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The flash-simulation of the LHCb experiment using the Lamarr framework

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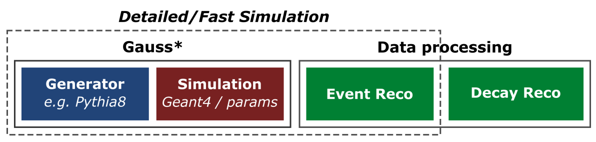
1. Motivation

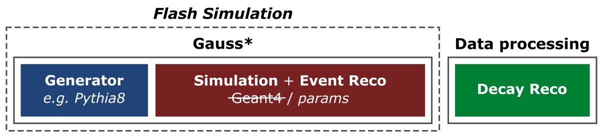
Detailed simulation of the interactions between particles and the LHCb detector requires significant CPU resources.

- LHCb has used **over 90% of CPU resources** for simulation during Run 2;
- Current approaches do **not scale** to future needs;
- Must develop ***faster* simulation options**!

2. Fast simulation VS. flash simulation



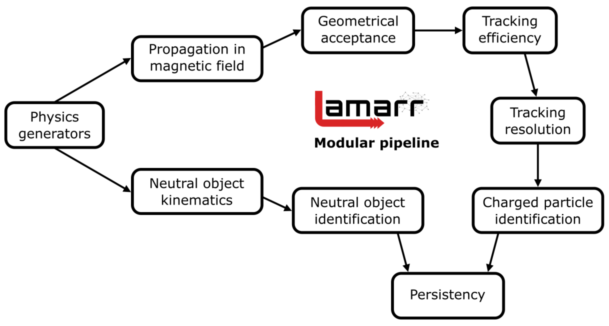
The **detailed simulation** of physics processes relies on Geant4 and is computed within Gauss*, the LHCb simulation software.
Fast simulation techniques aim to speed up Geant4 by parameterizing the energy deposits instead of relying on physics models.



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 branches:

1. **charged particles** require tracking and particle identification models;
2. **neutral objects** need to face the *particle-to-particle correlation* problem.

4. Models under the k-to-k hypothesis

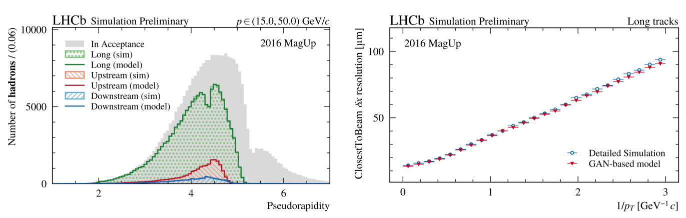
Assuming the existence of an **unambiguous** (k-to-k) **relation** between generated particles and reconstructed objects, the high-level detector response can be modeled in terms of **efficiency** and **"resolution"** (i.e., analysis-level quantities):

- **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 branch: 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*.



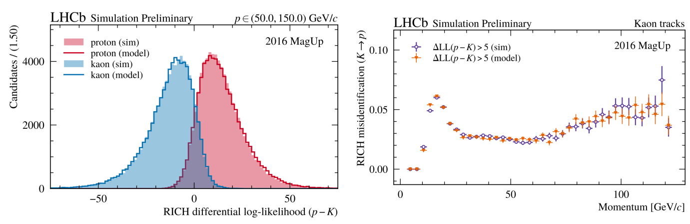
Validation plots for the DNN-based model of the tracking efficiency (left) and the GAN-based model of the spatial tracking resolution (right).

6. Charged particles branch: 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 flag:** 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 RICH response in terms of distributions (left) and proton selection misidentification (right).

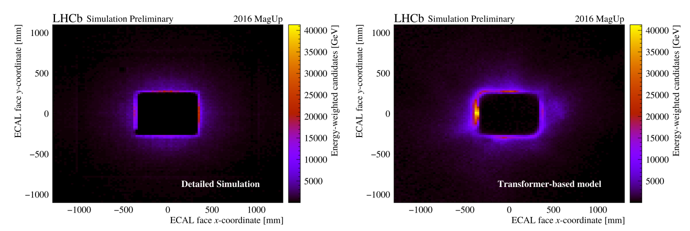
7. Neutral particles branch: the ECAL detector

The flash simulation of the LHCb ECAL detector is a non 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 ***Graph 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.

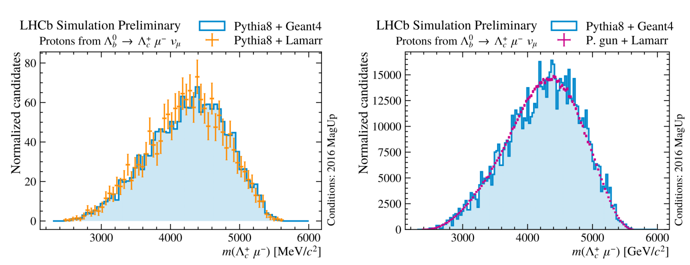
8. Validation campaign

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 those 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 $\Lambda_c^+\mu^-$ 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 could allow to reduce the CPU cost for the simulation of (at least) **two-order-of-magnitude**. Further reductions will require speeding up the generators.

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

Flash simulation: Pythia8 + Lamarr
1M events @ 0.5 kHS06.s/event ≃ 15 HS06.y

Flash simulation: ParticleGun + Lamarr
100M events @ 1 HS06.s/event ≃ 4 HS06.y

10. The role of ICSC for Flash Simulation

The **lifecycle of a generic flash-simulation model** includes designing, training, optimization, deployment, and validation, before to be put into production. While the development steps often involve **multiple GPU nodes** (*HPC paradigm*), the validation phase typically relies on the same distributed computing resources employed in the **production environment** (*HTC paradigm*).

The aim of **ICSC** (*Italian Center for SuperComputing*) is to create the national digital infrastructure for research and innovation, leveraging existing **HPC**, **HTC** and **Big Data** infrastructures and evolving towards a cloud data-lake model. The Lamarr framework is pioneering such **hybrid workloads on distributed and federated resources**, employing nodes from both WLCG data centers and pre-exascale supercomputers (e.g., Leonardo).

11. 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.

Acknowledgements

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