# ROOT modern HEP data analysis Vincenzo Eduardo Padulano (CERN, EP-SFT) for the ROOT team

Workshop on "Quasi-Interactive Analysis of Big Data with High Throughput" Bologna, Italy, 08.01.2025





- The ROOT project
- Current activities
- Focus on analysis





### Vincenzo Eduardo Padulano

- PhD in Computer Science, Universitat
   Politècnica de València
- Staff Computing Engineer, CERN, EP-SFT
- Working in the ROOT team since 2019





## https://root.cern

- Open-source software framework
  - **Storage**, data **analysis**, **processing**, visualization of **big** structured **datasets**
- Widely adopted in High Energy Physics and in other scientific and industrial fields
  - **Fits** and parameters estimations for discoveries (e.g. the Higgs)
  - **Thousands** of ROOT **plots** in scientific publications





# The ROOT team



- ROOT is an international collaboration
- Steady contributions
   coming from the
   community, and
   institutional responsibilities.



# The need for strategic thinking



QoS	ALICE	ATLAS	CMS	LHCb	Total
Disk [PB]	199	406	304	93	1002
Tape [PB]	283	666	673	250	1875

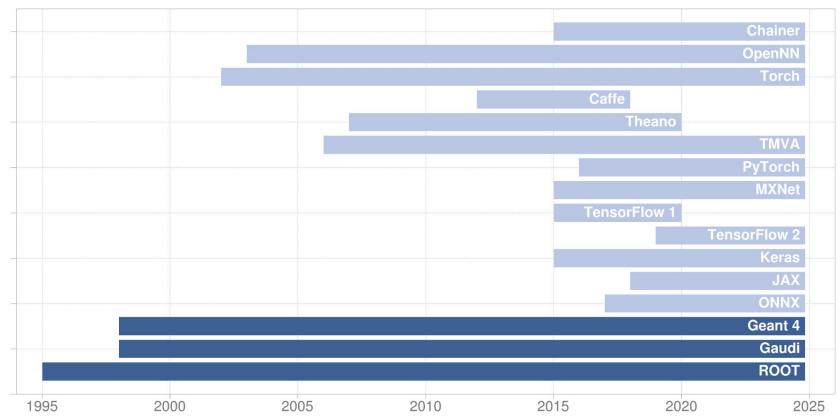
The full exploitation of the physics potential of present and future accelerators also passes through ROOT

`24 Pledges: source WLCG <u>CRIC</u>

## LHC Runs 1,2,3 → Today, >2 EB in ROOT format HL-LHC: ~30 EB in ROOT format?

# Long-term support model





Plot inspired by <u>M. Mazurek</u>

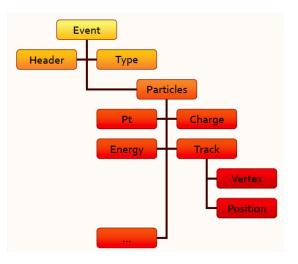
# Highlights of current activities

## Requirements and challenges of HENP datasets

1. Natural HENP data layout is

### jagged arrays of complex types with columnar access pattern

- HDF5 does not fit well due to its inherent tensor layout
- Otherwise only found in Big Data (but with limited type support)
- 2. HENP data organization: global federation of file sets
  - Requires **XRootD** and **HTTP** remote data access
  - Extra functionality to build data sets from files: fast merging, chains, joins
- 3. Integration in the HENP software landscape
  - Rich type system of experiment central EDMs with 10k+ columns
  - Multi-threaded reading and writing under tight memory constraints
  - Availability in the Python & C++ analysis ecosystem
- 4. >10 EB of data to be stored over decades
  - Requires excellent compression (lossy and lossless)
  - Data custodianship over time: backward & forward compatibility, schema evolution, bit-level checksumming



Dataset schema is the set of user-defined (C++) classes



- A new data format, based on 25+ yrs of experience with the established TTree data format, with a modern and efficient implementation:
  - **Smaller** files (typically **10% 50%**), higher throughput (often by factors)
  - More **robust**: binary format specification, modern API, fully checksummed
  - Efficient support of **modern storage systems**: NVMe, object stores, async & parallel I/O
  - Forward-looking limits: designed for **TB-sized events** and **PB-sized files**
- Feature-rich: works with complex experiment EDMs and with experiment frameworks
- Supported at HL-LHC timescale (2030-2040+)



# Rich type system support

Type Class	Types		EDM Coveraç	je	RNTuple Status
PoD	<pre>bool, char, std::byte, (u)int[8,16,32,64]_t, float, double</pre>				Available
Records	Manually built structs of PoDs	Flat n-tuple			
(Nested) vectors	std::vector, RVec, std::array, C-style fixed-size arrays		Reduced AOD		Available
String	std::string				Available
User-defined classes	Non-cyclic classes with dictionaries				Available
User-defined enums	Scoped / unscoped enums with dictionaries			Full AOD / ESD / RECO	Available
User-defined collections	Non-associative collection proxy				Available
stdlib types	<pre>std::pair, std::tuple, std::bitset, std::(unordered_)(multi)set, std::(unordered_)(multi)map</pre>			Available	
Alternating types	<pre>std::variant, std::unique_ptr, std::optional</pre>			Available	
Streamer I/O	All ROOT streamable objects (stored as byte array)				Available
Low-precision floating points	Double32_t, f16			Available	
	Custom precision / range (bfloat16, TensorFloat-32, other AI formats)	Optimization benefitting all E		g all EDMs	Available

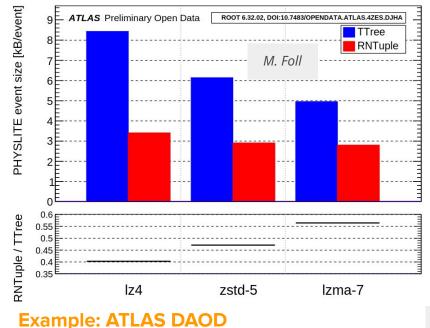


# Rich type system support

Type Class	Types		EDM Coverag	RNTuple Status	
PoD	<pre>bool, char, std::byte, (u)int[8,16,32,64]_t, float, double</pre>				Available
(Nested) vectors	<b>HDF5 and Big Data formats (e.g., Parquet)</b> std::vector, RVec, std::array, C-style fixed-size arrays	at n-tuple	Reduced AOD		Available
String	std::string				Available
User-defined classes	Non-cyclic classes with dictionaries			Full AOD /	Available
User-defined enums	Scoped / unscoped enums with dictionaries			ESD / RECO	Available
User-defined collections	Non-associative collection proxy				Available
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# RNTuple space savings



RNTuple in ATLAS [1] [2] [3]

Note that due to data preconditioning in RNTuple, the relative difference between compression algorithms fades.

### **Contributors to space savings**

- More compact on-disk representation of collections and booleans (trigger bits)
- Same page merging
- Type-based data encoding optimized for better compression ratio

### More performance studies

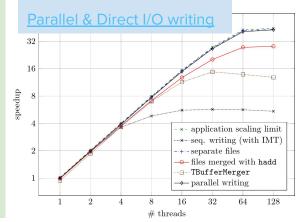
- <u>CMS</u>
- <u>LHCb</u>
- <u>Comparison with HDF5 & Parquet</u> (ACAT 21)

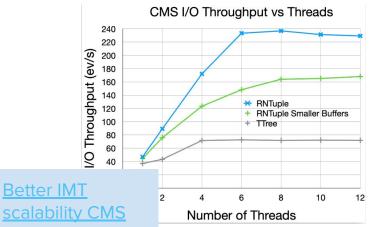


# **RNTuple throughput studies**

### **Contributors to higher throughput**

- Asynchronous prefetching
- Multi-stream disk access through io\_uring
- Code optimization
- New on-disk layout allows for higher degree of explicit and implicit parallelization
  - New analysis I/O scheduler



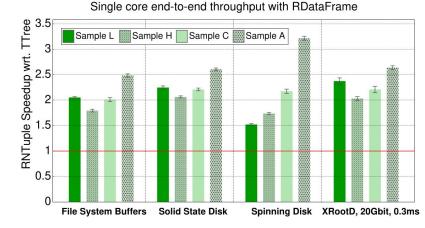


ntuple types and data access modes.

**Higher analysis** 

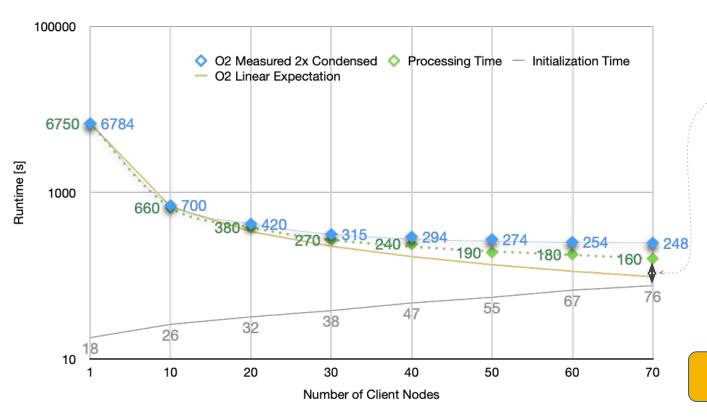
throughput across

various final-stage



## Large scale data analysis with RNTuple

### AGC analysis, 100x inflated dataset, 32-core nodes, 2240 cores max



With a 100x inflated AGC<sup>200</sup> dataset we observe that as the number of client nodes increases, the initialization time gets close the processing time, resulting in a breakdown of scalability.



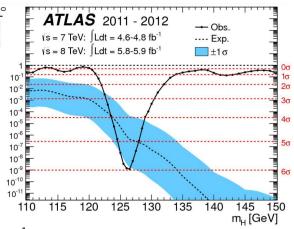
unle CHFP'24

Plenary

# Likelihood building and evaluation

RooFit: C++ library for statistical data analysis in ROOT

- Provides tools for model building, fitting and statistical tests
  - Sophisticated **binned** models with many nuisance parameters but few data entries
  - **Unbinned** fits of analytic shapes to huge datasets
- Recent development focused on:
  - **Performance** boost (preparing for larger datasets of HL-LHC)
  - More user friendly interfaces and high-level tools

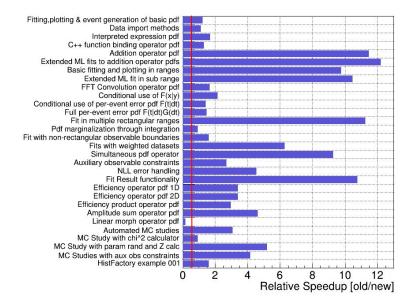




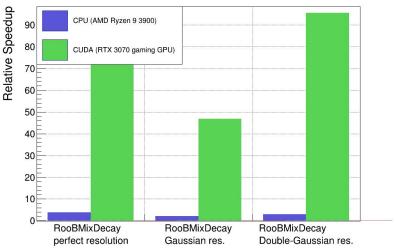
# **RooFit performance**

- Default CPU backend leverages vectorization (4.4x speedup on average, see plot on the left)
- The GPU backend can drastically speed up fits on large unbinned datasets
- See this <u>PyHEP 2023</u> presentation for more benchmarks
  - also compared to zfit and pyhf

RooFit/HistFactory stress tests: speedup of NLL minimization by using BatchMode("cpu")



RooFit: speedup in benchmark fits with BatchMode() relative to old RooFit (1 million events)



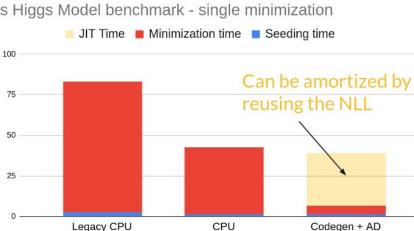
CPU and GPU speedup compared to legacy backend 17

(ROOT 6.30 default)

# Automatic Differentiation in RooFit

Time (seconds)

- **RooFit** is a **framework** to build computation graphs for function minimization, similar to ML frameworks such as TensorFlow or PyTorch
- Recently, a **new** RooFit **backend** was added which leverages an automatic differentiation engine, based on the <u>clad</u> technology
- Result: evaluating **analytic** likelihood gradients without compromises



(ROOT 6.32 default)

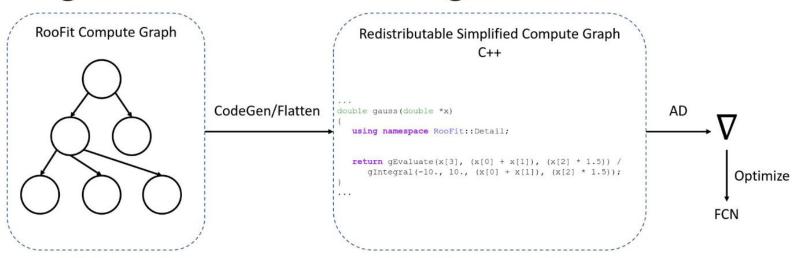


Atlas Higgs Model benchmark - single minimization



## RooFit + Clad

## How RooFit uses Clad to get analytic gradients: Code generation (aka. "codegen")



- 1. Mathematical concept
- 2. **RooFit** user code
- 3. Automatic translation of RooFit model to simple C++ code
- 4. Gradient of C++ code automatically generated with Clad
- 5. Gradient code **wrapped** back into RooFit object

*Note:* for the **nominal NLL** function, we **still use RooFits CPU backend** to benefit from vectorization and caching outside the gradients.

Rembser et al. ICHEP'24



# Python interface

# The quality of the ROOT experience for Python users is a priority

- Update to the latest version of <u>cppyy</u>, ROOT's C++-Py 'interoperability engine'
- Provide a demo infrastructure to <u>pip install ROOT</u>
- Improve the usage of several classes from Python through "pythonisations"
- Teach ROOT through its Python interface, especially for beginners courses

More actions are planned for the future, e.g.:

- Revisit Python tutorials and code examples
- Improve and extend the Python interface through pythonisations
- Steadily publish ROOT releases on conda
- Evolve pip install ROOT to Beta mode during 2025 (e.g. automatic publication of wheels, multiple wheels...)



# Seeing it in action

### pip install ROOT -i https://root-experimental-python-wheels.web.cern.ch

```
$:docker run --rm -it python /bin/bash
root@6f40406ea5f2:/# python -m venv myenv
root@6f40406ea5f2:/# source myenv/bin/activate
(myenv) root@6f40406ea5f2:/# pip install ROOT -i https://root-experimental-python-wheels.w
eb.cern.ch
Looking in indexes: https://root-experimental-python-wheels.web.cern.ch
Collecting ROOT
 Downloading https://root-experimental-python-wheels.web.cern.ch/ROOT-0.1a6-cp313-cp313-m
anylinux_2_28_x86_64.whl.metadata (5.3 kB)
Downloading https://root-experimental-python-wheels.web.cern.ch/ROOT-0.1a6-cp313-cp313-man
ylinux_2_28_x86_64.whl (215.0 MB)
                                      - 215.0/215.0 MB 113.7 MB/s eta 0:00:00
Installing collected packages: ROOT
Successfully installed ROOT-0.1a6
(myenv) root@6f40406ea5f2:/# python
Python 3.13.0 (main, Oct 8 2024, 00:06:32) [GCC 12.2.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import ROOT
>>> df = ROOT.RDataFrame(10)
>>> df.Count().GetValue()
10
```



ROOT provides a **C++ interpreter**, cling

- Based on LLVM's <u>clang</u> compiler, now available upstream as <u>clang-repl</u>
- But cling still builds on top of clang-repl, the goal is to simplify this infrastructure
- e.g. through <u>CppInterOp</u>, that exposes APIs from Clang and LLVM in a backward compatible way

Stay even more **up-to-date** with **LLVM** versions

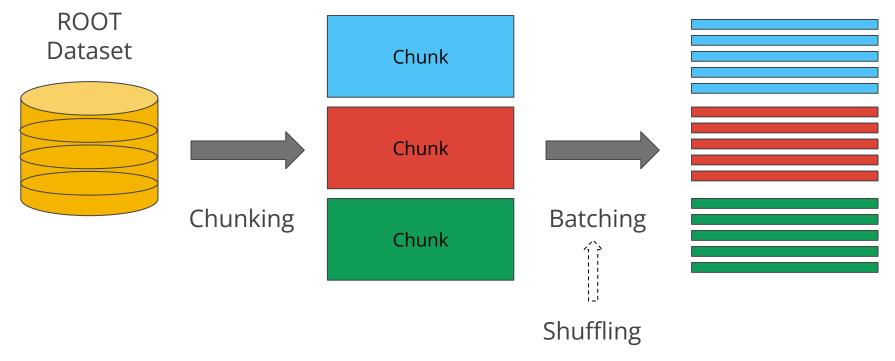
- ROOT 6.34 (November 2024) is based on LLVM 18.1 (March 2024)
- Exploit new features, e.g. performance, C++ standards
- Upstream Cling features to the LLVM repo with clang-repl

Continue research on C++ compilers and language interoperability



# Native ROOT data loading for ML

Provide a native data loading abstraction to pipe ROOT data (TTree, RNTuple) into ML training workflows (e.g. PyTorch, TF)



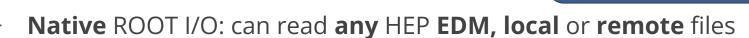


# Native ROOT data loading for ML

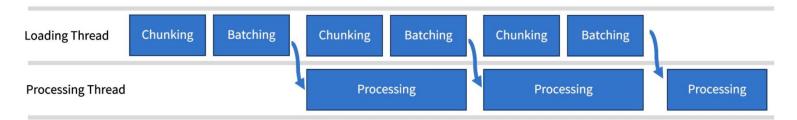
See CHEP'24 presentation

Provide a native data loading abstraction to pipe ROOT data (TTree, RNTuple) into ML training workflows (e.g. PyTorch, TF)

- Asynchronous loading (C++ thread)
- Supports scalar inputs as well as collections



- No need for **pre-conversion** step to other data formats thus **no duplication**
- Integrated with RDataFrame for batch preprocessing





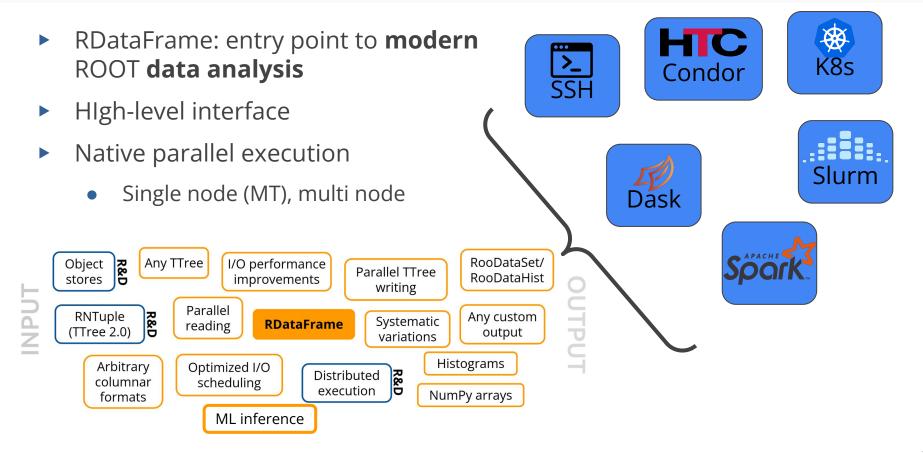
# Native ROOT data loading for ML

```
# Returns two generators that return training
# and validation batches as PyTorch tensors.
gen_train, gen_validation =
ROOT.TMVA.Experimental.CreatePyTorchGenerators(
    rdataframe, batch_size, chunk_size,
    columns=features+labels, target=labels,
    max_vec_sizes=100, validation_split=0.3,
  [...] Create PyTorch model
for x_train, y_train in gen_train:
    # Make prediction and calculate loss
    pred = model(x_train)
    loss = loss_fn(pred, y_train)
```

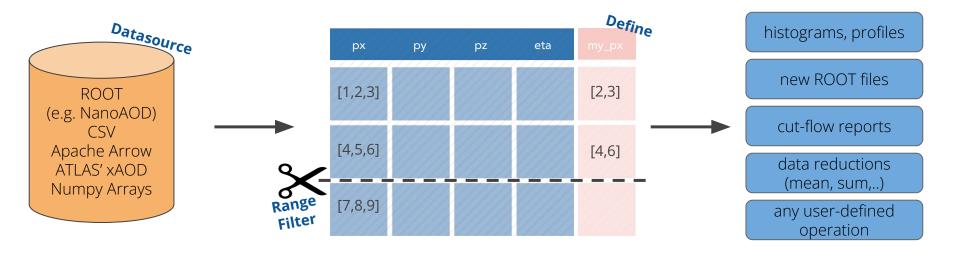
# Data analysis with ROOT



# Data analysis with ROOT



# RDataFrame analysis interface



# enable multi-threading ROOT.EnableImplicitMT()

df = ROOT.RDataFrame(dataset)

df = df.Range(2)

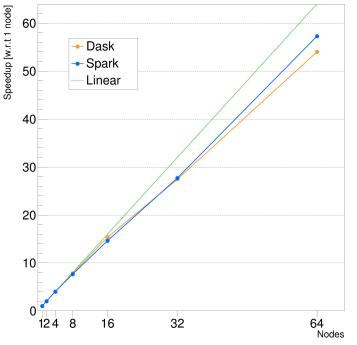
.Define("my\_px", "px[eta > 0]")

# filled in a single pass h1 = df.Histo1D("my\_px", "w") h2 = df.Histo1D("px", "w")

# RDataFrame + HPC centers

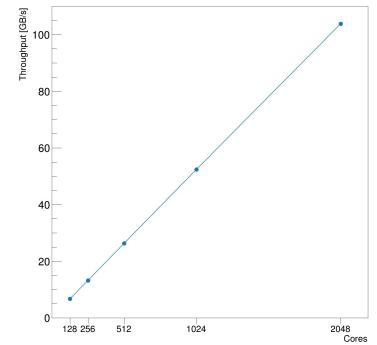
### CERN HPC

- Slurm jobs (Spark/Dask)
- ~100 GB/s on 2048 cores
- <u>JGC publication</u>



Jülich HPC

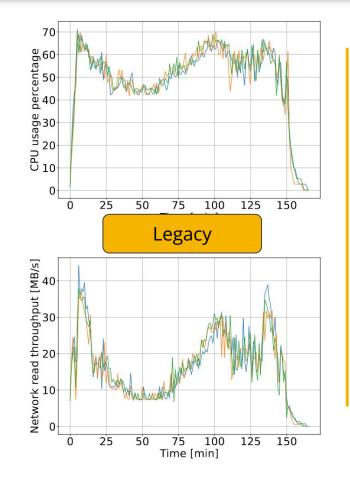
- Collaboration with OpenLab
- Slurm jobs (via Dask)
- <u>Presentation</u>

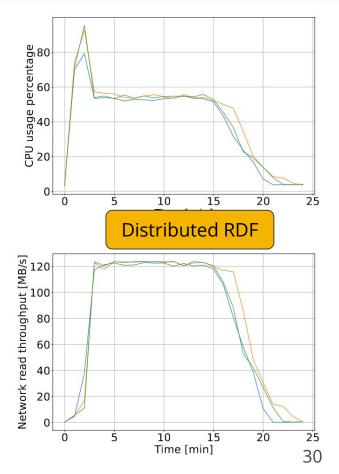




# RDataFrame + INFN analysis facility

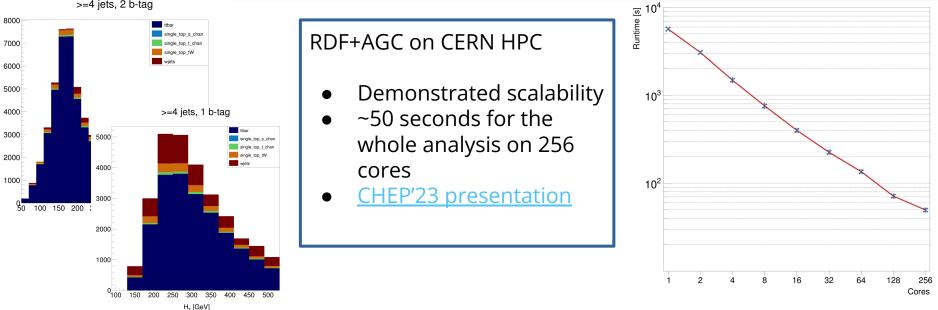
- CMS production analysis
- Before: Python for-loop with <u>NanoAODtools</u>, manual job submission
- After: Interactive distributed RDataFrame
- O(10) speedup
- T. Tedeschi et al.





# RDataFrame + Analysis Grand Challenge

>=4 jets, 2 b-tag

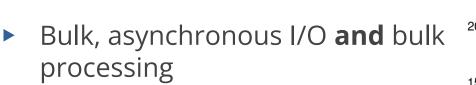


**New!** AGC on **SWAN**, scheduling with **Dask** on **CERN Condor** pools! Rediscovering **existing** infrastructures and services in a modern way

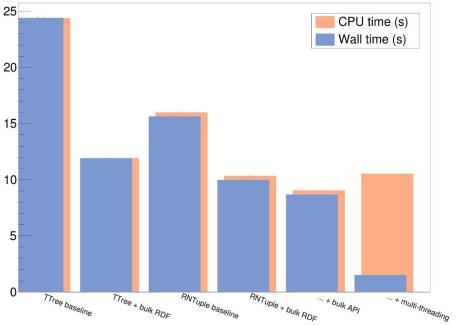
cvmfs + EOS + CERN batch + ROOT ≟ CERN AF



# RDataFrame + RNTuple



- Hide network latency
- Enable SIMD on CPU, GPU offloading



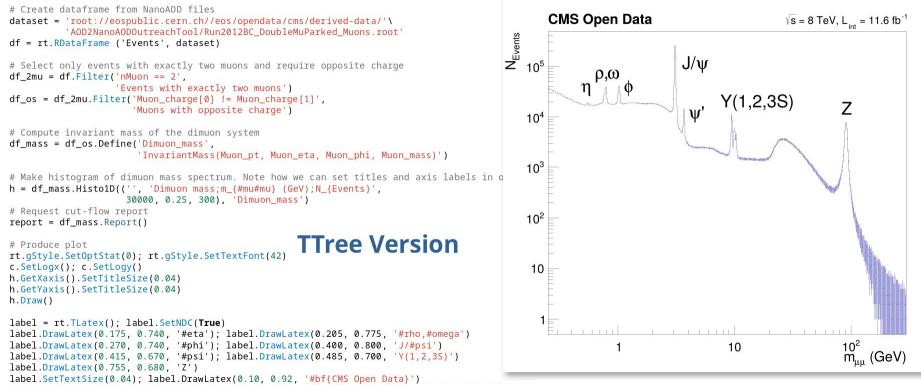
### Dimuon tutorial runtimes

# Moving to RNTuple with RDF: zero code changes

**Dimuon analysis tutorial** 

#### import ROOT as rt

#### rt.EnableImplicitMT()



label.SetTextSize(0.03); label.DrawLatex(0.63, 0.92, '#sqrt{s} = 8 TeV, L\_{int} = 11.6 fb^{-1}')

# Moving to RNTuple with RDF: zero code changes

#### import ROOT as rt

#### rt.EnableImplicitMT()

# Create dataframe from NanoAOD files
dataset = 'http://root.cern/files/tutorials/ntpl004\_dimuon\_v1rc2.root'

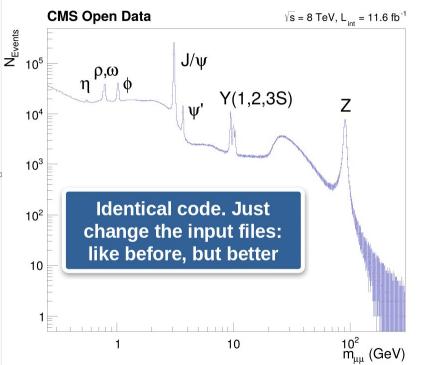
```
df = rt.RDataFrame ('Events', dataset)
```

```
# Request cut-flow report
report = df_mass.Report()
```

```
# Produce plot
rt.gStyle.SetOptStat(0); rt.gStyle.SetTextFont(42)
c.SetLogx(); c.SetLogy()
h.GetXaxis().SetTitleSize(0.04)
h.GetYaxis().SetTitleSize(0.04)
h.Draw()
```

1abel = rt.TLatex(); label.SetNDC(True)
1abel.DrawLatex(0.175, 0.740, '#eta'); label.DrawLatex(0.205, 0.775, '#rho,#omega')
1abel.DrawLatex(0.270, 0.740, '#phi'); label.DrawLatex(0.400, 0.800, 'J/#psi')
1abel.DrawLatex(0.415, 0.670, '#psi'); label.DrawLatex(0.485, 0.700, 'Y(1,2,3S)')
1abel.DrawLatex(0.755, 0.680, 'Z')
1abel.SetTextSize(0.04); label.DrawLatex(0.10, 0.92, '#bf{CMS Open Data}')
1abel.SetTextSize(0.03); label.DrawLatex(0.63, 0.92, '#sqrt{s} = 8 TeV, L\_{int} = 11.6 fb^{-1}')

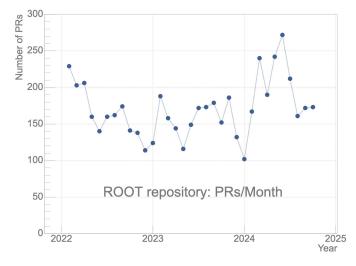
### Dimuon analysis tutorial



# Outreach

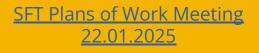
# An Open approach to boost collaboration

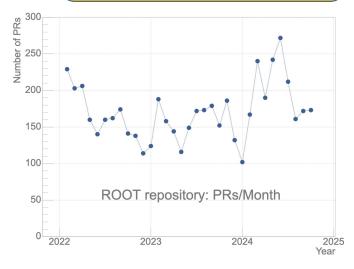
- Open-source and Open-development
  - On <u>GitHub</u>, LGPL 2.1
  - PR based model with public review process
  - Very visible authorship of contributions
- Open-planning: <u>https://cern.ch/root-pow</u>
- Yearly plan of work (PoW) formed internally, then discussed with users
- You can influence the PoW, with your input, active engagement and contributions!
- Formal reporting process engaging experiments



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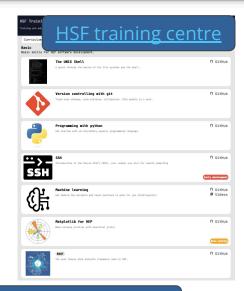




# Scaling up the ROOT training

- CERN Summer Student Course ~200 participants, ~5 per year
- With IRIS-HEP and HSF: Python for analysis course ~90 participants, ~3 per year
- Based exclusively on ROOT's Python interface and notebooks
- Besides the value of the trainings themselves:
  - Surveys: feedback received now incorporated in the material
  - Several ROOT devs involved: we trained to train!

The ROOT team is available to give trainings and help **train the trainers** 





• RDF is ROOT's high-level analysis interface.

2

- Users define their analysis as a sequence of operations to be performed on the data-frame object;
  - the framework takes care of the management of the loop over entries as well as low-level details such as I/O and parallelisation.
- RDataFrame provides methods to perform most common operations required by ROOT analyses:

# **ROOT Hackathons**

- - New in 2024!
  - An event born for ROOT core devs, open to everybody
  - A welcoming, positive and inclusive atmosphere
  - 1st Hackathon in February 2024
    - Nickname "Fixathon", aim at fixing various github issues
  - 2nd Hackathon 25-27 November 2024
    - Topic: Python, Docs, Tutorials
  - In presence only, very informal
    - Currently cannot provide sponsorships for attendance



ROOT::RHackathon

### Join us for the second ROOT Hackathon!

#### This edition, we are:

- Enhancing the Python documentation interfaces
- Extending ROOT's Python interfaces
  Modernising ROOT's collection of
- Modernising ROOT's collection of tutorials



Help us make an impact on HEP software, sign up today! Places are limited

#### Details

For whom	All levels of experience, from new users to seasoned contributors
When	November 25 - 27, 2024
Where	IdeaSquare, CERN
Good to know	Home cooked lunches are included!





- A welcoming, positive and inclusive atmosphere
- An opportunity to shape *together* the future of ROOT!
- A venue for ROOT users, world-class experts of scientific computing and the ROOT core team to *exchange ideas* and learn from each other
- A *rich program* of presentations, tutorials, and most importantly, discussions



In Europe 17-21 November 2025 Save the date!

# Conclusions





- The ROOT core team is here to support you, listen to your needs and make your data processing and analysis a success!
  - All sustained by a **long-term support model**, and a **rich** result-oriented **R&D** program
- Open approach: open-source, open-development, open-planning
  - For ROOT, collaborations and contributions are essential and highly valued!
- Forward-looking: a core set of modern features to support HL-LHC and future colliders



- ROOT web page: <u>root.cern</u>
- ROOT GitHub: <u>github.com/root-project/root</u>
- Careers at CERN: <u>https://careers.cern/</u>
- Email: <u>vincenzo.eduardo.padulano@cern.ch</u>