Machine Learning for Collider Theory

— Snowmass Summer Study 2022 —

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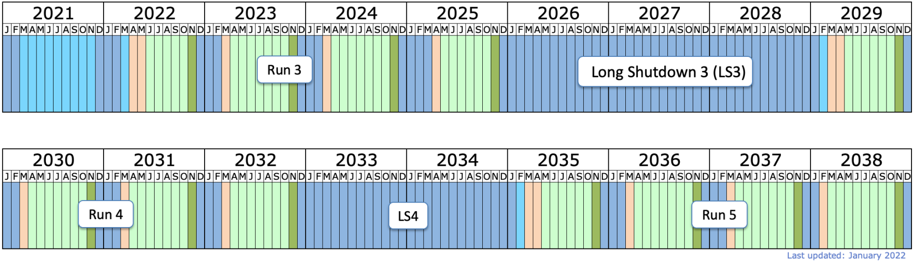
July 22, 2022

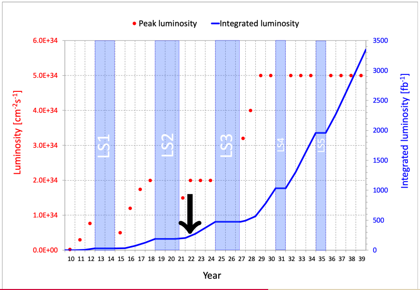
Based on the White Papers
Machine Learning and LHC Event Generation [2203.07460]
and
New directions for surrogate models and differentiable programming for HEP detector simulation [2203.08806]

We will have a lot more data in the near future.



Shutdown/Technical stop
Protons physics
Ions
Commissioning with beam
Hardware commissioning/magnet training

https://lhc-commissioning.web.cern.ch/schedule/LHC-long-term.htm



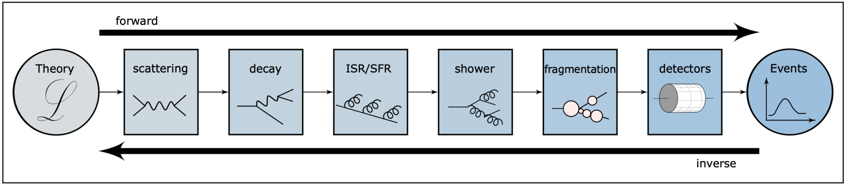
- We will have 20–25× more data.

$\Rightarrow$ We want to understand every aspect of it based on 1[st] principles!

We want to understand the LHC data based on 1^{st} principles.

What do we need to understand the data?

1. (a lot of) precise Simulations
2. optimized analyses for high-dimensional data



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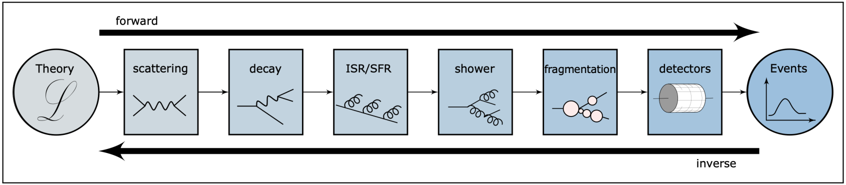

⇒ Machine Learning, as numerical tool, has a significant impact to every aspect of the simulation chain!

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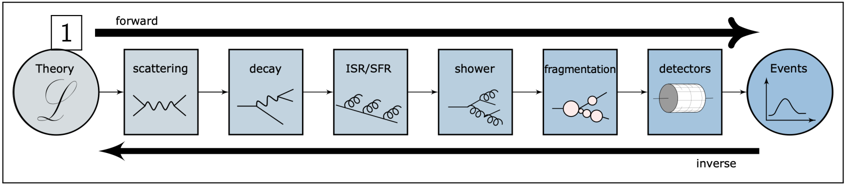

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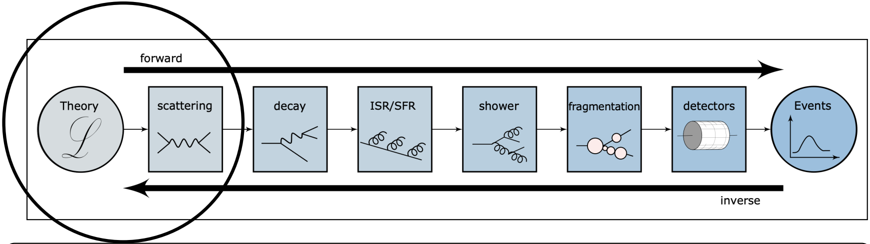
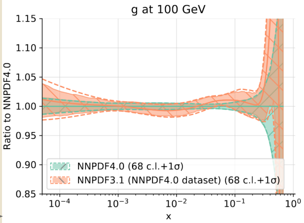
ML improves precise Simulations.



$$d\sigma \quad \sim \quad \text{pdf} \quad \times \quad \text{matrix element}^2 \quad \times \quad \text{phase space}$$

$\Rightarrow$ pdfs: ML reduces uncertainties.

- NNPDF uses NN for a long time (no parametric function assumed).
- Contemporary ML and hyperoptimizations reduced uncertainties from 3–5% to 1%.
- GAN-enhanced compression for delivery.



hep-ph/0204232, 1002.4407, 1410.8849, 2109.02671, 1907.05075, 2104.04535, . . . 2109.02653$\Rightarrow$

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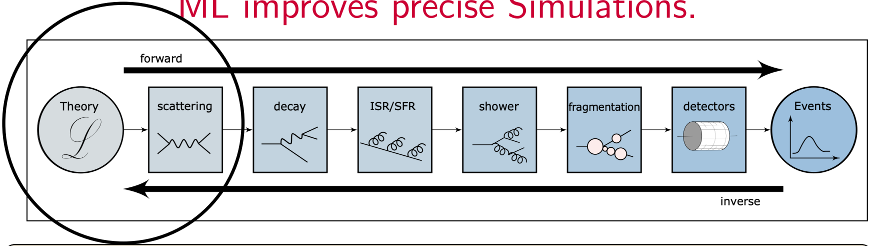


$$d\sigma \sim \text{pdf} \times \text{matrix element}^2 \times \text{phase space}$$

$\Rightarrow$ Amplitudes: Avoiding frequent calls to expensive matrix element.

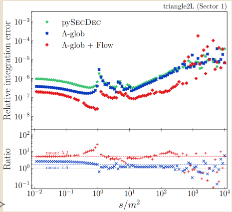
- as "simple" regression task,
- with uncertainties / boosted using a Bayesian NN,
- or using Catani-Seymour "basis" to reach per-mille level accuracy.

$\Rightarrow$ Loop integrals: increasing precision

- NN-assisted contour deformation

2109.11964, 1912.11055, 2002.07516, 2106.09474, 2206.14831, 2107.06625, . . .

2112.09145 $\Rightarrow$



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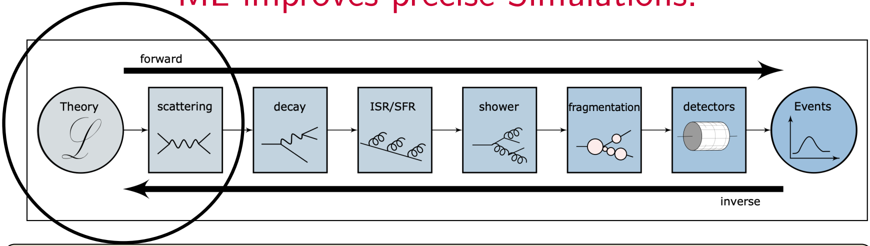


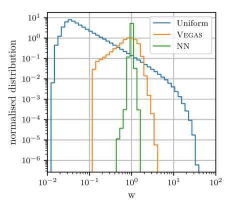
$$d\sigma \sim \text{pdf} \times \text{matrix element}^2 \times \text{phase space}$$

⇒ phase space: increase unweighting efficiency.

- improve Importance Sampling with normalizing flows
- learn channel weights in multi-channel integration
- learn distribution of events from event sample directly.

1707.00028, 1810.11509, 2001.05486, 2001.10028, 2009.07819, 2005.12719, 2011.13445, 1907.03764, 1903.02433, 1901.00875, 2102.11524, ...

2001.05478 ⇒



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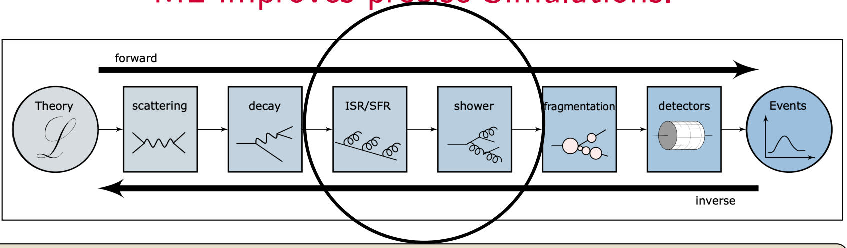

Semi-classical approximation good for small splitting angles.

$\Rightarrow$ parton shower: improve over semi-classical approach

- splittings are iterative, can be learned by RNN;
- using ML-based inference to improve splitting kernels.

- Many body final states can be tackled by graphs or sets and learned directly.

1906.10137, 2012.06582, 1804.09720, 1808.07802, 1701.05927, 1807.03685, 2009.04842, 2109.15197, 2111.12849, 2012.09873

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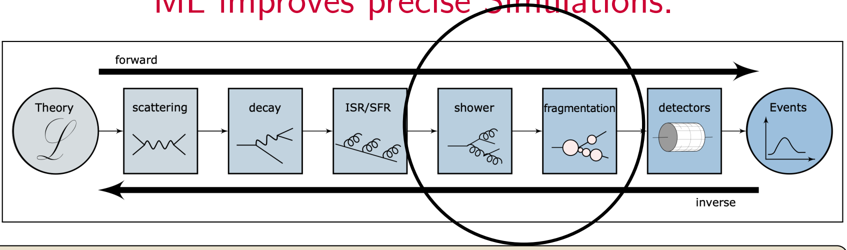
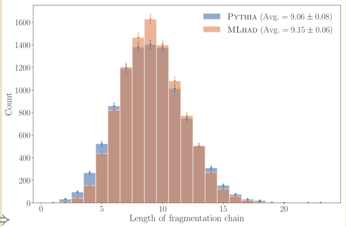


⇒ Fragmentation: Remove modeling bias.

- Same techniques as for pdfs.

⇒ Hadronization: better model non-perturbative effects.

- Either improve existing clustering and Lund string model
- or use ML for more generic approach.



2105.08725, 1706.07049, 1807.03310, 2202.10779, ...

2203.04983 ⇒

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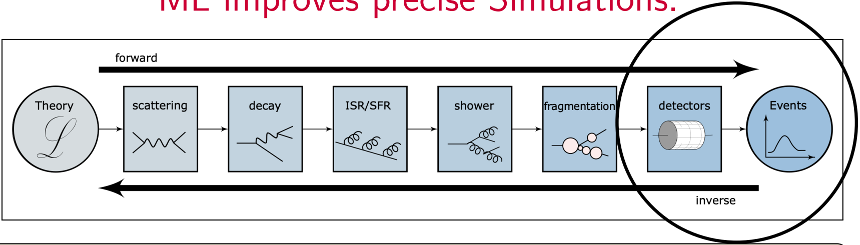


⇒ Detector Simulation: Speed-up full GEANT4

- Indistinguishable showers $10^4\times$ faster.
- More ideas developed in "CaloChallenge 2022".

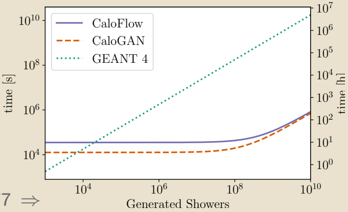
  https://calochallenge.github.io/homepage/

⇒ Trigger: more efficient storage and selection

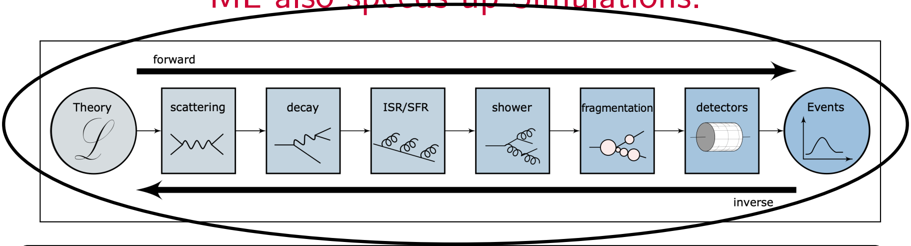
- Software for HLT, FPGAs for L1T

2109.02551, 1705.02355, 1712.10321, 1711.08813, 1802.03325, 1807.01954, 1912.06794, 2005.05334, 2102.12491, 2106.05285, PRL65.1321, 1712.07158, 1804.06913, 1903.10201, 2002.02534, 2104.03408, 2101.05108, 2110.13041, …

2110.11377 ⇒



ML also speeds up Simulations.



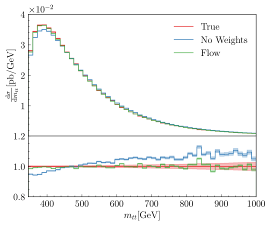
End-to-end ML-generators learn multiple steps at once. Advantages:

+ training on data combined with simulations,
+ post-processing of MC data for example to unweight events,
+ allows us to efficiently ship event samples,
+ provide datasets for phenomenological analyses,
+ enable inverted simulations,

⇒ Precise models with full control available!

2101.08944, 2110.13632, 1901.00875, 1901.05282, 1903.02433, 1912.02748, 2001.11103...

2011.13445 ⇒



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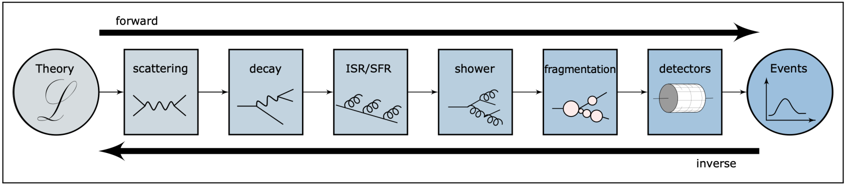

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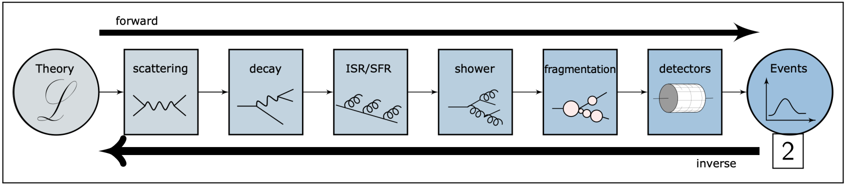

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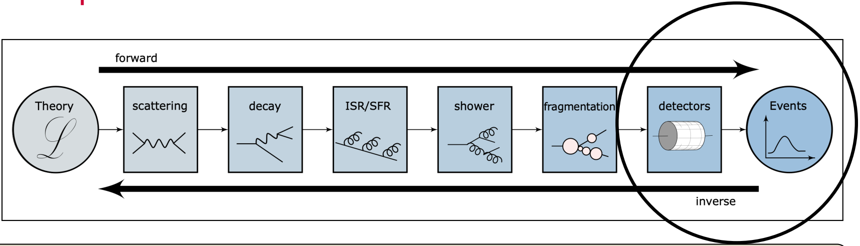
ML helps to invert the Simulation — for better inference.



⇒ Reconstruction in a busy detector

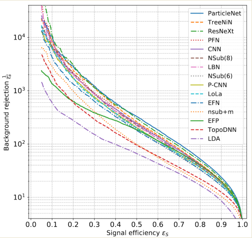
- going beyond traditional particle flow algorithms with GNNs
- improved tracking

⇒ Better particle identification

- e.g. Top Tagging Challenge

2003.08863, 2101.08578, 2106.01832,
2012.11944, 2012.04533, ...

1902.09914 ⇒



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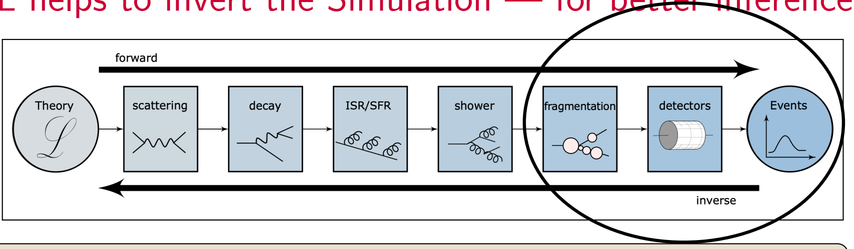
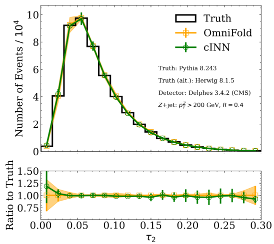


⇒ Unfolding of detector effects

- must be high-dimensional, unbinned, and statistically well-defined
- Classifier-based MC reweighting
- Conditional normalizing flow (cINNs)-based learn probability density per event



1806.00433, 2006.06685, 1911.09107, 2011.05836, 1912.00477, 2105.04448, 2105.09923, 2108.12376, . . . 2109.13243 ⇒

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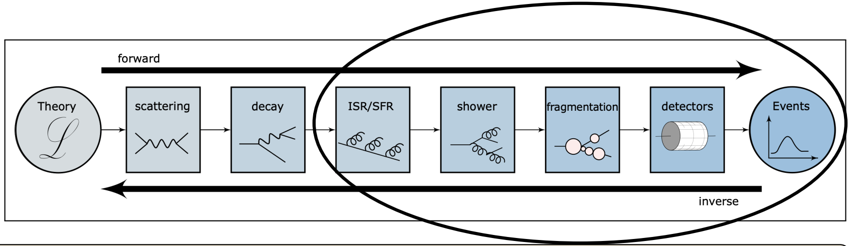
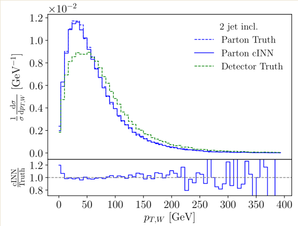


$\Rightarrow$ Inverting to parton level

- Inversion of QCD radiation and heavy particle (t, W, Z, h) decays
- Uses similar techniques like unfolding (cINNs and Classifiers)

1806.00433, 2109.13243, 1911.09107, 2011.05836, 1912.00477, 2105.04448, 2105.09923, 2108.12376, . . .

2006.06685$\Rightarrow$



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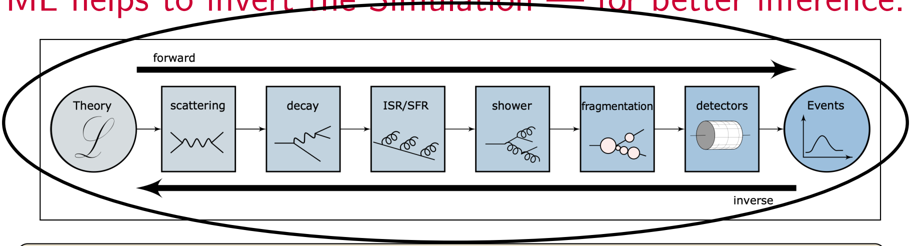


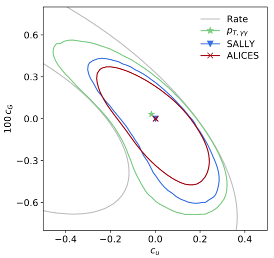
Simulation-based inference: inverting the full simulation chain

⇒ MadMiner

- can learn LL ratio or score by "mining" simulators.
- Having them differentiable would make it even more applicable.

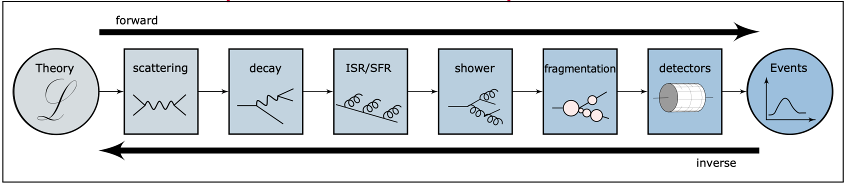
⇒ Matrix-Element Method (MEM)

- get LL from ME and unfolded events.
- More advanced (ML-based) unfolding yields better estimators.



1805.00013, 1805.00020, 1805.12244, 1808.00973, 2110.07635, 1506.02169, 1601.07913, . . . 1907.10621⇒

ML also improves model-independent searches.



Removing signal-model dependence to search for new physics:

⇒ Enhancing bump hunts

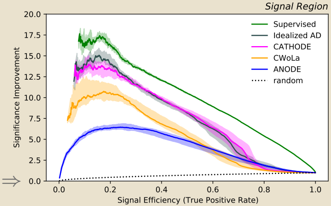
- methods now reaching results of idealized comparisons.
- lot's of active research in feature selection etc.

⇒ Anomaly detection

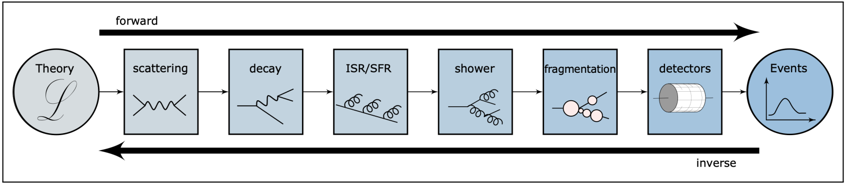
- searches for out-of-distribution events using various approaches
- see also "Dark Machines Anomaly Score Challenge"

1805.02664, 1902.02634, 1708.02949, 2001.04990, 2101.08320, 2105.14027, . . .

2109.00546 ⇒



The importance of ML for Collider Physics.



⇒ Modern ML is a new tool in our numerical toolbox — with applications to every step in the simulation/inference chain.

⇒ We've seen everything between "proof-of-concepts" to well established use cases.

⇒ There is an interesting interplay between HEP and the ML/AI community:

- Precise HEP simulations provide infinite, excellent training data for ML.
- HEP-specific application requirements (precision, symmetry, . . .) are different from industry applications (computer vision, etc.).