Detector Simulation White Paper

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1. Introduction

Detector simulation is an essential tool to design, build and commission the highly sophisticated detectors utilized in modern particle physics experiments and cosmology. It is also a fundamental tool for data analysis and interpretation of the physics measurements. The typical simulation software application in high-energy physics (HEP) experiments consists of a set of packages executed in sequence, usually starting with a generator of the physics processes under study. In particle colliders, event generators provide the final state particles observed as primary particles in the detector. A second module simulates the passage of the generated primary particles through the detector material and its magnetic field. In most contemporary experiments, this detector simulation module is based on the Geant4 simulation toolkit, a software package that provides the tools to describe the detector geometry and materials, and incorporates a number of models to simulate electromagnetic and hadronic interactions of particles with matter [1]. When appropriate, various fast simulation options are used to save computing time with some penalty on physics accuracy. The next module, often called digitization, simulates the readout process, including the signal processing by the detector electronics, as well as the calibration of individual channels. At the end of the chain, the same algorithms used to identify and reconstruct individual particles and physics observables in real data are applied to simulated events. In the case of accelerator-based neutrino experiments, the chain typically starts with a Geant4 module to model the interaction of a proton beam with a target to produce a neutrino beam which is driven to a detector where the physics interaction of interest occurs. The neutrino beam and the first neutrino-nucleus interaction in the detector is typically modeled with the GENIE [7] package, while Geant4 is utilized in a second step to simulate the nucleus de-excitation and subsequent hadron production. Readout modeling, calibration, and reconstruction is done as described for collider experiments. During the last three decades, simulation has proven to be of critical importance to the success of HEP experimental programs. For example, the detailed detector modeling and accurate physics of the CERN Large Hadron Collider (LHC) CMS and ATLAS experiments Geant4-based simulation softwηare helped these collaborations deliver physics results of outstanding quality faster than any previous hadron collider experiment. The FLUKA simulation package has also been used extensively for studies of shielding and radiation modeling, providing important input to the design of the original LHC experiments and their upgrades. Simulation software at the LHC experiments is more accurate and yet runs much faster than its predecessor at the Tevatron. Simulation samples of better quality and in larger quantities, evolving detector and computing technology, and a wealth of experience from pre-LHC experiments on calibration and data analysis techniques, improved significantly the precision of the measurements in the current generation of experiments. In parallel with this, simulation has been used to design a new generation of neutrino and muon experiments and in searches for beyond the standard model (BSM) physics in precision experiments.

For all its success so far, the challenges faced by the HEP field in the simulation domain are daunting. During the first two runs, the LHC experiments produced, reconstructed, stored, transferred, and analyzed tens of billions of simulated events. This effort required more than half of the total computing resources allocated to the experiments. As part of the high-luminosity LHC physics program (HL-LHC) and through the end of the 2030's, the upgraded experiments expect to collect 150 times more data than in Run 1. The 50 PB of raw data produced in 2016 will grow to approximately 600 PB in 2026 while the CPU needs will increase by a factor of about 60. Demand for larger simulation samples to satisfy analysis needs will grow accordingly. In addition, simulation tools have to serve diverse communities, including accelerator-based particle physics research utilizing proton-proton colliders, neutrino and muon experiments, as well as the cosmic frontier. The complex detectors of the future, with different module- or cell-level shapes, finer segmentation, and novel materials and detection techniques, require additional features in geometry tools and bring new demands on physics coverage and accuracy within the constraints of the available computing budget. More extensive use of fast simulation is a potential solution, under the assumption that it is possible to improve time performance without an unacceptable loss of physics accuracy.

Thus, the effort to improve detector simulation and modeling tools, including the accuracy of their physics while saving memory allocation and computing execution time, requires immediate attention. This chapter addresses the future development of full simulation (currently based on Geant4 [1], and in a few cases on Geant3) and fast simulation applications of HEP experiments for detectors and beam lines with a view to achieve improvements in software efficiency, scalability and performance, and to make use of the advances in processor, storage and network technologies. A plan must consider new approaches to computing and software that could radically extend the physics reach of the detectors, while ensuring the long-term sustainability of the software through the lifetime of the experiments running through the 2020's and 2030's. One example is the GeantV [2] R&D project, started in 2013. Another example is the ongoing effort to port simulation code to run on High Performance Computing (HPC) facilities, which provide massive CPU power and modern computing architectures.

Components of the HEP simulation chain, such as physics generators and event visualization tools are discussed in other chapters, while the modeling of the propagation and beam manipulation through accelerator lattices (i.e. CERN and Fermilab accelerator complexes) are considered to be outside the scope of this chapter. Space and medical applications are referred to briefly where appropriate.

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2. Challenges

The experimental programmes planned in the next decade are driving developments in the simulation domain; they include the High Luminosity LHC project (HL-LHC), neutrino and muon experiments, and studies towards future colliders such as the Future Circular Collider (FCC) and the Compact Linear Collider (CLIC). The requirement of improving precision in the simulation implies production of larger Monte Carlo samples, which scale with the number of real events recorded in future experiments, and this places an additional burden on the computing resources that will be needed to generate them. The diversification of the physics programmes also requires new and improved physics models.

The main challenges to be addressed if the required physics and software performance goals are to be achieved can be summarised as follows:

- reviewing the physics models assumptions, approximations and limitations in order to achieve higher precision, and to extend the validity of models up to FCC energies on the order of 100 TeV;
- redesigning, developing, commissioning detector simulation toolkits to be more efficient when executed on emerging computing architectures e.g. Single Instruction Multiple Data (SIMD) vectorisation, Non-uniform Memory Access (NUMA) hierarchies, Many Integrated Core (MIC) devices, Graphic Processing Unit (GPU), and Tensor Processing Unit (TPU) architectures;
- porting and optimising the experiment's simulation applications, or developing new ones to allow exploitation of High Performance Computing (HPC) facilities;
- exploring different fast simulation options, including common frameworks for fast tuning and validation using Machine Learning (ML) techniques;
- developing, improving, optimising geometry tools which can be shared among experiments to make the modeling of complex detectors computationally more efficient, modular, and transparent;
- developing techniques for background modeling, including contributions of multiple hard interactions overlapping the event of interest in collider experiments (pile-up);
- revisiting digitisation algorithms to improve performance by means of vectorisation and sub-system parallelisation techniques, and exploring opportunities for code sharing among experiments;
- recruiting, training, retaining, human resources in all areas of expertise pertaining to the simulation domain, including software and physics.

The complexity and diversity of future experiments results in an enormous demand for CPU, and detailed detector simulation already consumes the plurality of CPU resources of most current HEP experiments. Some progress has already been made in improving software performance, for example by adding multithreading capability to Geant4, and by redesigning the geometry library into the VecGeom package that exploits vectorisation. These R&D programmes need to continue in order to benefit from the various forms of parallelism offered by modern architectures. The goal of the GeantV R&D project is to build a realistic prototype application for a complex experiment with the aim of demonstrating a factor 2-5 gain in CPU time. The main architectural feature of this prototype is the implementation of particle-level, i.e. track-level, parallelization for more efficient use of SIMD vectorization and data locality. Whenever possible, sub-systems and libraries developed in this context should be made available for use with Geant4, as has been done with VecGeom, to maximize the benefits to experiments at the earliest opportunity.

An important constraint in any strategy is the need to support on-going experiments through continuous maintenance and improvement of the Geant4 simulation toolkit. This implies making minimal API changes visible to these experiments at least until production versions of potentially alternative engines, such as those resulting from ongoing R&D work, become available, integrated, and validated by experiments.

A flexible simulation strategy is needed that is capable of delivering a broad spectrum of options offering different levels of physics accuracy, from a pure full simulation approach to a combination of Geant4 showers, parametrized response functions, and shower libraries. R&D in the realm of fast simulation includes the use of Machine Learning (ML) techniques and embedded tools for tuning and validation in an effort to provide faster and more accurate physics and to be able to safely expand the use of fast simulation in the context of limited computing resources.

HPC facilities offer a valuable resource and work must continue to adapt simulation applications to run efficiently on these systems, which may produce a significant fraction of the simulation samples in future HEP experiments.

Work also needs to continue to improve the accuracy of the physics models, and the validity of the models needs to be verified for new detectors that include, for example, liquid argon time projection chambers (for DUNE) and silicon-absorber calorimeters (for CMS). The models need to be improved and validated for a large variety of incident particles and energy ranges, including muons, neutrinos, and the high energies accessible in a Future Circular Collider (FCC).

In producing new models of physics interactions and improving the fidelity of the models that exist, it is absolutely imperative that high-quality data are available. Simulation model tuning often relies on test beam data, and a program to improve the library of available data could be invaluable to the community. Such data would ideally include both thin-target test beams for improving interaction models and calorimeter targets for improving shower models. These data could potentially be used for directly tuning fast simulation models, as well. At the least it is important that the experiments carefully consider what measurements could be made that would be useful input to the community of Monte Carlo program developers and tuners.

High pile-up simulation for the high-luminosity environment in future data-taking at the LHC poses challenges in memory utilisation and data transfer (I/O) for generating the large statistics samples needed to compare with data from high trigger rates. It currently necessitates the generation and handling of large minimum bias samples in order to achieve an accurate description of high pile-up collision events (see Section 5). It would be desirable to have tools that allow overlay of both simulated and real data events. The latter poses a real challenge related to the collection of unsuppressed zero-bias data samples that reflect the luminosity profile of the physics run.

The digitization component of the simulation chain offers opportunities for parallelization, given that the code between sub-detector components is typically orthogonal. In the case of neutrino detectors based on liquid argon technology, this step is computationally expensive, as compared to other elements of the chain. Since digitization is often either memory- or I/O-intensive, there is a challenge to ensure that parallelism is efficient. Another issue is that digitization code, including containers, data types and data structures, is typically developed by the user. In order to exploit the SIMD opportunities intrinsic to the digitization process, digits must be constrained to a subset of the possible data structures, with priority given to data contiguity.

New areas of commonality across experiments need to be explored, for example in the domains of fast simulation and geometry. A great deal of common code is relied upon by many users for the benefit of the whole HEP community for the long term. It will be important to identify these pieces of code, remove the experiment dependency where appropriate, and ensure that the pieces that cannot be removed are either going to be maintained by a group that feels responsibility for them or will not become a bottleneck for any detector simulation in the future.

The large reliance on simulations implies the need for careful assessment of the systematic uncertainties associated to Geant4 predictions. New capabilities and tools are being developed to allow for the calculation of systematic uncertainties on the physics observables predicted by the Geant4 beam and detector simulations. In other words, kinematic distributions, efficiencies, and calibration constants will be predicted with systematic uncertainties resulting from the propagation of the uncertainties associated with the individual Geant4 physics models.

There are specific challenges associated with the Intensity Frontier experimental programme. Properly simulating a neutrino experiment like NOvA [3], MicroBooNE[4], MINERvA[5], or DUNE [6] involves a three-part software stack, the first and last of which are relevant to this paper; the second, event generators such as GENIE [7], is discussed elsewhere. The first element of the stack concerns the beamline and the neutrino flux prediction. Estimating the neutrino flux is a notorious problem because as weakly interacting particles, neutrinos offer no independent mechanisms for measuring the flux. A central problem is in the difficulty of accurately simulating the hadronic physics of meson production, especially in a thick target. Additionally, the simulated neutrino flux depends very strongly on minute details of the beamline, meaning that neutrino beam kinematic distributions must be described in great detail. Geant4 is the most commonly used software toolkit for this work, although FLUKA [8] and MARS [9] are also used. The final element of the stack is the detector simulation. Again there are numerous challenges in terms of efficiently simulating large numbers of events inside complex detector geometries and in handling subtle physics effects in the traversal of radiation across matter. Neutrino experiments in particular rely heavily on detector simulations to reconstruct neutrino energy, which requires accurate modeling of energy deposition by a variety of particles across a range of energies. Geant4 is the universal solution at this stage.

Muon experiments such as Muon g-2 and Mu2e also face large simulation challenges. Because they are searching for extremely rare effects, they must grapple with very low signal to background ratios, and the modeling of low cross-section background processes. Often the physics of these processes is not well understood, introducing large systematic uncertainties. Additionally, the size of the computational problem is a serious challenge, as large simulation runs are required to adequately sample all relevant areas of experimental phase space, even when techniques to minimize the required computations are used. Another aspect related to the background events is the need to simulate the effects of low energy neutrons, which requires large computational resources. For example, Mu2e used a total of approximately 60 million CPU hours, or 83 thousand core months, in a 2016 simulation campaign to produce the full simulation sample needed to complete a technical design report delivered in 2016. Geant4 is the primary simulation toolkit for all stages of these experiments. For comparison, the CMS experiment spent 860 thousand core months on simulation in the May 2015-May 2016 period.

Although the computing needs of the intensity frontier are currently small compared to the LHC experiments, they are expected to grow substantially in the next decade, and it is imperative that the intensity frontier experiments make use of modern computing architectures and algorithms. This transition will be complicated by the fact that the intensity frontier is fractured into many small experiments, some of which have as few as 50 collaborators, limiting the manpower available for updating detector simulations to use new tools. Efforts such as LArSoft[7] have recognized this challenge and aim to pool resources of many experiments for the benefit of all.

3. Geometry

The geometry modeler is a key component in Monte Carlo detector simulation, combining both solids modelling and efficient navigation techniques. Stringent requirements apply to provide the right level of flexibility, robustness and accuracy in modeling from the simplest to the most complex setups and to offer adequate precision and efficiency in the implemented algorithms. Geant4 [1] provides a wide variety of tools and solutions for describing geometry setups from simple to highly complex. Geometrical models of the LHC detectors, for instance, easily reach millions of geometrical elements of different kinds combined together in hierarchical structures. The geometry modeler provides techniques by which memory consumption can be greatly reduced, allowing regular or irregular patterns to be easily replicated and assembled. This, combined with navigation and optimization algorithms, allows the efficient geometry computation of the simulated tracks with the elements composing any geometry setup.

Recent extensions of the geometry modeler in Geant4 include specialized navigation techniques and optimization algorithms to aid also in medical simulation studies. This has allowed complex geometrical models of the human body to be developed. Extensions also include parallel navigation and tracking in layered geometries which allow geometry setups to be superimposed on one another with minimal impact on CPU time (Figure 1). An important and rather useful construct for shapes delimited by any kind of complex surface is offered by the tessellated-solid construct, which allows complex geometrical shapes to be described by approximating their surfaces as a set of planar facets (triangles), with tuneable resolution. This technique is used nowadays for importing geometries from CAD systems to generate surface-bounded solids. Recent developments introduced in Geant4 along with the implementation of the Unified Solids library [10] provide considerably improved CPU performance, making it possible to use such constructs for very detailed and realistic descriptions of surfaces, while optimally scaling with the number of facets in use. Further improvements to the tessellated solid construct are expected as part of the rewrite of most geometry primitives going on in the VecGeom [12] package, initiated within the GeantV project [2].

The Unified Solids Library started as an AIDA project in 2011, with the aim to unify and improve the algorithms provided by the Geant4 and ROOT [11] approaches to solids modeling. The library which comes with a large collection of primitives, has been extended and enhanced as part of the AIDA-2020 project, and is now integrated in VecGeom, which provides an independent geometry modeler library for use as alternative replacement in either Geant4 or ROOT. In VecGeom, the interfaces to geometrical primitives have been extended to support vector signatures, which are essential for GeantV, and allow for parallel processing of queries; algorithms are completely reviewed and in good part rewritten to make use of SIMD instructions wherever possible, and support different kernels and architectures, including accelerators such as Intel Xeon Phi® and GPU devices. The code has been reengineered to make use of C++ template techniques, allowing for more modular implementation and for specializing efficiently on different topologies.

The benefits in CPU time are clearly visible with ray-tracing scalar tests and also measurable in terms of few percent when full physics and electromagnetic field integration is applied.

The VecGeom geometry modeler includes a highly efficient navigation system. It has been developed and optimized to exploit vectorised transport on CPU, GPGPUs and Intel Xeon Phi®, making use of the full potential of the vectorised features of the library. It is planned in the near future to provide hooks within both Geant4 and ROOT for using the navigation system of VecGeom, eventually boosting speed further also for the scalar mode.

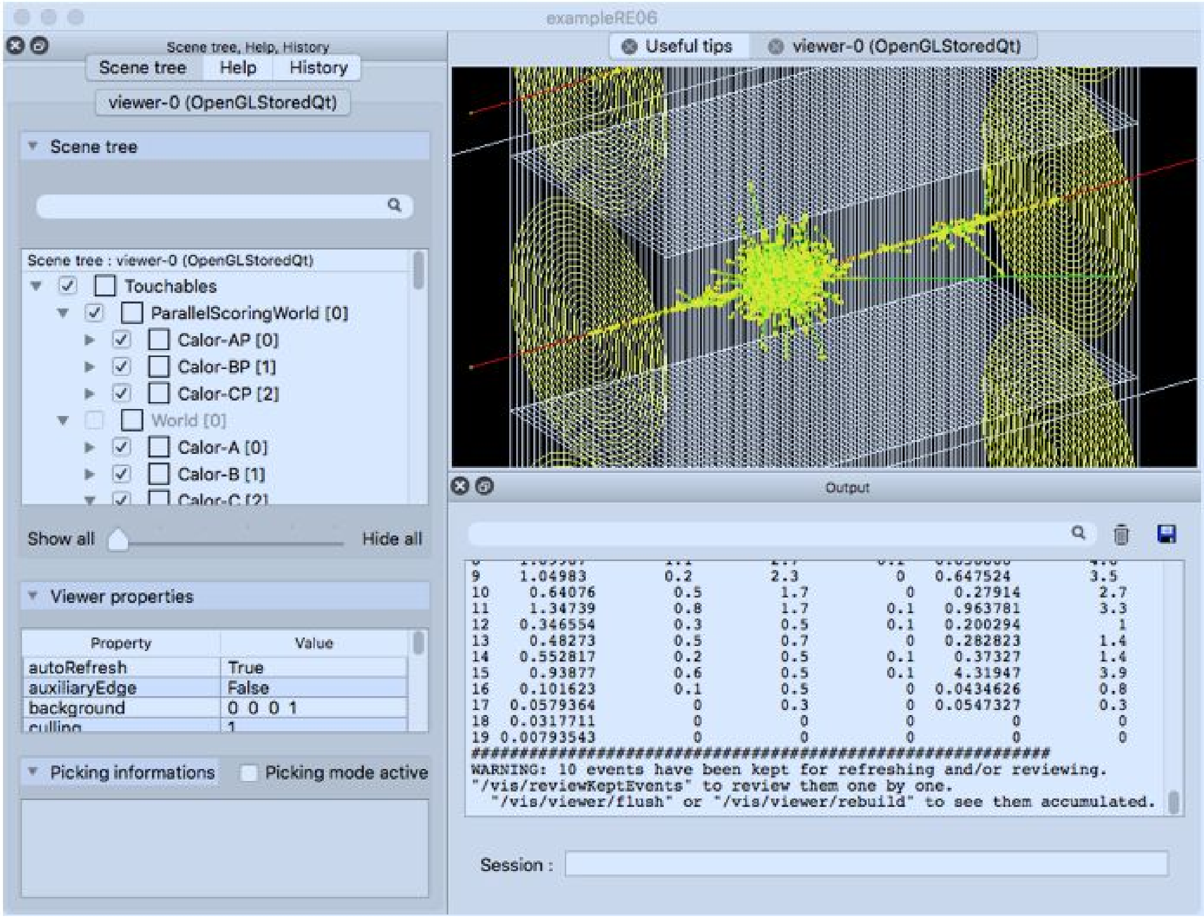


Fig. 1 - An interactive Geant4 example featuring parallel geometries and scoring with VecGeom primitives and parameterisations

Geant4 offers the ability to import and export Detector geometrical descriptions from text files according to the Geometry Description Markup Language (GDML) [13] based on XML; the exchange format is also supported by ROOT and the schema includes all the geometrical primitives currently in use. GDML supports the modularization of geometry descriptions to multiple GDML files, allowing for rational organization of the modules for complex setups. Verification of the GDML file against the latest version of the schema comes for free thanks to Xerces-C++ [14], with the possibility to turn it on or off in the Geant4 GDML parser.

The DD4hep Geometry Toolkit [15], being developed in the context of the AIDA and AIDA-2020 projects aims to provide a generic detector description toolkit built by reusing the existing components of widely used packages and provide the missing functional elements and interfaces, for offering a complete and coherent detector description solution to experiments.

Computations performed by a geometry modeler in a simulation program must be highly precise and efficient. Lots of effort has been spent in the past decades to achieve the level of precision and reliability offered today, still the evolution of the computing hardware, compilers and programming languages require algorithms and related implementations to evolve as well. It is therefore foreseeable that effort in this sense will have to continue, in a way as it is currently being done for the VecGeom package, to also favor modularity and reusability of the various components.

A better integration of the existing tools used in simulation and the adoption of CAD systems for designing and fast-prototyping the geometry models is also desirable. A variety of solutions tailored for simulation exist today, especially in tools developed for space science applications, although none or few of them are fully open source. In the past such a system was not desirable because of the difference in level of detail required in CAD programs compared to standard detector simulations. Individual pipes, bolts, and wires, often described in CAD, are normally grouped together and modeled as single large volumes in detector simulations. In some modern detectors, the precision of the physics program necessitates a level of detail in the detector geometry that is more comparable to that of a CAD design model.

Several of the systems for geometry description, while useful for detector simulation, lack important features for use in data reconstruction. The most important of these features is the ability to include detector (mis-)alignment effects, some of which may cause collisions between the 3-dimensional volumes in the detector. It is critical to include these effects in reconstruction software, but often in detector simulation such small alignment issues are omitted.

The programme of work for the near future in the field of geometry includes the following:

- Promote the adoption of VecGeom by the experiments and users community, by adiabatically integrate and validate its use through the interfaces now existing and provided in the latest versions of the Geant4 toolkit.
- Complete the porting and implementation in VecGeom of the missing shapes from the standard set of primitives of the GDML schema; deprecate the old scalar USolids implementation and tidy up code and configuration settings in VecGeom.
- Provide VecGeom documentation and user guides.
- Investigate adoption of VecGeom navigation algorithms in Geant4 and ROOT and provide first prototype implementations of a navigator adapter making full use of the scalar navigation capabilities in VecGeom.
- Provide implementation of a GDML reader/writer in VecGeom to allow for easy detector description geometry exchange.

4. Readout Modeling (Digitisation)

Simulation toolkits like Geant4, in the end, only provide energy depositions positioned in space and time in geometric elements. These simulators often do not include some effects like charge drift in an electric field, which would be prohibitively expensive (and often unnecessary) to model in detail, and they do not include models of the readout electronics of the experiments. They may not even have knowledge of the detailed readout structure of the detector, for example simulating charged particles passing through a block of silicon rather than individual pixels or strips that correspond to readout channels. Instead, these effects are normally taken into account in a separate step called digitization. The input to digitization is the “MC truth information” (see Sec. 6) and energy deposits from the simulation, and the output often includes a new, processed truth record, as well as a data format that is conceptually similar to the data from the detector (e.g. voltages, currents, times, and so on).

Digitization is inherently local to a given sub-detector, and often even to a given readout element, so that there are many opportunities for parallelism if the code and the data objects are designed optimally. Digitization is also normally the software in which pileup is introduced (see Sec. 5) and backgrounds, including detector noise, are included. Generally, without pileup, the digitization process is not particularly expensive in terms of CPU time or memory. With pileup included, however, there can be significant performance issues, particularly for HL-LHC configurations of digitization code. One exception to this performance rule are large drift detectors like the ALICE TPC, where significant “simulation” occurs in the digitization software. Again, parallelism can provide a path to performance improvements, both in terms of vectorization and multiprocessing or multi-threading.

Even without major performance challenges, digitization presents one of the most significant risks in terms of code aging and loss of expertise. The detailed understanding of the readout structure of a detector is normally most readily available when the detector is built, and as time goes on the experts in these read out systems may move on, making code maintenance and development, particularly for detector upgrades, problematic. Similarly, because these codes often do not result in major and obvious analysis-level issues, they are often left alone for many years, without being updated to newer standards and best practices. Such issues could be helped by greater code sharing, if it could be achieved.

Since digitization code includes a number of effects that are specific to the individual readout that is used, historically there has been very limited sharing of code among digitization frameworks. Recently, both hardware and software projects have benefitted from an increased level of sharing among experiments. LArSoft is an endeavor to provide common digitization code to all the experiments using large liquid argon detectors. Similarly, the development of next generation silicon detectors requires realistic simulation of the charge collection and digitization processes. Owing to the large variety of technologies, common software frameworks need to be flexible and modular to cater the different needs. The Allpix software and the more recent Allpix Squared framework provide generic algorithms shared between many silicon pixel detector projects, and Allpix Squared follows a modular approach and is thus also suited to simulate e.g. silicon-based calorimeters [16]. The frameworks also allow the implementation of effective radiation damage models and therefore enable the simulation of the detector response throughout the experiment's lifetime.

As both CMS and ATLAS expect to use similar readout chips in their future trackers, further code sharing might be possible. Such effects will be more important in the coming years, and the experiments both at the LHC and elsewhere are examining similar detector technologies for future upgrades or implementations, so the possibility of common code bases should not be ignored.

5. Modeling of Pileup

For the LHC experiments, in particular ATLAS and CMS, the modeling of pileup (proton-proton collisions simultaneous with, or almost simultaneous with, the collision of interest) represents a significant challenge over the next 10 years. The amount of pileup is expected to grow from an average of around 30 collisions for every proton-proton bunch crossing in 2016, to 50 in 2017, to almost 200 in the HL-LHC era around 2025. The individual detector elements of the experiments are sensitive to pileup in different ways, and over different time ranges. It is perhaps worth noting that the discussion of pileup here can equally apply to the high-multiplicity underlying event in central heavy-ion collisions at the LHC.

There are a number of ways to model the effect of pileup that the experiments have all examined. The conceptually simplest is to simulate a large number of inclusive proton proton collision events (usually called minimum bias events) with an event generator like Pythia8 [30] and to overlay the energy depositions from these events on top of the energy depositions from the event of interest. Normally these minimum bias events are kept in libraries to avoid frequent (and CPU intensive) re-simulation of all the required pileup. With the pileup expected at the HL-LHC, these libraries become very large if the re-use rate of events with high-pT jets is to be kept small, demanding large amounts of disk use for each job as they copy a sufficient number of events locally for use. The copying around of these libraries also strains networks when large numbers of jobs are running.

Another option is to “pre-mix” together the minimum bias collisions into individual events that have the full background expected for a single collision of interest. This has the advantage that the disk usage of a single event is reduced, but still runs a risk of re-use of background events for a large dataset.

The experiments have also explored the possibility of using data directly to model the pileup and detector noise, a technique normally called “overlay". This option has a number of advantages, including the correct modeling of detector noise over the full run period. There are, however, a few drawbacks that make this both technically and practically difficult. One can only model detectors for which data has been taken, so simulations of future layouts cannot be done this way. The detector misalignments and simulation misalignments may not be the same, but the events are normally run through a single reconstruction, so that hits shift positions if different alignments are used for both. The data used for overlay must also normally be taken without “zero suppression” in order to ensure that low energy contributions from both the signal event and background that are individually below the normal readout threshold for a detector can coherently add to a deposition above that threshold. In addition, some detector electronics have nonlinear responses to deposited energy, implying that their output data cannot be added trivially. Complications and approximations could be necessary in a data overlay scheme to deal with nonlinear electronics.

With very fast simulation come additional possibilities. For sufficiently fast simulation, it becomes feasible to perform the simulation (and even the generation) of the additional pileup events at the same time as the signal event. This ensures that the overlaid events are unique, but has the disadvantage of the fast simulation’s lower fidelity. Under normal circumstances, however, analyses are not sensitive to the details of the pileup simulation, and even a fast simulation that is not sufficiently accurate for a signal event simulation may be sufficient when simulating the pileup. Indeed, with generative adversarial networks like those discussed in the Fast Simulation Section 10.3, the background from pileup could be generated as a single background image, taking into account all backgrounds that don't require special handling. Such techniques are obvious candidates for exploration in the coming years.

Both experiments and theorists have also explored the possibility of parameterizations of either the pileup or the detector response to the pileup. Programs like DELPHES and PGS have simple parameterizations of the response and resolution of analysis objects, and in general the impact of pileup can be included, at least approximately, by modifying those resolutions and lowering identification and isolation efficiencies for leptons. Such techniques are rough, but are often good enough for analysis prototyping or for far-future feasibility studies before the experiments invest significant effort in the detailed simulation that might be needed for the analysis. Such techniques are often employed when performing large signal parameter space scans, as in the case of searches for Supersymmetry, before detailed simulation of specific signal models is undertaken.

In the parametric approach, any fast simulation technique used to model the pileup must have a sufficiently correct model of the physics of interest for the analysis at hand. For some analyses of, for example, long-lived particles, this may not be the case, so multiple solutions should always be kept in play.

As the LHC experiments further develop their data overlay techniques, it may be useful to hold occasional discussions of challenges overcome in these systems. Alignment issues, data-collection issues, and so on can be addressed with the same philosophical approach, even if the technical implementations differ somewhat. The development of fast simulations for pileup should be followed as a part of the fast simulation discussions explored in Section 10.3. As studies of physics analyses in high-luminosity environments become more common, some of the current parameterization and fast simulation techniques will improve their fidelity, but this will happen as a natural evolution with experimentalists and phenomenologists, and likely does not require any directed action.

6. Handling of MC Truth Information

All simulations keep some concept of “MC Truth”, a record of what was really going in the simulation of the detector, unaltered by the detector readout. This is in some cases as simple as the event record from the generator, which includes the particles that were input to the simulation as well as some of the upstream particles from which they derive. In most cases, however, more complex MC Truth is desired. Interestingly, the standards for these records exist as text formats and as C++ classes (HepMC and LHE), but there are not widely-used compressed binary storage formats for the classes. Having such a standard might facilitate the reusability of code and help the examples provided with simulation toolkits be more practically useful.

One standard addition to the event generator record is a record of a limited set of particle interactions in the detector. Often, for example, the hadronic interaction of a pion within the tracker volume is stored. There is not a standard format for such interactions, but it is common to add these interactions directly to the original event generator record, which is normally stored as a connected tree. This tree is unique for a given event, but if multiple particles are simultaneously in flight, as in the case of highly-parallel simulation, then they may need to make simultaneous modifications to this tree. This problem is not insurmountable, but requires some care.

The various other types of MC Truth are often detector-specific. These can include records of true energy deposition, as well as records of which particles in the generator record resulted in those energy depositions, for example. Such records are more straightforward to store in tracking detectors, where normally there is a one-to-one correspondence between a “hit” used for track reconstruction and an energy deposition by a particle from the event generator. Calorimeter records are inherently more complicated, as showers from many particles can overlap and merge.

The most significant challenge for MC Truth handling is keeping the memory and disk consumption minimal, while still storing all the information that is important to the analysis groups downstream. For example, Geant4 has a concept of a “Trajectory”, which can be useful for keeping a particle history as a part of the truth record. If such trajectories are kept for all particles produced in the calorimeter of an LHC experiment, however, then the memory usage would become prohibitive. Similarly, while most interactions can be stored in the truth record in the tracker, it would not be practical to do so in the calorimeter, where each event results in millions of secondaries generated. Ensuring that each experiment has the flexibility to save the required MC Truth information without inducing significant overheads in memory or CPU usage is critical for any future simulation toolkit.

For backgrounds that are included, as in the case of pileup (described in Sec. 5), it is also important for the experiments to be able to filter the truth information, and indeed filter it differently than is done for a signal event. What information is most of interest is both detector- and analysis-specific, but frameworks must ensure the flexibility required to satisfy even the most exotic use-case.

7. Physics Modeling

Geant4 physics libraries provide accurate simulation for a wide variety of applications in HEP, space science, medical physics and other scientific domains. HEP experiments tune their simulations by comparing simulation results with both test beam data and collision data. By and large, these comparisons show good agreement. Nevertheless, discrepancies in comparisons between the results of simulation and collider data do exist, and it can be extremely difficult to disentangle whether the differences arise from misrepresentation of the detector geometry and material or from inaccuracies in the physics modeling.

Big efforts continue to be invested by experimentalists to understand the performance of their detectors, as well as by the physics developers to improve and validate their physics simulation models. The comparison against thin-target data has been very successfully used to develop and to initially tune the physics models. However, it has been observed recently that further tuning leading to improvements against thin target data, does not necessarily lead to better simulation results when compared to the thick-target data. Beyond the lack of enough thin target data, this situation is, most likely, showing that the current models are reaching their limits and in order to improve the overall detector simulation, one needs to go beyond simple tuning of the existing models and to develop new, more sophisticated ones. Another modeling challenge that we will face at higher energies is related to the extreme closeness of the central trackers to the interaction points, allowing short lived particles such as hyperons to interact with the detector. Up to now, these particles are decayed by the generators without being transported by the simulation code as their decay happens in the vacuum of the beam pipe. As beam energies increase, the line between particles dealt with by generators and Geant4 will blur. These will survive long enough to pass through the first few layers of the detectors leading to "missing hits" in MC. As this situation becomes more common, the range of physics models available for such particles will need to be expanded.

Our goal in detector simulation in the coming decade is to cope with experimental needs for analysis of high-statistics data and for modeling the next generation detectors (ILC/CLIC, FCC). Higher statistics in future experiments will require smaller simulation errors, which in turn implies higher precision models and larger Monte Carlo (MC) events to be generated. This imposes two major challenges on physics modeling. The first priority is to improve physics models to limit the systematic error and match higher precision crucial for high luminosity HL-LHC. The second priority is the extension of the validity of the physics models up to FCC energies.

In the following, we summarize recent developments in electromagnetic and hadronic physics modeling. We discuss physics accuracy and performance improvements along with results of comparison of simulation with experimental data.

7.1 Electromagnetic Physics

Electromagnetic (EM) transport simulation is challenging as it occupies a significant part of the computing resources used in full detector simulation. More experimental data in the coming decade implies higher statistics and this implies the need for large and accurate simulation samples, which require both model accuracy and speed. Therefore the physics models need to be improved for achieving higher accuracy and the implementation of algorithms needs to be reviewed in order to optimize performance. Significant efforts have been made in the recent past to better describe the simulation of electromagnetic shower shapes, in particular to model the H -> γγ signal accurately at the LHC. This effort is being continued with emphasis on reviewing the models assumptions, approximations and limitations, especially at very high energy, and with a view to improving their respective software implementations. For LHC Run-1 simulation Geant4 version 9.4 was used [17].

For Run-2 significant improvements were introduced into the bremsstrahlung, pair production and multiple scattering [18, 19] further improving simulation of the EM shower shape; these improvements were made available in Geant4 9.5 and 9.6. For validation purposes, an extended set of tests versus data has been developed for high, moderate and low-energies using test-beam data and published thin target data. Comparisons with low-energy EM models from the Livermore and Penelope packages were also carried out.

The process of multiple scattering of charged particles is a key component of Monte Carlo transport codes. At high energy, it defines the deviation of charged particles from ideal tracks, limiting the spatial resolution of detectors. The scattering of low energy electrons defines the energy flow across volume boundaries. This affects the sharing of energy between absorbers and sensitive elements, directly affecting shower shapes. A comprehensive description of recent improvements of the Geant4 electromagnetic module can be found in [19]. Rather good agreement was found when Geant4 predictions were compared with experimental data collected at the LHC.

Figure 2 shows a comparison of CMS test beam data with predictions from two Geant4 physics lists, QGSP_FTFP_BERT_EML and FTFP_BERT_EMM. EML utilizes a simplified (faster) multiple scattering model for all detectors, while EMM uses the detailed multiple scattering model for sampling calorimeters and the simplified model for other detectors. The same figure also shows the ratio of Monte Carlo to data as a function of beam momentum. It is clear from the figure that the predictions from the physics list FTFP_BERT_EMM are closer to the data, in particular at higher beam energies, and therefore CMS has taken the decision to move to this list for its 2017 MC productions. Recent results from the CMS experiment were also presented showing discrepancies in the EM shower width in the endcap region as shown in Figure 3. This is a fresh observation that needs a much more detailed understanding, leaving us with an open question as to whether there is a problem in the physics model or an issue with the modelling of detector materials.

In the ATLAS experiment one area of disagreement concerns the measurement of lateral shower shapes in the EM calorimeter. Figure 4 shows a measurement of R_η for unconverted photons in the ATLAS EM calorimeter, where R_η is the ratio of shower energy deposited in 3x7 cells to 7x7 cells in the forward hadron calorimeter. There is a clear discrepancy between real data and the results of MC simulation with Geant4 9.6 (red line). Shower shapes in eta-direction are consistently wider in data than simulation, both for electrons and photons. Detailed investigations suggest that this is not a material issue and therefore work is continuing to better understand the impact of the EM physics modeling on the results of the simulation. A similar discrepancy is seen in the measurement of the lateral shower width for electrons in the first layer of the EM calorimeter, as can be seen from the lower plots in Figure 4 obtained with Geant4 9.2 and 9.4. Although the simulation in the upper plot can be adjusted to better match the data (“corrected”, in the figure), it is challenging to understand correlations between mis-modeled effects, and a more accurate simulation is desirable. A substantial amount of work and high level of coordination with experiments is therefore needed to investigate the pending discrepancies between data and simulation.

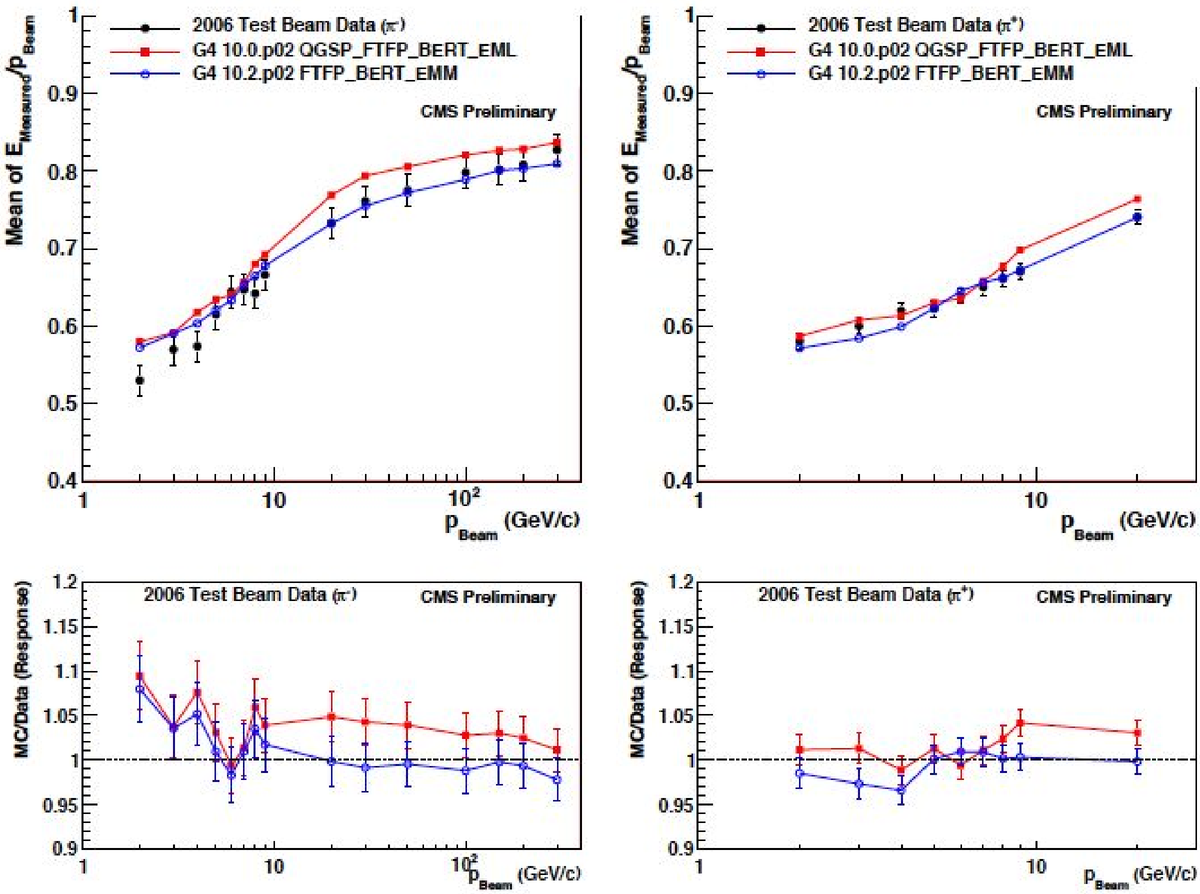


Figure 2. The top plots correspond to the mean energy response for p^- (left) and p^+ (right) as a function of the beam momentum. The bottom plots are ratios of Monte Carlo predictions to the data for pions as a function of beam momentum. The black points refer to the data, whilst the red and blue points are Monte Carlo predictions from physics lists QGSP_FTFP_BERT_EML of Geant4 10.0.p02 and FTFP_BERT_EMM of Geant4 10.2.p02 respectively.

The HL-LHC era will require higher precision simulations that can only be achieved by continuous improvement of the electromagnetic physics models used in the simulation. The further development of these models is therefore still being actively pursued in order to improve their precision and to extend their validity to higher energies. They include the following.

- A new Goudsmit-Saunderson “theory-based” model for describing the *multiple scattering* of electrons and positrons has been developed (Figure 5, blue line). It has been demonstrated to outperform, in terms of physics accuracy, the old theory-based model in Geant4 (grey line) and the Urban model that is the Geant4 default (Figure 5). The new implementation incorporates all the ingredients of the theoretical model resulting in extremely smooth angular distributions and has been developed with a view to fully exploiting track-level vectorisation in the future. At the same time it is important to note that this was achieved without incurring a speed penalty.

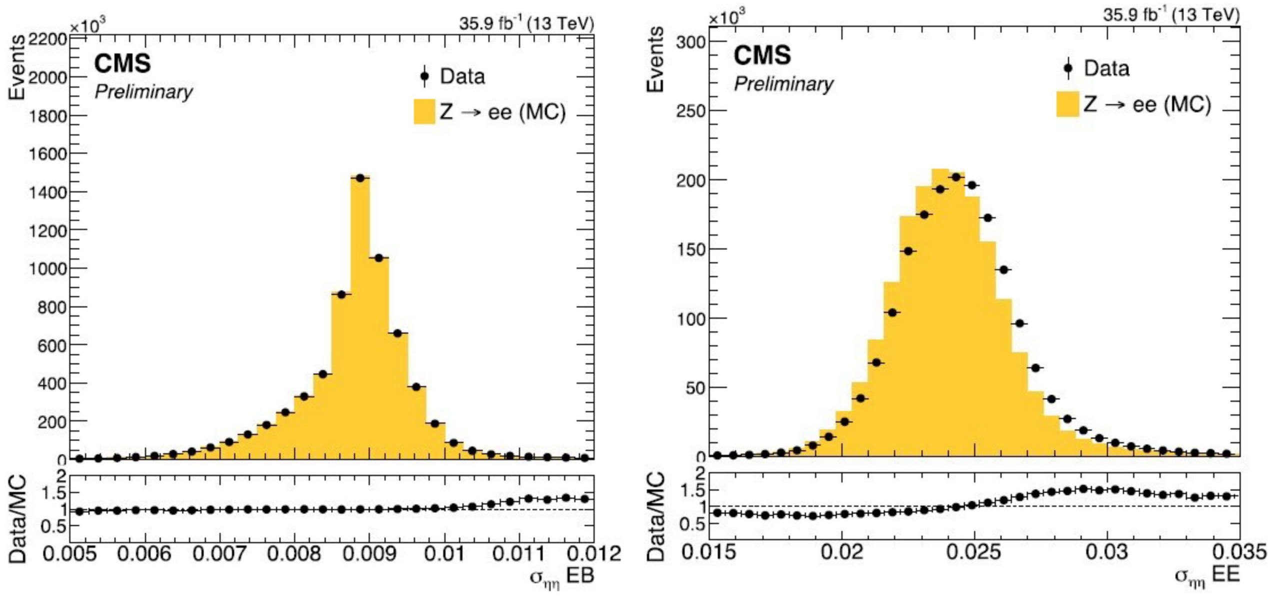


Figure 3. Crystal-based EM shower width from the CMS experiment in the eta direction in both the barrel and the endcap. Simulation and data are in good agreement in the barrel (figure on the left) but not in the endcap region (figure on the right) where there is more material.

- The models used to describe the *bremsstrahlung* process have also been reviewed for Geant4 9.5 allowing describe shower shape for CMS barrel (Figure 3). Recently an improved theoretical description of the Landau-Pomeranchuk-Migdal (LPM) effect was introduced which plays a significant role at high energies. We show in Figure 6 a comparison between the old (grey line) and improved bremsstrahlung implementations with respect to experimental data. The review of this model was beneficial and allowed excellent agreement with the data. Once again, these improvements were made without introducing any speed penalty. They are available with Geant4 10.3.
- The model describing the pair-production process has been reviewed. Similar improvements were introduced found in the LPM suppression functions. At very high energy improved pair production model shows a significant difference in the differential cross-section. The old implementation (green plot in Figure 7) was over-suppressing gamma conversion. In other words, the LPM effect was overestimated. There are currently no available experimental data for validation of our results. The use of the relativistic pair-production model is essential for accurate physics simulations for FCC.
- At extreme high energies (important for FCC studies), nuclear size effects become important. Different elastic scattering models with nuclear form factors taking into account finite nuclear size effects were developed. Figure 8 shows that the newly developed single scattering model agrees with experimental data at relatively low energy. Also at high energies, since precision becomes increasingly important, formfactor description may affect various EM processes. Such effects may be important for high energy muons, for shower shape, and for simulation of background for a dark matter search experiment.

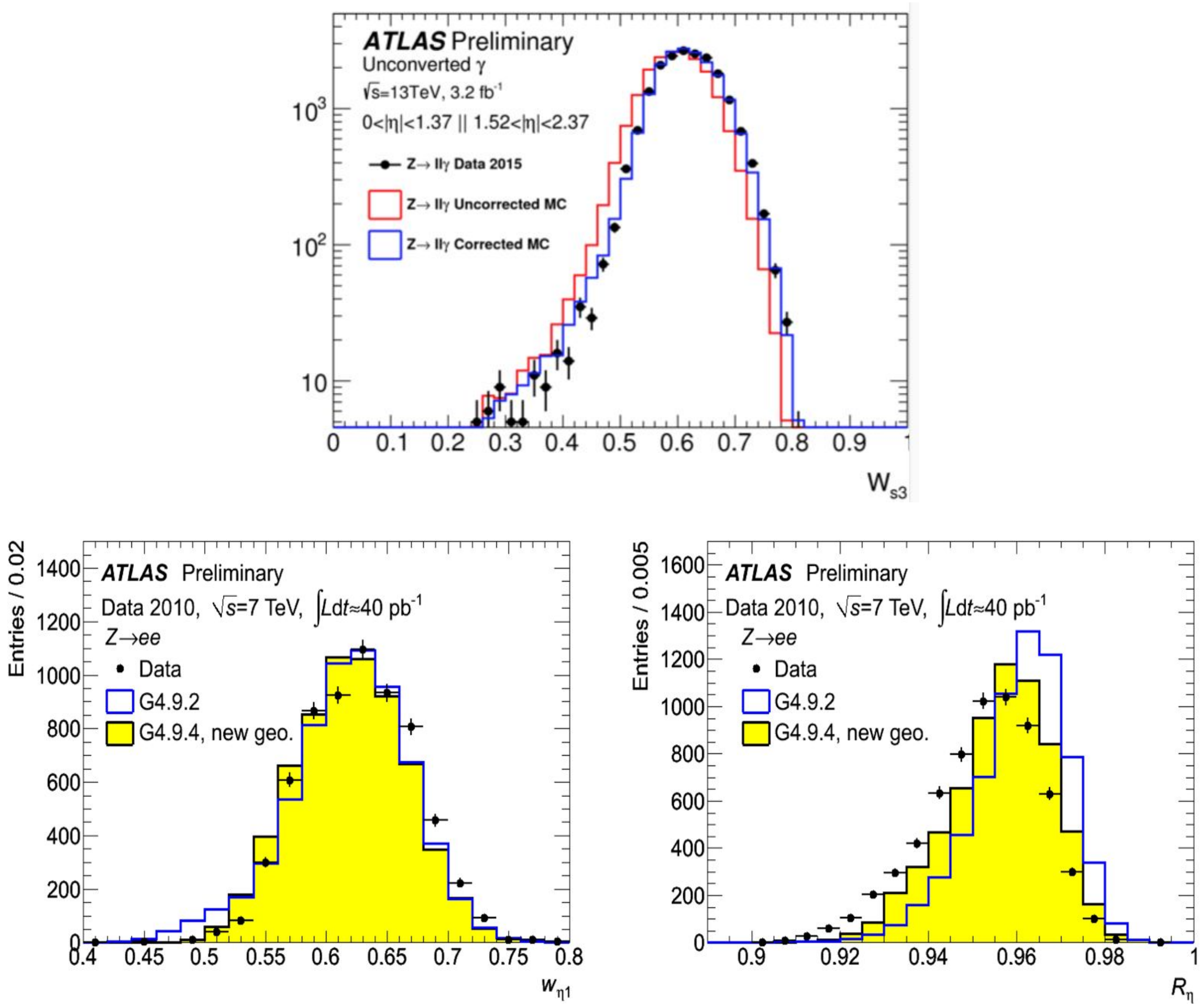


Figure 4. The upper plot plot shows a measurement of R_η *for unconverted photons in the ATLAS EM calorimeter, where* R_η *is the ratio of shower energy deposited in 3x7 cells to 7x7 cells in η-φ. The lower plot shows the lateral shower width,* $W_{\eta 1}$*, for electrons in the first layer of the EM calorimeter. Both plots show a clear discrepancy between real data and the results of MC simulation.*

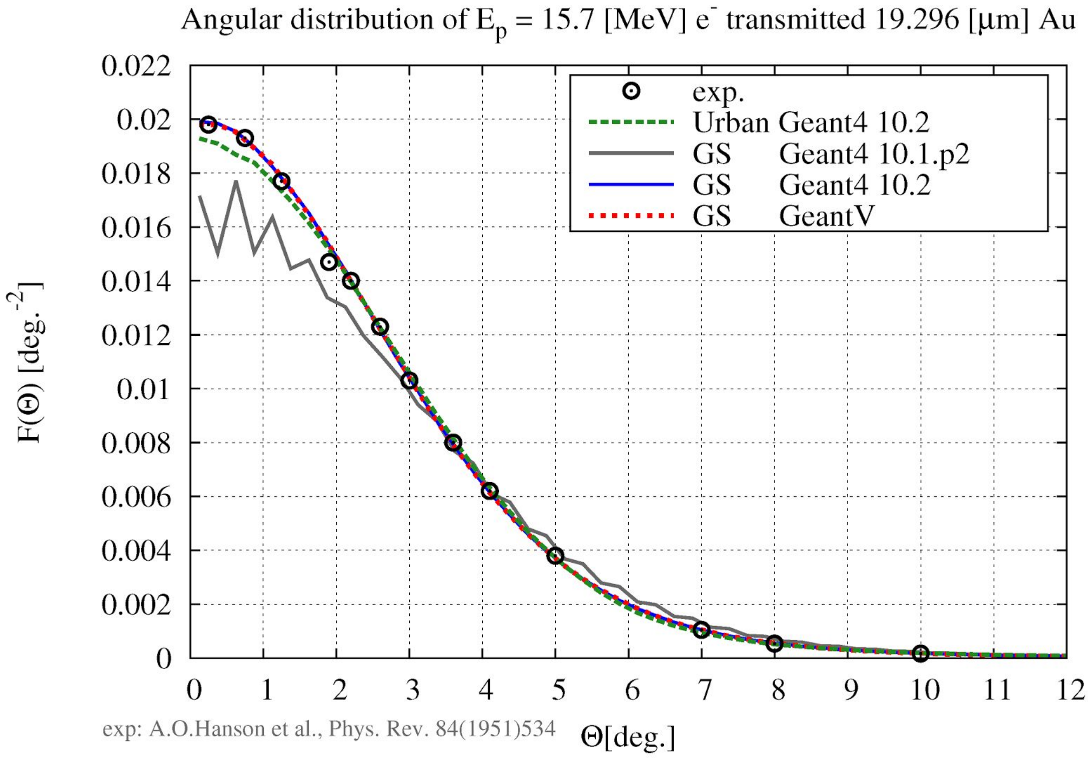


Figure 5. The new Goudsmit-Saunderson multiple scattering model implementation (GS - Geant4 10.2) shows no artefacts and excellent agreement with experimental data.

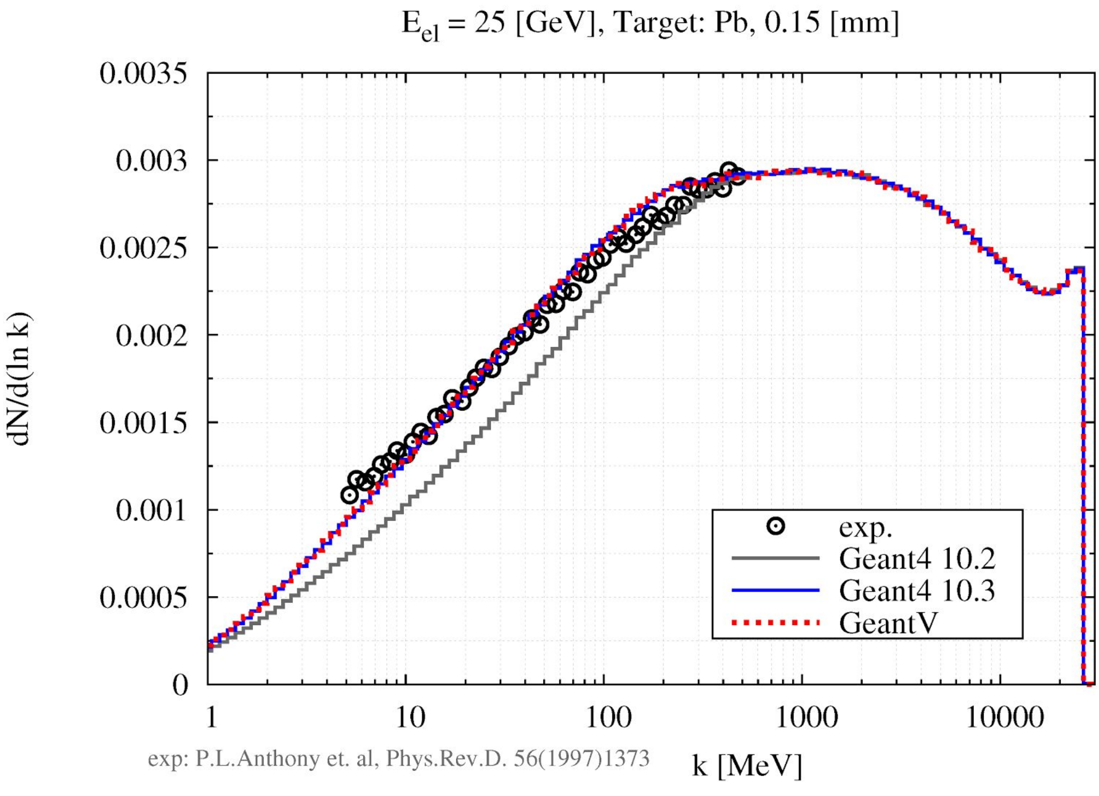


Figure 6. The improved bremsstrahlung model included in Geant4 10.3.beta and in GeantV shows better agreement with experimental data with respect to the existing implementation.

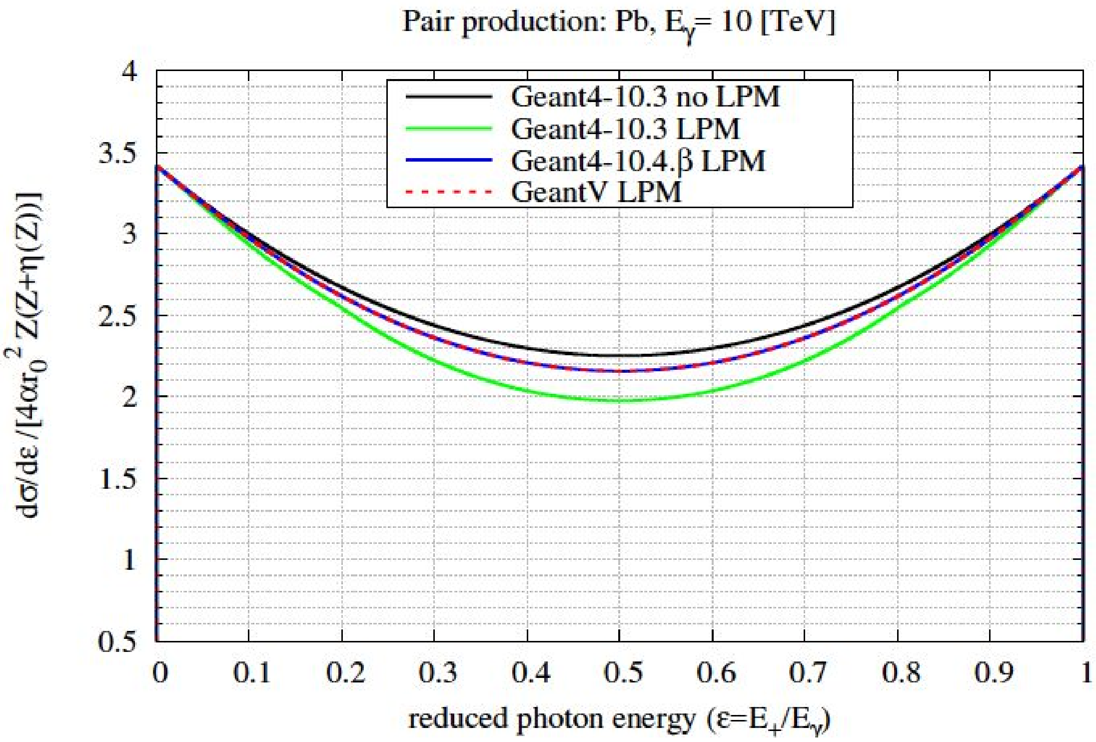


Figure 7. The improved pair production model included in both Geant4 10.4.beta and in GeantV is compared with the existing Geant4 implementation with and without LPM.

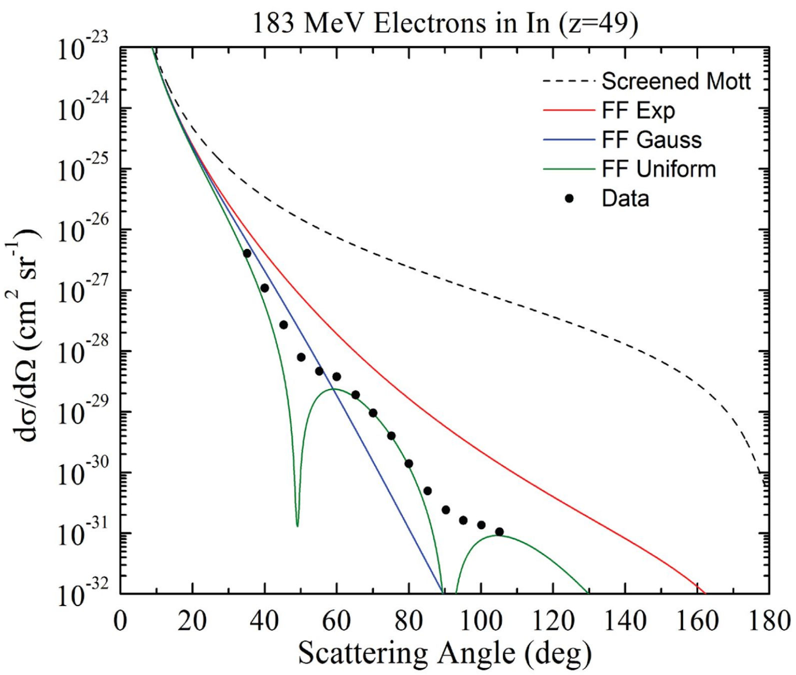


Figure 8. New models were developed in Geant4 taking into account finite nuclear size effect for elastic scattering of electrons at high energies.

Theoretical review of all electromagnetic models, including those of hadrons and ions is therefore of high priority both for HL-LHC and even more importantly for FCC studies. Efforts in this direction will continue, but completion of this task by 2025 will demand a substantial amount of work and continuous investments. Avenues that should be investigated include other channels that become important at extreme energies, such as triplet production taking into account nuclear recoil effects, size effects as well as γ conversion to muon and hadron pairs. Energy fluctuation models should be developed based on theory, not just parametrization. For Geant4 10.3 the upper energy limit for all EM physics models was extended to 100 TeV, that is important not only the HL-LHC programme but becomes crucial for the work being carried out in the context of the FCC detector design studies. At the same, further improvements for high energy EM models are possible. A substantial amount of work is needed for preparing simulations of next generation detectors. More personpower specialised in physics modeling would be required for the development and improvement of physics models to meet experiments needs.

7.2 Hadronic Physics

Hadronic physics simulation is loosely defined to cover any reaction producing hadrons in its final state. As such, it covers purely hadronic interactions, lepton- and gamma-induced nuclear reactions, and radioactive decay. In Geant4 the interaction is represented as a process which consists of a cross-section to determine when the interaction will occur, and a model which determines the final state of the interaction. Models and cross-sections are provided which span an energy range from sub-eV to TeV. More than one model is usually offered in any given energy range in order to provide alternative approaches for different applications. During the last several years, new models and cross-sections have been added to the toolkit, while others have been improved and some obsolete models have been removed.

it is not possible for a single model to describe all the physics encountered in a simulation due to the large energy range that needs to be covered and the simplified approximations that are used in hadronic models to overcome the difficulty of solving the full theory (QCD). A typical sequence of reactions may begin with a high energy hadron–nucleon collision within a nucleus (parton string model), followed by the propagation of the secondaries of the collision through the nuclear medium (intra-nuclear cascade model), followed by the de-excitation of the remnant nucleus (pre-compound model) and its evaporation of particles (evaporation and breakup models) until it reaches the ground state. Each of these stages is qualitatively different from the other. Wherever possible a theory-based approach to their implementation is followed as opposed to a phenomenological or parameterised approach. The main motivation is to have more confidence in the behaviour of the model outside the kinematic regions where it is validated and tuned with experimental data, and also to preserve the correlations between the different emitted particles.

Two models based on quark-parton concepts have been implemented in Geant4, the quark–gluon string (QGS) model and the Fritiof (FTF) model. There are also three intra-nuclear cascade models that are now offered: Bertini, Binary and INCL++. As of release 10.0, the toolkit provides nine reference physics lists whose names reflect the combination of models used to describe the hadronic interactions necessary for various applications over the whole energy range. Reference physics lists are extensively and routinely validated. Currently the most-used reference physics list for high energy and space applications is FTFP_BERT. It uses the Geant4 Bertini cascade for hadron–nucleus interactions from 0 to 5 GeV incident hadron energy, and the FTF parton string model for hadron–nucleus interactions from 4 GeV upwards. The letter P indicates that the Geant4 pre-compound model is used to de-excite the nucleus after the high energy FTF interaction has been completed. The FTFP-Bertini combination forms the backbone of many physics lists. It successfully extends the use of the string model at lower energies, down to 3 GeV, and at the same time the Bertini intra-nuclear cascade model has been validated up to 15 GeV. The net result has been that the need for using the LEP parameterised model at mid-range energies (around 10 GeV) has been eliminated. QGSP_BERT is a popular alternative which replaces the FTF model with the QGS model over the high energy range. It is important to note that the existence of more than one model (for each energy range) is very valuable in order to be able to determine the systematics effects related to the approximations used. The situation is similar to that of the Monte Carlo generators where the usage of different generators provides an assessment of the systematic errors.

Detector response is an effective test of any model combination. It is defined as the ratio of deposited energy visible to the detector, to the incident beam energy. For the above combination of models (as in the FTFP_BERT physics list), the general agreement between the simulated response and data for hadron-induced showers is at the level of a few percent. Other useful data, such as shower shapes and energy resolution are less precisely described and show agreement at a level of 10–20%.

The use of highly granular calorimeters such as the ones being designed by the CALICE collaboration for future linear colliders, allows a detailed validation of the development of hadronic showers with test-beam data. Preliminary results suggest that the lateral profiles of Geant4 hadronic showers are too narrow. Comparisons with LHC test-beam data have shown that a fundamental ingredient for improving the description of the lateral development of showers is the use of intermediate and low energy models that can describe the cascading of hadrons in nuclear matter and the subsequent de-excitation of the “wounded” nucleus. The longitudinal development of hadron showers mainly depends on the hadronic interactions at higher energies in the forward direction: quasi-elastic scattering and diffraction. An important effect recently introduced in Geant4 is the improvement of the neutron capture cross-sections and final state generator. Based on the high precision neutron library, it allows for an improved simulation of the time structure and the lateral profile of hadronic showers in neutron-rich materials [19]. Other recent developments include an improved and re-tuned Fritiof model.

The LHC experiments are preparing detector upgrades for PHASE 2 of the physics programme. For example, CMS will have a high granularity calorimeter replacing the endcap electromagnetic and hadron calorimeters. This will produce two main challenges. Firstly the EM calorimeter will be of sampling type and so the longitudinal shower profile becomes very important. Secondly, the sensitive detector elements will be a mixture of silicon and scintillators and some of them have hexagonal or half-hexagonal shape. This increases the complexity of the detector geometry and will present a new challenge for the CPU performance of the simulation code.

Work is ongoing to make a thorough review of the hadronics sector. Additional work is currently being invested in the further improvement of the QGS model, which is a more theory-based approach than the phenomenological FTF model, and therefore offers better confidence at high energies, up to a few TeV. This again is a large endeavour and requires continuous effort over a long time. Further extension of the coverage of hadronic interactions to higher energies, in the multi-TeV region, will be necessary for FCC detector simulation studies. Moreover, this would open a completely new domain of applications: the possibility to simulate very high energy cosmic ray showers in the Earth's atmosphere. The EPOS hadronic generator [20] offers currently the most accurate simulations in this domain, as a fresh C++ rewrite of the model, appears as a very interesting possibility for the future of hadronic simulations in high energy and cosmic ray physics.

For the intra-nuclear cascade models, while Bertini and Binary are likely to remain stable, further development is expected for the INCL++ model, besides the recent extension to higher energies (up to about 20 GeV). At the level of physics lists, the combined use of all the three intra-nuclear cascade models - choosing between them according to projectile hadron, projectile kinetic energy and target nucleus - will be explored to optimize physics accuracy or simulation speed.

Low-energy hadronic physics - pre-equilibrium, nuclear de-excitation and radiative decay models, as well as high-precision, data-driven transportation of low-energy neutrons and charged particles (deuteron, triton, He3 and alpha) - is and will remain a particular active area of development, mostly driven by medical and nuclear physics applications.

The way hadronic cross-sections are implemented is critical for the CPU performance of hadronic physics simulations and there are on-going efforts to review them and make them more efficient via the development of a common GeantV / Geant4 module. Total, inelastic and elastic cross-sections for hadron–nucleus, nucleus–nucleus and antinucleus–nucleus reactions are provided which cover energies up to TeV in some cases. Proton-, neutron- and pion-nucleus cross-sections at low to medium energies have been available in Geant4 since its beginning. Recent work has focused on development of cross-sections for other projectiles and at higher energies. The general behaviour of the optical models is to predict constant cross-sections for very high energies. However, experimental data show a moderate relativistic rise of hadron–nucleus cross-sections. For this reason the Glauber model is being used to describe hadron–nucleus cross-sections in the high energy region (above 90 GeV). The current implementation of this model is under review with a view to re-implementing it.

The above, ambitious program of development for the simulation of hadronic physics relies heavily on an updated, extended, robust and automated validation test-suite. Plenty of work has been done in the recent past in this direction, but a lot more remains to be done. In particular, a well-defined procedure to tune hadronic models needs to be defined and deployed.

7.3 Physics Modelling for the Intensity Frontier

Much of the text above concentrates on physics processes relevant to the LHC experiments. Much of this overlaps the needs of muon and neutrino experiments as well as dark matter and rare-decay experiments, which have typically used Geant4 physics lists tuned based on LHC requirements. But as the precision needs of these experiments increase, they increasingly need simulations responding to their particular needs, which vary significantly by experiment but broadly speaking are precise simulations of hadrons and electromagnetic particles from a few GeV to a few MeV. Precise neutron simulation is particularly critical for accelerator-based neutrino experiments that must reconstruct neutrino energy from final state particles. Also a radioactive decay model for modelling the decay chain of isotopes is essential for background studies.

Major components of the intensity frontier over the next decade will include liquid Argon TPC detectors and liquid Xenon calorimeters. Efforts to address common needs of the liquid Argon experiments including the post Geant4 phase of simulation are undertaken in projects such as LArSoft[21] and Qscan[22], while extending Geant4 EM physics models for liquid noble gases is undertaken by the NEST project [23]. Detectors with large numbers of wires and photo-sensors may naturally lend themselves to parallelization techniques, provided that the simulation frameworks are able to handle such cases in an efficient way. Additionally, the Wire Cell Toolkit [24] provides simulation, noise filtering, signal processing and reconstruction algorithms for LArTPC detectors. It includes experimental support for parallel processing following the data flow processing paradigm. More work and input from parallel processing experts is needed to bring this support to maturity.

Data-taking at current experiments, such as MicroBooNE, will greatly inform the simulation needs of the Intensity Frontier (IF) community moving forward. This might be most relevant for LArTPC technology as it is the newest and least familiar. For example, if significant non-uniformity of purity in data is observed in MicroBooNE, simulation of non-uniform purity will be a high priority simulation need of future LArTPC experiments.

Efforts are also underway to improve the accuracy of Geant4. While much of this effort was motivated by requests from Intensity Frontier experiments, especially the variation of the model parameters, it will be of use to the entire HEP community. This work includes:

- Validation of models: a validation database known as DoSSiER [25] that contains data from experiments measuring particle cross-sections (e.g. NA61) is being developed. It was started as a Geant4 project, but is now also used by GeantV and should be suitable for other MC toolkits such as e.g. GENIE [7].

- Development of new physics lists: Geant4 physics lists utilized by IF experiments were originally designed to meet the needs of LHC experiments. For example, a “Shielding” physics list was originally configured for radiation shielding studies and cavern background simulations for LHC experiments, but it is now widely used by underground dark matter experiments such as CDMS and LZ. A variant of this Shielding physics list (ShieldingM) was created to address the needs of Mu2e. Geant4 physics lists tailored for LHC were not adequate to the generation of neutrino beams, they disagree with existing hadron-production data by up to 40% in some areas of phase space. In light of this, a new physics list (“NuBeam”) has been created, aimed at meeting the specific needs of neutrino beam simulations.

- Variation of model parameters: Equally as critical as having an accurate beam or detector simulation is having an ability to quantify that accuracy. Neutrino experiments go to great effort to estimate and propagate uncertainties on Geant4 models to physics measurements.This is currently done experiment-by-experiment, but an initiative within Geant4 was recently begun to provide methods of assessing model parameters. Additionally, procedures are being developed to modify model parameters and compare with data, with the aim of producing uncertainties and covariance matrices on these parameters that can then be propagated to physics measurements.

7.4 Non-HEP use-cases

The extensibility of Geant4 has been appreciated also outside of the HEP domain and several applications and extensions have been created to perform simulations in some additional domains. It is worth to mention:

- Crystal extensions to model the property of crystalline structures. Applications include the use of bent crystals for beams manipulations, phonons and ultra-cold neutrons beams [26].
- Geant4-DNA: a Geant4 extension for the calculation of physico-chemical damage to DNA at a nanoscale level [27]

7.5 Radiation and Non-Collision Background Modeling

The LHC experiments have made use of the FLUKA simulation package, and to a lesser extent GCALOR and MARS, for modeling of the radiation backgrounds, primarily of low-energy neutrons and photons, present during and after the running of the LHC. Understanding these backgrounds is critical for estimating the required radiation hardness of on-detector electronics, for developing shielding that might reduce non-collision backgrounds in the detector, and for evaluating radiation safety procedures when servicing or upgrading the detectors. The FLUKA simulation package provides excellent modeling of these backgrounds, but to date has not been used for any significant high-energy collision modeling by any of the experiments. While its maintenance and continued functionality is critical for the future of the LHC experiments and for the development of the next generation of experiments, improvements in both performance and physics are not as critical as they are in the case of Geant4.

8. Software Performance

Simulation, including physics generation, interaction with matter (detailed analogue or parametrized simulation), digitization, reconstruction and analysis takes a large fraction of the computing resources utilized by HEP experiments. Depending on the experiments, and the complexity of the detectors, each of these components of the simulation chain contribute with different weights to the total. Setting aside the reconstruction of simulated events, the modeling of the interaction with matter is the most expensive module of a simulation application, as is certainly the case for the LHC experiments. Neutrino detectors are typically simpler, with a larger fraction of resources spent in the simulation of the readout. Physics generation usually takes the smallest fraction, except when generating signal samples that require a scan of large regions of theory parameter space or for cutting edge, high-accuracy calculations that are now becoming possible with new event generation tools.

As an illustration of the above, the CMS experiment, from start-up in 2009 through May 2016, the full simulation chain including all elements described above took 85% of the total CPU time utilized by the experiment, while the Geant4 module took about 40%. This information was obtained from the CMS Dashboard, which is a computing information monitoring source available to CMS members. The rest of the CPU cycles were primarily used to reconstruct and analyze real collider data. The assumption for the 85% figure is that the analysis of simulated data consumes 75% of the CPU time spent in analysis, including both simulated and real data, and excludes the generation of signal samples for BSM searches. The reason why the analysis of simulated data takes a larger fraction of the total analysis CPU time than the analysis of real collider data is that the design and optimization of the measurements, as well as the development and validation of data-driven methods, are all based on MC samples.

An analysis of jobs running on both the grid and on HPC systems in ATLAS, between July 2015 and July 2016, showed similar results with simulation utilising 65% of the total time available to the experiment. The breakdown shows that Event Generation (Evgen) took 25%, thanks to a big burst of Mira throughput, whilst Full Simulation (Geant4) took 39% and Fast Simulation (Atlfast-II) just 2%. In addition, Event Reconstruction of data and simulated events took 19%, whereas the production of derived datasets for use in analysis took 5% and user-level Analysis took 10% .

For comparison, the Geant4 module of the ALICE full simulation application takes 55% of the total detector simulation CPU time, excluding event generation and reconstruction, while digitization takes 35% of the time.

Although neutrino experiments are similar to LHC experiments in the fraction of computing resources used for simulation, NOvA spent 70% of their CPU cycles on simulation in 2016, the total amount of computing resources utilized by this experiment is two orders of magnitude less than those spent by CMS.

The main drivers of the need to improve computing performance in the next two decades are therefore the LHC experiments. It is expected that their computing needs will increase by a factor of 10 to 100 in the High-Luminosity LHC (HL-LHC) era depending on the solutions developed to face simulation, pileup, and reconstruction challenges arising from the high-luminosity environment. The challenge is daunting and the need to explore both evolutionary and breakthrough solutions through R&D programs to speed up simulation and reconstruction is essential. Computing needs of neutrino and muon experiments is expected to be a small fraction of that of the LHC experiments, but will grow substantially with time as more experiments come on-line and existing experiments accumulate data. These experiments will therefore need to make use of the solutions developed for the LHC.

The Geant4 Collaboration has invested significant effort into improving the toolkit computing performance in the past decade, as code was reviewed and optimized. In 2013, the release of event-level multithreading capabilities in Geant4 brought significant memory savings, as illustrated in Figure 10, which shows the CPU time (top) and memory (bottom) consumption of a simplified CMS standalone simulation application, based on Geant4 version 10.3.p01, runs for 50 GeV pions. Geant4 achieves almost perfect strong scaling (top plot) with the number of available cores (57) and still gains about +30% in hyperthreading regime [29,30]. The large memory reduction obtained with multi-threading is clearly visible (bottom). While a multi-process approach can reach the O(10GB) memory consumption with a relatively small number of threads (Geant4 version 9.6), it is only with a well designed multi-threading approach, which shares the read-only data among threads, that it is possible to run with the maximum number of threads remaining in a memory budget of approximately 1 GB. Recent versions of Geant4 has put emphasis on further reducing memory consumption to the current level of about 10MB needed for each additional thread.

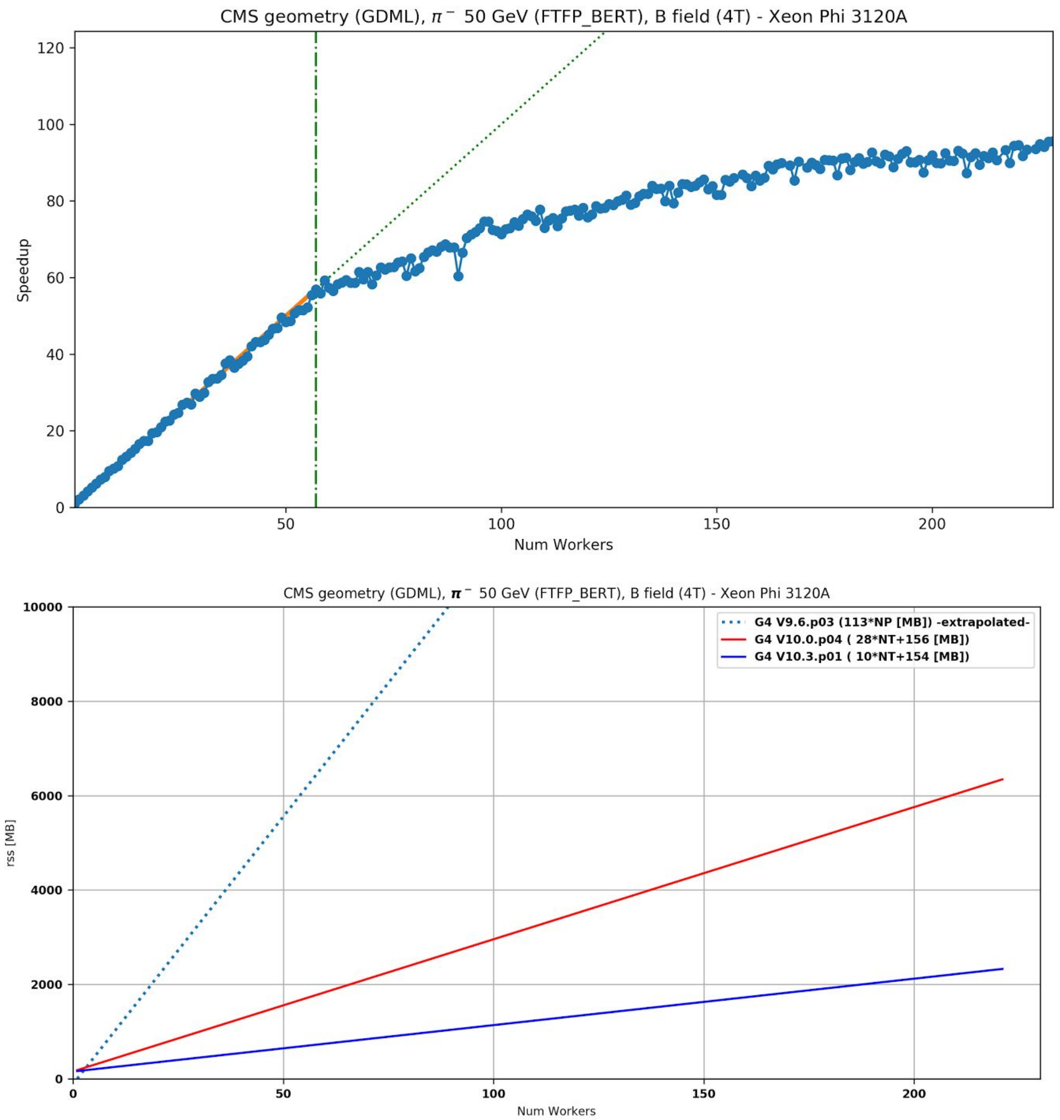


Figure 10: CPU time (top) and memory (bottom) consumption of a CMS standalone simulation application, based on Geant4 version 10.3.p01, run for 50 GeV pions. The strong scaling (top) as a function of the number of threads shows an almost perfect linearity (>90%) with the number of physical cores. The maximum number of cores (57) is denoted by the dot-dash vertical line. The use of hyper-threading improves the throughput by about 30%. The use of multi-threading allows optimal use of the limited memory budget of many-core systems. With multi-process approaches (Geant4 9.6.p03 and 10.0.p04 sequential) it is possible to use only a very limited set of the available parallelism. With multithreading the memory requirements are reduced by a factor 10.

Figure 11 shows the percentage change in CPU time performance taking Geant4 version 10.0 as a reference, starting with Geant4 version 9.4.p02 (2010) and ending with Geant4 version 10.2 (2015) for the standalone CMS application and a simple calorimeter configuration made of Cu-Scintillator in a 4 Tesla magnetic field [29].The study is performed for 50 GeV e^-, p^-, and protons, as well as for H → ZZ events. On average, the time performance improvement through the life of the LHC experiments (2010-2015) is of the order of 35%. All tests were performed on the same hardware

(AMC Opteron 6128 HE @ 2 GHz) using the same compiler and operating system (GCC4.9.2, Linux x86_64). Remarkably, the percentage time performance improvement during the period of time shown in the plots is in double digits, even as the physics models were improved significantly for accuracy, something that typically comes associated with a time performance penalty. Although CPU profiling is a good starting point to improve time performance, the biggest gains in Geant4 were achieved while focusing on reducing the memory usage. Important speedup was obtained as a direct result of both reducing the memory churn and improving the physics algorithms. For example, the rewriting of the Bertini physics model code yielded a reduced memory churn, making it substantially faster.

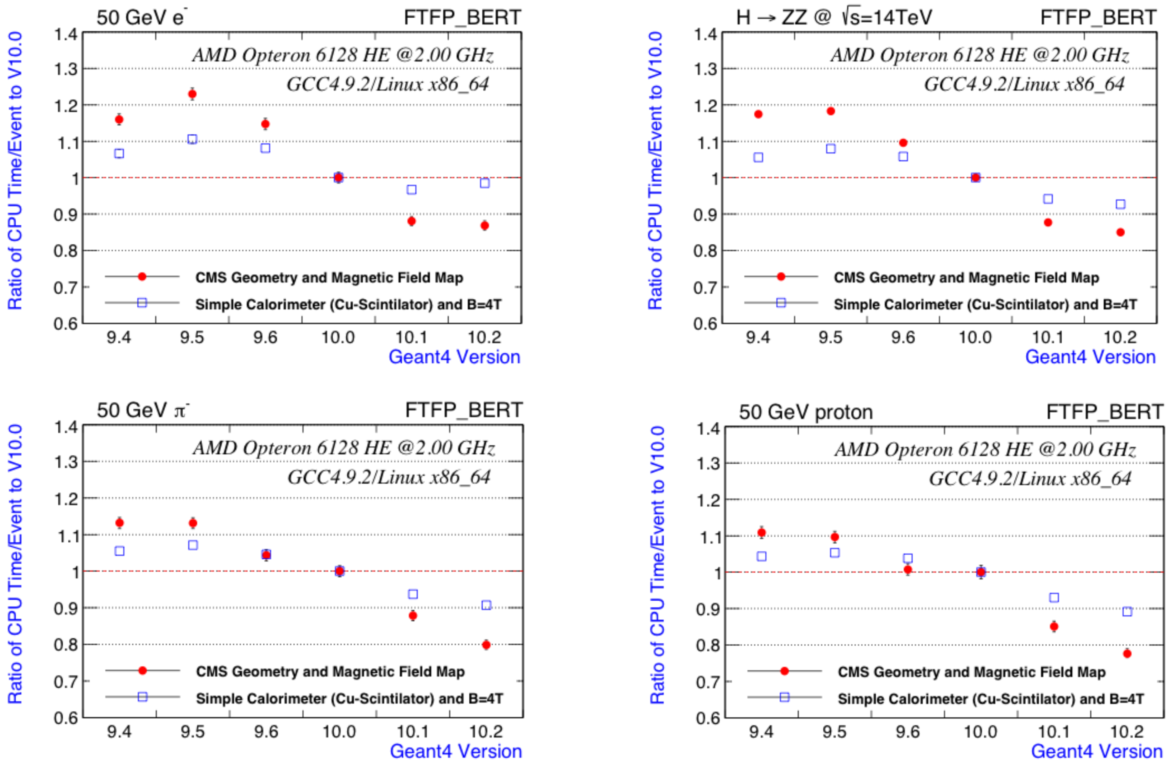


Figure 11: Percentage change in CPU time performance taking Geant4 version 10.0 as a reference, starting with Geant4 version 9.4.p02 (2010) and ending with Geant4 version 10.2 (2015) for the standalone CMS application and a simple calorimeter configuration.

Evolving compilers also offer opportunities for speed gains in simulation applications. Figure 12 illustrates the impact of the use of shared and static libraries in a simplified CMS application (HepExpMT public benchmark) [31]. In this example, static linkage yields a 20% gain, while Profile-Guided Optimization (PGO) gives another 20%. Multithreaded applications benefit more from static linkage and PGO, larger speedups as the number of threads increase. These options are particularly interesting because they do not change the physics output of the simulation. If this constraint can be relaxed additional speedups can be obtained using additional Geant4 flags to speedup the simulation.

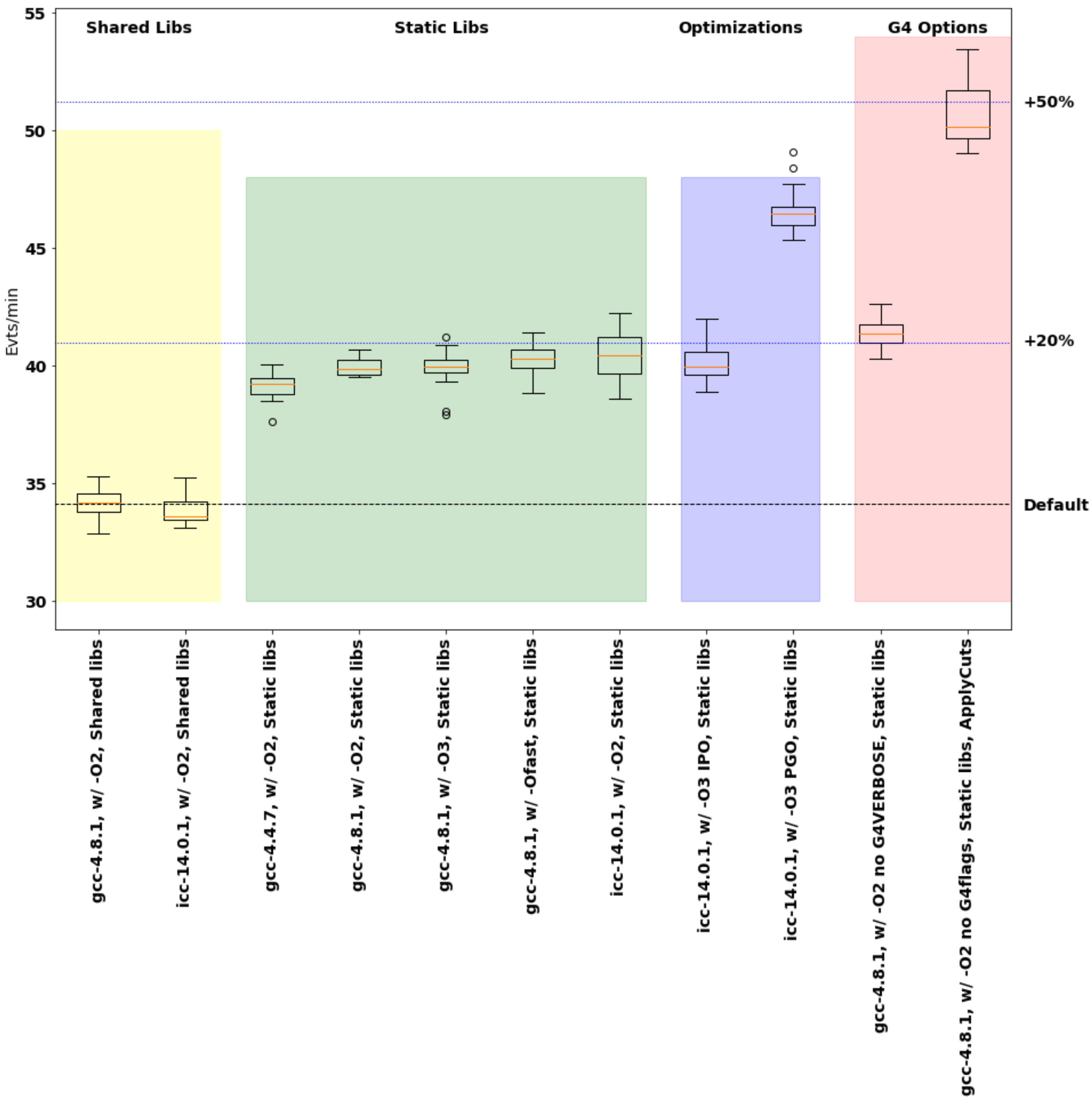


Figure 12: Impact of the use of shared and static libraries in a simplified HEP application. Results obtained with a simplified version of CMS with Geant4 version 10.0. Performances for different combinations of compilation options are compared. There is an important performance boost when using static builds (+20%), the main reason being the lack of PLT calls. Another +20% can be obtained using Profiler Guided Optimizations (PGO). These techniques do not change the physics output of the simulation, if this constraint can be relaxed compilation and runtime options of Geant4 can be used to obtain another +10% speedup.

In the following sections, we will discuss computing performance studies by different HEP experiments, as well as their diverse approaches to improve computing performance.

8.1 CPU Time and Memory Performance Measurements

The largest improvements to computing performance experienced by ATLAS and CMS have come from physics code reviews as part of the effort to reduce memory churn. The speedup has been a side effect of this effort. The lesson learned is that profiling is not a very useful exercise unless it is related to physics observables. The table in Figure 13 shows the number of Geant4 steps in each ATLAS sub-detector and for each particle type, providing useful quantitative information to optimize Geant4 tracking and therefore improve time performance. It is apparent that most of the steps occur in the forward and EM calorimeters, for electrons, photons, and neutrons. Based on the experience described above, the Geant4 Collaboration is developing a tool to monitor the number of steps and tracks, and the time spent in a given detector element. The tool will also provide this information for each Geant4 track in user defined energy ranges. The output will be displayed in the console, or saved in histograms or ntuples.

Number of G4Steps Units in 10^6	e^-	e^+	Photon	$\pi^\pm$	Proton	Neutron	Other	Total (%)
Px	2.32	0.24	2.37	0.68	0.14	0.30	0.21	0.3%
Sct	2.42	0.37	6.52	0.82	0.20	0.89	0.25	0.6%
Trt	5.37	1.05	40.20	1.82	0.50	5.46	0.53	2.9%
Sev	49.88	7.35	40.63	0.42	0.35	3.82	0.46	5.4%
Cry	48.92	6.48	49.01	0.34	0.40	7.38	0.41	6.0%
Pre	3.99	0.49	10.41	0.09	0.06	1.73	0.03	0.9%
EMB	79.94	11.76	66.26	0.74	0.56	32.59	0.38	10.2%
EMEC	137.13	22.73	114.97	1.34	1.03	63.34	0.65	18.1%
HCB	10.10	0.96	14.88	0.14	0.18	11.46	0.25	2.0%
HEC	17.49	1.67	23.01	0.23	0.30	20.79	0.58	3.4%
FC1	303.56	31.82	204.14	1.79	1.61	64.26	0.80	32.2%
FC23	90.15	13.18	42.67	0.91	0.83	87.99	0.72	12.5%
FCO	10.23	1.46	3.80	0.10	0.12	1.01	0.03	0.9%
LAr	2.50	0.25	2.97	0.06	0.11	0.54	0.05	0.3%
Mu	31.85	4.34	22.09	0.11	0.23	4.25	0.50	3.4%
Other	4.89	0.86	10.13	0.13	0.11	1.05	0.04	0.9%
Total (%)	42.4%	5.6%	34.6%	0.5%	0.4%	16.2%	0.3%	100%

Figure 13: Number of Geant4 steps in each ATLAS sub-detector and for each particle type. The sub-detector types are: Px (pixel tracker), Sct (strip tracker), Trt (straw-tube tracker), Sev (tracker services), Cry (calorimeter cryostat), Pre (calorimeter presampler), EMB (EM barrel calorimeter), EMEC (EM endcap calorimeter), HCB (hadronic barrel calorimeter), HEC (hadronic endcap calorimeter), FC1 (forward calorimeter EM module), FC23 (forward calorimeter hadronic modules), FCO (other parts of the forward calorimeter), LAr (other parts of the liquid argon calorimeter system), Mu (muon system), and other (those not otherwise accounted for).

Figure 14 shows a chart of CPU time for the G4 module of the CMS full simulation application [32]. About 60% of the time is spent on functions associated with the propagation of particles through the detector geometry and magnetic field, while about 15% is spent on EM physics, and about 10% followed by hadronic physics. Figure 15 shows the CMS throughput and memory per event utilization for QCD and ttbar simulated events [32]. Maximum CPU efficiency is achieved after simulating about 500 events, when contribution of initialisation of Geant4 and CMSSW become negligible.

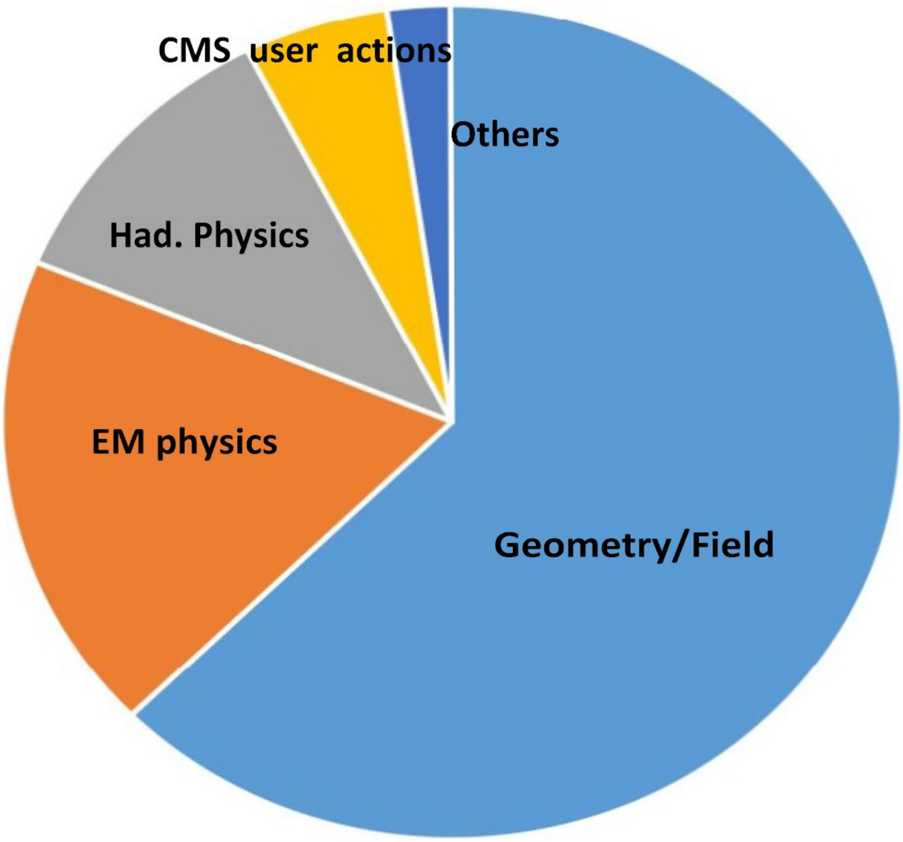
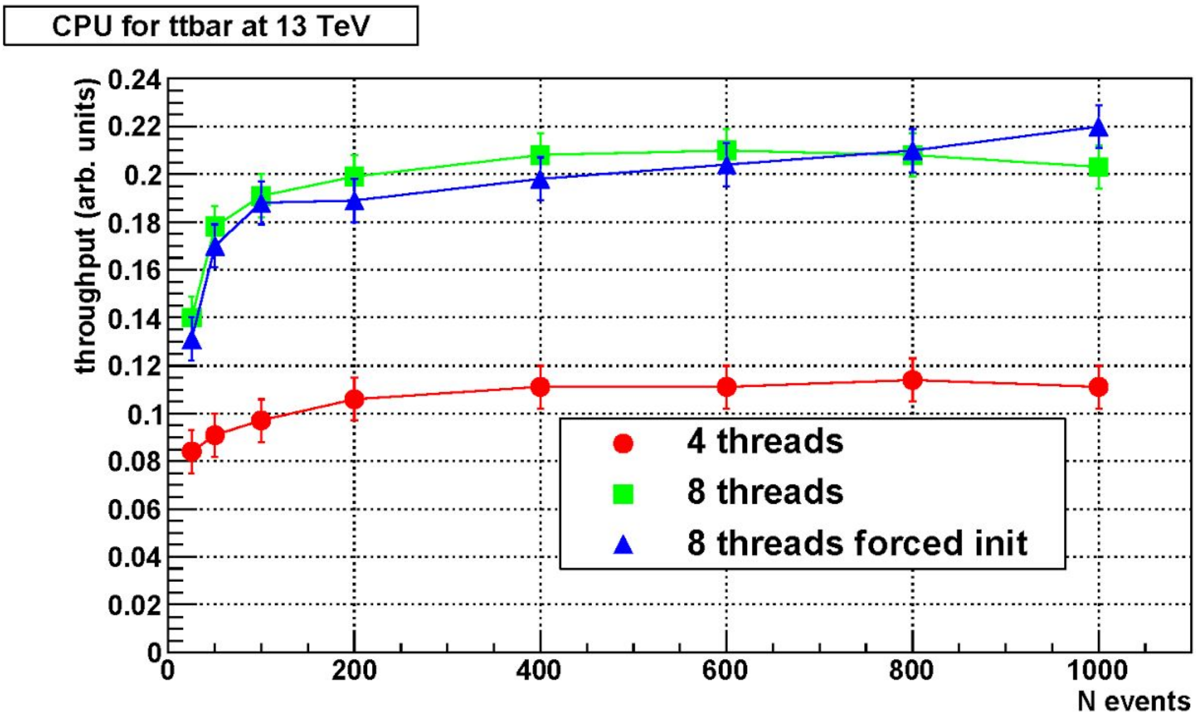


Figure 14: Chart of CPU time spent in different tasks of the CMS full simulation application for Run-2 simulation



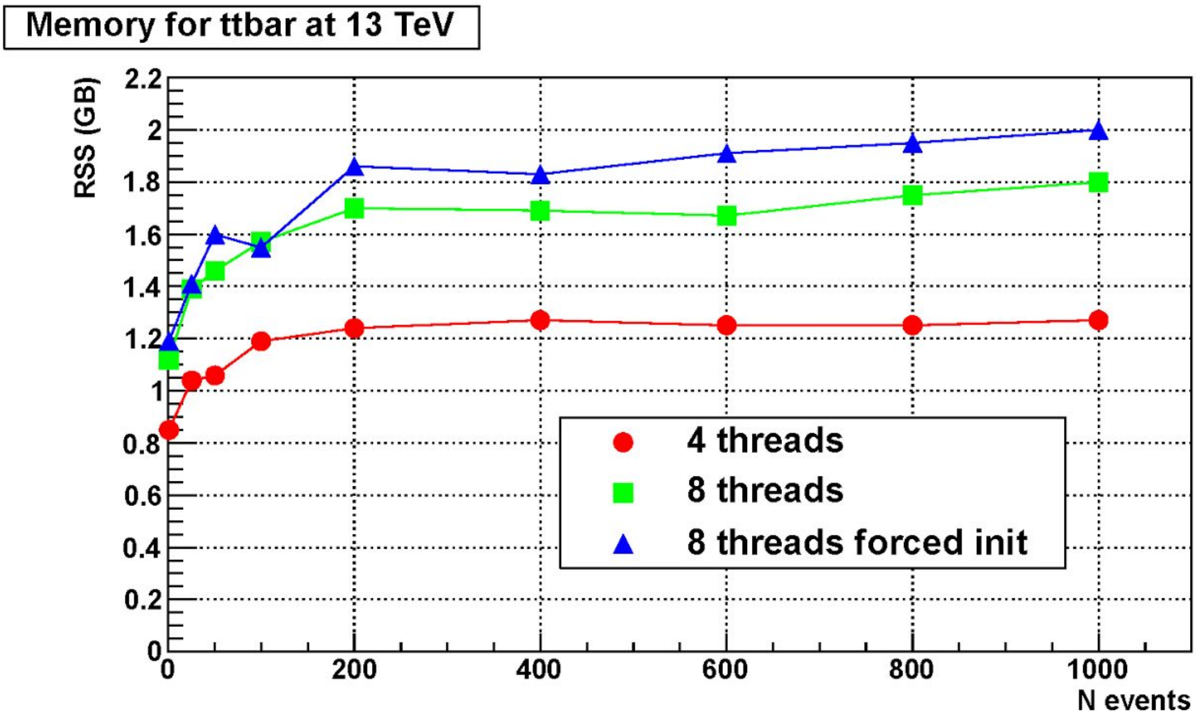


Figure 15: Throughput and memory per event for ttbar simulated events in CMS as a function of the event number. The version of Geant4 is 10.2p02, run in multi-threaded mode with 4 and 8 threads. Forced init refers to the case when all data for photon evaporation is read at initialisation time.

Optimizing particle production cuts and replacing particle showers in detectors with pre-generated showers or parameterizations are also part of the strategy to improve computing performance. Both ATLAS and CMS have these “frozen showers” or “shower library” options, particularly to replace full simulation in the forward calorimeters. GFLASH [33], a Geant4 module for the fast simulation of electromagnetic and hadronic showers using parameterizations for the longitudinal and lateral profile, is not used at the moment due to the peculiarities of the ATLAS accordion calorimeter and the limitations of this approach to model longitudinal shower leakage in the CMS calorimeters.

Geant4 offers the option to utilize the “Russian Roulette” technique (see Sec. 10.1) to kill N-1 out of N particles within an ensemble of neutrons and gamma below few MeV thresholds inside calorimeter geometry regions. The surviving particle is assigned a weight of N. The use of this technique by the CMS experiment yields significantly CPU time savings as discussed in Sec. 8.2.

8.2 ATLAS and CMS

Given that ATLAS and CMS are expected to be the largest consumers of computing resources a decade from now, the two experiments have decided to develop a computing performance assessment program that includes the Run 1 and Run 2 detectors as a reference, the different HL-LHC detector scenarios to predict future needs, and an evaluation on how much can be gained by utilizing state of the art techniques, such as re-optimizing simulation parameters and replacing Geant4 showers with libraries of frozen showers. Towards that end, ATLAS and CMS agreed on a set of simulation configurations and physics input samples:

- Machine: olhswep16.cern.ch (CERN’s OpenLab), one thread runs
- Compiler: gcc 6.3
- Geant4: version 10.2, FTFP_BERT physics list
- Pythia [34] events: 13 TeV Pythia minimum bias (300 events) and ttbar (300 events), pseudo rapidity cut $|\eta|<5.5$
- Particle gun: 50 GeV e’s, muons, pions with a flat η,φ distribution in $\eta=[-0.8,0.8]$, $\eta=[2,2.7]$, and $\varphi=[0,2\pi]$
- Geometry: 2015 or 2016

From this reference configuration, various options are incorporated to study the impact on time and memory performance, including Russian Roulette, shower libraries, timing cuts, and particle production cuts per region. For the reference configuration, each experiment uses its own timing and production cuts, as well as its own choice of stepper and tracking parameter values. The experiments also study the evolution of the time and memory performance of the full simulation application as the detectors are upgraded from the Run 1 and Run 2 configurations to several potential HL-LHC configurations.

The differing structures of the ATLAS and CMS detectors means that even in stand-alone Geant4 the simulation times are very different. Different detectors imply different CPU demands. This is clearly demonstrated by the information from CMS in Table 1. This shows the CPU time and memory measurements for different CMS HL-LHC candidate detector configurations with respect to the 2015 reference geometry. HL-LHC CMS configurations demand 28-36% more CPU cycles than 2015 or 2016 configurations to simulate minimum bias events, while they require 57-65% more for ttbar events. Given that the physics of the simulation at the core of the CMS HL-LHC upgrade, the High Granularity Calorimeter (HGCAL), is still not fully validated awaiting further test beam experiments, new physics accuracy requirements might push the CPU needs higher. The reason is that the HGCAL is a significantly more complex apparatus than the current detector using different technology and materials, covering the [1.5,3] pseudorapidity range, consisting of 40 layers of silicon and copper/tungsten, brass, or steel, with a total of 6 million channels with cell sizes of 0.5 cm^2 and 1 cm^2. Owing to much more modest detector revisions, the difference in simulation performance for the current Run 2 and upgraded ATLAS detector is 5% for ttbar events and 15% for minimum bias events. This is simply a reflection of the geometry differences in the inner detector and muon system, in the case of ATLAS, and no additional penalty is expected from significant revisions to physics models.

Tables 2, 3 show the CMS time performance of the Geant4 module of the full simulation application, that is excluding physics generation, digitization, and reconstruction, for the default configuration and several options to reduce CPU time consumption in production of Pythia [34] generated minimum bias and ttbar events. Table 2 lists the individual impact of each of the options, while Table 3 shows the cumulative effect. The conclusion is that small gains may be achieved by utilizing static libraries and by re-optimizing timing or particle production cuts. In the CMS simulation Geant4 time cuts and tracking cuts are optimized per detector region. The cut in range value for the production of secondary particles is 1 mm in the electromagnetic and hadronic calorimeters, 0.01 mm in the pixel detector, 0.1 mm in the strip tracker, 0.002 mm in the muon sensitive volumes, and 1 cm in the support structures. The propagation time cut is 500 ns. The tracking cut is applied for charged particles below 2 MeV inside the vacuum chamber to avoid looping electrons or positrons. The Russian roulette technique applied inside calorimeter regions gives a 33% speedup and is already utilized in current detector configurations for Run-2, as is also the case of the HF shower library, which yielded a 68% gain in time performance. Additional CPU time savings are achieved by optimizing parameters associated with particle tracking in EM fields and production of secondary particles.

Tables 4 and 5 shows the relative CPU performance of a number of configurations of the ATLAS simulation application. The largest gain comes from introducing shower libraries in the forward calorimeter, which comes at a cost of 430MB of VMEM per job. No other option applied here has an appreciable effect on memory requirements of the application. The neutron time cut shows only a small CPU improvement, but was shown to reduce the size of the output file by almost a factor of two in previous tests. This file size issue can also be mitigated by various approaches to hit storage, however. Removing range cuts decreases the simulation time per event, because the thin volumes of the sampling calorimeter demand a tighter range cut, including 30um in the forward calorimeter and 300um in the EM calorimeters, to provide an accurate physics description. This penalty is not present in the CMS simulation, since the CMS EM calorimeter has much larger active volumes. Still, the effect of range cuts on the two applications is similar.

Having exhausted the most obvious optimisations, CMS is exploring various opportunities to improve computing performance in various ways e.g. by testing the newest Geant4 versions, by using the most advanced compilers, and by implementing an energy dependent “smart tracking” algorithm for propagation of particles in EM fields. However, the biggest gains will most probably come from ongoing R&D efforts, such as the vectorized geometry library, VecGeom, which was recently released for use with Geant4. Although VecGeom is optimized for GeantV, where it promises a significant speedup by benefiting from data locality and SIMD vectorization, preliminary tests with Geant4 in CMS give a 5-10% time performance gain coming from improvements in the geometry algorithms. In other words, although VecGeom can only be run in scalar mode with Geant4, it still delivers significant time performance gains. The GeantV project will offer more opportunities in the future, with the possibility of integrating navigation and EM physics libraries to the Geant4 CMS simulation application. The promise of a factor of 2-5 time performance improvement using GeantV's full track-level parallelization approach and SIMD vectorization is very enticing, and plans are being made for a potential migration within the timeframe of the start of the HL-LHC run in 2026, if the GeantV computing performance targets can be met.

ATLAS is also exploring a number of technical and physics options to improve simulation performance. Several of these options were delayed in order to complete a migration to a new multi-threading friendly infrastructure and to use a cmake build system. Russian Roulette for neutrons and static library building are both currently being explored, and it is expected that PGO will be investigated after those are complete. Some further optimization of range cuts is to be validated in order to gain a few percent of CPU performance. ATLAS has also investigated the new geometry modules available in the Geant4 10.4 beta release and found in some cases significant CPU improvements resulting from these (5%-level). They are expected to be validated and moved into production soon. VecGeom will be investigated as well.

When considering which optimizations to implement (or even the order in which they should be attempted) the total amount of effort required to bring each one into production should be taken into account as well as the overall impact on resource requirements.

An assessment of the effort required, in addition to the obvious cost of how much person-power is required to implement an optimization, should also include how complicated it is to validate. For example static compilation of Geant4 should come with no change in physics, so it is easy, in principle, to validate. Conversely changing range cuts will very often change the physics and so will require a lot more careful examination by a larger group of experts before it can be signed off. A modest CPU improvement may not be worth the risk of reproducing a large Monte Carlo dataset if a problem is found with the physics of the simulation.

When making an assessment of the overall impact on resources, the potential gains in CPU usage and potential reductions in disk usage should be considered along side other potential issues. For example, if samples simulated with the new optimization cannot be combined with older samples, then a new simulation campaign with new calibrations might be required to benefit from the new optimization.

	Minimum Bias		Top Pair	
	CPU Time	Memory (RSS)	CPU Time	Memory (RSS)
2015	1.00	0.75 GB	1.00	0.79 GB
2016	1.01	0.75 GB	1.01	0.75 GB
2017	1.21	0.70 GB	1.13	0.75 GB
2023D4	1.28	0.87 GB	1.65	0.83 GB
2023D17	1.36	0.78 GB	1.57	0.78 GB

Table 1: Time and memory performance of the Geant4 module of the CMS full simulation application for minimum bias and ttbar events in current and future detector configurations. The Geant4 version used in the test is 10.2p02. With respect to the 2015 and 2016 configurations, which are very similar, 2017 adds an upgraded pixel detector and modifies the forward calorimeter layer configuration, 2023D4 and 2023D17 are different versions of the HL-LHC CMS detector with an upgraded tracker and a High Granularity end cap calorimeter (HGCAL), the latter sub-detector involving a significant increase in the number of Geant4 volumes.

Configuration	MinBias	ttbar
CMS default (FTFP_BERT_EMM)	0.87	0.83
FTFP_BERT	1.00	1.00
no Russian roulette	1.33	1.41
no HF shower library	1.68	1.36
no tracking cuts	1.45	1.13
no time cuts	1.05	1.03
no cuts per region	1.07	1.03
no static build	1.05	1.07

,

Table 2: Relative time performance of the Geant4 module of the CMS full simulation application for minimum bias and ttbar production. Measurements of the individual effect of several options to

reduce CPU time consumption are listed. The Geant4 version used in the test is 10.2.p02. Values of range cuts and tracking cuts are specified in the text.

Configuration	MinBias	ttbar
CMS default	1.0	1.0
no Russian roulette	1.28	1.37
no Russian roulette + no tracking and time cuts	1.84	1.63
no Russian roulette + no tracking and time cuts + FTFP_BERT	2.25	2.04
no Russian roulette + no tracking and time cuts + FTFP_BERT + no HF shower library	4.43	3.22
no Russian roulette + no tracking and time cuts + FTFP_BERT + no HF shower library + no cuts per region	4.73	3.41

Table 3: Relative time performance of the Geant4 module of the CMS full simulation application for minimum bias and ttbar production. Measurements of the cumulative effect of several options to reduce CPU time consumption are listed. The Geant4 version used in the test is 10.2p02. Values of range cuts and tracking cuts are specified in the text.

Configuration	MinBias	ttbar
Nominal production configuration: shower libraries in the forward calorimeter, nominal range cuts, NystromRK4 stepper, FTFP_BERT_ATL physics list, 250ns neutron time cut, simulation of primary particles with pseudo-rapidity below 6.0	1.0	1.0
No shower libraries	1.5	1.3
ClassicalRK4 stepper instead of NystromRK4	1.09	1.07
No neutron time cut	1.02	1.01
FTFP_BERT instead of FTFP_BERT_ATL physics list	No change	No change
No simulation of primaries with pseudo-rapidity above 5.5	0.94	0.95
All range cuts set to 1mm	0.92	0.90

Table 4: Relative time performance for various configurations of the ATLAS simulation for minimum bias and ttbar production events. The Geant4 version used for this test was G4 10.2p03. No significant performance improvements were introduced in patch 03 with respect to patch 02.

Configuration	MinBias	ttbar
Nominal production configuration:	1.0	1.0
No shower libraries	1.5	1.3
No shower libraries + use ClassicalRK4 stepper	1.6	1.4
No shower libraries + use ClassicalRK4 stepper + No neutron time cut	1.6	1.4
No shower libraries + use ClassicalRK4 stepper + No neutron time cut + use FTFP_BERT physics list	1.6	1.4
No shower libraries + use ClassicalRK4 stepper + No neutron time cut + use FTFP_BERT physics list + All range cuts set to 1mm	1.5	1.3
No shower libraries + use ClassicalRK4 stepper + No neutron time cut + use FTFP_BERT physics list + All range cuts set to 1mm + No simulation of primaries with pseudo-rapidity above 5.5	1.4	1.2

Table 5: Relative time performance for various configurations of the ATLAS simulation for minimum bias and ttbar production events. Measurements of the cumulative effect of several options to reduce CPU time consumption are listed. The Geant4 version used for this test was G4 10.2p03. No significant performance improvements were introduced in patch 03 with respect to patch 02.

8.3 LHCb and Alice

Although the use of CPU grid resources by LHCb is two orders of magnitude below ATLAS', the expectation for the 2020 LHC run and beyond is to use up to 90% of its allocation for Monte Carlo simulation. In Run2 the experiment has adopted the concepts of split High Level Triggers (HLT) and of the TURBO stream that integrate real-time calibration and alignment into the data taking process, thereby performing an online reconstruction that is equivalent to offline. Nevertheless LHCb is currently exploiting all resources at its disposal for simulation, including the use of its Online Farm when idle. The full readout of the detector at 40 MHz in the LHCb upgrade will have a major impact on trigger and offline computing systems and the experiment will have to cope with higher rates, up to 2-5 GB/s from the detector. Hence the concepts above will be further exploited moving the event reconstruction and selection as close as possible to the online farm. The experiment plans to match the amount of physics events collected with the same order of simulated events. Exploring faster simulation options is therefore a primary focus of the LHCb software efforts. The experiment has yet to evolve its framework for parallelization and is currently migrating to a version of Geant4 that supports multithreading, with the promise to achieve significant memory savings. Potential gains from static library linkage and re-optimization of simulation parameters will also be investigated. The plan is to evolve the software into an integrated simulation framework which allows to choose and combine different fast simulation options. Table 4 shows the percentage of the CPU time spent on each sub-detector systems for different particle types in a given version of the software The RICH detector took almost 50% of the time followed by the Ecal with about 26%. Optical photons took the largest fraction of the total time, followed by photons, and electrons. Re-optimization of the RICH modeling has already been performed reducing the time of the RICH simulation to 20-30% in future production versions.

	Velo	TT	IT	OT	RICH1	RICH2	SPD&PRS	ECAL	HCAL	Muon	Other	All
opticalphoton	0.1	0.0	0.0	0.0	10.9	32.6	0.0	0.0	0.0	0.0	0.0	43.6
e+/e-	0.3	0.1	0.1	0.2	0.3	0.9	1.2	9.9	2.7	0.9	4.0	20.6
gamma	0.5	0.1	0.3	0.3	0.1	0.3	1.6	12.7	3.0	0.8	2.2	21.9
pi+/pi-	0.9	0.1	0.1	0.1	0.1	0.3	0.1	1.1	0.6	0.2	1.1	4.7
neutron	0.1	0.0	0.0	0.1	0.0	0.1	0.2	1.7	2.0	0.3	0.2	4.7
proton	0.4	0.0	0.0	0.0	0.0	0.3	0.0	0.5	0.5	0.1	0.8	2.6
K+/K-	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.3	0.5
mu+/mu-	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1
other	0.0	0.0	0.0	0.0	0.4	0.0	0.0	0.0	0.0	0.0	0.2	0.6
All	2.4	0.3	0.6	0.7	12.0	34.6	3.1	26.3	9.0	2.4	8.6	100.0

Table 4: Percentage of the CPU time spent on each sub-detector systems for different particle types for a given version of the software.

ALICE also consumes two orders of magnitude less CPU resources than ATLAS. Figures 16 and 17 show charts of the percentage of time spent in different elements of the detector simulation chain, including the Geant4 and digitization modules, and in the different library components, respectively. The challenge for ALICE is to reduce the time spent in Geant4 simulation (55% of the total simulation time), particularly in the geometry package and math functions, and re-optimize the stepping algorithms. Digitization takes a large fraction of the CPU resources in ALICE (35%) and is therefore also a target of ongoing R&D to improve the modeling of the TPC readout and the IO, and to explore the benefits from SIMD vectorization.

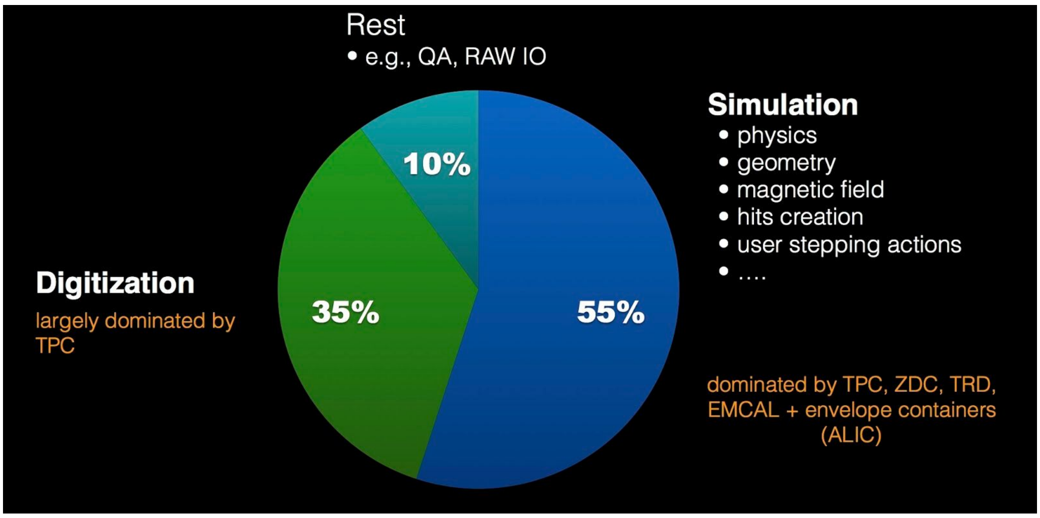


Figure 16: Approximate percentage of time spent in different components of the ALICE detector simulation chain, including the Geant and digitization modules (for a representative Pb-Pb Hijing event)

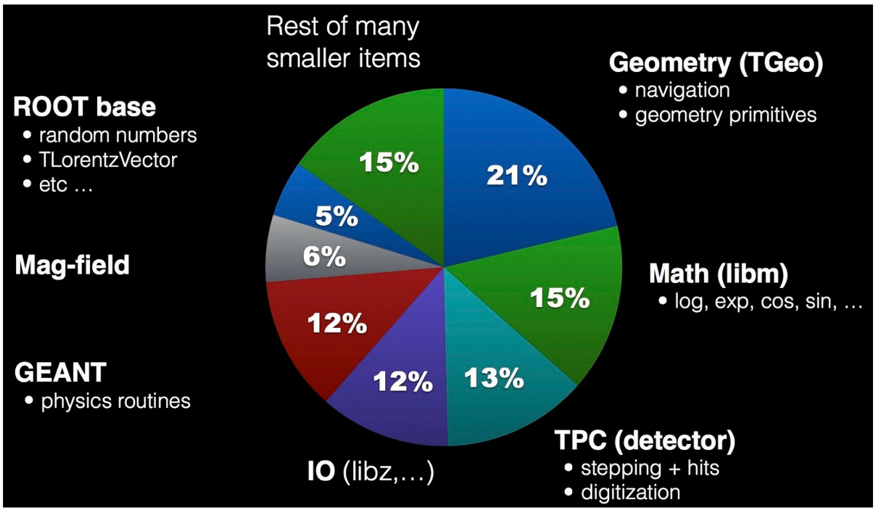


Figure 17: Approximate percentage of time spent in the different library components of the ALICE detector simulation chain for the same setting as in Figure 16.

8.4 Neutrino Experiments

Accelerator-based neutrino experiments use “detector” simulation tools in two different places. Beam simulations are used to model primary proton beam interactions with the target and the creation, integration and decay of hadrons that produce neutrinos. For this step, most experiments use Geant4, although some use Fluka [8] or MARS [9]. Neutrino-nucleus interactions inside the detectors are taken care of by neutrino generator tools, such as GENIE [7]. The actual Geant4-based detector simulation stage takes over from the generator to propagate the final state particles through the detectors. Neutrino detectors divide into three broad categories: segmented scintillator detectors, liquid argon TPC’s, and Cherenkov detectors.

Beam simulations generally do not require significant computing resources. A total of 100 million events, produced at a rate of 0.01 sec/event and using much less than 1 GB per job, is generally sufficient for a production pass. More resources are needed for assessing beam uncertainties, simulating muons in muon monitors, and for beam design optimization.

For the MINERvA experiment, the whole simulation chain from neutrino beam modeling to the production of the analysis files take about 20 sec/event, with 25-35% of this time spent in the Geant4 module. The required memory is typically less than 2 GB per job. The NOvA experiment used 13 million CPU hours in 2016, 70% of which were spent on simulation, and less than 2 GB of memory per job.

For liquid argon TPC detectors, all Fermilab experiments use the LArSoft software [21], which contains the simulation and reconstruction packages. LArSoft includes both the Geant4 module and a “DetSim” module that handles the conversion from energy to ionization charge, the scintillator light, and the propagation of charge and photons. The MicroBooNE experiment spends approximately 3 min/event in the Geant4 module and 1 min/event the DetSim module, with a memory footprint per job of 4.6 GB and 2.3 GB respectively. Table 5 shows a summary of CPU time measurements for the ProtoDUNE and DUNE Far Detector (DUNE FD) simulation applications. Although the DUNE FD is much larger (40 kTon) than ProtoDUNE (770 tons), ProtoDUNE will operate on the surface and requires simulation of cosmic backgrounds. It is also not necessary to simulate the entire 40 kTon DUNE FD in every event. For these reasons, Geant4 simulation of the DUNE FD is substantially faster than ProtoDUNE. Memory consumption is 2 (3) GB per job for the Geant4 module and 1.3 (1) GB per job for the DetSim module.

In summary, computing performance is not the dominant challenge for the simulation of scintillator-based neutrino experiments. However, the TPC’s liquid argon and segmented detector technology under consideration for the DUNE near detector (DUNE ND) may pose significant new demands on computing resources. The issue of liquid argon simulations requiring large amounts of memory will be mitigated by evolving the *art* software framework [35] to support multithreading.

Experiment / Simulation Stage CPU (in sec/event)	**Generation**	**Geant4**	**Geant4 with space charge**	**DetSim**	**Reco**
ProtoDUNE (Cosmic events with Corsika [36])	10	180	480	25	1000
DUNE FD (ν_e events with GENIe [7])	0.04	4		44	160

Table 5: Summary of CPU time measurements for the different modules associated with the ProtoDUNE and DUNE Far Detector (DUNE FD) simulation applications.

8.5 Direct dark-matter search experiments

As is the case for neutrino and muon experiments, the direct dark-matter search experiments do not face significant computing performance challenges. Given the typical event topology (very few tracks of limited energy), CPU and memory consumption are not considered a particular concern, with the exception of some specific requirements. There is, instead, a large interest in improved and extended physics modeling.

The issues associated with physics modeling can be summarized as:

- For the liquid noble gas experiments an extension to Geant4 scintillation process [37] is usually employed
- For cryogenic crystal detectors the simulation of phonons and their interaction becomes important. Geant4 has been extended to support these processes [38]

The specific CPU-related elements are:

- High-precision neutron transport may be needed in some cases. The associated physics models are computationally more intensive than the default Geant4 models.
- Optical photon transportation may become a CPU bottleneck for experiments with a detailed and complex optical model. Advanced techniques leveraging GPUs are under investigation [39].

9. R&D Towards Improving Software Performance

Here we will discuss the activities that use the latest state of the art techniques to improve computing performance. In other words, we will include R&D efforts other than optimization of compiler or library settings, shower library replacements, and optimization of Geant4 tracking parameters or production cuts. The use of fine grained parallelization techniques, novel computing architectures, and HPC systems are within the scope of this section.

When considering the question of code modernization, it is often the case that developers are confronted with the dilemma whether to adiabatically evolve the current code or start an entirely new product. Advantages and disadvantages of the two approaches are obvious, but they tend to balance each other, so that it is common wisdom that there is really no good solution. Adiabatic evolution of an existing code is by nature slow and gradual, particularly in the case of a code like Geant4 which is of critical importance for HEP. Users demand at the same time improvements and stability, which means that profound architectural changes are challenging and any change, before entering production, has to be thoroughly validated, which is a very long process. The development of an entirely new code draws precious and scarce resources from the developer community and its validation is a daunting task that may be beyond the resources of the experiments. This may delay the transition and reduce the uptake of the new code. The simulation community is pioneering an interesting new approach introduced by the GeantV project. While a new transport engine is developed to allow vectorized transport, the accompanying modules (e.g. geometry, physics, fast simulation) are developed as independent modules that can be used also by Geant4. Of course when used with Geant4 they will not expose their full performance potential, since transport in Geant4 is sequential, but this allows their full validation and comparison with the existing Geant4 counterparts. This approach offers a number of benefits: the GeantV project is continuously producing added value to the simulation users and its critical modules are thoroughly validated in the existing framework. When GeantV is fully developed, only the multithreaded vectorized transport will be entirely new, while all the other components will be validated by the experiments. This approach seems to offer the best of both worlds, avoiding to split the communities of users and developers and maximizing synergy and sharing of experience.

9.1 GeantV and detector performance

The CPU time that is spent in the simulation of LHC detectors is typically dominated by the physics components, and in particular by the electromagnetic part. The development of electromagnetic showers in calorimeters plays a major role for the CPU performance of simulations. This is also true for jets because hadronic showers, induced by the hadron components of jets, have electromagnetic components coming from the decays of neutral pions. The geometry component as well as particle propagation in fields fill also important slices in the overall performance pie-chart of simulation, as can be observed in Figure 14. These observations are showing in which areas the R&D effort should be mainly focused in the short and medium term from the perspective of detailed simulation.

Improving the CPU performance is a major milestone of simulation R&D and the related program of work is mainly bound to the LHC schedule for the high luminosity phase. Adapting the simulation workflow and algorithms to make better profit from the FLOPS potential of modern architectures is very important. The R&D undertaken by the GeantV project to increase the data and instruction locality has shown [40] that performance improvements by large factors are within reach even in highly complex frameworks such as particle transport simulation.

Making use of the SIMD pipelines available today even in commodity PC's has been already investigated at large in GeantV. An important lesson resulting from this R&D is that vectorizing the computing intensive algorithms of the program is required but not sufficient for enabling significant overall gains due to SIMD pipelines. The entire simulation workflow needs to be adapted to provide the multiple data required by vectorization. GeantV prototyped an approach that splits the stepping procedure for tracks into stages, aiming to accumulate many particles before actually performing the actions involved by the stage. As illustrated In Figure 18, the generation of the final states from discrete physics processes can be such a simulation stage. Particles entering it are directed to different physics model handlers that accumulate tracks into baskets, executing the different model algorithms in multi-particle mode. This kind of design changes the traditional stack-based execution into a multi-stream execution pattern. It creates the premises for increasing the code and data locality while allowing to feed multiple data to possibly vectorized code.

Such reshaping of the simulation approach has several practical implications, out of which many are affecting directly the user code. Mixing tracks from multiple events is required for sustaining the basketized flow. To be noted that several current or future experiment frameworks will support track-level parallelism as well. This will affect the data management and I/O on the user side, requiring concurrent bookkeeping and management of multiple events in flight. Extending the user API with vector signatures will allow vectorised user code to exploit the particle-level parallelism supported by the framework..

The support for an alternative approach to particle transport will affect also the strategy for the development and long term maintenance of physics models. An important objective of the physics developers is therefore to review the physics algorithms and their implementation in order to better adapt them to a multi-particle flow. This will allow a better use of the system caches even without vectorized algorithms. For such revisited models, GeantV is offering a testbed allowing to turn on the basket flow and benchmark the impact of vectorization. It is of utmost importance that newly developed or revisited physics models are easily ported to both Geant4 and GeantV, and this would need to be reflected in the program of work. The main reason is delivering the new models to the community while having them tested and shaped for an evolution of the particle transport toolkit. This would also facilitate the validation of the new developments and benchmarking their performance in a basket flow environment.

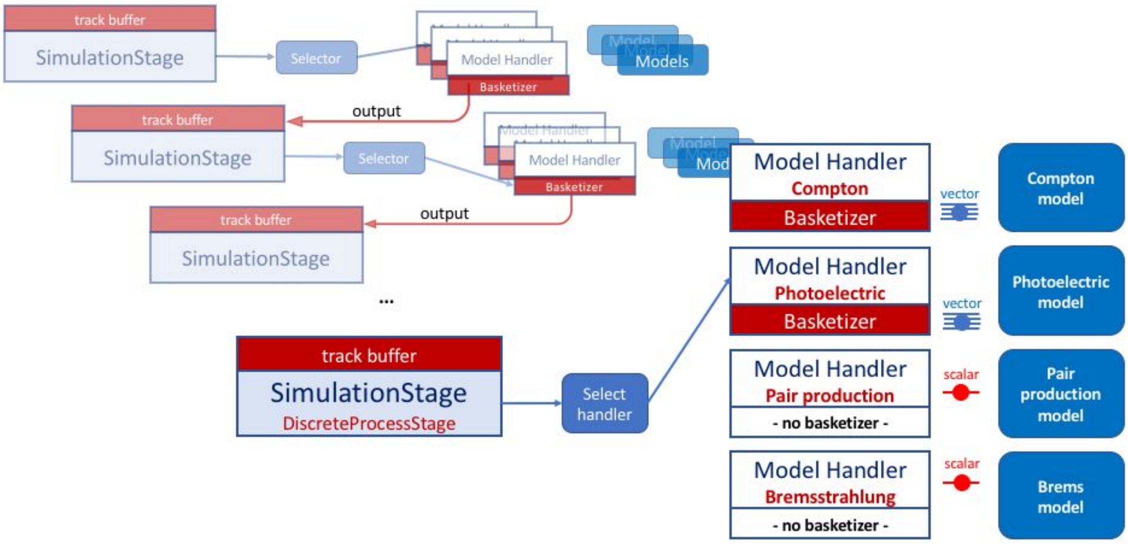


Figure 18: *The stepping procedure in particle transport is the sequence of actions allowing to propagate a particle from a starting point to the next point where the state of the particle changes meaningfully (e.g. physics process occurrence or geometry crossing). In GeantV stepping is decomposed into stages, each stage selecting among a set of models. Tracks can be buffered and sent in form of baskets to vectorized models, which are allowed to coexist with scalar models. This approach improves the locality and cache coherency compared to the classical stack-based approach.*

The required increase in CPU performance cannot be achieved only from algorithmic improvements, structural changes and multiparticle flow. This also involves the development of fast sampling algorithms as well as Fast Simulation approaches that bypass the simulation of full showers. The project aims to investigate further the ways in which Full and Fast simulation capabilities can be integrated in a single detector simulation framework.

At the moment, the GeantV team is focused on the initial goal to test the transport engine with the vectorised geometry package and demonstrate a significant speedup factor. For simplicity, the project started by following a “tabulated physics” approach using values derived from Geant4, thus enabling equal footing comparisons between the two. Tests under this approach are performed to ensure the consistency and validity of the time performance results. Tabulated physics is being now replaced with a physics framework using improved and vectorised physics models, which are being validated as they become available. Full-scale physics validation will be performed both on available “thin target” data and in the context of realistic detector applications and in collaboration with the experiments.

The vectorized components developed by GeantV show substantial speed-ups with respect to the corresponding code in Geant4, sometimes exceeding by one order of magnitude. This is the case for certain solids within the VecGeom geometry package [41], and is planned to be extended to field propagators and certain EM physics models. While this result is very promising, it still does not constitute an authoritative benchmark, although it gives confidence that the stated project goal of reaching a global speedup of a factor five is well within reach.

Some of the speed-up of GeantV will come from optimized, vectorised physics models, which are being developed with the objective of improving physics accuracy and to respond to the requirements of HL-LHC and the future intensity and energy frontier experiments. Numerous branches in the physics code, especially in hadronics physics, pose a major challenge to vectorisation. Because EM processes dominate showers and have relatively fewer branches, they are the first targets of optimization and vectorization. Low energy neutron and elastic hadron scattering processes are also more amenable to vectorization.

The estimate for the remaining work to complete the first version of the GeantV EM physics library is of order of 1.5 FTE-years, while the work to implement a complete first version of hadronic physics is much larger. The GeantV team is currently planning to “wrap” an existing Geant4 hadronic physics model to allow meaningful physics and time comparisons. This effort is estimated at 2 FTEs.

9.2 Hybrid Computing and simulation

Hybrid computing refers to sharing work across a mixture of computers with different architectures. This computing model seeks to exploit the benefits of multithreading and fine grained parallelism, and needs a software framework for writing code that executes across heterogeneous platforms, which at the moment may include CPUs, GPUs, MICs, etc. In detector simulation, parallelism is achieved at the level of events, as in Geant4, or at the level of tracks, as in GeantV. Monte Carlo techniques for detector simulations are implemented as sequential algorithms because each *step* depends on the *history of previous steps*. Although the use of these emerging technologies in detector simulation remains a challenge R&D efforts are to be aggressively pursued, given the potentially large gains to be obtained.

One of the most time consuming components common to the majority of detector simulation applications is neutron tracking, which needs to be precise. Neutron tracking has some characteristics that make it a good candidate to explore acceleration with the use of co-processors:

- there are many particles of the same type in the simulation;
- the number of physics branches (e.g. different physics processes) involved in the simulation of these particles is limited;
- each particle goes through a large number of steps though the detector material before being absorbed or leaving the detector;
- when eventually an interaction occurs, the number and species of generated secondary particles that will further contribute to the signal is relatively limited.

Previous experience [42] has shown that large speedup factors can be achieved for tasks that are well-suited to GPGPU technology: simplified geometry with only few materials, limited number of particle species and physics processes. One example is the R&D effort started by the Geant4 Collaboration to extend the existing code to the transport of neutrons. One of the unique characteristics of this approach is that this system can be integrated in existing applications, replacing only the specific components with independent libraries. This approach is particularly effective for HEP experiments because it allows for a non-disruptive evolution of the simulation code that extends the thoroughly validated current versions of the Geant4 neutron physics models (see Figure 19).

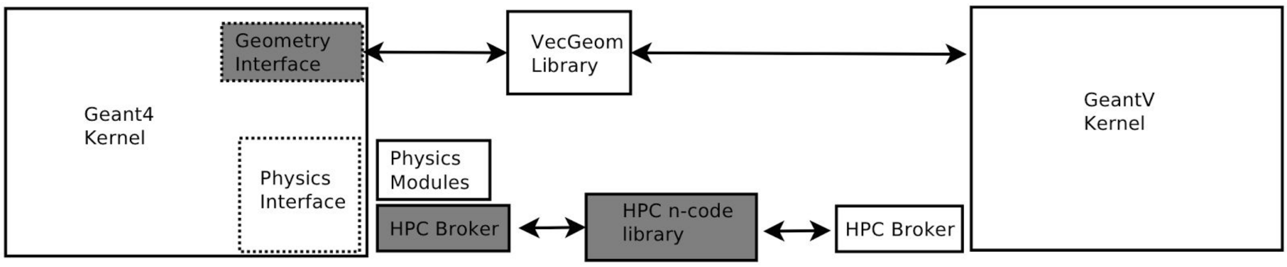


Figure 19: Proposed architecture of a specialized library to leverage GPU for neutron transport.

The first target of the described approach is the use of GPUs for thermal neutron transportation. While the CPUs continue to process the rest of the particles, the processing of all secondary thermal neutrons would be offloaded to GPUs. Thermal neutrons propagate in the detector and cavern for a long time before eventually interacting and generating detector signals. Given that the latency is large, from 10 seconds to minutes, thermal neutron depositions cannot always be associated with the original event such that the neutron flux is the only meaningful output information from thermal neutron transport. As granular I/O is known to be one of the dominant obstacles against efficient use of GPUs, a hybrid simulation with minimal I/O utilization offers an ideal opportunity for making efficient use of GPUs.

Along the same lines, the GeantV project achieved speedup factors of up to 30 with respect to Geant4 when processing a basket of electrons and photons in a GPU [43]. This is explained by the fact that EM interactions in a detector evolve into a self-contained cascade of electrons and photons that can exploit the benefits of vectorized code, SIMD, and data locality. In other words, electrons and photons traversing the same volume and getting applied the same instructions are bundled in a single basket processed in a single thread on a GPU. The caveat is that the baskets need to contain at least ten thousand tracks in order for the factor of 30 to be achieved, due to the long transfer times to and from the GPU.

9.3 Simulation on High Performance Computing Systems

HPC resources at supercomputer centers can provide a substantial fraction of the needed computing power to address HL-LHC needs. The Geant4 Collaboration has started an R&D program of code optimization for a more efficient utilization of HPC resources. One of the main features of the next generation of supercomputers is the use of massively parallel architectures that require the combination of novel techniques to achieve scalability. The release of multi-threaded Geant4 in 2013 has shown that it is possible to obtain almost perfect linear scaling, whilst keeping memory usage under control. Subsequent research has focused on extending the parallelism to multi-node with HPC-friendly techniques (MPI), using a mixed MT/MPI approach. A recent result has shown that scaling for hundreds of thousands of concurrent threads can be achieved for a semi-realistic HEP-Geant4 application. A test performed on the MIRA supercomputer at ANL successfully ran a modified version of Geant4 spawning more than 3 million threads [44]. The test concluded that the main bottleneck to achieve scaling linearity is concurrent access to I/O resources (see Figure 20). Extensions to Geant4 capabilities to improve the scalability of the code are underway. These include:

- parallel merging of scorers/histograms and ntuples via MPI;
- redesign of RNG Seeding in large parallel applications;
- investigation of use of HPC-friendly data-storage for input data-base libraries.

A custom version of Geant4 developed for tests on MIRA showed scalability for up to 3 million threads. This version is the basis for further development to be included in future Geant4 public releases. A spinoff result from the MIRA tests has been the validation of Geant4 physics to $1/10^5$, a level of precision never achieved before.

ATLAS is actively pursuing HPC resource utilization to supplement grid resources for simulation production. Multi-process jobs distributed with YODA have been running successfully in production on supercomputers at NERSC and machine utilization is being studied [45]. ATLAS is currently migrating its simulation application to multi-threading to ensure good scaling performance on HPC architectures with minimal memory footprint. Current measurements of multi-threaded event throughput and memory consumption scaling on Intel Xeon Phi Knights Landing chips are very promising, demonstrating ability to scale well up to the maximum number of threads on a device with a factor five decrease in the per-worker memory consumption relative to multi-process jobs [46]. Overall throughput performance falls short of traditional Xeon architectures, however, so studies are ongoing to identify and remove the performance bottlenecks.

CMS has also been studying how best to exploit HPC resources by running combined multi-step jobs that cover Generation, Simulation, Digitization and Reconstruction in a single workflow. The results when scaling to high-pileup scenarios have shown that limitations are primarily due to the reconstruction step, rather than the simulation step. Studies have been made of various ways of filling a whole KNL many-core node with Generation and Simulation jobs of varying sizes and the highest total node event throughput was achieved with two jobs using 128 threads each. The simulation application and its underlying simulation engine, Geant4, is not limiting scaling behaviour.

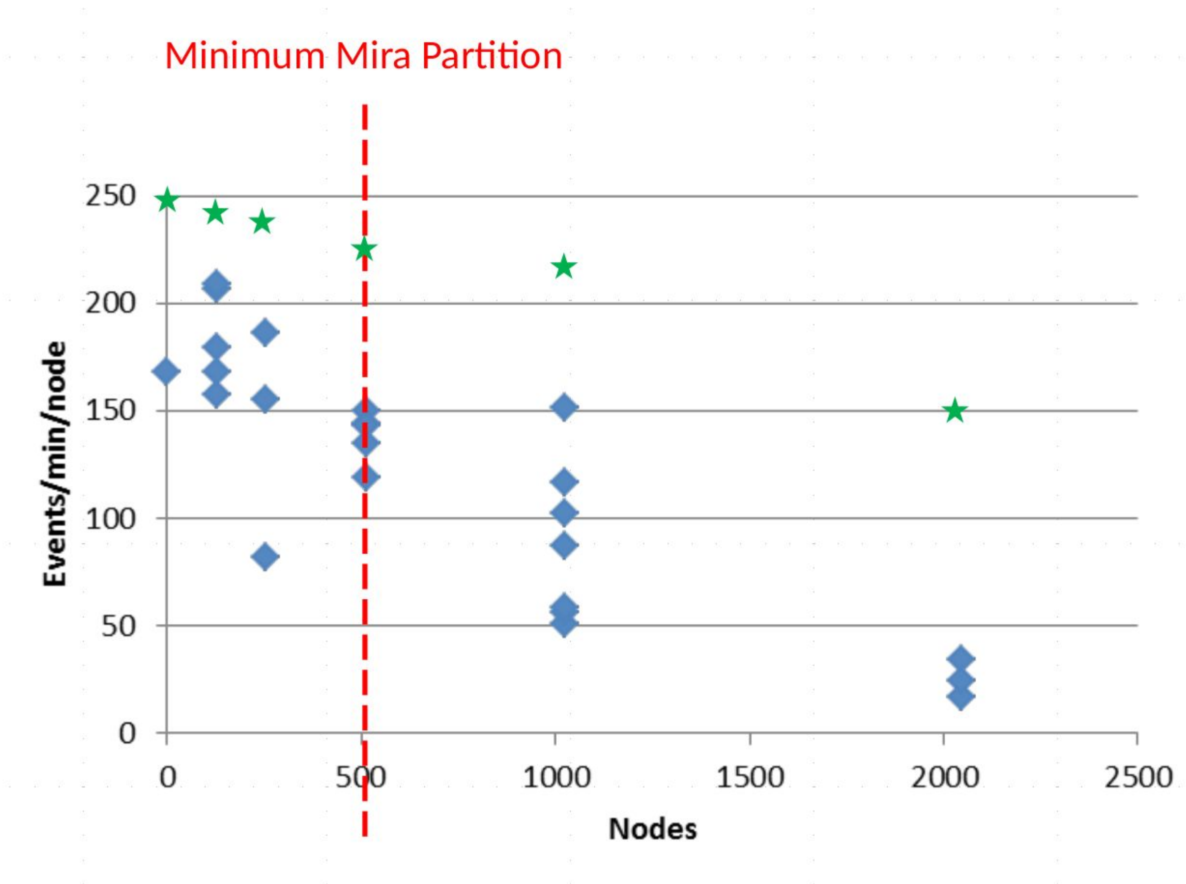


Figure 20: Top: Initial testing of Gean4 on MIRA (blue diamonds) and VESTA (green stars). Each node has 80 threads. The loss of scalability is due to I/O and intra-node communication limitations (MIRA nodes do not have disks and rely on MPI for every I/O operation). VESTA, a smaller test-bed, shows better results because the number of I/O nodes is larger.

10. Fast Simulation

As pointed out earlier, simulation consumes the majority of the CPU time used by many experiments. Optimization studies on detailed simulation codes are ongoing and can provide helpful performance improvements, but in order to satisfy the needs of an entire experiment, other options must be explored. The increase in size of the MC samples needed to match those of the data collected by upgraded or future experiments, as well as the increase in the complexity of the events, will put additional strains on the CPU needs. While the availability of an accurate detailed simulation will remain of paramount importance, often the full high-fidelity description of the detector implemented by the experiments is not necessary. There are many cases, including detector upgrade studies, tests for evaluation of systematic uncertainties in physics measurements, scans of large signal phase spaces in the context of new theories, and prototyping of new analysis ideas, where the demand on simulation physics accuracy may be relaxed. Even within a given physics analysis, it may be good enough to evaluate some quantities with high accuracy in a small MC sample and other quantities with lower accuracy in larger samples. A combination of different fast simulation approaches targeting parts or the whole simulation application are the optimal solution for saving computing resources in these cases.

In general, simulation time scales with the energy of the particles being simulated, and with the minimum energy down to which they are simulated. This means that by far the most time is taken by showers in calorimeters, where large numbers of low-energy electromagnetic particles are produced and propagated by the simulation. Because the simulation time scales with energy, rather than transverse energy, the time consumed by LHC simulations is dominated by the forward regions, which are the target of the highest energy particles in most collider events. Fast simulations options for calorimeter showers have the side-effect of reducing significantly the number of low energy neutrons in the simulated event, which contribute significantly to the simulation time due to their relatively long lifetimes. Particle propagation in tracker detectors is typically the next most time-consuming step in a simulation. This step consists mostly of charged particle propagation, and the geometry detail is the most important aspect to be addressed by the a fast simulation. Heavy Flavour physics experiments utilize Ring Imaging Cherenkov (RICH) or Detection of Internally Reflected Cherenkov light (DIRC) detector technology. The transport of Cherenkov photons through optical processes needs to be simulated in detail in these cases, and requires more CPU time than regular trackers. Fast simulation of these processes is in general tied to the reconstruction technique used in a given detector.

There are two main types of “fast” simulations. One is the replacement of a particular physics process or set of processes with a module that contains faster code. The other approach is the simulation of an entire particle trajectory or shower, or even a more complex object like a hadronic jet, with a faster software module. These faster modules often consist of parameterized models of the physics processes or particle trajectories. While the technique could be shared, the exact implementation would be different for each experiment. Much of this section focuses on the second technique, while the first is discussed further in Sec. 10.3, which is about machine learning.

It is worth noting that the fast simulation techniques and software have relevance outside the HEP domain. For example, radiation transport techniques are extremely important for a wide range of applications:

- radiation protection in all industrial fields using ionizing radiations (sterilization, imaging etc.);
- radiation protection for space flights;
- design and optimization of imaging medical instruments;
- treatment planning for radiation therapy;
- radiation safety for nuclear power and fuel processing plants;

All these applications would greatly benefit from an increase in the simulation speed with important benefits to their respective fields.

A way to achieve an additional speedup is to customize the simulation to the needs of a specific physics analysis. This would allow to target a given sub-detector or part of the event.

10.1 Fast Simulation techniques and examples

There are many techniques to make simulation faster. Some of them are applied to Geant4-based full simulation applications, such as for example Russian Roulette and shower libraries, to speedup simulation in a given sub-detector. In the literature, these applications are still labeled full simulation and Geant4-based. Some experiments have developed alternative fast simulation frameworks, based on fast track propagation through a simplified geometry and parametrized showers, which are less accurate and are typically used in detector upgrade studies and to produce “signal” samples that require scans of a large region of theory parameter space. Generally, the faster the simulation, the more imprecise the physics is. Examples of fast simulation techniques, used to speedup Geant4-based applications or in fast simulation frameworks, are:

- **Russian Roulette:** Some fraction of the simulated particles are discarded and a weight is applied to the others to compensate for this effect. It is commonly used in the simulation of thermal neutrons, which have long lifetimes and consume a significant amount of CPU time while propagating through matter before being absorbed. Russian Roulette is used in CMS’s full simulation application and yields 25% (30%) CPU savings when processing minimum bias (ttbar).

- **Shower libraries:** A particle of a given type and in a given energy range and geometry region is replaced with the simulation information of a similar particle stored in a library of showers pre-simulated with a detector simulation tool such as Geant4. Shower libraries are typically used to replace full simulation in sub-detectors with high particle occupancy, such as forward detectors in colliders. The are efficient to model high-energy showers where a large number of low-energy secondary particles are produced. If applied to the entire detector, they achieve speedup factors of 2-5. Both in ATLAS and CMS, shower libraries are used by default in the forward hadronic calorimeters, yielding a 25%-40% time performance gain in the case of CMS and a 30-50% performance gain in the case of ATLAS. ATLAS tests indicated previously that extending the use of these libraries to the remainder of the calorimetry could bring gains of an additional 50%. LHCb is currently exploring its use.

- **Parametrization of calorimeter showers**: The simplest implementation of a parametrized particle shower involves the parametrization of the shower shapes of high- and low-energy

EM particles. In sampling detectors with complex geometries, these parameterizations are difficult to tune. Additionally, with a relatively thick inner detector, and in the case of ATLAS a cryostat and solenoid in front of the active calorimeter region, there may not be many high-energy electromagnetic particles available to the fast simulation. This simplest approach, based on Ref. [34], was abandoned by ATLAS about ten years ago. Current approaches used by both ATLAS and CMS involve more complex modeling of the showers than can be achieved by a simple parameterization. Although not part of the current default simulation, CMS implemented shower parameterizations using GFLASH [33] to model the shower after the first interaction of each primary particle with matter, by tuning a set of parameters to fit the geometric distribution of the associated energy depositions obtained from a Geant4 simulation. The ATLAS approach uses histograms with energy deposit and shower shape information to directly treat particles before they enter the cryostat. All these approaches have the advantage that they can ignore, during energy deposition, the detailed geometry of the calorimeter, and deal only with the readout geometry. All have the option of building objects similar to the energy depositions from Geant4 or attempting to directly build summary-like objects that are used in digitization. Typically, parametric simulation achieves speedup factors of 100-1000 in the part of the detector treated by the parameterization.

- **Low energy background parameterization**: Muon detectors are located behind the calorimeter system preventing most high energy particles of a different nature to reach them. The main contribution to the occupancy in these detectors, apart from muons, is due to leakage from calorimetric showers and thermal neutrons. In order to obtain fully realistic occupancies in the muon system, photons, electrons and neutrons need to be transported to very low energy, and the surrounding infrastructure and accelerator elements must be modeled. In the LHCb experiment, the addition of this detail to the full Geant4 simulation would result in a CPU time increase of the order of a factor of 10. Instead, this low energy background is simulated via a parametrization of the difference between a full simulations with and without the low energy processes. A similar method is being validated by the ATLAS collaboration.

- **Fast tracker simulation**: Both ATLAS and CMS have custom fast track simulation algorithms based on simplified geometries. The time consumed by the full simulation of a tracking detector is primarily spent on the propagation of charged particles in a magnetic field, which is directly related to the number of times the field must be sampled. By simplifying the geometry, for example by considering infinitely thin layers, the number of samples is significantly reduced, resulting in a faster overall simulation. The other way to speed up the tracker simulation is by introducing fast, parameterized models for material interactions, particularly for the more common electromagnetic interactions. The fast track simulation code used by ATLAS has been made public as a part of the common tracking software project ACTS [47], adopted by the FCC [48]. These fast track simulations offer speed improvements of 10-1000x over a detailed simulation, though for a fast simulation including both fast tracking and fast calorimeter simulation, tracking is typically the dominant resource consumer.

- **Fast digitization and reconstruction**: Especially for higher pileup at the LHC, once fast calorimeter simulation is used, and certainly when fast tracker simulation is included, digitization and reconstruction become the dominant consumers of CPU time in the simulation chain. As a result, both CMS and ATLAS have implemented fast modules for specific pieces of the digitization and reconstruction code that are most time-consuming, primarily in fast inner detector digitization and fast tracking. Fast tracker hit reconstruction uses template hit smearing functions derived from full reconstruction, whereas fast tracking often uses generator (truth) particles as seeds to avoid the combinatorial issues of standard track reconstruction software. The speed improvements from these algorithms varies with pileup but are generally more than one order of magnitude. [49]

- **Fully parameterized simulation:** Many programs are available in the public domain for the implementation of very fast parameterized simulation, the most popular being DELPHES and PGS [50,51]. These tools are extremely fast, running at hundreds of events per second, but they lack the accuracy of the alternatives discussed before. These programs are heavily used by phenomenologists for re-interpretation of LHC results, and by ATLAS, CMS, and LHCb for upgrade detector performance studies.
- **Ultra fast self-tuning non-parametric simulations:** A re-emerging alternative trend in simulation is to develop ultra fast, self-tuning simulators based on lookup tables that directly map generator events into simulated events. The lookup tables in this case are formed directly from fully simulated events. A past example was Turbosim [52] developed at the Tevatron for the D0 and CDF experiments. A prototype for a redesign called Falcon [53] was recently released, with a more efficient algorithm for the multi-dimensional mapping of particle properties.

A natural evolution of having separate full and fast simulation frameworks in experiments is the concept of “hybrid” simulation (see Sec. 9.2), where a single framework allows to treat some aspects of the event with a fast or very fast simulation technique and others with a detailed simulation approach. Such configurations might be useful for handling pile-up and also for B-physics, where only a few particles are of great interest to the analysis while it is helpful to have the others simulated with some minimal accuracy. The difficulty with the hybrid approach is that the optimal configuration is analysis dependent and requires the derivation of customized calibration and efficiency factors, activities which are person-power intensive.

LHCb has developed simulation code for reuse of the underlying event in the case where only a few particles are of interest and the contribution of the rest only degrades the ‘signal’ measurement. The technique consists of fully simulating the underlying event once, while the ‘signal’ is simulated N times independently and recombined with the one underlying event. It allows a reduction in CPU time consumption proportional to the number of times the underlying event is re-used.

10.2 Physics Performance of Fast Simulations

The fastest of the fast simulations are typically useful for situations in which only approximate answers are needed, or where large uncertainties are not a serious concern. Such situations are surprisingly common: e.g. studies of BSM limits on new particles in LHC upgrade scenarios, where cross-sections fall rapidly with mass, can afford a 100% uncertainty on the analysis efficiency as it results in a relatively small uncertainty on the excluded mass. The slower simulation techniques generally provide higher fidelity, but they are more resource intensive.

The performance of fast simulation in ATLAS, CMS, and LHCb is evaluated with respect to the Geant4-based full simulation. For the fastest version of ATLAS FastSim, and for CMS FastSim, the agreement is on average quite good for kinematic distributions such as the momentum and pseudo rapidities of high level event objects such as light jets, b jets, missing transverse energy, muons, electrons, photons and taus. Larger discrepancies are observed when comparing variables that depend on the structure or shape properties such as jet particle composition or variables used for electron and photon identification. Fast simulations have difficulty reproducing the detailed structure of hadronic shower shapes, which create issues in modelling boosted objects and jet substructure, which are very relevant signatures at higher energies. Another common issue is in the treatment of exotic particles. Particles with high charge (e.g. Q-balls), strange propagation (e.g. Quirks), unusual nuclear interaction patterns (e.g. R-hadrons), and almost any particles with late decays that result in displaced vertices or disappearing tracks, for example, are difficult to treat with fast simulations because of the assumptions built into the parameterizations. For example, most fast simulations assume that particles are pointing, while particles from late-decaying heavy particles may not be.

Fast simulations do have the advantage that they are generally more tuneable than a detailed simulation toolkit like Geant4. The knobs for tuning are generally better exposed to users (particularly for cases like PGS and DELPHES), and they have a more clear connection with physical observables. Thus, it can be easier to tune a fast simulation to match the data than it is to tune a detailed simulation toolkit.

Figure 21 shows the speed of CMS fast simulation factorized into different subprocesses as a function of the number of pileup interactions. The sub-processes are defined as follows:

- *Trajectory sim.* refers to fast simulation of the particle trajectory through the detector, and formation of tracker and muon simulated hits.
- *Calorimeter sim.* refers to fast calorimeter simulation.
- *Tracker hits* refers to a FastSim specific simplified hit reconstruction in the tracker.
- *Pileup mixing* refers to the process of mixing hits from a physics process of interest with those from a minimum bias sample representing pileup.
- *Tracking* is the MC truth based, fast track finding algorithm.
- *Digitization* is the simulation of readout, which is the same in fast and full simulation in CMS.
- *Calorimeter reco.* is the reconstruction of calorimeter hits, which is standard for all simulation and data.
- Muon reco (not shown in the plot): is the reconstruction of muon detector hits, and takes on average ~0.01s/event.
- Finally, *Object reco.* is the standard CMS reconstruction of all objects including vertices, jets, electrons, photons, muons and taus used in data and simulation.

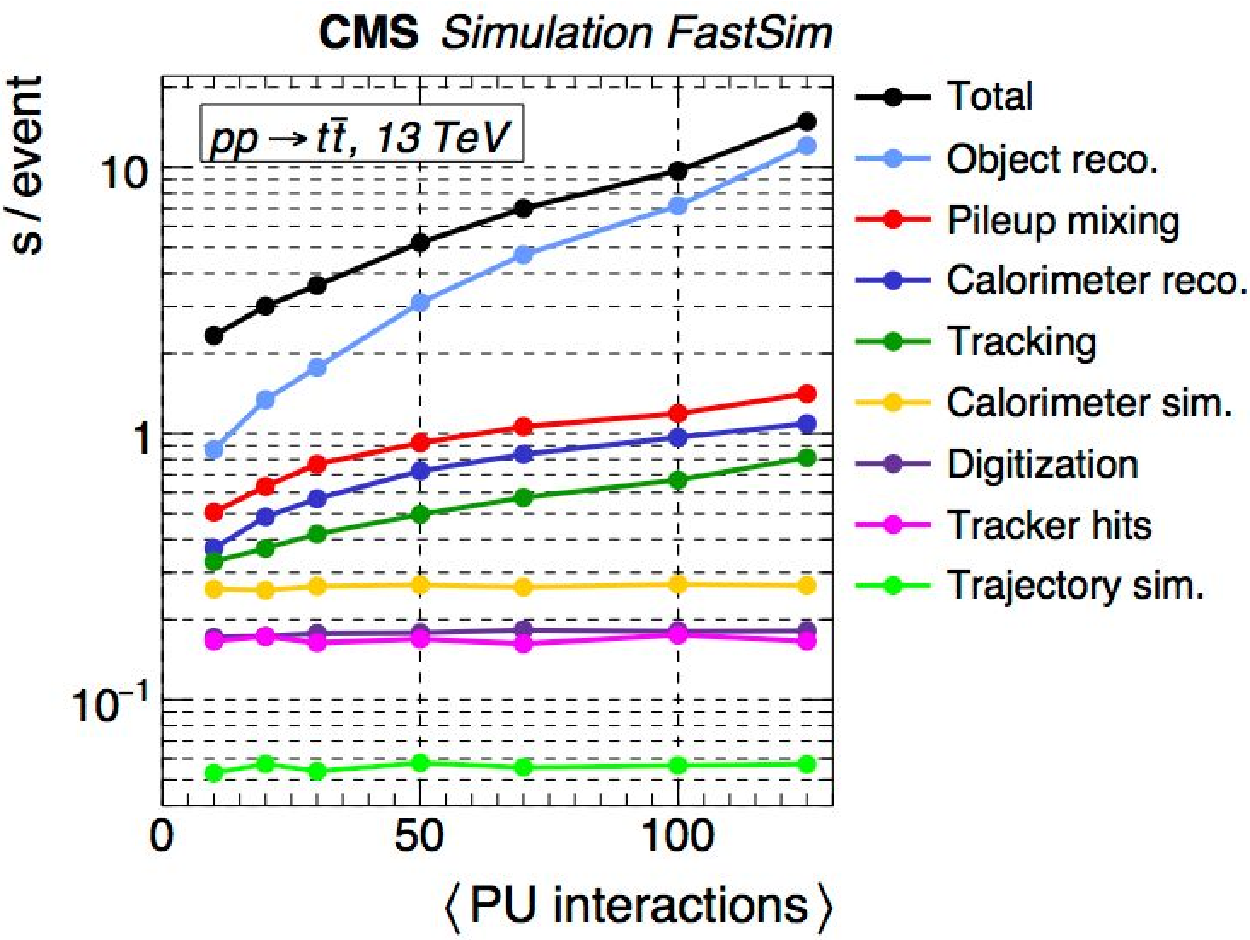


Figure 21 Speed of CMS fast simulation factorized into different subprocesses, as explained in Sec. 10.2, versus number of pileup interactions.

10.3 Machine Learning in Fast Simulations

There has recently been a great deal of interest in the use of machine learning in fast simulation, most of which has focused on the use of multi-objective regression [54] and generative adversarial networks (GANs) [55,56,57]. Since use of GANs allows for non-parametric learning in cases such as calorimetric shower fluctuations, it is a promising avenue for generating non-Gaussian and highly correlated physical effects. This is an obvious area for future expansion and development, as it is currently in its infancy. Just as with fast simulation in general, one can imagine two types of machine learning applications to simulation. One is the replacement of a particular physics process or set of processes with a machine learning module. Such an approach has the clear advantage that it can be shared among the experiments as a part of a general simulation toolkit like Geant4. The approach has the disadvantage that, while it can be used to directly replace a specific module of the toolkit by training against the standard model, it otherwise might be rather difficult or cumbersome to produce training data that can be used for the development of a clearly distinct new model of physics. The other approach is the replacement of a fast simulation technique with a machine learning module - that is, a machine learning module that performs the entire simulation of a particle, or even a more complex object like a hadronic jet. Machine learning approaches also offer the opportunity for end-to-end simulation where the output can represent composite objects resulting from multiple simulation steps. While the technique, and perhaps even some details of the network and training methods, could be shared, the exact implementation would most likely have to differ among the experiments. Discussions and sharing involved in this latter scenario is more appropriate in an inter-experiment “forum” like the recently developed Inter-experiment Machine Learning Working Group at CERN [58]. The sharing of code and other technical details, in addition to ideas and results, is essential in order to expand the benefits to the entire community.

Most current work is focused on using multi-objective regression and generative networks on simple events, such as single particle calorimeter showers. Even though these are the most basic events to simulate, more complex observables can be built as straightforward combinations of single particle showers. In all cases, one must choose an output, whether a general type like an energy deposit that might be common to many experimental simulation applications, or a specific type like the detector response that would presumably be applicable to only one experiment. The technique and methodology, however, can be shared among experiments even when their output formats differ.

The applications of machine learning are numerous, and the coming period will involve a detailed exploration of many different approaches to improving or speeding up the simulation using machine learning tools. Within ATLAS, for example, neural networks are being explored as a replacement for the histograms used in fast calorimeter simulation mentioned earlier. This type of machine learning tool could also be applicable to the storage of cross-sections within Geant4, for example.

While these techniques are quite promising, these are early days, and detailed speculation about the adoption of machine learning across the field is difficult. The fact that machine learning tools like SciKitLearn [59] and TensorFlow [60] are being developed by professionals and in an open-source community means that if the simulation community takes full advantage of these publicly available tools then the optimizations and developments of the broader community will be immediately useful. Already, the parallelism of standard machine learning tools used to implement GANs have made it possible to foresee significant improvements from parallelism and vectorization, even with current simulation frameworks based on Geant4.

The first neural network-based fast simulations are now publicly available, along with code, documentation, and training data [56,57]. These first results are very promising and establish a baseline for continuing to improve the performance in preparation for integration into real experimental settings. Dialog between and within the experiments has been, and will continue to be, important to push these techniques forward.

There are two related approaches for replacing or augmenting fast simulations with generative models. One approach is to construct tailored architectures that are specifically designed for all or part of a particular detector geometry and detector response. Another approach is to develop generic tools that can be adapted for universal or common aspects of simulation in many experiments. It is likely that a synergy of both approaches will be required to extract the most performance from state-of-the-art methods. The GeantV collaboration already has an active program to develop generic tools for this second approach. Within the GeantV project, it is planned to develop a general interface where a user can specify a physics process and detector type and get back an optimal trained machine-learning model that will simulate the detector response. Such a tool, once developed and validated, will be usable with any transport Monte Carlo, including

Geant4 with its well-developed fast simulation interface. The GeantV R&D program also includes tests of the generative neural networks in the context of Geant4. The tool will incorporate various trained machine learning models, predictive clustering trees and generative neural networks. Early studies have shown that choosing heuristically a network layout and then training it may not lead to the expected results. The fundamental parameters of the network need to be adapted to the problem under study. This opens the possibility of introducing some of the parameters defining the network structure among the quantities to optimize in the training process. Although this moves the whole optimization process one step further by introducing a meta-optimization that can be accomplished in the same step or in alternate steps to the more traditional network training, it offers the possibility to go beyond the one-size-fits-all in Machine Learning. This will remove part of the arbitrariness in choosing a given network structure, and will provide the opportunity to control the trade-offs between accuracy of the results and training and computation time. In ML parlance, this is called an embedded algorithm, where the information from the feature performance is fed back to the algorithm building stage together with the meta-optimization, usually called *hyper-parameter tuning*, leading to problem-specific optimized classifiers. If successful, this could provide an opportunity for shared not only techniques but also work among the experiments, as the meta-optimization could account for some of the differences between detectors and targets.

While the focus in this section and in the literature so far has been on using machine learning to do fast simulation (e.g. learn Geant4), it may be possible to train a generator directly on data to replace or augment full simulation. This would require high fidelity testbeam data for a variety of particles and energies. While this is beyond the scope of this CWP, we suggest that this be pursued in parallel to improving the speed and accuracy of fast simulators.

10.4 Sharing of Fast Simulation and Interfaces

At the moment, simulation toolkits like Geant4 provide interfaces for the experiments to “hook in” their fast simulation code. These have proven sufficient for very simple fast simulations. Because many aspects of fast simulation depend on experiment specific issues (not just in terms of detector technologies, but in terms of actual C++ types used, as in many cases intermediate classes are bypassed to save time), it can be difficult to find commonalities. However, the techniques, approaches, and methods, as well as some of the issues encountered during implementation or understanding of the tuning of fast simulation, can be common among the experiments. A forum in which such issues could be discussed would be very useful, particularly as machine learning techniques become more widely adopted.

In GeantV, fast simulation is being integrated as a user process, offering the same flexibility as in Geant4 to combine fast with full simulation. The fast simulation processes will get as input the full track state information, allowing to limit the step length and therefore select particles for performing the user-defined fast simulation based on arbitrary selection criteria, such as particle type, energy, detector, etc. As in the case of Geant4, it will be possible to have physics lists per region, which in case of fast simulation gives extra flexibility for implementing some use cases. The main difference however will be the possibility to put fast simulation in the multi-particle vectorized flow. As any physics model, fast simulation will provide not only a scalar interface (allowing the user code working with Geant4 to work also with GeantV), but also multi-particle interfaces. The fast simulation user models that are vectorized will be able to benefit from data and code locality, as well as instruction level parallelism as any other component of GeantV, while the scalar models will be still usable.

11. Pseudorandom number generators

The use of sequences of pseudo-random numbers is critical for all Monte Carlo simulations. In simulating particle and radiation transport the use of pseudorandom number generators is a vital component. The large number of random numbers required in the simulation of LHC and other High Energy and Nuclear Physics (HENP) detector events, as well as simulation in other fields, and the need to obtain statistically correct estimate while simulating with a large or very large degree of parallelism present challenges in the selection and use of pseudorandom number generators (PRNGs).

Reproducibility is a key requirement of HENP simulation i.e. when repeating the simulation of an event with the same input particles, with the same state of a PRNG (in the same geometry and with the same physics models), the simulation must provide exactly the same results, i.e. the same values for all observed quantities. Moreover it is required because it allow problems to be located and debugged. It enables the verification of new experiment software versions when based on the same simulation release (e.g. Geant4 release 10.3 patch 1) and even of new hardware, given the same binaries.

The results must be statistically equivalent for all PRNG, and obtaining different results with any PRNG is a clear signal that at least one of the PRNGs is not adequate for the simulation. Correct results require that the sequences do not contain correlations.

Sequential runs of detector simulation in one process, e.g. using Geant4, only require a single initialisation of a PRNG at the start of a simulation run. The state of the PRNG at the start of an event can be recorded, and stored with the event, to enable its reproduction.

In event-parallel multi-threaded simulation, such as multi-threaded Geant4, reproducibility means that each event must be provided with a deterministic seed (or state), typically created at the start of the simulation. This method is a simple extension of event seeding used in experiment grid productions.

Nevertheless only some PRNGs offer guarantees for the correlation of such sequences. Thus tests to ensure that all simulation results are unaffected by changing the type of PRNG engine is strongly advised. This use is similar to the research on parallel PRNG for use in other fields [61]. A recent survey [62] covers developments for parallel PRNGs, including ones for GPUs.

When each track of an event can be simulated in different order, as in the case of the GeantV simulation design, the state of the PRNG must be attached to a track. This requires memory proportional to the size of the state of the PRNG and to the number of tracks in flight. This excludes the use of PRNGs with large state. A number of potentially suitable PRNG classes have been identified, including counter-based PRNGs, such as Random123 [63], Combined Multiple Recursive Random number Generators (CMRGs) [64] and the newest extension of the MIXMAX PRNGs [65] with small matrix size.

These new families of PRNGs are largely untested in radiation transport simulation, yet are at the forefront of PRNG 'technology' for use in parallel applications. Thus a key aim should be to obtain implementations compatible with current interfaces (CLHEP and ROOT) so that they can be tested in large scale simulations, before their use become necessary in the transition to large-scale or fine-grained parallelism.

One of the methods for seeding parallel threads is to create sub-sequences from a single PRNG with a very long period. The mechanism for choosing a subsequence, whether it depends only on the sequencing of tracks or on additional transport parameters, and its computational cost are areas of active investigation. The resulting algorithms to generate a new state for each daughter track, must be validated in trial simulations.

In addition, the new C++11 <random> interface and its implementations must be considered. These have not yet seen widespread use in simulation. Trials within the Root project raised an issue with the performance of distributions that output floating point numbers (single and double precision) for several popular generators. If these findings are confirmed, we must seek to create faster, lower precision, distributions for floating point numbers for particular generators. In current practice a single function call is used to obtain many variates (output numbers) in performance critical code. Investigations will be made as to whether it is possible to create similar functionality by designing and implementing a new type of distribution object, or obtain similar performance benefits in a different way.

The future programme of work in the field of PRNGs includes the following:

- Ensure that performant implementations of additional state-of-the-art PRNGs are made available, in particular PRNGs which have been shown to have none or minimal correlations between separate sequences or subsequences.
- Promote the replacement of obsolete PRNGs currently in use in HEP experiments, including HepJamesRandom, RanECU, whose periods are small by the standards of today's computing power, and the number of output numbers required in typical event simulations.
- Create vectorised implementations of PRNGs for use in sequential, event-parallel and track-parallel (fine grained) simulations.
- Develop a single library containing sequential and vectorised implementations of the set of state-of-the-art PRNG, to replace the existing Root and CLHEP implementations within 3 years. This includes counter-based methods, the MIXMAX family of generators, improved implementations of RANLUX, implementations of CMRGs and other categories of sequential and parallel PRNGs. Promote a transition to the use of this library to replace existing implementations in ROOT, Geant4 and GeantV.
- Collaborate with the authors of the state of the art PRNG testing suites, and in particular TestU01[66], encouraging and seeking to contribute to the extension to increase the statistics of testing, extend testing to 64-bit variates, and expand the testing of correlations between sub-sequences.
- Follow and contribute to the evolution of the field of PRNGs for parallel and highly parallel applications, collaborating with researchers in the development of PRNG, seeking to obtain generators which address better our challenging requirements.

- Investigate whether poor PRNGs, or PRNGs with few, known deficiencies can create erroneous results in the particle-transport simulation of simple setups.

12. Summary and outlook

In this note we have attempted to describe the main challenges and opportunities for Full and Fast simulation applications of HEP experiments in view of planned future experimental programs in the next decade; these include the HL-LHC, neutrino and muon experiments, and studies towards future colliders such as FCC and CLIC. The combination of additional physics models and higher precision in the simulation with the need of larger Monte Carlo samples, which scale with the number of real events recorded in future experiments, place an additional burden on the computing resources that will be needed to generate them.

A multi-prong approach is being followed as a strategy for responding to these challenges. Firstly Geant4 will continue to deliver new or refined functionalities both in physics coverage and accuracy, whilst introducing software performance improvements whenever possible. At the same time, an R&D programme is investigating new approaches that aim to benefit from modern computing architectures. Its main feature is track-level parallelisation, bundling particles with similar properties from different events to process them in a single thread. This approach combined with SIMD vectorisation coding techniques and use of data locality is expected to yield large speed-ups, which are being measured in a realistic prototype under development. In addition, the work on Fast Simulation is accelerating with a view to producing a flexible framework that permits Full and Fast simulation to be combined for different particles in the same event. The overriding requirement is to ensure the support of experiments through continuous maintenance, support and improvement of the Geant4 simulation toolkit with minimal API changes visible to these experiments at least until production versions of potentially alternative engines, such as those resulting from ongoing R&D work, become available, integrated, and validated by experiments. The agreed ongoing strategy to meet this goal is to ensure that new developments resulting from the GeantV R&D programme can be deployed immediately in Geant4.

Improving the speed of simulation codes by an order of magnitude represents a huge challenge. However the gains that can be made by speeding up critical elements of the common Geant4 toolkit can be leveraged for all applications that use it and therefore will have a big impact on computing resource requirements. It is important to note that the current effort level available in the community is barely sufficient to keep up with the maintenance and improvements required by current and future experiments. It is therefore of critical importance that the whole community of scientists working in the simulation domain continue to work together in as efficient way as possible in order to deliver the required improvements. Very specific expertise is required across all simulation domains, such as the physics modeling, tracking through complex geometries and magnetic fields, and building realistic applications that accurately simulate highly complex detectors. Continuous support is needed to recruit, train, and retain the person-power with the unique set of skills needed to guarantee the development, maintenance, and support of simulation codes over the short, medium, and long timeframes foreseen in the HEP experimentals programmes.

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