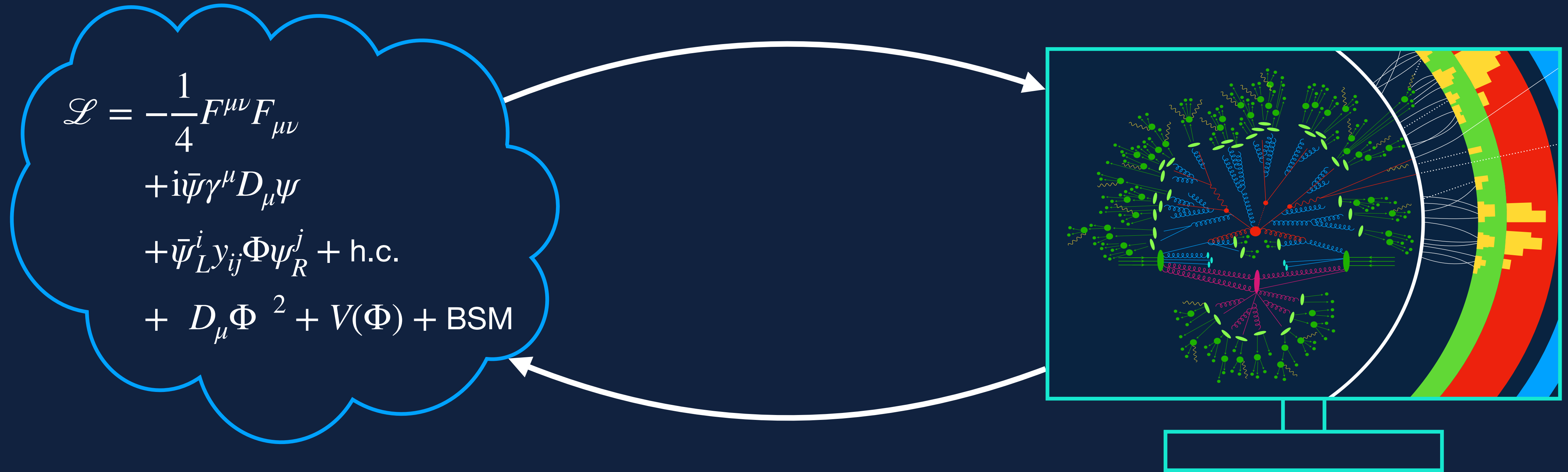


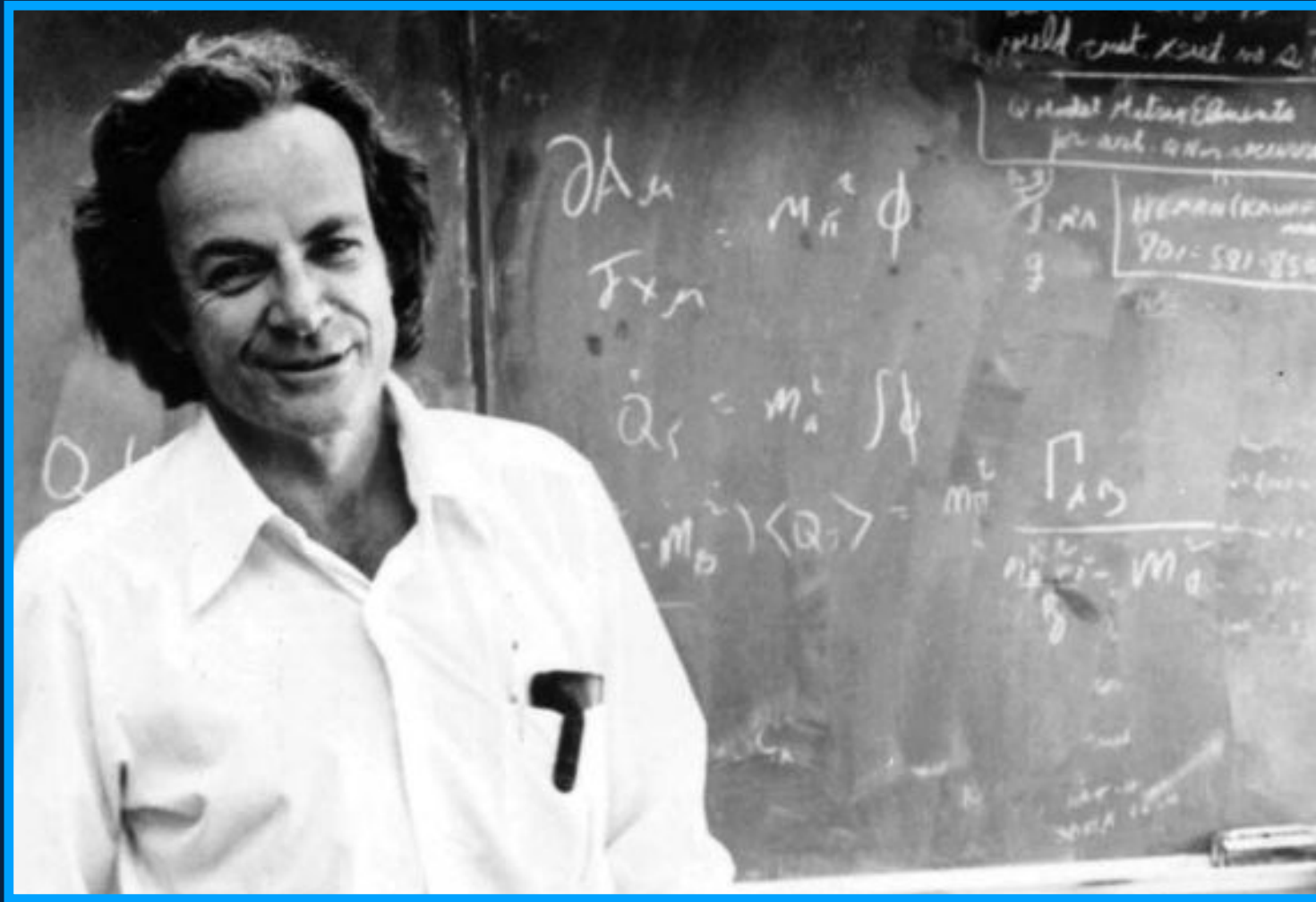
Modern Machine Learning for the LHC Simulation Chain



Why do we talk about simulations?

A theorist perspective...

Why do we talk about simulations?

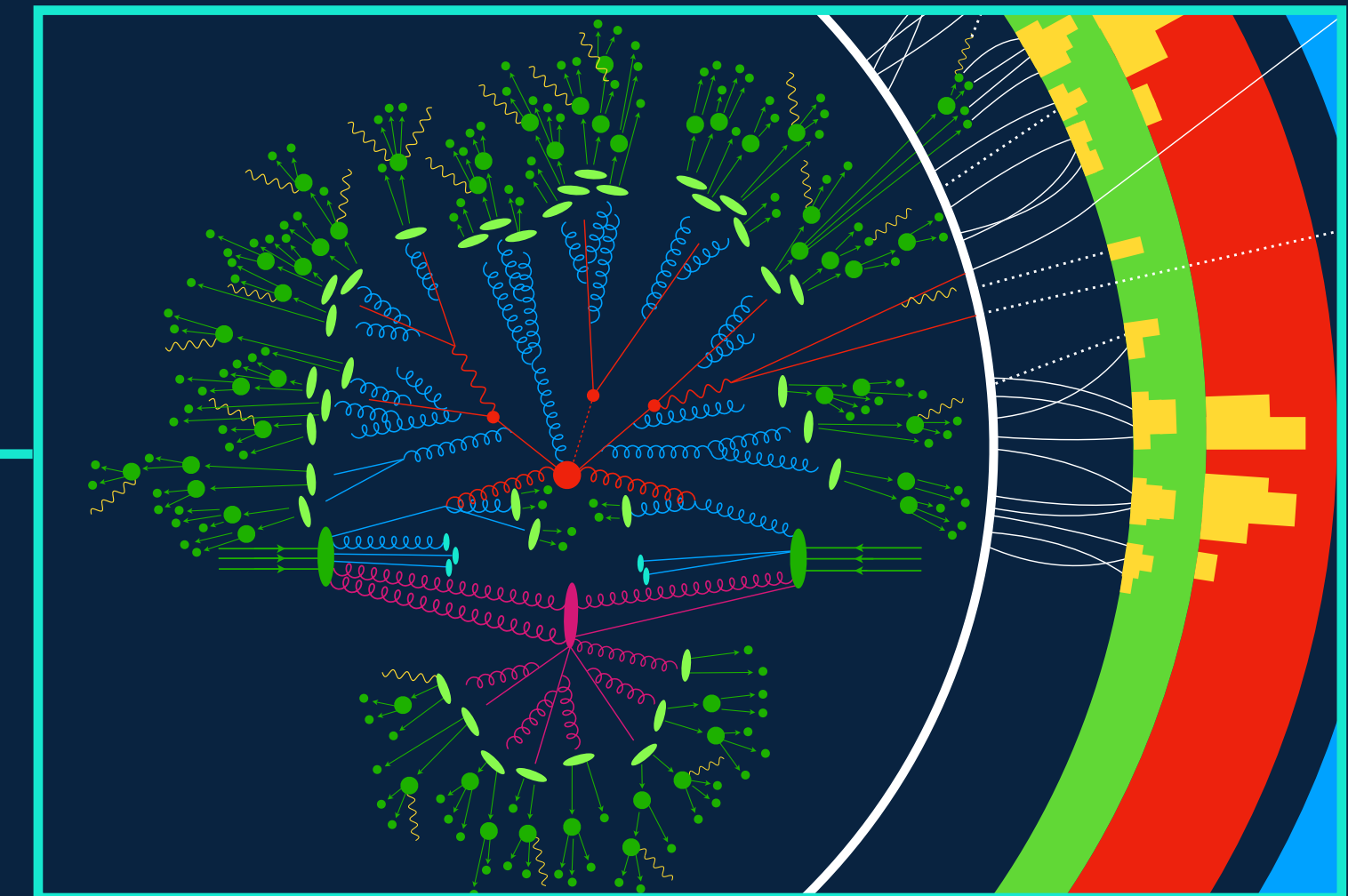


“What I cannot create, I do not understand”

Richard P. Feynman

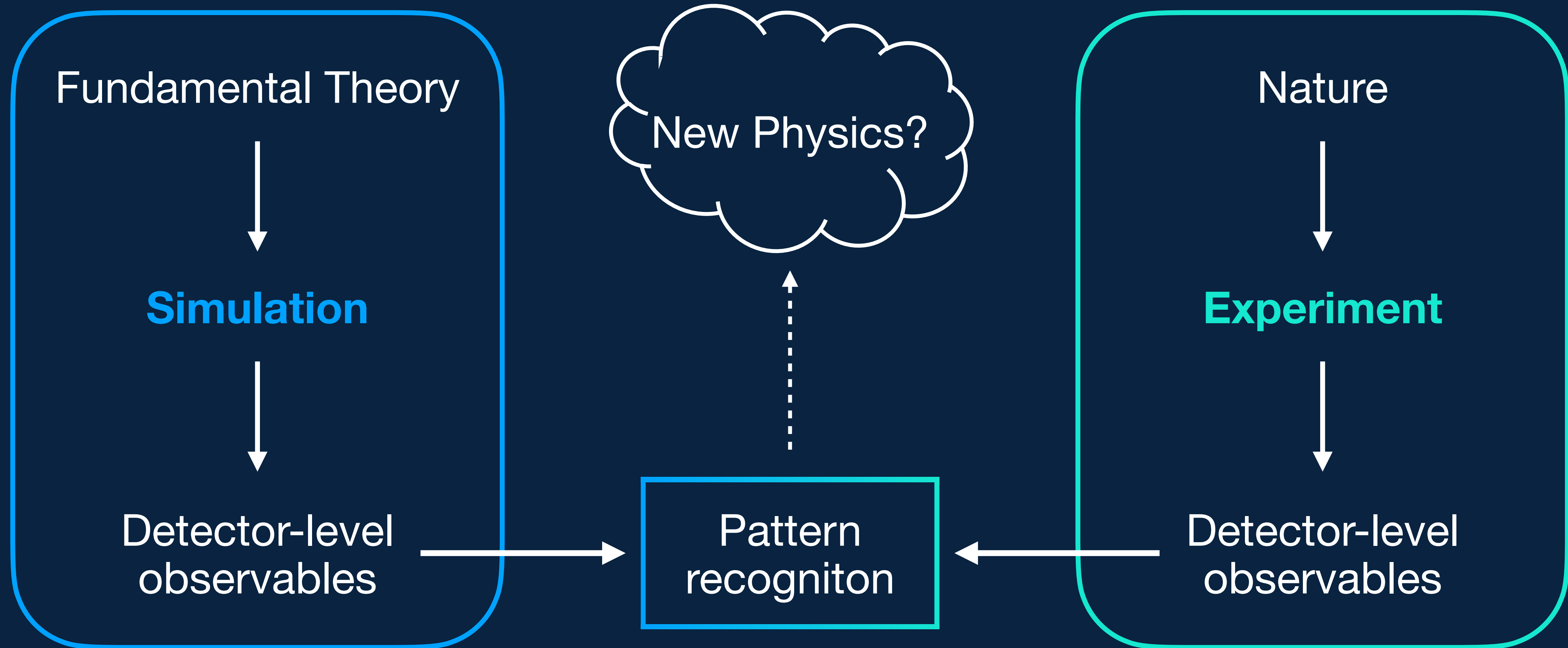
“What I understand, I can create”

LHC Simulations & Generative Modelling

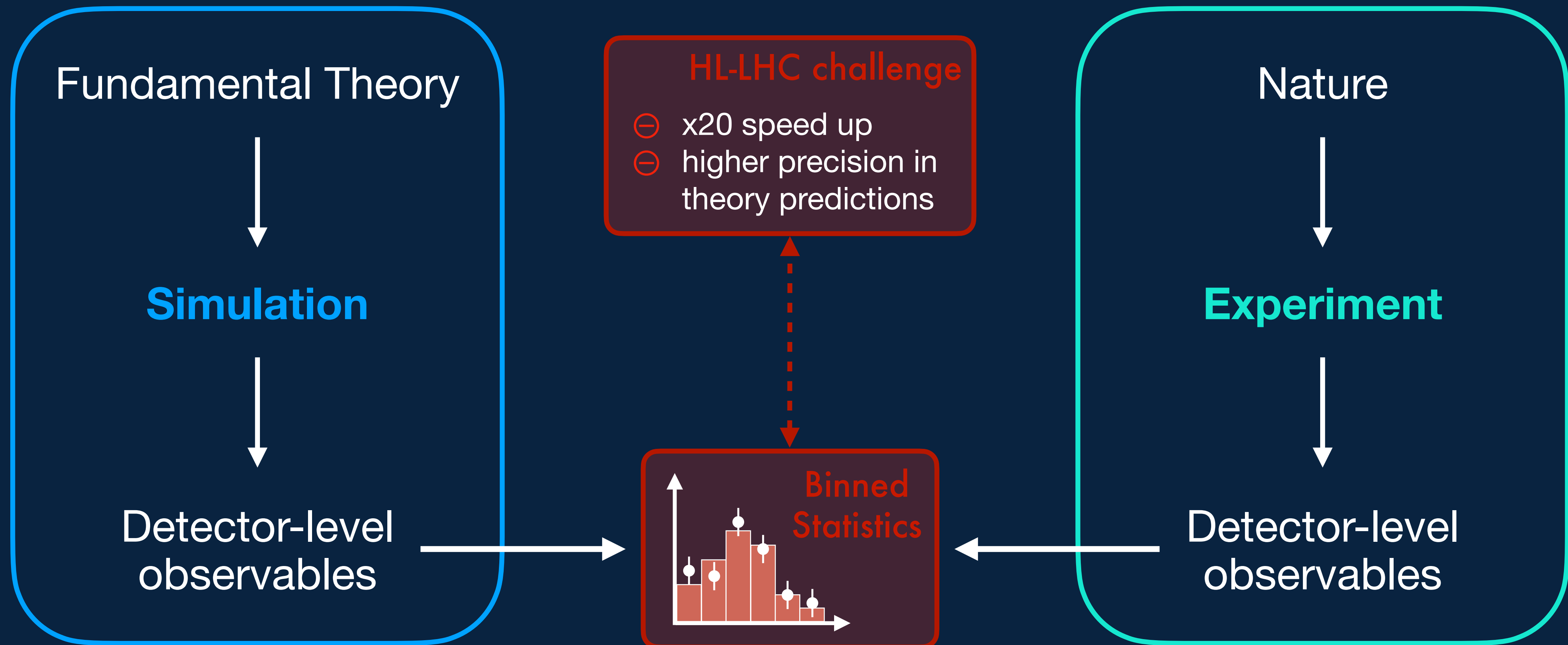


Why do we need them for LHC physics?

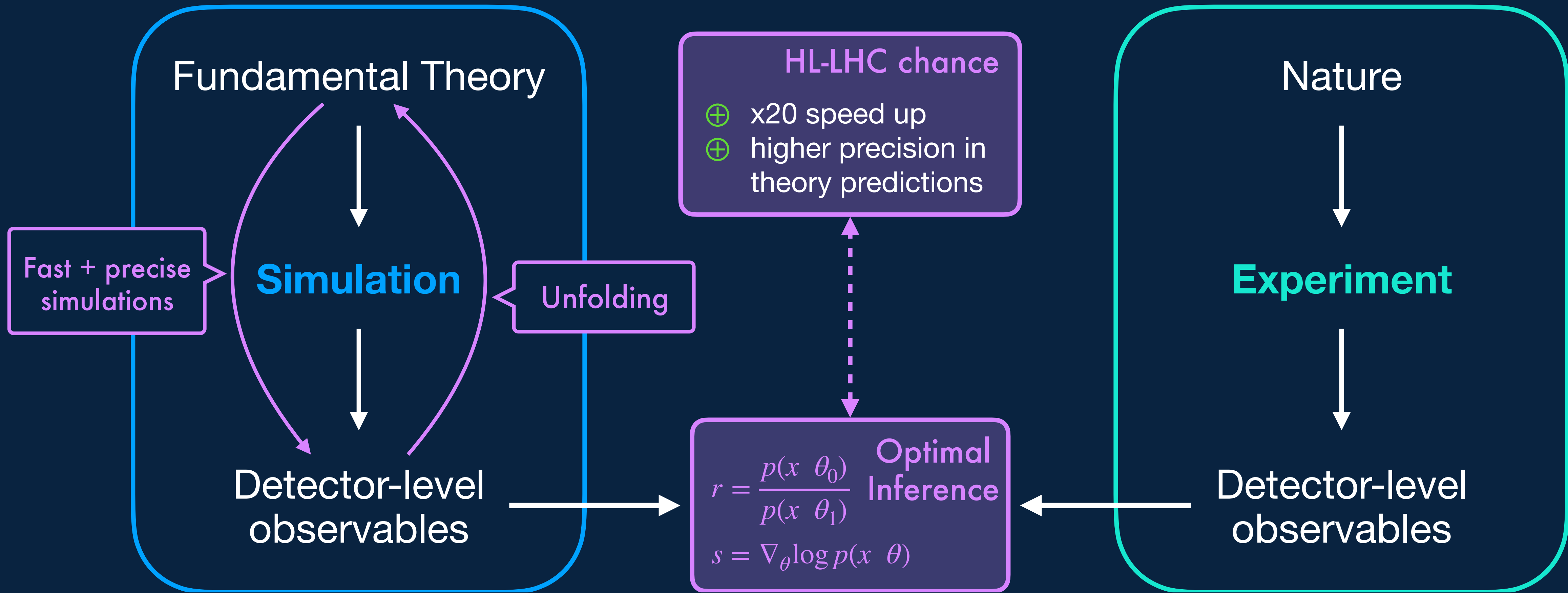
LHC analysis (oversimplified)



Problem: Information bottleneck



Solution: LHC analysis + ML



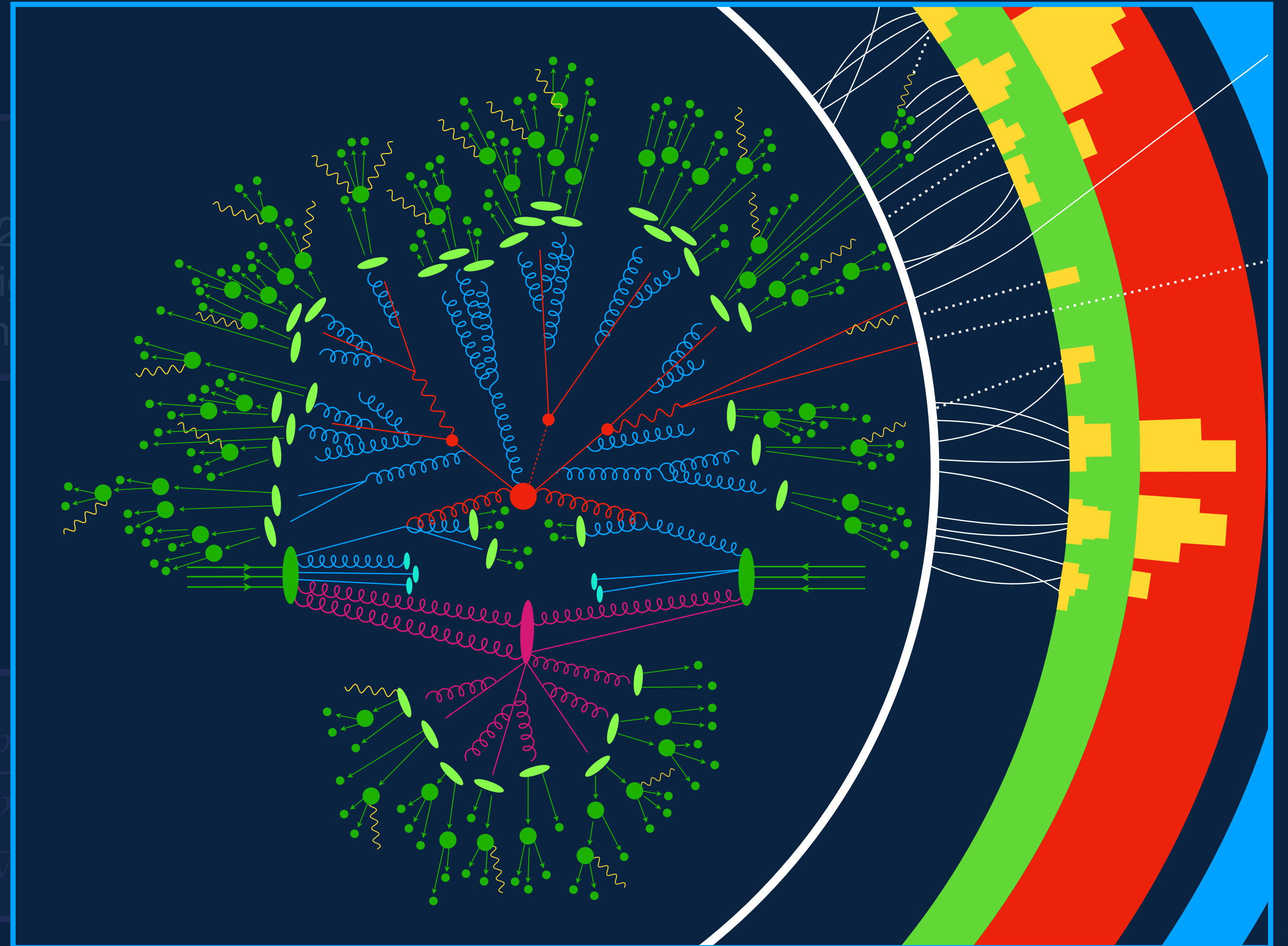
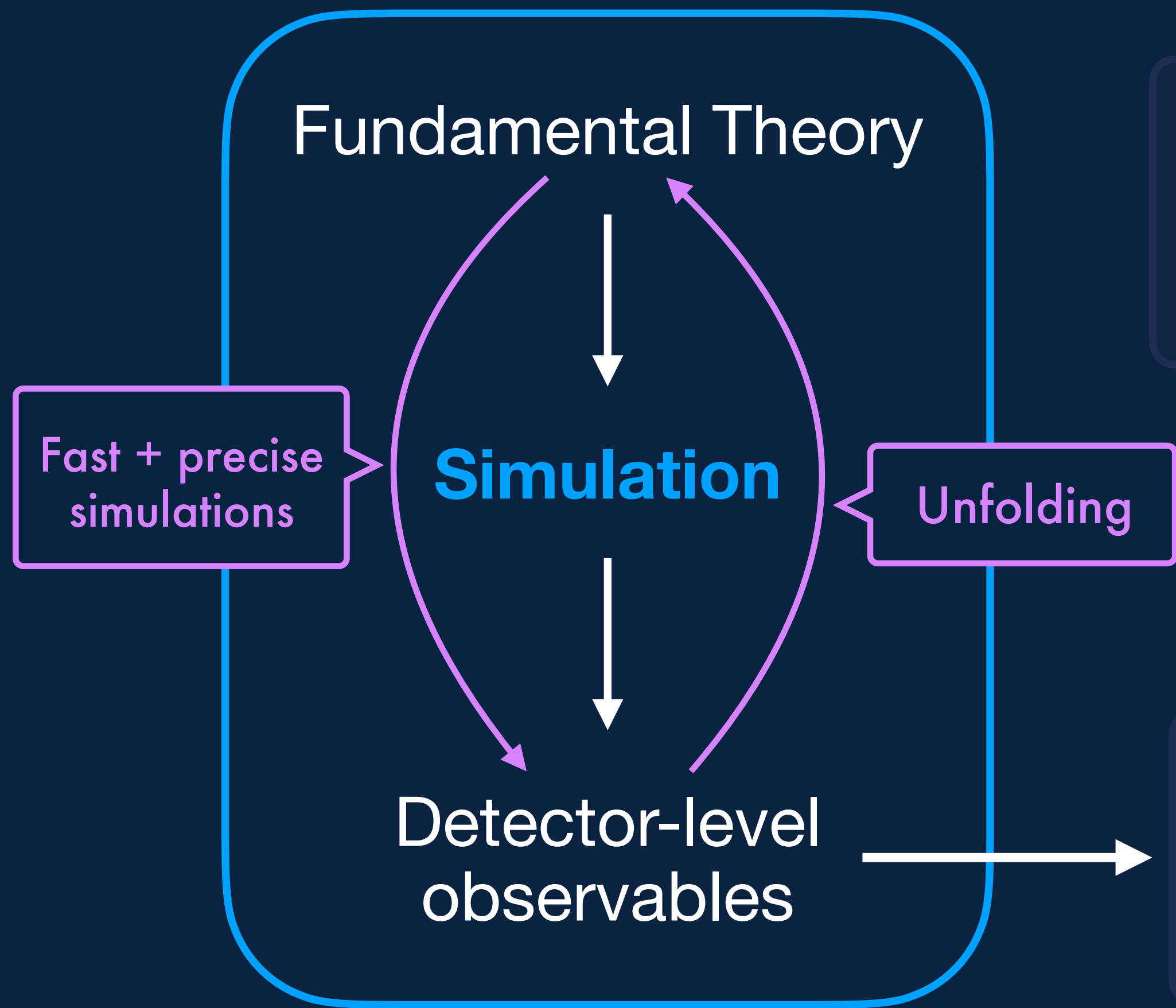
Likelihood-free inference (e.g. MadMiner)

Talk by Jakob Macke
[1506.02169, 1507.03000, 1507.03002, 1507.03003, 1507.03004, 1507.03005, 1507.03006, 1507.03007, 1507.03008, 1507.03009, 1507.03010, 1507.03011, 1507.03012, 1507.03013, 1507.03014, 1507.03015, 1507.03016, 1507.03017, 1507.03018, 1507.03019, 1507.03020, 1805.12244, 1907.10621, 2101.07263, 2210.01680, 2305.10500, 2308.05704,...]

Matrix element method (MEM)

Talk by Theo Heimel
[hep-ex/9808029, hep-ex/9810031, hep-ex/0605118, 1003.1316, 1007.3300, 1010.2263, 1211.3011, 1304.0414, 1502.02485, 1511.05980, 1511.06170, 1512.03429, 1606.03107, 1710.10699, 1712.03266, 1805.08555, 2008.10949, 2210.00019, 2310.07752,...]

Solution: LHC analysis + ML



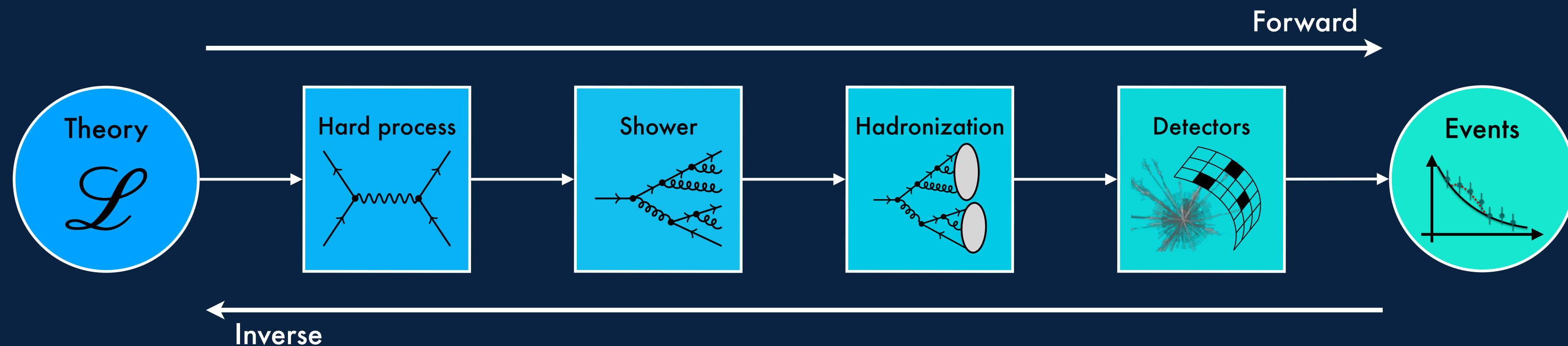
➡ We want to understand **all aspects of data** based on **first principles!**

Understanding LHC data based on 1st principles



What do we need to understand the data?

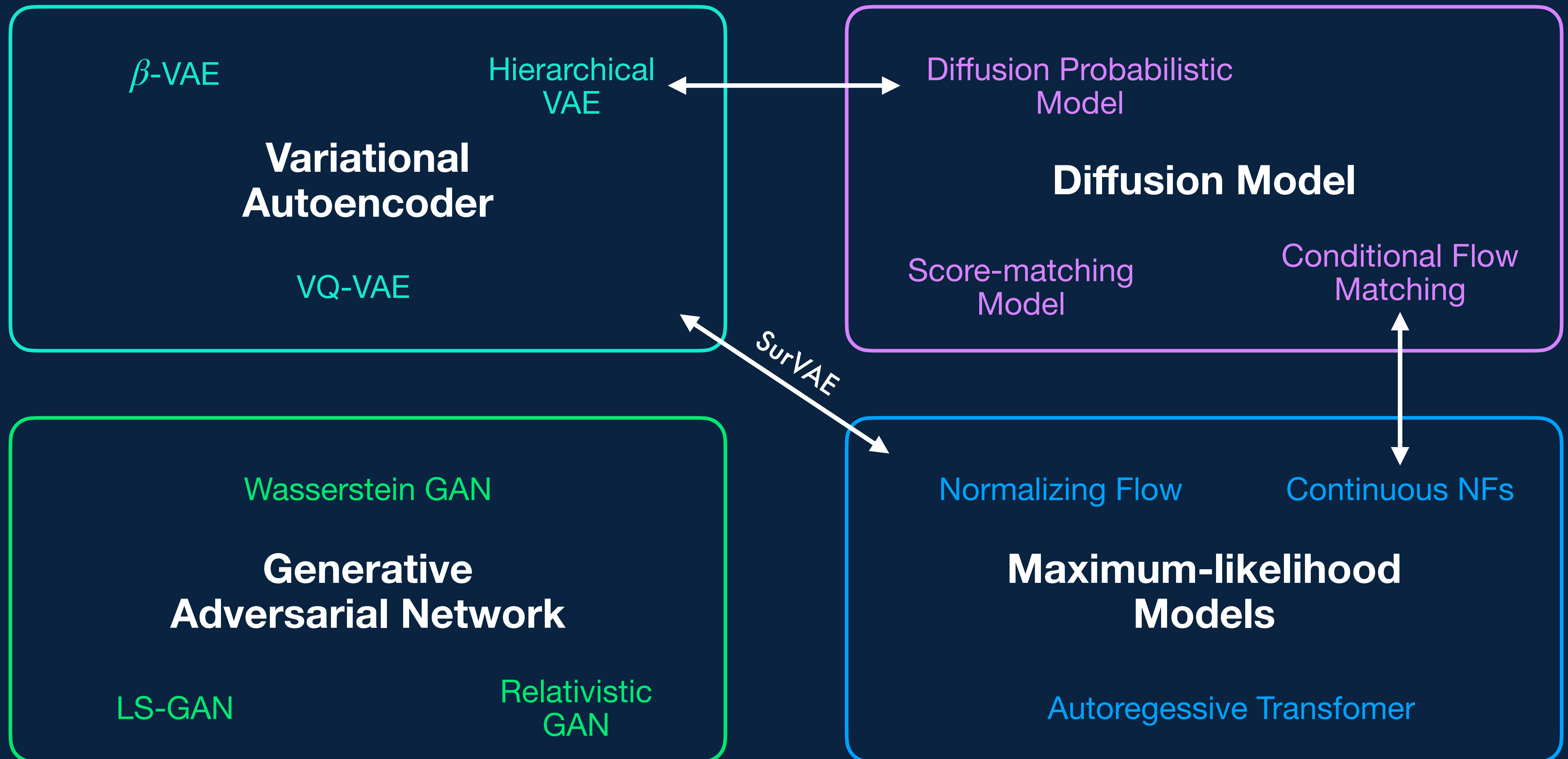
1. Precision simulations (a lot) ← this talk
2. Optimized analyses for high-dimensional data ← Talks by Jakob Macke, Theo Heimel



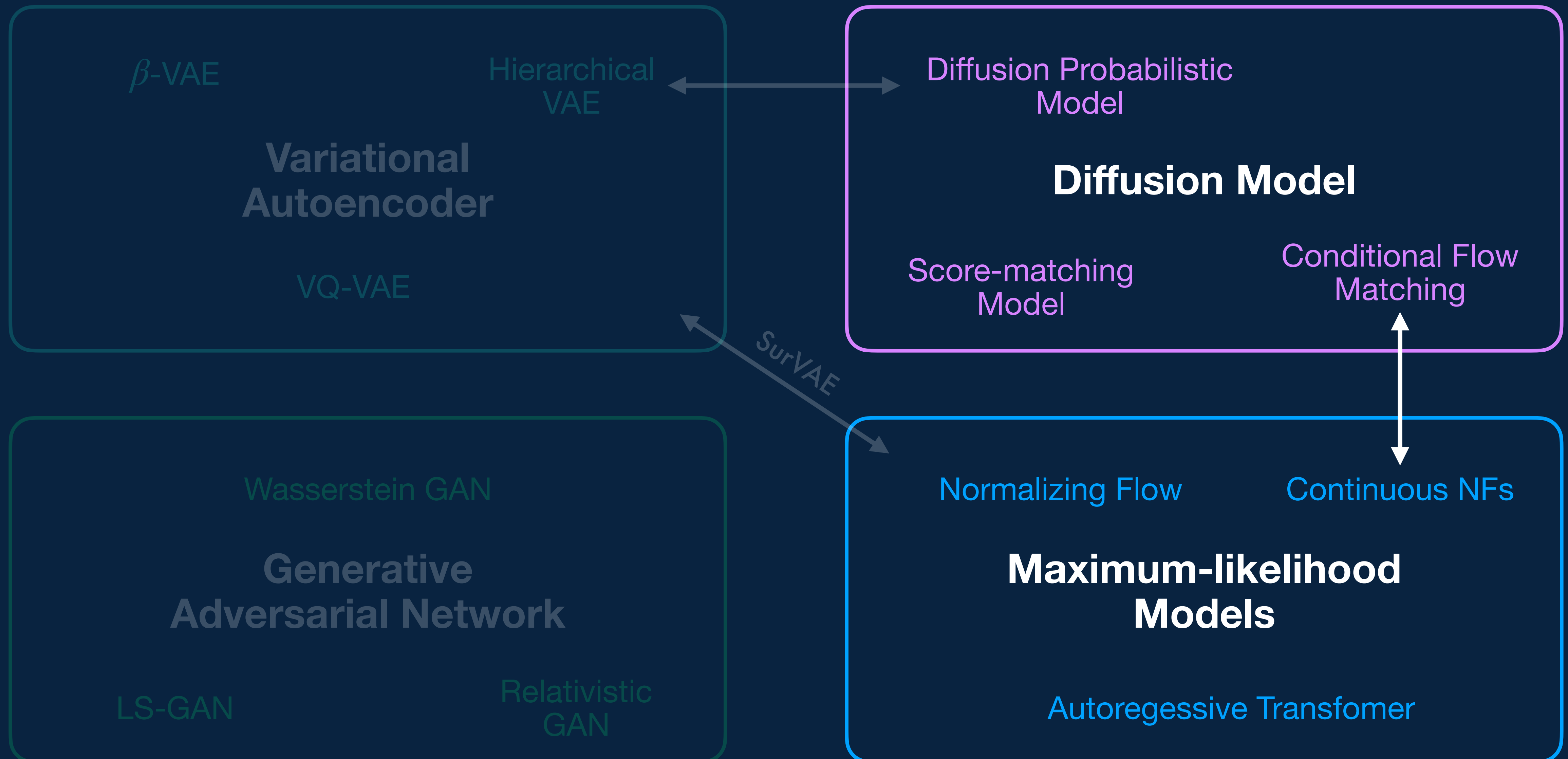
→ **Machine Learning** has significant impact on all aspects

Deep generative models

Deep generative models



Deep generative models



Deep generative models

- ⊕ State-of-the-art in precision
- ⊕ Fast and stable training
- ⊖ Slow likelihood estimation

Application dependent

- ⊕ Fast training and evaluation
- ⊕ Tractable and fast likelihoods
- ⊖ Reduced flexibility and expressivity

Diffusion Probabilistic Model

Diffusion Model

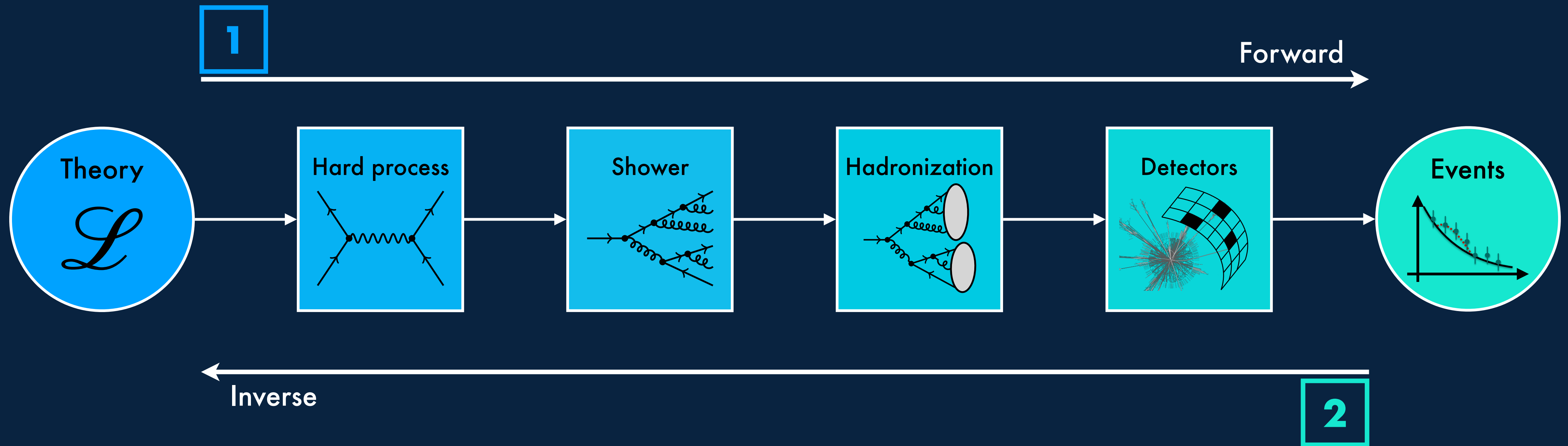
Score-matching Model Conditional Flow Matching

Normalizing Flow Continuous NFs

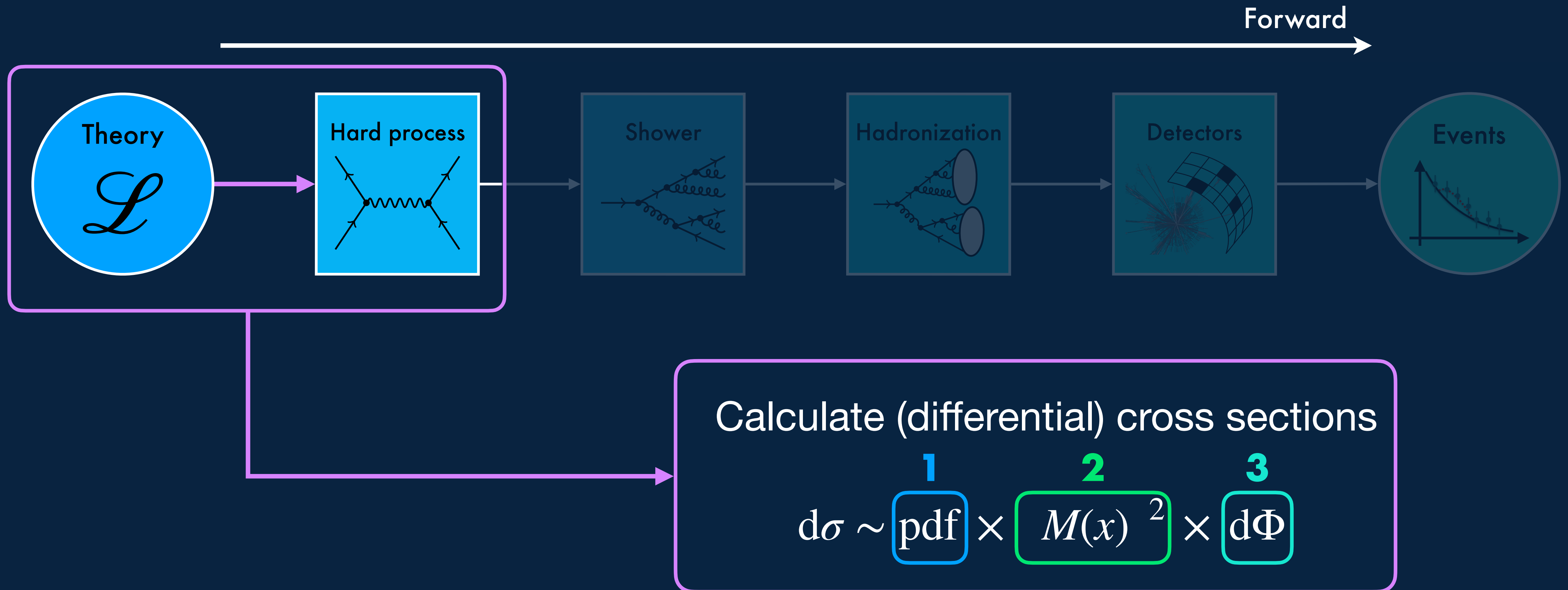
Maximum-likelihood Models

Autoregressive Transformer

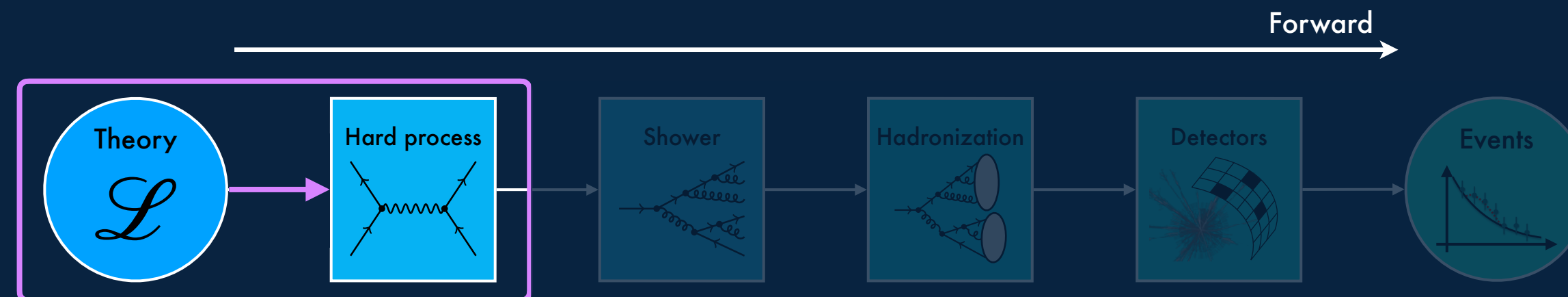
ML aided simulation chain



ML for forward simulations



ML for forward simulations

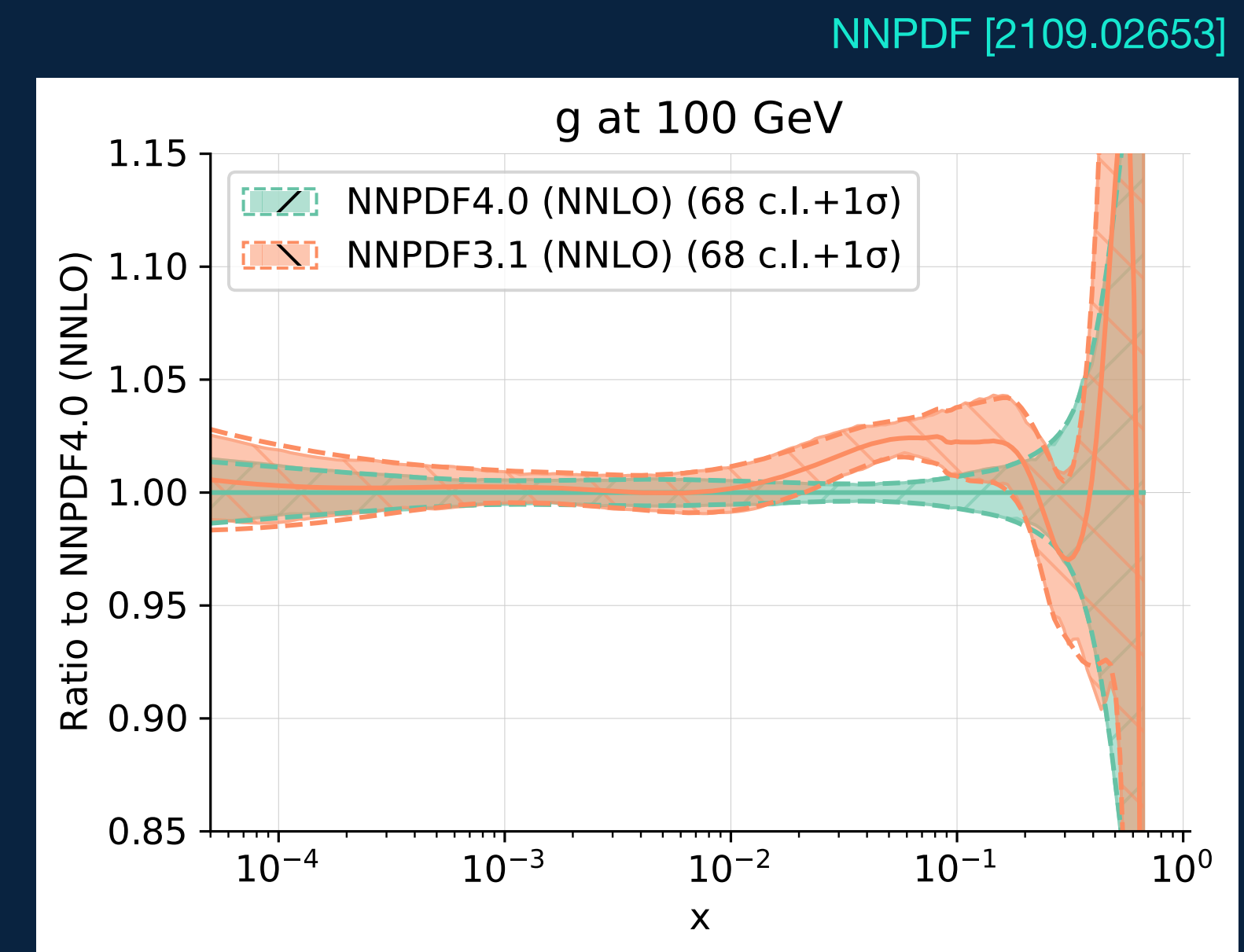


$$d\sigma \sim \boxed{\text{pdf}} \times M(x)^2 \times \text{phase space}$$

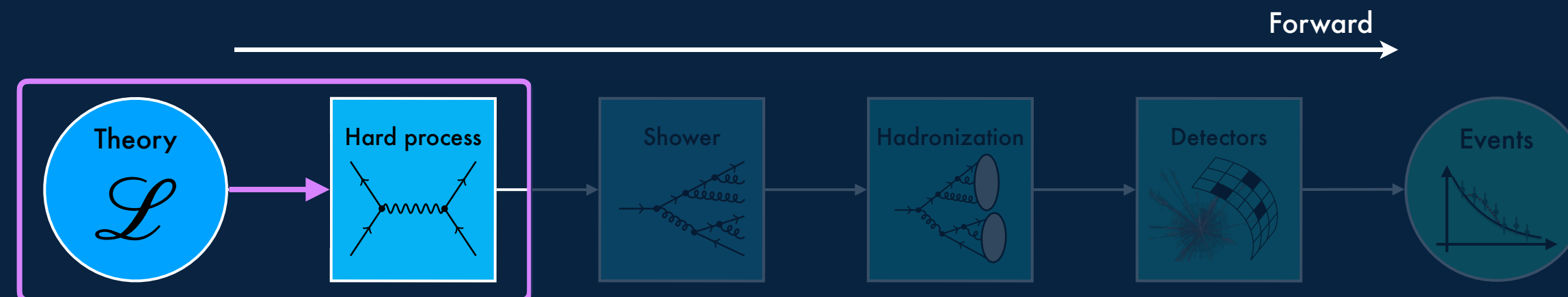
PDFs: ML reduces uncertainties

- **NNPDF** uses NN for a long time (no parametric function)
- Modern ML and hyper-opt
→ reduced uncertainties: **3-5% → 1%**
- **GAN**-enhanced PDF compression

[[hep-ph/0204232](#), [1002.4407](#), [1410.8849](#), [1907.05075](#), [2010.03996](#), [2012.08221](#), [2104.04535](#), [2109.02653](#), [2109.02671](#), [2201.07240](#), [2211.01094](#), [2212.12569](#), [2302.08527](#), [2303.06159](#), [2307.05967](#),.....]



ML for forward simulations

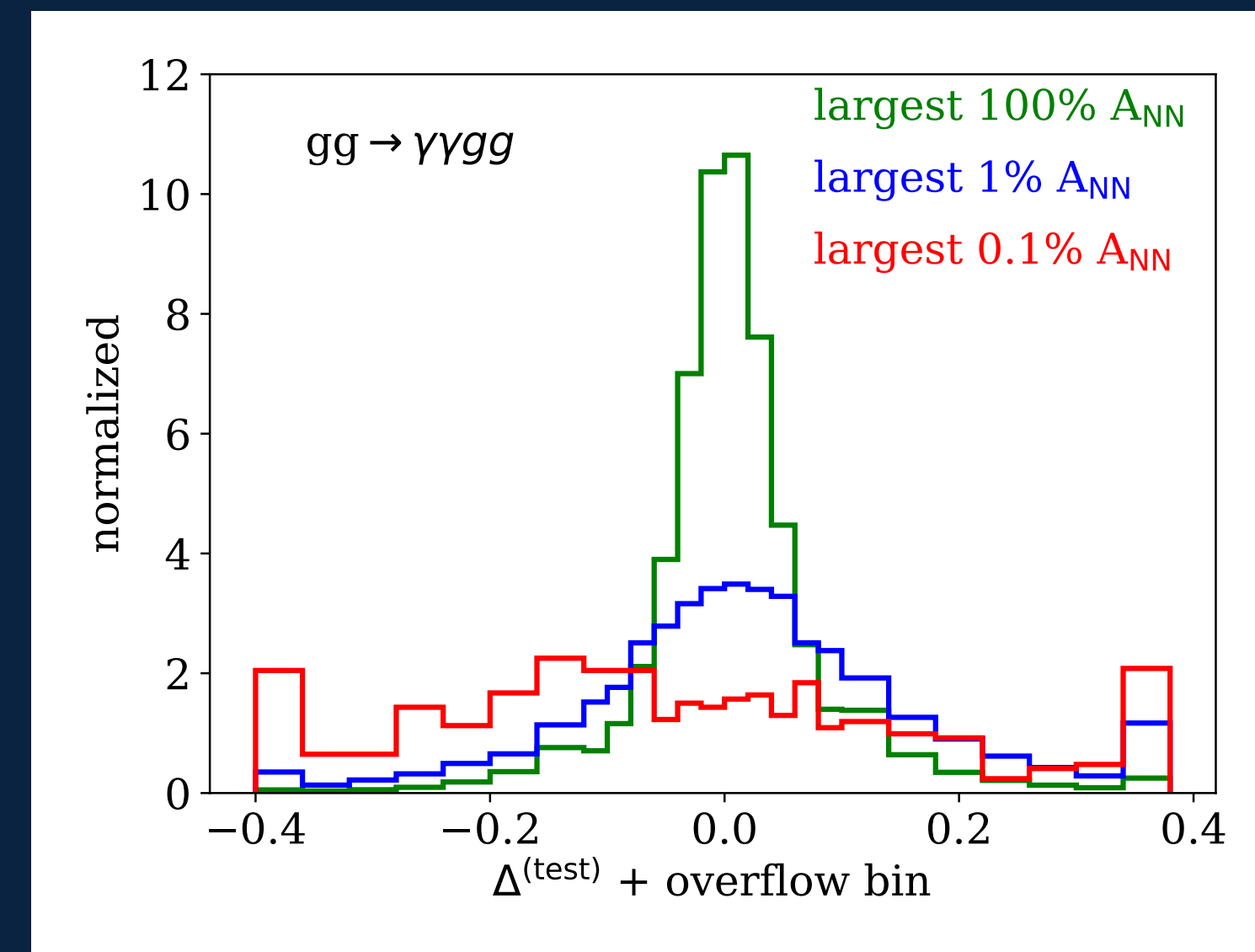


$$d\sigma \sim \text{pdf} \times M(x)^2 \times \text{phase space}$$

Amplitudes: avoid expensive matrix element

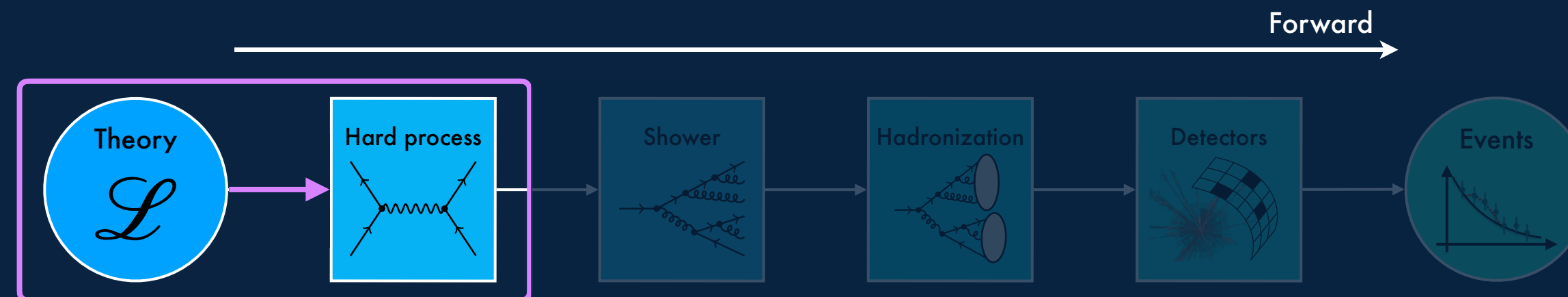
- As “simple” **regression** task
- With uncertainties/boosting using **Bayesian NN**

Badger, Butter, Luchman, Pitz, Plehn [2206.14831]



[1912.11055, 2002.07516, 2006.16273, 2008.10949, 2104.14182, 2105.04898, 2106.09474, 2107.06625, 2109.11964, 2112.09145, 2201.04523, 2206.08901, 2206.04115, 2206.14831, 2301.13562, 2302.04005, 2306.07726,.....]

ML for forward simulations

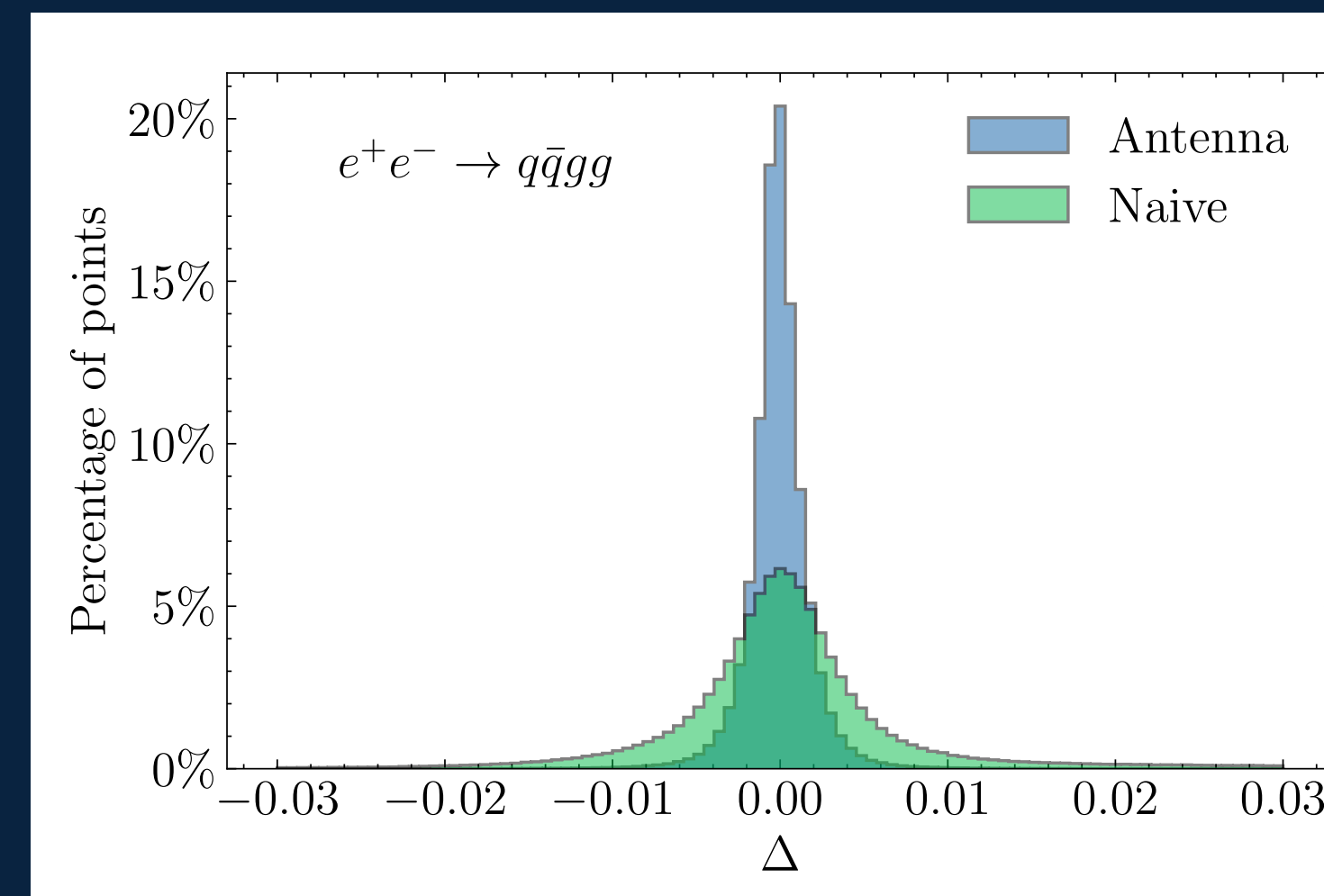


$$d\sigma \sim \text{pdf} \times M(x)^2 \times \text{phase space}$$

Amplitudes: avoid expensive matrix element

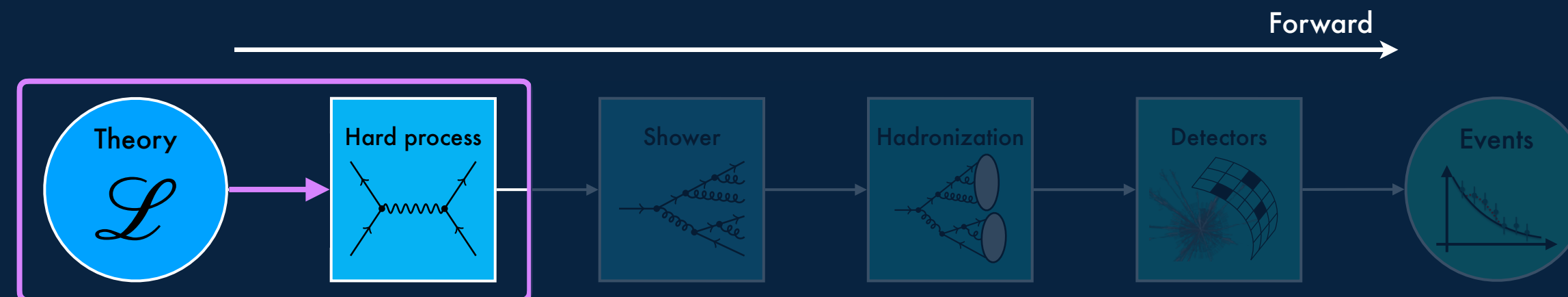
- As “simple” **regression** task
- With uncertainties/boosting using **Bayesian NN**
- Using factorisation ansatz to reach **% level** accuracy

Maire, Truong [2302.04005]



[1912.11055, 2002.07516, 2006.16273, 2008.10949, 2104.14182, 2105.04898, 2106.09474, 2107.06625, 2109.11964, 2112.09145, 2201.04523, 2206.08901, 2206.04115, 2206.14831, 2301.13562, 2302.04005, 2306.07726,.....]

ML for forward simulations

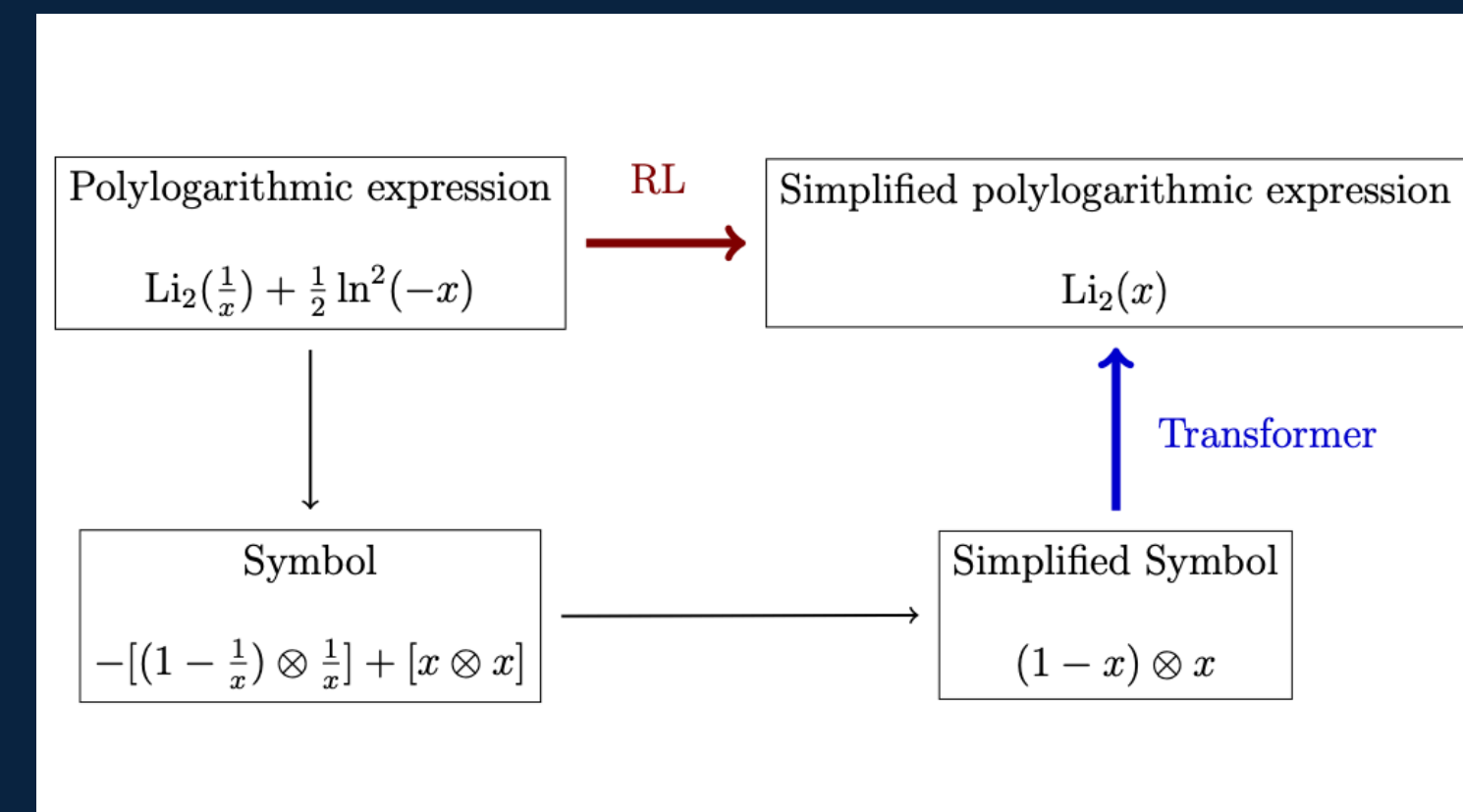


$$d\sigma \sim \text{pdf} \times M(x)^2 \times \text{phase space}$$

Amplitudes: avoid expensive matrix element

- As “simple” **regression** task
- With uncertainties/boosting using **Bayesian NN**
- Using factorisation ansatz to reach **% level** accuracy
- **RL and/or Transformer** for simplifications of Polylogarithms
- NN-assisted **contour deformation** (Loop integrals)

Dersey, Schwartz, Zhang [2206.04115]



[1912.11055, 2002.07516, 2006.16273, 2008.10949, 2104.14182, 2105.04898, 2106.09474, 2107.06625, 2109.11964, 2112.09145, 2201.04523, 2206.08901, 2206.04115, 2206.14831, 2301.13562, 2302.04005, 2306.07726,.....]

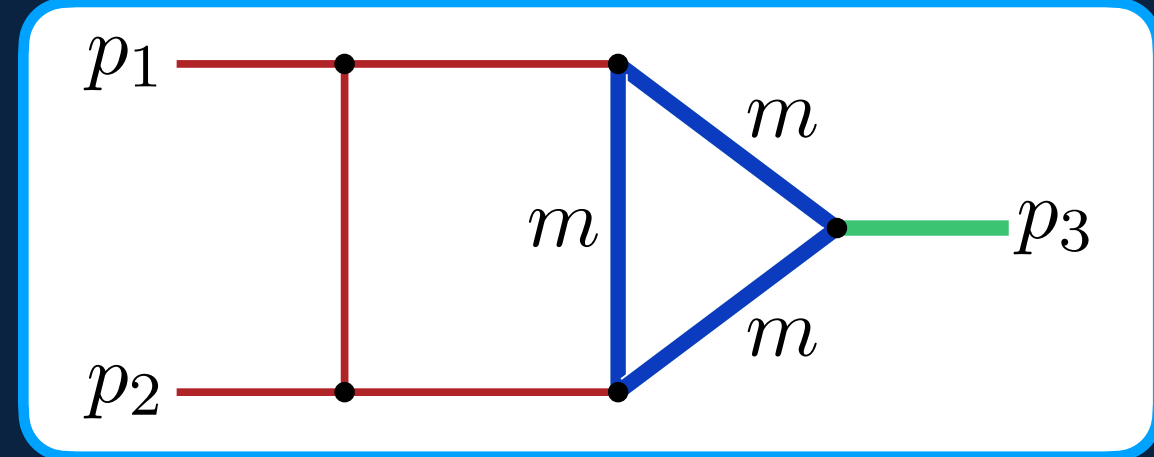
NNContour

ML for loop integrals

NNContour — ML for loop integrals

RW et al. [2112.09145]

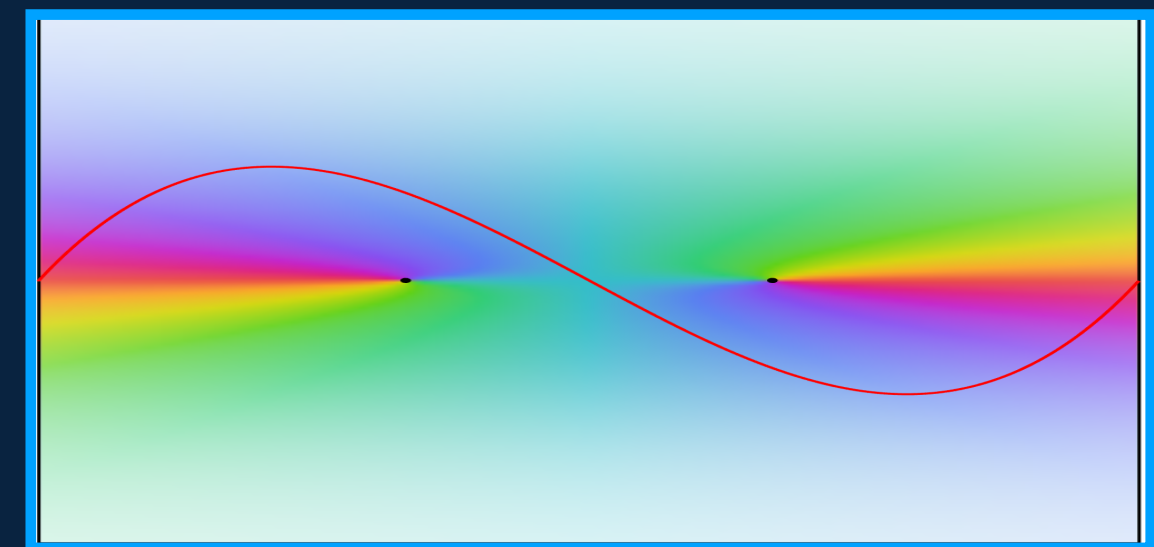
$$G \propto \int_0^1 \prod_{j=1}^{N-1} dx_j x_j^{\nu_j-1} \frac{U^{\nu-(L+1)D/2}}{F^{\nu-LD/2}}$$



Contains singularities

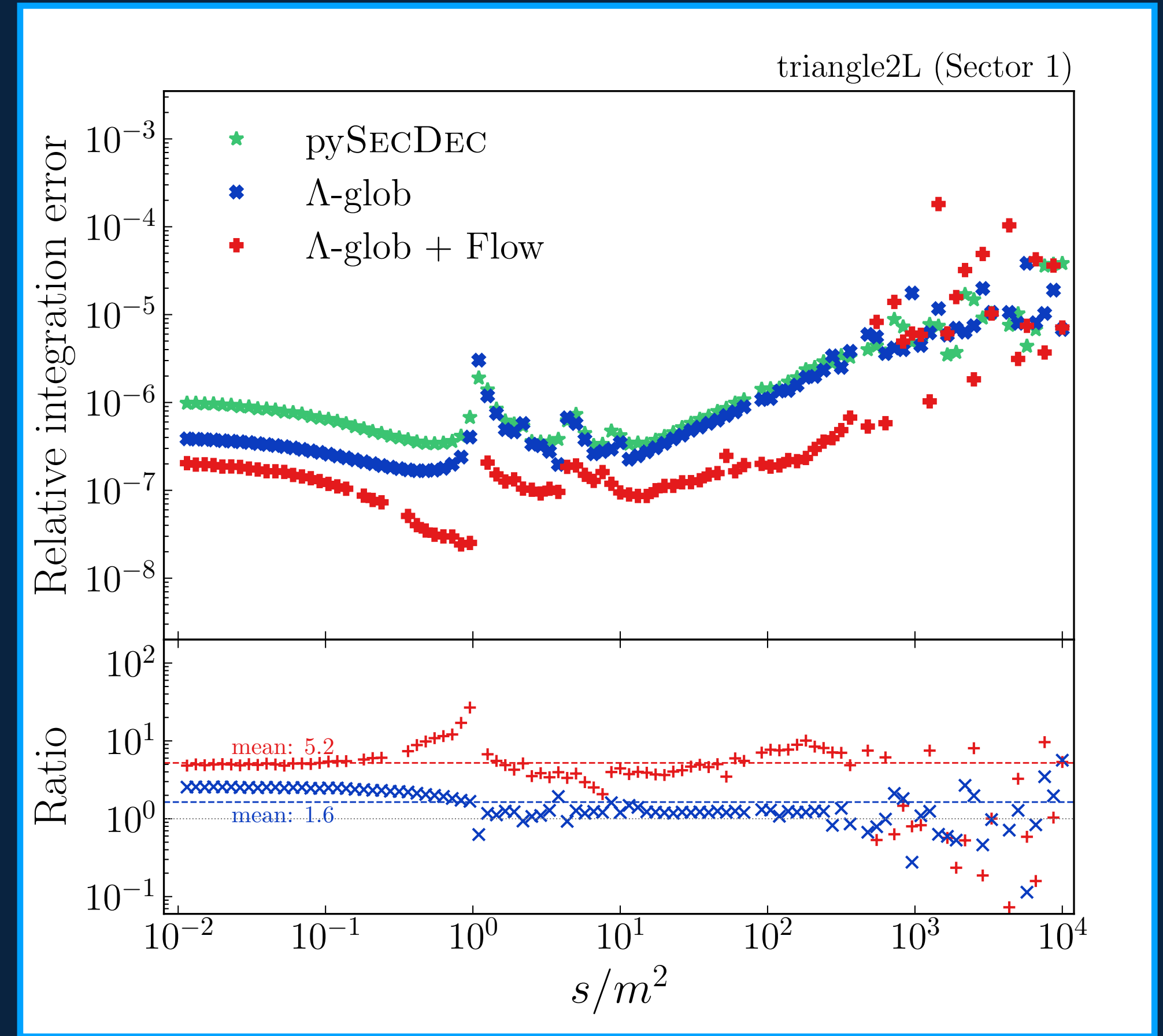
Cauchy-Theorem → Contour deformation

$$\int_0^1 \prod_{j=1}^N dx_j I(\vec{x}) = \int_{\gamma} \prod_{j=1}^N dz_j I(\vec{z})$$



Parametrize with **NF + NN**

→ Optimal parametrization = small variance

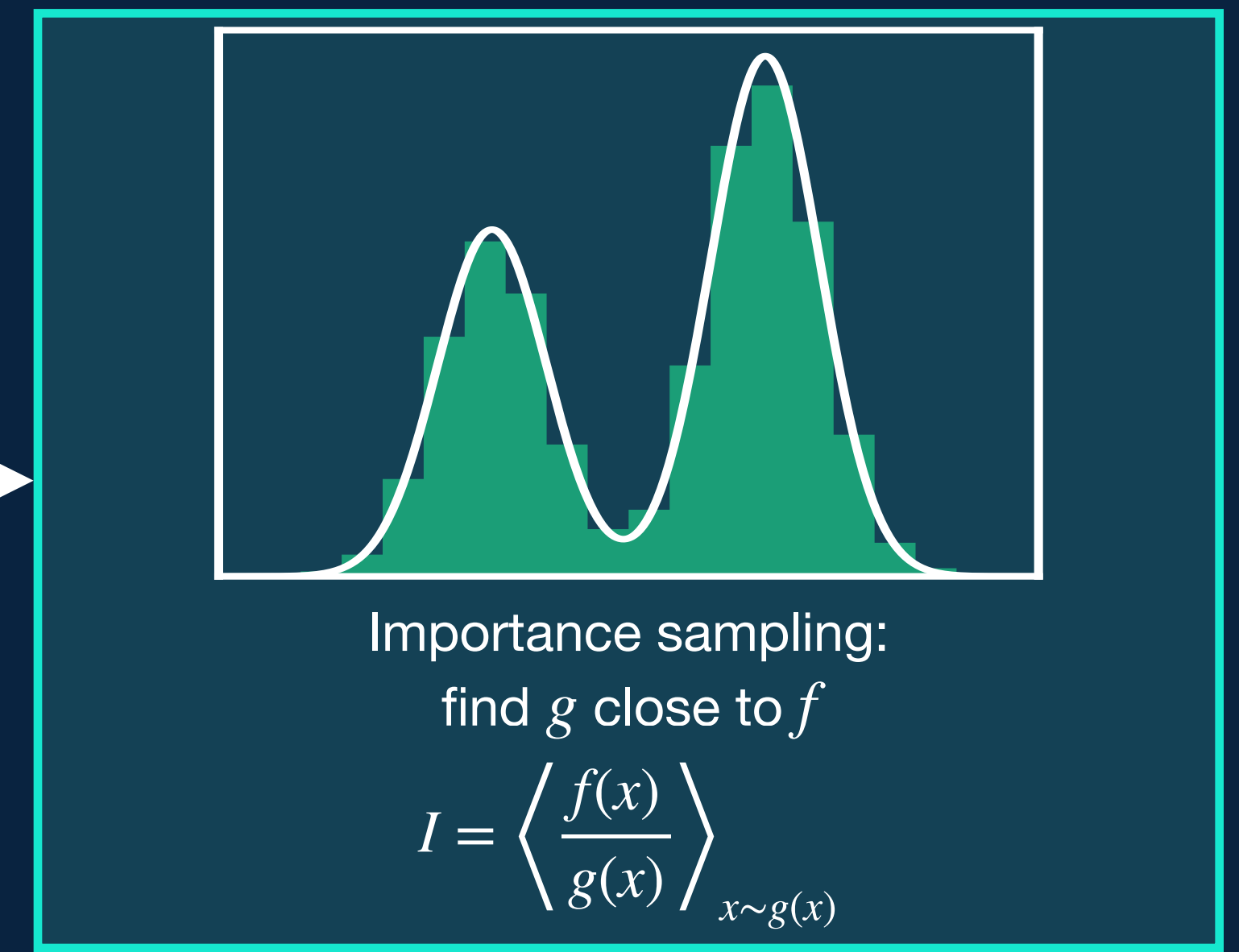
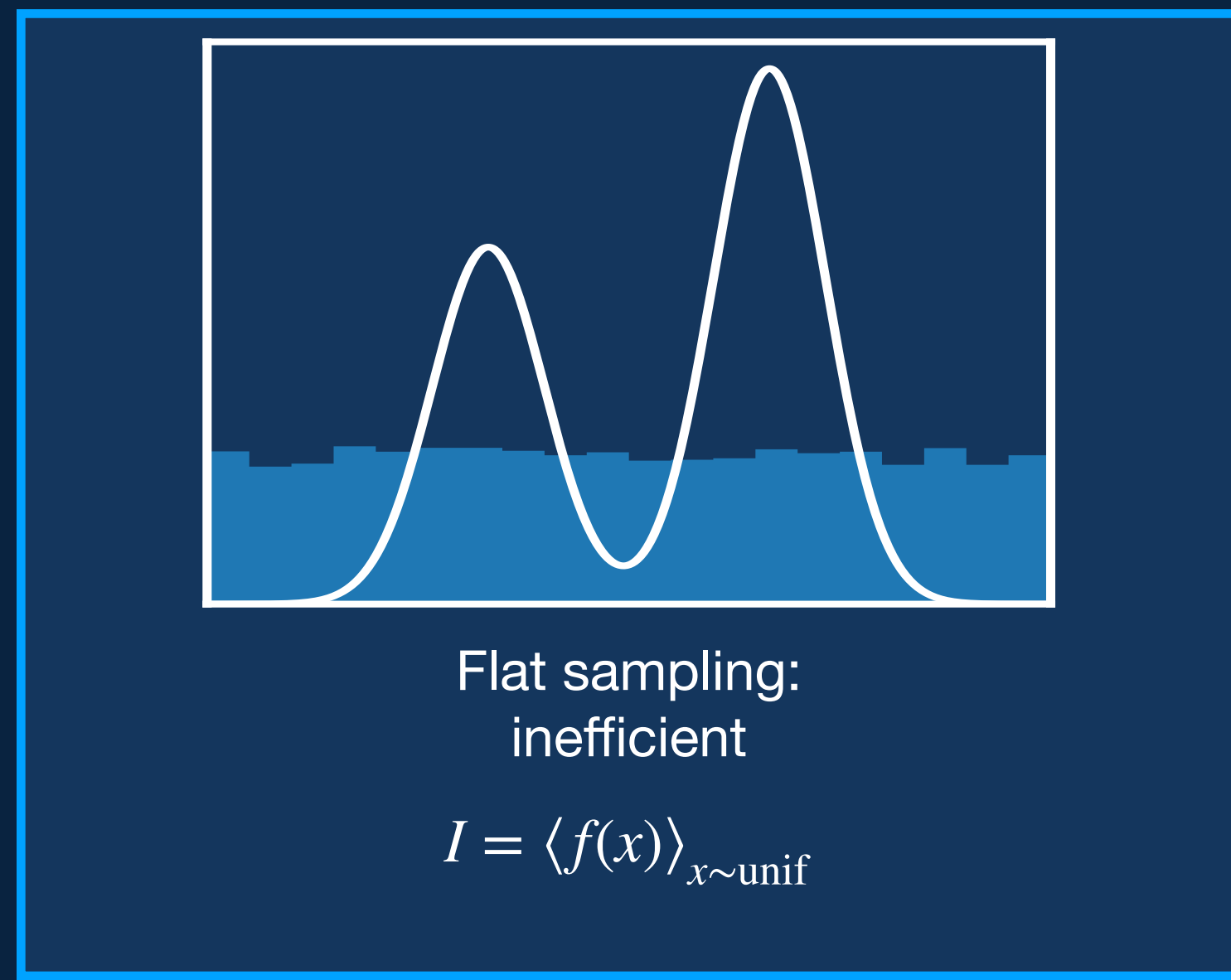


ML for forward simulations

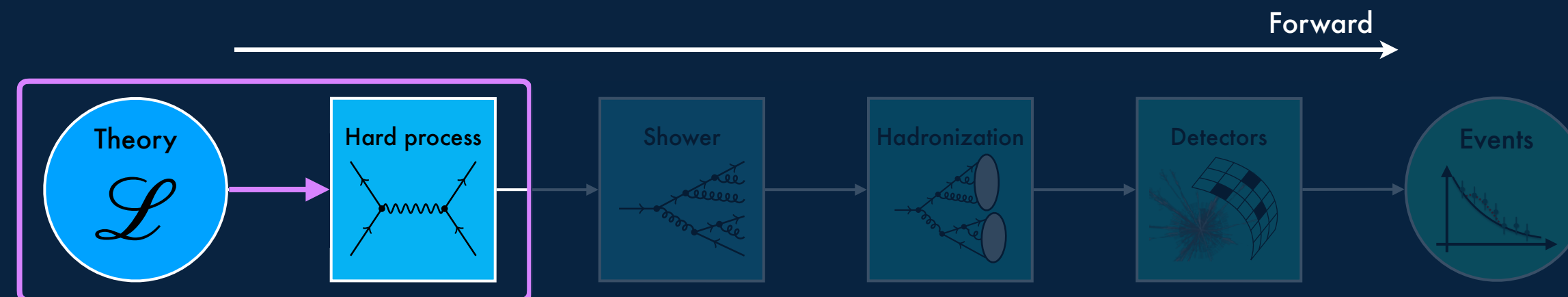


$$d\sigma \sim \text{pdf} \times M(x)^2 \times \text{phase space}$$

Phase space: increase unweighting efficiency



ML for forward simulations



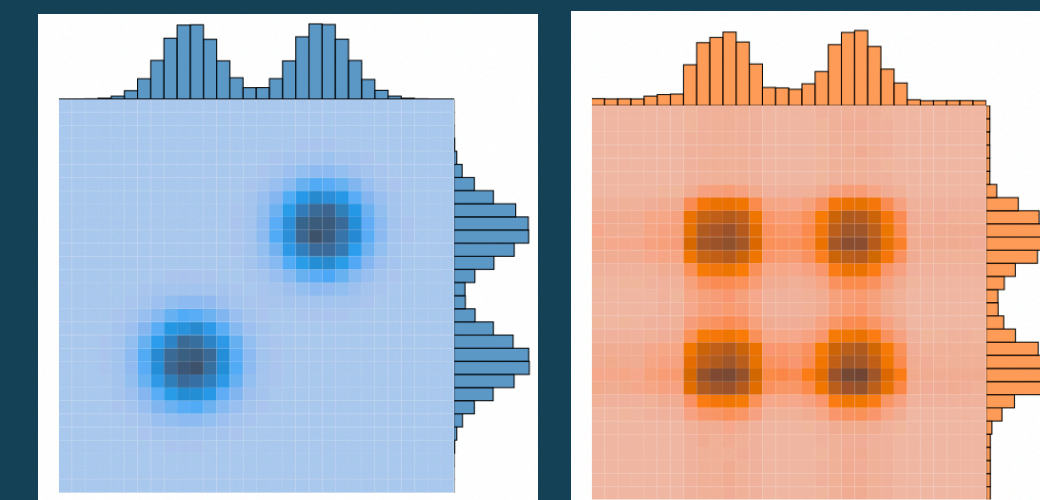
$$d\sigma \sim \text{pdf} \times M(x)^2 \times \text{phase space}$$

Phase space: increase unweighting efficiency

- Standard **VEGAS** approach → **fast** but **no correlations**
- Improve with **NN** → **correlations** but **unstable**

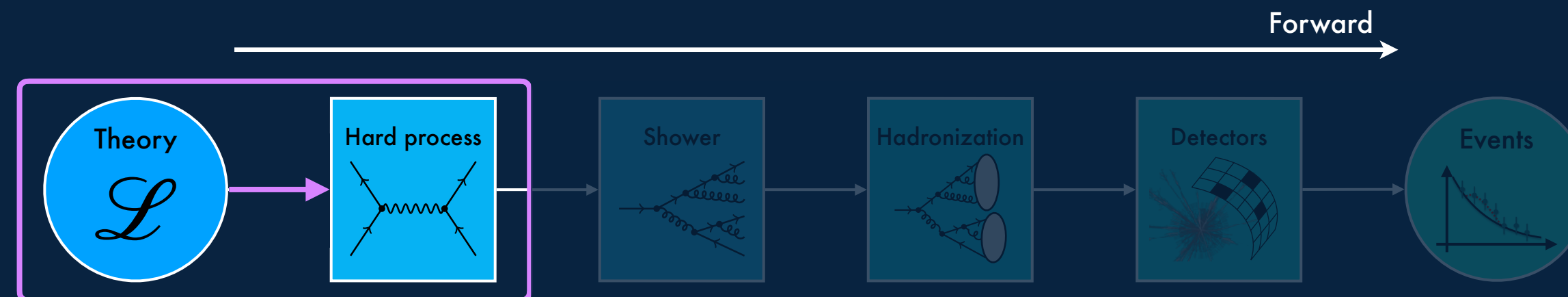
[G. P. Lepage, 1978]

- ⊕ Computationally cheap
- ⊖ High-dim and rich peaking functions → **slow convergence**
- ⊖ Peaks not aligned with grid axes → **phantom peaks**



[1707.00028, 1810.11509, 2001.05478, 2001.05486, 2001.10028, 2005.12719, 2009.07819, 2011.13445, 2112.09145, 2212.06172, 2309.12369,.....]

ML for forward simulations

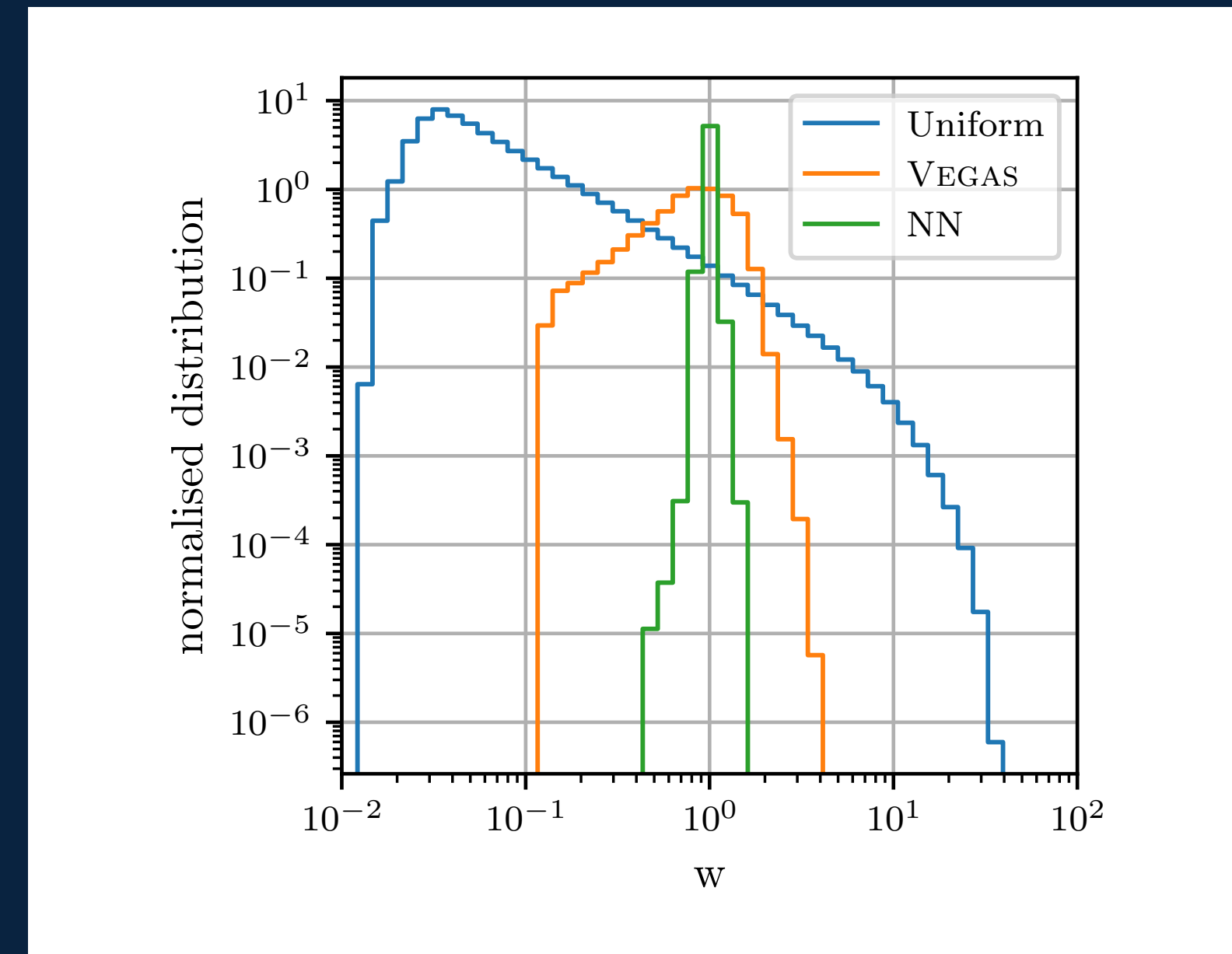


$$d\sigma \sim \text{pdf} \times M(x)^2 \times \text{phase space}$$

Phase space: increase unweighting efficiency

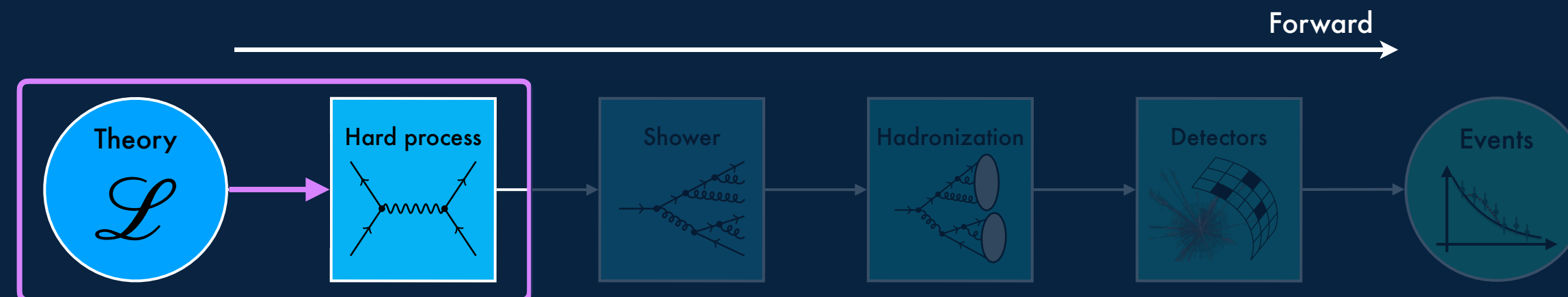
- Standard **VEGAS** approach → **fast** but **no correlations**
- Improve with **NN** → **correlations** but **unstable**
- Use **normalizing flows** → **correlations** and **stable**

Bothmann, Janßen, Knobbe, Schmale, Schumann [2001.05478]



[1707.00028, 1810.11509, 2001.05478, 2001.05486, 2001.10028, 2005.12719, 2009.07819, 2011.13445, 2112.09145, 2212.06172, 2309.12369,.....]

ML for forward simulations

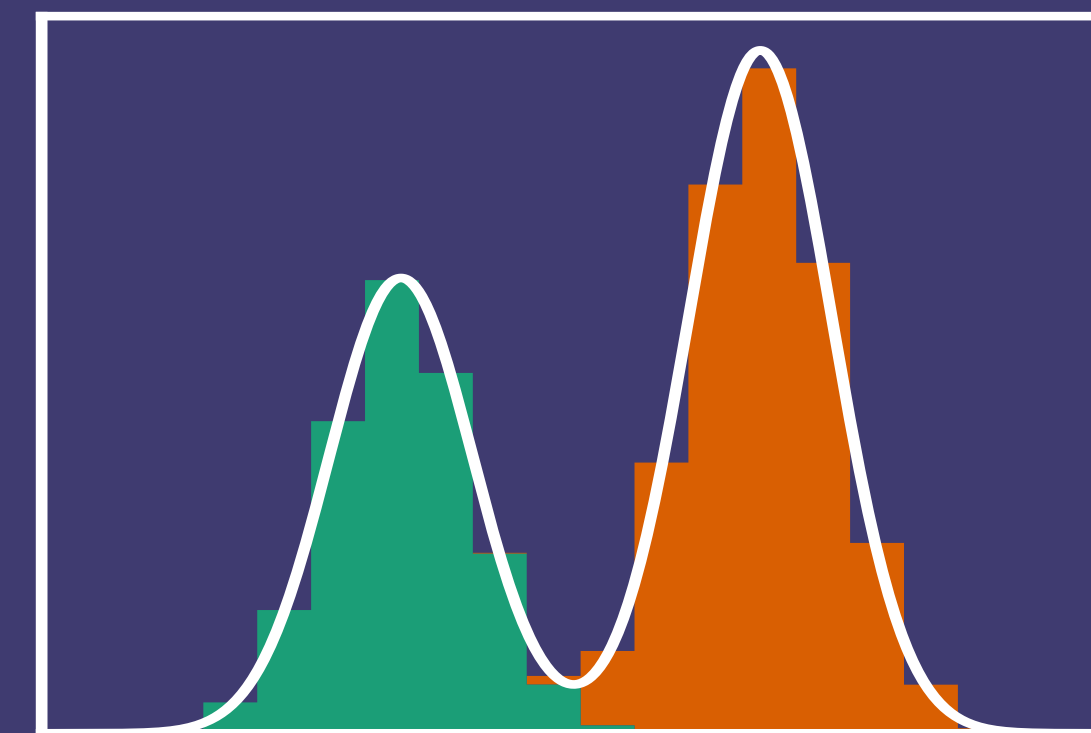


$$d\sigma \sim \text{pdf} \times M(x)^2 \times \text{phase space}$$

Phase space: increase unweighting efficiency

- Standard **VEGAS** approach → **fast** but **no correlations**
- Improve with **NN** → **correlations** but **unstable**
- Use **normalizing flows** → **correlations** and **stable**
- **Multi-channel** approach → split the integral
- Combine all (VEGAS, learned α_i , NF, symmetries,..) → **MadNIS** framework

Kleiss, Pittau [hep-ph/9405257], Maltoni, Stelzer [hep-ph/0208156]



Multi-channel:
one map for each channel

$$I = \sum_i \left\langle \alpha_i(x) \frac{f(x)}{g_i(x)} \right\rangle_{x \sim g_i(x)}$$

[1707.00028, 1810.11509, 2001.05478, 2001.05486, 2001.10028, 2005.12719, 2009.07819, 2011.13445, 2112.09145, 2212.06172, 2309.12369,.....]

MadNIS

Neural Importance Sampling

Heimel, Huetsch, Maltoni, Mattelaer, Plehn, RW [2311.XxxxX]

Heimel, RW, Butter, Isaacson, Krause, Maltoni, Mattelaer, Plehn [[2212.06172](#)]

MadNIS — Basic functionality

$$I = \sum_i \left\langle \alpha_i(x) \frac{f(x)}{g_i(x)} \right\rangle_{x \sim g_i(x)}$$

Use physics knowledge to construct channel and mappings

Normalizing flow to refine channel mappings

Fully connected network to refine channel weights

Update simultaneously with variance as loss function

MadNIS — Loss function

Minimize total variance

$$\sigma_{\text{tot}}^2 = N \sum_i \frac{\sigma_i^2}{N_i} \quad \text{with}$$

$$\sigma_i^2 = \left\langle \alpha_i^2(x) \frac{f^2(x)}{g_i^2(x)} \right\rangle_{x \sim g_i(x)} - \left\langle \alpha_i(x) \frac{f(x)}{g_i(x)} \right\rangle_{x \sim g_i(x)}^2$$

Total variance depends on N_i

↓
affects optimal $\alpha_i(x)$

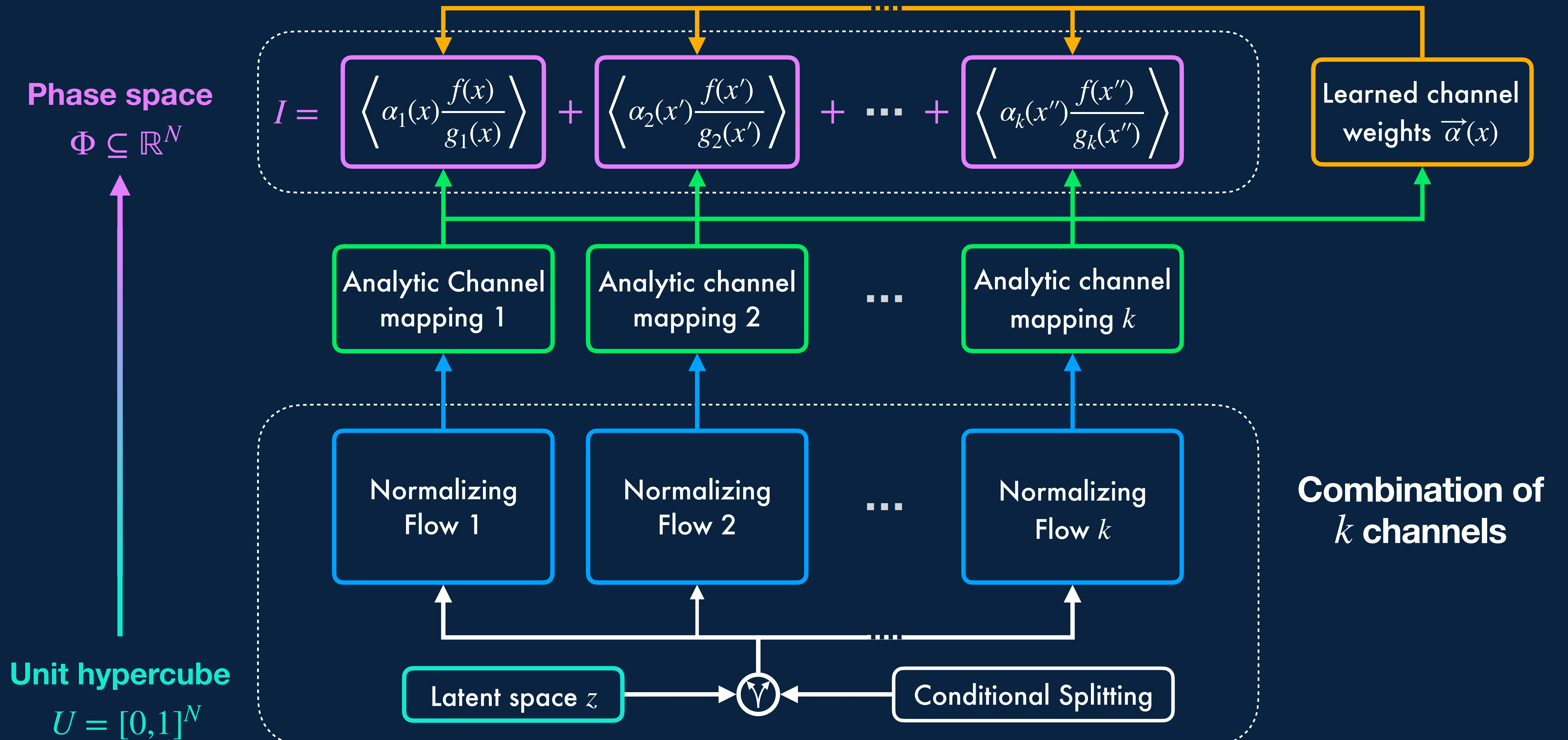
↓
use stratified sampling

$$N_i = N \frac{\sigma_i}{\sum_k \sigma_k}$$

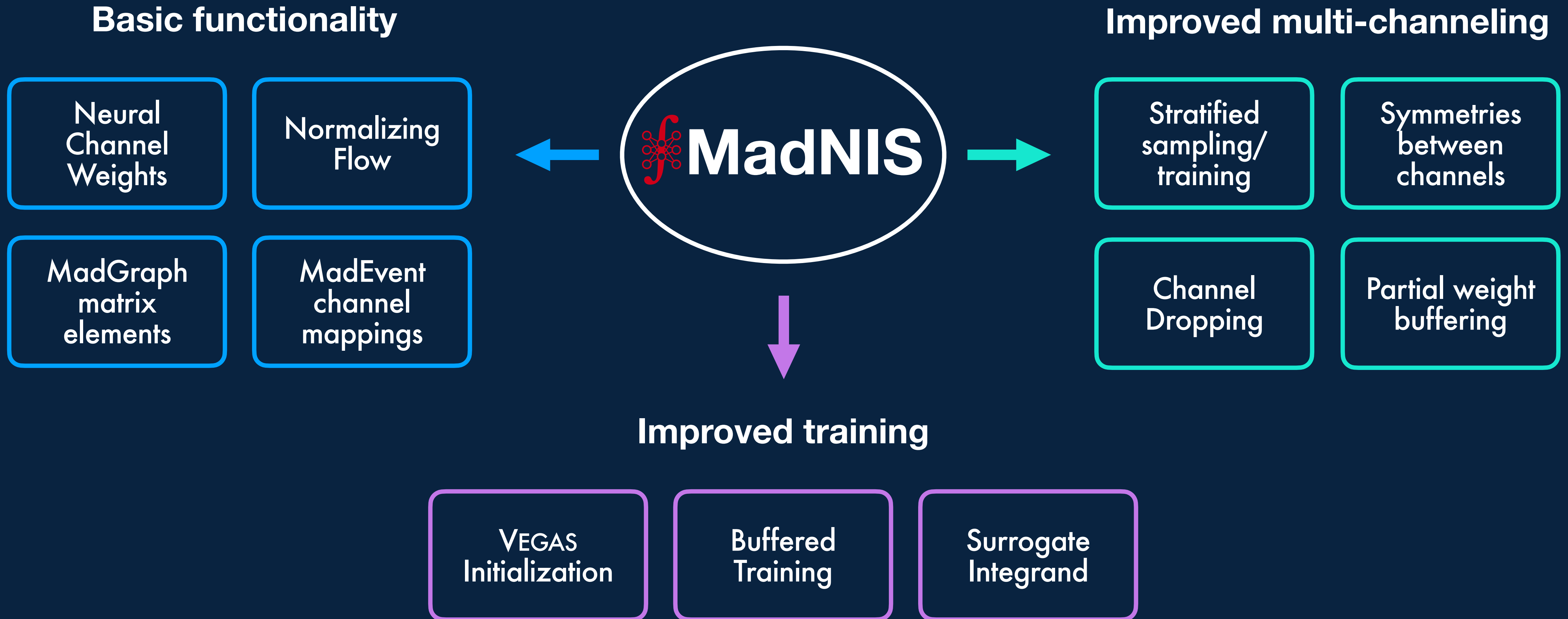
MadNIS loss function

$$\mathcal{L} = \sigma_{\text{tot}}^2 = \sum_{i,k} \sigma_i \sigma_k = \left[\sum_i \sigma_i \right]^2$$

MadNIS – Basic functionality



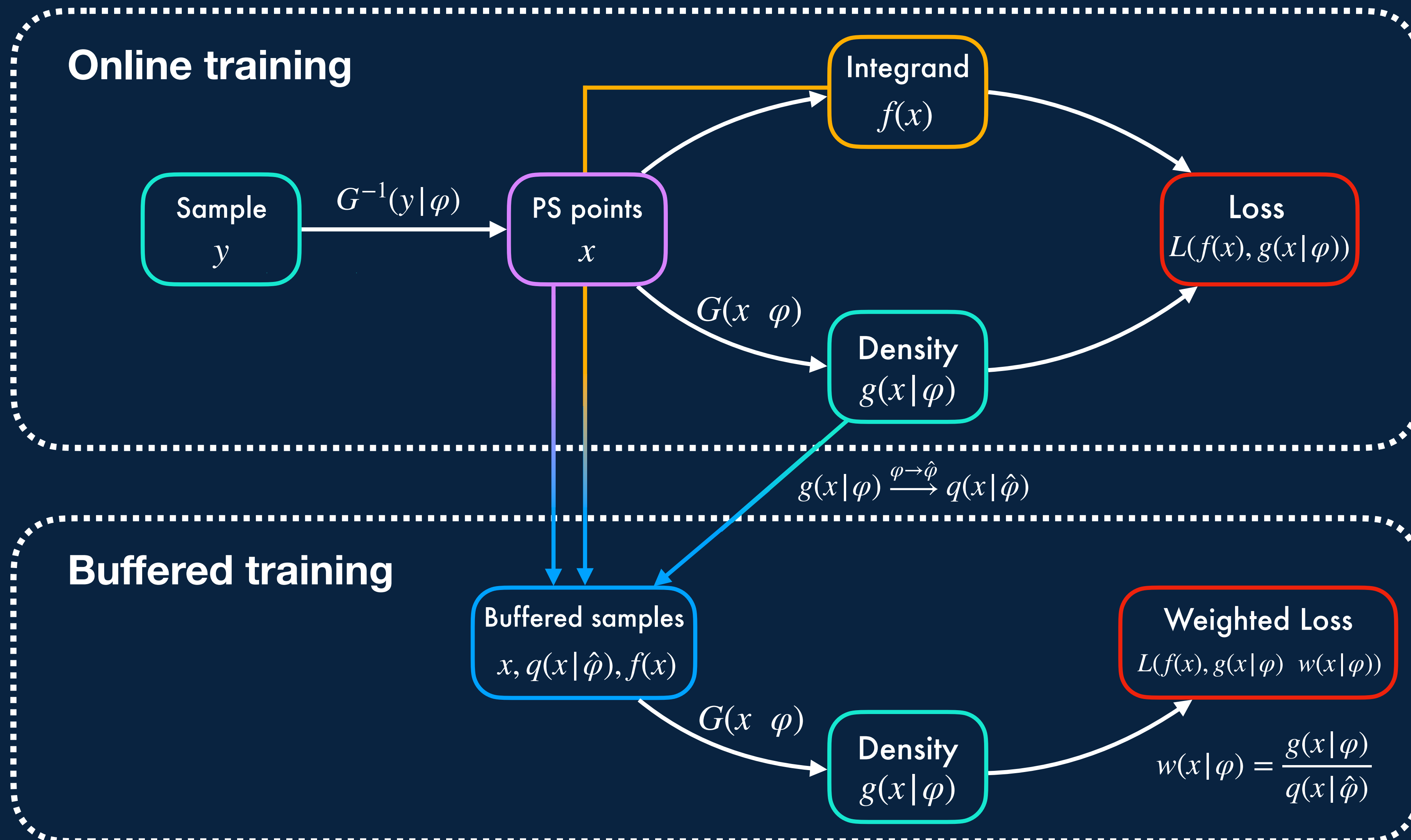
MadNIS — Overview



MadNIS — Buffered training



MadNIS – Buffered training



MadNIS — Buffered training

Training algorithm

generate new samples, train on them,
save samples



train on saved samples n times

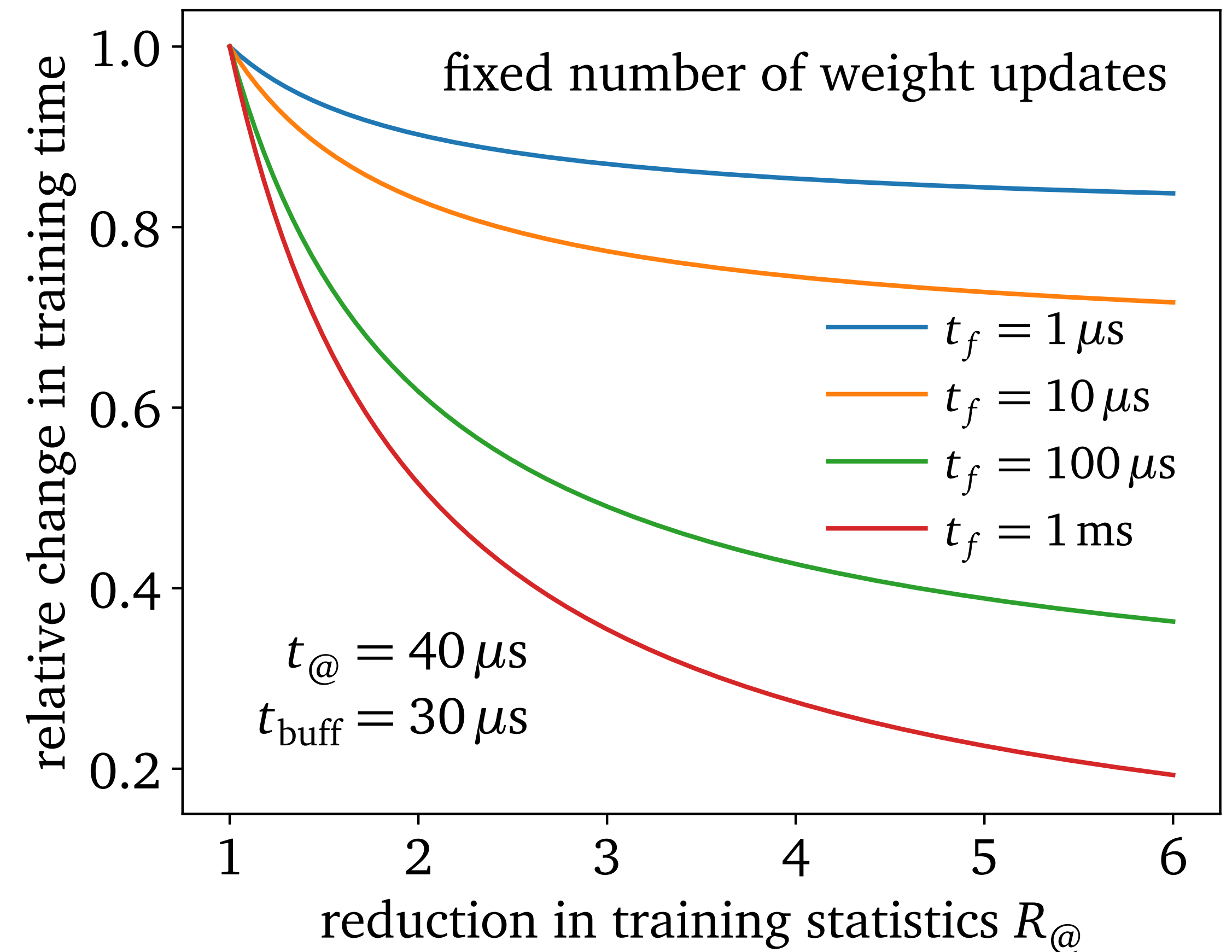


repeat



Reduction in training statistics by

$$R_{@} = n + 1$$



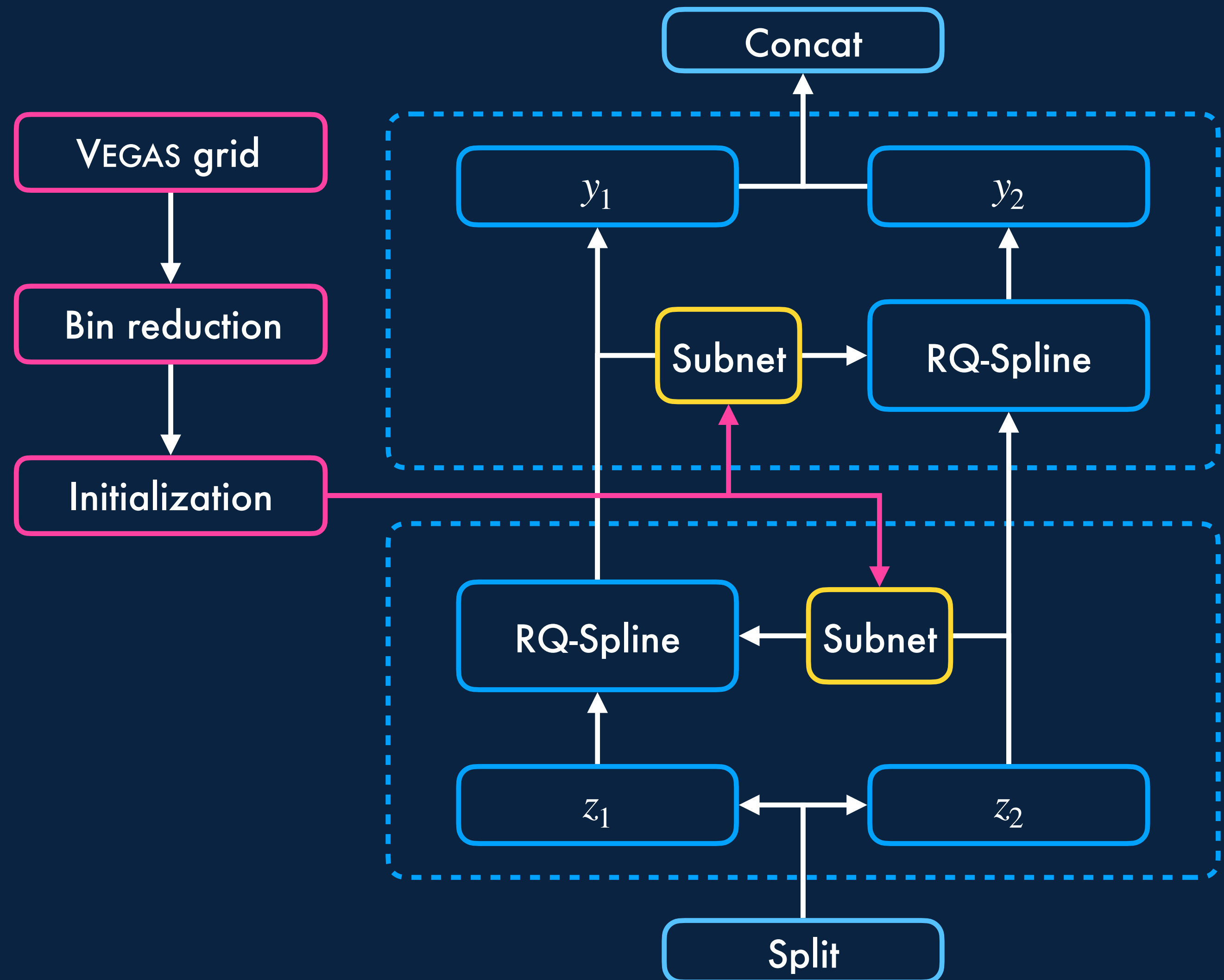
MadNIS — VEGAS initialization



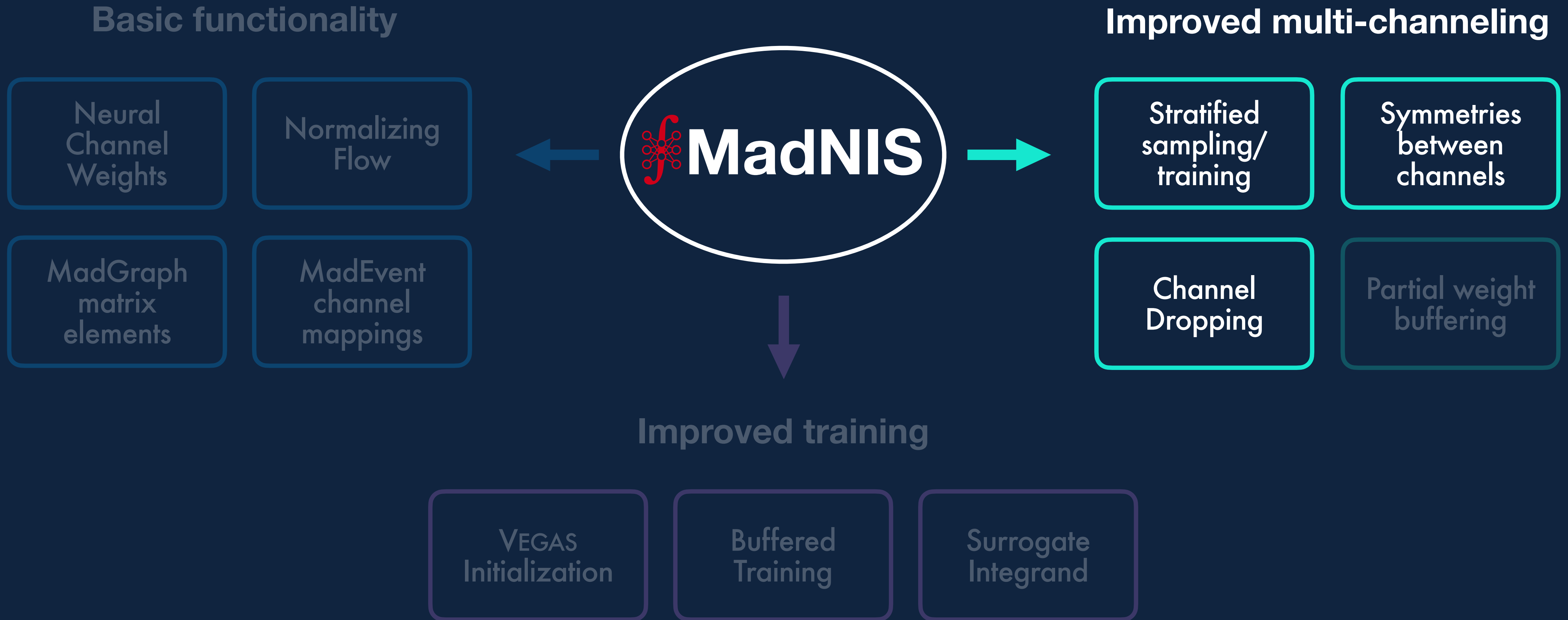
MadNIS — VEGAS initialization

	VEGAS	Flow
Training	Fast	Slow
Correlations	No	Yes

Combine advantages:
Pre-trained VEGAS grid as
starting point for flow training



MadNIS – Improved multi-channeling



MadNIS – Improved multi-channeling

37

Use symmetries

Groups of channels only **differ by permutations** of final state momenta



use **common** flow **combine** in loss function

Stratified training

Channels have different **contributions** to the total variance



more samples for channels with **higher variance** during training

Channel dropping

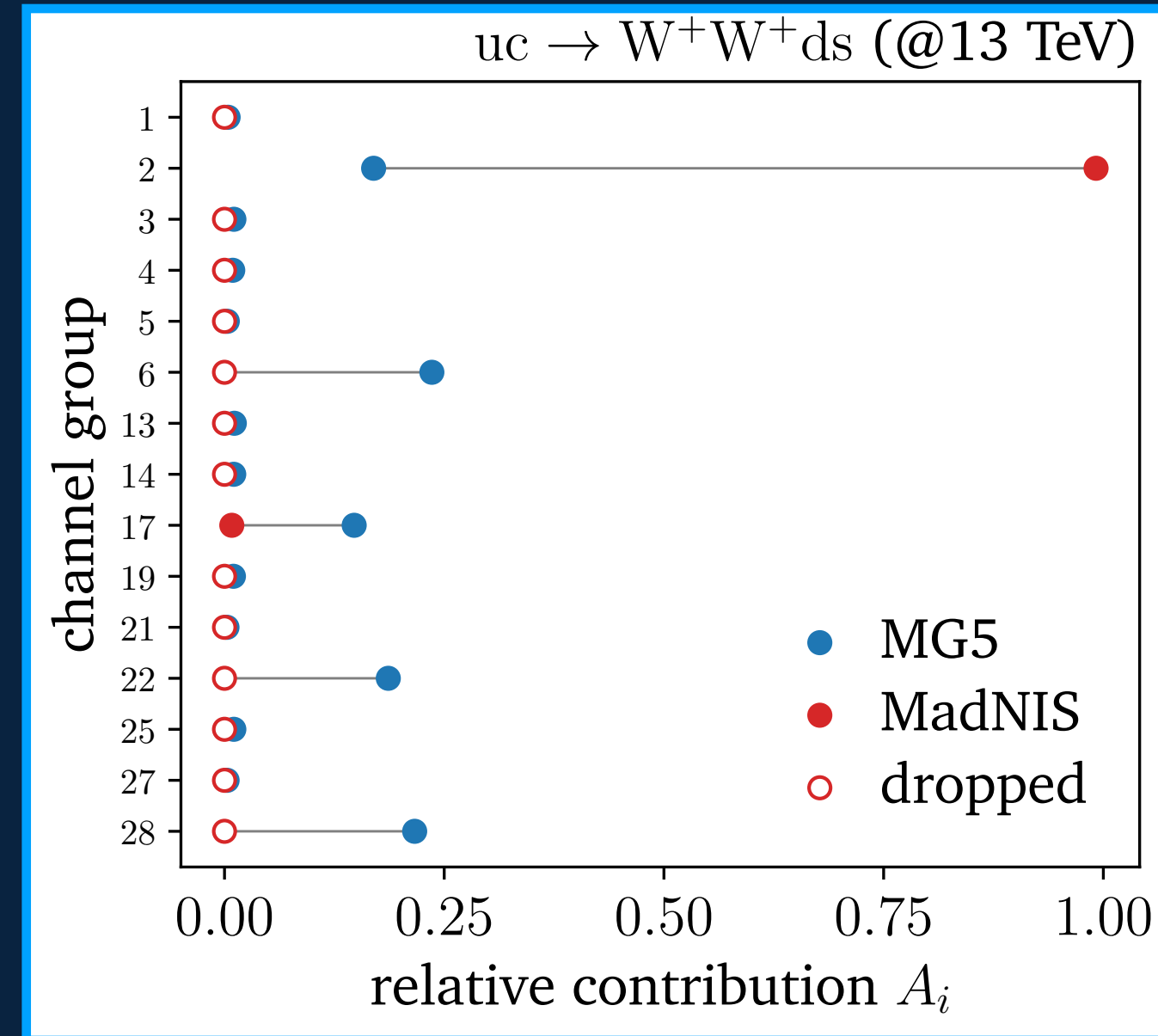
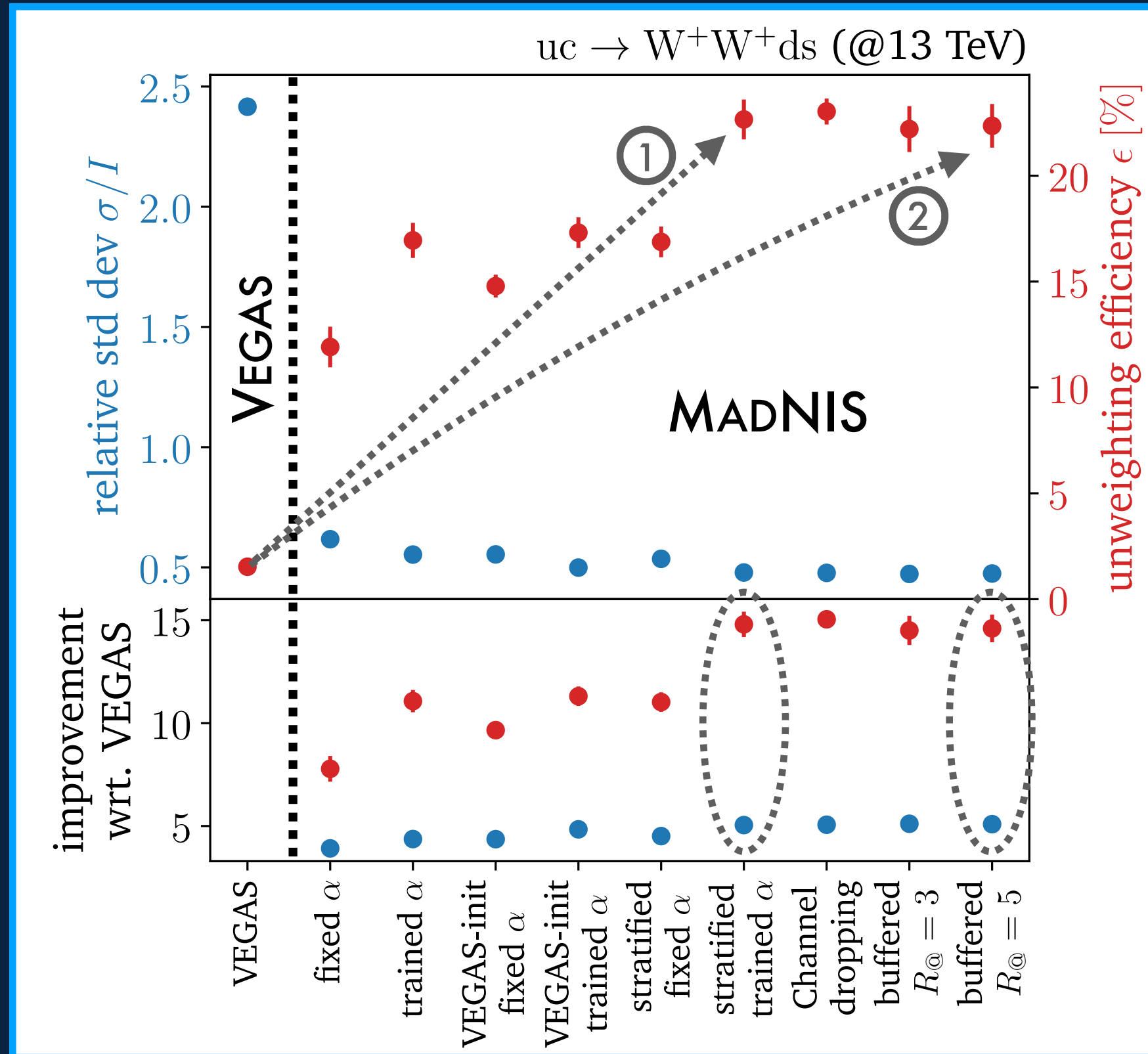
MadNIS often **reduces contribution** of some channels to total integral



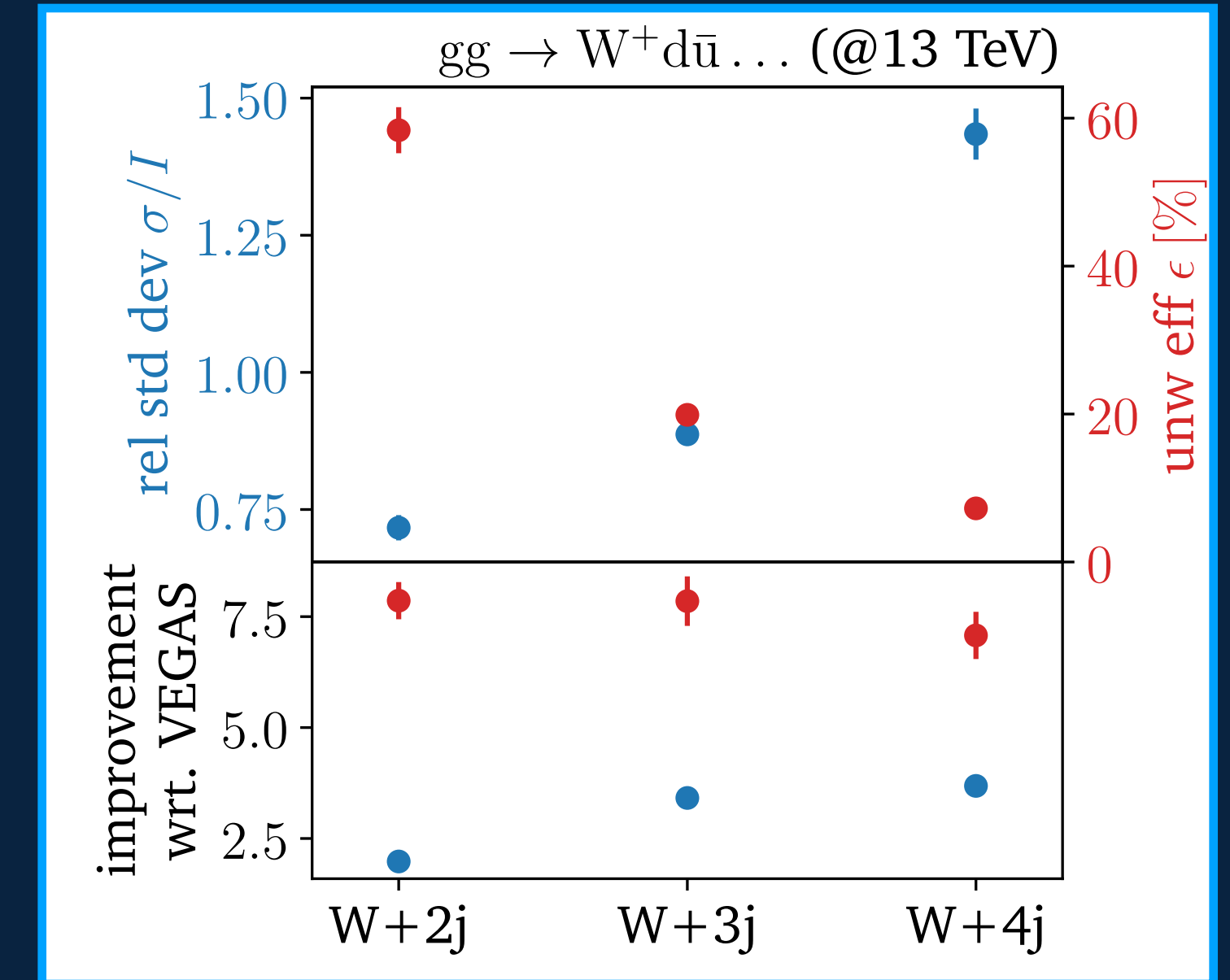
remove these channels from the **training** completely

Reduced complexity
Improved stability

MadNIS — Results



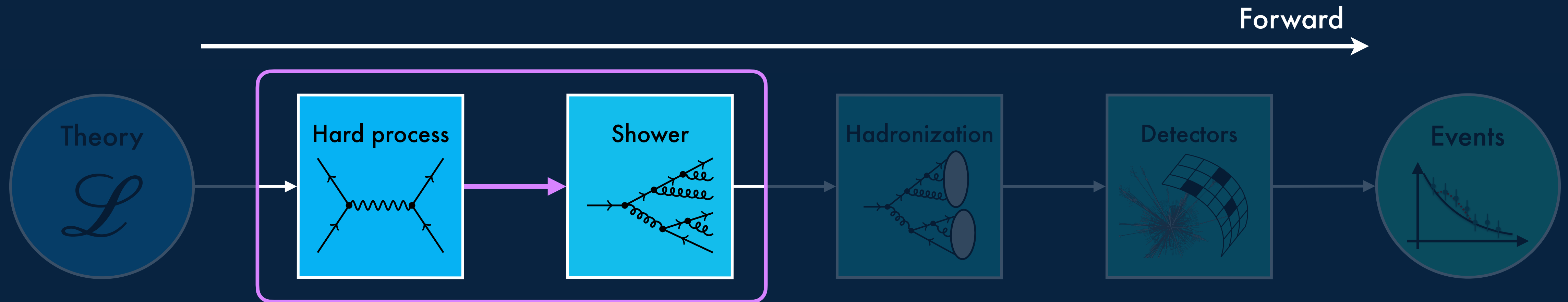
many channels **are zero**
 ↓
 dropping channels



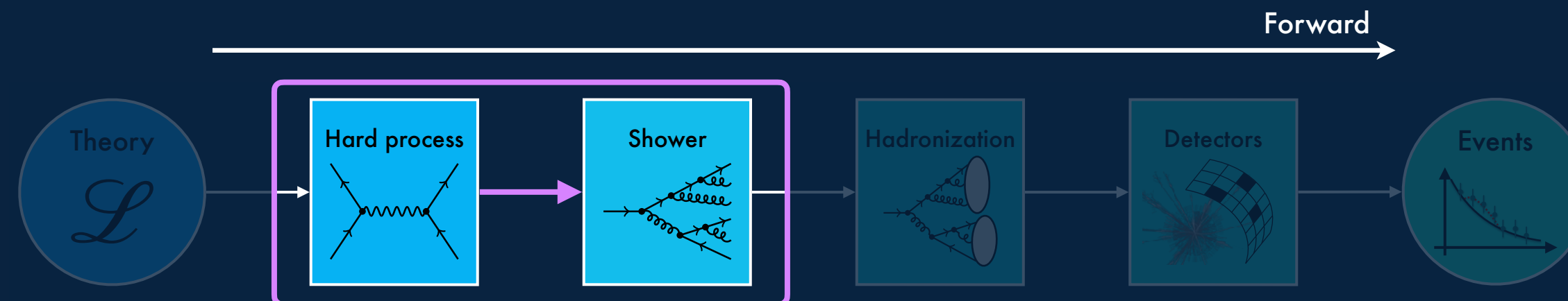
gg \rightarrow W⁺dūgg
 384 channels, 108 symm.
 $\eta = 7.5\% = 5.9 \eta_{\text{VEGAS}}$
 ↓
 scales well with high multiplicity and many channels

1. excellent results with all improvements
2. same performance with buffered training

ML for forward simulations



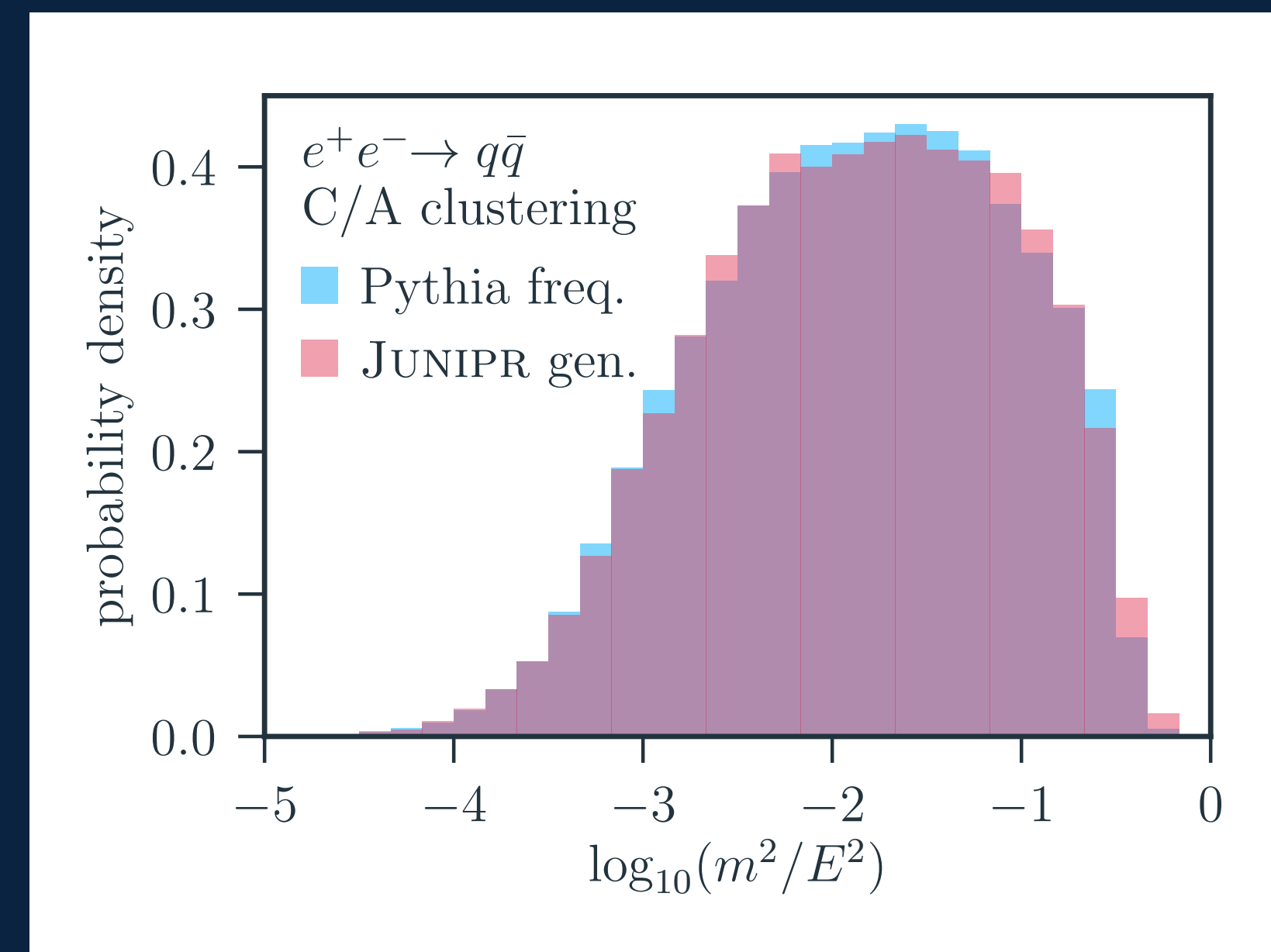
ML for forward simulations



Parton shower: improve over semi-classical approach

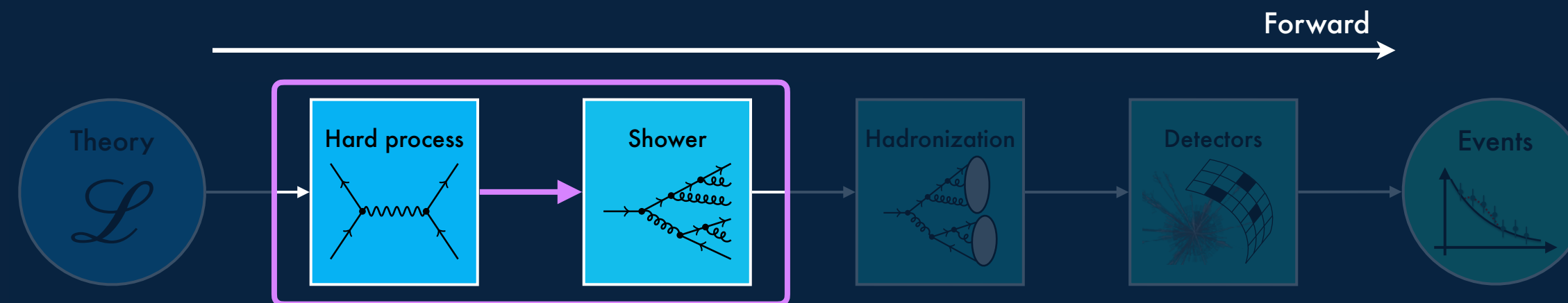
- Splittings are iterative
→ can be learned with RNN (**JUNIPR**)

Andreassen, Feige, Frye, Schwartz [1804.09720]



[1701.05927, 1703.06114, 1804.09720, 1807.03685, 1808.07802, 1810.05165, 1906.10137, 2009.04842, 2012.06582, 2012.09873, 2106.11535, 2109.15197, 2111.12849, 2211.06406, 2211.10295, 2212.08751, 2301.08128, 2303.05376, 2304.01266, 2307.06836, 2310.00049,....]

ML for forward simulations

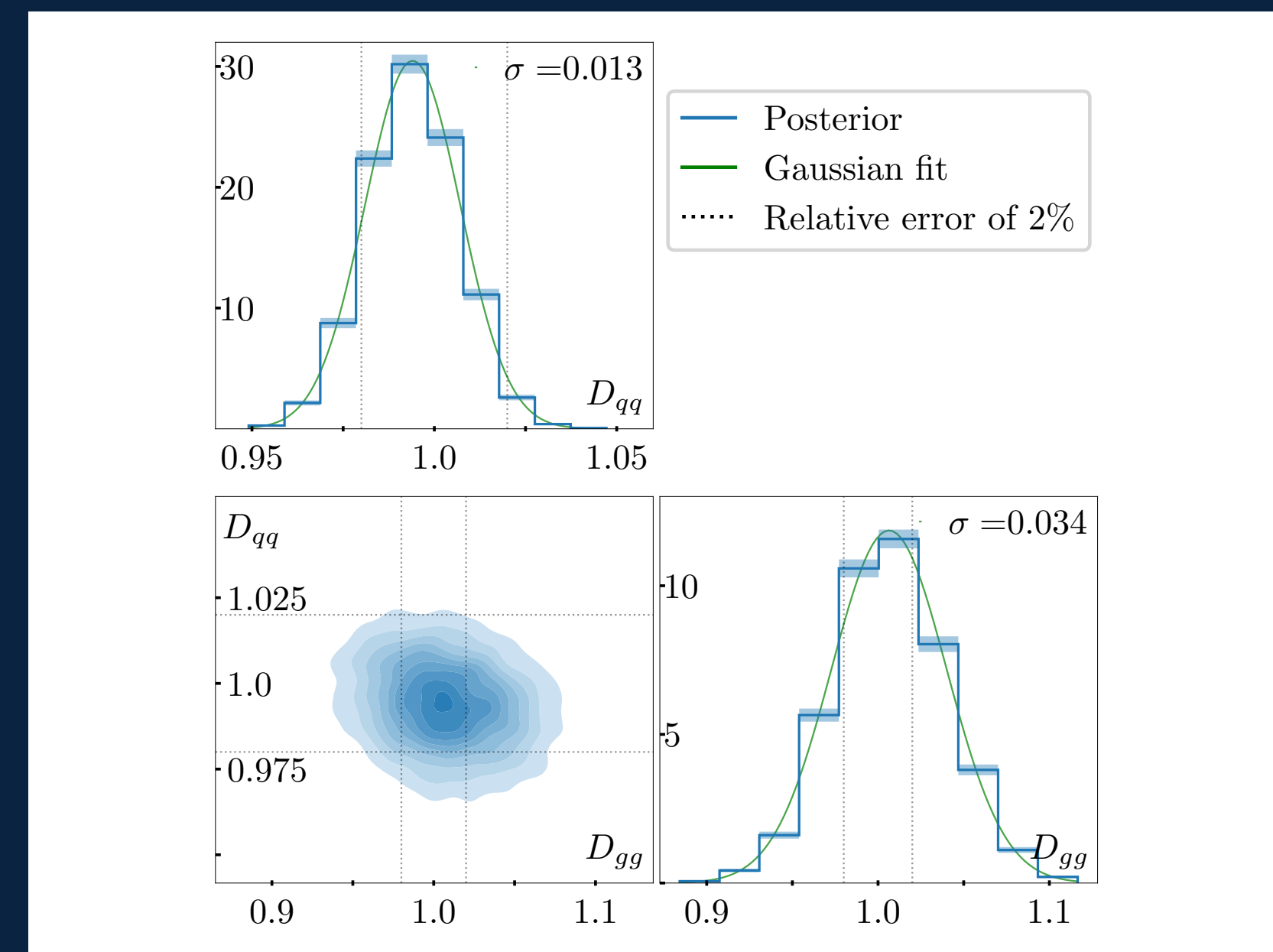


Parton shower: improve over semi-classical approach

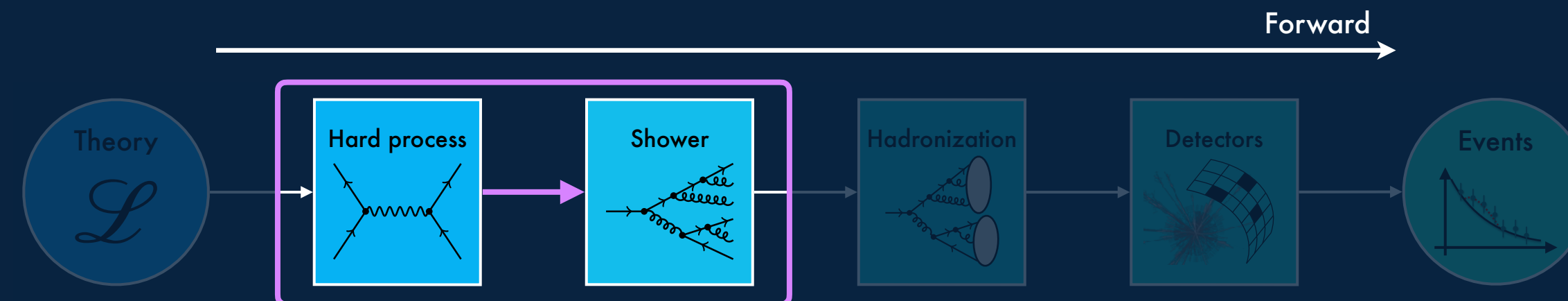
- Splittings are iterative
→ can be learned with RNN (**JUNIPR**)
- Using **ML-based inference** to improve splitting kernels

Bieringer, Butter, Heimgel, Höche, Radev, Köthe, Plehn [2012.09873]

[1701.05927, 1703.06114, 1804.09720, 1807.03685, 1808.07802, 1810.05165, 1906.10137, 2009.04842, 2012.06582, 2012.09873, 2106.11535, 2109.15197, 2111.12849, 2211.06406, 2211.10295, 2212.08751, 2301.08128, 2303.05376, 2304.01266, 2307.06836, 2310.00049,....]



ML for forward simulations

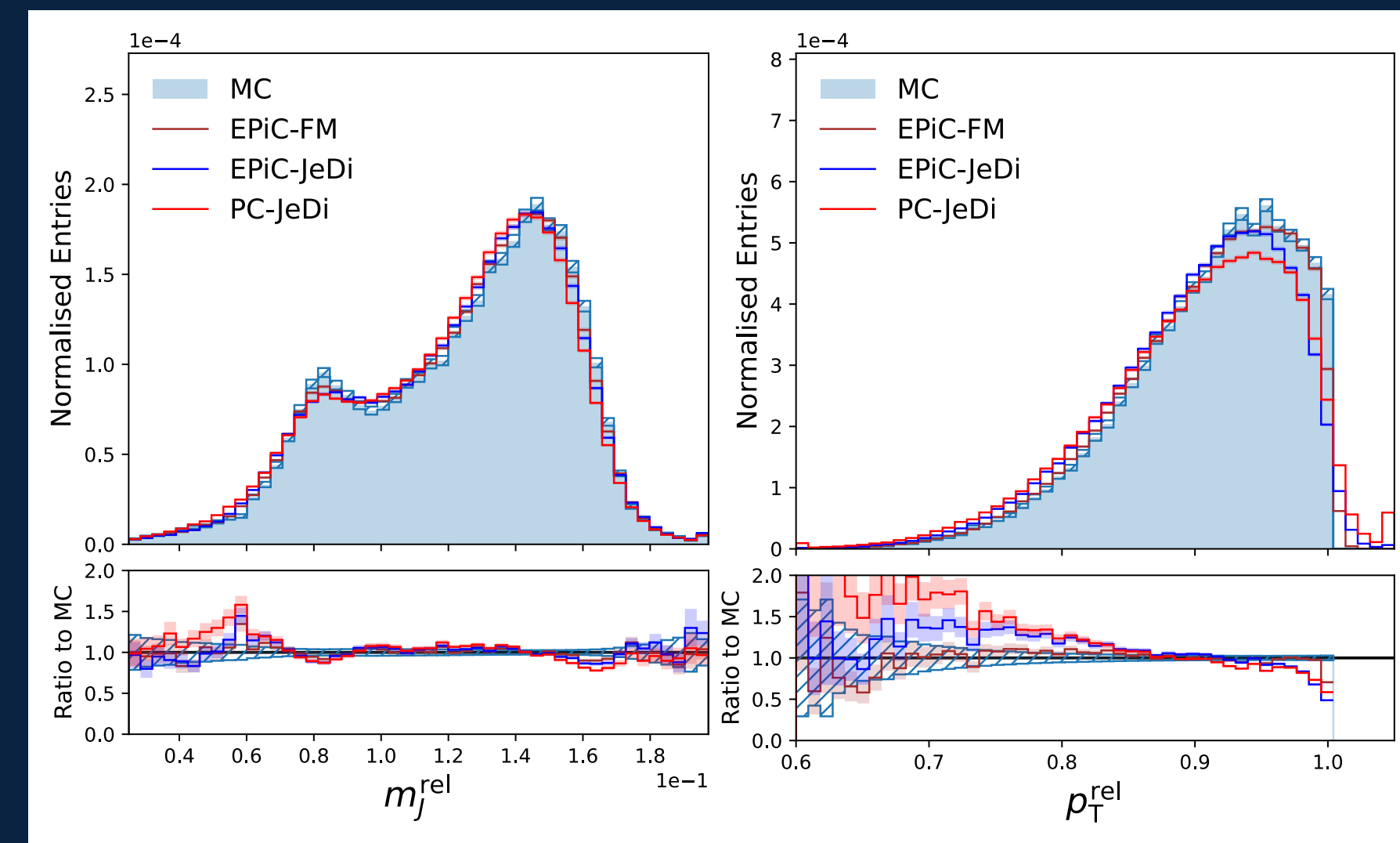


Parton shower: improve over semi-classical approach

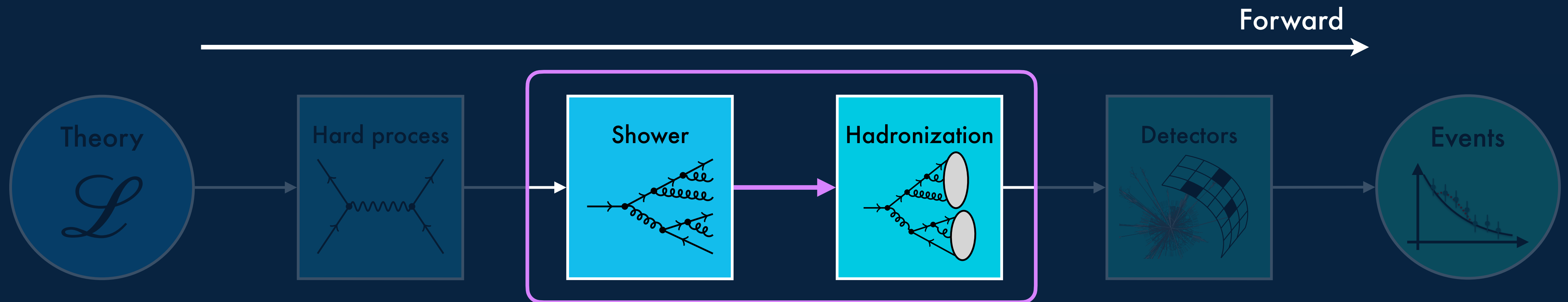
- Splittings are iterative
→ can be learned with RNN (**JUNIPR**)
- Using **ML-based inference** to improve splitting kernels
- End-to-end generation with **particle clouds**
→ SOTA based on **diffusion models**

[1701.05927, 1703.06114, 1804.09720, 1807.03685, 1808.07802, 1810.05165, 1906.10137, 2009.04842, 2012.06582, 2012.09873, 2106.11535, 2109.15197, 2111.12849, 2211.06406, 2211.10295, 2212.08751, 2301.08128, 2303.05376, 2304.01266, 2307.06836, 2310.00049,....]

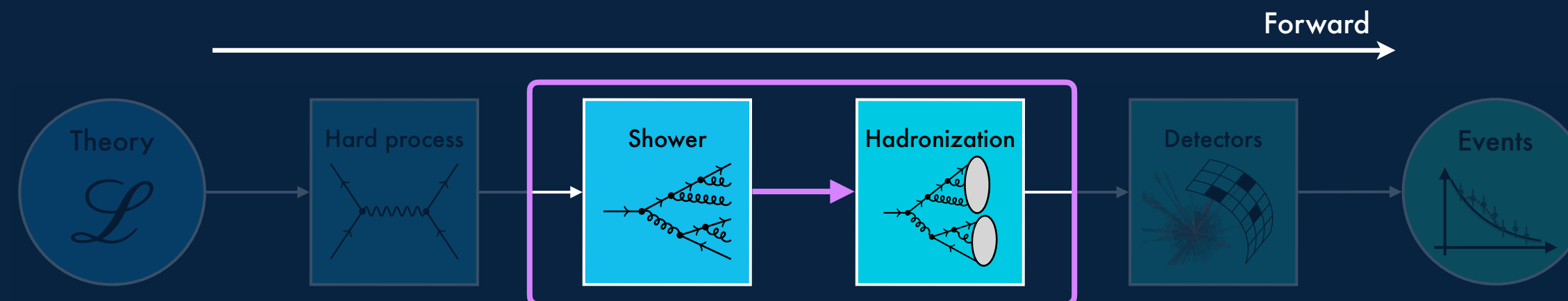
Buhmann et al. [2310.00049]



ML for forward simulations



ML for forward simulations



Fragmentation: remove modelling bias

- Same technique as for PDFs

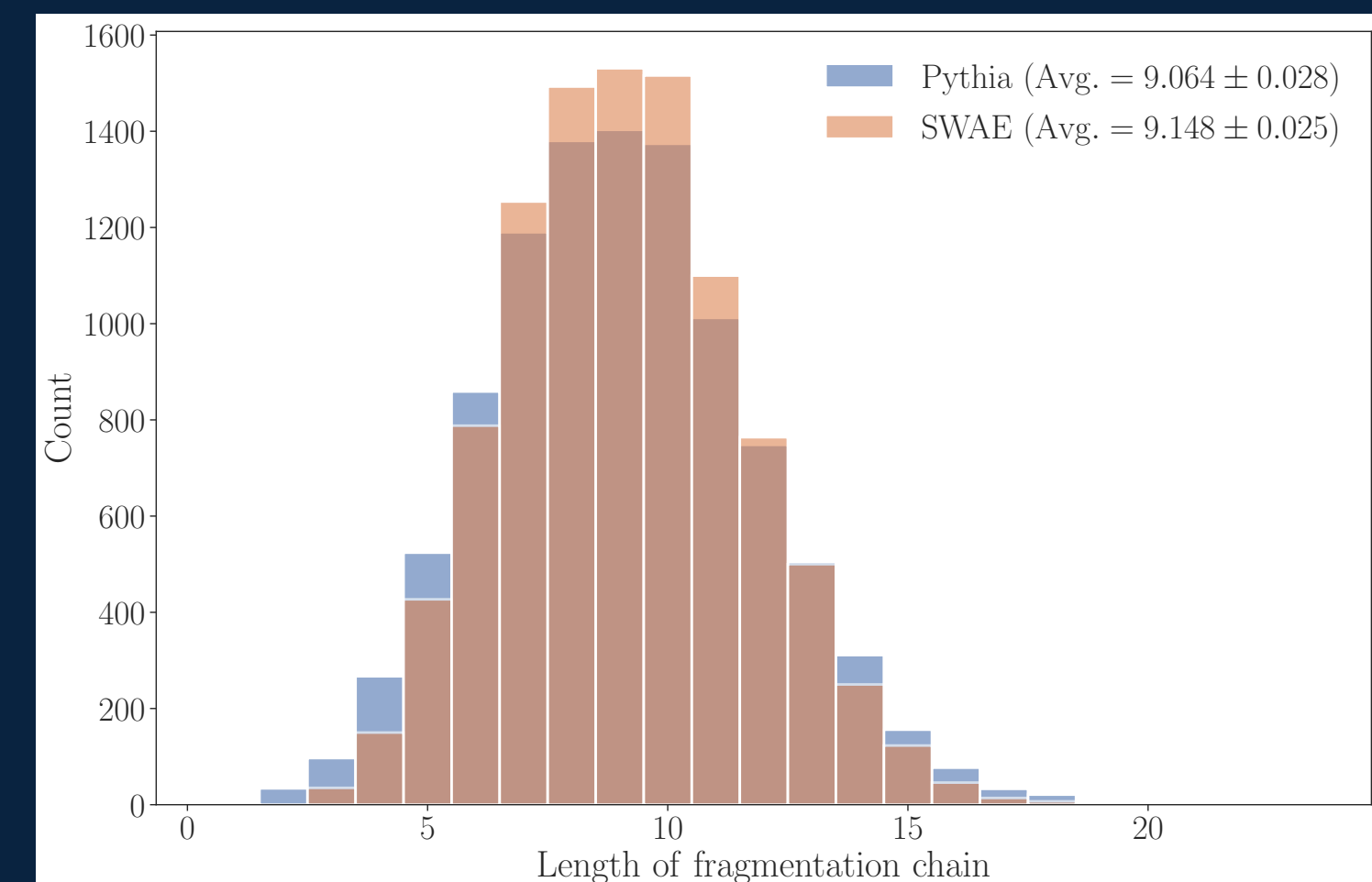
[1706.07049, 1807.03310, 2105.08725, 2202.10779.....]

Hadronization: better model non-perturbative effects

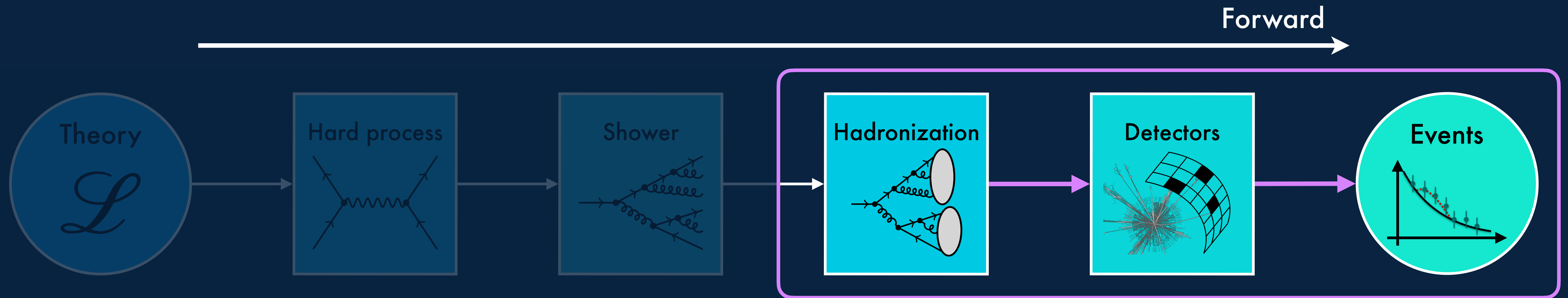
- Improve existing **clustering or Lund string** model
- **Generative ML** for more generic approach

[2203.04983, 2203.12660, 2305.17169,.....]

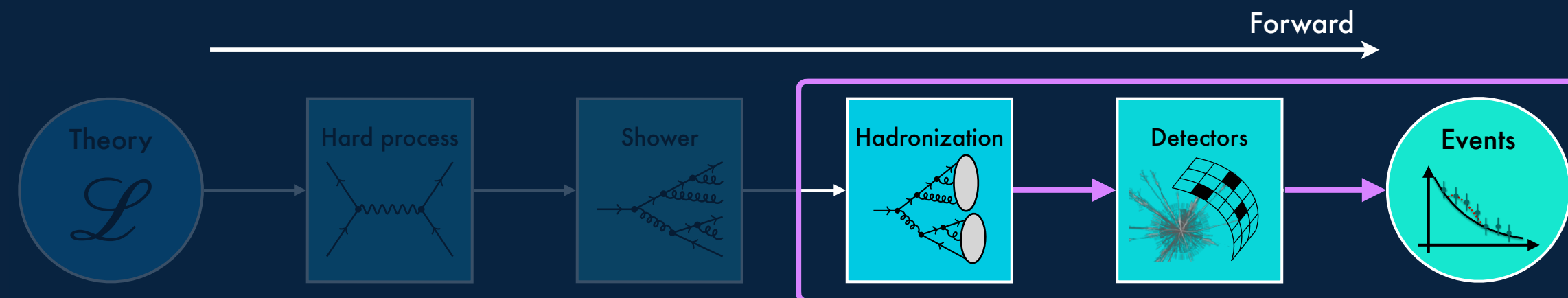
Ilten, Menzo, Youssef, Zupan [2203.04983]



ML for forward simulations



ML for forward simulations



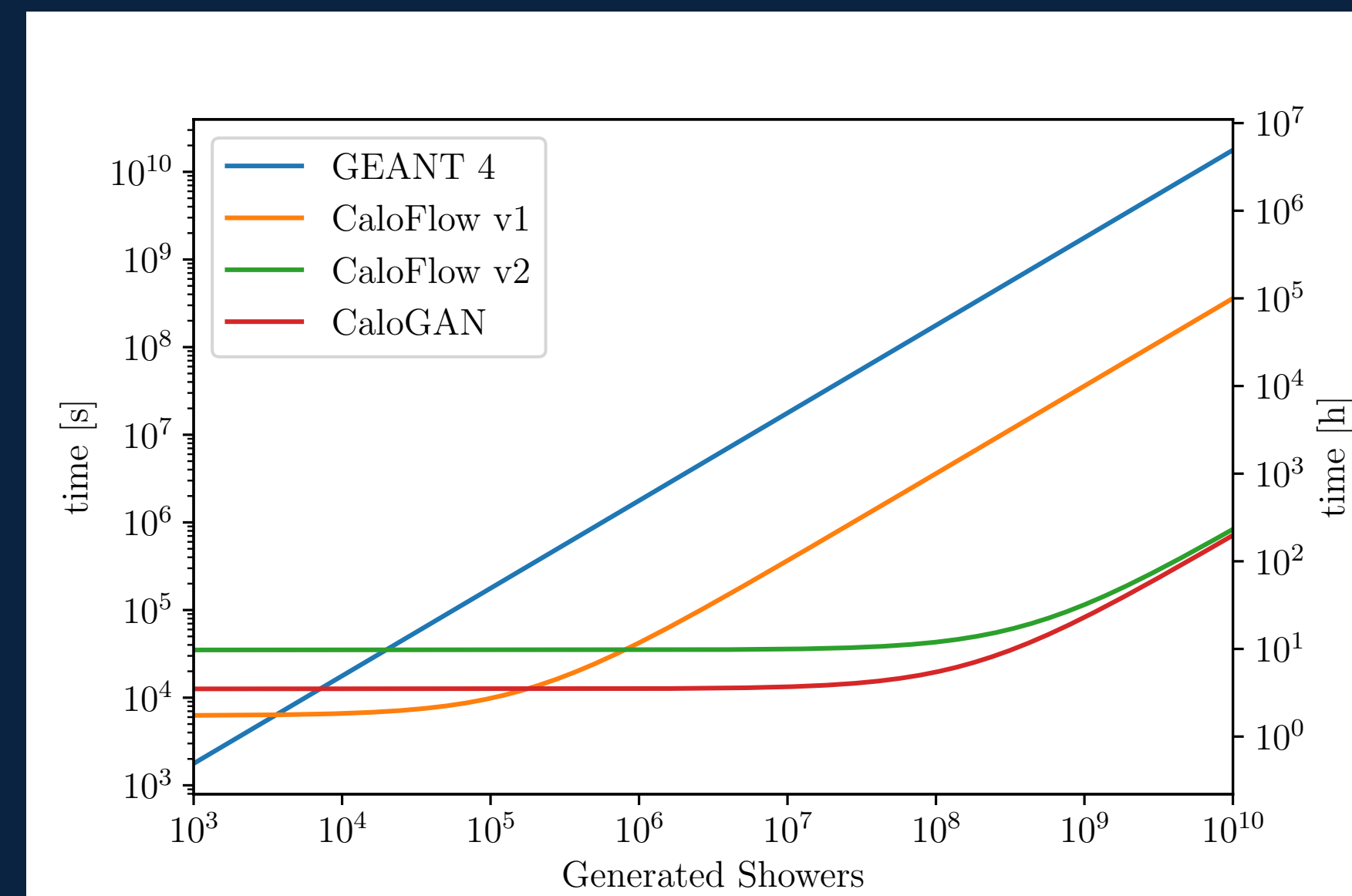
Detector simulation: speed-up GEANT4

- Up to $\sim 10^4$ faster
- More ideas developed in **CaloChallenge 2022**

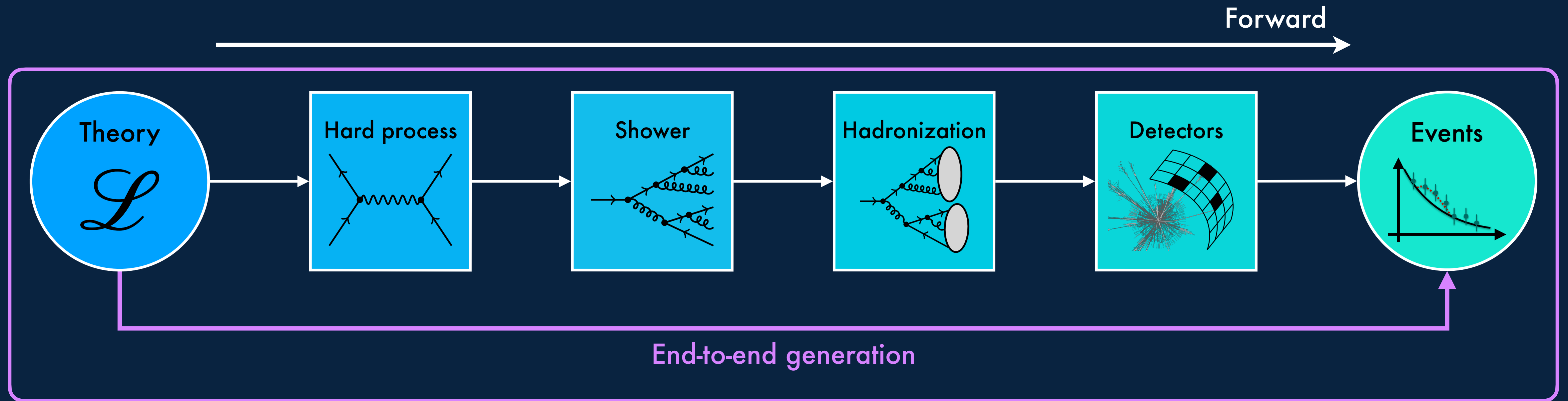
<https://calochallenge.github.io/homepage/>

[1705.02355, 1711.08813, 1712.10321, 1802.03325, 1807.01954, 1912.06794, 2102.12491, 2106.05285, 2109.02551, 2110.11377, 2206.11898, 2211.15380, 2302.11594, 2305.04847, 2305.11934, 2305.15254, 2307.04780, 2308.03876, 2308.11700, 2309.06515, ...]

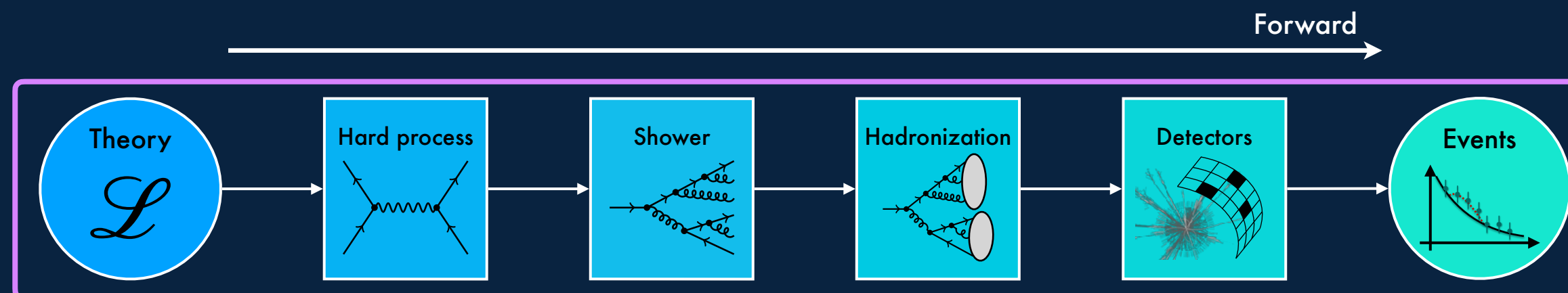
Krause, Shih [2110.11377]



ML for forward simulations



ML for forward simulations

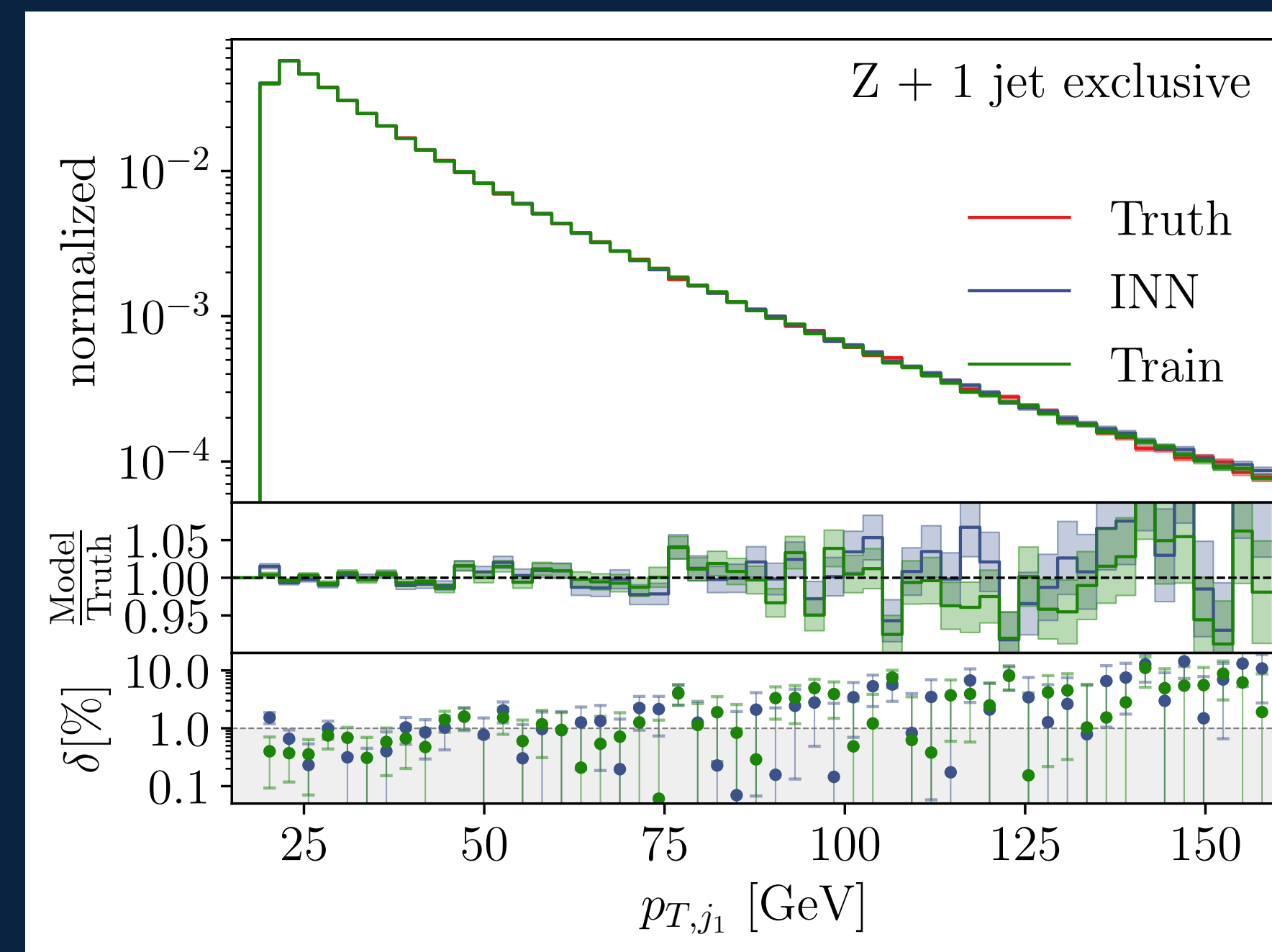


End-to-end generators learn multiple steps at once

Butter, HeimeI, Hummerich, Krebs, Plehn, Rousselot, Vent [2110.13632]

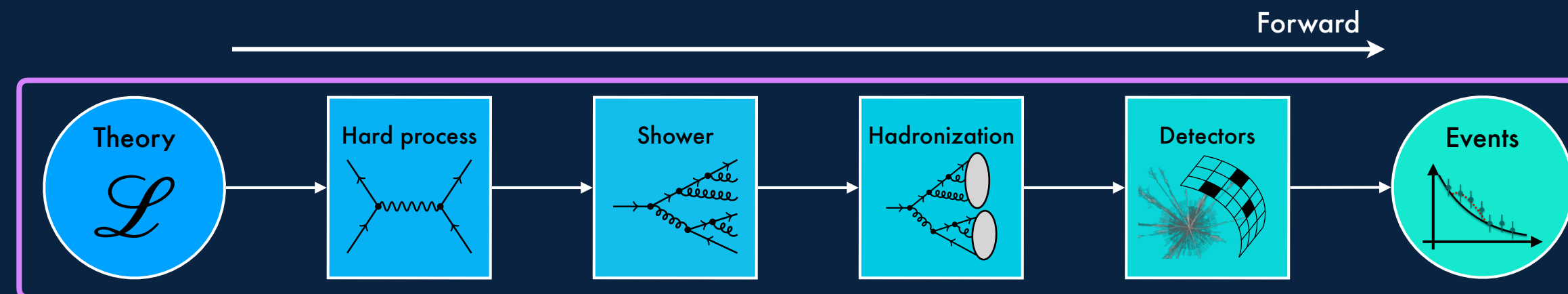
Precision generation

- First attempts based on **GANs and VAEs**
- Improved speed and efficiency with **Flows**



[1901.00875, 1901.05282, 1903.02433, 1907.03764, 1912.02748, 2001.11103, 2011.13445, 2101.08944, 2110.13632, 2211.13630, 2303.05376, 2305.07696, 2305.10475, 2305.16774, 2307.06836]

ML for forward simulations



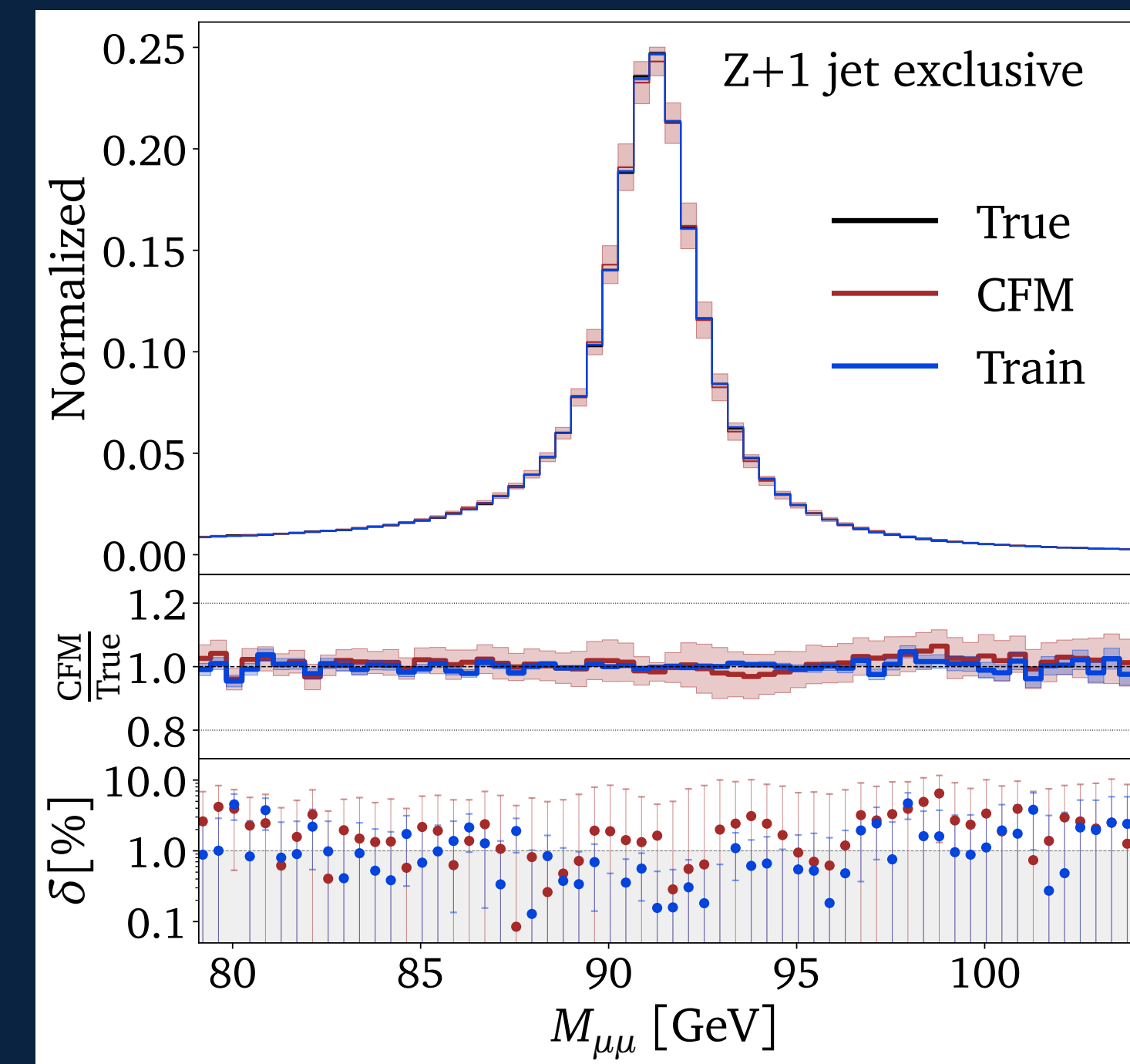
End-to-end generators learn multiple steps at once

Precision generation

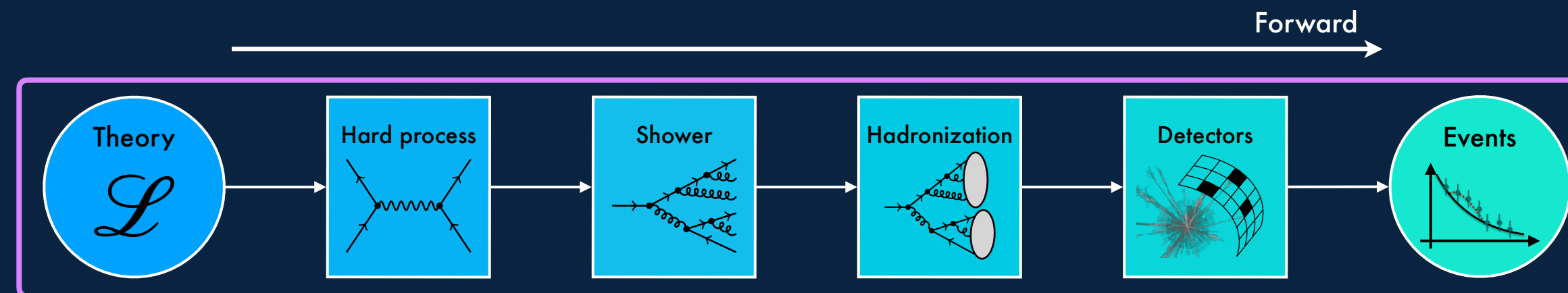
- First attempts based on **GANs and VAEs**
- Improved speed and efficiency with **Flows**
- High precision with **Diffusion** and **Transformer** models

[1901.00875, 1901.05282, 1903.02433, 1907.03764, 1912.02748, 2001.11103, 2011.13445, 2101.08944, 2110.13632, 2211.13630, 2303.05376, 2305.07696, 2305.10475, 2305.16774, 2307.06836]

Butter, Huetsch, Schweitzer, Plehn, Sorrenson, Spinner [2110.11377]



ML for forward simulations



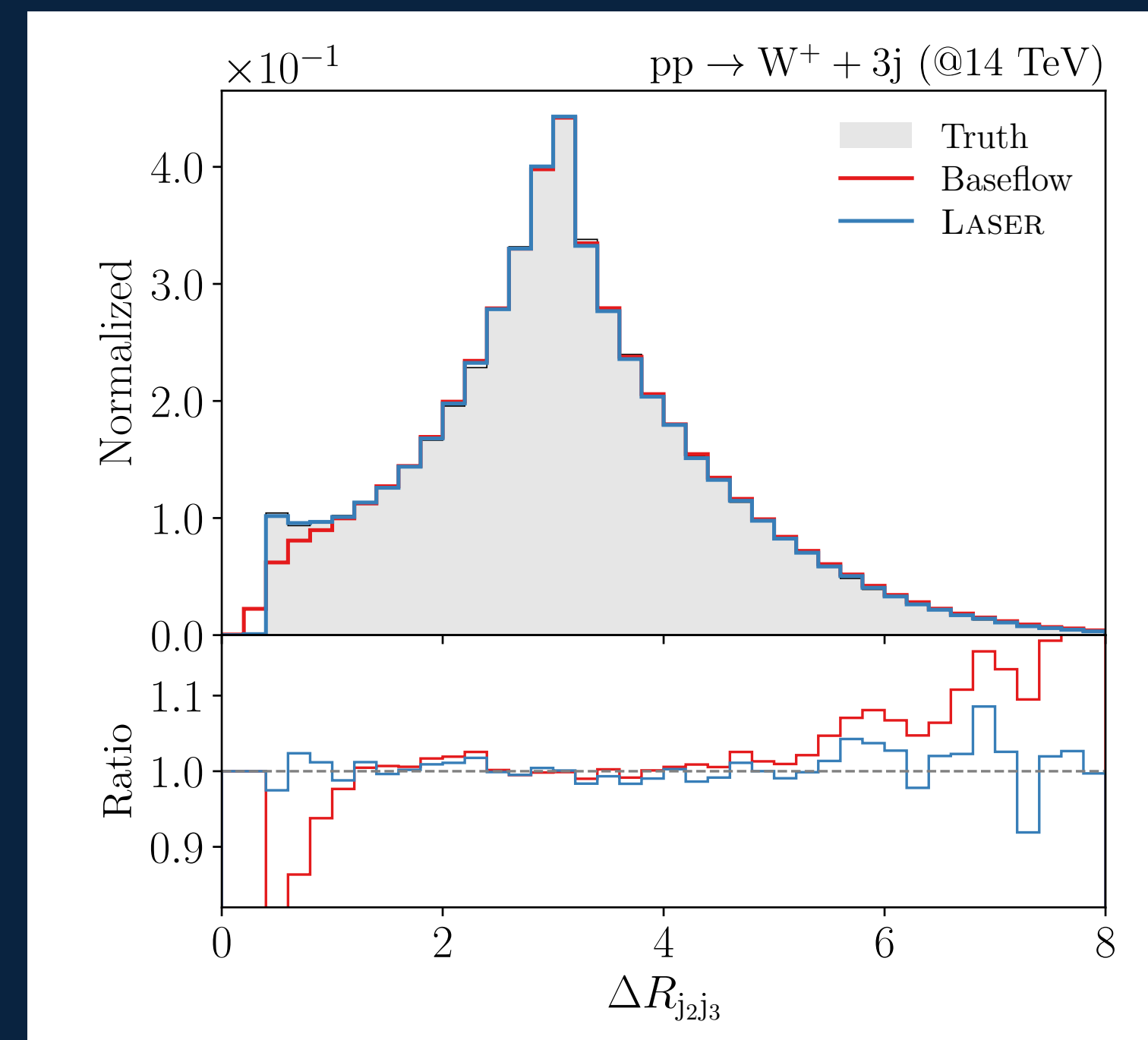
End-to-end generators learn multiple steps at once

Precision generation

- First attempts based on **GANs and VAEs**
- Improved speed and efficiency with **Flows**
- High precision with **Diffusion** and **Transformer** models
- **Bayesian NN** and **classifiers** for full control

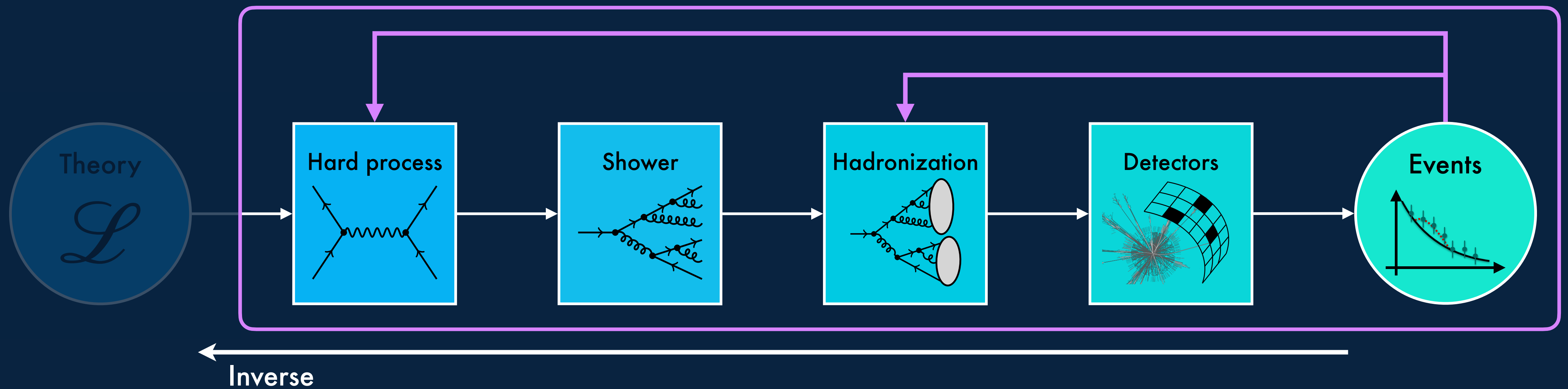
[1901.00875, 1901.05282, 1903.02433, 1907.03764, 1912.02748, 2001.11103, 2011.13445, 2101.08944, 2110.13632, 2211.13630, 2303.05376, 2305.07696, 2305.10475, 2305.16774, 2307.06836]

Nachman, RW [2305.07696]



ML for inverse simulations

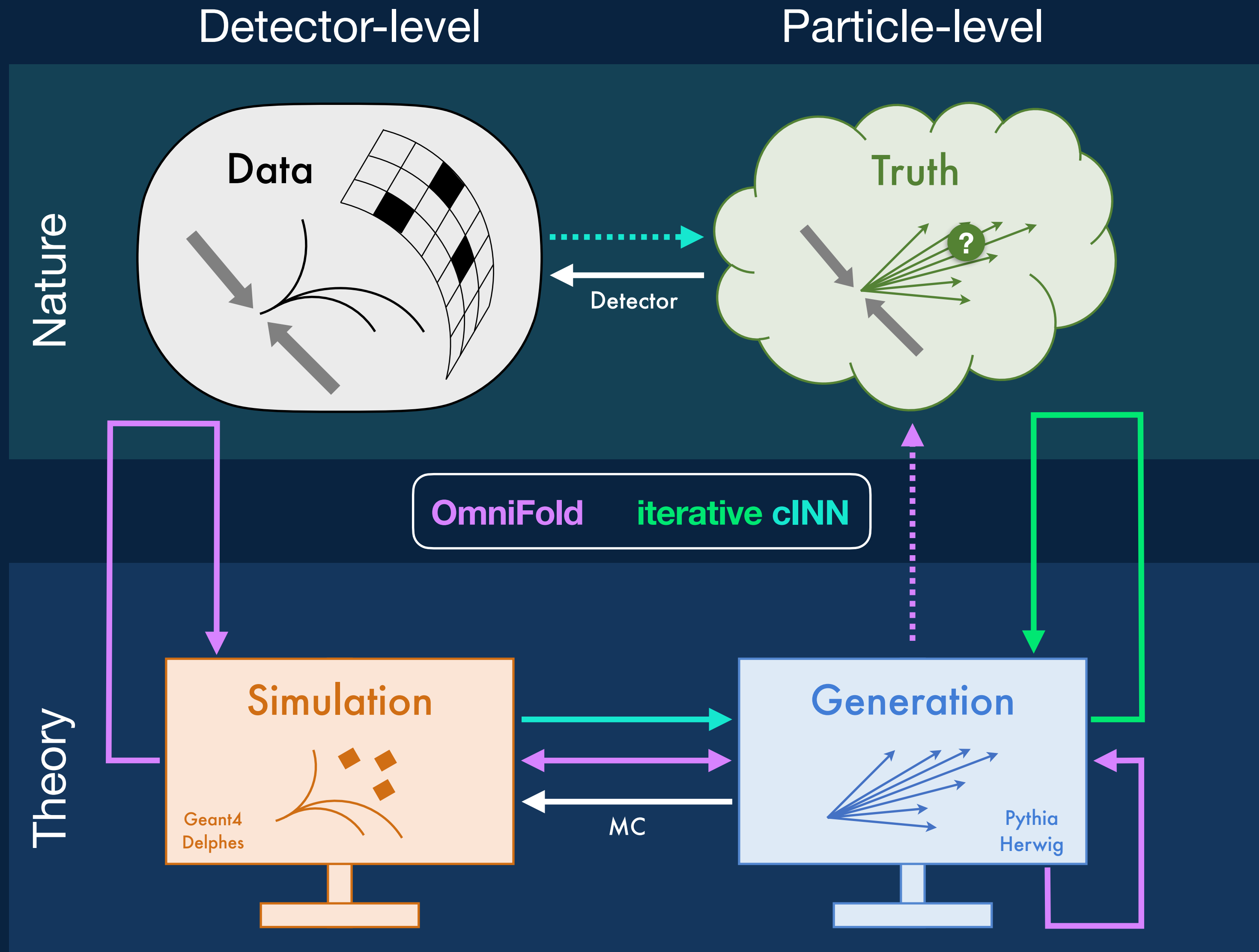
Unfolding



Unfolding

Classifier-based ↔ **Density-based**
reweighting generative

Unfolding – Basic concept



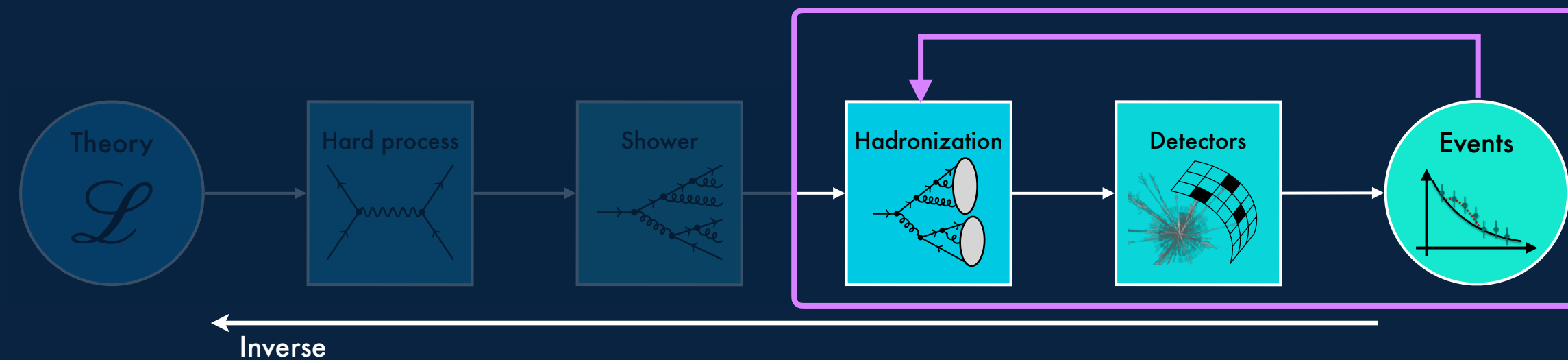
- Requirements:
- ✓ High dimensional
 - ✓ Unbinned
 - ✓ Statistically well defined

Omnifold [1911.09107]
Andreassen, Komiske, Metodiev, Nachman

cINN [2006.06685]
Bellagente, Butter, Kasieczka, Plehn, Rousselot, RW, Ardizzone, Köthe

lcINN [2212.08674]
Backes, Butter, Dunford, Malaescu

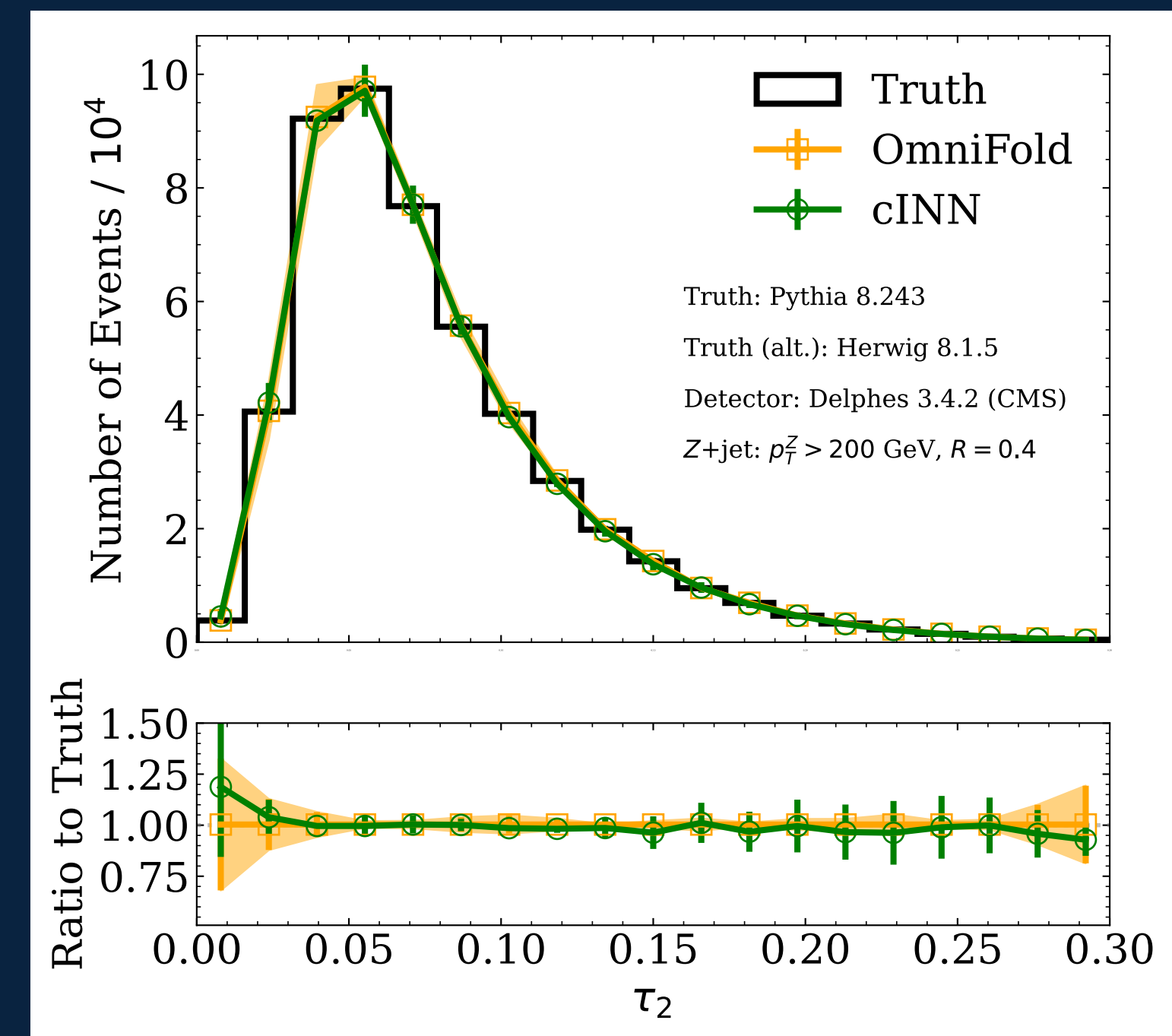
ML for inverse simulations



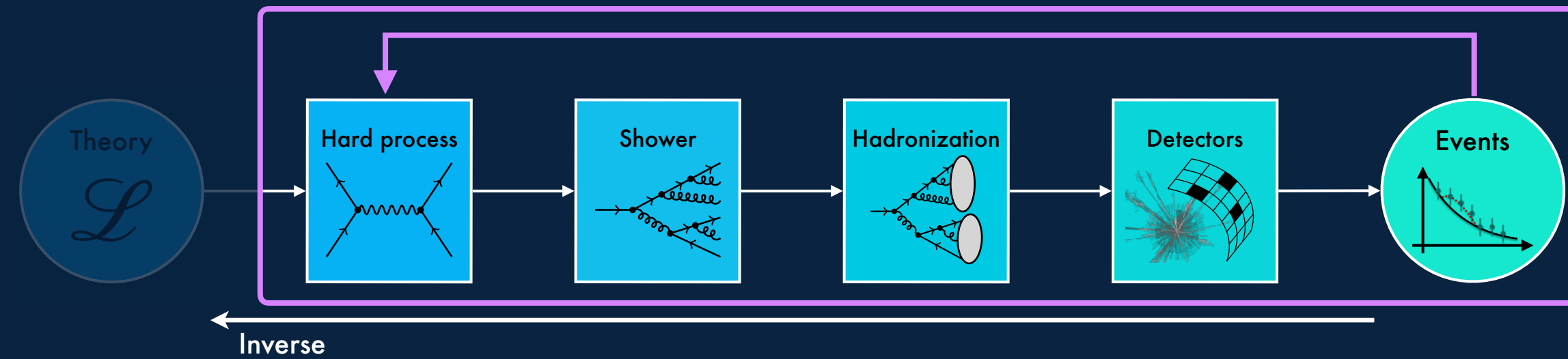
Unfolding of detector effects

- Must be high-dimensional, unbinned, and statistically well-defined
- **Classifier-based** MC reweighting
[1911.09107, 2105.04448, 2105.09923, 2109.13243, 2302.05390]
- **Density-based** generative unfolding
[1806.00433, 1912.00477, 2006.06685, 2101.08944, 2109.13243, 2207.00664, 2212.08674, 2305.10399, 2307.02405, 2308.00027, 2308.12351, 2310.17037]

Arratia et al. [2109.13243]



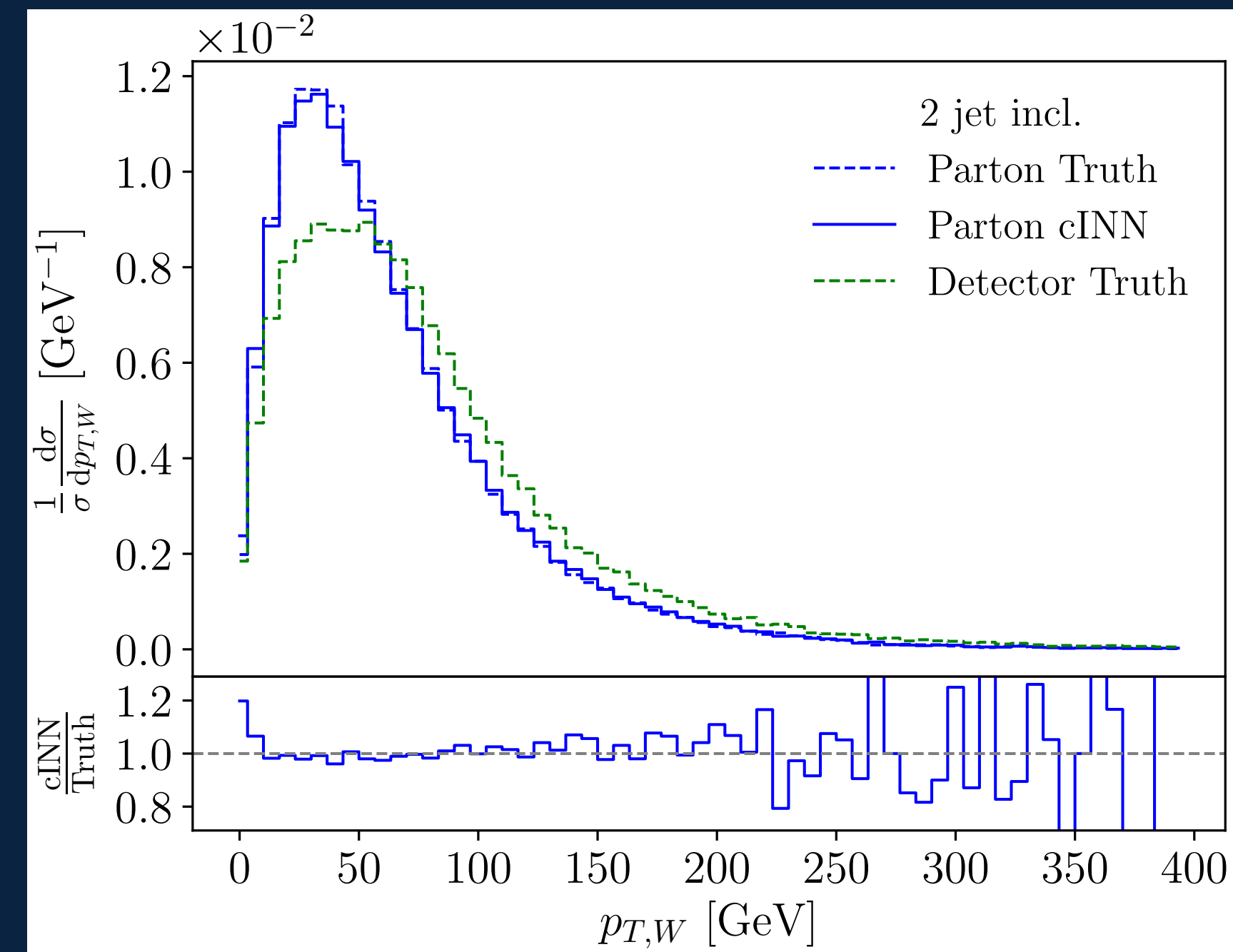
ML for inverse simulations



Inverting to parton level

- Inversion of **QCD radiation** and heavy particle (t,W,Z,h) decays
- Use same techniques as before (**cINNs**, **Classifiers** + others)

Bellagente, Butter, Kasieczka, Plehn, Rousselot, RW, Ardizzone, Köthe [2109.13243]



[1912.00477, 2006.06685, 2101.08944, 2207.00664, 2210.00019, 2307.02405, 2308.00027, 2310.07752]

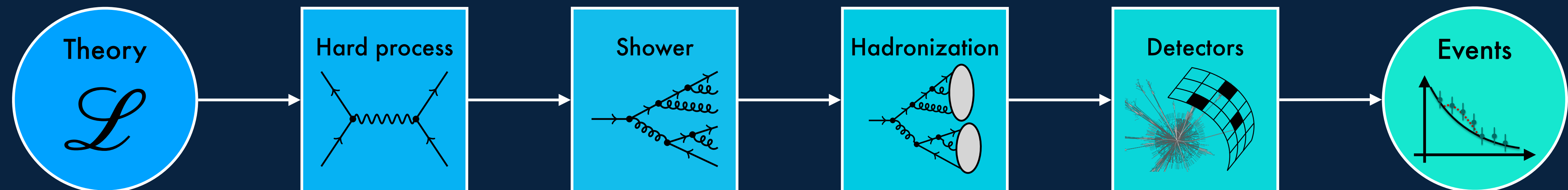
Summary and Outlook

Take-home message

- ML beneficial in **every step** in the simulation chain
- We find both **proof-of-concepts** as well as established use cases (→ **MadNIS**)
- Interesting **interplay** between **HEP** and **ML**
 - HEP simulations provide **~infinite data** for ML
 - HEP requirements (**precision, symmetries,...**) **different** than industry applications

Future tasks

- **Full integration** of ML-based simulations into standard tools → **MadGraph,....**
- Make everything run on the **GPU and differentiable** (MadJax - Heinrich et al. [[2203.00057](#)])
- Foster deeper collaboration between **theory, experiment,** and **ML** community



Summary and Outlook

Machine learning and LHC event generation

Anja Butter^{1,2}, Tilman Plehn¹, Steffen Schumann³, Simon Badger⁴, Sascha Caron^{5,6}, Kyle Cranmer^{7,8}, Francesco Armando Di Bello⁹, Etienne Dreyer¹⁰, Stefano Forte¹¹, Sanmay Ganguly¹², Dorival Gonçalves¹³, Eilam Gross¹⁰, Theo Heimel¹, Gudrun Heinrich¹⁴, Lukas Heinrich¹⁵, Alexander Held¹⁶, Stefan Höche¹⁷, Jessica N. Howard¹⁸, Philip Ilten¹⁹, Joshua Isaacson¹⁷, Timo Janßen³, Stephen Jones²⁰, Marumi Kado^{9,21}, Michael Kagan²², Gregor Kasieczka²³, Felix Kling²⁴, Sabine Kraml²⁵, Claudius Krause²⁶, Frank Krauss²⁰, Kevin Kröniger²⁷, Rahool Kumar Barman¹³, Michel Luchmann¹, Vitaly Magerya¹⁴, Daniel Maitre²⁰, Bogdan Malaescu², Fabio Maltoni^{28,29}, Till Martini³⁰, Olivier Mattelaer²⁸, Benjamin Nachman^{31,32}, Sebastian Pitz¹, Juan Rojo^{6,33}, Matthew Schwartz³⁴, David Shih²⁵, Frank Siegert³⁵, Roy Stegeman¹¹, Bob Stienen⁵, Jesse Thaler³⁶, Rob Verheyen³⁷, Daniel Whiteson¹⁸, Ramon Winterhalder²⁸, and Jure Zupan¹⁹

Abstract

First-principle simulations are at the heart of the high-energy physics research program. They link the vast data output of multi-purpose detectors with fundamental theory predictions and interpretation. This review illustrates a wide range of applications of modern machine learning to event generation and simulation-based inference, including conceptual developments driven by the specific requirements of particle physics. New ideas and tools developed at the interface of particle physics and machine learning will improve the speed and precision of forward simulations, handle the complexity of collision data, and enhance inference as an inverse simulation problem.

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- Foster deeper collaboration between **theory, experiment, and ML** community
- More details in our **Snowmass report**



Summary and Outlook



Future tasks

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- Make everything run on the **GPU and differentiable** (MadJax - Heinrich et al. [2203.00057])
- Foster deeper collaboration between **theory, experiment,** and **ML** community
- More details in our **Snowmass report**
- Stay tuned for many other **ML4HEP applications**

