

8th Round table on Deep Learning @ DESY

Report of Contributions

Contribution ID: 1

Type: **not specified**

Observable Optimization for Precision Theory: Machine Learning Energy Correlators

Friday 14 November 2025 14:15 (10 minutes)

The practice of collider physics typically involves the marginalization of multi-dimensional collider data to uni-dimensional observables relevant for some physics task. In any cases, such as classification or anomaly detection, the observable can be arbitrarily complicated, such as the output of a neural network. However, for precision measurements, the observable must correspond to something computable systematically beyond the level of current simulation tools. In this work, we demonstrate that precision-theory-compatible observable space exploration can be systematized by using neural simulation-based inference techniques from machine learning. We illustrate this approach by exploring the space of marginalizations of the energy 3-point correlator to optimize sensitivity to the top quark mass. We first learn the energy-weighted probability density from simulation, then search in the space of marginalizations for an optimal triangle shape. Although simulations and machine learning are used in the process of observable optimization, the output is an observable definition which can be then computed to high precision and compared directly to data without any memory of the computations which produced it.

Author: BHATTACHARYA, Arindam Sonali Amar (T (Phenomenology))

Co-authors: Dr FRASER, Katherine (UC Berkeley); Prof. SCHWARTZ, Matthew (Harvard University)

Presenter: BHATTACHARYA, Arindam Sonali Amar (T (Phenomenology))

Session Classification: Session 1

Contribution ID: 2

Type: **not specified**

CaloClouds3; Diffusion and Flows

Friday 14 November 2025 13:25 (10 minutes)

Presenting a generative model for detector simulation, that utilities normalising flows for macro-information, and iid diffusion models for fast details.

This is the third iteration of the CaloClouds series, which surpasses previous limits in inference speed. New, upgraded, capacities allow simulation of photons throughout the barrel of the detector. By integrating the model into the key4hep workflow we are able to produce realistic use-case results.

Authors: KOROL, Anatolii (FTX (FTX Fachgruppe SFT)); GAEDE, Frank (FTX (FTX Fachgruppe SFT)); KASIECZKA, Gregor (UNI/EXP (Uni Hamburg, Institut fur Experimentalphysik)); DAY-HALL, Henry (FTX (FTX Fachgruppe SFT)); KRUEGER, Katja (DESY (FTX Fachgruppe DTA)); VALENTE, Lorenzo (UNI/EXP (Uni Hamburg, Institut fur Experimentalphysik)); MOZZANICA, Martina (UNI/EXP (Uni Hamburg, Institut fur Experimentalphysik)); MCKEOWN, Peter (CERN); MADLENER, Thomas (FTX (FTX Fachgruppe SFT)); BUSS, Thorsten (Universität Hamburg)

Presenter: DAY-HALL, Henry (FTX (FTX Fachgruppe SFT))

Session Classification: Session 1

Contribution ID: 3

Type: **not specified**

Agents of Discovery

Friday 14 November 2025 11:35 (10 minutes)

Particle physics and other sciences are becoming more and more data centric, requiring increasingly complex analysis methods. Often large parts of these methods belong to standard procedures which have to be implemented by hand again and again, taking time away from more interesting and innovative work. With the rise of agentic AI systems, driven by the rapid improvement of large language models (LLMs) in the last years, other approaches become feasible: Tasking AI agents with implementing those known parts, making workflows more efficient. In this work we present a framework allowing a team of AI Agents to work autonomously on a given task, including capabilities for writing code, code execution, error correction and logic checks.

The setup uses state-of-the art OpenAI LLMs and has been tested in the realm of anomaly detection with a task based on the LHC Olympics challenge. The performance was monitored throughout many different technical and physical metrics, allowing us to draw detailed conclusions on the capabilities of the different LLMs: Most are capable of solving the given task, while the best were able to match human level performance.

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Presenter: LUKAS, Tim (Desy)

Session Classification: Session 1

Contribution ID: 4

Type: **not specified**

A Differentiable Physics Model for Automated Inverse Design in Optics

Friday 14 November 2025 13:05 (10 minutes)

Designing complex optical coatings, such as dispersion-managed mirrors for ultrafast lasers, is a high-dimensional inverse problem traditionally relying on iterative, expert-guided methods. We present a machine learning framework that automates this process by employing an autoencoder with a differentiable, physics-based decoder. This decoder, which analytically solves Maxwell's equations via the Transfer Matrix Method, allows the network to learn the design mapping from target specifications alone. The framework successfully generated a multi-objective dispersive mirror design with performance metrics that match those produced by established commercial optimization software, offering a powerful alternative for rapid and automated design exploration.

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Presenter: TUENNERMANN, Henrik (FS-LA (Research))

Session Classification: Session 1

Contribution ID: 5

Type: **not specified**

PanShower: One model for all calorimeter showers

Friday 14 November 2025 13:45 (10 minutes)

Accurate and efficient detector simulation is essential for modern collider experiments. To reduce the high computational cost, various fast machine learning surrogate models have been proposed. Traditional surrogate models for calorimeter shower modeling train separate networks for each particle species, limiting scalability and reuse. We introduce PanShower, a unified generative model that simulates calorimeter showers across multiple particle types using a single generative model. PanShower is a continuous normalizing flow model with a Transformer architecture, enabling it to generate complex spatial and energy correlations in variable-length point cloud representations of showers. Trained on a diverse dataset of simulated showers in the highly granular ILD detector, the model demonstrates the ability to generate realistic showers for electrons, photons, charged and neutral hadrons over a wide range of incident energies and angles without the need for retraining.

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Presenter: BUSS, Thorsten (Universität Hamburg)

Session Classification: Session 1

Contribution ID: 6

Type: **not specified**

Workshop idea: "How to use AI tools to make your research more efficient"

Friday 14 November 2025 10:50 (10 minutes)

More and more AI tools written by non-physicists such as ChatGBT, CoPilot and Cursor are becoming available. These tools allow researchers to perform their work more efficiently. Yet, many are not using them (properly), though they can be very useful for literature research, writing texts, coding, etc.

To ensure that scientists at DESY have a basic understanding of what is possible and where to start, our idea is to offer a half-day workshop on these AI tools. Besides introducing the tools and how to best use them, ethical aspects such as citation of tools, which data to share and how trustworthy the tools are shall be covered.

Authors: BRUEERS, Ben (Z_ATUP (ATLAS-Upgrade)); SPITERI, Dwayne (IT (IT Scientific Computing)); MADLENER, Thomas (FTX (FTX Fachgruppe SFT))

Presenter: SPITERI, Dwayne (IT (IT Scientific Computing))

Session Classification: Session 1

Contribution ID: 7

Type: **not specified**

LLM-Powered Issue Analysis for High-Availability Laser Operations

Friday 14 November 2025 11:25 (10 minutes)

Ensuring 24/7 operation of the laser systems for DESY's free-electron lasers requires detailed analysis of operator logbooks and RT-tickets, a task currently limited by labor-intensive manual methods that lack statistical granularity. As part of a DASHH collaboration with the University of Hamburg, we investigate the application of Large Language Models (LLMs) to automate this analysis. We benchmarked LLMs on binary issue detection in logbooks and multi-class categorization of intervention tickets, achieving strong performance with an F1 score of approximately 0.84 and a Macro-F1 of 0.42, respectively. This automated classification enables fine-grained, real-time statistical analysis of fault patterns for data-driven identification of subsystems requiring targeted upgrades. This work provides the foundation for developing advanced operational tools, including system health dashboards, expert support chatbots, and proactive diagnostic agents.

Authors: KARIMI, Afshin; TUENNERMANN, Henrik (FS-LA (Research))

Co-authors: Prof. LAUSCHER, Anne (UHH); PRESSACCO, Federico (FS-LA (Injector and Heater Lasers)); MAYET, Frank (MXL (XFEL)); HARTL, Ingmar (FS-LA (Lasergruppe))

Presenters: KARIMI, Afshin; TUENNERMANN, Henrik (FS-LA (Research))

Session Classification: Session 1

Contribution ID: 8

Type: **not specified**

Automating beam alignment at the European XFEL

Friday 14 November 2025 12:45 (10 minutes)

Large-scale facilities like European XFEL consist of numerous subsystems, where precise real-time tuning is essential for maintaining stable and optimal performance. Automation techniques can be leveraged to reduce operators' time investment and potentially increase the exploitation of allotted beamtime, both in quantity and quality. In this talk, we will discuss our ongoing efforts to automate the alignment of optical components across multiple subsystems.

Author: BIRNSTEINOVA, Sarlota (Eur.XFEL (European XFEL))

Co-authors: GARCIA-TABARES, Ana; DAVTYAN, Arman; ENOQUE FERREIRA DE LIMA, Danilo; DOBLAS-JIMÉNEZ, David; SOBOLEV, Egor; BISHARA, Fady; SOHN, Florian; KARPICS, Ivars; WRIGLEY, James; KOLIYADU, Jayanath; BIELECKI, Johan; SZTUK-DAMBIETZ, Jolanta; GELISIO, Luca; SIKORSKI, Marcin; KUJALA, Naresh; ZALDEN, Peter; DE WIJN, Raphaël; BEAN, Richard; LETRUN, Romain; HAUF, Stefan; MICHELAT, Thomas

Presenter: BIRNSTEINOVA, Sarlota (Eur.XFEL (European XFEL))

Session Classification: Session 1

Contribution ID: 9

Type: **not specified**

Differentiable Physics-Based Feedback for Adaptive Laser Pulse Shaping

Friday 14 November 2025 13:15 (10 minutes)

Precise control of the temporal profile of laser pulses is essential for optimizing beam emittance in photoinjectors. Achieving this through spectral shaping is particularly challenging due to nonlinear effects, temporal drifts, and experimental nonidealities. To address this, a two-step feedback mechanism based on differentiable physics modeling is developed for adaptive experimental control. The approach combines a differentiable model that captures the system's behavior within its operating regime with gradient-based optimization to efficiently achieve desired pulse shapes. This framework demonstrates how differentiable models can bridge physical understanding and data-driven optimization, offering a versatile strategy for controlling complex experimental systems.

Authors: ILIA, Denis (FS-LA (Research)); HARTL, Ingmar (FS-LA (Lasergruppe)); MAHNKE, Christoph (FS-LA (Laser Operations & User Support)); PRESSACCO, Federico (FS-LA (Injector and Heater Lasers)); TUEN-NERMANN, Henrik (FS-LA (Research))

Presenter: ILIA, Denis (FS-LA (Research))

Session Classification: Session 1

Contribution ID: 10

Type: **not specified**

Neural networks for FEL diffraction image separation

Friday 14 November 2025 12:55 (10 minutes)

Newly available soft X-ray two-color FEL pulse mode at European XFEL opens a new way to the structural and plasma studies of the nano-scaled object. The first pulse, designated as the pump, characterizes the initial state of the object, whereas the second probe pulse captures the system's evolution following its interaction with the pump. The pulses are separated by an extremely short time interval of less than a picosecond. Due to the short delay between the pump and probe pulses, the state-of-the-art detector is unable to capture two separate diffraction images corresponding to the pump and probe pulses. Instead, it records a single image that is a superposition of both, making it difficult to analyze the effects of each pulse individually. The analysis would ideally provide the electron density of the sample before the interaction with the X-ray and afterwards, which allows us to examine the impact of the excitation in a time-resolved manner.

This talk presents a machine learning-based solutions for separating the overlapping components in such images. We propose two methods: one based on diffusion probabilistic models, a recent and powerful approach in image generation, and another using feed-forward convolutional neural networks to solve the same task.

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Presenter: MOROZOV, Nikita (Eur.XFEL (European XFEL))

Session Classification: Session 1

Contribution ID: 11

Type: **not specified**

OmniJet- α for Calorimeters

Friday 14 November 2025 13:55 (10 minutes)

We present a second-generation transformer for simulating calorimeter showers as point clouds in high-granularity detectors. As in OmniJet- α , showers are modeled as variable-length sequences, capturing realistic shower development without conditioning on the number of hits. New in this version, we remove the VQ-VAE entirely and directly tokenize the detector geometry. This geometry-aware tokenization simplifies training and delivers higher fidelity, better stability, and markedly improved scalability to larger and more complex calorimeters.

Author: ROSE, Henning (UNI/EXP (Uni Hamburg, Institut fur Experimentalphysik))

Presenter: ROSE, Henning (UNI/EXP (Uni Hamburg, Institut fur Experimentalphysik))

Session Classification: Session 1

Contribution ID: 12

Type: **not specified**

CaloHadronic: a diffusion model for the generation of hadronic showers

Friday 14 November 2025 13:35 (10 minutes)

Simulating showers of particles in highly-granular calorimeters 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 approaches that do not rely on a fixed structure, but instead generate geometry-independent point clouds, are very efficient. We present a transformer-based extension to previous architectures which were developed for simulating electromagnetic showers in the highly granular electromagnetic calorimeter of the International Large Detector, ILD. The attention mechanism now allows us to generate complex hadronic showers with more pronounced substructure across both the electromagnetic and hadronic calorimeters. This is the first time that machine learning methods are used to holistically generate showers across the electromagnetic and hadronic calorimeter in highly granular imaging calorimeter systems. Improvements to this model will also be shortly presented.

Author: MOZZANICA, Martina (UNI/EXP (Uni Hamburg, Institut fur Experimentalphysik))

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Presenter: MOZZANICA, Martina (UNI/EXP (Uni Hamburg, Institut fur Experimentalphysik))

Session Classification: Session 1

Contribution ID: 13

Type: **not specified**

Cross-Geometry Transfer Learning in Fast Electromagnetic Shower Simulation

Friday 14 November 2025 14:05 (10 minutes)

Accurate particle shower simulation remains a critical computational bottleneck in high-energy physics. Traditional Monte Carlo methods, such as Geant4, are computationally prohibitive, while existing machine learning surrogates are often tied to specific detector geometries and require full retraining for each design change or alternative detector configuration.

We present a transfer learning framework for generative calorimeter simulation that enables efficient adaptation across diverse geometries with high data efficiency. Using point cloud representations and pre-training on the International Large Detector (ILD), our approach handles new configurations without re-voxelizing showers for each geometry.

On the CaloChallenge dataset, transfer learning with only 100 target-domain samples achieves a 44% improvement in Wasserstein distance over training from scratch. Parameter-efficient fine-tuning using bias-only adaptation attains competitive performance while updating only 17% of model parameters.

This study provides insight into adaptation mechanisms in particle shower development and establishes a baseline for future progress in point cloud-based calorimeter simulation.

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Presenter: VALENTE, Lorenzo (UNI/EXP (Uni Hamburg, Institut fur Experimentalphysik))

Session Classification: Session 1

Contribution ID: 14

Type: **not specified**

The Helmholtz Model Zoo: Enabling AI Model Sharing and Inference in the Helmholtz Cloud

Friday 14 November 2025 11:45 (10 minutes)

The Helmholtz Model Zoo (HMZ) is a cloud-based platform providing remote access to deep learning models within the Helmholtz Association via web interface and REST API. Scientists from all 18 Helmholtz centers can contribute models through a streamlined GitLab submission process, with HMZ automatically generating the interface, testing, and deploying the model.

HMZ runs on GPU nodes at DESY Hamburg using NVIDIA Triton Inference Server, ensuring data sovereignty by keeping all data within the Helmholtz Cloud. The platform offers unrestricted inference capacity with fine-grained access control through Helmholtz Virtual Organizations, and supports external researcher collaboration. Development is led by the Helmholtz Imaging Support Team at DESY with support from HIFIS and Helmholtz AI.

Author: WERNERS, Hans William (IT (Research and Innovation in Scientific Co))

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Presenter: WERNERS, Hans William (IT (Research and Innovation in Scientific Co))

Session Classification: Session 1

Contribution ID: 15

Type: **not specified**

AI Copilot for FEL Experiments at European XFEL

Friday 14 November 2025 11:15 (10 minutes)

As part of an effort to integrate generative AI into operation, a project focusing on establishing an AI Copilot to help guide experiments at the European XFEL has been initiated. Initially, a survey was designed and implemented to investigate which issues beamline staff face during operation, and that they think could benefit from an AI co-pilot. The results of the survey indicated that interactions with the data acquisition (DAQ) system during beamtimes was a common source of problems. Consequently, the first use case for this tool will focus on the DAQ. To this end, a device was developed, that subscribed to events in the control system, informing us on what data a model could expect to have access to from the live system. The AI Copilot would then consist of a model to detect anomalies, which a RAG-based knowledge assistant would then forward to the Zulip chat client, enabling scientists to communicate effectively with the Copilot through an interface that has already proven efficient in other internal applications. In this contribution we present the results of the survey and initial results from classifying the control system data the model may have access to. These activities fit into a larger effort of investigating generative AI to support facility operation.

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Presenter: Mr AJAMI, Mahmoud (Eur.XFEL (European XFEL))

Session Classification: Session 1

Contribution ID: 16

Type: **not specified**

AI-assisted retrieval and visualization of control-system data from the InfluxDB time-series database at the European XFEL

Friday 14 November 2025 12:05 (10 minutes)

Historic data of settings and operational conditions within the Karabo SCADA system at the European XFEL is stored in an InfluxDB time-series database and facilitates trend analysis, anomaly detection and performance optimization. Frequently, the data serves as a foundation for data-driven decision-making, allowing researchers and engineers to analyze past events, validate system behavior, and refine experimental processes for improved efficiency and reliability. In this contribution, a prototype of a chat-based AI assistant for retrieval and visualization of data from the database is presented, which provides an easier and quicker access to the data than the traditional Grafana-based frontend.

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Co-author: HAUF, Steffen (Eur.XFEL (European XFEL))

Presenter: SOHN, Florian (Eur.XFEL (European XFEL))

Session Classification: Session 1

Contribution ID: 17

Type: **not specified**

Early experiences with agentic generative AI for EuXFEL operations support

Friday 14 November 2025 11:55 (10 minutes)

Generative AI is increasingly playing a role in supporting the operation of light sources, e.g. through support assistants or tools that cover certain recurring tasks. While LLM-based coding assistants are somewhat established, and RAG-based knowledge assistants are reaching production-readiness levels in well-defined domains, agentic generative AI, to which operational tasks are handed off, are still in an emergent state, with prototypes being tested. In this contribution, we present currently ongoing evaluations at the EuXFEL on using the model context protocol (MCP) to provide contextual awareness for agentic LLMs in a scientific operational setting. The technology stack presented utilizes FastMCP and mcp_use for MCP integration, QdrantDB as a vector database, and explores Zulip as a front-end.

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Presenters: SOHN, Florian (Eur.XFEL (European XFEL)); HAUF, Steffen (Eur.XFEL (European XFEL))

Session Classification: Session 1

Contribution ID: 18

Type: **not specified**

FSR recovery with a GNN-based supervised tagger

Friday 14 November 2025 14:25 (10 minutes)

Efficient capture of final state radiation (FSR) is crucial for a high mass resolution in BSM QCD searches. Using kinematic observables of dijet processes, we want to develop a GNN-based supervised tagger that improves the FSR resolution and is able to distinguish BSM processes from a dijet background.

Authors: Dr LIU, Bingxuan; SANDER, Christian (ATLAS); FUSTE COSTA, Max (ATLAS (ATLAS-Experiment)); ISHIKAWA, Ryotaro (Department of Physics, Graduate School of Science, Tokyo Metropolitan University); HEIM, Sarah (ATLAS (ATLAS Dark Matter with Higgs)); DREYER, Sascha (ATLAS (ATLAS Beyond Standard Model))

Presenter: FUSTE COSTA, Max (ATLAS (ATLAS-Experiment))

Session Classification: Session 1

Contribution ID: **19**

Type: **not specified**

Welcome

Friday 14 November 2025 09:30 (10 minutes)

Presenter: HEUSER, Philipp (DESY/Helmholtz Imaging)

Session Classification: Session 1

Contribution ID: 20

Type: **not specified**

AI in Climate Research - How LLMs and its Platforms make a Difference

Friday 14 November 2025 10:05 (45 minutes)

Climate research often requires substantial technical expertise. This involves managing data standards, various file formats, software engineering, and high-performance computing. Translating scientific questions into code that can answer them demands significant effort. The question is, why? Data analysis platforms like Freva (Kadow et al. 2021, e.g., gems.dkrz.de) aim to enhance user convenience, yet programming expertise is still required. In this context, we introduce a large language model setup and chat bot interface for different core e.g. based on GPT-4/ChatGPT or DeepSeek, which enables climate analysis without technical obstacles, including language barriers. Not yet, we are dealing with climate LLMs for this purpose. Dedicated natural language processing methodologies could bring this to a next level. This approach is tailored to the needs of the broader climate community, which deals with small and fast analysis to massive data sets from kilometer-scale modeling and requires a processing environment utilizing modern technologies, but addressing still society after all, such as those in the Earth Virtualization Engines (EVE - eve4climate.org). Our interface runs on an High Performance Computer with access to PetaBytes of data - everything just a chat away.

Presenter: Dr KADOW, Christopher (DKRZ)

Session Classification: Session 1

Contribution ID: 21

Type: **not specified**

Setting the stage: User's intro to LLMs

Friday 14 November 2025 09:40 (25 minutes)

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Session Classification: Session 1