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Fast Simulation for ATLAS: Atlfast-II and ISF

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Abstract. Monte Carlo simulations of physics events, including detailed simulation of the detector response, are indispensable for every analysis of high-energy physics experiments. As these simulated data sets must be both large and precise, their production is a CPU-intensive task. Increasing the recorded luminosity at the Large Hadron Collider (LHC), and hence the amount of data to be analyzed, leads to a steadily rising demand for simulated MC statistics for systematics and background studies. These huge MC requirements for more refined physics analyses can only be met through the implementation of fast simulation strategies which enable faster production of large MC samples. ATLAS has developed full and fast detector simulation techniques to achieve this goal within the computing limits of the collaboration. We present *Atlfast-II* which uses the *FastCaloSim* package in the calorimeter and reduces the simulation time by one order of magnitude by means of parameterizations of the longitudinal and lateral energy profile, and *Atlfast-IIF* with the fast track simulation engine *Fatras*, which achieves a further simulation time reduction of one order of magnitude in the Inner Detector and Muon System. Finally we present the new *Integrated Simulation Framework* (ISF) which is based on the requirement to allow to run all simulation types in the same job, even within the same sub-detector, for different particles. The ISF is designed to be extensible to new simulation types as well as the application of parallel computing techniques in the future. It can be easily configured by the user to find an optimal balance between precision and execution time, according to the specific physics requirements for their analysis.

1. Introduction

Monte Carlo simulations of physics events, including detailed simulation of the detector response, are indispensable for every analysis of high-energy physics experiments. This ever-growing task involves the accurate description of the elementary physics processes as well as the simulation of interactions of particles with a detailed model of the detection apparatus. Due to the tiny cross-sections of the signatures of potential new physics with respect to background processes, and the need to study systematic effects with increasing precision, a large number of events needs to be generated for Monte Carlo (MC) studies. The major fraction of dedicated computing time can be accounted to the simulation of particle interactions with the active and passive detector material and the determination of the detector response.

The response of the detector is traditionally simulated in the most accurate way possible, by modeling any small structures which could affect traversing particles, no matter whether they originate from the interaction point in the center of the detector, from subsequent reactions and decays, or from cosmic radiation. However, this approach is very time-consuming and therefore not always feasible. In order to study rare processes, systematics and background effects, some analyses require a large number of collision events to be simulated. In many cases this can only

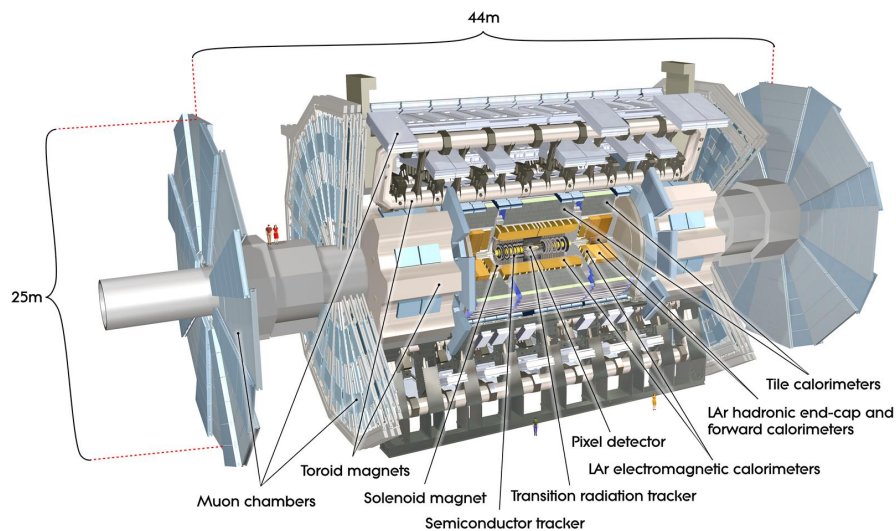


Figure 1. The ATLAS detector at the LHC, full overview.

be done with a fast simulation using parameterizations and/or a simplified approach of modeling the detector material and the response of active detector elements. The obvious drawback of any such fast simulation strategy is reduced accuracy, which may be acceptable for some but not all particles and sub-detector regions.

This distinction between simulation strategies traditionally implies a mutually exclusive choice between high precision and fast execution time. However many physics studies are only interested in time-consuming high precision simulation of certain particles and regions, while the remaining particles and regions require much less precision. In order to reconcile these demands of (1) varying degrees of simulation precision for different particles and/or sub-detector regions, and (2) as fast execution time as possible, the most promising approach for the future is a new *Integrated Simulation Framework* (ISF) which allows the flexible combination of different simulation strategies within a single event.

2. The ATLAS Experiment

The ATLAS experiment [1] of the Large Hadron Collider (LHC) at CERN is the largest volume general-purpose particle detector ever constructed in particle physics as of today. Several different sub-detectors, one solenoidal and one toriodal magnet system, as well as cabling and cooling infrastructure, form an immensely complicated apparatus, measuring 25 m in height and 44 m in length and weighing about 7000 tons. The ATLAS detector has been built to collect data from proton-proton collisions with center-of-mass energies of up to 14 TeV, as well heavy ion (Pb-Pb) collisions with up to 5.5 TeV per nucleon pair. A cut-away view of the detector is shown in Fig.1.

The primary focus of the ATLAS detector, which is located about 100 m below the surface of the French and Swiss countryside close to CERN, is the search for new physics, such as Supersymmetry or the Higgs Boson. The apparatus can be divided into three main parts:

- Inner Detector
- Calorimeters
- Muon System

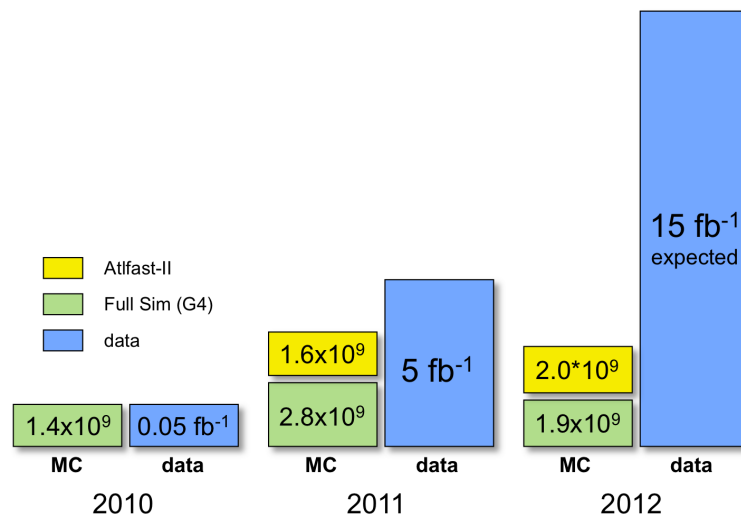


Figure 2. Schematic comparison of the number of simulated MC events with the amount of data recorded by the ATLAS detector in terms of integrated luminosity. The projected number of MC events is smaller in 2012 than 2011 due to larger simulation CPU time and event sizes. The simulation strategies *Attfast-II* and *Geant4* (G4) are explained in the following sections.

The Inner Detector and Muon System are tracking systems, responsible for precisely measuring the momenta of charged particles. The Inner Detector is also responsible for the precise vertex measurement. The calorimeters are used for determining the energies of traversing particles. Together these sub-detector components also allow for precise particle identification.

3. Simulation strategies in ATLAS

The modeling of the detector response with Monte Carlo methods is an integral component of many high energy physics studies. The complex detector instruments have to be commissioned and fully understood, also with respect to the results of previously conducted simulation efforts.

Physics analyses often require large MC data sets for the estimation of systematic effects, the modeling of background processes, and the study of rare processes with small cross sections. This MC production to the finest simulation detail is usually a very CPU-intensive task. The high demand for MC samples rises further as the recorded luminosity at the LHC, and hence the amount of ATLAS data to be analyzed, increases over time (see Fig.2). The ATLAS collaboration has developed full and fast detector simulation techniques to achieve the goal of large-scale MC production within the computing limits of the collaboration [2].

The Monte Carlo sample generation process is generally divided into four steps, which may be combined into a single job:

1. event generation in standard HepMC¹ format
2. physics and detector response, hit collections
3. digitization
4. reconstruction² and production of final output

¹ The HepMC package is an object oriented event record written in C++ for High Energy Physics Monte Carlo Generators. (see <http://lcgapp.cern.ch/project/simu/HepMC/>) [3]

² The event reconstruction step, which includes the reconstruction of vertices, particle tracks and energies as well

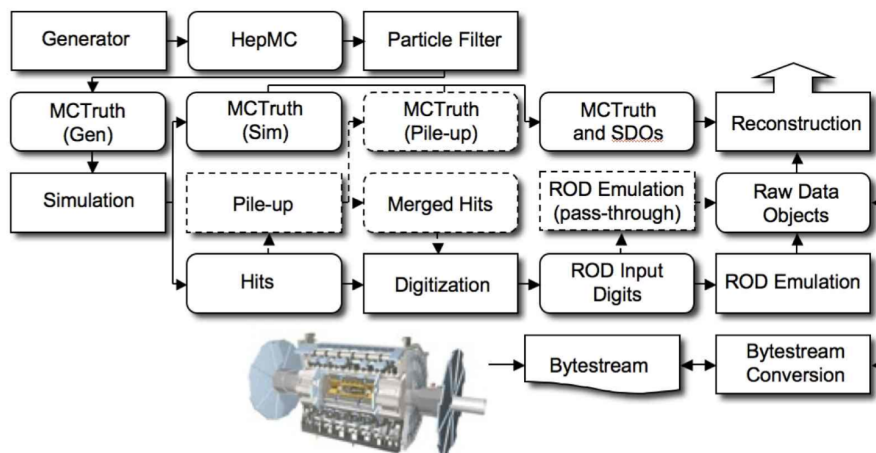


Figure 3. The flow of the ATLAS simulation software, from event generators (top left) through reconstruction (top right). Algorithms are placed in square-cornered boxes and persistent data objects are placed in rounded boxes. The optional pile-up portion of the chain is dashed.

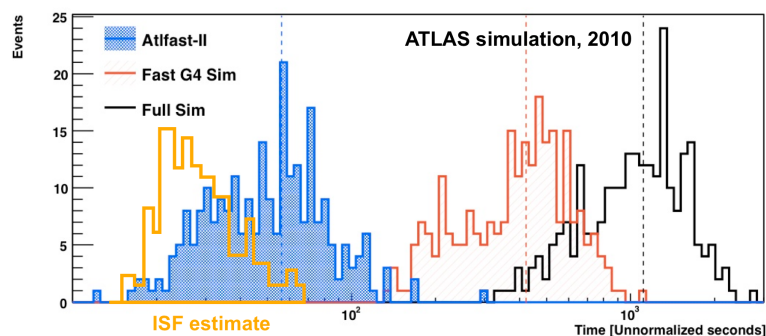


Figure 4. Comparison of CPU time spent for the simulation of $t\bar{t}$ events, with an overlay of the estimated ISF timing. The vertical dotted lines show the mean CPU time of each simulation flavor.

Fig.3 shows the flow of ATLAS Simulation software from event generation (top left) to reconstruction (top right). The event generation (step 1 in the simulation chain) is achieved by general purpose generators such as PYTHIA [4][5], HERWIG [6] and Hijing [7], which produce complete primary particle collections of collision events, starting from a proton-proton, proton-nucleus or nucleus-nucleus initial state.

The simulation of the physics processes and detector response (step 2 in the simulation chain) can be performed with different simulation strategies, which can be characterized by varying degrees of accuracy and simulation speed:

- (i) Full G4 Simulation (using Geant4 and a fully detailed detector description)
- (ii) Fast G4 Simulation (using Geant4 and pre-simulated particle showers in the calorimeter)
- (iii) Atlfast-II (using a parameterized calorimeter simulation (FastCaloSim))
- (iv) Atlfast-IIIF (using the FastCaloSim and a fast track simulation (Fatras))

An overview of the CPU time of different simulation flavors for $t\bar{t}$ events, with an overlay of the estimated timing of the Integrated Simulation Framework (ISF), is shown in Fig.4.

as particle identification, measurement of missing transverse momentum etc., can take as an input either raw data objects (RDO) from simulation or actual data recorded by the detector.

3.1. Full G_4 Simulation

The standard simulation strategy of ATLAS is based on the Geant4 (G4) particle simulation toolkit [8] and uses a highly detailed detector description. Geant4 provides detailed models for physics processes and the infrastructure for particle transportation through a geometry. The detector geometry itself is constructed in the Geant4 format. Physics models, which include the interactions of particles with matter, are typically chosen as physics lists (e.g. QGSP_BERT which includes the Quark-Gluon String Precompound model (QGSP) and the Bertini intranuclear cascade model (BERT)). The ATLAS simulation has provided a challenging test-bed for the Geant4 toolkit, and Geant4 has been extensively evaluated and validated during large-scale simulation production.

Because of the complicated detector geometry and detailed physics description used by the full Geant4 simulation, it is impossible for many physics studies to achieve the required simulated statistics without faster simulation strategies. To that end, several flavors of fast simulation techniques have been developed to complement the full Geant4 simulation.

3.2. Fast G_4 Simulation

Almost 80% of the full simulation time with Geant4 is spent simulating the progression of particle showers traversing the calorimetry, mainly caused by electromagnetic particles such as electrons and photons, which produce large secondary particle cascades in the complex electromagnetic calorimeter. The Fast G4 Simulation aims to speed up this slowest part of the full simulation by replacing low energy electromagnetic particles in the calorimeter with pre-simulated *frozen showers* stored in memory as libraries. Using this approach, the CPU time is reduced by a factor of three in hard scattering events (e.g. $t\bar{t}$ production) with little physics penalty.

3.3. *Atlfast-II* and *FastCaloSim*

The full Geant4 simulation time can be reduced by more than one order of magnitude by using the *Atlfast-II* fast simulation, which uses *FastCaloSim* in the calorimeter [9]. Here the energy of single particle showers is deposited directly using parameterizations of their longitudinal and lateral energy profile. The reconstructed *Atlfast-II* output includes the energies in the calorimeter cells. Because the standard reconstruction is run, it is possible to work with a combination of events obtained from Geant4 and *Atlfast-II* without modifying the analysis code.

The approach taken by *FastCaloSim* is intrinsically less accurate, but the parameterizations can be tuned against data. It has been used since 2011 for the production of large MC samples needed for new physics searches as well as precision measurements. *Atlfast-II* has been validated against the Geant4 based full simulation for electrons, jets and missing transverse energy (E_T). Validation plots of the calorimeter shower shapes of high E_T electrons are shown in Fig.5. In these plots, data taken in 2010 at a center-of-mass collision energy of $\sqrt{s} = 7$ TeV is compared with Geant4 version 9.4 (yellow histogram) and *Atlfast-II* (dashed red histogram) for $Z \rightarrow ee$ events. The left plot shows the distribution of ratios of energy deposited in a 3×7 versus 7×7 cluster of cells containing a particle shower in the bulk electromagnetic calorimeter layer 2. The right plot shows a distribution of the particle shower width in the high granularity strip layer 1 of the electromagnetic calorimeter, determined in a window corresponding to the cluster size (typically 40 strips in η), around the strip of the first local maximum of energy deposition.

3.4. *Atlfast-IIF* and *Fatras*

Compared with *Atlfast-II*, another order of magnitude in simulation time can be gained in *Atlfast-IIF* using the Fast ATLAS Tracking Simulation (*Fatras*) for the Inner Detector and Muon System [11][12]. *Fatras* produces a Monte Carlo simulation based on the software modules and the simplified geometry used by the standard ATLAS track reconstruction algorithms (see Fig.6). It also uses simplified parameterizations of physics processes. The combination of *Fatras*

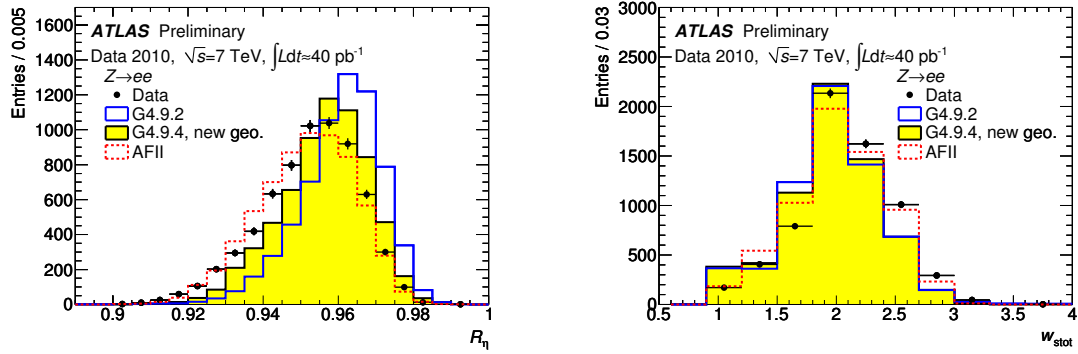


Figure 5. Left: deposited energy ratio R_η in a $\Delta\eta \times \Delta\phi = 3 \times 7$ cells cluster with respect to a 7×7 cells cluster size in the bulk EM calorimeter layer 2. Right: shower width W_{tot} determined in a window corresponding to the cluster size in the high granularity strip layer 1. In both validation plots the MC samples have been normalized to match the number of entries in the data. The agreement between 2010 data (black markers) and Atfast-II (AFII, dashed red histogram) in comparison with Geant4 (G4.9.2 and G4.9.4, blue and yellow filled histograms) indicates that Atfast-II can be tuned to match the data with good accuracy. [10]

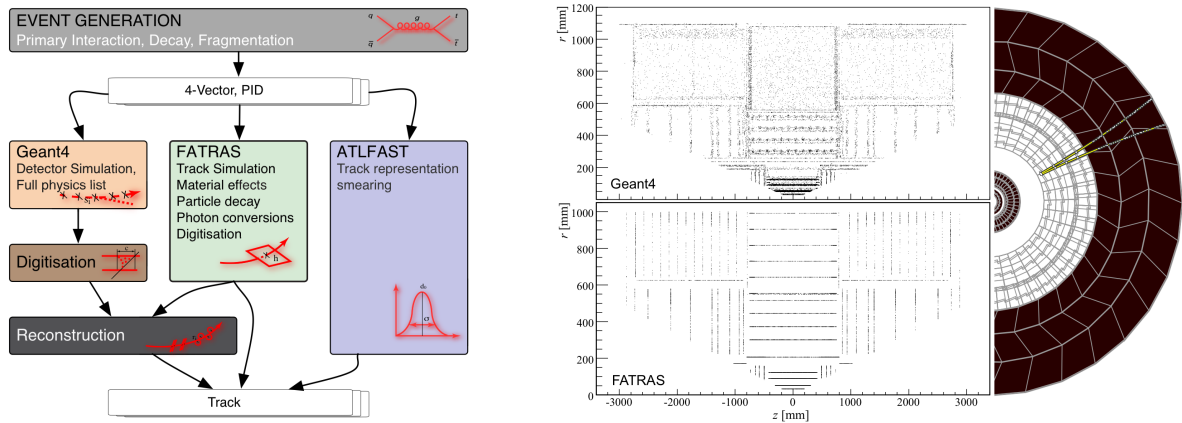


Figure 6. Left: overview of the different ATLAS track simulation strategies and different subtasks done in Fatras. Right: visualization of the simplified geometry used by the standard ATLAS track reconstruction and Fatras, derived from photon conversion vertices.

with FastCaloSim in Atfast-IIF shows a high level of agreement with the Geant4-based full simulation, while reducing the overall amount of computing time by two orders of magnitude.

Fatras was designed to provide a fast feedback cycle for tuning the MC simulation to real data, including the material distribution inside the detector, the integration of misalignment and current conditions, as well as calibration at the detector hit level. Fatras can also be tuned against data, making it a useful tool for validation studies, fast material calibration and rapid large-scale MC production. An example for the validation of Fatras with 900 GeV collision data, comparing the number of hits in the Pixel detector, is shown in Fig.7.

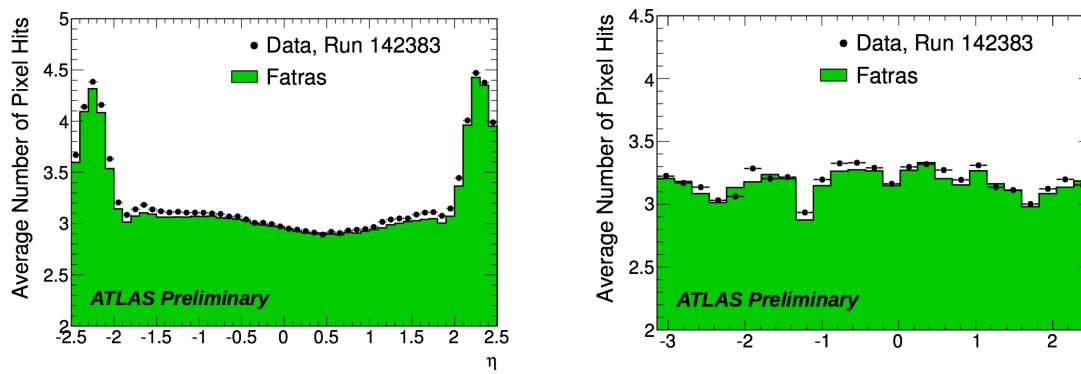


Figure 7. Comparison of the geometric distribution of pixel detector hits in η (left) and ϕ (right) in 900 GeV collision data (black points) and MC simulated with Fatras (histogram). The agreement indicates that Fatras can be tuned to match the data with good accuracy. [12]

4. The Integrated Simulation Framework (ISF)

Many physics studies require large MC samples for which time-consuming high precision simulation of certain particles and regions is necessary, while the remaining particles and regions require much less accuracy. The most sensible approach to the multitude of such use cases is the development of an Integrated Simulation Framework that allows for a flexible combination of different simulation strategies.

The new Integrated Simulation Framework is based on the requirement to allow to run all simulation types in the same job, even within the same sub-detector region, for different particles. The principle of the ISF is visualized in a use-case example of one simulated event in Fig.8. This framework is designed to be extensible to new simulation types as well as the application of parallel computing techniques in the future.

The ISF is fully embedded in the ATLAS software framework (Gaudi-Athena [13]). The general simulation flow (see Fig.9) is based upon these main components of the ISF core:

- SimKernel
- ParticleBroker
- Simulators

The general simulation flow is steered by the SimKernel, which is a single Athena algorithm being called in the execute chain of the Athena AlgSequence. It holds Simulator services for the sub-detectors, a ParticleBroker service and the truth service. The SimKernel retrieves particles from the ParticleBroker and routes them to their associated simulation engines. All simulators fill a common set of hit collections for the different sensitive detectors, which are then processed in the same digitization and reconstruction chain.

Each particle processed by the ISF is passed by the ParticleBroker through configurable routing chains for the current sub-detector. The particle is associated to a simulator according to the first filter rule that applies to its current properties. Prior to the simulation launch, users can configure these filter rules according to their specific physics analysis requirements. In this way they can find an optimal balance between precision and execution time by selecting faster simulation flavors for all parts that do not require full detail.

An example for the visualization of an ISF event which uses different simulation engines (Full Geant4 Simulation, FastCaloSim and Fatras) is illustrated in Fig.10 as a projection in the x-y plane. In the Inner Detector all electrons and photons as well as their secondaries are simulated

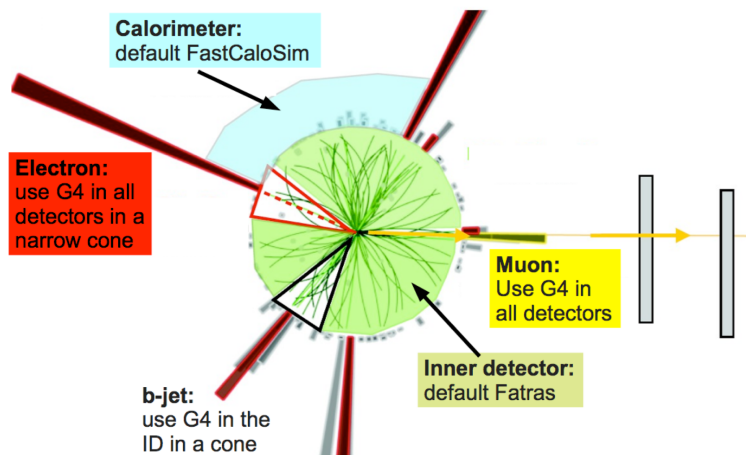


Figure 9. General simulation flow of the ISF. A central ParticleBroker associates a simulator to each particle via configurable routing chains. The SimKernel retrieves particles from the ParticleBroker and sends them to their associated simulators, which hand the outcoming particles back to the ParticleBroker.

with the full Geant4 simulation, while tracks of muons and pions are simulated with Fatras, and for all particles the energy deposition in the Calorimeter is modeled with the FastCaloSim. The layers of Pixel and SCT modules around the interaction point are shown in green and dark blue, while the TRT hits are represented by red markers.

5. Summary

In order to meet the increasing physics demands on MC samples, the Integrated Simulation Framework (ISF) is being developed. It allows the flexible combination of full and fast simulation strategies in a single event to provide an optimal balance between precision and execution time, depending on the required accuracy.

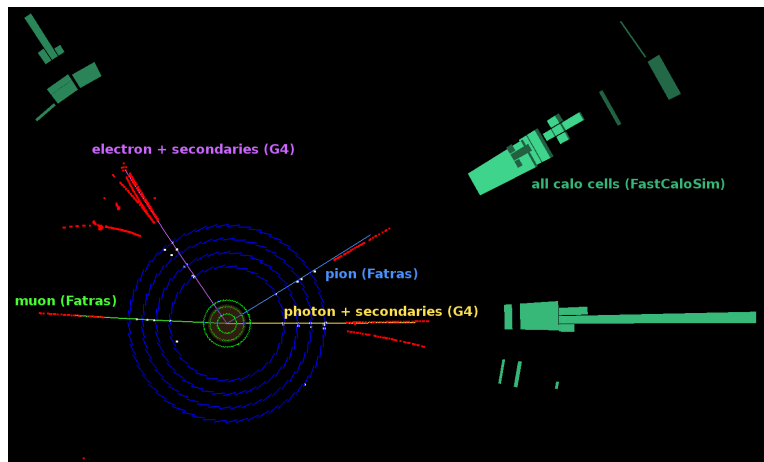


Figure 10. Event visualization in the x-y plane of an ISF event, which is using different simulation engines (Geant4, FastCaloSim and Fatras) according to the particle type and detector region.

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