

Monte Carlo

The Monte Carlo method was invented by scientists working on the atomic bomb in the 1940s. Its core idea is to use random samples of parameters or inputs to explore the behavior of a complex system or process. Nowadays, MC are essential part of both theoretical and experimental particle physics research. This chapter gives an overview of ATLAS experiment simulation scheme, simulation methods and software used. Also, a technique for speeding up this simulation will be discussed. At the end list of the MC samples, used in the analysis will be described.

1.1 MC simulation at ATLAS experiment

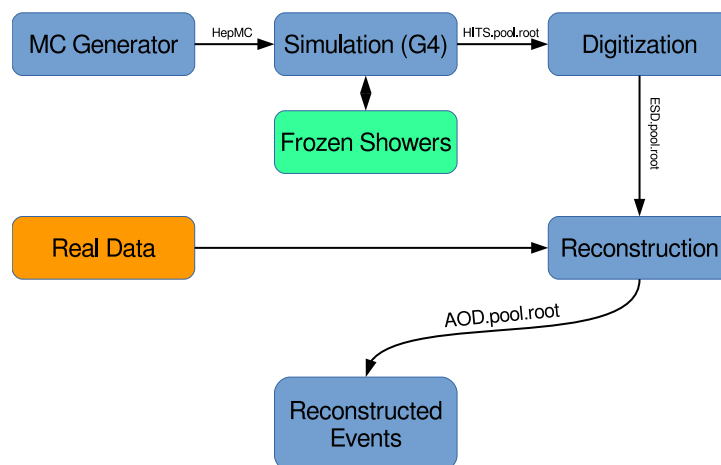


Fig. 1.1: Diagram of the ATLAS MC production chain

Monte Carlo is allowing to make different analysis, such as compare data with predictions, study detector or selection algorithms performance. This means, that MC precision is important. Simulation needs to use precise models of physics for sampling and have large enough statistics, to exclude statistical uncertainties (usually 5-10 times more, than expected in a data). ATLAS simulation software is integrated into Athena and usually used during large production of events. Simulation chain is generally divided into 4 main steps (Figure 1.1):

Event generation Simulation of hard interaction and a resulting high-energy particles parameters. This step is independent of ATLAS detector geometry.

Simulation Simulation of energy depositions ("hits") done by final state particles in ATLAS detector.

Digitalization Simulation of detector response using "hits" information: first, inputs to the read out drivers (ROD's), called "digits" are constructed, then, ROD functionality is emulated. Detector noise effects are added at this stage.

Reconstruction Production of the Analysis Object Data (AOD) files, which are containing sufficient information for physics analysis. This stage is identical for both data and MC

This scheme is allowing to use computing resources efficiently, than with a single-step simulation, and simplifies software validation, since it is possible to use files from the previous steps with different software version. In the following sections event generation and simulation will be described more detailed

1.1.1 Event generators

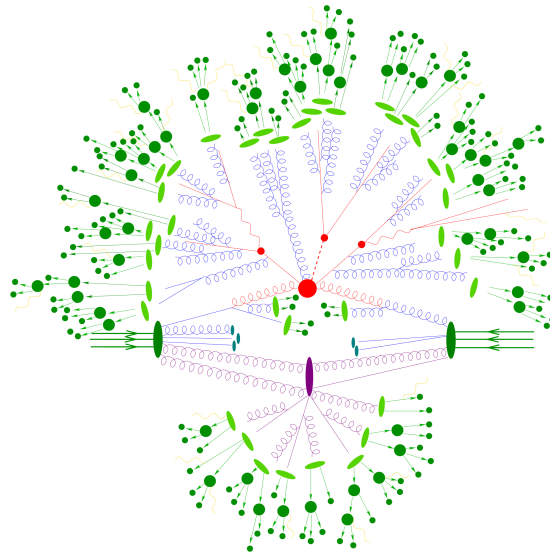


Fig. 1.2: Schematic view of a $t\bar{t}H$ event produced in a pp-collision: the hard scattering is shown as a red blob with the solid and dashed lines as the resulting three particles. Independently happening multi-particle interactions are indicated by the violet blob. Parton showers are shown with curly lines. Hadronization yields hadrons as shown in light green, while the final state particle are dark green.

The outcome of the hard interaction could be simple scattering, their annihilation or a combination of two. In any case, the final state consist of a large multiplicity particles. The main goal of event generator is to provide a complete picture of this final states: description of the particle types and momentia on event-by-event basis. The factorisation theorem allows to make event generation in independent stages, which are dominated by different dynamics:

Modelling of hard subprocess Hard subprocess is happening at the smallest scales of times and distance, where all of the colliding partons are considered free and their initial momentia are given by selected PDF set. Process of interest is simulated by selecting production channels and calculating corresponding matrix elements (ME) in the desired level of accuracy in pertrubation theory . Most of the generators have leading order or next to leading order ME in α_s . Scale of α_s

is can be determined through renormalisation of factorisation. Also, inclusion of higher-order correction reduces scale dependency, however it makes calculations technically more difficult.

Parton showering Quarks and gluons from hard process can QCD radiation, resulting on the dozens of additional partons associated with the event. This process calculated as step-by-step evolution of momentum transfer scales from highest (hard subprocess), to the lowest (around 1 GeV). There is a possibility of double counting between showers and hard subprocess. This can be avoided using matching approach, for which higher order corrections to ME are integrated with parton showers, or merging strategy, where jet resolution scale is used as an threshold between matrix elements and parton showers.

Hadronisation Final stable color-neutral particles, what can be detected in experiment, are formed during hadronisation. This occurs at larger nonperturbative scales and usually implemented using different phenomenological models.

Modelling underlying event Parallel to the main process other collisions of partons can occur, called underlying event. These additional interaction can produce partons which contribute to the final state. This is one of the least understood aspect of hadronic collisions.

Schematic plan of simulation of $t\bar{t}$ event is shown on a figure 1.2. The hard scattering itself is shown as a red blob with the solid and dashed lines indicating the resulting particles, which themselves decay further. Underlying event is indicated by the violet blob. Parton showers are shown with curly lines. Hadronization yields hadrons as shown in light green, while the final state particles are dark green.

The current analysis uses samples generated with the following generators:

Powheg Powheg is generator with NLO ME, that can be interfaced with other generator(such as Pythia or Herwig) for higher precision of showering.

Pythia Pythia is a general purpose generator for hadronic, hadron-lepton and leptonic collisions. It can model initial and final state showers, hadronisation and decays, underlying event (via multi parton interactions). Pythia contains library with around 240 processes with LO ME. It uses Lund String model for hadronisation.

Herwig Herwig is a LO general purpose event generator for simulation lepton-lepton, hadron-lepton and hadron-hadron collisions. The main difference between Pythia and Herwig is that it uses angular ordering in the parton showers and also models the hadronisation step based on the cluster fragmentation

Sherpa Sherpa is a generator with tree level of matrix elements, featuring its own implementation of parton shower and hadronisation models.

Photos Precision tool for QED radiative corrections in W and Z decays.

Tauola Generator, used to describe leptonic and semi-leptonic τ -decays.

1.1.2 Simulation in Geant4

After event generation, the final state particles have to be propagated through the detectors to obtain the corresponding hardware responses. The main method used by ATLAS, referred to as *Full Simulation*, makes use of the Geant4 toolkit [?]. This package has a wide range of applicability and it

is used not only for LHC (ATLAS, CMS, LHCb) experiments, but in other high energy, nuclear physics experiments, for medical and space sciences.

One of the main advantages of Geant4 is an ability to simulate complex detector structure, both sensitive material (e.g. scintillator) and corresponding detector infrastructure. For sensitive material it holds information "hits" - snapshots of physical interactions. They are used afterwards during digitalization. Geometry package allows to make a model with large number of components, that are stored in a hierarchical tree. Properties of material, like radiation and interaction length, excitation energy loss etc are automatically calculated for each volume. It is also possible to manually describe surface properties for tracking of optical photons. Physics models, used in simulation can be set using physics lists. They are using different models and parametrisations and are adjusted for better CPU performances. ATLAS is using FTFP_BERT list, that has fritiof model for high energy particles and bertini-style cascade for hadrons. This physics list is roughtinegly validated for each Geant4 release. All of the physics processes simulated by step-by-step.

It is required to have mass MC production (called MC campaign) for each data taking. Usually full simulation requires huge computational resources and most of the run-1 CPU time have been used for simulation. Typical time spend to simulate 1 QCD event is around 20 or more minutes. In order to optimize CPU usage, some improvements for a Run-2 have been performed, such as tuning physics lists to reduce simulation of unwanted particles or rework of B-field access. Also there are long term developments for multi-threading and vectorisation of the code. However it is still impossible to achieve required statistics without faster approach to simulation. Several fast simulation techniques have been developed in ATLAS experiment.

There are several approaches to fast simulation: use of simplified geometry, optimizing transport and navigation, use of parametrisation for material interaction, etc. Almost 80% of the time is spend on simulation of calorimeters, so fast calorimetry is crucial. There are two main methods used in ATLAS:

- Parametrisation. Basic idea of this method is that we are killing all of the particles (except for a muons) in the entry of calorimeter and simulating calorimeter cell response using parametrisation of longitudinal and lateral shapes of shower. This is also allowing to tune shower shape variables to data.
- Frozen Showers. This technique will be described more detailed in the following section

1.1.3 Frozen Showers

Main principle of this library is described by it's name. It is using pre-simulated "frozen" showers instead of full simulation. This process is schematically shown on a Figure 1.3. The library itself organized as follows: it contains basic simulation parameters, like Geant4, geometry and atlas software release version and physics list used. It stores information about position of initial particle in a bins, energy remains unbinned. For showers it has list of hits, that are containing four vector (time and position) and energy deposition. There is also additional information about lateral and transverse size of the shower.

Production use of Frozen Showers

During a simulation, if an energy of particle falls below cut-off energy, particle is stopped and killed and substituted by shower from library. Also, it is checked, that particles is far away from the edges of calorimeter, so what resulting shower will be by 90% contained in a calorimeter. This check is

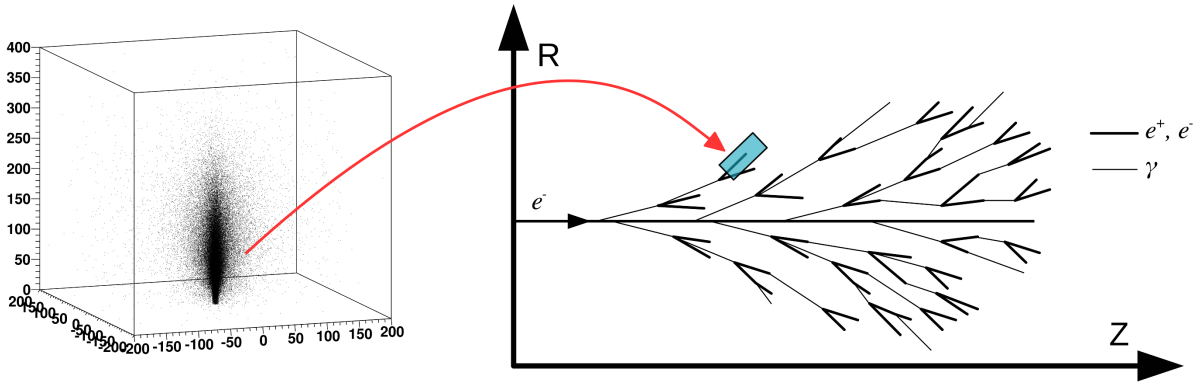


Fig. 1.3: Diagram showing the shower substitution of the low-energy particle, during the high-energy particle simulation.

energy dependent, since shower sizes are growing with the energy. When particle is removed, it is substituted by shower taken from corresponding eta and distance bin with the closest energy found. Energy of the hits in shower is scaled to fully correspond to particle energy. Also, shower direction is changed to the direction of the shower.

Frozen Showers have been used in Atlas Monte-Carlo production since run-1. This method is applicable for all LAr calorimeters in ATLAS, but currently it is enabled for simulation of forward calorimeters (FCAL), since it is showing the smallest differences, compared to the other fast simulation methods (e.g parametrization). This is happening because of large of non-uniformly distributed sensitive material (citation to previous chapter). Energy resolution of calorimeter on a fixed energy depends only on a two statistical factors: fluctuations of the energy loss and number of produced charged particles. Additional binning variables are allowing to capture this non-uniformities. Example of this is in picture Sum of the deposited in a sensitive material "hits" divided by initial particle energy is shown on picture. Gap position is shown by the red lines. It is clear, that showers, what have been born inside sensitive material tend to have higher energy response (SumE/E) and thicker tails, than showers in a dead material. This is causing larger constant term. Introducing additional spacial binning, that is defined as distance to the closest rod center is allowing to capture this fluctuations. It can be also shown, that size of this fluctuation is depending on initial particle energy (pic.). For electrons with energy greater than 500 GeV they are almost negligible. This is why upper limit for frozen showers was set to 1000 MeV. This method is allowing to capture well shower-shape variables, that are later used for identification of the forward electrons. Distribution of shower energies, used for production of high-energetic electron (1000 GeV in that case), is shown on a Figure . More than 50% of them are having energy less than 20 MeV. Studies have showed, that Frozen showers are slower, than a standard Geant4 simulation for showers with energy 3 MeV. This is happening due to library non-binned structure for energy. This makes search of closest energy shower in a library slower, than simulation of shower with zero or one hit in a sensitive detector.

Generation of Frozen Showers library

In a Frozen Shower method there are separate libraries for each particle and subdetector used. Showers should cover fully energy and pseudorapidity region and be able to describe data, that is needed during simulation. This is why 2 stages simulation approach have been used. The first stage is to take initial particle parameters, that later will be used in a library from a physical process. This

The general frozen showers parameters	
Detectors used	FCAL1, FCAL2, FCAL3
Type of the particle	photons, electrons, neutrons
Energy range	$E_\gamma < 10 \text{ MeV}$, $E_e < 1000 \text{ MeV}$, $T_n < 100 \text{ MeV}$
Containment requirement	$\Delta E_{\text{shower}} > 98\%$
The library post-processing parameters	
Generation clustering cutoff	$(\Delta R_{\text{cluster}})^2 < 25 \text{ mm}$
Generation truncation cutoff	$R_{\text{hit}}^2 < 50000 \text{ mm}$, $\Delta E_{\text{shower}} < 1\%$

Table 1.1: Main parameters used for the frozen shower libraries in FCAL

is done using simulation of some process (e.g. ttbar or single electron). Every time, when particle becomes eligible for Frozen Showers, it is saved as a starting point. Particles tend to cluster tightly around original track, so in order to achieve a better detector coverage on a smaller sample, this primary points are randomly truncated. On the second stage, simulation for this primary vertexes is performed, using standard Atlas simulation infrastructure. This is allowing to take into account sampling fluctuations and charge-collection effects on a hit information automatically. Furthermore, in order to save disc space as well as a memory consumption, hit information is compressed. This compression is done in a two steps, hit merging and truncation:

- if the distance between any two hits is smaller, than a given parameter R_{min} , then hits are merged into one deposit at the energy weighted center of them. This process is done iteratively.
- hits whose energies are below the fraction f of the total energy sum of all hits, are truncated. The energy of remaining hits is rescaled back to preserve the total deposited energy.

Unfortunately, for a Frozen Showers, generated for Run-1 monte-carlo, additional tuning of electron libraries was needed. This was done using reconstructed energy of electrons. Frozen Showers tend to underestimate fluctuations of energy loss, that is leading to a smaller electron resolution for a high energies. Correction is done by enlarging bin, corresponding to a gap position. Also, correction of the mean shift is done by scaling energy response of all showers. After this frozen showers are showing good agreement with full simulation. This procedure needs to be done every time, when something is changing in software. Because tuning is done manually, lots of a manpower is needed for each Monte Carlo mass production campaign.

Distance binning problem

As it was mentioned before, process of library generation can be complicated and take a lot of the time because of the needed tuning. In this subchapter possible ways to improve frozen showers performance have been studied. As it was mentioned before, that there are two type of material used in a FCAL and showers within them are giving different response, what is affecting overall reconstructed electron energy resolution. At the first generations distance bin have been corresponding to LAr gap or dead material positions. During tuning bin with LAr was enlarged to gain a better agreement with full simulation. So, one of the basic ideas to improve frozen showers performance is to change a binning, that is used during Frozen Showers library generation. It was decided to treat showers, that have been born near LAr gap and crossed it on a radiation length, in a same way with showers in

sensitive material gap, and call them sensitive material showers. Oppositely, showers, that haven't crossed LAr gap, are called dead showers. This model leads to a bigger gap width by a definition. One of the possible ways to find this bin position automatically is to use machine learning tools.

Machine Learning is a set of algorithms, what allows computers to learn and give a predictions without being specifically programmed. This is a modern field of computer science, that is wildly used in a different fields like computer vision, natural language processing, data science etc. There are two main types of machine learning algorithms: supervised, where example of desired output is given by the "teacher" and the goal is to learn a general rule, that maps inputs to outputs and unsupervised learning, then there are no labels given to algorithm, and algorithms is discovering hidden patterns in data. Initial data parameters of interest, that are used in algorithm to learn are called features. It is important to have right proper set of features and good training sample. From a geometrical point of view, one of the main parameter is a direction of the shower. Eta momentum distribution is showed on a Figure . Most of the showers are collinear to an electron direction. Because of this it was decided to use as a training sample simulation results for electrons with energies less than 1 GeV and momentum uniformly distributed between eta 3.0 and 4.0. This allowing to study equally low and high energy showers equally.

From out definition of 2 classes of showers, it is simple to construct a pre-labelled training sample. This is done by reducing initial sample and taking showers near rod center and inside liquid argon gap. Output of this classifier, that was trained on with sample with shower features, such as energy responce and number of hits, than can be used to expand our labels to a full distance range. Than it can be used as an input to a second classifier, which will separate two types of showers using particle parameters, such as energy and distance to a rod center. For a first step decision trees have showed good classification efficiency (around 97%). For a second classifier support vector machines have been used. This method is trying to reconstruct a hyperplane, that is dividing two classes. Outputs of both of this classifiers are shown on a figure . New gap position is determined using borders of hyperplane. This procedure is giving expected from the initial model results. Gap is wider, than and original one. It is also getting bigger with bigger energy, because of the radiation length growth. Validation results for two different eta bins are shown on figure a) and b). In a bin this new binning is performing better, than original one without any additional tuning. Unfortunately this is not true for all of the bins, as we can see on a figure b). This eta bin have showed worst performance for a new binning, but it is performing still better, than original binning without tuning.

This binning was used in a production of new libraries for Monte Carlo in a Run-2. It is planned to use more precise training sample for a future iterations of this procedure for improving performance of outlying eta bins.

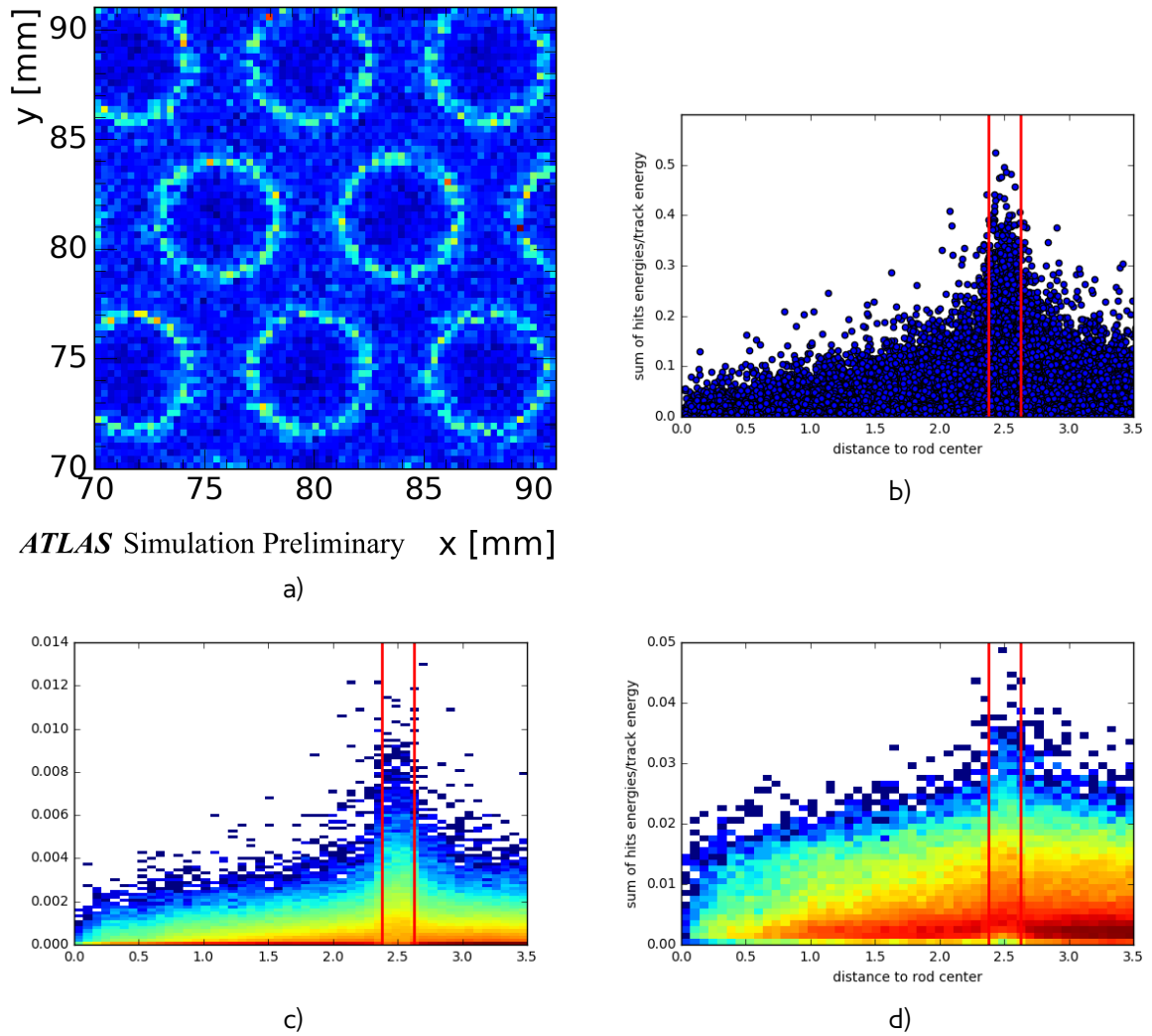


Fig. 1.4: Energy response for electrons in a calorimeter a) in a x vs y plane and in a distance plane for b) all electrons in a library c) electrons with energy less than 100 MeV d) electrons with energy bigger, than 100 MeV

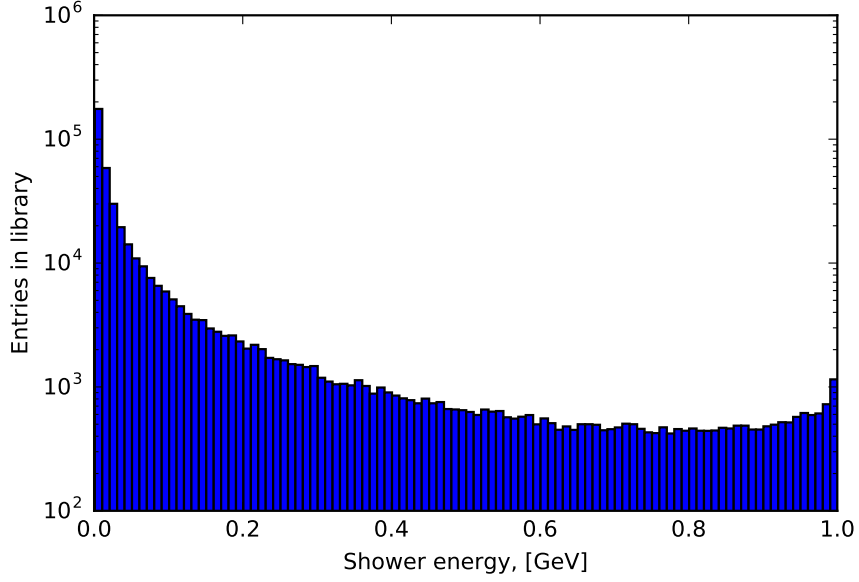


Fig. 1.5: Distribution of shower energy used in production of 1000 GeV electrons.

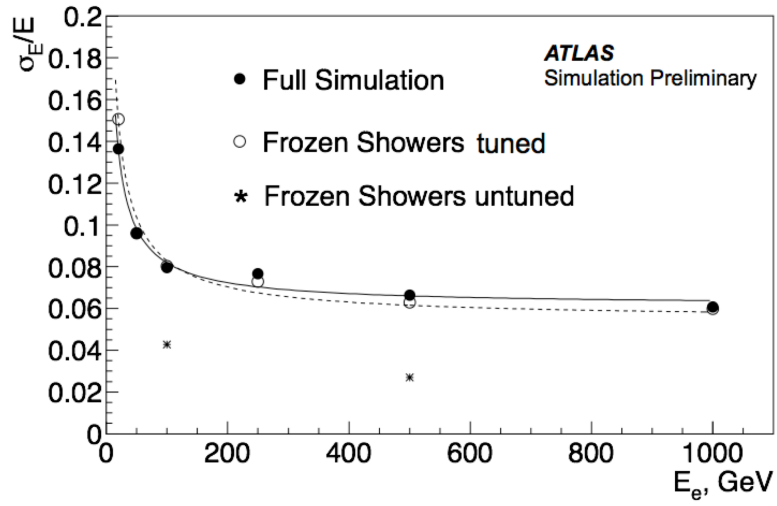


Fig. 1.6: Electron resolution for full simulation, tuned and untuned frozen showers

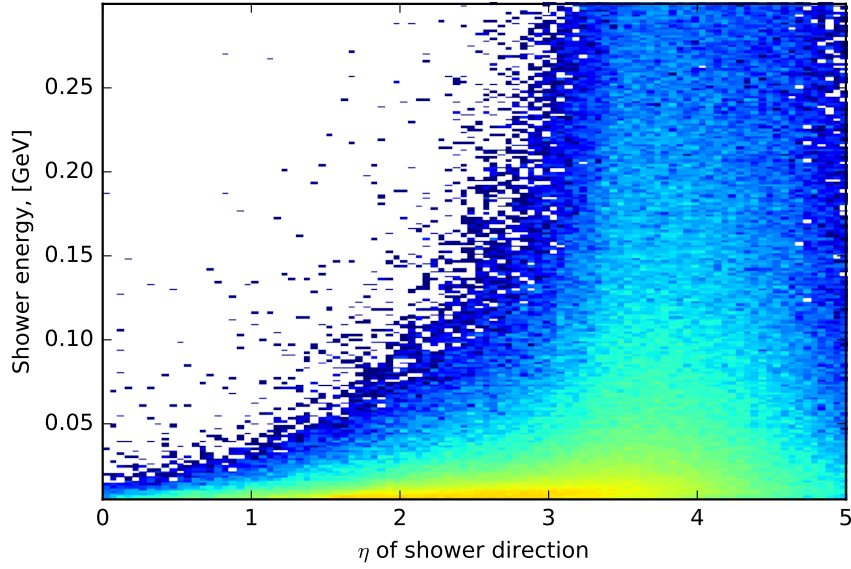


Fig. 1.7: Distribution of showers used in production of 1000 GeV electrons on shower energy vs η_{momentum} plane.

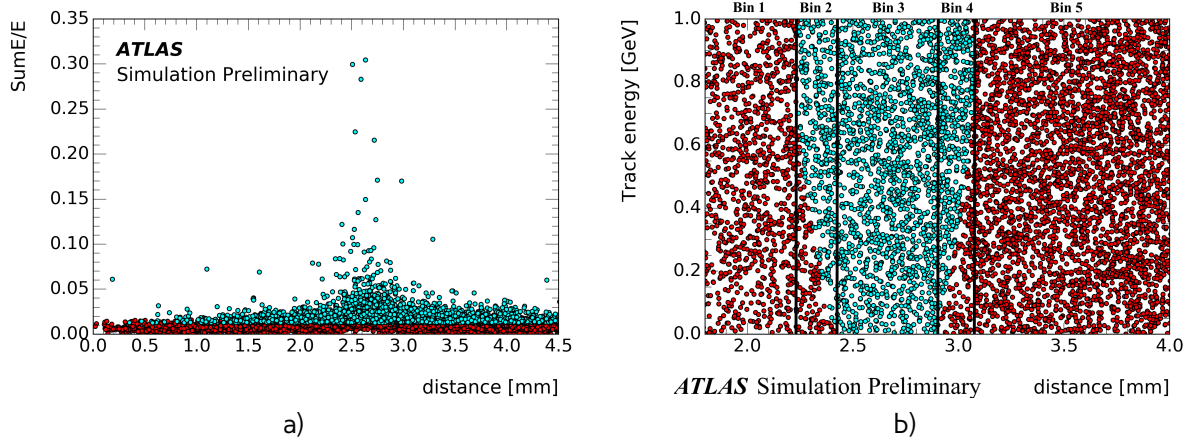


Fig. 1.8: Results of machine learning for a) first classifier b) second classifier. Cyan dots are corresponding to sensitive material showers, red - dead material showers

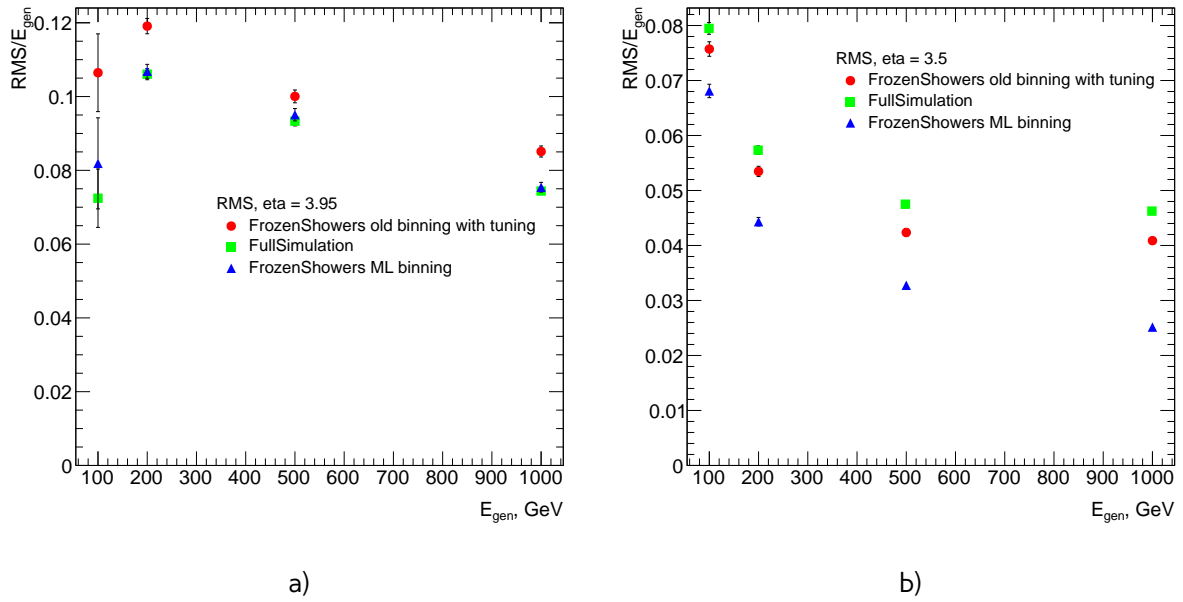


Fig. 1.9: Resolution of reconstructed electrons for full simulation, new libraries with ML binning and old tuned libraries with original binning for a) $\eta = 3.95$ b) $\eta = 3.5$