A Vision on the Status and Evolution of HEP Physics Software Tools

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1 Introduction

This paper represents the vision of the members of the Fermilab Scientific Computing Division’s Computational Physics Department (SCD-CPD) on the status and the evolution of various HEP software tools such as the Geant4 detector simulation toolkit, the Pythia and GENIE physics generators, and the ROOT data analysis framework.

We do not intend to present here a complete and balanced overview of current development, planned or potential R&D activities associated with the HEP software tools, since we would need to get many individuals and institutions around the world involved in the process for the summary to be representative of the thinking of the whole HEP community. Instead, we present a vision that expresses opinions and interests of the members of the SCD-CPD at Fermilab.

The goal of this paper is therefore to contribute ideas to the Snowmass 2013 process toward the composition of a unified document on the current status and potential evolution of the physics software tools which are essential to HEP.
2 Generator

2.1 Introduction

Monte Carlo event generators have long been an essential tool in high-energy physics. They are applied at almost every stage of an experimental program: for design, for collecting data, and for interpreting data. An example of their impact is the fact that the manual for the *PYTHIA* event generator was the most highly-cited publication in high-energy physics for 2012.

A primary goal of particle physics is to determine the Lagrangian which describes particle interactions at short distances. Since the effects of long-distance physics cannot be calculated from first principles, the event generator must invoke models and parametrization in the translation from short- to long-distance physics.

In developing an experimental program, event generators are often important for determining what kind of accelerator (beam types and energy) is necessary for answering a particular theoretical question. Enough was known about the \( Z \) boson to determine that a high-energy hadron collider was the best machine for discovery and a lepton collider tuned to the measured mass was the best machine for measuring its detailed properties. However, the case for how to understand electro-weak symmetry breaking is not as clear. The fact that many viable proposals for physics beyond the Standard Model involve weakly-interacting particles further complicates the issue. Event generators allow physicists to run toy experiments and make judgments on the most promising experimental program.

Event generators also play a part in detector design, especially when extrapolations must be made to unexplored energies. Educated guesses must be made regarding the production of charged and neutral energy in time and space. For example, the occupancy of a silicon detector must be known to determine an optimal distance from the beam pipe.

When running an experimental program, decisions must be made on how to collect data. Event generators give estimates of the production of event topologies that can be used as trigger signatures and evaluation of alternative schemes.

Most detectors have limited angular and energy coverage. Particles can be lost because they are produced particular directions, or at too low of an energy or because of detector inefficiencies. Event generators are used to estimate these acceptance effects.

2.2 Software

Event generators are integrated into the computational framework of an experiment so that their predictions can be treated on an equal footing with data. This means that the software should act as a library. For some given configuration data, which specify the parameters of the physics model, the event generator returns a list of particles (including information about the particle type, momentum, production vertex, etc.) that can be used as an input for a detector simulation.

In the past, event generators were mainly written in *FORTRAN*. Currently, *C++* versions of the major event generators exist, though they are used interchangeably with some of the older *FORTRAN* codes. The main reason for this is that the *FORTRAN* codes have been validated and tuned to data to provide reliable predictions. Thus, despite the computational advantages of using programs written in a modern language, the physics content of the program is an important consideration.

The codes produce theoretical (or Monte Carlo truth) event records of the underlying interactions, a combinations of the incoming particles, intermediate states and the long lived final state particles leaving the interaction. Usually a number of events are generated and then propagated through a detector simulation. The output of the detector simulation is a record that is mostly indistinguishable from the recorded data. The event generator can operate in such a fashion because many of the physics processes can be simply coded and sampled using Monte Carlo techniques. However, this structure has become less attractive as more advanced and detailed calculations are required.

In some instances it is sufficient to generate lots of events and use more crude smearing, rather than detailed detector simulations, to explore the potential for discovery in various physics scenarios. In such cases it is important that the generator be efficient. In some experimental setups, such as neutrino experiments, the interaction region is diffuse and not a central crossing point; in such cases the generator is needed to determine where the neutrino probe interacts with the target nucleon within the detector apparatus.

Most of the recent advancements in predicting Standard Model processes has come at the stage of the event de-
development where fixed-order, perturbation theory can be applied. This piece is known as the hard interaction, and the predictions coded into the event generators are typically those at the lowest order of perturbation theory. The higher-order, more-accurate predictions are computationally intensive and often require specialized code. The other pieces of event generation, such as the parton shower, multi-parton interactions, hadronization, nuclear breakup and decays must also be handled by the event generator models.

For generators used by collider experiments much work has gone into interfacing the calculation of the hard interaction beyond the lowest order with the event generators. Mostly, this is accomplished by passing the output of the higher-order calculation into the event generator through files. This adds the complication that the hard-interaction files must be coordinated with the running of the event generator.

Alternatively, software can be rewritten to perform both the calculation of the hard interaction and the other aspects of event generation. This has certain practical limitations. One is that executable must increase in size as the calculations become more extensive. This can become an issue on computing platforms with limited memory. A second is that many of the codes to calculate hard interactions are not engineered to fit easily into this model.

Examples of event generators used by HEP physics programs are PYTHIA and GENIE. The PYTHIA code is widely used in the collider programs both past and present and is continually being updated to supply users with desired simulations of numerous extensions to the physics models. The GENIE code was developed to consolidate a number of competing neutrino event generators and provide a framework for adding extensions and modeling of more complex or rare processes.

2.3 Future

As more detailed calculations are required to better understand the theoretical implications of HEP data, the event generators will face the problem of complexity and timing. Timing is usually not considered an important issue, because detector simulations are usually orders-of-magnitude slower. However, there are several reasons why the execution speed of the event generators matter. First, code can be developed and validated in proportion to execution speed. Second, the tuning process – when the parameters of the event generator are varied to match data – is facilitated by speed. Thirdly, the calculation of systematic uncertainties for an analysis typically requires running the event generators several times, each with different configurations.

The problem of complexity may be solved by optimizing code design. Currently, the theorists who develop code do not coordinate with computing or experimental experts. We should promote communication between these different communities.

Improvements in timing can arise from the intelligent application of multi-core processors or GPU’s. Already, GPU’s have been successfully employed in calculating many-parton Feynman diagrams, and we should look for other, practical uses. The possibility of performing multi-core calculations does not currently look fruitful, because the event generator codes are structured serially – typically one step of a calculation must be completed before the next. However, this could be the result of the code design. A successful merging of the theory and computing communities may find avenues for improving the design of event generator codes.
3 Root

3.1 Introduction

ROOT \([1]\) is an object-oriented C++ framework that is designed to store huge amounts of data in an efficient way optimized for very fast data analysis. Any instance of a C++ class can be stored, in a machine independent compressed binary format, into a ROOT file. The ROOT TTree object container is optimized for statistical data analysis over very large data sets by using vertical data storage techniques. The TTree containers can span a large number of files. These files may be on local disks, on the web or on a number of different shared file systems. The users have access to a very wide set of mathematical and statistical functions, including linear algebra, numerical integration and minimization. For example the RooFit library allows the user to choose the desired minimization engine. In addition, the RooStat library provides abstractions for most used statistical entities, supporting all their operations and manipulations. ROOT also provides 1D, 2D and 3D histograms that support any kind of operation and can be displayed and modified in real-time using either a interactive C++ interpreter, other interactive language like python or a graphical user interface. The final result can be saved in high-quality graphical formats like PostScript and PDF or in bitmap formats like JPG that are easier to include into a web page. The result can also be stored into ROOT macros that can be used to fully recreate and rework the graphics. Users typically create their analysis macros step by step, making use of the interactive C++ interpreter, by running over small data samples. Once the development is finished, they can then run these macros, at full compiled speed, over large data sets by either using ACLiC (the automatic compiler interface) to build a shared library that is then automatically loaded and executed, or by creating a stand-alone batch program. Finally, if processing farms are available, the user can make full use of the inherent event parallelism by running their macros using PROOF, that will take care of distributing the analysis over all available CPUs and disks in a transparent way.

ROOT is at the heart of almost all HEP experiments world wide. From simulation to data acquisition, from event processing to data analysis, from detector monitoring to event displays, it provides essential components and building block for the experiments to assemble their framework. In particular all the experiment’s data is stored in ROOT files. At the time of writing there were already more than 177 PBs of data for just the Large Hadron Colliders experiments. The use of ROOT extend beyond HEP to many sciences, including nuclear physics, biology, astronomy and even in the private sector where many finance firms use ROOT in their own data analysis and market trend prediction software tools.

3.2 Root for the Future

Building on years of success, ROOT is in the mist of a significant migration to future proof its architecture and code base. ROOT is replacing its existing home-grown C++ interpreter (CINT) \([2]\). CINT has been since its inception in the early 1990s, the premier solution for C++ interactivity, offering access to most of the features of the C++ 2003 standard while providing a very simple and portable to use solution to access any compiled code from the interpreter session. Upgrading CINT to support the large number of extensions in the 2011 C++ standard would have required a very large efforts. In addition CINT architecture was not designed to support heavily multi-tasking processing.

To address CINT’s limitations, ROOT is leveraging the rise of a very flexible and very programmable compiler framework, LLVM \([3]\), which includes a fully C++ 2011 standard compliant compiler (clang). Clang and LLVM have become industry standard tools supported and relied upon by a large set of commercial companies including Apple, Google, Nvidia, etc. Using clang and its versatile libraries, ROOT is developing a new C++ interpreter (cling) to replace CINT.

Migrating to the new interpreter will open up a host of new opportunities. Since it is based on a flexible and expandable compiler framework, cling can easily be extended to support additional languages, including objective C or NVidia’s CUDA programming language. Rather than a classical interpreter, Cling’s implementation is closer to an interactive compiler. Once processed, any code input on the command line is slightly transformed and then compiled in memory using the Clang compiler, the same compiler currently used to build all of MacOS’ components. The seamless availability of just-in-time compilation of C++ code enables a large set of possible optimizations, including boosting I/O performance by optimizing specific uses cases of the currently running application, improving the minimization’s algorithm’s performance by customizing and recompiling the hot-spots of the current search. In addition, the migration will enable the library and the users to start using the many performance and code improvements allowed by the new 2011 C++ standard.

In conjunction with this major migration, ROOT is also preparing for the newest set of hardware platforms. Several
efforts are in place to leverage general graphical processor units, in particular to speed up minimization algorithms. The internal mathematical libraries are being upgraded to take advantage of vectorized processing units, including incorporating and using the VC (Vector Classes) library [4]. ROOT has been recently ported to both the ARM and Xeon Phi architectures which should both benefit from the on-going vectorization efforts.

As the number of individual cores offered in each processing unit is increasing rapidly, the need for multi-threading and multi-processing solutions is becoming greater. ROOT is planning on offering multiple alternative for parallelizing the Input and Output. One medium term alternative is to provide for fast merging of files produced in parallel. In this scenario rather than write the files locally and wait until all producers are finished to start the merging process, the merging process is started as soon as the producers have created a medium size chunks of data (dozens of megabytes). Once the merging process has started, rather than writing the data to local disk, the data is send directly to the server to be written into the final file and then to disk, avoiding many unnecessary reads. Longer term solutions include upgrading the infrastructure to support the seamless writing from multiple producing stream within the same process into a single file. Solutions will be developed in close collaboration with the main users in order to ease their transition to the many-cores era.

### 3.3 Conclusions

ROOT is at the core of HEP software as well many other science and industry frameworks. Its migration into the many-core era is an essential stepping stone to enable the eco-system that has been built upon its libraries to flourish and benefit from the newest hardware generations. Many of its features, including a unique customizable framework to efficiently store and retrieve extremely large data back and forth between persistent storage and live representation in C++ while supporting significant schema evolution, are fundamental to many currently running and upcoming experiments and any improvements in ROOT libraries will greatly benefit them.

Upgrading ROOT infrastructure is a challenging balancing act of enabling new technologies while supporting existing use patterns to avoid disruption to running experiments. However any investment and progress towards using, enabling and promulgating modern, multitasking coding patterns will flow through all software layers involved in the experiments. Both framework developers and individual researchers will benefit from the examples and leads that ROOT can provide.
4 Geant4 R&D

4.1 Introduction

Precise modeling of particle interactions with matter in systems with complex geometries is essential in experimental high-energy physics (HEP) and certain accelerator and astrophysics applications. Because of the impact of this type of simulation, it is imperative that the HEP community has access to computational tools that provide state-of-the-art physical and numerical algorithms and run efficiently on modern computing hardware. Geant4 [5] is a toolkit for the simulation of particle-matter interactions that has been developed for almost twenty years by an international collaboration of physicists and computer scientists. The most commonly used simulation tool in experimental HEP, Geant4 incorporates physics knowledge from modern HEP and nuclear physics experiments and theory.

The computing landscape continues to evolve as technologies improve. Modern-day computers used to support High Energy Physics (HEP) experiments now have upwards of 32 processors on a single chip, and that trend will only continue. Furthermore, new generations of computing hardware such as Graphics Processing Units (GPUs) are emerging for markets like the enhancement of end-user experience in gaming and entertainment. Their highly parallel structure makes them often more effective than general-purpose central processing units (CPUs) for compute-bound algorithms, where processing of data is done in highly parallel manner. This technology has great potential for the high-energy physics community.

The current implementation of Geant4 contains many features that hinder our ability to make use of modern parallel architectures since Geant4 relies heavily on the object-oriented features of C++ for developing class hierarchies. Of particular significance is the use of global resources and the complexity they introduce into the management of program and processing state. Such an arrangement makes parallelism through threading difficult. Other contributing factors are its heavy reliance on C++ inheritance, abstract interfaces, and organization of of data structures.

The diversity among these forthcoming machines presents a number of challenges to porting scientific software such as Geant4 and achieving good performance. Extrapolating to the situation over the next several years, we anticipate more cores per chip, and these will likely be a heterogeneous mix of processors, with a few optimized to maximize single thread throughput, while most are designed to maximize energy efficiency with wide SIMD data paths. The Advanced Micro Devices (AMD) Fusion family of Accelerated Processing Units (APU), blending Opteron CPUs and Radeon GPUs, is just the beginning. This trend will not only exacerbate performance optimization challenges, but also simultaneously promote the issues of energy consumption and resilience to the forefront. Moreover, as new memory technologies (e.g., phase change, resistive, spin-transfer torque) begin to appear, computational scientists will need to learn to exploit the resultant asymmetric read/write bandwidths and latencies.

4.2 Geant4 Research and Development for the Future

To address both the scientific and the computing challenges facing Geant4, it will be essential to bring together expertise in physics simulation and modeling with specialists in software systems engineering, performance analysis and tuning, and algorithm analysis and development. The overall goal is to move Geant4 into the era of multi-core and many-core computing, effectively utilizing existing and future large-scale heterogeneous high-performance computing resources for both core science simulation data-set generation and also data-set storage, retrieval, and end-user validation and analysis.

Significant exploration and study is needed in order to move the Geant4 toolkit toward the long term goal of being able to utilize large-scale, heterogeneous computing systems, as it was designed for much simpler platforms. Thus the need for complete studies and work towards a re-engineering of the underlying system software framework that retains connections to crucial existing applications and physics libraries while permitting migration and transition to a new improved construction. An extensive reorganization of the underlying coordination framework will allow for more diverse processing options (e.g., GPUs) and allow for greater flexibility as computing resources evolve.

While exploring concurrency, part of the focus should be on abstracting the overall structure of the Geant4-based codes in terms of computational flows, algorithms and models. This analysis can be used to enable the development of code generation schemes and execution strategies targeting future high-performance architectures.

To enable the use of multiple concurrent and heterogeneous execution units, Geant4 needs to be re-engineered to have at its core a concurrent particle propagation engine. Integration of the equations of motion and determination of particle interaction has very different structures and computational requirements. Thus a smart dispatcher is
required that can dynamically adapt to its run-time environment, scheduling bundles of work for resources best
suited for the operation to be performed. The coordination framework must also permit asynchronous interactions
amongst the internal components and with the surrounding application software infrastructure necessary for event
processing. Such an arrangement allows for more rare and complex particle interactions to not interfere with more
common, less resource-intensive ones.

Figure 1 depicts a possible structure for such a concurrent particle propagation engine. A track bundle is a set
of tracks that can be conveniently and efficiently scheduled to go through the same set of processes which could
potentially include propagation. The role of the track dispatcher is to assemble the tracks in bundles in such a way
as to maximize the efficiency of the processes that run on them. The dispatcher also selects which processor or
group of processors or cores, for example a GPU enhanced PC cluster, to schedule the execution of the processes
for a specific track bundle. In order to leverage the on-chip and on-core caches of general purpose CPUs, the
dispatcher might decide to associate a set of geometrical elements with a specific processor/core and to send to
this processor/core only the bundle of tracks that are traversing these geometrical elements. It might also gather
together tracks that need to go through processes that have been optimized for GPUs and send them to one of the
graphics cards. Once the tracks are done going through the simulation, they are added to another stack, which can
also be handled in parallel, to run processes that require all the finished tracks for a given simulation event, for
example to digitize the energy deposit on the detector elements.

![Figure 1: Simplified view of Geant4 re-engineered processing entities.](image)

Real-world Geant4 program traces can be used to drive prototype propagation components. A fundamental change
in strategy will be required, removing the event-by-event and particle-by-particle processing ensconced in the
current framework. A new strategy will remove these boundaries and allow large particle vectors to be assembled
across event boundaries where this would enhance processing efficiency on the target hardware architecture.

A key aspect of this work is adherence to science constraints. Two important ones are validation of the physics
and reproducibility. Validation tells us that the modules we are working with give answers that are in statistical
agreement with experimental measurements, or at least in agreement with answers from the previously validated
code. Reproducibility means that results can be regenerated within a tolerance defined by the scientific community
of users a bit-for-bit agreement where possible. Both validation and reproducibility are likely to be affected by
parallelism and non-deterministic processing characteristics. Reproducibility will need to be precisely defined by
working with the physics collaborations. One area of difficulty will be in random-number stream management. A
strategy could be defined to prevent bottlenecks where random numbers are used and to record necessary seeds to
allow replication of results. Deviations in results, including measurement uncertainties should be studied.

Geant4 would also benefit from research required to optimize I/O in heavily multi-threaded systems. In particular,
it is important to understand what data-organization tasks can be achieved by the simulation itself and what tasks
would be more efficiently performed by separate IO run-time services focused on data collection and organization.
4.3 Conclusions

Geant4 is an important software tool for the HEP community as well as many other communities. As experiments evolve, the demands on both the amount of simulated data as well as precision of the simulations will grow. Geant4 must evolve in order to both take advantage of the emerging computing technologies and to be able to meet the future simulation demands in a cost effective way. Furthermore, this evolution of Geant4 will enable HEP experimental scientists to take advantage of current leadership class computing that is available but not utilized by this community.

Transforming Geant4 will require research to overcome a broad range of challenges of which categories include systematically improving the sequential performance of Geant4; re-factoring the code for emerging, highly parallel computing systems; improving data access, management, and analysis; exploring novel new programming abstractions, and reducing the human effort required to handle the upcoming, Exabyte-scale, globally distributed, data sets generated by Geant4.

There appear to be opportunities for near-term performance enhancement on individual processors, as well as more profound, long-term changes that would lead to a new Geant4 that effectively exploits a variety of future multi-core systems. Taking Geant4 to the next level in terms of parallelization is paramount for HEP scientists. The next generation of experiments will demand it and the current ones would profit greatly.
References

[1] Rene Brun and Fons Rademakers, ROOT - An Object Oriented Data Analysis Framework, Proceedings AIHENP'96 Workshop, Lausanne, Sep. 1996, Nucl. Inst. & Meth. in Phys. Res. A 389 (1997) 81-86. See also http://root.cern.ch/

[2] See http://root.cern.ch/drupal/content/cint

[3] See http://llvm.org/

[4] See http://code.compeng.uni-frankfurt.de/projects/vc

[5] http://geant4.cern.ch
Stream A (independent work flow)

Preprocessing (Mixing, Noise, ...)

Geant4 module

Generator Event Stream

Subsystem communication boundary

Each can use multiple threads

Can execute in parallel

Tracks from one event

Stream B (independent work flow)

Preprocessing (Mixing, Noise, ...)

Geant4 module

One event: one readout of the entire detector