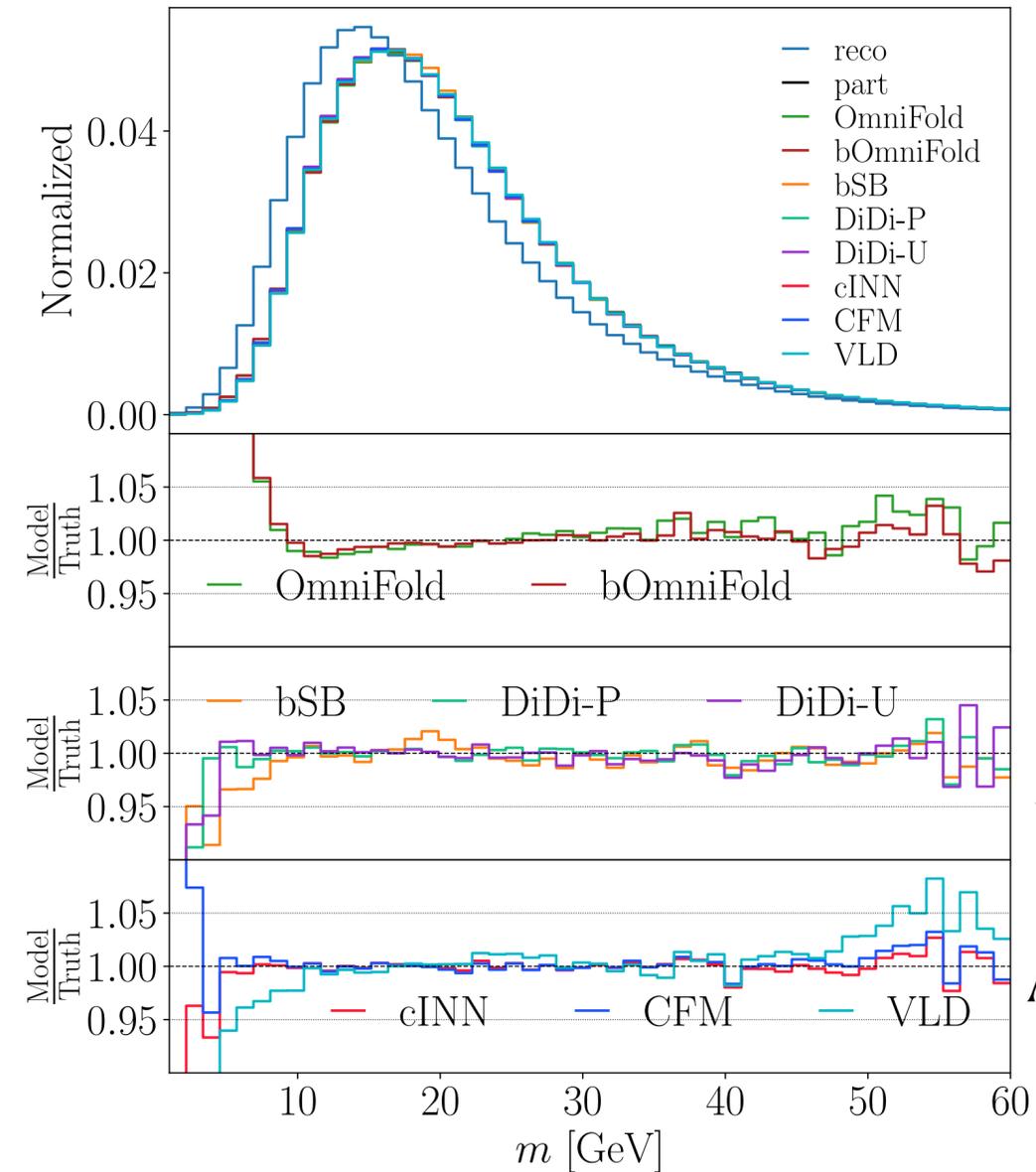
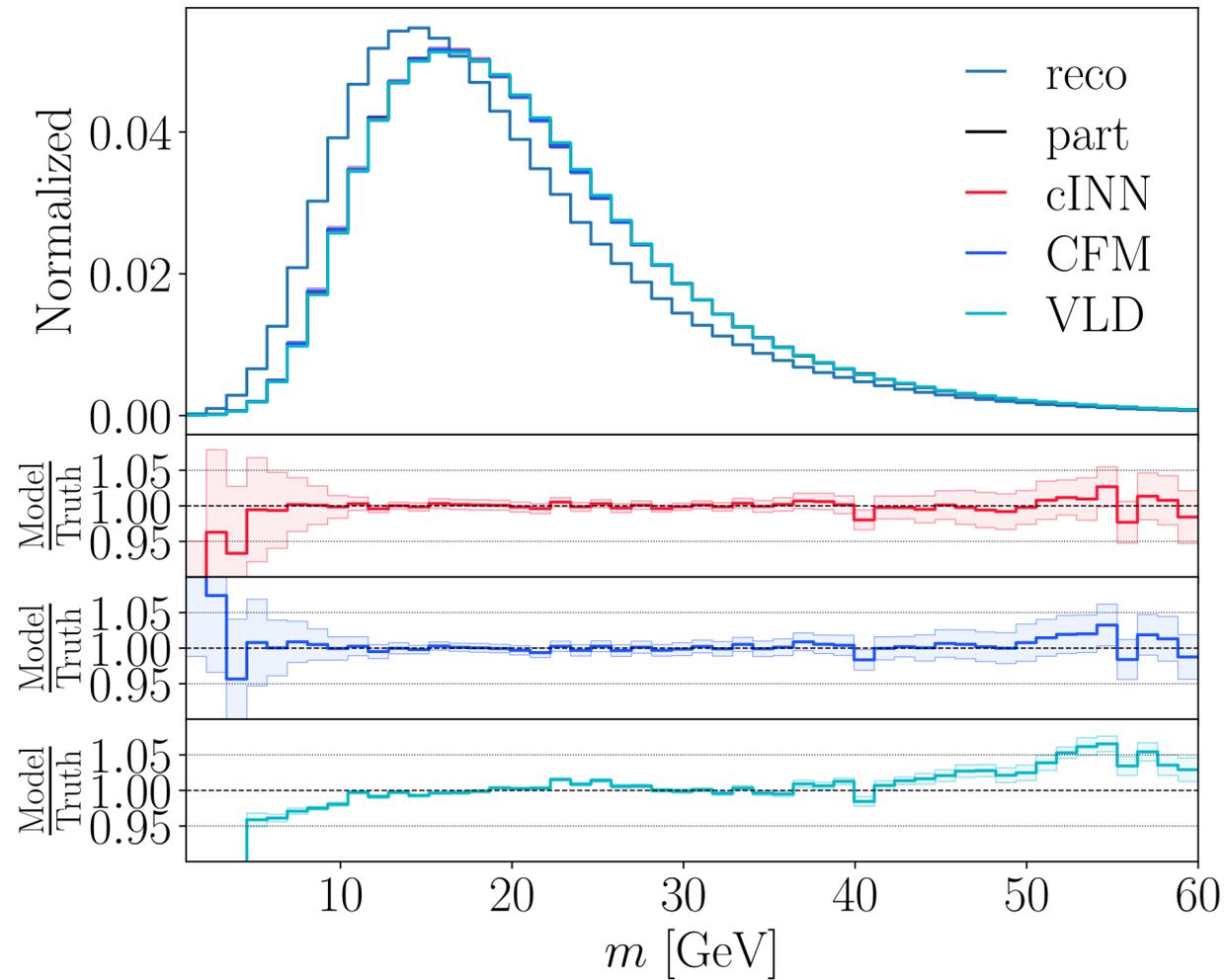
High-dimensional. Bin independent. Robust.

Given a reconstructed event:  
What is the probability distribution at particle level?



# Unfolding $Z$ +jets events

Observables  $m, \tau_{21}, w, N, \log \rho, z_g$



[1911.09107]

A. Andreassen, et al.

[2411.02495]

AB, S. Diefenbacher, et al.

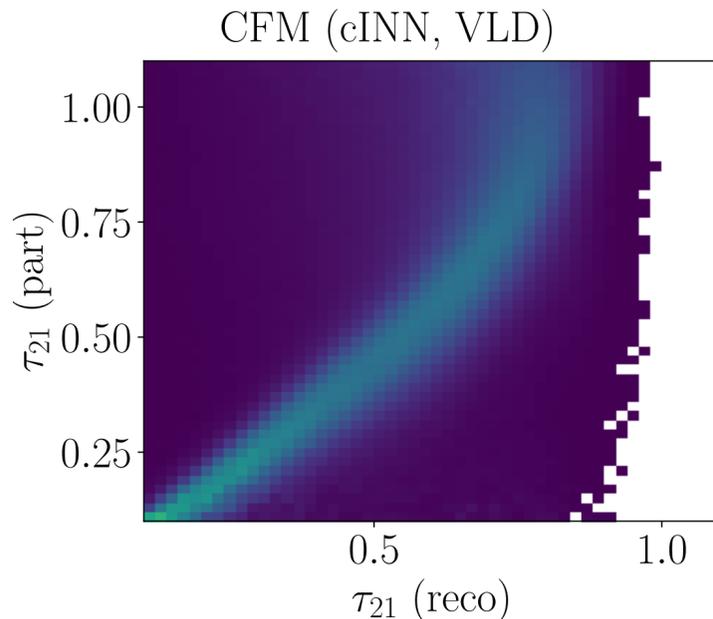
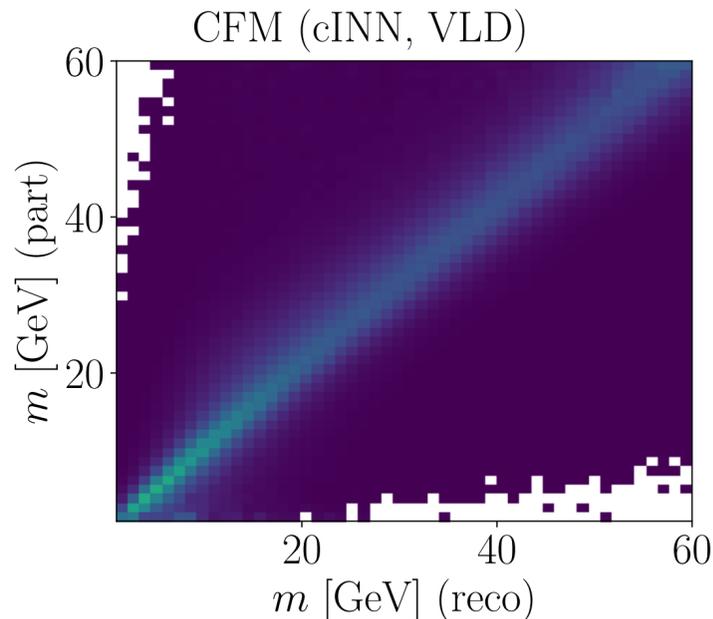
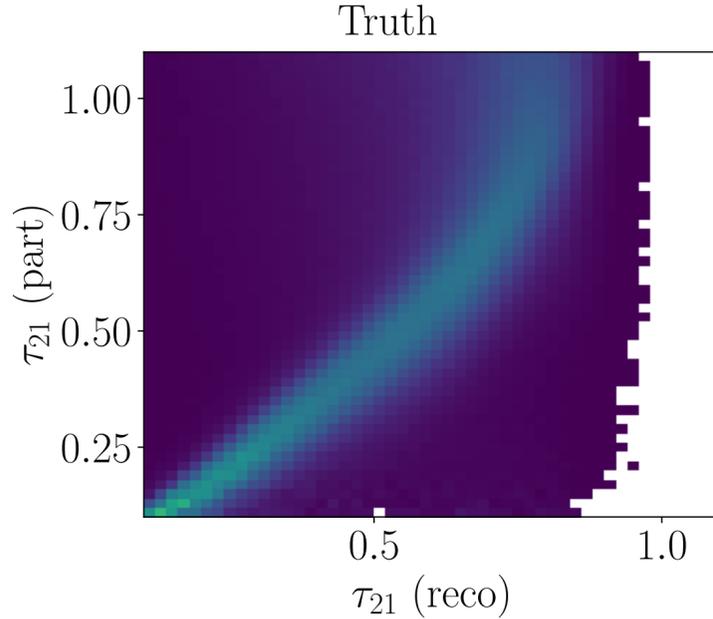
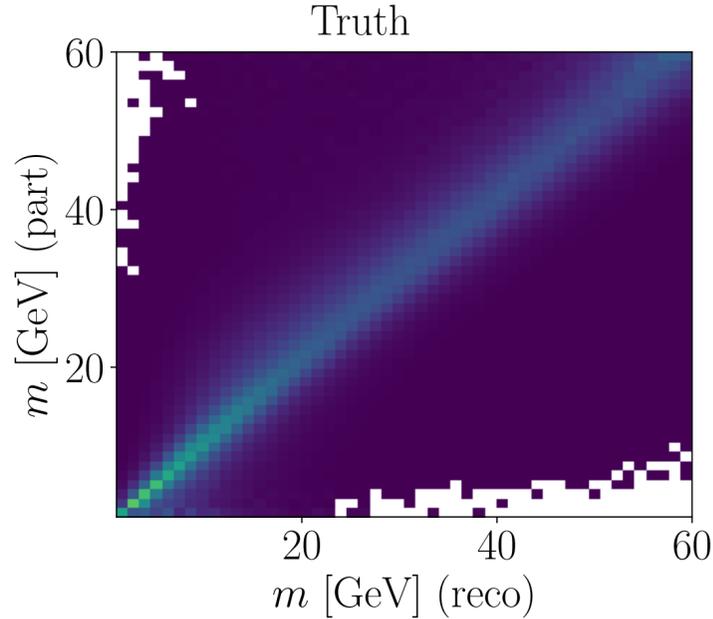
VLD: [2305.10399]

A. Shmakov, K. Greif, et al.

**The Landscape of Unfolding with ML [2404.18807] N. Hütsch, et al.**

# Correlations

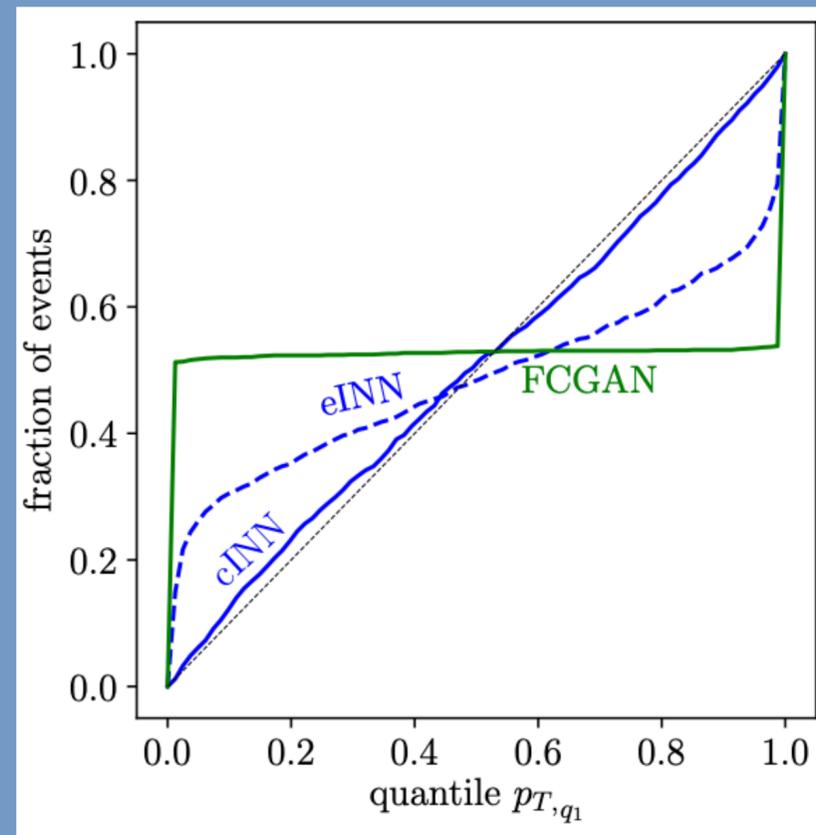
## Z+jets: reco vs particle level, jet mass & subjettiness ratio



# Correlations

**Calibrated!**

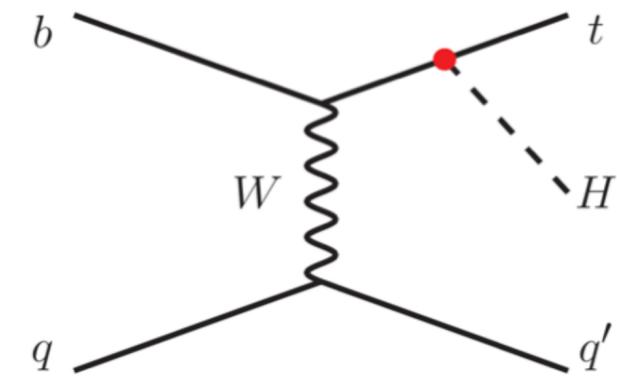
**[2006.06685] M. Bellagente, AB, G. Kasieczka, et al**



**[2404.18807] N. Hütsch, et al.**

# Beyond unfolding: Enabling the MEM

[2210.00019, 2310.07752]



Single Higgs production

with anomalous non-CP conserving Higgs coupling

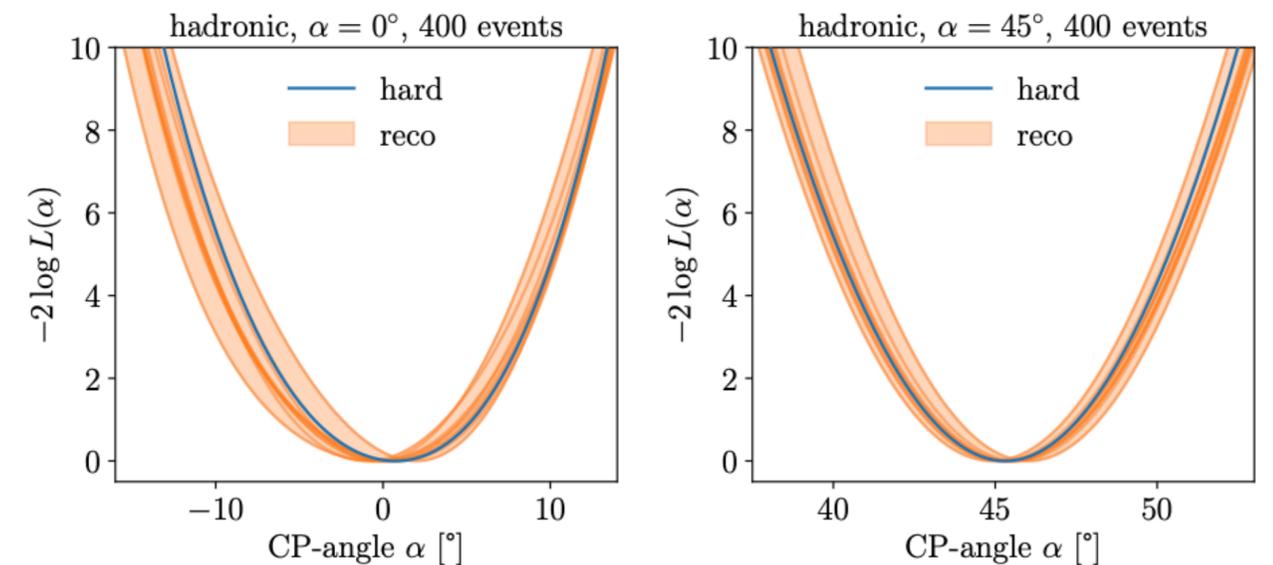
Matrix element method is based on untractable likelihood

$$p(x_{\text{reco}}|\alpha) = \int dx_{\text{hard}} \underbrace{p(x_{\text{hard}}|\alpha)}_{\text{diff. CS}} \underbrace{p(x_{\text{reco}}|x_{\text{hard}}, \alpha)}_{\text{estimate with network}}$$

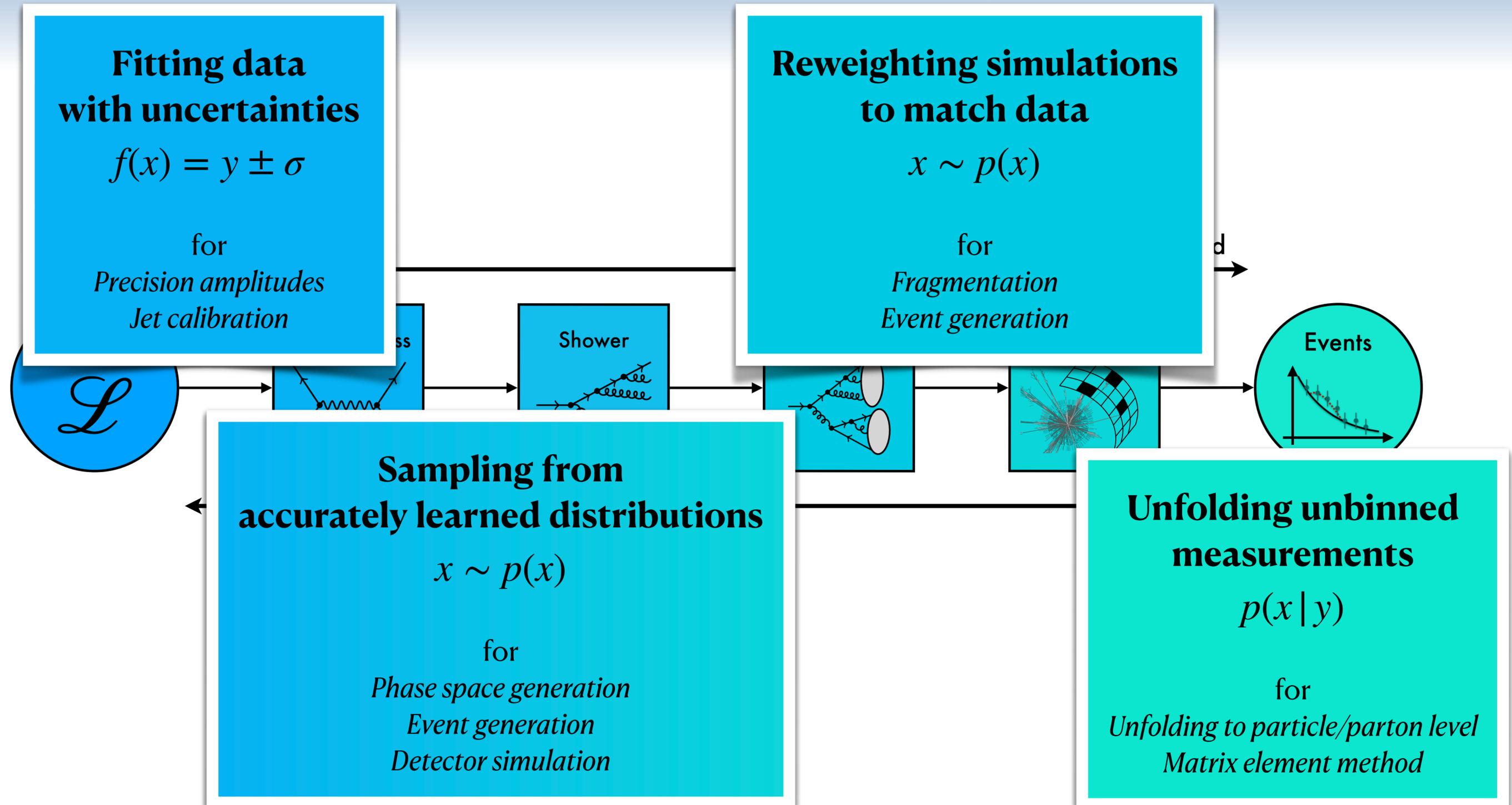
Problem: integration over full phase space of the hard scattering

Solution: Use unfolding cINN to sample  $x_{\text{hard}}$

$$p(x_{\text{reco}}|\alpha) = \left\langle \frac{1}{q(x_{\text{hard}})} p(x_{\text{hard}}|\alpha) p(x_{\text{reco}}|x_{\text{hard}}, \alpha) \right\rangle_{x_{\text{hard}} \sim q(x_{\text{hard}})}$$



# ML enables



# What's next?

# What's next?

## MadAgents

Tilman Plehn<sup>1,2</sup>, Daniel Schiller<sup>1</sup>, and Nikita Schmal<sup>1</sup>

<sup>1</sup> Institut für Theoretische Physik, Universität Heidelberg, Germany

<sup>2</sup> Interdisciplinary Center for Scientific Computing (IWR), Universität Heidelberg, Germany

February 11, 2026

### Abstract

We uncover an effective and communicative set of agents working with MADGRAPH. Agentic installation, learning-by-doing training, and user support provide easy access to state-of-the-art simulations and accelerate LHC research. We show in detail how MADAGENTS interact with inexperienced and advanced users, support a range of simulation tasks, and analyze results. In a second step, we illustrate how MADAGENTS automatize event generation and run an autonomous simulation campaign, starting from a pdf file of a paper.

<https://github.com/heidelberg-hepml/MadAgents>

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Automate repetitive tasks

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Automate repetitive tasks

## Theoretical Physics Benchmark (TPBench) - a Dataset and Study of AI Reasoning Capabilities in Theoretical Physics

Daniel J.H. Chung<sup>1</sup>, Zhiqi Gao<sup>2</sup>, Yurii Kvasiuk<sup>1</sup>, Tianyi Li<sup>1</sup>, Moritz Münchmeyer<sup>1,5</sup>, Maja Rudolph<sup>3</sup>, Frederic Sala<sup>2</sup>, and Sai Chaitanya Tadepalli<sup>4</sup>

<sup>1</sup>Department of Physics, University of Wisconsin-Madison

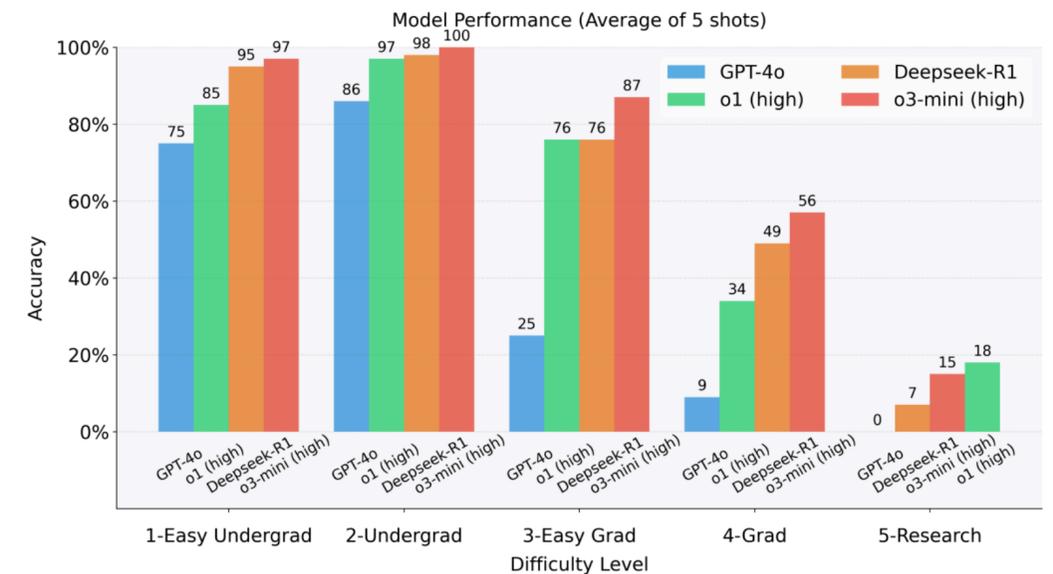
<sup>2</sup>Department of Computer Science, University of Wisconsin-Madison

<sup>3</sup>Data Science Institute (DSI), University of Wisconsin-Madison

<sup>4</sup>Department of Physics, Indiana University, Bloomington

<sup>5</sup>NSF-Simons AI Institute for the Sky (SkAI), Chicago

February 25, 2025



# What's next?

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Tilman Plehn<sup>1,2</sup>, Daniel Schiller<sup>1</sup>, and ...  
<sup>1</sup> Institut für Theoretische Physik, Heidelberg, Germany  
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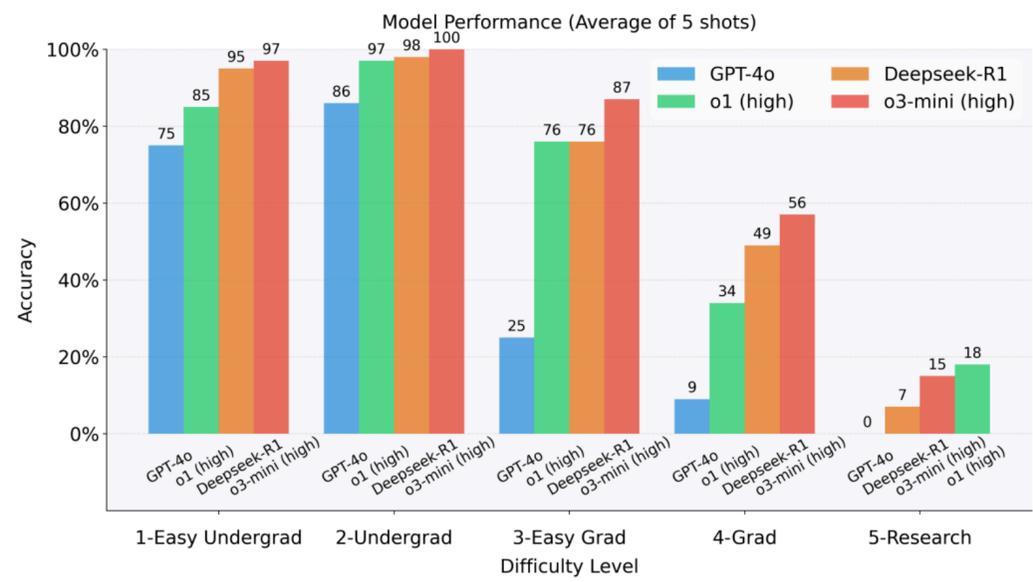
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*Automate repetitive tasks*

Theoretical Physics Benchmark (TPBench) Dataset and Study of AI Reasoning Capabilities in Particle Physics  
Daniel J.H. Chung<sup>1</sup>, Zhiqi Gao<sup>2</sup>, Yu ...  
<sup>1</sup> Department of Physics, University of Wisconsin-Madison  
<sup>2</sup> Department of Physics, University of Wisconsin-Madison  
<sup>3</sup> Data Science Institute, University of Wisconsin-Madison  
... Indiana University, Bloomington  
... Institute for the Sky (SkAI), Chicago

February 25, 2025

*Reasoning at student level*



# What's next?

**MadAgents**

Tilman Plehn<sup>1,2</sup>, Daniel Schiller<sup>1</sup>, and ... hmal<sup>1</sup>

1 Institut für Theoretische Physik, Heidelberg, Germany  
2 Interdisciplinary Center for Scientific Computing, Heidelberg, Germany

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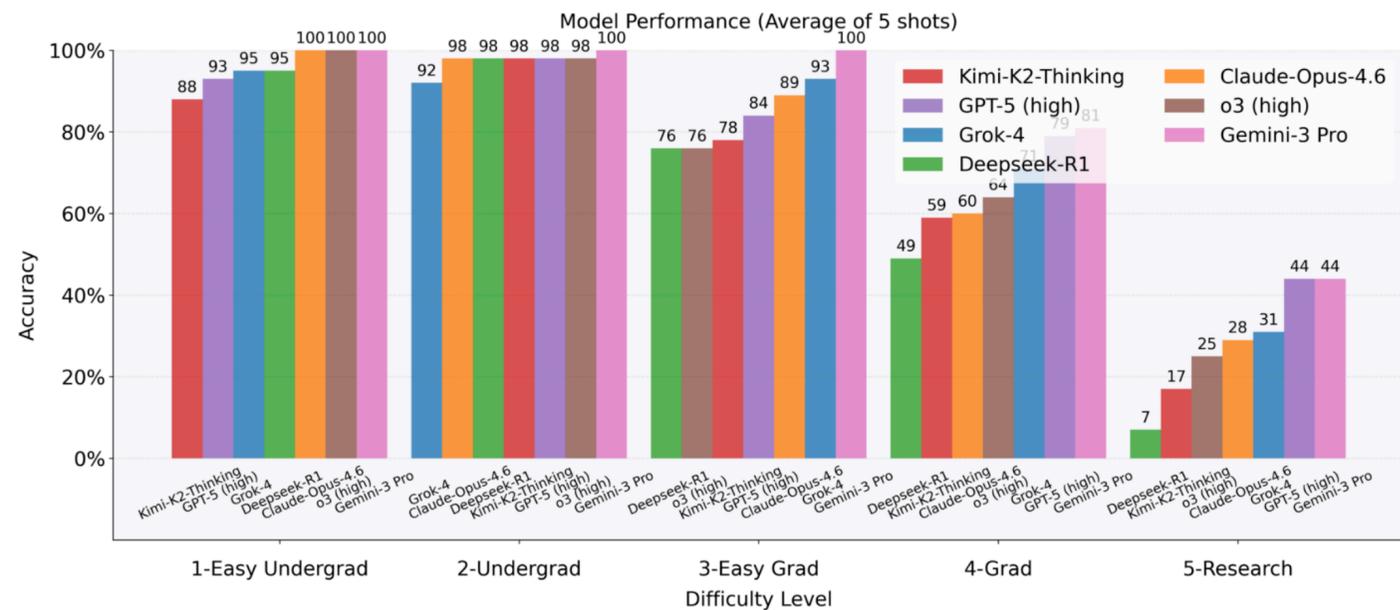
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1Department ... Wisconsin-Madison  
2Department ... University of Wisconsin-Madison  
3Data ... University of Wisconsin-Madison  
4 ... Indiana University, Bloomington  
5 ... Institute for the Sky (SkAI), Chicago

February 25, 2025

Reasoning at student level



# What's next?

**MadAgents**

Tilman Plehn<sup>1,2</sup>, Daniel Schiller<sup>1</sup>, and ... hmal<sup>1</sup>

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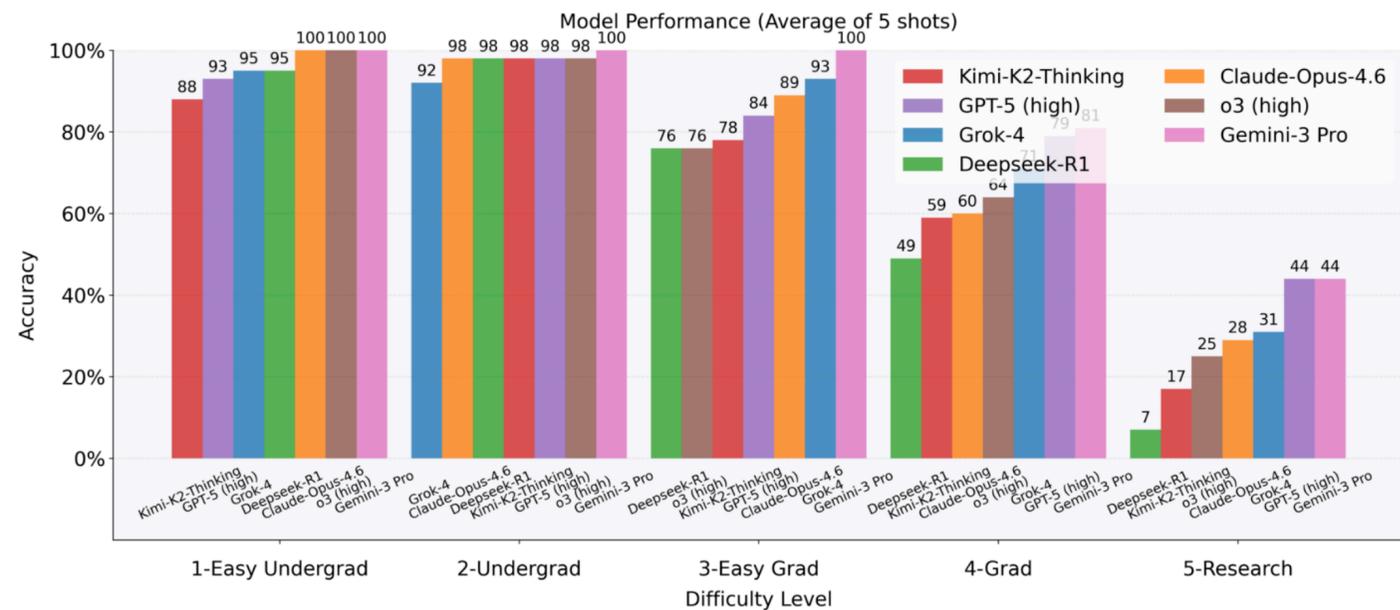
Theoretical Physics Benchmark (TPBench) and Study of AI Reasoning Capabilities in Physics

Daniel J.H. Chung<sup>1</sup>, Zhiqi Gao<sup>2</sup>, Yu ... Münchmeyer<sup>1,5</sup>, Maja Rudolph<sup>3</sup>, Frederic ... Tadepalli<sup>4</sup>

1Department ... Wisconsin-Madison  
2Department ... University of Wisconsin-Madison  
3Data ... University of Wisconsin-Madison  
4 ... Indiana University, Bloomington  
5 ... Institute for the Sky (SkAI), Chicago

February 25, 2025

2026 Reasoning at researcher level



# What's next?

Tilman Plehn<sup>1,2</sup>  
 1 Institut für Theoretische Physik  
 2 Interdisciplinary Center for Science and Technology

## Abstract

We uncover an agentic workflow for automated research. Agentic installations, using-by-default state-of-the-art simulations and AI assistants, interact with inexperienced researchers on tasks, and analyze results. In a series of experiments, we demonstrate event generation and run an automated workflow for the production of a paper.

<https://github.com/heidelberg-hep/ai-research-assistant>

Automated

## Resummation of the C-Parameter Sudakov Shoulder Using Effective Field Theory

Matthew D. Schwartz<sup>1,2</sup>

<sup>1</sup>Department of Physics, Harvard University, Cambridge, MA 02138, USA

<sup>2</sup>Institute for Artificial Intelligence and Fundamental Interactions (IAIFI)

[schwartz@g.harvard.edu](mailto:schwartz@g.harvard.edu)

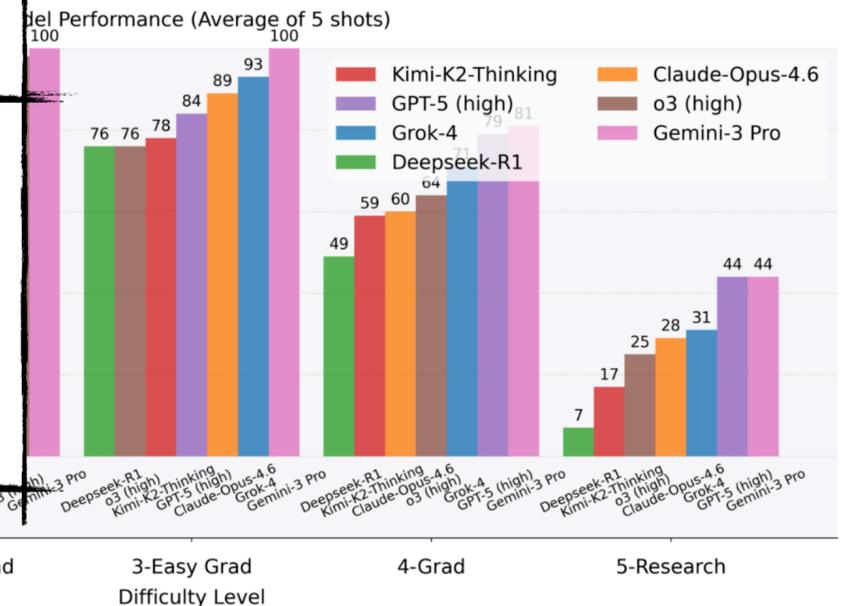
AI RESEARCH ASSISTANT: Claude Opus 4.5 (Anthropic)

January 7, 2026

## Author Contributions

M.D.S. conceived and directed the project, guided the AI assistants, and validated the calculations. Claude Opus 4.5, an AI research assistant developed by Anthropic, performed all calculations including the SCET factorization theorem derivation, one-loop soft and jet function calculations, EVENT2 Monte Carlo simulations, numerical analysis, figure generation, and manuscript preparation. The work was conducted using Claude Code, Anthropic's agentic coding tool. M.D.S. is fully responsible for the scientific content and integrity of this paper.

Benchmark (TPBench) and Study of Capabilities in Physics  
 b<sup>2</sup>, Yury... Münchmeyer<sup>1,5</sup>, Maja... Tadepalli<sup>4</sup>  
 Wisconsin-Madison  
 University of Wisconsin-Madison  
 University of Wisconsin-Madison  
 Indiana University, Bloomington  
 Institute for the Sky (SkAI), Chicago  
 February 25, 2025



# What's next?

Tilman Plehn<sup>1,2</sup>  
 1 Institut für Theoretische Physik  
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**Abstract**

We uncover an... con...  
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<https://github.com/heidelberg-hep>

Automated

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schwartz@physics.harvard.edu

AI RESEARCH ASSISTANT Claude Opus 4.5 (Anthropic)

February 25, 2025

AI research assistant?

### Author Contribution

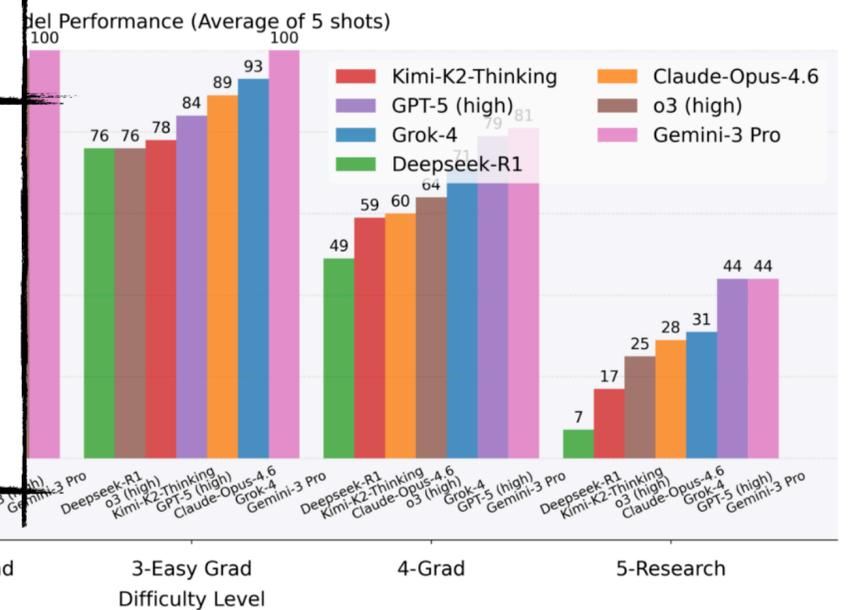
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Benchmark (TPBench) and Study of Capabilities in Physics

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February 25, 2025

Coming at researcher level



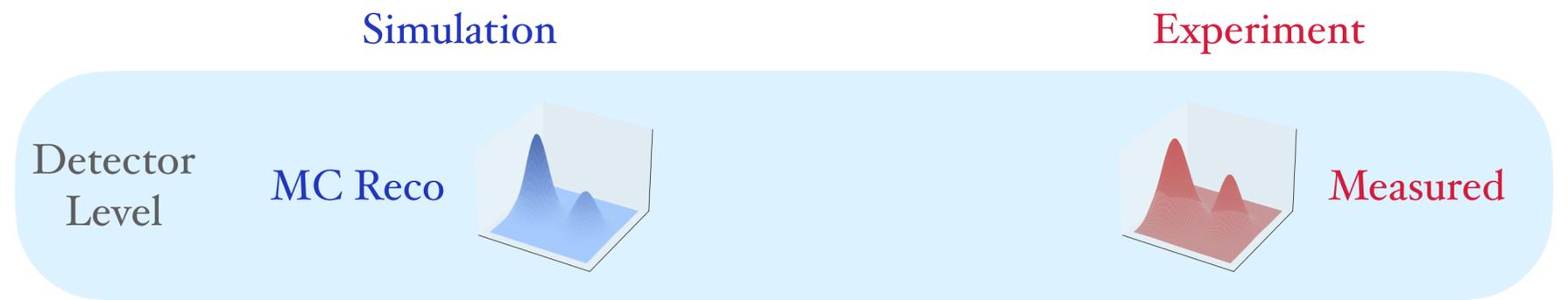
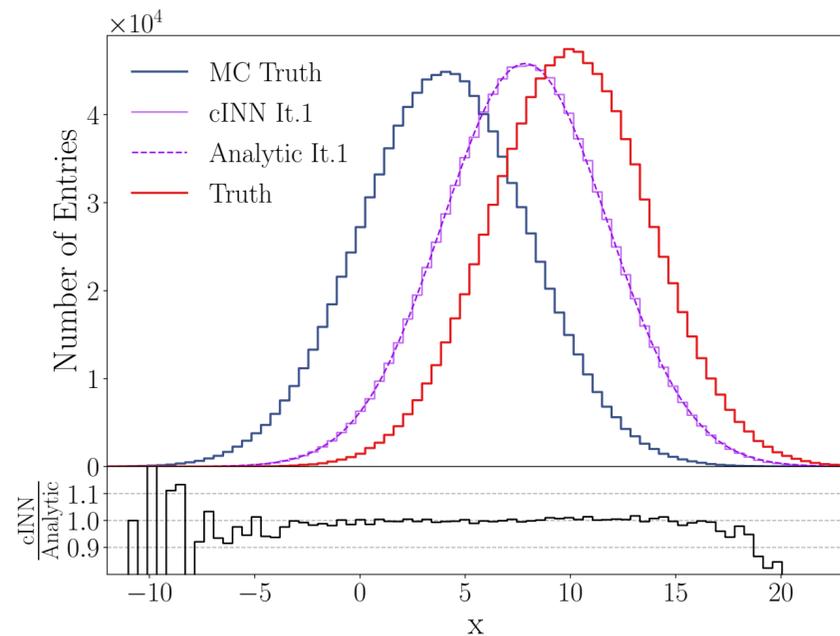
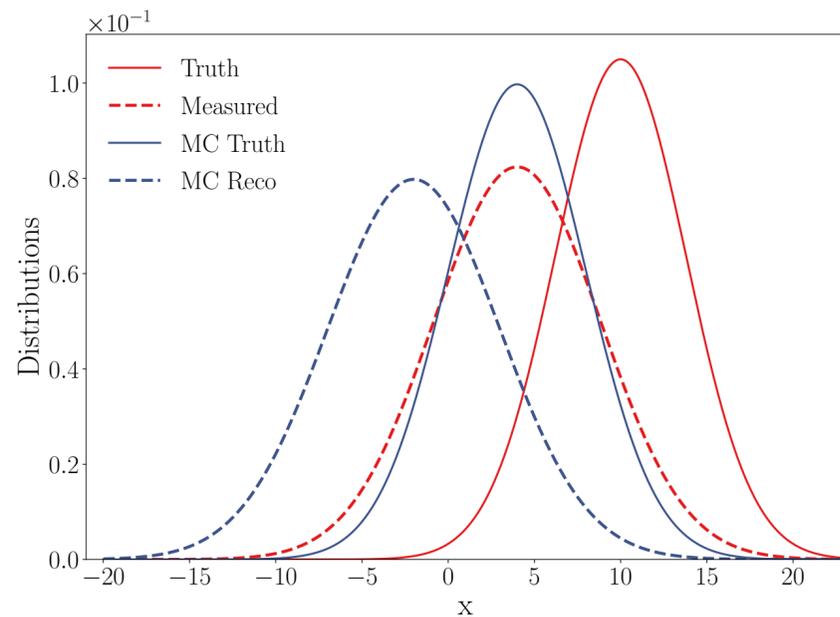
*If everything is uncertain,*

*anything is possible*

*Margaret Drabble*

# Limitations of direct unfolding with generative NNs

## Prior dependence



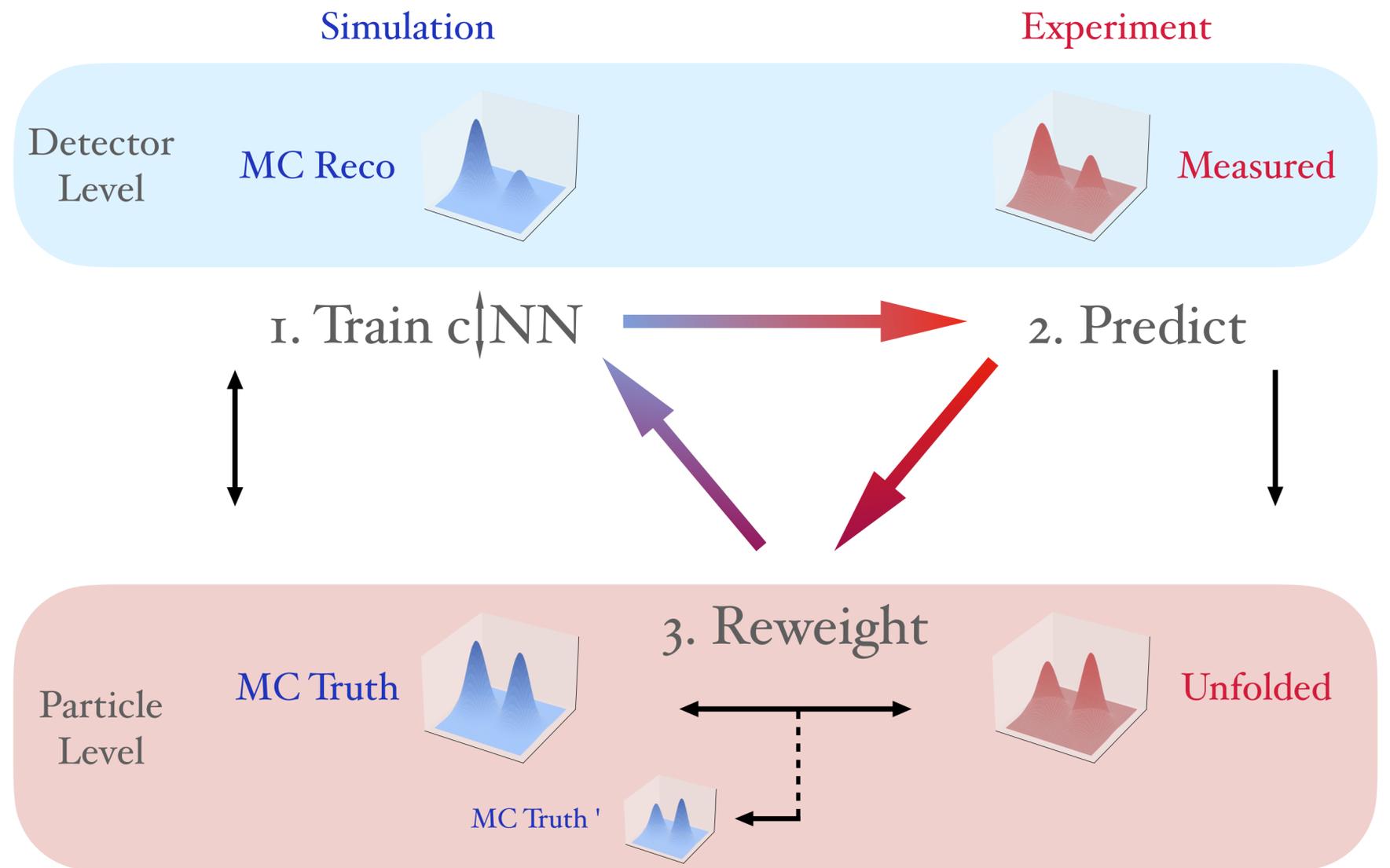
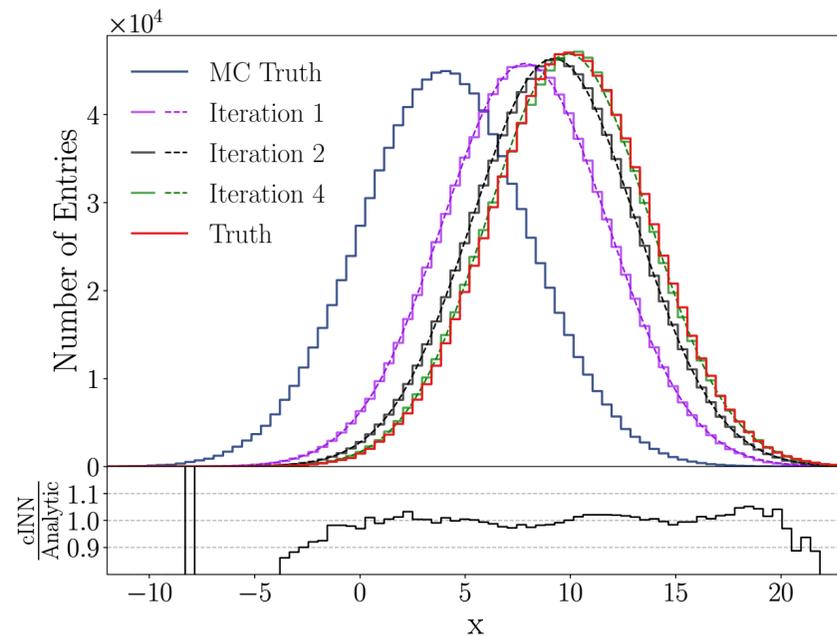
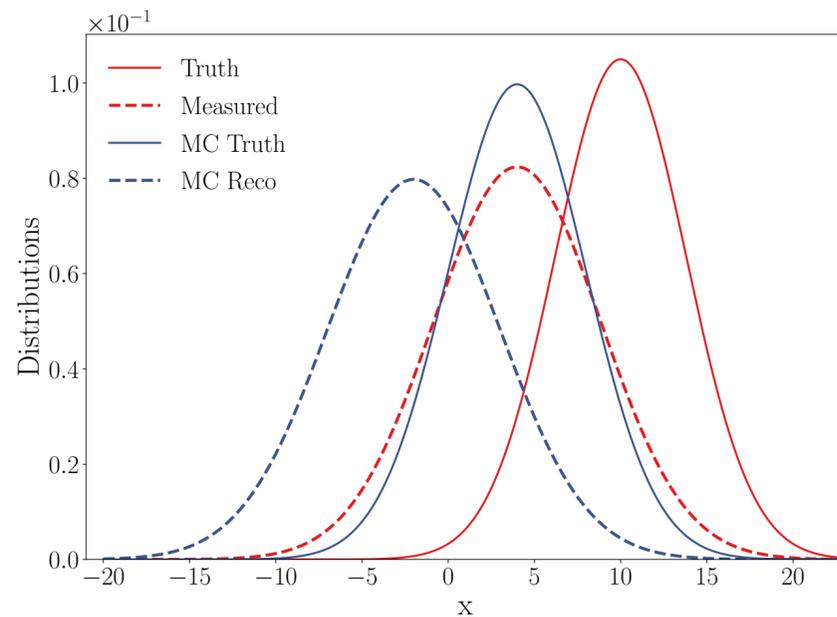
1. Train  $c|NN$   $\longrightarrow$  2. Predict



$$p(\text{part} | \text{det}) = \frac{p(\text{det} | \text{part}) \cdot p(\text{part})}{p(\text{det})}$$

# Conditional iterative unfolding

[2212.08674] M. Backes, et al.



# SPINUP

## Simulation-Prior Independent Neural Unfolding Procedure

[2507.15084] AB, T Heime1 , N. Huetsch1 , M. Kagan, T. Plehn

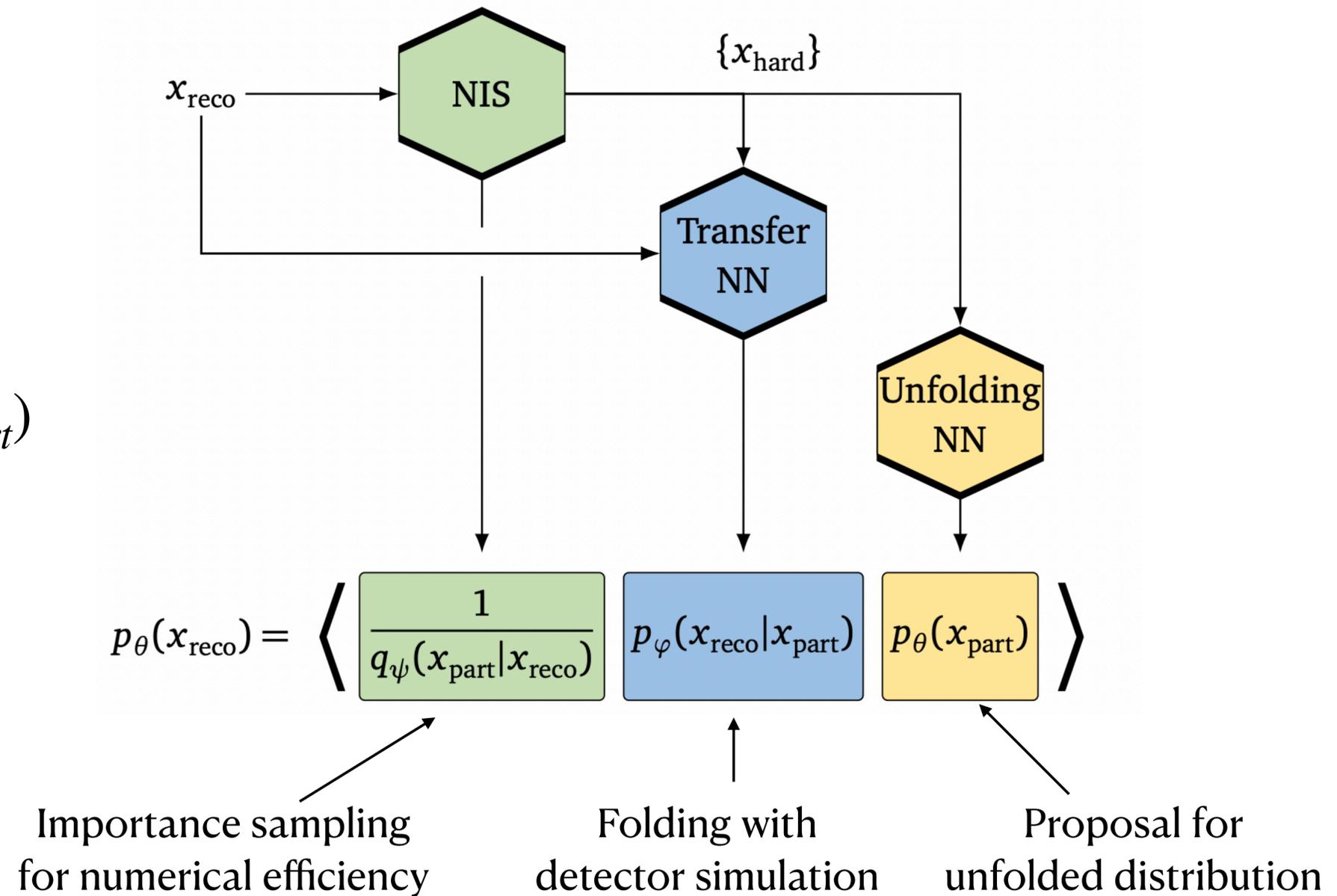
Ansatz

DATA

“folded” unfolded distribution

$$\begin{aligned} P_{data}(x_{reco}) &= P_{\theta}(x_{reco}) \\ &= \int dx_{part} P(x_{reco} | x_{part}) P_{\theta}(x_{part}) \end{aligned}$$

→ Minimize KL divergence



# SPINUP

## Simulation-Prior Independent Neural Unfolding Procedure

Ensembling for lower bound on uncertainty from information loss

Drastic example:

Forward mapping  $x_{reco} = |x_{part}| + \mathcal{N}(0, 0.2)$

