Lamarr: implementing a flash-simulation paradigm at LHCb

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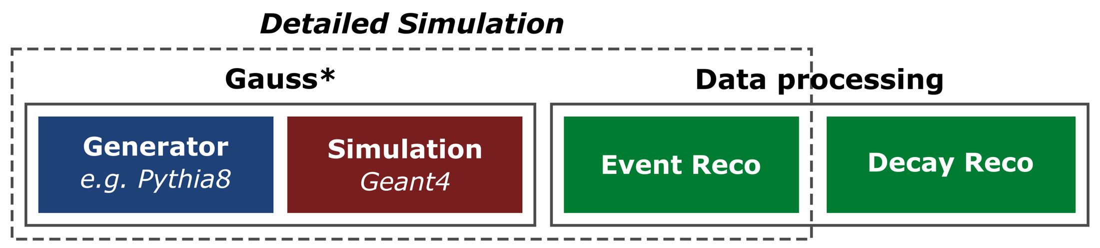
L. Anderlini[1], M. Barbetti[2], S. Capelli[3,4], G. Corti[5], A. Davis[6], D. Derkach[7], M. Martinelli[3,4], **M. Mazurek**[8]

[1]INFN-Firenze, [2]INFN-CNAF, [3]INFN-MiB, [4]University of Milano-Bicocca, [5]CERN, [6]University of Manchester, [7]HSE University, [8]NCBJ

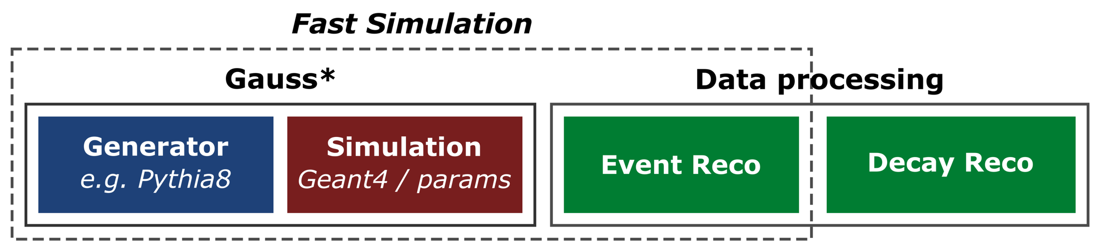
1. Motivation

Detailed simulation of the interaction between the traversing particles and the LHCb active volumes is the major consumer of CPU resources. During the LHC Run2, the LHCb experiment has spent **more than 90% of the pledged CPU time** to simulate events of interest. Matching the upcoming and future demand for simulated samples means that the development of **faster simulation options** is critical.

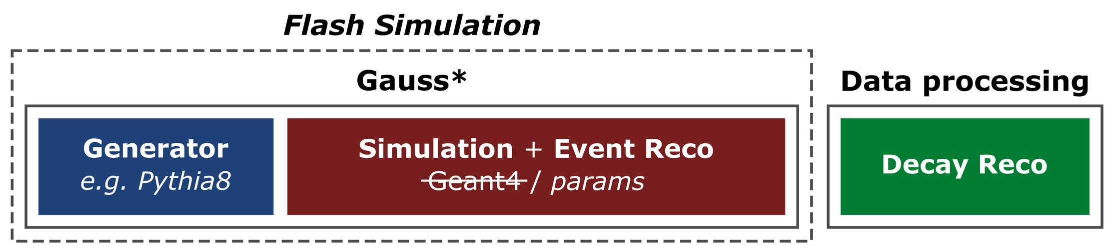
2. Fast simulation VS. flash simulation



Detailed simulation relies on Geant4 to reproduce the radiation-matter interactions that are computed within Gauss*, the LHCb simulation software.



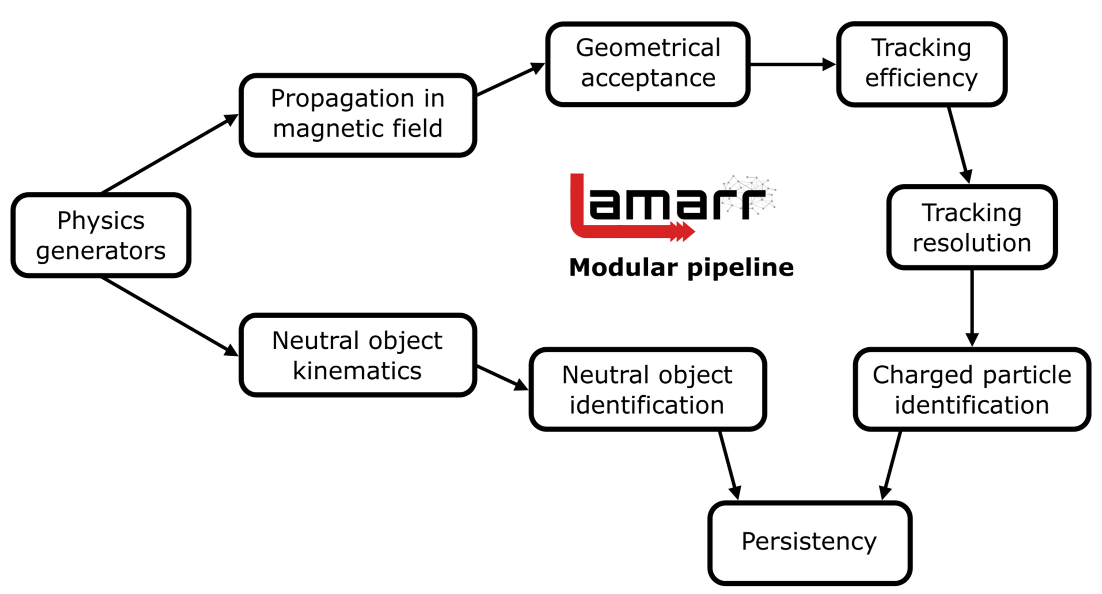
Fast simulation techniques aim to speed up the Geant4-based simulation production by parameterizing the energy deposits instead of relying on physics models.



Flash (or *Ultra-Fast*) ***simulation*** strategies aim to directly transform generator-level particles into analysis-level reconstructed objects.

3. What is Lamarr?

Lamarr is the novel flash-simulation framework of LHCb, able to offer the fastest option to produce simulated samples. Lamarr consists of a **pipeline of** (ML-based) **modular parameterizations** designed to replace both the simulation and reconstruction steps.



The Lamarr pipeline can be split in two chains:

1. a branch treating **charged particles** relying on tracking and particle identification models;
2. a branch facing the *particle-to-particle correlation* problem innate in the **neutral objects** reconstruction.

4. Models under the k-to-k hypothesis

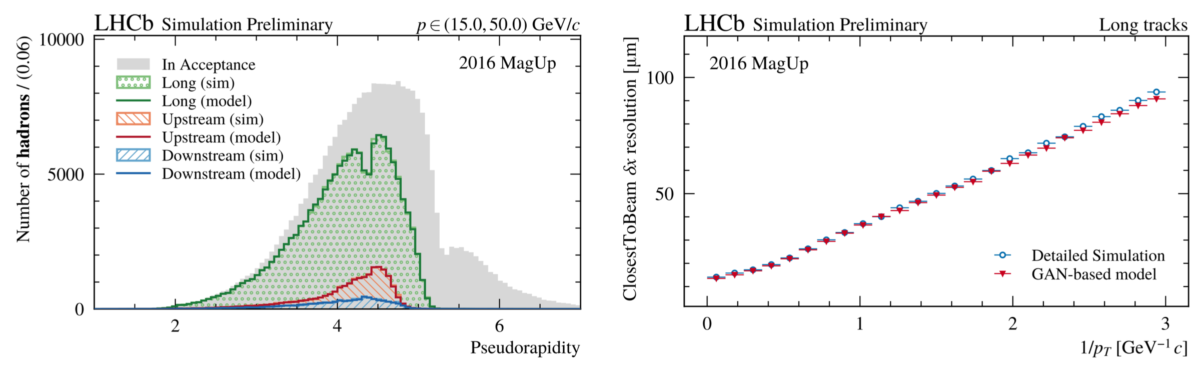
Assuming the existence of an **unambiguous** (k-to-k) **relation** between generated particles and reconstructed objects, the high-level detector response can be modeled in terms of **efficiency** and **"resolution"** (i.e., analysis-level quantities):

- **Efficiency:** *Deep Neural Networks* (DNN) trained to perform classification tasks so that they can be used to parameterize the fraction of "good" candidates (e.g., accepted, reconstructed, or selected).
- **Resolution:** Conditional *Generative Adversarial Networks* (GAN) trained on detailed simulated samples to parameterize the high-level response of LHCb detector (e.g., reconstruction errors, differential log-likelihoods, or multivariate classifier output).

5. Charged particles pipeline: the tracking system

Lamarr parameterizes the high-level response of the **LHCb tracking system** relying on the following models:

- **propagation:** approximates the trajectory of charged particles through the dipole magnetic field → *parametric model*;
- **geometrical acceptance:** predicts which of the generated tracks lay within a sensitive area of the detector → *DNN model*;
- **tracking efficiency:** predicts which of the generated tracks in the acceptance are properly reconstructed by the detector → *DNN model*;
- **tracking resolution:** parameterizes the errors introduced by the reconstruction algorithms to the track parameters → *GAN model*;
- **covariance matrix:** parameterizes the uncertainties assessed by the Kalman filter procedure → *GAN model*.



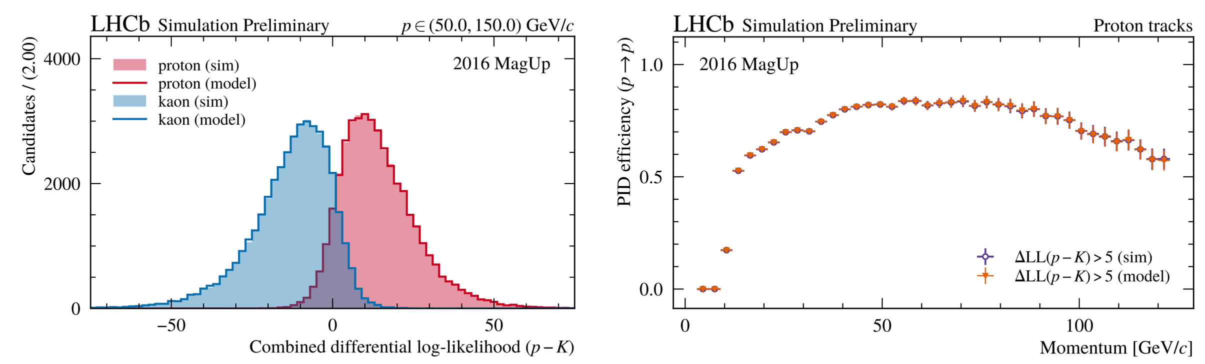
Validation plots for the DNN-based model of the tracking efficiency (left) and the GAN-based model of the spatial tracking resolution (right).

6. Charged particles pipeline: the PID system

Lamarr parameterizes the high-level response of the **LHCb PID system** relying on the following models:

- **RICH PID:** parameterizes DLLs resulting from the RICH detectors → *GAN model*;
- **MUON PID:** parameterizes likelihoods resulting from the MUON system → *GAN model*;
- **isMuon:** parameterizes the response of a FPGA-based criterion for muon loose boolean selection → *DNN model*;
- **Global PID:** parameterizes the global high-level response of the PID system, consisting of CombDLLs and ProbNNs → *GAN model*.

Lamarr provides separated models for **muons**, **pions**, **kaons**, and **protons** for each PID set of variables.



Validation plots for the proton-kaon separation parameterized with the GAN-based models of the Global PID response in terms of distributions (left) and proton selection efficiency (right).

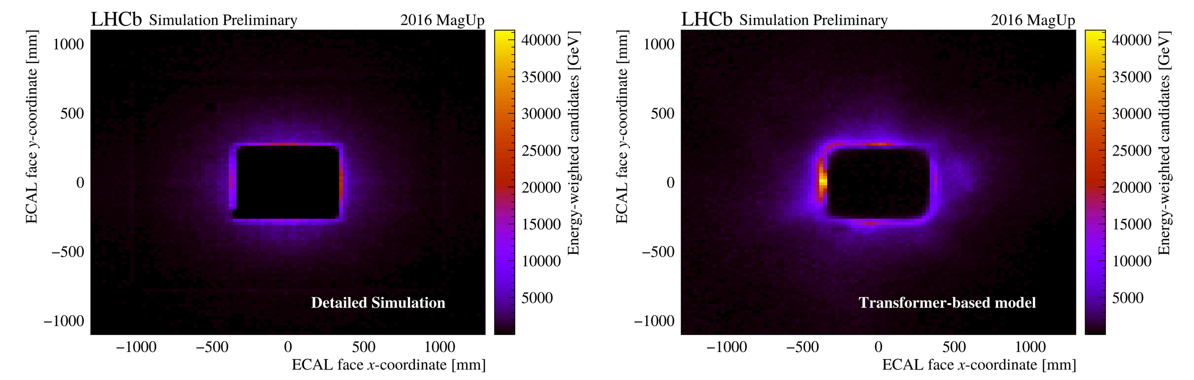
7. Neutral particles pipeline: the ECAL detector

The flash simulation of the LHCb ECAL detector is not trivial task:

- bremsstrahlung radiation, converted photons, or merged π^0 may lead to have n **generated particles** responsible for m **reconstructed objects** (in general, with $n \neq m$);
- the ***particle-to-particle correlation*** **problem** limits the validity of strategies used for modeling the unambiguous k-to-k detector response.

To parameterize a generic n-to-m response of the ECAL detector, solutions inspired by the natural language **translation problem** are currently under investigation:

- the aim is to define an **event-level description** of the ECAL response;
- assuming ordered sequences of photons/clusters, the problem can be modeled with a ***Transformer*** model;
- complying with the problem topology, the ECAL response can be modeled with a ***Grapha Neural Network*** (GNN) model



Validation plots for the (x, y)-position of the ECAL clusters as reconstructed by detailed simulation (left) and a Transformer-based model (right). Each bin entry is properly weighted to include also the energy signature.

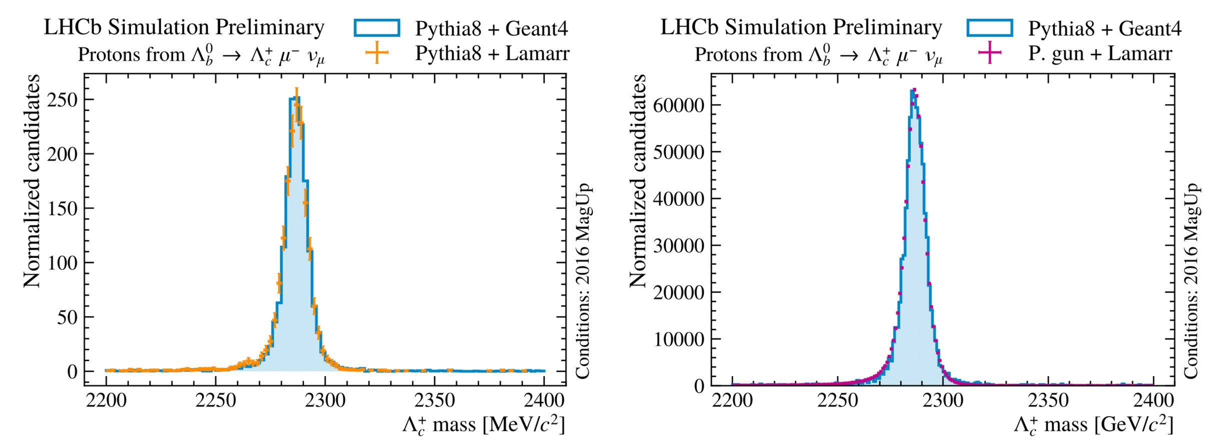
8. Validation campaign

Lamarr provides the high-level response of the LHCb detector by relying on a **pipeline of** (subsequent) **ML-based modules**. To validate the charged particles chain, the distributions of a set of **analysis-level** reconstructed quantities resulting from Lamarr have been compared with that obtained from detailed simulation for $\Lambda_b^0 \to \Lambda_c^+ \mu^- X$ decays with $\Lambda_c^+ \to pK^-\pi^+$.

The deployment of the ML-based models follows a ***transcompilation approach*** based on `scikinC`. The models are translated to C files, compiled as *shared objects*, and then dynamically linked in the LHCb simulation software (Gauss).

The integration of Lamarr with Gauss enables:

- interface with all the **LHCb-tuned physics generators** (e.g., Pythia8, EvtGen);
- compatibility with the **distributed computing middleware** and production environment;
- providing **ready-to-use datasets** for centralized analysis.



Validation plots for the Λ_c^+ mass obtained from Pythia8 (left) and particle-gun (right) generators by Lamarr VS. detailed simulation. Reproduced from LHCB-FIGURE-2022-014.

9. Preliminary timing studies

Overall time needed for producing simulated samples has been analyzed for detailed simulation (Geant4-based) and Lamarr. When Lamarr is employed, the generation of particles from collisions (e.g., with Pythia8) becomes the new **major CPU consumer**.

Lamarr allows to reduce the CPU cost for the simulation phase of (at least) **two-order-of-magnitude**. Further timing will require speeding up the generators.

Detailed simulation: Pythia8 + Geant4
1M events @ 2.5 kHS06.s/event ≈ 80 HS06.y

Ultra-fast simulation: Pythia8 + Lamarr
1M events @ 0.5 kHS06.s/event ≈ 15 HS06.y

Ultra-fast simulation: Particle Gun + Lamarr
100M events @ 1 HS06.s/event ≈ 4 HS06.y

10. Conclusions and outlook

Great effort is ongoing to put a **fully parametric simulation** of the LHCb experiment into production, aiming to reduce the pressure on computing resources.

DNN-based and GAN-based models succeed in describing the high-level response of the LHCb tracking and PID detectors for **charged particles**. Work is still required to parameterize the response of the ECAL detector due to the **particle-to-particle correlation problem**.

Future development Lamarr aims to support both integration within the LHCb software stack and its use as a **stand-alone** package.

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