UNIVERSITY OF CALIFORNIA SAN DIEGO

Understanding the High Energy Higgs Sector with the CMS Experiment and Artificial Intelligence

A dissertation submitted in partial satisfaction of the
requirements for the degree Doctor of Philosophy

in

Physics

by

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2024

The Dissertation of Raghav Kansal is approved, and it is acceptable in quality and form for publication on microfilm and electronically.

University of California San Diego

2024

DEDICATION

To my family.

EPIGRAPH

तम आसीत्तमसा गूह्ळमग्रे प्रकेतं सलिलं सर्वाऽइदम् ।
तुच्छ्येनाभ्वपिहितं यदासीत्तपसस्तन्महिनाजायतैकम् ॥३ ॥

- नासदीय सूक्त

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ACKNOWLEDGEMENTS

My interest in physics was ignited in the 10th grade by the discovery of the Higgs boson and Stephen Hawking's *The Universe in a Nutshell*. These past five years, dedicated to understanding the Higgs and the mysteries of our early universe, have been a fulfillment of dreams then born and will be a part of my life I cherish forever.

I have many people to thank for allowing my childhood passion to flourish into this dissertation. I start first and foremost with my parents and little Kli for their love and support at every step. I thank as well my entire extended family for making me feel at home around the world, from Delhi to Pondicherry and California to Texas. I am especially grateful to all my grandparents, whose wisdom, selflessness, and memory inspire me always.

I would not have survived this PhD — particularly the two long years of lockdown and two long quarters of E&M, without my amazing friends, old and new, in San Diego: Aneesh, Biswa, Chris, Davide, Dro, Elliot, Gerald, Hulk, and Varun (to name a few). I thank as well my fellow CMS students, Farouk and Yanxi, with whom I moved across continents and conducted an ancillary PhD in ping pong. Along with them, I thank my friends in Geneva and Chicago, including Fifi, Jay, Priyanka, and the LPC crew, for making my two years working at CERN and Fermilab so memorable. Most of all, I thank Praniti, for her sweetness and support throughout.

Like the universe, my journey in high energy physics (HEP) began with a bang: the CERN Openlab summer student program. It was a breathtaking experience, and I am grateful to Cliff, Frank, and my supervisor Maurizio for their support then and throughout my career since. Maurizio, in particular, introduced me to the (Nobel-prize winning!) potential of AI in HEP, and I have been hooked ever since.

More importantly, he introduced me to Javier right as we were both, perhaps serendipitously, joining UCSD in the Fall of 2019. Javier has been the most brilliant, kind, and supportive advisor I could have asked for, and I thank him for teaching me a lot more than just physics. Along with him, I thank many awesome postdocs and scientists, including Cristina, Daniel, Nhan, Petar, and Si for their mentorship through the years.

Parts partI—**??** are primarily original work for this dissertation, discussing the standard model, the CMS experiment and the LHC, AI and ML, and statistics, and building on several references listed therein. On the topic of statistics, I thank Javier and Nick Smith for countless discussions (as well as their much-needed help with analysis software and the CMS combine tool)!

Part partII presents novel methods for producing and validating fast simulations of the CMS detector using AI. I thank Maurizio for introducing me to this topic as a summer student and his guidance since, and Javier for supporting this work, and all the research directions it bloomed, since the beginning of my PhD. I also thank my fellow students on the topic, Mary and Breno; Nadya for her support during my time at CERN; Kevin Pedro for lending his expertise on CMS simulations; and the IRIS-HEP institute and the Fermilab LPC for supporting this work through the IRIS-HEP fellowship and the LPC AI fellowship and graduate scholarship, respectively.

Part **??** describes searches for high energy Higgs-boson pair production in the $\mathrm{b\bar{b}VV}$ channel using data collected by the CMS experiment during Run 2 of the LHC. I thank Cristina for her hands-on guidance on both the physics and technical aspects from the start and her patience as I refactored our codebase every week. I thank as well Javier, Petar, Si, and the rest of our boosted double-Higgs working group, as well as Nhan and the DASZLE team, for their advice and support. I thank finally Nick, Lindsey, and all the Coffea and Scikit-HEP developers for building a wonderful and supportive Pythonic HEP ecosystem.

Part **??** on the JetNet library and Lorentz-equivariant ML represents a collection of work [2–4] on which I mentored some amazing students at UC San Diego and more. I thank them all for choosing me as their mentor, and Javier for encouraging and supporting us graduate students in engaging in so many rewarding mentorship opportunities.

Chapter **??** is, in part, a reprint of the materials as they appear in R. Kansal. "Symmetry Group Equivariant Neural Networks," (2020); and NeurIPS, 2021, R. Kansal; J. Duarte; H. Su; B. Orzari; T. Tomei; M. Pierini; M. Touranakou; J.-R.

Vlimant; and D. Gunopulos. Particle Cloud Generation with Message Passing Generative Adversarial Networks. The dissertation author was the primary investigator and author of these papers.

Part partII is, in part, a reprint of the materials as they appear in the NeurIPS ML4PS Workshop, 2020, R. Kansal; J. Duarte; B. Orzari; T. Tomei; M. Pierini; M. Touranakou; J.-R. Vlimant; and D. Gunopulos. Graph generative adversarial networks for sparse data generation in high energy physics; NeurIPS, 2021, R. Kansal; J. Duarte; H. Su; B. Orzari; T. Tomei; M. Pierini; M. Touranakou; J.-R. Vlimant; and D. Gunopulos. Particle Cloud Generation with Message Passing Generative Adversarial Networks; and Phys. Rev. D, 2023, R. Kansal; A. Li; J. Duarte; N. Chernyavskaya; M. Pierini; B. Orzari; and T. Tomei; Evaluating generative models in high energy physics; and the NeurIPS ML4PS Workshop, 2024, A. Li; V. Krishnamohan; R. Kansal; J. Duarte; R. Sen; S. Tsan; and Z. Zhang; Induced generative adversarial particle transformers. The dissertation author was the primary investigator and (co-)author of these papers.

Chapters **??** and **??** and Part **??**, in part, are currently being prepared for the publication of the material by the CMS collaboration. The dissertation author was the primary investigator and author of these papers.

Part **??** is, in part, a reprint of the materials as they appear in JOSS, 2023, R. Kansal; C. Pareja; Z. Hao; and J. Duarte; JetNet: A Python package for accessing open datasets and benchmarking machine learning methods in high energy physics; and Eur. Phys. J. C, 2023, Z. Hao; R. Kansal; J. Duarte; and

N. Chernyavskaya; Lorentz group equivariant autoencoders. The dissertation author was the primary investigator and (co-)author of these papers.

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PUBLICATIONS

Note: as a member of the CMS collaboration, I have been an author on all CMS papers since 2019. The following includes only the CMS publications to which I made significant contributions during my PhD.

1. CMS Collaboration, “Search for Nonresonant Pair Production of Highly Energetic Higgs Bosons Decaying to Bottom Quarks and Vector Bosons”, in prep, CMS-HIG-23-012 (2023).

2. CMS Collaboration, "Search for a massive scalar resonance decaying to a light scalar and a Higgs boson in the two b quarks and four light quarks final state", in prep, CMS-B2G-23-007 (2023).

3. A. Li*, V. Krishnamohan*, R. Kansal, J. Duarte, R. Sen, S. Tsan, and Z. Zhang, "Induced generative adversarial particle transformers", NeurIPS ML4PS Workshop (2023), arXiv:2312.04757.

4. R. Kansal, C. Pareja, Z. Hao, and J. Duarte, "JetNet: A Python package for accessing open datasets and benchmarking machine learning methods in high energy physics", **JOSS** 8, 5789 (2023).

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ABSTRACT OF THE DISSERTATION

Understanding the High Energy Higgs Sector with the CMS Experiment and Artificial Intelligence

by

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Doctor of Philosophy in Physics

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Javier Duarte, Chair

This dissertation describes efforts towards understanding the Higgs boson at the highest energies humanly accessible, using the CMS experiment at the Large Hadron Collider and advances in artificial intelligence (AI) and machine

learning (ML). We present searches for resonant and nonresonant Higgs-boson (H) pair production in the all-hadronic two beauty-quark and two vector boson (V) final state, using a novel strategy to measure the quartic HHVV coupling and search for new Higgs-like bosons. By targeting highly Lorentz-boosted Higgs pairs, we probe effects of potential new physics in the high energy Higgs sector, which could hold answers to fundamental mysteries of nature such as baryon asymmetry.

To enable these and future searches, we introduce as well significant developments in AI/ML, including in the identification of boosted $H \rightarrow VV$ decays with deep transformer networks and advances in AI-accelerated fast simulations of the CMS detector. The latter notably includes the development of the first, highly performant generative models for point-cloud data in high energy physics, which have the potential to improve CMS' computational efficiency by up to three orders of magnitude. We also highlight novel solutions to the important and challenging problems of calibrating and validating these ML techniques. Finally, we present new approaches to search for new physics in a model-agnostic manner, using physics-informed ML methods equivariant to Lorentz transformations.

The quartic HHVV coupling is observed (expected) to be constrained to $[-0.04, 2.05]$ ($[0.05, 1.98]$) at the 95% confidence level relative to the standard model prediction, representing the second-most sensitive measurement of this coupling by CMS to date. Exclusion limits on the production cross section of new heavy resonances decaying to two Higgs-like bosons are expected to be as low as 0.3 fb for high resonance masses.

Introduction

The story so far: In the beginning the Universe was created. This has made a lot of people very angry and been widely regarded as a bad move.

- Douglas Adams, The Restaurant at the End of the Universe

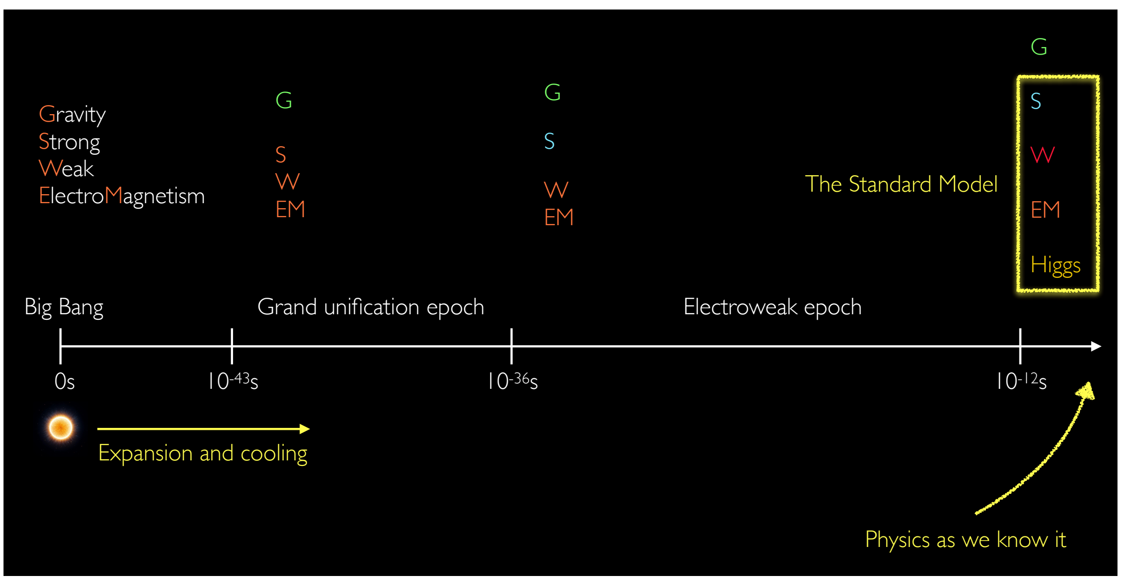

Figure 1. The timeline and evolution of forces in the early universe.

The universe started with a bang. A massive burst of energy, temperature, and pressure, with all four fundamental forces — electromagnetism, nuclear weak, nuclear strong, and gravity — as one. Immediately after, the universe expanded and cooled, and after about 10^{-43} seconds, gravity parted ways. 10^{-36}s later, the strong force separated as well and finally, by around 10^{-12}s, so did the weak and electromagnetic forces,"turning on" the Higgs field in the process and leaving us with the fundamental forces and laws of physics as we know them today (Figure figure1).

Electromagnetism, the nuclear weak and strong forces, the Higgs field, and all known elementary particles can be elegantly described by the standard model (SM) of particle physics. Over the last 60 years, it has proven a monumentally successful theory, both explaining and predicting physical phenomena up to energies produced naturally only within a nanosecond of the Big Bang. These include the prediction of the Higgs boson 50 years before its discovery, explanations for radioactive decay and the binding of atomic nuclei, and the unification of the electromagnetic and weak forces. However, despite its triumphs, there remain fundamental mysteries that the SM cannot explain.

The most glaring of these is its reconciliation, or lack thereof, with gravity, for which a quantum, SM-compatible theory has proven elusive. There is also abundant cosmological evidence of "dark" matter and energy, constituting 95% of the universe and yet finding no justification from the SM. Other subtle mysteries include the inconsistency between the matter-antimatter *a*symmetry we observe and the symmetry the SM predicts, the mechanism for neutrino masses, and the origin of flavor.

The work in this dissertation is motivated by the strong possibility of many of the answers being tied to the Higgs boson. It is our newest discovered and least understood elementary particle, and the unique nature of the Higgs field and its interactions leaves open vast potential for intriguing new physics in this sector. As electroweak symmetry breaking, i.e., the separation of the weak and electromagnetic forces, is intimately connected to a phase transition of the Higgs field, many theories naturally link this transition with the breaking of the matter-antimatter [5] and flavor symmetries [6] as well. The Higgs boson may also be the connection between the SM and the dark sector [7], while the "Higgs-Saw" [8] mechanism is a promising explanation for dark energy.

Predictions of these theories include new, rare, Higgs-like particles and/or minute deviations to the interactions of the Higgs boson from the SM. However, as many of the phenomena therein would have occurred during the electroweak epoch or earlier (see Figure figure1), these effects would manifest only at the highest energies, comparable to that of < 1ps after the Big Bang. This dissertation presents two complementary efforts to probe such effects, by (1) searching for new, highly energetic Higgs bosons, and (2) measuring Higgs interactions uniquely sensitive to new, high energy physics.

We do so using the Large Hadron Collider (LHC) at CERN. The LHC accelerates and collides extremely high-speed protons, producing energies comparable to the early universe just 10ps after the Big Bang. We observe these collisions with the Compact Muon Solenoid (CMS) experiment, one of four massive detectors at the LHC, and one of the two that discovered the Higgs boson in 2012. Crucially, we emphasize that, with the exponentially increasing rate of collisions and data at the LHC, the CMS experiment is entering an era of unprecedented potential for scientific discovery.

To fully realize this, however, and maximize the impact of our new data, significant computational innovation is required. To this end, we also present in this dissertation several novel AI techniques to identify high energy Higgs bosons, accelerate simulations of the CMS detector, and complement traditional data analysis techniques with model-agnostic searches for new physics. Particular emphasis is placed on the development of physics-informed machine learning (ML) algorithms, which uniquely leverage biases of high energy physics (HEP) data to improve their performance and robustness. Namely, we introduce the first generative models for *point-cloud* data in HEP, which respect the sparsity and high granularity of detector data, and the first anomaly detection models equivariant to Lorentz transformations.

We also describe significant efforts towards *validating* such AI techniques, which is critical for them to ultimately have an impact in the field. Specifically, we apply a novel method for calibrating ML algorithms targeting Higgs to vector boson decays, which has proven effective not only for the analyses presented in this dissertation but for the broader CMS physics program as well. We additionally present several studies and new statistical techniques for evaluating fast simulations. The combination of these and our new AI models has the potential to revolutionize the computing paradigm in CMS, improving the computational efficiency of our simulations by up to three orders of magnitude, and ensuring trust in their modeling of the underlying physics.

This dissertation is organized as follows. Part partI introduces the theoretical basis for this dissertation, starting with the mathematical framework behind symmetries in physics (Chapter **??**) and of quantum field theory (Chapter **??**) before detailing the SM of particle physics (Chapter **??**). Part **??** then describes the experimental apparatus used in this dissertation: the LHC (Chapter **??**) and the CMS experiment (Chapter **??**). Part **??** concludes the background material with an introduction to ML in HEP (Chapter **??**), as well as the data analysis and statistical framework used in this dissertation (Chapter **??**).

Parts partII—**??** comprise the novel contributions of this dissertation. Part partII presents new methods for producing and validating fast simulations of the CMS detector using ML, which will be critical to maximizing the scientific output of the LHC in the coming decade. These methods leverage advancements in generative modeling to develop novel, physics-informed simulation techniques that are orders of magnitude faster than traditional methods. We also discuss new techniques for robust evaluation of such fast simulation techniques, and the outlook for their use in CMS.

Part **??** then presents two novel searches to understand the high energy

Higgs sector of the SM, targeting the production of Lorentz-boosted Higgs boson pairs, which decay into two beauty quarks and two vector bosons. Such searches are critical to understanding the properties of the Higgs boson and searching for the effects of new physics at very high energies. We discuss the analysis techniques used in these searches, particularly the use of deep transformer networks to identify Higgs-boson decays to two vector bosons for the first time, and competitive constraints achieved on new physics models and the two-Higgs-two-vector-boson coupling.

Finally, Part **??** outlines the development of new software to facilitate research in ML and HEP and ML techniques that respect the symmetries of the high energy collisions that we study. Namely, we introduce the JetNet Python package, which has proven impactful in this field, and a novel ML algorithm for searching for new physics while remaining robust to Lorentz-transformations of our data.

Part I

Theoretical Background

Chapter 1

Introduction to the Standard Model

God used beautiful mathematics in creating the world. — Paul Dirac [9]

The standard model (SM) of particle physics is perhaps the greatest scientific theory of all time. It is a mathematical representation of three fundamental forces, all known elementary particles, and their collective interactions. In a broader sense, it is also the culmination of centuries of iterative, syncretic experimental results and theoretical advances, from Newton's laws of motion up to the discovery of the Higgs boson. That such a wide array of seemingly idiosyncratic physical phenomena and theories — electricity, magnetism, radioactive decays, quantum mechanics, special relativity, the structure of the atom, the binding of the nucleus, the behavior of elementary particles, and more — can all be encapsulated at their most primordial level into a single theory exemplifies the beauty of the SM.

This beauty is perhaps most apparent when viewing the SM through the lens of *symmetries*. Symmetries provide an elegant way to precisely describe the extremely complex physics mentioned above. Indeed, superficially, the SM can be viewed simply as a classification of elementary particles and their interactions according to their behavior under different symmetries of the universe and its mathematical description.

This is illustrated in Figure figure1.1, listing the SM particles and their properties. They are first divided into two classes, fermions and bosons, based on how they behave under Lorentz transformations — a fundamental physical symmetry of nature. This simple distinction has profound implications: fermions constitute matter, i.e. what all the "stuff" in the universe is made out of, while bosons are the particles responsible for forces and their interactions. Specifically, the photon mediates electromagnetism, the $W^{\pm}$ and Z bosons the weak force, and gluons the strong force. There is also the Higgs boson, which is special: it does not mediate a force in the classical sense, but its interactions with elementary particles are what imbues them with mass.

Each force is intimately tied to a symmetry in the SM, and particles are further distinguished by their behavior under these symmetries — or, equivalently, how they are affected by this force. Fermions are divided by those interacting (quarks) and not interacting (leptons) with the nuclear strong force, while each of their rows in Figure figure1.1 further separates them by different "charges" under the weak force. Additionally, each particle's mass and electric charge rep-

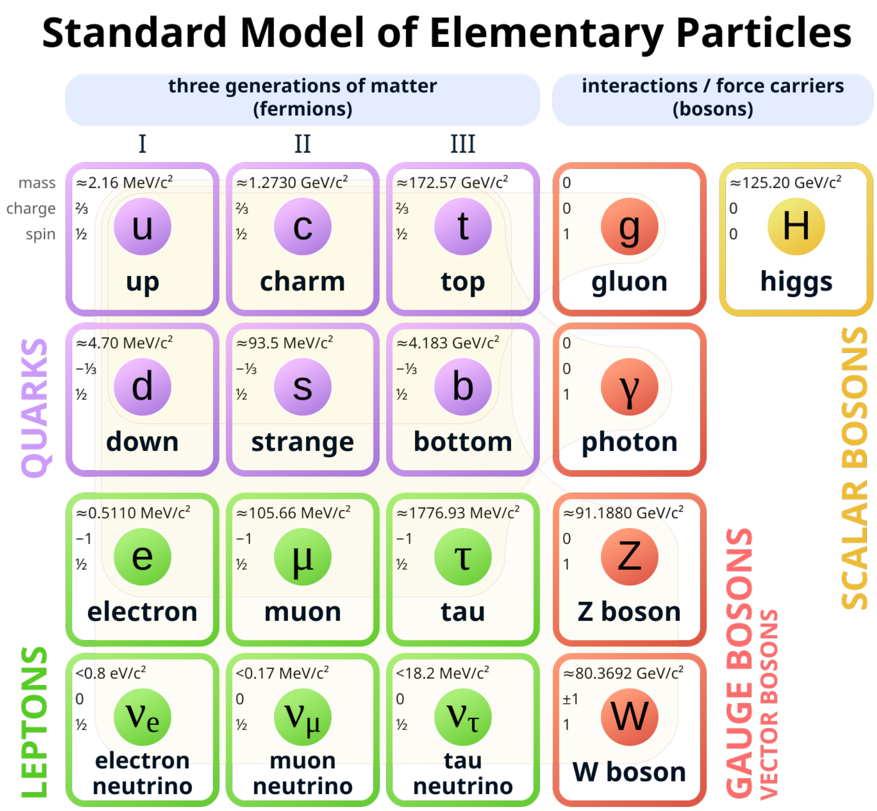

Figure 1.1. Particles and their classifications in the SM, reproduced from Ref. [1].

resent the strength of its interaction with the Higgs and electromagnetic fields, respectively. Finally, we can see a mysterious *almost*-symmetry: there are three copies, or "flavors" or "generations", of each fermion, which are entirely identical but for their masses (e.g. the electron, muon, and tau family of particles). Such a structure may suggest the presence of new, yet-to-be-discovered forces tied to this symmetry.

The goal of Part partI is to make this picture more precise, and lay the theoretical foundation for the work discussed in this dissertation. The mathematical frameworks needed to do so are called group theory and quantum field theory (QFT), and are the subjects of Chapters **??** and **??**, respectively. Equipped with these tools, we then describe the SM in Chapter **??**, including the interactions discussed above and, of most relevance to the subject of this dissertation, the phenomenon of jets, the Higgs sector, and Higgs boson pair production within and beyond the SM.

These chapters build off of several great resources, including:

- David Tong's extremely useful and insightful lecture notes on QFT [10], gauge theories [11], and the standard model [12];
- John McGreevy's great course on symmetry in physics [13] (which I had the pleasure of attending in the Fall of 2020);
- Frederic Schuller's precise lectures on the geometric anatomy of theoretical physics [14];
- Tony Zee's *Group Theory in a Nutshell for Physicists* [15] and *Quantum Field Theory in a Nutshell* [16];
- Peskin and Schroeder's classic *An Introduction to Quantum Field Theory* [17];
- Gavin Salam's lectures on *Elements of QCD for hadron colliders* [18];
- and Hong Liu [19] and Ricardo Matheus' [20] clear, recorded lectures on QFT.

Part II

Accelerating Simulations with AI

Chapter 2

test chapter

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