# HL-LHC Analysis With ROOT

ROOT Project Input to the HL-LHC Computing Review Stage 2

# The ROOT Team, September 2021

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This document was prepared by ROOT Collaboration using the resources of the Fermi National Accelerator Laboratory (Fermilab), a U.S. Department of Energy, Office of Science, HEP User Facility. Fermilab is managed by Fermi Research Alliance, LLC (FRA), acting under Contract No. DE-AC02-07CH11359.

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## 1 Introduction

The HL-LHC analysis is expected [1] to be similar to Run 3 analyses, with more events (data and simulation), possibly higher number of samples (multiple background channels, side-band channels from data, comparing more collision event generators, higher number of data skims), higher complexity of fits due to more precise models with higher parameter counts, and more common usage of Machine Learning to improve the physics performance of analysis algorithms. As a consequence of more complex fits and the usage of machine learning, ROOT expects a further increase in the usage of GPUs and possibly other accelerators such as TPUs.

ROOT is preparing for HL-LHC analyses through a series of R&D tasks started several years ago, to be able to address these challenges in the form of an integrated solution. It will do this in time for HL-LHC, given the resources and ROOT's experience with a sustainable feedback and development velocity, and the adoption rate in the physics community. Several of these undertakings are massive (in ROOT's scale) with respect to the required effort and expected impact.

Until now, ROOT has provided the core ingredients for virtually all LHC analyses. Because of its role as "integrated analysis foundation library", much of ROOT can be used by ROOT itself, increasing the impact of its own developments: all of ROOT's features are optimized with respect to  $I/O$ ; many make use of ROOT's visualization abilities; fundamental features such as just-in-time compilation and network calls are enabling fundamentally new features such as remote event displays.

Being a central element of the HEP software ecosystem, ROOT sees many contributions, from volunteer, occasional improvements to institutionalized cooperation. Whatever the contribution, it will become part of ROOT only if the contribution is relevant to the community as a whole. Or, conversely, any successful contribution to ROOT has a large impact on the community, multiplied through the tens of thousand physicists and virtually all HEP experiments, world-wide.

Given the experience and expertise of the ROOT project, ROOT believes the main HL-LHC analysis challenges to be:

- Data: high-throughput, local and remote data access to reduce the impact of analyses' traditional I/O bottleneck.
- Efficiency and simplicity: making it obvious for physicists how to write an analysis with faster time-to-results.
- Robustness and correctness: providing results that can be trusted and published
- Interoperability: enabling physicists to use the language of choice, with the packages of choice, without sacrificing performance or simplicity.
- Sustainability and Innovation: investing in solutions that the community can benefit from for the next decades.

This part of the document introduces the main analysis challenges as perceived by the ROOT project, alongside their potential remedies with associated risks.

# 2 Analysis Ecosystem

ROOT continues to be a catalyzer for an analysis ecosystem around it. At the same time, Python is expected to become the dominating HL-LHC analysis language, and ROOT is further integrating into a wider Python ecosystem. ROOT works towards strengthening both aspects - by providing the integrated, fundamental ingredients targeted at HEP that enable ecosystems to grow around it, and by providing smooth interoperability to the Python analysis ecosystem in a reusable way for easy integration with emerging ecosystems such as Julia.

## 2.1 Machine Learning

Most primary machine learning (ML) interfaces are written in Python, encouraging the transfer of large amounts of data for instance to GPUs which then internally run non-Python code. ROOT works towards the integration with such frameworks, specifically PyTorch and TensorFlow's generator interface, to have simple and highly efficient user-facing interaction between ROOT's analysis interface RDataFrame and ML tools. This benefits from ROOT's ability to optimize the HEP I/O layer. Examples include ROOT's ability to arrange for in-memory data layout and alignment that corresponds to on-disk layouts, reducing or removing the need for CPU cycles when transferring data into GPUs.

Investment in this area (1.5 FTE over 3 years) is needed for the analysis community to benefit from ROOT's I/O layer, and to create a performance and usability benefit so significant that analysts do not migrate to less performant options due to a perceived increase of productivity. It is trivial for physicists to find examples for use of machine learning for instance from data in text format. Without additional benefits and clear, communicated advantages, large parts of the community will adopt less efficient (in terms of CPU and storage-space requirements) approaches simply because of their much higher online presence. This is an inherent risk of the wider adoption of Python as the preferred analysis language, with a transformation away from the single, community-agreed, consistently designed, integrated and performance-conscious analysis framework, to an ecosystem of literally thousands of potential building blocks  $[https://pypi.org/]$  $[https://pypi.org/]$  $[https://pypi.org/]$ . Investment in this area  $(0.5$  FTE over 4 years) can help reduce the residual risk that comes with Python becoming the primary analysis language, which is nowhere as visible as in the context of machine learning, and which we expect to continue during HL-LHC.

ROOT's role with ML must thus be to integrate external machine learning libraries with ROOT's I/O and analysis facilities. This requires expertise in Python and C++, ML, GPUs, as well as code and memory layout optimization, as an ongoing effort (0.5 FTE/y). ROOT's R&D on [RNTuple](https://indico.cern.ch/event/999647/) (1 FTE/y over 3 years), [LLAMA](https://github.com/alpaka-group/llama) (0.5 FTE/y over 4 years), [cling-CUDA integration](https://resources.nvidia.com/events/GTC2020s21588) (0.1 FTE/y over 3 years) and [au](https://github.com/vgvassilev/clad)[tomatic differentiation](https://github.com/vgvassilev/clad) (0.5 FTE/y over 4 years) are significant building blocks in that respect. First results for RDataFrame-based training on GPUs are expected in 2022; ML-optimized RNTuple-to-GPU transfer leveraging above mentioned R&D will be implemented by 2024 (0.75 FTE over 2 years).

The optimization of machine-learning models is an interactive, user-facing activity. ROOT used to provide a GUI for the visual inspection of the training quality (for instance versus epoch). This has many users, but needs to be improved and ported to ROOT's new web-based GUI, with all its advantages. Work for this is underway  $(0.25 FTE/y)$ , and should complete by 2024.

Dissemination of optimal analysis approaches again underlines the necessity for ROOT's experts to be trusted and visible in the HEP ML and analysis community. It requires the continuous investment of a significant training effort, by said ROOT ML experts  $(0.25$ FTE/y).

#### 2.2 Python

Python is seeing a constantly increasing adoption rate as language of choice for analyses. It is important to understand that this is the *surface* layer: just as bash scripts steer programs for the computational work, Python code is ideally delegating resource-intense work to for instance  $C/C++$  libraries. With PyROOT, ROOT provides the "glue" used by HEP to make HEP's C++ libraries accessible transparently through Python. With significantly more than ten years of experience, ROOT has learned how to design C++ interfaces in a way that makes them good Python interfaces, too. A good example is ROOT's analysis interface RDataFrame, where virtually identical user code is written, be it in  $C++$  or Python [2]. While much of the (pseudo-) object oriented interfaces match nicely across languages, some idioms are language-specific and need to be adapted. PyROOT enabled this through a mechanism called "pythonizations": features added on top of the default bindings to make ROOT easier to use from Python, or in a more intuitive way for Python programmers.

PyROOT relies on a project called cppyy [3], a tool used for instance in computational biology. Cppyy in turn relies on ROOT's type description system and cling, ROOT's interpreter / JIT, to dynamically create the binding between Python and  $C_{++}$ . This binding layer needs to evolve with  $C_{++}$ , supporting new language features and data types. Significant expertise is required for this, in the areas of Python, and in cling and ROOT's type description system, which provide PyROOT with an answer to questions such as "which methods does edm::Collection <edm::Jet > have". Due to a lack of past investment, this layer has accumulated significant technical debt. The current state is hindering gradual evolution with minimal investment, and [limits PyROOT's performance and functionality.](https://bitbucket.org/wlav/cppyy/issues/5/requirements-for-use-of-roots-cling) Addressing this would require an investment of 1 FTE over 4 years.

The experiments' frameworks are aggressively embracing new C++ standards, cling and PyROOT are expected to support new features as quickly as possible. The continuous investment of  $0.5 FTE/y$  is necessary to prevent a reduction of functionality from Python, which in turn can mean usage migrating away from performant C++ libraries.

ROOT's interoperability with Python libraries such as NumPy is crucial for high performance data processing. ROOT plans to invest in a C++ container that allows data transfer directly into NumPy arrays. This work (0.25 FTE over 1 year) is expected to conclude by 2023.

ROOT remains a C++ program and library; yet - seeing the widespread use of Python in analyses - needs to ensure that ROOT can be used "naturally" from Python, in terms of interoperability (data formats such as NumPy), interface style, Python syntax, object ownership. This requires investment in existing and future C++ interfaces. It even stipulates the re-design of interfaces such as RooFit. Without such an investment, a fair part of the community is expected to migrate to alternative solutions. The number of available alternatives - even today - will cause a fragmentation of the community. This reduces the benefits of central investment; all known solutions have feature limitations, risking a reduced physics reach for analyses; solutions will not be easily applicable to other problems due to the expected feature segregation. To counter these risks, ROOT has invested significantly in PyROOT and for instance RooFit, to improve ease of use, stability, performance, support, documentation - in short: to reduce the physicists' need to migrate away. This effort needs to be maintained  $(1 FTE/y)$ , for ROOT to be able to continue to compete, and to reduce the residual risk of community fragmentation. At the same time, competition needs to be fostered, especially in the Python ecosystem, which sees much innovation (especially in interfaces) and can be a fruitful, effective ground for software experiments. This competition is input to ROOT's evolution, and allows to benchmark ROOT against alternatives.

For several of years now, ROOT has been [released also through Conda.](https://root.cern/install/#conda) This gives many Python users trivial access to ROOT. The notion of "ROOT is  $C_{++}$  and thus awkward to use in Python" needs to be overcome, by continuing to invest in simple distribution mechanisms and perfect embedding in Python ecosystems, making ROOT accessible in Python ecosystems as easily as any other Python packaged  $C++$  library (continuous 0.1 FTE/y).

What has been done for Python with PyROOT can be (and has been) done for other languages, in a similar way. ROOT's C++ interpreter / JIT compiler cling allows ROOT to create such language bindings dynamically for languages that might become relevant to HEP analyses in the future.

#### 2.3 Data Format

Up until Run3, the LHC experiments used ROOT files and TTrees; several, mostly small-scale, studies have questioned that and proposed alternatives. A more complete and in-depth review showed the advantages of ROOT's file format and TTree [4]. Nonetheless, these studies and for instance ROOT's experience with supporting I/O in multi-threaded environments have shown limitations to TTree. As ROOT's I/O subsystem guarantees backward compatibility (old ROOT files can be read with new ROOT versions) as well as forward compatibility (new ROOT files can be read with old ROOT versions), evolution of TTree is severely limited.

R&D on potential benefits of a new data layout for HEP, called RNTuple [5], showed improvements to transfer rate, storage size efficiency (see Fig. 1), robustness, and flexibility that are sufficiently significant to warrant the introduction of a new, evolved I/O subsystem for HL-LHC, see the *Foundation* part of the ROOT input. ROOT caters both to frameworks and analysis physicists. It was thus paramount to make RNTuple work exceptionally well also for analyses. RNTuple is expected to have a significant performance effect on machine learning (more than a factor 10 read throughput in training compared to TTree) and RDataFrame, ROOT's modern analysis interface (factor 2 in read throughput). These two standard ingredients of analyses are traditionally I/O limited and will benefit directly from RNTuple.



Figure 1. Fraction of storage size RNTuple vs. TTree for identical data content (CMS NanoAOD); lower is better.

ROOT expects to provide a tool converting TTrees to RNTuples in 2021 (0.2 FTE). For several years now, ROOT has been advocating and training physicists in the use of RDataFrame, also as an abstraction of the underlying data layout and to ease the migration from TTree to RNTuple. RDataFrame can process ROOT files containing TTrees just as well as ROOT files containing RNTuples. ROOT will continue to maintain the TTree interfaces. Nonetheless we expect to see a migration away from the use of low level TTree interfaces to RDataFrame, enabling optimizations and concurrency. After all, the data format will be defined by the experiments; it is ROOT's task to ensure a smooth migration is possible for physicists.

Alternative data formats continue to be used in HEP, although it is unclear whether their adoption is increasing. As analyses are probably the most agile part of HEP's software environment, they are expected to continue to try alternatives (HDF5, Parquet, etc), also in function of the tools and libraries used by analyses [6]. ROOT's goal is to preempt such re-formatting, which has consistently proven as a bottleneck for analyses' agility, preventing smooth integration of optimizations in the ROOT-part of the analyses, and increasing the storage needs for analyses. During the coming years, ROOT will continue to work on providing efficient and easy to use interfaces. Examples include interfaces to ML [7], for transparent use of multi-core and GPUs [2, 8], for distributed computing [9], to Python [10], and for data visualization.

#### 3 Empowering Physicists

ROOT's role is to facilitate analyses. Helping physicists get analysis results quickly, reliably, and with less resources, is what ROOT is striving to improve, constantly.

## 3.1 Analysis as Effective Use of Luminosity, Efficiency of Physicists, Time to Publication

There are two drawbacks in high turn-around times of analyses: on one hand, this simply delays the results, pushing what could be published in 2025 to 2026. This used to be perceived as a mere optimization issue. Being first or a runner-up seems to be of increasing significance to funding agencies, the public, and experiments as a whole.

On the other hand, the analysis throughput of physicists is a limited resource. Making physicists more productive simply means better use of luminosity. Or in other terms, the analysis efficiency should be considered as an integral part of the experiments' overall efficiency: it should not stop at reconstruction.

Increasing the physics reach of a typical PhD analysis should thus be an important goal for the community. This can be considered as part of the overall efficiency, and included in optimizations and upgrades. As detailed below, ROOT has the proven potential to measurably increase the effectiveness of analyses by factors, at a cost that is shared between experiments and that is far lower than investment in detector parts.

#### 3.2 Multi-Platform Support

Being mostly written in C++, ROOT's code can make efficient use of CPUs. This brings a certain platform dependence: compiled  $C++$  code will only work on a given set of architectures; optimized code might restrict this even more. ROOT strives to support as many platforms and operating systems as reasonably possible. It certainly intends to support all architectures and operating systems that are in production use, by experiments or a significant number of physicists. It currently supports GCC and clang compilers, up to the latest released versions; work is ongoing to also support the Microsoft Visual Studio Compiler (0.2FTE/y). The supported operating systems are Linux (Fedora, CentOS, Ubuntu, Debian) and macOS (up to the latest version, including the ARM M1 version); work is ongoing to support Windows. Architectures include Intel and AMD 64bit, Intel 32bit, ARM Aarch64; work is ongoing to ensure continued support of Power8 and Power9. ROOT is released by Linux distributions (or rather their package maintainers) on Fedora and CentOS EPEL, through Conda, Homebrew, and Snap. This service has been provided by the community for many years, and seems to demonstrate that ROOT is part of a solid, sustainable software ecosystem. To facilitate all of this, ROOT maintains a Continuous Integration and Testing / Continuous Release system  $(0.5 FTE/v)$ .

In the past, being multi-platform caused ROOT to contain architecture-specific code, such as X11 for Linux; Cocoa (including ObjectiveC code) for macOS, and GDK for Windows. This is expertise not needed elsewhere in ROOT, and the evolution of these platforms (such as macOS dropping X11 and GL support) forces ROOT to invest in these areas of (for ROOT) niche expertise. To address this, ROOT is developing HTML-based web-GUI and web-graphics systems, to succeed and eventually replace the architecture-specific GUI and graphics backends.

This was again tested and validated by Apple's recent move to its ARM-based M1 architecture: within a few days, ROOT was passing most of its own, extensive

test suite (>600'000 lines of code) on M1. In that respect, ROOT's Achilles' heel is the set of platforms supported by llvm and clang. It is reasonable to expect that clang, one of the major C++ compilers and tooling ecosystems, will always support HEP's main architectures. So far this has always been the case; for instance, Power9 support and Apple ARM M1 support appeared in clang/llvm before they were needed by ROOT. Nonetheless, ROOT's extensive and special use requires expertise to adapt to these new architectures and their support in clang/llvm.



Table 1. Operating systems and their architectures as supported by ROOT.

#### 3.3 Code Reuse and Preservation

Reuse of analysis code is common practice in HEP. Being a community-agreed standard tool with a strong focus on backward compatibility, ROOT helps with making code reusable. Frameworks that attempt to formalize analyses, claiming to ease analysis reuse and preservation, often increase the effective analysis complexity: they add multiple ingredients to define an abstract analysis on top of a wealth of libraries and software tools. ROOT prefers to reduce complexity, thereby guaranteeing evolution and support of future architectures.

The platform independence and backwards compatibility of ROOT's data format helps analysis preservation: old ROOT files can be read without issues by the most recent ROOT versions, even on the most recent chips such as Apple M1. By supporting as many platforms as possible, ROOT aims to help with preservation: new platforms will likely be similar to what ROOT already supports; migration should thus be feasible.

Being able to run ROOT on a future platform is not sufficient for preservation and longevity. The community must also retain sufficient technical expertise to address future challenges, such as for reading ROOT files into a new memory layout. The ROOT project's core team of long term contributors is essential in this respect.

The move towards event data models (EDMs) that can be read without accompanying experiment libraries is helping with preservation: this data can be read with ROOT alone, across decades. This approach has been beneficial to HEP already since PAW and ZEBRA - file formats that can be read and processed still today.

ROOT is engaging in discussions on a [common likelihood interchange format for](https://indico.cern.ch/event/896473/) [HEP.](https://indico.cern.ch/event/896473/) On one hand, such a format is a useful and effective documentation feature, for instance for publications. On the other hand, it allows for optimized implementations of likelihood functions outside of the highly general RooFit framework, which inspires the continuous development and optimization of RooFit itself.

ROOT believes that analysis frameworks will continue to thrive: ROOT's role is to provide the building blocks that enable physics groups to tailor mini-frameworks to their use. ROOT is continuing to ingest common functionality where it is of general use to the community. This is especially called for where ROOT can implement these tools in a better way, for instance regarding performance, maintainability, or accessibility. Examples only from the RooFit context include the RooCrystalBall and RooJohnson probability density functions; RooStats and HistFactory; ongoing efforts to integrate RooFit extensions developed within ATLAS; CMS's and ATLAS's higher-level likelihood building tools; and RooUnfold.

#### 3.4 Open Science

ROOT participates in CERN's Open Science Policy Working Group. This is only the most recent example of a long history of ROOT engaging with open science and open data.

ROOT is engaged in the experiments' open data efforts, consulting on issues with their data and analyses efficiencies  $(0.1 FTE/y)$ . ROOT also benefits itself tremendously from said open data efforts: these open data samples play a crucial role for ROOT's training sessions, example code, benchmarks and tests. One of the limiting factors appears to be the available personpower from the experiments on the open data side, and ROOT would be happy to intensify its involvement.

All of ROOT's code is public. All changes to ROOT's code are public; they can be reviewed by anyone in the world. ROOT's website is providing everything from an introduction to ROOT up to the technical documentation of all of its interfaces. ROOT sees contributions from high school students to university professors, with changes in 2020 in ROOT itself that correspond to a diff file of 31MB, with about 2800 lines changed each working day. ROOT follows the [FAIR-Software](https://fair-software.nl/) approach, making it as open as best practices recommend.

Multiple R&D projects are taking place in the context of ROOT, for instance with the [LLAMA / Alpaka](https://www.hzdr.de/db/Cms?pNid=2097) group of the Helmholtz Center Dresden, Germany. While CERN is providing the backbone of ROOT's resources, crucial long-term contributions for specific areas come from Fermilab, GSI, Princeton, UCSD, and University of Nebraska. Additional temporary commitments happen on a regular basis, in 2020 for instance by LAL, through Google Summer of Code as well as Season of Docs.

ROOT's developments have an impact on other fields. A good example is ROOT's interpreter cling, which is famously serving as the engine behind [Jupyter's](https://github.com/jupyter-xeus/xeus-cling) [C++ kernel](https://github.com/jupyter-xeus/xeus-cling) and whose [integration into llvm](https://reviews.llvm.org/D96033) is ongoing; or ROOT's work on an improved, platform-independent RANLUX implementation [11] that we expect to integrate into GCC's standard library and the GNU Scientific Library. ROOT has strong ties with the  $C++$  committee; experience from HEP's use of  $C++$  frequently leave traces in modifications of C++ std::simd [12], std::variant [13], C++ reflection  $[14, 15]$  and – due to the well-established connections – in the C++ implementations such as  $\text{std}$ ::any and  $\text{std}$ ::unique\_ptr. ROOT's I/O format for the HL-LHC, RNTuple, will be accessible through a library that does not rely on ROOT or its interpreter, with limited functionality. Nonetheless we expect that this approach makes ROOT's I/O layer significantly more interesting for other sciences.

This means ROOT is itself an active element of open science. At the same time, ROOT is used also outside HEP, for instance through BioDynamo [16] or in quantitative finance research [17].

#### 3.5 Training, Education, Support

ROOT's advances will only have an impact on the community if the community is aware of them. Dissemination is a core responsibility of ROOT; creating training material and presentations for new features is time consuming. At the same time it is extremely beneficial also for the evolution of ROOT's new interfaces, for instance through feedback received during training sessions. In general there is a constant tension between investing in ROOT's evolution, or investing in talking about it; a suitable balance has to be kept  $(1 FTE/y)$ .

The ROOT team has started a "Train the Trainer" series of events which will be resumed after the COVID-related travel bans are reduced. Its purpose is to scale training out: if the ROOT team cannot train the community the way it should, then the ROOT team should train trainers who will then multiply the effectiveness of ROOT's training material. These "ambassadors" are community connections, expected to give multiple trainings per year, and collect feedback on ROOT and the training material, to commonly advance it. Keeping the material with the project allows ROOT to evolve the material together with ROOT, addressing new demands quickly and sharing new features early. Nobody knows ROOT as well as its developers; both the community and the ROOT project benefit from these close ties to the trainers and the trained communities. Even once the ambassadors take over, ROOT expects to continue to give introductory ROOT courses, for instance to summer students (traditionally three per year) and as part of the experiments' introductory courses for PhD students.

ROOT has engaged with the Masterclasses project, for instance [with ALICE](https://alice-masterclass.web.cern.ch/MasterClassInstallation.html) and tries to support them both on a technical level and by making HEP more visible outside the CERN member states: following ROOT's workshop in Sarajevo, including a public lecture to local students, the Sarajevo University joined the Masterclasses program.



Figure 2. Distribution of monthly ROOT forum postings in recent history.



Figure 3. Distribution of consolidated ROOT forum pageviews in recent history.

The ROOT forum sees vivid interaction from young physicists to senior statistics experts, with monthly numbers that are usually significantly higher than 300 thousand page views and thousand messages posted (see Fig. 2 and 3). Over the last 12 months, the average response time to questions is below one hour (3 FTE/y shared among the project members). The forum is a knowledge base for ROOT and HEP analysis in general, and a fantastic indicator of where the community's problems are, and where the ROOT project needs to invest.

With the creation of a new generation of ROOT interfaces, the ROOT team expects to asymptotically reduce the investment in support. Robust, simple interfaces with good documentation, excellent tutorials, and good defaults deploying expert optimizations "behind the scenes" are expected to reduce boilerplate code that gets "inherited" over generations of PhD students. This will result in analysis code that is simpler to understand, more robust, and can serve as a better starting point for future PhD generations.

# 4 Analysis Data

## 4.1 Data Models Optimized for Analysis

Today's CPUs and GPUs, such as available through exascale systems, benefit greatly from large amounts of data, allocated consecutively in memory, that an algorithm can iterate over. This favors "structs of arrays" (SoA) rather than the more traditional object-oriented "arrays of structs" (AoS). Modern ROOT features enable SoA as input, handle memory as SoA internally, and pass memory as SoA to GPUs.

This is further facilitated by ROOT's I/O format: TTree and RNTuple store data in a columnar way. Reading this into memory provides, by default, SoA layout. With TTree this was a lucky coincidence that became relevant only after the interface design of TTree. RNTuple on the other hand can immediately benefit from this, and makes columnar data access as SoA a first-class interface.

While for many programs, AoS-to-SoA transformation is a costly operation, HEP does it as part of ROOT I/O serialization. This means HEP and ROOT have decades of experience with it, with the experiments' analysis data formats migrating to columns (TTree "branches") of simple data types. These "simple aods / ntuples" simplify data discovery and reading, as they can rely purely on ROOT without the need for extra libraries, reading data into the beneficial SoA in-memory layout.

SoA layout of simple data types has the additional advantage of being language agnostic (or compatible): virtually all languages can handle arrays of ints or doubles. This improves very efficient language interoperability. The language boundary is crossed not once per value, but once per array, making interoperability significantly faster as can be seen by [ROOT's benchmarks](https://github.com/root-project/rootbench/) with handing data into NumPy, machine learning libraries, or GPU processing.

## 4.2 Machine Learning

As described in section 2.1, ROOT plays a role as a data source for training and inference of machine learning models. Currently, ML (whether run on GPU or not) benefits from large arrays as input data. These data "structures" are simple enough that ROOT - and here especially RNTuple - will be able to provide them with virtually no overhead. With the advent of graph neural networks, data must be "reformatted" into more complex memory data structures. Most state-of-the-art ML algorithms are fairly young, also in relation to when HL-LHC is supposed to start. The whole sector of quantum-computing inspired ML has not seen production use yet. Given these expected fundamental changes, it is essential for ROOT to have the capability to adjust in-memory data structures, more than to optimize to current requirements. Here, LLAMA can be a fundamental ingredient, together with RNTuple's ability to handle custom data layouts and ROOT's C++ interpreter and just-in-time compiler (JIT) cling enabling optimized transformation of memory layouts.

ROOT is expected to contribute to ML advances indirectly, with its  $C++$  interpreter and JIT: As an example, trained models can be read and converted to  $C_{++}$ code at runtime, with state-of-the-art optimizers (provided by the compiler technology community) significantly accelerating and simplifying inference [18]. Similar technology advances can be expected also in the future. Leveraging those, ROOT can increase its visibility and relevance also outside HEP, and provide benefits to HEP with little additional investment, by building on ROOT's existing core components.

Many of these tasks require expertise in ROOT's key enabling technologies that are part of and used by ROOT, such as clang, ROOT's Python binding, or the I/O system. They also require an excellent understanding of the ML application side and its requirements, as well as credibility and community trust. This enables conception, design and implementation of solutions with sufficient lead time ahead of demand, and gradual ("agile") adoption. Given the required expertise and development effort, ROOT can significantly impact efficient use of compute resources, including GPUs, for analyses and other workflows employing ML (reconstruction, simulation). This happens directly through software technology advances relevant to HEP using ROOT's technologies, and by encouraging and guiding the use of efficient analysis designs.

RDataFrame-based training on GPUs is completed by 2023 and ML-optimized RNTuple-to-GPU transfer by 2025. Much of the evolution cannot be planned ahead and needs to adapt to the evolving requirements of physics analyses and ML research. The inherent risk is the lack of predictability of ML's future evolution. We hope that a versatile setup like ROOT's (and here especially that of RNTuple and RDataFrame) allows us to adjust quickly to ML's upcoming requirements. Lack of delivering said adjustments in a timely manner will drive ML research, and as a consequence also analyses involving state-of-the-art ML, into other ecosystems, causing segregation by use of different tools that are potentially less suited, optimized, or adapted for HEP.

#### 4.3 Data Movement to GPU

GPUs are ideal for instance for ML training; ROOT is working to accelerate data movement from storage to GPUs. R&D areas include memory layout particularly suitable for GPU algorithms [19]; [direct transfer](https://developer.nvidia.com/blog/gpudirect-storage/) from storage to GPU, bypassing of CPU; use of [compression algorithms](https://developer.nvidia.com/blog/optimizing-data-transfer-using-lossless-compression-with-nvcomp/) optimized for GPUs; and total throughput optimization of these different options, possibly combining them. Much of this sees very recent and ongoing technology evolution such as [nvCOMP](https://github.com/NVIDIA/nvcomp) and [DirectStorage;](https://searchstorage.techtarget.com/news/252503292/Nvidia-finalizes-GPUDirect-Storage-10-to-accelerate-AI-HPC) ROOT is following these developments, making sure that they can be captured for production use in the context of RNTuple, ROOT's future I/O library. Here, RNTuple is expected to initiate and schedule the data transfer to GPUs, making use of its abilities to provide high-bandwidth  $I/O$  in a flexible way including, most importantly here, its scheduling.

As this is a highly evolving area, risks are mostly associated with a design that prevents HEP from benefiting from these performance improvements. Even after considering current R&D in the design of RNTuple, residual risks are associated with much of the GPU ecosystem being closed source. As this is in the high performance area of computing, ROOT expects that  $C_{++}$  will continue to play an important role. This should allow ROOT to benefit from its  $C++$  core, possibly after adapting RNTuple, its supported compression algorithms, and its scheduler to requirements of future high-bandwidth storage-to-GPU interfaces.

#### 4.4 Data Location, Transfer, Caching

On the other extreme of data transfer is remote I/O, where data is transmitted from a data lake or any other non-local, medium to high latency storage service. This plays a role in centralized storage, possibly separating storage and computer centers geographically, as well as in (on- and off-premises) cloud computing.

ROOT's approach is to make use of application-side knowledge to drive I/O before the data is needed: after an initial latency cost, subsequent data should arrive before it is needed by the processing code. This was already exercised by TTree's asynchronous prefetching which was not commonly used in production, likely due to insufficient investment in the feature's robustness. With asynchronous I/O being at the heart of RNTuple's design, this is supported from the get-go and the default mode of operation.

To reduce the impact of remote I/O latency, ROOT combines transfer requests across an entry range. This was exercised with TTree's TTreeCache for many years, enabled by default since 2015. RNTuple utilizes a similar mechanism for grouping I/O requests; its performance is being tuned in the context of HPC file systems such as [Ceph/Lustre](https://indico.cern.ch/event/1009424/contributions/4246120/attachments/2204442/3748030/Benchmarking%20HPC%20-%20openlab%20technical%20workshop%2021.pdf) and remote I/O through Davix. Remote I/O through Xrootd is expected to be implemented by 2023, in close cooperation with CERN's Xrootd developers.

Determining which columns need to be read can be based on past usage or can be configured by the application. With efficient "read what you need" and asynchronous I/O, pre-placement of jobs and data files should be superseded by ROOT reading only those bytes that the application needs, ahead of time, reducing I/O requirements and increasing CPU efficiency.

ROOT allows for gradual production of derived data columns, such as calibrated jet pTs derived from uncalibrated jet pTs, among others, and extending an original dataset. These additional columns can be stored in dedicated files, extending the original tree ("friend trees"). This together with columns existing only for certain entries allows a storage efficient creation of sub-samples, where overlaps between samples are not duplicated.

Analyses see repeated runs on identical input data. ROOT is working on a transparent, multi-tier caching layer to be deployed on batch systems such as Spark clusters: ROOT's upcoming Distributed RDataFrame will favor the "sticky" distribution of jobs' input data to enable node-local data caches. This has been shown to accelerate processing [20]. Given sufficient resources, ROOT hopes to extend this to an automatic data cache of intermediary analysis results, to short-cut and dramatically accelerate the re-running of analyses. Such a mechanism is considered for deployment in analysis facilities [\("ServiceX"\)](https://iris-hep.org/projects/servicex) that come with their very distinct software ecosystems.

Given the relevance of object stores in next-generation data centers (such as [Aurora\)](https://www.alcf.anl.gov/aurora) as an alternative to conventional filesystems, there are ongoing efforts to support alternative backends in RNTuple, such as Intel DAOS [21] or Amazon S3. The use of object stores as a cache for accessed data is also being investigated [22].

The risks associated with remote I/O are suboptimal usage of network and CPU resources - corresponding to the key resources of HEP computing. For the ROOT project it is of paramount importance that its  $I/O$  layer is capable of making adequate use of these resources; benchmarks are TTree's behavior as well as raw network speed and CPU usage. Given the pace of technology evolution in the network and remote storage environments, ROOT does not expect technology evolution to be a significant risk on the HL-LHC timeframe.

"Black-box" systems optimized for re-processing of analyses can be a motivation for analysis physicists to migrate to alternative ecosystems. This is a residual risk that ROOT tries to reduce through technology advances and acceleration of repeated analysis. From ROOT's experience, these optimizations are rarely applicable to multiple analyses, for instance on the level of an analysis facility: reuse of data and especially intermediary analysis results are expected to be specific for a given analysis.

## 5 Analysis Design

The "old" ROOT forced physicists to deal with the data source, reading, and the event loop. This prevented many optimizations, for instance multithreading. PROOF tried to formalize analyses, enabling ROOT to process the analysis concurrently. Still, for optimal efficiency, the analysis was commonly interacting directly with the I/O layer, and handling the values read from storage, and their types, explicitly.

In 2018, RDataFrame became ROOT's modern analysis interface, revolutionizing how physicists write analyses today. As can be seen from ROOT's user forum, RDataFrame is now a topic as popular as "tree" or "histogram". This can be seen as a recent major success and a crucial contribution that the community seems to have been longing for. The significance for the community is certainly similar to RooFit.

Unlike alternative approaches, ROOT believes that analyses should be allowed to be conceived and written "event-centric": the minimum number of jets per event, maximum missing ET, number of jets associated with a muon - all these parameters are traditionally per event. ROOT expected it to be much easier for physicists to not give this up when writing their analysis, but instead to handle arrays of events (and arrays of arrays of jets and muons) "behind the scenes", where concurrent and batch processing can run on the user declared analysis, without physicists having to think about the array-ness of certain values such as jet pT.

## 5.1 Declarative Analysis

RDataFrame's main benefit is its declarative interface style, where physicists declare what needs to be done, allowing ROOT to take care of how to do this optimally. As an example, to consider only events with more than two jets reads  $\text{Filter}("n\text{jets} >$ 2"). This is done with minimal overhead, yielding a very efficient, multi-threaded analysis, which evaluates a complex analysis graph in a single pass through all input data.

The community has built several "mini-frameworks" on top of RDataFrame, for instance [bamboo](https://indico.cern.ch/event/948465/contributions/4324161/), [CROWN](https://github.com/KIT-CMS/CROWN), and [TIMBER](https://github.com/lcorcodilos/TIMBER). This by itself is a good sign, showing that ROOT has successfully provided another fundamental building block significant enough to be picked up. ROOT is following closely what these frameworks provide, and what they have difficulties in providing, to "fill the gaps" and - where it is adequate - to provide centrally maintained facilities. Examples of current developments include the variation of event weights and other analysis parameters, to determine the effect of uncertainties. This will be possible without re-running the whole analysis for each variation. This, too, is expected to have significant effects on how HL-LHC analyses will be written.

While RDataFrame supports multithreaded analyses from the start, multi-node support is introduced by Distributed RDataFrame. The latter works together with schedulers and job submission backends (Spark, Dask, etc) for an optimal distribution of input data and compute tasks to clusters of machines. Such clusters are often institute clusters, benefiting from a much higher data-reuse and code-rerun rate than for instance the grid. This motivates ROOT's work on backend-specific work placement, which will allow for analysis acceleration through node-local caches. In order to enable support for a variety of use cases, distributed RDataFrame features a modular backend design. In the future, users will be able to distribute the same computation graph over a set of different cluster frameworks by changing a single line of code. Usability is a key ingredient for such a distributed analysis feature, and configuration of underlying scheduler backends, authentication, data placement, and writable disk space and result collection is generally complex. ROOT plans to address this with a community-wide, community-maintained database of available configurations, such that physicists can use Distributed RDataFrame with their local resources simply by providing the cluster identification.

As with any new ROOT interface, RDataFrame is written with Python in mind; Distributed RDataFrame is only possible because of this. Several optimizations are

pending, for instance for optimized just-in-time compile code; compiled code generated from Python code to be run in the "hot" event loop; more efficient bulk processing. Much of this requires understanding of RDataFrame, ROOT's C++ interpreter and just-in-time compiler called cling, PyROOT, and Python in general.

```
ROOT :: EnableImplicitMT () ;
ROOT:: RDataFrame df (dataset);
auto df2 = df.Finter("x > 0"). Define ("r2", "x*x + y*y");
auto rHist = df2.HistolD("r2");
df2. Snapshot ("newtree", "out.root");
```
Listing 1. RDataFrame C++ code example.

```
ROOT . EnableImplicitMT ()
df = ROOT . RDataFrame ( dataset )
df2 = df.Finter("x > 0"). Define ("r2", "x*x + y*y")rHist = df2.HistolD("r2")df2 . Snapshot (" newtree ", "out. root ")
```
Listing 2. RDataFrame Python code example.

As can be seen from the uncertainty variation of parameters, investment can have a significant performance impact for analyses  $(O(10)$  speed-up for regular analysis, compared to TTree, with an investment of 0.5 FTE for 2 years), running the analysis once instead of once per variation. ROOT plans to invest in RDataFrame to make it significantly easier to use with ML, RooFit, and GPUs  $(O(10)$  speed-up for average analysis, with an investment of 2 FTE for 4 years). Together with snapshotting of intermediary results, optimizations of the Python and just-in-time interfaces, and internal bulk processing of RNTuple data, common analyses will be accelerated by at least an order of magnitude. We expect that by the time of HL-LHC, the vast majority of analyses will be using RDataFrame - especially as already now, RDataFrame is as popular on ROOT's user forum as ROOT's histograms or TTree. Such investment thus scales out to a very large number of analyses, with a significant community impact. It also fosters ecosystems to be built around RDataFrame - tools that can be shared and integrated into ROOT if they are of general use.

This acceleration can bring analyses that are too time consuming into reach; it can improve analyses' ability to optimize their parameters. This is beneficial for traditional analyses with iterative analysis optimization, and a prerequisite for differentiable analysis [23] approaches.

#### 5.2 Accelerators

At the HL-LHC timescale, ROOT expects GPUs to be the commonly available accelerators. For analysis, their main use will certainly continue to be ML training. Also because of the expected ubiquitous use of ML for HL-LHC analyses, ROOT expects GPUs to be ubiquitous for analyses, and is working on R&D to integrate GPU acceleration in RooFit which builds upon prior work on architecture-specific vectorization [24]. This shows very promising results. To be of general use, such acceleration must be enabled by default, when available and advantageous. Much of the R&D goes into determining mechanisms that transparently turn on such acceleration.

ROOT's future I/O subsystem RNTuple is designed to utilize (de-)compression accelerators, which can play a crucial role in analysis throughput. These have already been available in past Xeon generations.

## 6 Analysis Algorithms

## 6.1 Histogramming

ROOT's histogramming package has been the core ingredient for most analyses, for decades. Hardware performance characteristics have changed since its original conception, and much of the design is limiting today's and tomorrow's use. The interfaces of ROOT's histograms are not designed for their usage from Python, nor their interoperability with the Python ecosystem such as NumPy. Alternatives, such as [Boost histograms,](https://github.com/boostorg/histogram) have been created. They lack commodity features expected from a ROOT-provided histogram package, and are optimized more towards raw performance than usability. ROOT's histograms must provide graphics, serialization, and fitting facilities.

The creation of alternative packages and the "impedance mismatch" of modern code with ROOT's histograms (including ownership, lack of generalization, more than 300 member functions, no support for atomic bins) clearly signal that this code part needs to be revisited. Thanks to a partial FTE contribution from LAL, ROOT made much progress with a new [histogram library.](https://github.com/root-project/root/blob/master/tutorials/v7/simple.cxx) Nonetheless, without sustained effort for two years, a new ROOT histogram library cannot be advanced to the minimal feature level required for adoption. The community risks continued work around the ownership discrepancies of ROOT's histograms, paying a performance price for analyses, and additional fragmentation in the experiments' online and offline framework, where even today, experiment specific histogramming facilities have been reintroduced to not use ROOT's histogram library [25]. CMS has provided a [review](https://indico.cern.ch/event/697389/contributions/3108820/attachments/1714101/2764583/cms-dqm-rootworkshop.pdf) of issues of ROOT histograms for DQM. Despite these issues, ROOT histograms currently remain the most commonly used histogramming library. Without investment, usage will further segregate, with no obvious place to invest for the whole community.

This new generation of histograms will allow ROOT to implement long requested features, such as concurrent filling, consistent availability of arbitrary dimensions, or special axes such as circular axes or logarithmic axes with a custom base, efficiency axes (pass versus all), or axes for multiplicity studies. While some of these features merely simplify writing an analysis, some other features counter commonly seen correctness issues with histograms, such as floating point precision issues with multiplicity axes, or can help reduce memory use in concurrent analyses such as analysis trains.

## 6.2 Modeling and Fitting

RooFit is high energy physics's standard tool for modeling statistical distributions and building likelihood functions. It is used in most LHC analyses for estimating physical parameters, confidence intervals and discovery significances. The minimization of a likelihood function defined in the RooFit framework is central in most LHC analyses. With the HL-LHC, the number of parameters and observables in the likelihood function is expected to increase. Usually, minimization time grows superlinear with the number of parameters, meaning technical innovation in likelihood minimization is necessary.

Thanks to modern deep-learning frameworks such as TensorFlow or PyTorch, it is increasingly easy to minimize a function expressible as a chain of linear algebra operations. However, the mathematical operations in a typical LHC likelihood fit are often much more complex, requiring for instance the numerical integration of probability densities for normalization purposes or looking up the result of an auxiliary measurement in a histogram. The RooFit library was designed with such general likelihood functions in mind, supporting unbinned minimization. As RooFit is written in C++, there is still ample room for performance optimization at all the levels of the likelihood evaluation and minimization, making it ready to face the challenges of the HL-LHC data volume.



Speed up using vectorisation

Figure 4. Acceleration from vectorized functions in RooFit.

The ROOT developers pursue several paths to optimize RooFit's performance: speeding up the likelihood gradient calculation, accelerating specific computations with GPUs, writing more vectorizable code (see Fig. 4), general optimization of expensive operations, and improving the interoperability with other libraries that can handle large datasets. The larger the number of parameters in the likelihood function, the more expensive it is to numerically determine the gradient by varying one parameter at a time. In late 2021, RooFit will introduce functionality to parallelize the gradient calculation over multiple CPU cores. In the following year, R&D on auto-differentiation for gradient computation in constant time will move into the focus (see Minimization section). To increase the throughput of computations, much of RooFit was recently rewritten to support auto-vectorization. This path will also be followed in the future, alongside the continuous optimization of CPU code in general. In 2021, the foundational work to offload computations to a GPU was done. Next, the remaining likelihood-building blocks that are frequently used for HL-LHC analyses have to be implemented.

With the increasing dataset sizes, it is crucial to improve RooFit's interoperability with other libraries meant to deal with big data. This concerns other ROOT components (RDataFrame and RNTuple) and libraries from the Python ecosystem (e.g. NumPy and Pandas).

A redesign of the RooFit interfaces based on value semantics instead of RooFit's current reference semantics would make RooFit significantly easier to use, simplify ownership management, and enable the same straight-forward interfaces from C++

and Python. This will attract physicists who would otherwise use Python-AST based interfaces with reduced performance and feature characteristics.

#### 6.3 Minimization



Figure 5. Speed-up of multi-parameter minimization due to automatic differentiation.

Minimization is another area that can benefit greatly from the use of GPUs. The evaluation of minimizer functions can be accelerated on GPUs, especially when operating on large amounts of data. Use of analytical gradients, or automatic gradient calculation for instance with [clad](https://github.com/vgvassilev/clad) can provide further acceleration, see Fig. 5. Some of the algorithmic challenges remain hard, such as normalization of probability density functions when evaluating likelihood functions as seen with RooFit models; we are confident that continued R&D investment will pay off.

Advances in minimizers will provide immediate benefits to RooFit. Even the side-effects from these R&D efforts are useful to the community and outside, with the C++ automatic differentiation tool clad being a perfect example.

ROOT continues to try state-of-the-art minimizers, benchmarking them against MINUIT and other production minimizers. Production-grade, general purpose minimizers are rare; ROOT does not expect that major development effort will need to be invested here, except for the above-mentioned GPU minimization.

# 7 Visualization and Graphical Interfaces

ROOT's graphics style and abilities have defined the visual language of HEP. With the ever increasing complexity of architecture specific graphics and the web taking over GUI and graphics, ROOT has opted for a redesign of its graphics and GUI systems based on HTML, CSS and JavaScript.

## 7.1 Scientific Graphics

ROOT's graphics system allows extreme configurability while creating graphics in publication quality. Several of the defaults would be chosen differently today, for instance the font size being relative to the window size, or the line widths of histograms, or histograms' default colors.

The complexity of maintaining highly efficient graphics on all platforms has increased enormously: Linux is migrating from X11 to Wayland (and alternatives); macOS offers Cocoa and Metal; Windows offers GDI+ or DirectX. Luckily, web browser engines have established themselves as a platform independent abstraction layer. The Chrome / Chromium Embedded Framework for instance is used by many programs such as Mattermost, the Atom editor, and Spotify. This means ROOT's architecture specific libraries can be succeeded by libraries maintained by the open source community.

Any scientific graphics library is built around primitives such as axes, lines, greek letters and formulae, and the ability to zoom. Luckily, these features are available in open source JavaScript graphics frameworks that ROOT was able to adopt and build upon for its usage. JSROOT is ROOT's JavaScript interface that draws for instance histograms in a browser window, with virtually the same configurability and performance as the previous architecture-specific implementations. Hundreds of histograms can be shown interactively, with smooth interaction.

The move to web graphics enables embedding of ROOT graphics in custom GUI applications such as Qt applications. Before, embedding of ROOT graphics depended to a large extent on platform-specific features (and, as a consequence, stopped working on macOS unless using legacy X11 implementations). Today, virtually all GUI systems allow embedding of browser windows, or are written themselves as browser GUIs.

With this new technology in its hands, ROOT is now working on making the user facing implementation of ROOT's graphics much simpler to use. New interfaces allow ROOT to define new defaults and to streamline the graphics interfaces, simplifying for instance ownership management and separating data structure from graphics abilities. This work is ongoing and expected to deliver a robust, simpler graphics interface in time for HL-LHC. Prototyping new graphics programming models is expected to conclude in 2022. Implementation of the new default style and CSSbased style customization is expected to be available by 2024. Grid deployment (for instance with the above mentioned Chrome Embedded Framework available through LCG) is expected to be achieved by 2022.

#### 7.2 Graphical User Interfaces

With the graphics system moving to web technology, moving ROOT's custom GUI system along was an obvious next step. ROOT has decided to use the featurerich, open source Web GUI library named OpenUI5. Communication of the browser window with the ROOT process happens through an open source web server library called civetweb, which is developed independently of ROOT. The ROOT process communicates through its interpreter / JIT compiler cling, passing data both ways, and calling the appropriate methods on the  $C++$  or JavaScript side. ROOT's I/O subsystem is used to transform C++ objects into JSON and back, to transport state between the ROOT process and the browser.

This shows that ROOT is able to re-use its own core components to generate a wealth of fundamental tools specific for HEP. While ROOT's GUI itself is important (for instance ROOT's new RBrowser, or the new fit panel), it is equally important that ROOT and its interactivity can be embedded in "foreign" GUI systems, and retain its functionality and interactivity. The current setup based on web technology allows just that, as demonstrated for instance by the ROOT masterclasses or Eve7.

#### 7.3 Jupyter Notebooks

For "exploratory analysis", i.e. the first steps into discovering data, fundamental distributions, or even for training of machine learning models and the evaluation of their quality, Jupyter has established itself as one of the interfaces. Being based on web technology itself, it integrates nicely with ROOT's web graphics already today,

ROOT's C++ interpreter / JIT compiler cling is the engine behind the official C++ Jupyter kernel. ROOT provides an enhanced version of this, making many ROOT features more accessible through its own, dedicated kernel.

Work is ongoing to integrate ROOT's web GUI system with the new Jupyter GUI system. Given sufficient demand from physicists, this feature is expected to be available in 2024.

## 7.4 Event Display

ROOT's event display EVE was in production use in many experiments, for instance CMS, ALICE, Belle II, T2K, HyperK, ILC, NA62 and several smaller experiments in neutrino, nuclear, and medical physics. Being exposed to the same problems and limitations as ROOT's legacy graphics and GUI libraries, Eve has been redesigned as Eve7, to work with ROOT's new, web-based graphics and GUI system, too; see Fig. 6. This has increased its versatility dramatically: Eve7 works on all platforms, can present events remotely, and is thus a perfect implementation for everything from online monitoring to outreach.

Apart from JSROOT and ROOT's GUI system, Eve7 also uses ROOT's C++ interpreter / JIT compiler internally for filter expressions, for instance to display



Figure 6. ROOT event display with object selection.

only jets satisfying certain cuts. As these expressions can use the full power of  $C_{++}$ , the event display is highly customizable and extremely versatile, useful for instance to understanding effects of detectors or detector algorithms.

Event displays play a role in analyses, too: they allow a visual inspection of selected events, for sanity-checking and to determine for instance different topologies of samples. As such they are inherently an analysis feature, where usability and performance is a key requirement.

Being developed in close collaboration with CMS and currently deployed as a prototype in CMS, the feature set and performance of Eve7 has already impressed several users of event displays. A first experiment, Mu2e at Fermilab, has officially announced their interest in using Eve7 in production in the coming years. ROOT has every reason to expect community adoption of Eve7 to be at least on par with the adoption of the legacy Eve.

We expect that the majority of effort will be invested into Eve7 satisfying the requirements of CMS, which can serve at the same time as a proof of being feature complete. This work is expected to conclude in time for HL-LHC, and driven mostly by CMS itself.

## 8 Project Requirements

#### 8.1 Organization

The ROOT project is in its core a group of contributors to a common open source project. Decisions are taken publicly at a weekly team meeting, upon discussion and by consensus. Consensus building happens through good arguments; ROOT is thus in practice a meritocracy, where new, capable contributors can quickly acquire significant influence.

ROOT development was traditionally split in several loosely coupled parts - both regarding libraries and regarding development subgroups, for instance for the I/O or the statistical part of ROOT. In recent years, these delineations have reduced, to encourage both sharing of expertise, and exposing of problems and solutions to a wider audience, with a more diverse background of technical expertise.

ROOT continues to be a successful integrated "hub" for R&D; several grants were attributed to work in the context of ROOT. Examples include the R&D on the hrefhttps://reviews.llvm.org/D96033integration of ROOT's C++ interpreter / JIT compiler cling into llvm / clang ("upstreaming"), compression studies [26], PhD students' work on topics such as [LLAMA](https://github.com/alpaka-group/llama) and data caching for distributed computing [20]. Some R&D - such as the core RNTuple work, or RDataFrame - requires sustainability that goes beyond the time frame of PhD student or grant requests, and needs to be taken up by long-term contributors.

Besides this R&D aspect, ROOT has a strong responsibility for sustainability and support. ROOT's interfaces need to be backward compatible, to facilitate sharing of analysis code across ROOT versions. This requires an "interface vision": designing interfaces now that allow optimizations behind the scenes in ten or 20 years from now is an expertise that is required by the core ROOT developers.

Support is a significant workload for ROOT's core developers, with hundreds of messages needing to be processed per day; issue reports and code contributions requiring attention; infrastructure work (configuration, continuous integration and benchmarking systems); and the ROOT team presenting ROOT's advances at physics conferences, for instance [iCHEP 2020,](https://indico.cern.ch/event/868940/contributions/3814685/) [EIC,](https://indico.jlab.org/event/247/contributions/3063/) [CEPC 2020,](https://indico.ihep.ac.cn/event/11444/session/12/contribution/170) [EPS-HEP 2021,](https://indico.desy.de/event/28202/contributions/105604) and during training sessions. This load can generally not be shouldered by contributors who have dedicated R&D goals, but is carried by those developers with long-term contracts.

ROOT has virtually constant interaction with the experiments, from early discussions on ROOT's development plans to high-priority issue processing. The ROOT team engages with the experiments' software and computing experts at a dedicated ROOT / Experiments meeting series; at the Librarian and Integrators Meeting; and at the Architects' Forum. Office visits between core experiments' developers and ROOT are common (or rather, were common before the pandemic), as was pair debugging. Requirements for the experiments' core software is collected through the discussion of the plan of work and through issues opened by the experiments.

This constant interaction leaves traces with all parties involved. ROOT has contributed to the definition of the ALICE analysis model of Run3, to the interplay of ATLAS XAODs and RDataFrame, and to optimizing CMS nanoaods. Multithreading bottlenecks are addressed in cooperation; I/O performance improvements are guided by measurements from the experiments, often with tools provided by ROOT. With for instance RNTuple, ROOT further increases its investment in benchmarking campaigns with the experiments, to guide design and development by realistic, early feedback.

Requirements for the experiments' analyses are generally much harder to define. ROOT invites to workshops (e.g. in [2018](https://cern.ch/root2018) and [2015\)](https://root.cern/blog/workshop_2015/) to solicit combined feedback, makes use of the forum and GitHub issues as feedback platforms, and presents where physicists are (see the list of recent contributions at physics conferences above, regular invitations at experiments' meetings, engagement / participation for introductory ROOT courses) to engage in discussions.

ROOT owes much of its stability to the experiments' investment: all experiments test all main ROOT releases, or even their branches; some even report with low latency (about one week) on issues found in ROOT's main development branch ("master"). This allows ROOT to carry out major changes, in a coordinated way with the experiments. Recent examples include the migration to a new PyROOT implementation; or updates of LLVM. Another example of ROOT's engagement with experiments is the [integration of RNTuple in CMSSW,](https://github.com/cms-sw/cmssw/pull/33825) a combined effort of CMS and ROOT. The experiments trust ROOT to maintain Vc, VecCore, and VecMath, packages used by the experiments directly or indirectly, for instance through Geant4.

#### 8.2 Development Team

ROOT's development is driven by R&D contributions, where short term contracts dominate by number. ROOT currently hosts one technical student, one PhD student paid by CERN; one PhD student funded externally; 2.5 FTE CERN fellows; one CERN EP R&D fellow; and one externally funded fellow, i.e. in total 7.5 FTEs.

Sustainability, guidance, accretion and integration of expertise is guaranteed by developers with long-term positions, totalling 8.25 FTEs, see Table 2.

A fair fraction of these developers (marked "R&D" in above table) cannot contribute to the project's baseline load of supporting users on the ROOT forum, infrastructure work (such as maintenance of ROOT's continuous integration system or build system), or issue processing. Much of the recent ROOT developments and expertise associated with those developments - notably RDataFrame and RooFit rely on fellows. RNTuple is an exception from this, where the main developer was rewarded with an IC and expects to migrate to ROOT for the vast majority of his working hours.

The age profile of ROOT's development team versus its recent massive renovation is one issue; the lack of gender diversity is another. ROOT has succeeded in capturing

<b>FTE</b>	Expertise	Funding source
$5.5$ , incl $4.5 \text{ ICs}$	$I/O$ , statistics, ML, C++ interpreter / JIT compiler cling, ROOT's type description system, PyROOT, build system, documentation, platform support and continuous integration infrastructure, support	CERN
0.5	I/O	Fermilab
	R&D and support: event display	<b>UCSD</b>
0.5	R&D: $C++$ interpreter / JIT compiler cling; $C++$ automatic differentiation	Princeton
0.5	$R&D$ : compression, I/O	UNLincoln
0.25	R&D: web-based GUI and graphics	GSI

Table 2. Current long-term contributions to ROOT.

physicists and computer scientists; developers from diverse national backgrounds. But with currently zero female team members paid by CERN it has failed to achieve a reasonable gender balance. This is an issue that ROOT expects to address in the coming years, by investing in recruitment, reaching out to universities and job fairs. Improving this requires a noticeable effort from the ROOT project. This effort can only be effective in a sustainable way as appropriate positions become available.

## 8.3 Sustainability

For ROOT as a long-term software project, sustainability is a key requirement. Apart from technical sustainability such as I/O and interface backward compatibility, separation of stable user interfaces from evolving optimizations behind the scenes, and multi-platform support, ROOT needs to also guarantee sustainability on a non-technical, "cultural" level. Worth mentioning are ROOT's long-term common vision for a ROOT evolution that matches HEP's requirements. ROOT's expertise is the basis for the community's trust in ROOT and its continuing evolution. The successful and established mode of working of ROOT's development team guarantees productivity and integration of many kinds of contributions, sources of contributors, and an active, vivid, and continuously challenging ecosystem with constant communication with ROOT's stakeholders.

ROOT's significant investment in support is addressed with a new generation of coherently designed, well integrated, robust interfaces that are simple to use correctly, and difficult to use incorrectly. This should asymptotically lower the support load

for ROOT.

Over the past years, ROOT has deprecated and removed interfaces, and even large parts of ROOT. They either have seen insufficient use to warrant the project's continuous investment; or they have not seen general adoption from the community, thus benefiting from a lifecycle independent of ROOT. Some interfaces (such as TLorentzVector) see continuing wide-spread adoption but are nonetheless seen as problematic; the ROOT team is working through documentation and training to migrate usage to recommended interfaces (such as PtEtaPhiMVector).

At the same time, ROOT targets development and investment in a very focused way. With about 5 million source lines, ROOT needs to choose what to evolve, and what to "freeze". Many parts of ROOT have existing usage, nonetheless much of their motivation is not applicable anymore today. Examples include ROOT's collection classes which were needed because no general C++ standard library support existed 20 years ago; or parts written to bridge between ROOT's previous, limited C++ interpreter and non-ROOT libraries; or internal tools that have been replaced by other, open-source tools such as the transition from THtml to doxygen, or TThread to tbb. Much of this legacy code has been written with a past understanding of "software development's best practices", making any more fundamental investment a challenge and of dubious value. Instead of causing friction and additional work for the community, ROOT maintains these parts with low cost, by moving their code to new C++ standard versions, platforms, and compiler versions as needed. Where sensible, ROOT [marks](https://root.cern/doc/master/classTLorentzVector.html) these parts as legacy, to clearly communicate that now new adoption of these features should happen, and what the recommended alternatives are.

Lines of code changed per week, 2020	2800
Number of contributors, 2020	Approx. 100
Number of architectures and package managers per ROOT version	-28
New issues (bug reports) in 2020	690
Closed issues (bug reports) in 2020	660

Table 3. Key ROOT development metrics.

## 8.4 Generational Handover

For ROOT to be successful in perpetuating its flourishing developments and converting them into sustainable, trusted software building blocks for HEP, the upcoming generational handover must succeed. There is a strong risk that with the retirement

of a large fraction of very visible ROOT developers, expertise or at least visibility and community trust get retired with them. To reduce this imminent risk considerably, a small number of currently well-known young experts of ROOT should be retained until they have a chance to apply for long-term contracts, succeeding the retired core developers.

## 8.5 Cooperation & Innovation

Cooperation is essential for ROOT's evolution and a crucial source of contributions. Fostering cooperation, i.e. an open ROOT project that newcomers feel invited and welcome to contribute to, is paramount for this. Being open source and with open discussions and project meetings is a prerequisite, but in and by itself is not sufficient.

We see how innovation serves as an incentive to contribute. It creates attention, causes alternatives to be tried by the community, which is an incentive to benchmark, compare, and improve. The better solutions generally get integrated into ROOT, where it is of high relevance to the community and where it matches ROOT's evolution and responsibilities. Even where innovation does not get integrated because it is outside of ROOT's scope, it generally backfeeds requirements and ideas, and by doing so triggers innovation. Cooperation can thus exist on many levels, from formal ones such as ROOT's current and past CERN knowledge transfer projects, to informal ones where physicists give presentations to the ROOT team to share ideas or propose solutions (e.g. [Bamboo,](https://indico.cern.ch/event/963454/contributions/4052766/) [TTreeIterator,](https://indico.cern.ch/event/1042946/) [CROWN\)](https://indico.cern.ch/event/1045394/).

ROOT is working towards making cooperation easier, also on a more formal level. While this is ongoing, a major milestone in this regard is expected to be reached in 2023.

## 8.6 Creating Opportunities for Externally Funded Projects

With ROOT's responsibility towards the community and the ongoing need to compete with alternative solutions, core development is generally shouldered by longterm contributors. Many of the peripheral developments that are still crucial but less time critical can be owned by specific R&D projects.

ROOT tries to increase the availability and visibility of sizable, open R&D projects that are not on ROOT's critical path. The HEP community interested in software does not have established mechanisms to facilitate this; ROOT's past efforts to engage with this community have had very little successes. ROOT does not yet see the [HEP Software Foundation](https://hepsoftwarefoundation.org/) or CERN's [SIDIS](https://sidis.web.cern.ch/welcome) effort serving as a forum for laboratories or university software R&D groups to engage. While investment in software exists, the HEP community might benefit more from synergies and a more coordinated investment.

In its yearly published [plan of work,](https://root.cern/for_developers/program_of_work/) ROOT will continue to include tasks that are not foreseen to be covered by existing contributions. The hope is to trigger discussions on these topics, to identify interested parties, and to engage in more coordinated R&D. Having a forum or a set of entities to address this to would certainly help.



#### 8.7 Summary of Risks, Functionality Gaps, Dependencies

Figure 7. Milestones and associated effort: ROOT I/O

Part of ROOT's core responsibilities is the I/O system, as covered in detail by the Foundation part of the ROOT input. Its milestones and associated effort are shown in Fig. 7. Other areas and associated risks are as follows.

#### Analysis interfaces: efficient, robust and obvious



Figure 8. Milestones and associated effort: RDataFrame



Figure 9. Milestones and associated effort: PyROOT, cling C++ Interpreter / JIT



Figure 10. Milestones and associated effort: Distributed RDataFrame



Figure 11. Milestones and associated effort: Histogramming

If evolved properly, ROOT's prime analysis interface, RDataFrame (see Fig. 8), can make use of the impressive uptake from physicists, by guiding them towards automatically efficient analyses that use all available resources (network, CPU, GPU). This will enable physicists to work within a common ecosystem, together build features and tools on top of RDataFrame, and thus increase and share the benefits of an analysis environment tailored for HEP. It is paramount to delimit the R&D surface: where the open source data analysis community provides efficient tools that are easy to use, ROOT must invest in interoperability, with a focus on smooth, efficient usage and highest possible data transfer bandwidth.

ROOT must invest in interoperability of the expected HL-LHC data format RNTuple with tools from the open source data analysis ecosystem, specifically for machine learning (training), NumPy and future (likely Python-based) data exchange interfaces.

RDataFrame needs to be extended to handle systematic variations within the same event loop, providing a significant speed-up for the average analysis. Bulk processing of data must be enabled for RDataFrame, to benefit from RNTuple's new data layout and to benefit from significantly higher throughput on CPUs and GPUs.

PyROOT will play an even increasing role in HEP's data analysis environment. It critically depends on ROOT's C++ interpreter / JIT compiler cling, and ROOT's type description system, see Fig. 9. Future  $C_{++}$  standards, performance and feature bottlenecks must be addressed in ROOT's type description system. Python-specific adapters to widely used ROOT interfaces must be implemented to ease their usage also from Python.

With RDataFrame, ROOT has mostly addressed the issue of "how to write an analysis accelerated by multithreading". This needs to be extended to a multi-node environment, currently developed as Distributed RDataFrame, see Fig. 10. This will reduce the need for the community to develop adapters for running analyses on clusters such as Spark, for instance by reading ROOT files in Java. It will make university clusters accessible to interactive analysis, significantly reducing the turnaround time for analyses.

ROOT's new histogram library will address usability and performance issues, while providing the feature set expected by HEP analyses, see Fig. 11.

#### Machine learning models and likelihood functions with ROOT data



Figure 12. Milestones and associated effort: Machine Learning



Figure 13. Milestones and associated effort: RooFit

Many analyses can benefit significantly from direct RNTuple to GPU data transfer, for instance for machine learning, see Fig. 12. This requires work on data layout and GPU-compatible compression algorithms. Inference from machine learning models must be simple to use from RDataFrame; results from RDataFrame must be easily and efficiently usable as ML training input.

RooFit (see Fig. 13) needs to continue its renovation for increased efficiency, for instance by processing arrays of input data also on GPUs. A significant hurdle of RooFit is the pointer-based interface with implicit ownership rules; a redesign based on value semantics and thus similar for Python and  $C++$  is needed for future evolution of RooFit.



## State-of-the-art visualization

Figure 14. Milestones and associated effort: UI and Visualization

Further investment (see Fig. 14) will ensure smooth transition from the legacy graphics and GUI interfaces to the new architecture independent, web-based graphics and GUI implementations [27]. For this to succeed, the new libraries must provide the minimal feature set needed by analyses, before the legacy libraries will cease to function on commodity analysis systems, due to these systems deprecating and penalizing X11, GL, Cocoa, GDI, etc, a process that is currently ongoing.

ROOT must invest in a productivity layer of its very configurable and currently complex graphics interfaces. This allows graphics to be well integrated with the rest of ROOT, still highly configurable, but with defaults that correspond to physicists' expectations. It will guarantee that the community keeps and commonly evolves its "visual language", for instance regarding plots showing multiple uncertainty bands, efficiencies, or higher-dimensional distributions.

ROOT's developing event display seems to satisfy a real community need, with its high-performance, highly customizable web graphics interface. ROOT is not aware of any viable alternative with similar functionality and usability. ROOT expects that this event display will see wide-spread adoption, if development continues, and is backed by investment in its constituents such as ROOT's HTTP data transfer (based on ROOT's I/O) and ROOT's C++ interpreter / JIT compiler cling, and ROOT's web-based graphics and GUI system.



<sup>&</sup>lt;sup>1</sup>FTE is average per year from 2022 to feature completion; about 50% senior  $/$  50% junior developer







Table 4: Summary of benefits, priorities, efforts, and risks of mainwork areas.

For ROOT, RNTuple has the highest priority and is most time critical, as adoption depends on production readiness well before the start of HL-LHC. Analysis interfaces (RDataFrame, RooFit, machine learning and Python interoperability, histogramming) are the second most important development, defining the future of ROOT-based HEP analysis, with a significant benefit for the efficiency of physicists and the impact of delivered luminosity. Progress is defined by a combination of these priorities and available expertise and developer effort. In general, ROOT must provide continuous effort for support and maintenance of all these fields, which in turn guarantees a sustained development progress in all these fields.

## 9 Summary

Several years ago, ROOT had identified the HL-LHC as a welcome timeline to reinvent itself. Today's ROOT can still function as it did ten or twenty years ago, thanks to its backward compatibility. But many physics analyses have moved away from that, embracing ROOT's new features that come with a much increased usability and efficiency. This endeavor has attracted many R&D contributions, helping with fundamental innovation and fast progress in ROOT's evolution. All of ROOT's core areas have benefited from this investment: the I/O system, likelihood evaluation, machine learning, data analysis interfaces including distributed analysis, Python bindings and ROOT's "Python personality", ease of installation and deployment.

Part of ROOT's evolution speed is due to technology advances being accessible to other parts of ROOT: the web graphics system and the event display benefit from ROOT's JavaScript interface JSROOT, the I/O subsystem and the interpreter; RooFit's vectorization efforts benefit from experience in vectorizing ROOT's fitting algorithms; the development teams shares commonly accrued expertise on writing high-performance, highly concurrent code; ROOT's Python-specific interfaces benefit from in-house experience of data transfer into Python other features of PyROOT and the C++ interpreter / JIT compiler. ROOT is itself an ecosystem, re-using its own innovations to multiply their effect.

At the same time, ROOT is embedded in an ecosystem of tools built on top of ROOT, or bridging into other data science ecosystems. ROOT works on providing these bridges itself, arguing that efficiency and separation of concerns are best taken care of by experts who can guide the analysis physicists in their use of for instance ROOT data with machine learning tools. ROOT's technologies and the continuing relevance of C++ will likely allow ROOT to also satisfy interoperability needs for the next 20 years.

Yet, ROOT cannot reinvent itself without providing sustainability for those new features, which in turn requires long-term commitment of developer resources, and the ability of these developers to also invest significantly in work not related to R&D. The currently ongoing peak of innovation will need to transition into an era of optimizations and support, during the HL-LHC data taking years. To guarantee this, retaining expertise and community trust is paramount.

## 10 Conclusion

ROOT is not only a software project: it is a team of technical experts and innovators, communicators with the HEP community, people that this community trusts and knows to rely on. At age 28, ROOT is currently reinventing itself, to benefit from the team's and the community's experience and support, and to adjust to tomorrow's challenges and requirements, in time for the HL-LHC.

ROOT's evolution is driven by a rich bouquet of innovation with steady progress over the last couple of years. The goal is to bring ROOT to the level of usability, efficiency, robustness, and community trust required for HL-LHC analyses. Efficiency improvements in orders of magnitude have been seen across the board; adoption by physicists has been impressively rapid, likely because of the features' quality, but also due to increased efforts invested in communication of these new features, and involvement of the analysis community already during the development of the new features, following ROOT's tradition.

Even though ROOT is working on filling several feature, performance, and productivity gaps, it needs to be able to do so in a sustainable way: today's new features are tomorrow's source of bugs. ROOT relies on continued assistance from the community and contributors to provide user support and maintenance for HL-LHC. It especially needs this assistance to transition from the current active R&D phase into a support phase, with retained expertise.

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