Machine Learning for LHC Simulations

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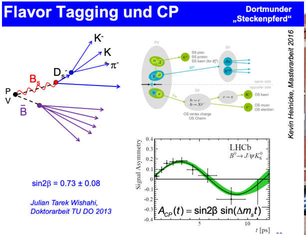
Universität Heidelberg

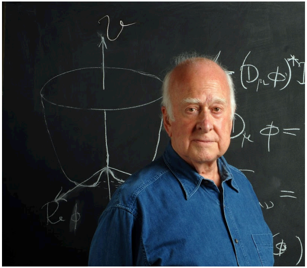
Snowmass, July 2022

Modern LHC physics

Classic motivation

- dark matter
- baryogenesis
- Higgs VEV





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LHC physics

- fundamental questions
- huge data set
- complete uncertainty control
- first-principle precision simulations

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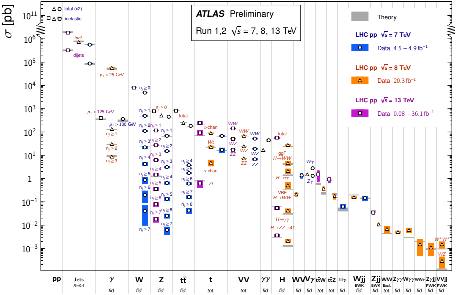
Time to kiss good-bye

- discover in rates
- unveil little black holes
- find supersymmetry
- travel extra dimensions
- measure couplings



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First-principle simulations

- start with Lagrangian
- calculate scattering using QFT
- simulate events
- simulate detectors

$\rightarrow$ LHC events in virtual worlds

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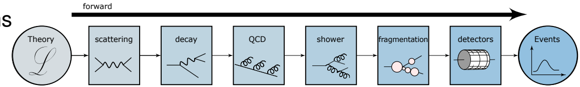
Dual goal of HL-LHC

- avoid modeling
- compare simulations and data
- analyze data systematically [SMEFT]

$\rightarrow$ understand LHC data completely

$\rightarrow$ find new particles



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LHC questions

- How to get from $3 \cdot 10^{15}$ Bytes/s to $3 \cdot 10^{8}$ Bytes/s?

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  . . .

  More than off-the-shelf solutions?

Shortest ML-intro ever

Turning fits into science

- approximate $f(x)$ using $f_\theta(x)$
- no parametrization, just many θ
- minimize loss to find best θ

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- regression $x \to f_\theta(x)$
- classification $x \to f_\theta(x) \in [0, 1]$
- generation $r \sim \mathcal{N} \to f_\theta(r)$
- conditional generation $r \sim \mathcal{N} \to f_\theta(r|x)$

$\to$ One tool, many applications

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LHC-specific AI challenges

- vast datasets
- precision
- uncertainties
- simulation-based inference

$\to$ LHC-specific ML

Event generation

ML-goals in event generation

- general goals

  1- improve established tasks
  2- develop new tools for established tasks
  3- transform through new ideas

- LHC-specific goals

  1- ML in established generators
  2- end-to-end ML-generators
  3- inverse simulation and inference

→ Make best out of HL-LHC

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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 conceptional 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.

Submitted to the Proceedings of the US Community Study
on the Future of Particle Physics (Snowmass)

ML in Established Generators

HL-LHC generators

- 25 times Run 2 dataset
- increased precision
- increased speed

$\to$ Improvement, no revolution

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HL-LHC generators

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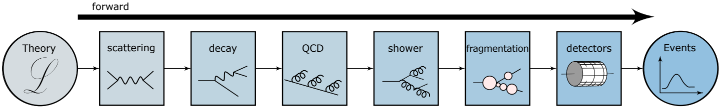
→ Improvement, no revolution

ML-Pythia/Madgraph/Sherpa/Herwig

- phase space sampling
- fast loop amplitudes
- fast loop integrals
- optimal multi-channeling
- data-driven parton shower
- precision parton densities
- precision hadronization/fragmentation
- fast detector simulation ...



End-to-end ML-Generators

ML-Generators

- fast events at parton and reco level
- comparison VAE-GAN-NF-INN
- amplification through implicit bias
- control of learned features
- precision of learned density

→ Generative network benchmark

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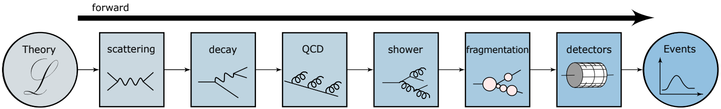
Challenges and applications

- shipping large datasets
- combined training on data and simulations
- subtraction/unweighting of event samples
- step towards detector simulations
- step towards inverted simulations

→ Trigger of new ideas?



Inverse Simulation and Inference

Inference

- particle reconstruction
- ML-particle flow
- likelihood/score extraction
- enhanced bump hunt
- symbolic regression

→ Playground for ML-ideas

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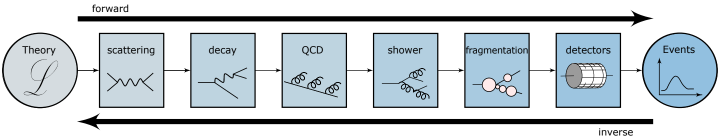
Inverted simulation

- detector unfolding
- unfolding to parton level
- matrix element method

→ Inference at optimal simulation stage



Outlook

Short ML-story [also see Claudius Krause's talk]

- just a fit, but much better
- transforming all numerical science
- LHC physics unique in many ways
- LHC event generation obvious case
- excitement and progress everywhere in ML
- check out ML4Jets at Rutgers in November

→ hep-ml key part of our future