T 76: Data, AI, Computing, Electronics VII (Generative AI, MC Generators)

Time: Thursday 16:15–18:45 Location: VG 2.101

T 76.1 Thu 16:15 VG 2.101

Correcting the mis-modeling of photon energy deposits in the calorimeter using normalizing flows and flow matching — Caio Daumann, Johannes Erdmann, and •Lars Schiffeler — III. Physikalisches Institut A, RWTH Aachen University

Simulated events are key ingredients for almost all high-energy physics analyses. However, imperfections in their configuration can result in mis-modelling and discrepancies between the data and simulations. Normalizing flows are used in CMS to correct the high-level inputs to the photon identification algorithms, which have a low dimensionality. Improved identification algorithms, on the other hand, use information with an increased dimensionality, such as individual energy deposits in a calorimeter. This poses a challenge to normalizing flows, as they are more effective in lower-dimensional spaces. We investigate the influence of this increase in dimensionality on normalizing flows and compare their effectiveness to flow matching. To study these effects, simulations of a CMS-inspired toy calorimeter are used.

T 76.2 Thu 16:30 VG 2.101

Belle II PXD background generation with diffusion models — •Fabio Novissimo, Nikolai Hartmann, and Thomas Kuhr — Ludwig-Maximilians-Universität München

The Pixel Vertex Detector (PXD) is the innermost detector of the Belle II experiment. Information from the PXD, together with data from other detectors, allows to have a very precise vertex reconstruction. The effect of beam background on reconstruction is studied by adding measured or simulated background hit patterns to hits produced by simulated signal particles. This requires a huge sample of statistically independent PXD background noise hit patterns to avoid systematic biases, resulting in a huge amount of storage due to the high granularity of the PXD sensors. As an efficient way of producing background noise, we explore the idea of an on-demand PXD background generator realised using diffusion models. In order to evaluate the quality of generated background we measure physical quantities which are sensitive to the background in the PXD.

T 76.3 Thu 16:45 VG 2.101

Study of deep generative models for the enhancement of simulated ATLAS datasets — Boris Flach, Andre Sopczak, and •Lukas Vicenik — Czech Technical University in Prague

Numerous searches for new particles and precision measurements crucially depend on the amount of available simulated data, which has an impact on the resulting analysis uncertainties. For instance, machine learning algorithms for separating signal and background events could significantly profit from enlarged simulated datasets. We propose advanced generative models based on variational autoencoders, generative adversarial networks, and diffusion-based deep generative models to address the limitations of current simulated datasets. These models generate synthetic data that capture complex, non-homogeneous features observed in particle physics. Evaluation metrics from particle physics and machine learning are employed to assess the accuracy, diversity, and physical validity of the generated data. The augmented datasets are subsequently used to enhance signal and background separation, reduce uncertainties in analyses, and improve the overall reliability of the results.

T 76.4 Thu 17:00 VG 2.101

PointL2LFlows: How to generate Hadronic showers in ECal and HCal with CNFs — •Thorsten Buss — Institut für Experimentalphysik, Universität Hamburg, Germany

In collider experiments, Monte Carlo (MC) simulations are the essential tool for comparing experimental findings with theory predictions. However, they have a high computational demand, and future developments, such as higher event rates, are expected to increase this demand beyond availability.

Generative models provide a way of augmenting MC simulations, speeding them up, and overcoming this bottleneck. Recent works have successfully applied this approach to electromagnetic showers in electromagnetic calorimeters (ECal) and to pion showers in low-granular homogeneous calorimeters. However, applying it to pion showers developing in a highly granular ECal and continuing in a highly granular HCal remains a challenge due to their rich substructure.

This work shows how point-cloud-based continuous normalizing flows (CNF) can jointly generate pion showers in ECal and HCal. As in our L2LFlows model for EM showers, we generate one calorimeter layer at a time conditioned on the previous layers. This reduces the size of the point clouds reducing computational costs and making it easier for the model to focus on the most important structures in the showers.

T 76.5 Thu 17:15 VG 2.101

Point-Clouds based Diffusion Model on Hadronic Showers — •Martina Mozzanica — University of Hamburg

Simulating showers of particles in highly-granular detectors is a key frontier in the application of machine learning to particle physics. Achieving high accuracy and speed with generative machine learning models can enable them to augment traditional simulations and alleviate a major computing constraint. Recent developments have shown how diffusion based generative shower simulation approach that do not rely on a fixed structure, but instead generates geometry-independent point clouds, are very efficient.We present a novel attention mechanism based extension to the CaloClouds 2 architecture that was previously used for simulating electromagnetic showers in the highly granular electromagnetic calorimeter of ILD with high precision. This attention mechanism allows to generate complex hadronic showers from pions with more pronounced substructure in the electromagnetic and hadronic calorimeter together. This is the first time that ML methods are used to generate hadonic showers in highly granular imaging calorimeters.

T 76.6 Thu 17:30 VG 2.101

Generative transformers for learning point-cloud simulations — Joschka Birk[1], Frank Gaede[2], Anna Hallin[1], Gregor Kasieczka[1], Martina Mozzanica[1], and •Henning Rose[1] — [1]Institute for Experimental Physics, Universität Hamburg, Hamburg — [2]Deutsches Elektron-Synchrotron DESY, Hamburg

We successfully demonstrate the use of a generative transformer for learning point-cloud simulations of electromagnetic showers in the International Large Detector (ILD) calorimeter. By reusing the architecture and workflow of the OmniJet-α model, this transformer predicts sequences of tokens that represent energy deposits within the calorimeter. This autoregressive approach enables the model to learn the sequence length of the point cloud, supporting a variable-length and realistic shower development. Furthermore, the tokenized representation allows the model to learn the shower geometry without being restricted to a fixed voxel grid.

T 76.7 Thu 17:45 VG 2.101

AIDO - A Generalized Detector Optimization Framework using Surrogate Models — •Kylian Schmidt, Jan Kieseler, and Nikhil Krishna — Institute of Experimental Particle Physics (ETP), Karlsruhe Institute of Technology (KIT)

The design of modern high-energy physics detectors is a highly intricate process, aiming to maximize their physics potential while balancing various manufacturing constraints. As detectors become larger and more sophisticated, it becomes increasingly difficult to maintain a comprehensive understanding of the entire system. To address this challenge, we aim to translate the design process into an optimization task suitable for Machine Learning by treating the parameters of the simulation as hyper-parameters of the model.

The AIDO framework is a generalized tool for the optimization of continuous and discrete detector parameters. We train a diffusion-based surrogate model on parallel Geant4 simulations with varying detector geometries, enabling the model to interpolate the expected performance across different configurations. This allows for gradient descent on the generated parameter space and identification of the optimal combination of parameters that maximizes a specific physics goal. As a demonstration, we show how this approach can be applied to generate an optimal sampling calorimeter by maximizing its energy resolution starting from a random initial composition.

T 76.8 Thu 18:00 VG 2.101

Navigating Phase Space for Event Generation: interfacing Sherpa with BAT.jl — Cornelius Grunwald[1], Timo Janssen[2], Kevin Kröninger[1], •Salvatore La Cagnina[1], and Steffen Schumann[2] — [1]TU Dortmund University, Dortmund, Germany — [2]Georg-August-Universität Göttingen, Germany

The generation of Monte Carlo events is a crucial step for all particle collider experiments. A major challenge in event generation is the efficient sampling of the phase spaces of hard scattering processes due to the potentially large number and complexity of Feynman diagrams and their interference and divergence structures. In this presentation, we address the challenges of efficient Monte Carlo event generation and demonstrate improvements that can be achieved through the application of advanced sampling techniques. We highlight that using the algorithms implemented in BAT.jl for sampling the phase spaces given by Sherpa offers great flexibility in the choice of sampling algorithms and has the potential to significantly enhance the efficiency of event generation. By interfacing BAT.jl, a package designed for Bayesian analyses that offers a collection of modern sampling algorithms, with the Sherpa event generator, we aim to improve the efficiency of phase space exploration and Monte Carlo event generation. We combine the physics-informed multi-channel sampling approach of Sherpa with advanced sampling techniques such as Markov Chain Monte Carlo (MCMC) and Nested Sampling.

T 76.9 Thu 18:15 VG 2.101

Geant4 Optimizations in ATLAS — •Mustafa Schmidt für die Mu2e-Kollaboration — Bergische Universität Wuppertal, Deutschland

The ATLAS experiment at the LHC heavily depends on simulated event samples produced by a full Geant4 detector simulations. These Monte Carlo simulations based on Geant4 were a major consumer of computing resources during the 2018 data-taking year and will remain one of the dominant resource users in the HL-LHC era. Consequently, ATLAS has continuously been working to improve the computational performance of this simulation for the Run 3 Monte Carlo campaign.

This report highlights the recent implementation of Woodcock tracking in the Electromagnetic Endcap Calorimeter and provides an overview of other implemented and upcoming optimizations that still have to be validated. These improvements include enhancements to the core Geant4 software, strategic choices in simulation configuration, simplifications in geometry and magnetic field descriptions, as well as technical refinements in the interface between ATLAS simulation code and Geant4.

Overall, a performance improvement of around 50% regarding CPU time was achieved compared to the baseline simulation configuration utilized during Run 2.

T 76.10 Thu 18:30 VG 2.101

Exploring tomorrow's Monte-Carlo generators: MC Validation in ATLAS with PAVER — •Johanna Kraus, Anna Bingham, Frank Ellinghaus, Dominic Hirschbühl, and Mustafa Schmidt — Bergische Universität Wuppertal

Monte-Carlo (MC) simulations play a key role in high energy physics, for example at the ATLAS experiment. MC generators evolve continuously, so a periodic validation is indispensable for obtaining reliable and reproducible physics simulations. For that purpose, an automated and central validation system was developed: PMG Architecture for Validating Evgen with Rivet (PAVER). It provides an MC event generator validation procedure that allows a regular evaluation of new revisions and updates for commonly used MC generators in ATLAS as well as comparisons to measured data. The result is a robust, fast, and easily accessible MC validation setup that is constantly developed further. This way, issues in simulated samples can be detected before generating large samples for the collaboration, which is crucial for a sustainable and low-cost MC production procedure in ATLAS.