https://doi.org/10.1142/9789811280184_0001

Chapter 1

New Theory Paradigms at the LHC

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The success of particle physics rests on precision measurements combined with precision predictions, to answer burning fundamental physics questions. Modern LHC physics combines searches for physics beyond the Standard Model with a first-principle understanding of the vast LHC dataset. Building on the Higgs discovery and a detailed understanding of weak-scale physics, the upcoming LHC runs will keep incorporating new concepts, for instance from data science, to probe the properties and interactions of all known and to-be-discovered new elementary particles.

The Puzzles of Particle Physics The defining features of particle physics are the big and exciting fundamental physics questions, for which we try to find answers (for example, at the LHC). Some of these questions come from the mathematical structure of quantum field theory, others are posed by cosmological observations combined with a fundamental model describing elementary particles and their interactions.

The consistency of the Standard Model (SM) as a quantum theory for the electroweak interactions has lead us directly to the discovery of the Higgs boson. The renormalizability of the electroweak gauge theory, experimentally confirmed by many LEP measurements, predicts a new scalar with a mass in the electroweak range. The Higgs boson arises as quantum excitation of the Higgs field with non-zero vacuum expectation value (VEV), which generates the masses of the gauge bosons and fermions in the SM. This has to be separated from the hadron masses, which are generated by the non-abelian structure of QCD, which is also probed at colliders.

The mechanism of generating mass through spontaneous symmetry breaking has been observed in other systems and other fields of physics. One big open question that remains after the Higgs discovery is how electroweak symmetry breaking is realized in our Universe, and if Nature really follows its most economic realization with one fundamental scalar particle.

Cosmology allows us to probe physics over a vast range of energy scales by combining observations with a fundamental understanding of the thermal history of the universe. Because our Universe is a somewhat complex system, we have not been able to pin down the fundamental, dynamic mechanisms behind, for example, the observed dark matter relic density and the observed matter-antimatter asymmetry from cosmological data. However, dark matter and the matter-antimatter asymmetry have to be put into the context of elementary particle physics. Provided that these mechanisms affect physics below the TeV scale, we can test them in the controlled environment of particle physics experiments. Here, multi-purpose experiments at hadron colliders are an especially promising path to search for dark matter particles and to probe the symmetry structures behind baryogenesis.

Most generally, we need to ask the question: whether we can describe all physics effects and all measurements at the LHC in terms of a fundamental quantum field theory or its effective field theory (EFT) extension. At the parton level, we can describe the hard scattering precisely in the Standard Model or possible extensions; we also know that we can use resummed QCD predictions to describe, for instance, parton showers; in both cases the challenge is to match the experimental precision with perturbative or resummed calculations. Open questions in QCD include hadron spectra, dynamic hadronization, and parton densities from first principles. QCD should be the correct fundamental theory to describe all these effects, but for effects out of reach of perturbation theory, we would need to close the gap with non-perturbative computations and lattice gauge theory. At hadron colliders these aspects of fundamental QCD can be targeted by electron-hadron or heavy-ion collisions. The symmetry structure of the QCD Lagrangian is the main motivation for new light axions, which would, in turn, provide a portal to dark matter and link quantum field theory, collider physics, and cosmology.

Hadron Colliders and Theory Experimental collider physics and theory are two inseparable sides of the same coin — the path to the fundamental structure of Nature. Back in the days of the LEP, the Tevatron, and HERA, the common wisdom was that hadron colliders were discovery machines, while electron-position and electron-proton colliders were needed for precision measurements and to really understand new particles or interactions. Looking back at the discoveries in the heavy, electroweak sector this judgement is sensible. The W and Z-bosons were discovered in 1983 at the SPS, the top quark was discovered in 1994 at the Tevatron, and the Higgs boson in 2012 at the LHC. In addition, LEP has established the electroweak SM as a predictive, renormalizable quantum field theory, predicting the Higgs discovery at the LHC. This list defines a similar task for the LHC: to discover, if at all possible, new particles by understanding all LHC data and starting from the full Standard Model.

Because of the complexity of the experimental environment, the large data sets with correspondingly small statistical uncertainties, and the long list of effects which need to be described by theory, a close interaction between theory and experiment is crucial for hadron collider physics. At a time when advanced particle physics experiment and theory (each tackling their respective challenges) tend to drift apart, a unified approach is more important than ever.

Strictly speaking, an experimental measurement targets a rate or kinematic correlations in a given fiducial phase space. Already, this measurement requires theory input for calibration or to transfer knowledge from control regions to the signal region. However, from a physics perspective a QCD-dominated total rate measurement is not interesting. What we want to measure are fundamental parameters, which need to be extracted from the original rate measurement through additional kinematic handles. This means any relevant physics measurement rests on a fundamental physics interpretation framework, and any inference requires a well-defined hypothesis which relates a measured rate to an interesting physics question.

The workhorse in theoretical predictions for the LHC are fast event generators combined with detector simulations. Multi-purpose generators take fundamental Lagrangians as inputs and generate events as we expect them in the virtual world defined by a given Lagrangian. These generators are maintained by the theory community and provide the main pipeline for realising theory ideas into experiments. Simulation-based inference then compares measured and simulated events and extracts information on the underlying theory, probing the particle content, the interactions, or the fundamental symmetry structure. This kind of fundamental analyses, combined with a precisely controlled experimental environment and equally precise theoretical prediction, has turned the LHC into the first precision hadron collider, breaking the historic split between precision-lepton-collider physics and discovery-proton-collider physics.

The appeal of future hadron colliders is driven by the immense success of the LHC. As we will discuss below, the experimental and theoretical LHC program established the notion of precision-hadron collider physics. Experimentally, the proposed HE-LHC and FCChh are defined by significant increases in energy and luminosity beyond the full LHC dataset. The LHeC and FCCeh attempt to combine the advantages of hadron collider physics with electron beams that have enough energy to induce scattering of electroweak gauge bosons. Their setup benefits from the success of modern hadron colliders, but shifts the focus from QCD to electroweak scattering. The benefits from increased luminosity are key to all future colliders, a serious challenge to the entire underlying methodology, and a trigger for exciting developments already for the final phase of the LHC.

Precision Predictions A key ingredient to the success story of the LHC lies in theoretical developments since around 2000.[1] The prediction of hard scattering amplitudes is now dominated by automated next-to-leading order (NLO) calculations in QCD, available essentially for all relevant signal and background processes.[2] These calculations are not only available for total rates, but for the full event kinematics, thanks to advanced subtraction schemes for soft and collinear phase space regions. Automated NLO QCD calculations as part of standard event generators are the final step of decade-long developments of analytical[3] and numerical methods and tools.[4] The next challenge will be to systematically provide NLO electroweak corrections[5] and next-to-NLO (NNLO) QCD corrections to experiment, and cover the relevant channels to next-to-NNLO (NNNLO), including as many kinematic distributions as possible. Current state of the art predictions in precision theory includes: NLO predictions to $t\bar{t}b\bar{b}$ production with all off-shell effects included,[6] NNLO for exclusive jet production[7] or Higgs production and decay in weak boson fusion,[8] combined NNLO-QCD and NLO-electroweak corrections to top pair production,[9] or first NNNLO predictions for Higgs production.[10]

In addition, Monte Carlo event generators have taken precision predictions significantly beyond the simple hard process. Complex hard processes with many particles in the final state can be described by helicity amplitudes, avoiding the CPU-consuming task of squaring scattering amplitudes analytically, and instead computing them numerically and then squaring these single numbers.[12] Multi-purpose generators like PYTHIA,[13] MadGraph,[14] Sherpa,[15] and Herwig[16] now describe events with high and variable jet multiplicities, arguably the one big challenge for LHC

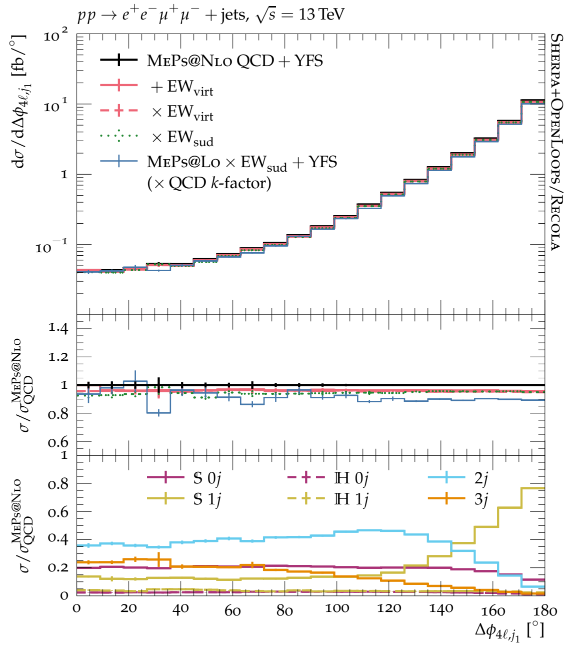

Fig. 1. Correlation for ZZ+jets production based on precision MC, including fixed-order QCD and electroweak corrections, as well as Sudakov logarithms. Figure from Ref. 11.

simulations. The combination of a hard matrix element with logarithmically enhanced jet radiation is solved by so-called jet merging, first solved by introducing the CKKW[17] method. In Fig. 1 we show what state of the art programs can analyse, including NLO-QCD and NLO-electroweak corrections as well as Sudakov logarithms and jet radiation in Sherpa.[11]

While this is not true for all current analyses, modern simulation-based inference approaches, as will be discussed in more detail below, require simulations of SM-backgrounds and any new physics hypotheses with the same precision. The additional challenge is that precision predictions for signal hypotheses have to cover a large model space. Here, MadGraph and Sherpa drove the development of flexible and automated event generation based on a given Lagrangian,[18] while still with the same access to automated higher-order corrections.

Finally, there still exists a part of the LHC simulation chain where our access to first-principle predictions is limited, for instance, parton densities or fragmentation. In these cases the event generators combine data and theory input using modern data science methodologies. This does not mean that we have given up on understanding these aspects through first principles forever, but that, at this stage, modelling them provides a better basis for experimental analyses.

Higgs Discovery and EFT Properties As mentioned above, the existence of the Higgs boson can be derived as a purely formal prediction based on the description of the massive electroweak sector in terms of a renormalizable quantum field theory.[19–21] In that sense the starting point of all Higgs physics are the precision measurements of the electroweak SM at LEP. These measurements and their interpretation went beyond the usual leading order in perturbation theory and probed quantum corrections systematically for the first time in collider-based particle physics. This legacy lives on at the LHC, where we systematically describe hadron collider data including quantum effects for the first time. Given the combined LEP results, the existence of some kind of Higgs boson was never really a question, because it is needed to ensure unitary predictions for scattering processes.

Weak boson fusion and weak boson scattering are sensitive processes at the LHC, consequently forming the core of the electroweak physics program at the LHC. The main question answered by the Higgs discovery in 2012 was about its mass. Nature's choice of 125 GeV[22,23] is perfect for the LHC program, because it is right in the middle between the light-Higgs regime with dominant Higgs decays to fermions and photons, and the heavier-Higgs regime with dominant Higgs decays to weak bosons. This means that Higgs physics, as described in this book, could move immediately from the Higgs discovery to Higgs measurements.[24,25] These measurements combine different production and decay channels to a global analysis, initially described in terms of Higgs couplings and by now upgraded to a consistent, effective quantum field theory.

Following the Higgs discovery in Run 1, the LHC Run 2 has been the first comprehensive precision program at a hadron collider. Experimentally, this refers to, for instance, the large number of measured Higgs production and decay channels and their comprehensive treatment of statistical and systematic uncertainties. On the theory side it is driven by precision predictions of rates as well as precision simulations of the entire phase space for, essentially, all LHC measurements. Additional key ingredients are precision predictions for parton densities and all other aspects of the event generation chain.

Responding to the precision of the Run 2 measurements and their sensitivity to higher orders in perturbation theory, a major shift in the theoretical interpretation has been to move from an ad-hoc and theoretically inconsistent modification of Higgs couplings to a proper description of modified interactions in terms of an effective Lagrangian. Effective field theory tracks deviations through higher-dimensional Higgs operators, induced by unspecified heavy new particles. This SM effective field theory (SMEFT) had already been established at LEP, to describe anomalous electroweak gauge couplings, and was easily extended to the gauge and Higgs sector at the LHC.[26] One of the great successes of the LHC is that the SMEFT precision measurements of electroweak Wilson coefficients outperform the corresponding LEP measurements,[27] turning the LHC into a discovery-and-precision machine. The successful SMEFT description of the electroweak and Higgs sector[28–31] has, by now, been extended to the top sector,[32–34] a combination of the two,[35,36] anomalous QCD couplings,[37] and the link between top quark and bottom quark physics.[38]

The SMEFT interpretation framework for the LHC comes with many benefits. Firstly, quantum field theory properties like renormalizability allow us to formulate the underlying hypotheses including quantum effects, or higher orders in perturbation theory. If LEP has established perturbative quantum field theory as the correct description of elementary particles, the LHC has turned this description into a systematic interpretation framework for all its data. Secondly, higher-dimensional operators do not only modify total production rates, they also affect kinematic distributions, specifically high-energy tails. This way, SMEFT allows us to describe and analyze potential deviations in a wide range of kinematic observables. Finally, SMEFT does not just modify individual sectors of physics, rather, it expands the entire SM-Lagrangian using higher-dimensional operators. This means that we can use it to answer the big global question: how well does the SM describe all LHC measurements, as well as measurements from other experiments probing similar mass scales? Figure 2 illustrates the situation in the Higgs sector after the LHC Run 2.

These features imply that a global SMEFT analysis serves as a first step towards a comprehensive analysis of the entire SM facing the full LHC dataset, as we will discuss below. On the other hand, given what we know about the shortcomings of the SM and given the success of renormalizable field theory, we should really consider global SMEFT analyses a useful limit setting tool. Once the LHC experiments observe a significant anomaly, the corresponding theory interpretations will use all our phenomenological and conceptual background knowledge to identify the fundamental structures behind such an anomaly.

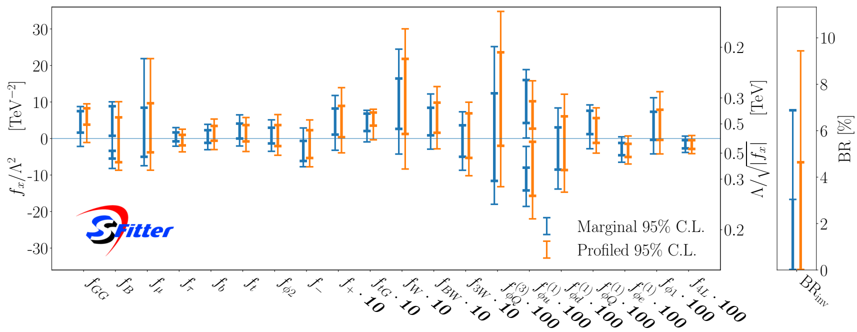

Fig. 2. Global SMEFT analysis of the Higgs and electroweak gauge sector. The two colors correspond to consistent likelihood and Bayesian marginalization frameworks for the nuisance parameters and Wilson coefficients. Figure from Ref. 39.

Physics beyond the Standard Model The ultimate goal of the LHC community is not to confirm the Standard Model, but to find cracks in this description and to discover new particles and interactions. Towards this goal, the discovery of a fundamental Higgs scalar does not only give us faith in the renormalizability of the SM and its structural validity to high energies, it also provides us with a framework to tackle two fundamental questions related to cosmological observations: the nature of dark matter and the origin of the matter-antimatter asymmetry of the universe. Neither of them can be answered within the SM, and both point towards renormalizable extensions of the SM. Such models predict new particles and a modified symmetry structure, and the Higgs or scalar sector is a prime candidate to accommodate these features.[40–42]

While we know that the SM does not explain all the observations we expect it to explain, the LHC has not yet found any sign of new particles. The constraints from these LHC searches either push new particle masses to larger values or their couplings to SM particles to very small values. While indirect probes of heavy new particles can often be described by an effective field theory, there will be observables, like the relic dark matter density, for which we need to work with the full models and new particles on their mass shell. Such light and weakly interacting new particles will also be produced on-shell at the LHC.[43]

Going beyond effective field theories towards well-defined renormalizable models requires a solid understanding of the underlying quantum field theory. It allows us to predict LHC signatures by studying the interplay between UV-complete models and effective field theories. The very specific questions about dark matter and baryogenesis then suggest what to look for at the LHC. For dark matter to be produced during the thermal history of the universe, it has to interact with the SM in some way. Thermal freeze-out production forms the general basis of weakly interacting massive dark matter. While the W and Z-bosons are ruled out as mediators, the Higgs sector provides an attractive portal to dark matter.[44] A direct consequence of such a Higgs portal could be an invisible decay of the SM-like Higgs boson, more general dark matter searches target missing transverse energy in association with jets or other SM production processes.

Alternatively, extended scalar sectors with a spectrum of Higgs particles can serve as a direct link to gauge-singlet dark matter particles. Any such additional mediators couple to the Standard Model and to dark matter, which means we can search for them as missing energy or as resonances, for example, in di-jet or di-lepton production.

Extended Higgs sectors also play an important role for baryogenesis, as they can promote the electroweak phase transition to strong first order with the SM-like Higgs boson remaining at a mass of 125 GeV. This way the matter-antimatter asymmetry can be generated dynamically through electroweak baryogenesis,[46] illustrated in Fig. 3, if besides the departure from thermal equilibrium the remaining two of the three Sakharov conditions[47] are fulfilled. These are charge (C) and charge-parity (CP) violation and baryon number violation. The first condition entails additional Higgs bosons that can be lighter or heavier than the SM-like Higgs boson. They can be searched for at the LHC. CP-violation in the Higgs sector can be probed at the LHC, either through CP-sensitive or optimal observables, or by searching for heavy Higgs decays into two SM-like Higgs bosons and into a SM-like Higgs boson plus a Z-boson, simultaneously.[48,49]

Coming back to a global interpretation of LHC data, model-based searches for new particles and SMEFT searches are closely related in their theory interpretations. At some point we always need to match the two theory hypotheses in phase space regions where both of them are valid. This matched description covers all channels where the new particle can be produced on its mass shell, but also light new particles remaining off-shell in t-channel exchange. Precision matching beyond leading order can uncover potential shortcomings of the SMEFT approach when we truncate the series at operators dimension six,[50] and it introduces a matching scale uncertainty.[51,52] Model-based searches and SMEFT are also related on the analysis side. While an observed resonance can, obviously, not be interpreted in terms of SMEFT, limits from such resonance searches for example

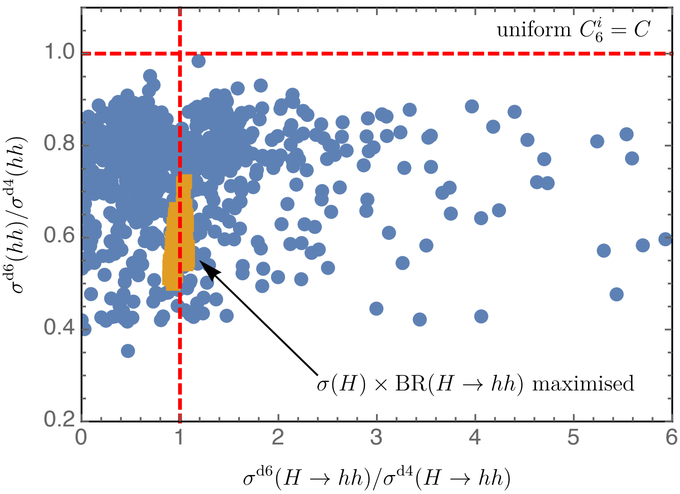

Fig. 3. Modification of Higgs pair production $gg \to hh$ and its correlation with resonance production $gg \to H \to hh$ in a 2HDM including scalar dimension-6 operators to achieve a strong first order electroweak phase transition. The Wilson coefficients are chosen uniformly, $C_6^i = C$. Highlighted are the Higgs-philic scan result points. Figure taken from Ref. 45.

in WW, WZ, or WH production provide some of the most useful inputs to SMEFT analyses.[27,28] No matter if we are more interested in global analysis strategies or in finding fundamentally motivated new physics models, SMEFT and model-based searches are two sides of the same medal.

Predictions and inference for the HL-LHC In many ways the expected size, complexity, and precision of the HL-LHC dataset challenge our established methodology, starting from data acquisition to data processing, analysis, and theory predictions. The 10-fold increase in the integrated luminosity as compared to the combined Runs 1-3 reduces many statistical uncertainties to a level where systematic and theory uncertainties will dominate the vast majority of analyses. For theory this means that we need to avoid a situation where theory uncertainties become the limitation to experimental measurements, these measurements become purely data-driven, and this way turn to modelling rather than understanding fundamental physics. One way to tackle this challenge is to employ ideas and methods from modern data science to improve theory predictions as well as the way we make them available to analyses.[53] This task sounds technical at first, but it links two of the most exciting aspects of modern science: fundamental questions from physics and cosmology and the revolutionary tool box from data science.

The immediate motivation to use data science methods at the LHC is the combination of the size of the LHC dataset with the availability of precision simulations based on first principles. Any LHC analysis and any comparison between data and predictions already employs multi-variate methods and simple neural networks. The natural and necessary next step is to update these methods and make use of the transformative developments in data science research over the last 20 years.

The more abstract motivation for data science methods in LHC physics is that modern data science provides a common language for theory and experiment. It not only builds bridges between data science and theory or experiment individually, it also allows us to build the bridges between experiment and theory, exactly what we need to make the HL-LHC a success. Furthermore, modern machine learning provides new interdisciplinary opportunities between fundamental science and data science.

For particle theory, modern machine learning (ML) has the potential to improve all aspects of our established theory computation and simulation chain, as illustrated in Fig. 4. Standard network architectures we can employ for theory predictions include simple regression, but also classification and generative models. Critical regression tasks in LHC theory include loop integrals, libraries of standard functions, or surrogates for loop amplitudes. The NNPDF parton densities[54] have shown how machine learning does not only increase the speed of the evaluation, it should also allow for controlled precision by avoiding biases from non-perfect theory assumptions. Other modules in the forward simulation chain which we expect to benefit from machine learning are phase space sampling, parton showers, and, especially, hadronization or fragmentation models.

A second strategy to improve LHC simulations involved generative networks for event generation[53] and for detector simulations.[56] Here we

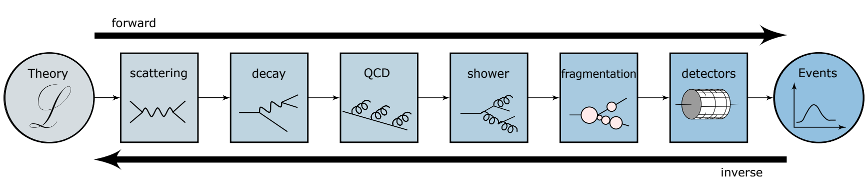

Fig. 4. Illustration of the forward simulation and the inverted simulation or unfolding-inference direction for the LHC. Figure from Ref. 53.

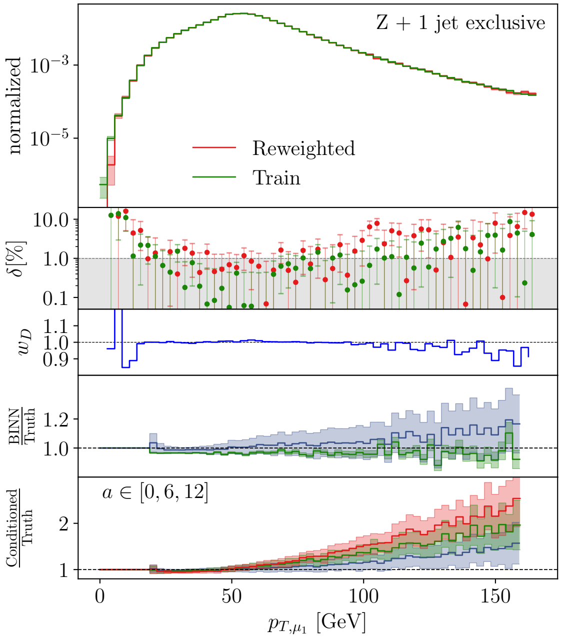

Fig. 5. Results from a INN-based NN-event generator including a comprehensive uncertainty treatment. Figure from Ref. 55.

attempt to replace the entire chain shown in Fig. 4 by a generative network. Such a ML-generator can be trained on Monte Carlo or on measured events, it can combine positive events and subtraction terms, be used to subtract entire event samples or to unweight events, transform events in control regions into events in signal regions, and it can provide an efficient way to distribute standardized event samples. The key challenge for all networks employed in LHC physics, but especially generative networks, is to ensure that they have learned all relevant phase space features and can reproduce them within a given uncertainty.[55] Results from Bayesian and conditional normalizing flows are shown in Fig. 5. Conceptually, an interesting question is how many events we can simulate with a generative network trained on a limited number of events. Just like a parameterized fit, the implicit bias of the network will lead to an amplification effect, but the exact amount of amplification is an unsolved problem,[57] where particle physics should give answers the data science community has not provided.

Obviously, we can use data science concepts for LHC inference. An orthogonal approach to model-based searches and the logical next step from global SMEFT analyses is to analyze the LHC dataset by directly comparing measured and simulated events.[58] For this strategy, detailed precision simulations are crucial, because they allow us to cover the full phase space and search for features which we would not see in rate measurements. This means that the main challenge in simulation-based inference are not the experimental setup, but suitable theory predictions.

Finally, LHC inference can be transformed by data science through inverse simulations, as illustrated in Fig. 4. One of the problems of precision LHC physics is that it is almost impossible to use the most recent theory predictions if they cannot be implemented in event generators. To identify the best simulation or data processing stage to compare theory and experiment we can add inverse simulations to the forward simulation chain. Stochastically defined inverse problems can be solved using multi-dimensional classifier reweighting[59] or conditional generative networks.[60] Inverted simulations are already used at the LHC, but as localized efforts with limited and ad-hoc techniques. They include: detector unfolding of simple kinematic distributions, jet algorithms, unfolding to the parton level process, and the matrix element method. For all of them, machine learning applied to simulations and to simulation-based inference provides us with a consistent and powerful framework to make the best use of the vast HL-LHC dataset.

A Bright Future There is no crisis in modern particle physics. On the contrary, the future of particle physics is bright, because we have exciting and fundamental physics questions to answer and datasets which allow us to do so. Here, we should really consider the HL-LHC as a new experiment, with a proper name, with new strengths, and with new challenges, in both theory and experiment. Modern hadron collider physics will benefit from the HL-LHC because it is all about precision measurements, precision predictions, and a theoretical interpretation in terms of fundamental Lagrangians. Exciting discoveries will be driven by these unique strengths in the particle physics and science landscape.

When interpreting LHC data we need to keep in mind that there is nothing to learn from modelling data without a fundamental interpretation framework. While it might be necessary to model effects or background kinematics to then be able to search for physics beyond the SM, a purely data-driven approach would potentially leave us with an outcome where the HL-LHC discovers no new particles, and we do not learn anything fundamentally interesting from the SM dataset either. This is illustrated by the not very well-known fact that the LHC has not only discovered the Higgs boson, but it has discovered more than 60 new particles. However, all but one of these particles are hadronic resonances without revolutionary theory implications. Only the Higgs tells us something new and structural about fundamental physics; the existence of a background field in the vacuum that is responsible for particle masses.

The fact that in this discussion of hadron collider physics and theory the invention of models for physics beyond the Standard Model hardly shows up is often interpreted as a problem for particle physics. However, what it really implies is that particle physics has entered an exciting, data-driven era. Theory is crucial, as it formulates the fundamental questions, provides precision predictions, defines consistent interpretation frameworks, and allows us to combine LHC results with a wide range of particle physics and cosmological insights. What theory cannot provide is the answers to our fundamental questions — theoretical models without data to test them make for a fun game, but physics needs relevant datasets like the one provided by the HL-LHC.

In this new, data-driven era, successful LHC physics relies on a wide range of experimental and theoretical techniques. It derives its excitement from new ideas, concepts, and tools, and their huge impact on detectors, analysis techniques, theory calculations, and simulations. Looking at the expected size of the HL-LHC dataset (and future collider designs), we have to make use of modern machine learning wherever we can. Some data science concepts might be directly applicable to LHC physics, but in most cases we will have to develop methods and tools which guarantee the control, precision and uncertainty treatment needed for the LHC. And no matter what we do, particle physics is defined by its physics questions and the close ties between experiment, analysis, and fundamental theory. These ties give us great hope that, eventually, we will discover new effects leading to new, unexpected, and exciting insights into the Nature of fundamental particles.

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