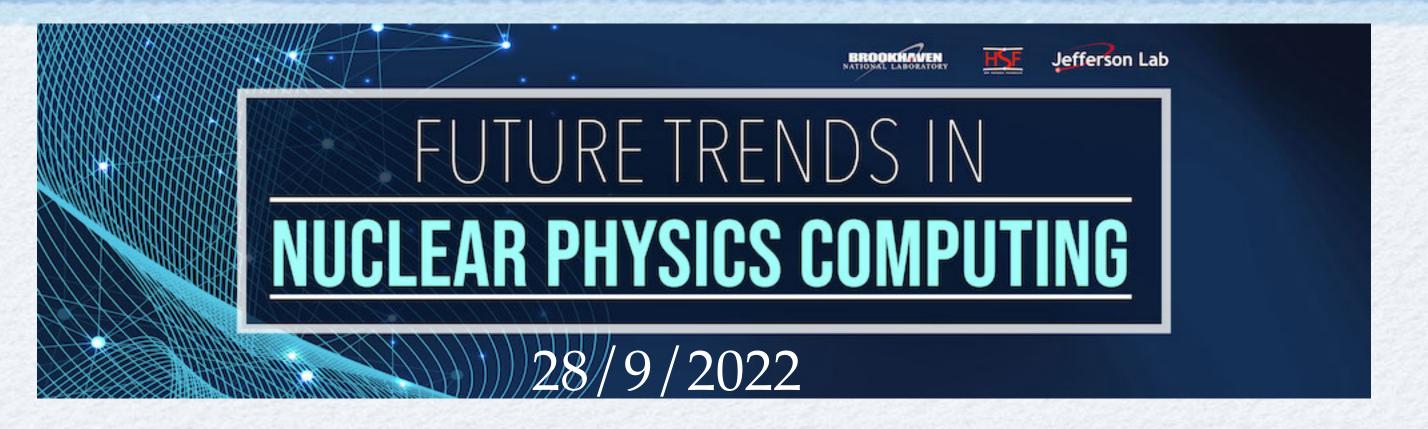




# Status and Future of Analysis The ROOT Perspective (covering Python and C++)

Lorenzo Moneta (CERN/EP-SFT)

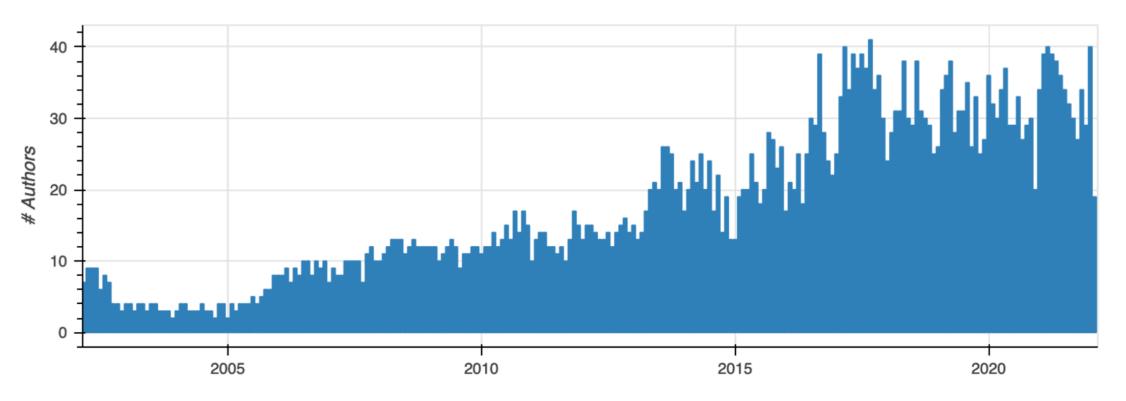




## Introduction



- ROOT is an open source, community-driven project
  - C++ under the hood, but looks like a Python module
- ROOT is used by all HEP experiments
  - more than 1EB of data stored in ROOT I/O format.
- Serving both analysis and experiments software
  - excellent interactions with users (~1000 Root Forum post/month)
- Despite existing for many years ROOT is still very active
  - high number of contributors/month
- Ongoing massive innovation
  - I/O, analysis interfaces, python, RooFit, ML, web-graphics, etc..





# ROOT Core Components



- I/O : reading and writing data efficiently
- Analysis interfaces: histograms and RDataFrame
- Interactivity: C++ interpreter and Python bindings
- Math libraries: PRNG, numerical algorithms (e.g. Minuit)
- Statistics and modeling: fitting
- Graphics: scientific visualization
- Machine learning: TMVA, model evaluations and interoperability

Major recent developments in some of these components and the future plans



## Outline



- Analysis landscape:
  - I/O developments
    - RNtuple
  - Python interfaces:
    - PyROOT
  - data exploration, declarative analysis
    - RDataFrame
  - machine learning, interoperability and analysis integration
    - TMVA/SOFIE
  - statistical analysis and modelling
    - RooFit
- What we have in ROOT now and the planned future developments



# Future Analysis Landscape



- Expect a higher number of events and more complex problems
  - larger data sets
  - higher dimensional problems requiring more CPU (or GPU)
- ROOT is well suited for this
  - ROOT columnar data (TTree and new RNTuple) designed for analysis on large data sets
  - New versatile analysis interfaces (RDataFrame)
  - Language and tool interoperability (e.g. with ML libraries)
  - Statistical analysis of complex problems (RooFit)



# RNTuple



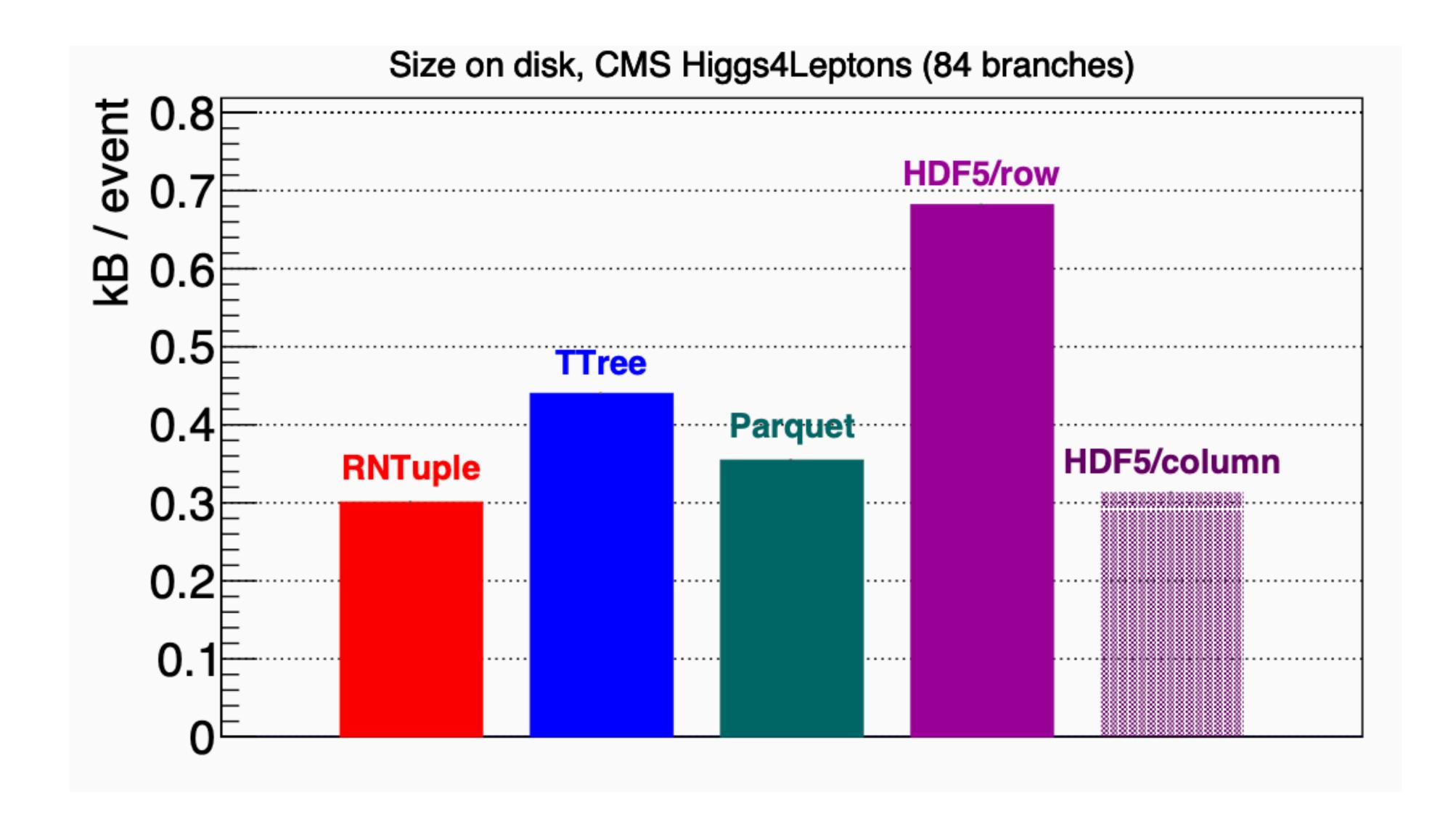
- Successor of TTree
  - columnar storage of event data optimised for selective reads
- Integration with LHC experiments is ongoing, to be production ready for HL-LHC
- Based on 25+ years of TTree experience,
- Redesigned I/O subsystem providing:
  - Less disk and CPU usage for the same data content
  - 15% smaller files, × 2–5 better single-core performance
  - 10 GB/s per box and 1 GB/s per core sustained end-to-end throughput
- And also:
  - Systematic use of exceptions to prevent silent I/O errors
  - Efficient support of modern hardware (built for multi-threading and async I/O)
  - Native support for object stores

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## RNTuple Performances: I/O Size





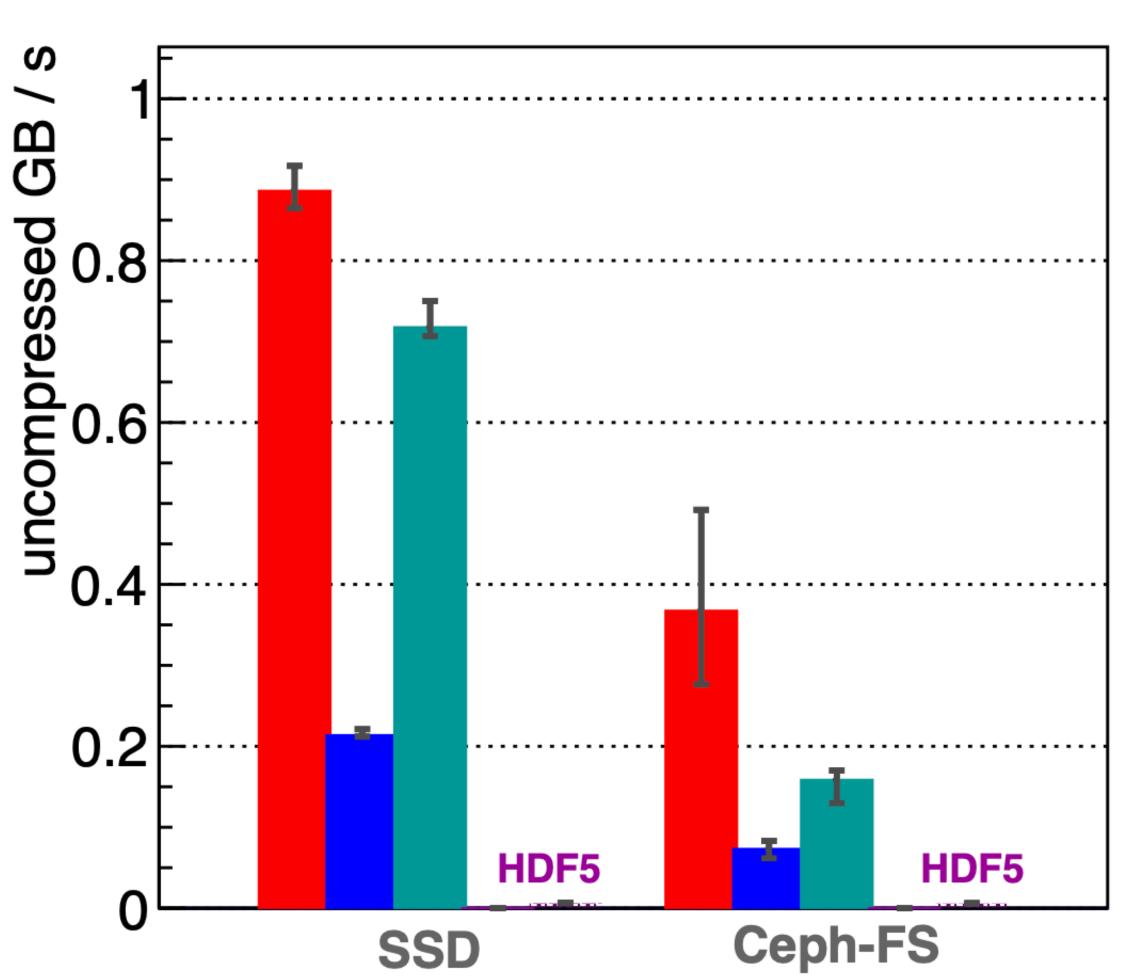


## RNTuple Performances: I/O Speed

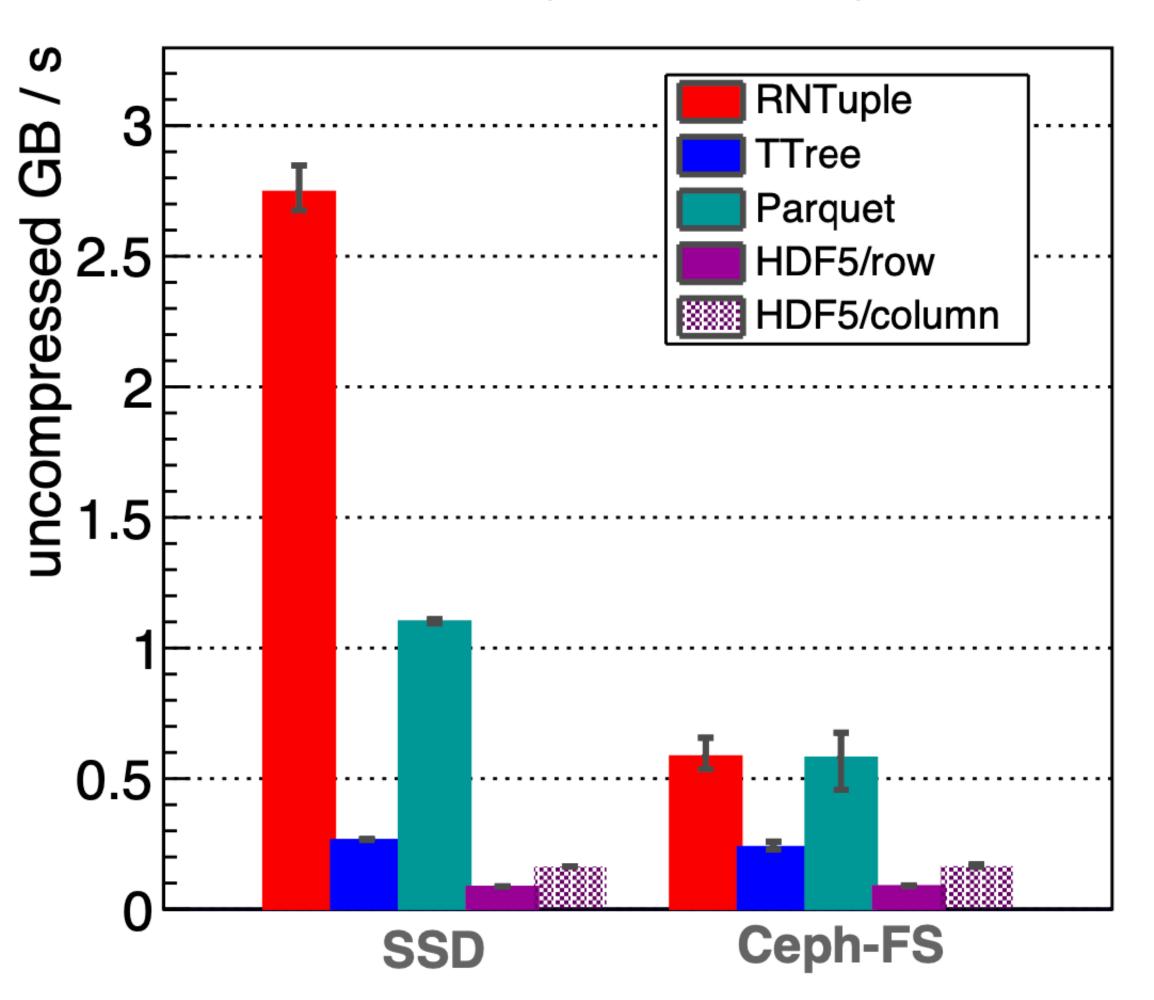


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#### LHCb B2HHH (10/26 branches)





# RNTuple Plans



- Smaller files and significantly faster reads compared to TTree
- Modern and robust API
- Capable of making efficient use of modern devices and storage systems (such as SSD, object stores, and many cores)
- More results and developments will be presented at the coming ACAT22
- RNTuple is work in progress in ROOT::Experimental
  - the on-disk format is still subject to small changes!
  - happy to get your feedback!





# PyROOT



- ROOT is not only C++
- It can be used as a Python module thanks to Python-C++ bindings
  - > import ROOT
  - > h1 = ROOT.TH1D("h1","my hist",100,0.,10.)
- All C++ functionality is available in Python
  - can also access user-defined C++ code from Python
- ROOT-specific pythonizations added on top of C++ API
  - make ROOT classes more "pythonic" to use
- PyROOT is now built on top of Cppyy (from W. Lavrijsen)
  - based on Cling and ROOT type system
  - support modern C++



# ROOT Pythonizations



- Make C++ classes easier to use in Python
- Available for some classes:
  - TFile, TTree
  - RDataFrame, RVec
  - Main RooFit classes
  - TMVA

#### **PyROOT**

In the same way as for **TDirectory**, it is possible to inspect the content of a **TFile** object from Python as if the directories and objects it contains were its attributes. For more information, please refer to the **TDirectory** documentation.

In addition, TFile instances can be inspected via the Get method, a feature that is inherited from TDirectoryFile (please see the documentation of TDirectoryFile for examples on how to use it).

In order to write objects into a TFile, the WriteObject Python method can be used (more information in the documentation of TDirectoryFile).

PyROOT modifies the TFile constructor and the TFile::Open method to make them behave in a more pythonic way. In particular, they both throw an OSError if there was a problem accessing the file (e.g. non-existent or corrupted file).

This class can also be used as a context manager, with the goal of opening a file and doing some quick manipulations of the objects inside it. The **TFile::Close** method will be automatically called at the end of the context. For example:

```
from ROOT import TFile
with TFile("file1.root", "recreate") as outfile:
   hout = ROOT.THIF(...)
   outfile WriteObject(hout, "myhisto")
```

- Documented in reference guide (in class documentation)
- Working on pythonizations of Histograms and Graph classes
  - better inter-operability with Numpy
  - implementing <a href="UHI">UHI indexing</a>: hist[bin1:bin2]



# **Examples of Pythonizations**



TTree and TFile

Process with RDataFrame and convert to Numpy arrays

```
from ROOT import RDataFrame
df = RDataFrame('myTree', 'file.root')

# Apply cuts, define new columns
df = df.Filter('x > 0').Define('z', 'x*y')

cols = df.AsNumpy() # cols is a dict of NumPy arrays
```

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# Analysis Landscape



#### **Analysis life cycle**

skimming, ntuple production

quick exploration, first implementation systematics, scale out

statistical analysis

#### **Platforms**

laptop or PC

many-core machine

computing cluster + job submission

#### **Analysis languages**

**↓** ~50% C++

**1** ~50%

Python

#### Storage

local disk fast-access network storage EOS or other not-so-fast backend



## RDataFrame



## A Swiss army knife for data analysis

#### **Analysis life cycle**

skimming, ntuple production

quick exploration, first implementation systematics, scale out

#### **Platforms**

laptop or PC

many-core machine

computing cluster + job submission

#### **Analysis languages**

**♣** ~50% C++

**1** ~50%

Python

#### Storage

local disk fast-access network storage EOS or other not-so-fast backend

**ROOT.RDataFrame** is a modern analysis interface that addresses all these use cases with one high-level programming model that performs well, scales well and enables HEP-specific ergonomics, in C++ and Python.



## RDataFrame Code



#### Example of RDF code in Python

df = ROOT.RDataFrame (dataset)······	on this (ROOT, CSV,) dataset	
df = df.Filter("x > 0")	only accept events for which $x > 0$	event selection
.Define("r2", "x*x + y*y")	define $r^2 = x^2 + y^2$	derived quantities, object selections
rHist = df.Histo1D("r2")	plot r2 for events that pass the cut	
df.Snapshot("newtree", "out.root") ·········	write the skimmed data and r2 to a new ROOT file	data aggregations

Users can inject **arbitrary code** at all steps, which makes this relatively simple API extremely versatile.

Physicists describe analysis ingredients, ROOT handles technicalities



## RDataFrame Code: MT



#### Switch to multi-thread execution (Python):

ROOT.EnableImplicitMT()	Run a multi-thread event loop
df = ROOT.RDataFrame(dataset)·····	on this (ROOT, CSV,) dataset
df = df.Filter("x > 0")	only accept events for which $x > 0$
.Define("r2", "x*x + y*y")	define $r2 = x^2 + y^2$
rHist = df.Histo1D("r2")	plot r2 for events that pass the cut
df.Snapshot("newtree", "out.root") ······	write the skimmed data and r2 to a new ROOT file

from E. Guiraud: RDF@ICHEP 2022



# RDataFrame Code: DistRDF



#### Switch to distributed execution (Python):

cluster = dask\_jobqueue.HTCondorCluster(n\_workers=64)

df = RDataFrame(dataset, daskclient=Client(cluster)).....

connect to HTCondor via Dask

df = df.Filter("x > 0")

.Define("r2", "x\*x + y\*y")

other code stays the same

rHist = df.Histo1D("r2")

df.Snapshot("newtree", "out.root")

**Available since v6.26 (experimental)** 

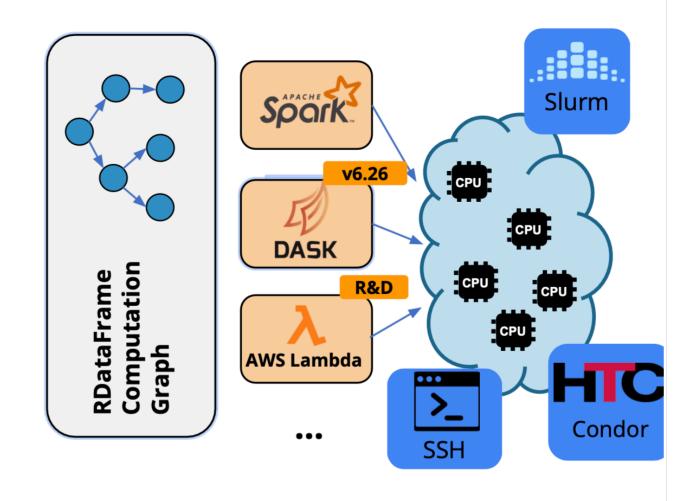
Also see this tutorial, the docs, the recent ATTF talk

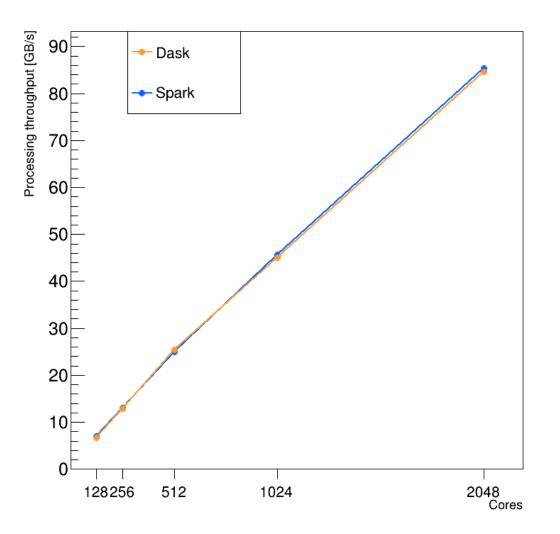


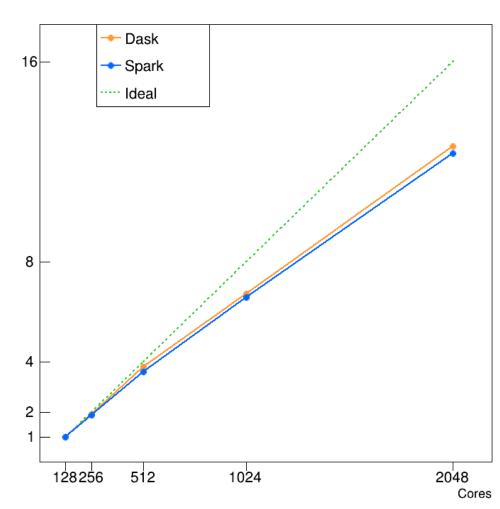
## Distributed RDF



- Enables interactive large-scale distributed data analysis
- Uses Python RDF API(C++ event loop)
- High throughput with native ROOT I/O
- Spark/Dask/HTCondor/Slurm/
   SSH.... take care of scheduling and resource management
- Transparently merges results coming from different computing nodes







Distributed RDF benchmark (dimuon, 4000x data)
See this talk

from E. Guiraud: RDF@ICHEP 2022

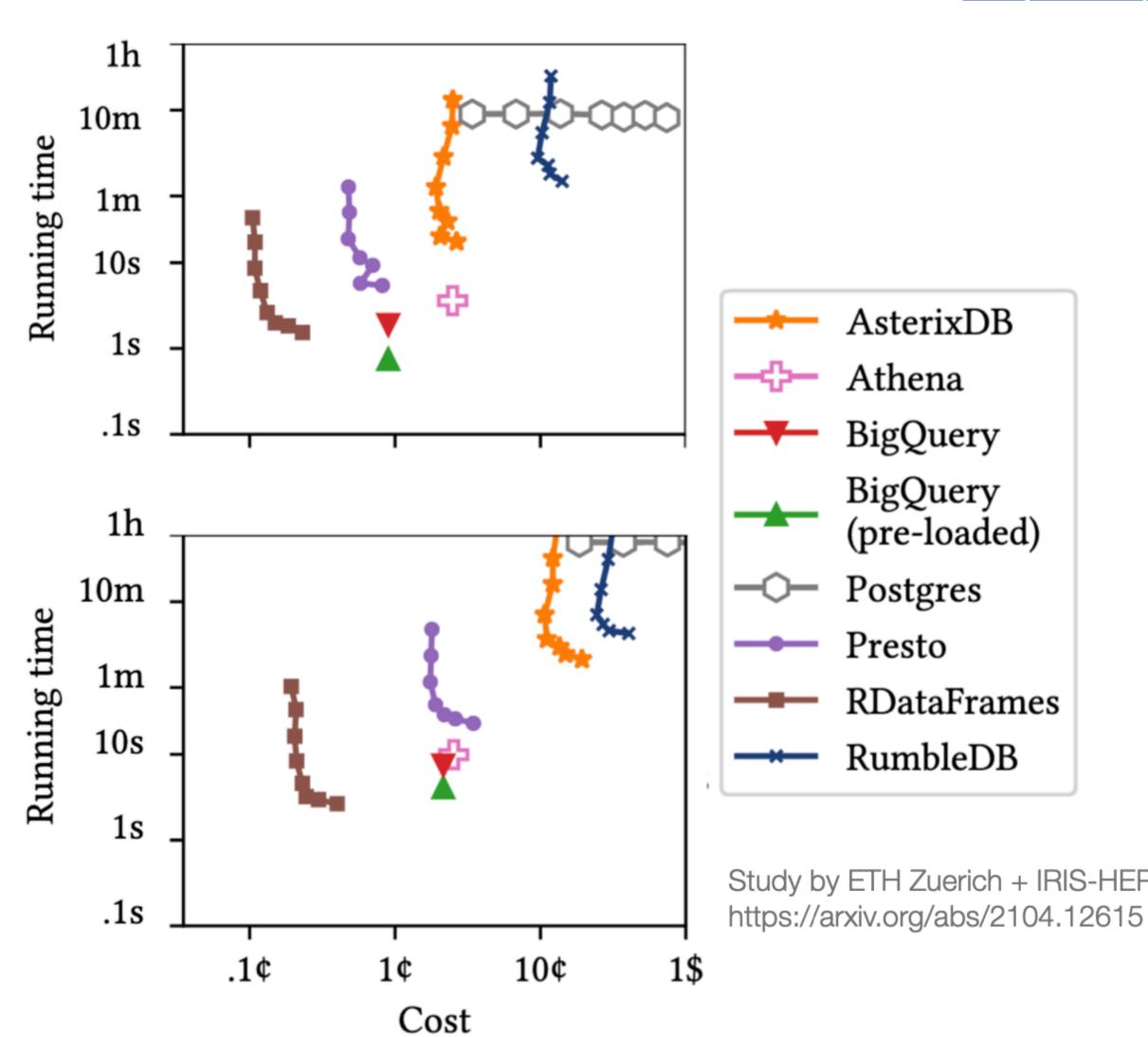
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## RDF Performances



- RDF enables fast turnaround for complex analysis use cases
- scales well to many cores, many nodes, many histograms
- Independent study shows RDF analysis to be significantly faster
- Performance is always ongoing work:
  - we are constantly looking for feedback/use cases





# Systematic Variations



```
Python
                                  attach an up/down variation to "pt"
                nominal hx =
                  df.Vary("pt", "RVecD{pt*0.9, pt*1.1}", ["down", "up"])
                    .Filter("pt > k")
proceed as usual,
                    .Define("x", someFunc, ["pt"])
as if working with
nominal values only
                     .Histo1D("x")
                hx = ROOT.RDF. VariationsFor(nominal_hx)
                                            obtain all variations
                hx["nominal"].Draw()
                hx["pt:down"].Draw("SAME")
```

Variations automatically propagate to selections, derived quantities and results.

Multi-thread and distributed execution just works.

Only needed quantities are re-computed, all in one event loop.

from E. Guiraud: RDF@ICHEP 2022



## RDF: Status and Plans



- and many more features, e.g.
  - transparent support for RNTuple
  - machine learning inference:
    - SOFIE, RBDT
  - interoperability with Numpy
- and coming soon:
  - bulk (batch) processing of data
    - improved performance
    - batch generator for ML tools
- RDF keeps evolving
  - cooperation with user community
- Critical to focus on the right features
  - need your feedback and help!

Lazy action	Description
Aggregate()	Execute a user-defined accumulation operation on the processed column values.
Book()	Book execution of a custom action using a user-defined helper object.
Cache()	Cache column values in memory. Custom columns can be cached as well, filtered entries are not cached. Users can specify which columns to save (default is all).
Count()	Return the number of events processed. Useful e.g. to get a quick count of the number of events passing a Filter.
Display()	Provides a printable representation of the dataset contents. The method returns a ROOT::RDF::RDisplay() instance which can print a tabular representation of the data or return it as a string.
Fill()	Fill a user-defined object with the values of the specified columns, as if by calling Obj.Fill(col1, col2,).
Graph()	Fills a <b>TGraph</b> with the two columns provided. If multi-threading is enabled, the order of the points may not be the one expected, it is therefore suggested to sort if before drawing.
GraphAsymmErrors()	Fills a TGraphAsymmErrors. If multi-threading is enabled, the order of the points may not be the one expected, it is therefore suggested to sort if before drawing.
Histo1D(), Histo2D(), Histo3D()	Fill a one-, two-, three-dimensional histogram with the processed column values.
HistoND()	Fill an N-dimensional histogram with the processed column values.
Max()	Return the maximum of processed column values. If the type of the column is inferred, the return type is double, the type of the column otherwise.
Mean()	Return the mean of processed column values.
Min()	Return the minimum of processed column values. If the type of the column is inferred, the return type is double, the type of the column otherwise.
Profile1D(), Profile2D()	Fill a one- or two-dimensional profile with the column values that passed all filters.
Reduce()	Reduce (e.g. sum, merge) entries using the function (lambda, functor) passed as argument. The function must have signature T(T,T) where T is the type of the column. Return the final result of the reduction operation. An optional parameter allows initialization of the result object to non-default values.
Report()	Obtain statistics on how many entries have been accepted and rejected by the filters. See the section on <b>named filters</b> for a more detailed explanation. The method returns a <b>ROOT::RDF::RCutFlowReport</b> instance which can be queried programmatically to get information about the effects of the individual cuts.
Stats()	Return a TStatistic object filled with the input columns.
StdDev()	Return the unbiased standard deviation of the processed column values.
Sum()	Return the sum of the values in the column. If the type of the column is inferred, the return type is double, the type of the column otherwise.
Take()	Extract a column from the dataset as a collection of values, e.g. a std::vector <float> for a column of type float.</float>
Instant action	Description

action	Description			
Foreach()	Execute a user-defined function on each entry. Users are responsible for the thread-safety of this callable when executing with implicit multi-threading enabled.			
ForeachSlot()	Same as Foreach(), but the user-defined function must take an extra unsigned int slot as its first parameter. slot will take a different value, 0 to nThreads - 1, for each thread of execution. This is meant as a helper in writing thread-safe Foreach() actions when using RDataFrame after ROOT::EnableImplicitMT(). ForeachSlot() works just as well with single-thread execution: in that case slot will always be 0.			
Snapshot()	Write the processed dataset to disk, in a new TTree and TFile. Custom columns can be saved as well, filtered entries are not saved. Users can specify which columns to save (default is all). Snapshot, by default, overwrites the output file if it already exists. Snapshot() can be made lazy setting the appropriate flag in the snapshot options.			

#### Querie

These operations do not modify the dataframe or book computations but simply return information on the RDataFrame object.

Operation	Description
Describe()	Get useful information describing the dataframe, e.g. columns and their types.
GetColumnNames()	Get the names of all the available columns of the dataset.
GetColumnType()	Return the type of a given column as a string.
GetColumnTypeNamesList()	Return the list of type names of columns in the dataset.
GetDefinedColumnNames()	Get the names of all the defined columns.
GetFilterNames()	Return the names of all filters in the computation graph.
GetNRuns()	Return the number of event loops run by this RDataFrame instance so far.
GetNSlots()	Return the number of processing slots that RDataFrame will use during the event loop (i.e. the concurrency level).
SaveGraph()	Store the computation graph of an RDataFrame in DOT format (graphviz) for easy inspection. See the relevant section for details

from E. Guiraud: RDF@ICHEP 2022



# Machine Learning in ROOT



- TMVA: Toolkit for Multi-Variate Analysis
  - Provides a collection of several ML algorithms including Decision Trees, but also Deep Learning tools with GPU support
- Shifted Focus now on :
  - interoperability with Python ML libraries
    - developing glue between ROOT I/O and Python ML ecosystem
    - designing also new interfaces in TMVA for better interoperability
  - optimal model inference
    - enable physicists to deploy easily their ML models on large datasets
    - integration of model inference with analysis tools (RDF)

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## SOFIE: Fast ML Inference in ROOT



- New ROOT tool for inference code generation for DL models
  - input, a trained ML model:
    - ONNX (new standard for ML)
    - TF/Keras
    - PyTorch
  - Output:
    - C++ code
      - minimal dependency (BLAS)
      - can be compiled on the fly (e.g. with Cling)

ROOT 6.26 (experimental)

```
C++ source

ONNX

PyTorch

SOFIE

Inference function

Keras

using namespace TMVA::Experimental::SOFIE;

RModelParser_ONNX parser;

RModel model = parser.Parse("Model.onnx");
```

// generate text code internally (with some options)
model.Generate();
// write output header file and data weight file
model.OutputGenerated();

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# ML inference with RDataFrame



- ML model evaluation can be integrated in RDF event loop
  - SofieFunctor: adapter for using SOFIE within RDF

- support for multi-threaded evaluation
- see full Example tutorial code in <u>C++</u> or <u>Python</u>

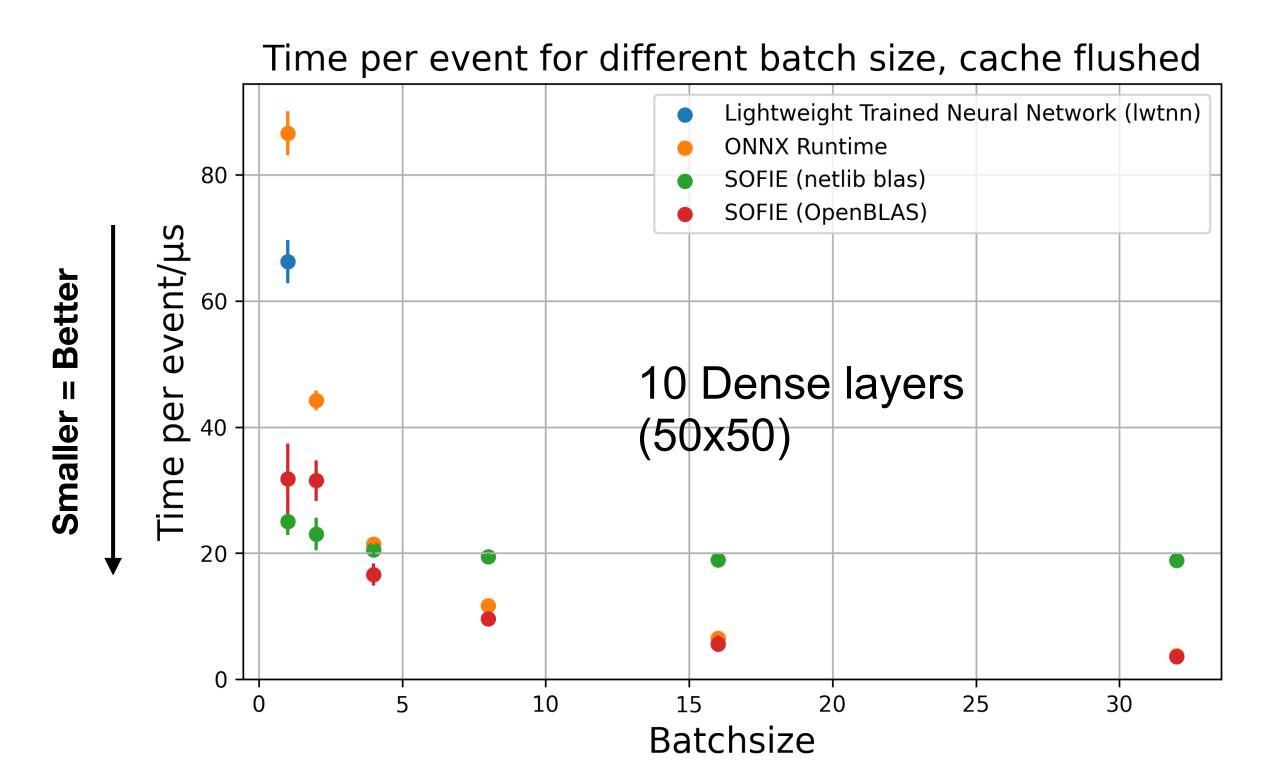


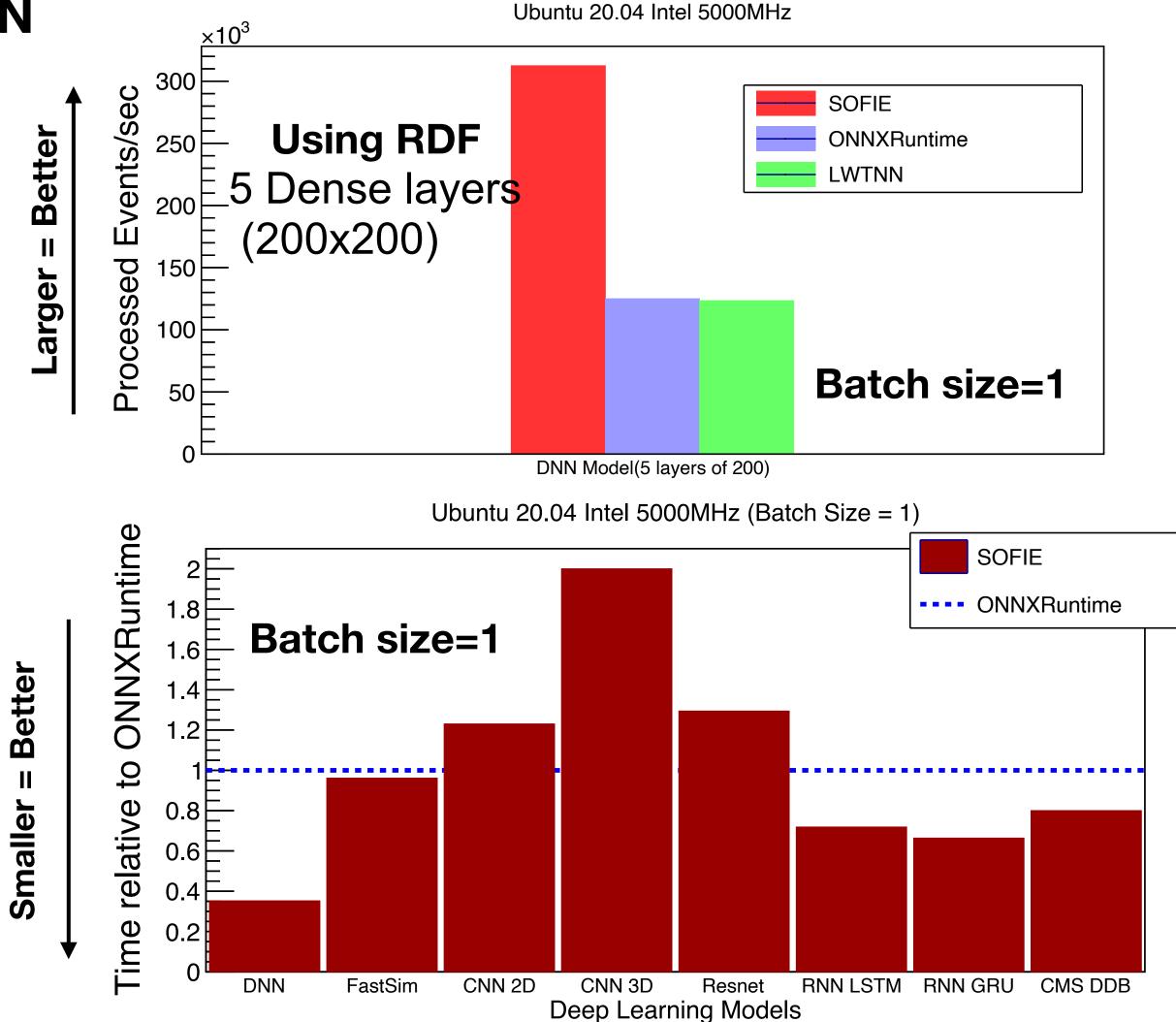
## SOFIE Benchmarks



#### Comparison with ONNXRuntime and LWTNN

- 2-3 faster than ONNXRuntime for DNN with batch size=1
- 20% faster for RNN operators
- slower for CNN (20% for 2D, x2 for 3D)





varying batch size...



# Supported Operators in SOFIE



Perceptron: Gemm	Implemented and integrated (ROOT 6.26)
Activations: Relu, Seul, Sigmoid, Softmax, LeakyRelu	Implemented and integrated
Convolution (1D, 2D and 3D and ConvTranspose	Implemented and integrated
Recurrent: RNN, GRU, LSTM	Implemented and integrated
BatchNormalization	Implemented and integrated
Pooling: MaxPool, AveragePool, GlobalAverage	Implemented and integrated
Layer operations: Add, Sum, Mul, Div, Reshape, Flatten, Transpose, Squeeze, Unsqueeze, Slice, Concat, Identity	Implemented and integrated
User-defined operator	Implemented and integrated
Gather (for embedding) and more depending on user needs	Planned for next release
Direct GNN support (NEW)	Planned for next release

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# Fast Decision Tree Inference



- Inference engine taking model parameters from externally trained models
- Features:
  - Simple to use from Python and C++
  - Thread-safe
  - Zero-copy
  - Fast for single event and batch inference
  - External training and model conversion

```
xgb = xgboost.BDTClassifier(options)
xgb.fit(x, y)
ROOT.TMVA.SaveXGBoost(xgb, "myBDT", "model.root")
```

#### Python application

```
xgb = xgboost.BDTClassifier(options)
xgb.fit(x, y)
ROOT.TMVA.SaveXGBoost(xgb, "myBDT", "model.root")
```

#### C++ application

```
TMVA::RBDT bdt("myBDT", "model.root");
auto y1 = bdt.Compute({1.0, ...});

auto x = TMVA::RTensor<float>(data, shape);
auto y2 = bdt.Compute(x);
```

```
New BDT inference (jitted)

New BDT inference (jitted)

New BDT inference (jitted)
```

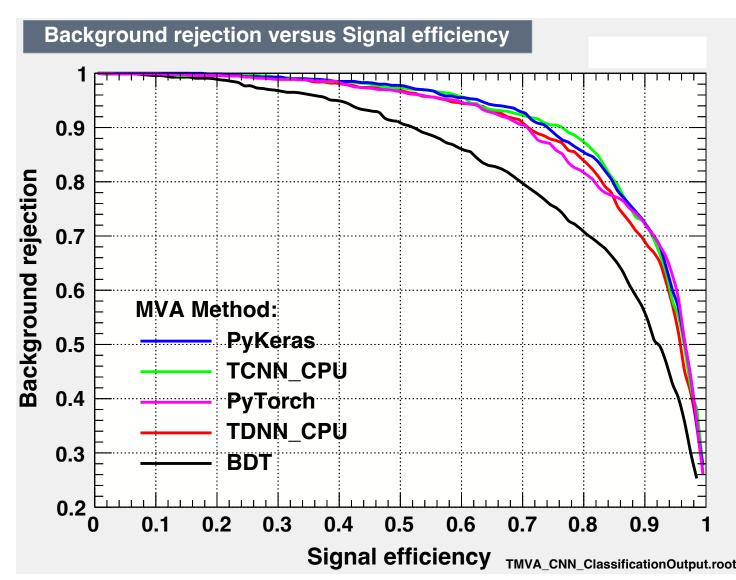
New BDT inference



# Interoperability of TMVA



- Pythonization of TMVA interfaces
  - from string API to python keyword args
- Training of Python ML tools within TMVA workflow
  - interfaces to scikit-learn, Keras and PyTorch
- Working on generic data-loader for ML workflows
  - Generator doing batching and shuffling from ROOT files on the fly
  - Allows for efficient training of datasets larger than RAM sizes
  - Direct feeding of data from disk to GPU



```
Example of a possible ML workflow loading batches
```

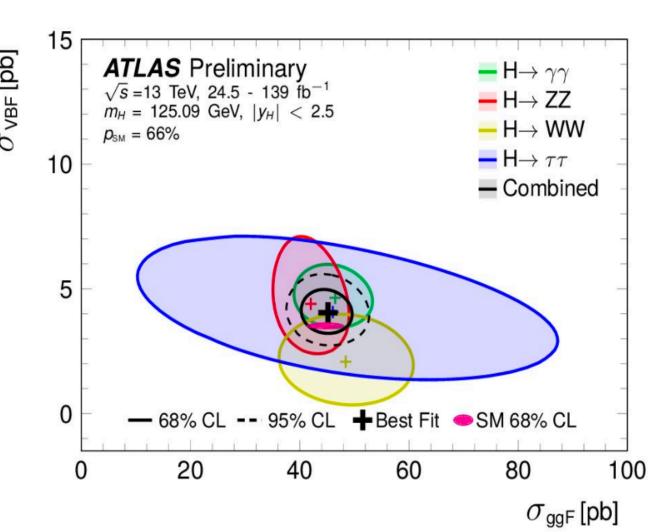
```
df = ROOT.RDataFrame("Events", "http://file.root")
generator = TMVA.BatchGenerator(df, cols, batchSize)
for step in gradientSteps:
    x = generator()
    model.fit(x)
```



# Statistical Modeling



- Physics analyses continuously generate increasingly complex likelihood models to describe their data
  - Higgs combination fits, EFT interpretations
    - O(1000) parameters
    - O(100) likelihood components
    - O(100) datasets



Recent ATLAS Higgs combination fit result [1]. This fit took about five hours to complete.

- Only one tool capable of handling such models: RooFit
- Recent development give possibility to bring down fitting time from hours to minutes
  - from a work day to a coffe break!



## Roofit Evolution



### RooFit is evolving on many different areas:

Vectorization

Gradient parallelization

Higher-level interfaces

**GPU Implementation** 

Fit precision and correctness

Pythonizations

Automatic differentiation

Testing and benchmarking

Interoperability

Performance optimization

Targeted optimizations for expensive workflows

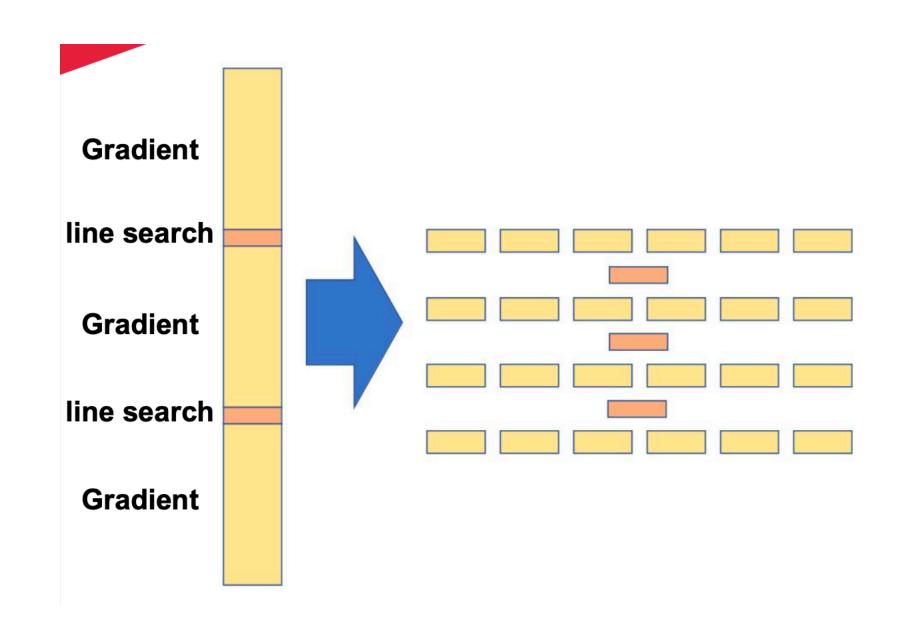
User interface and experience

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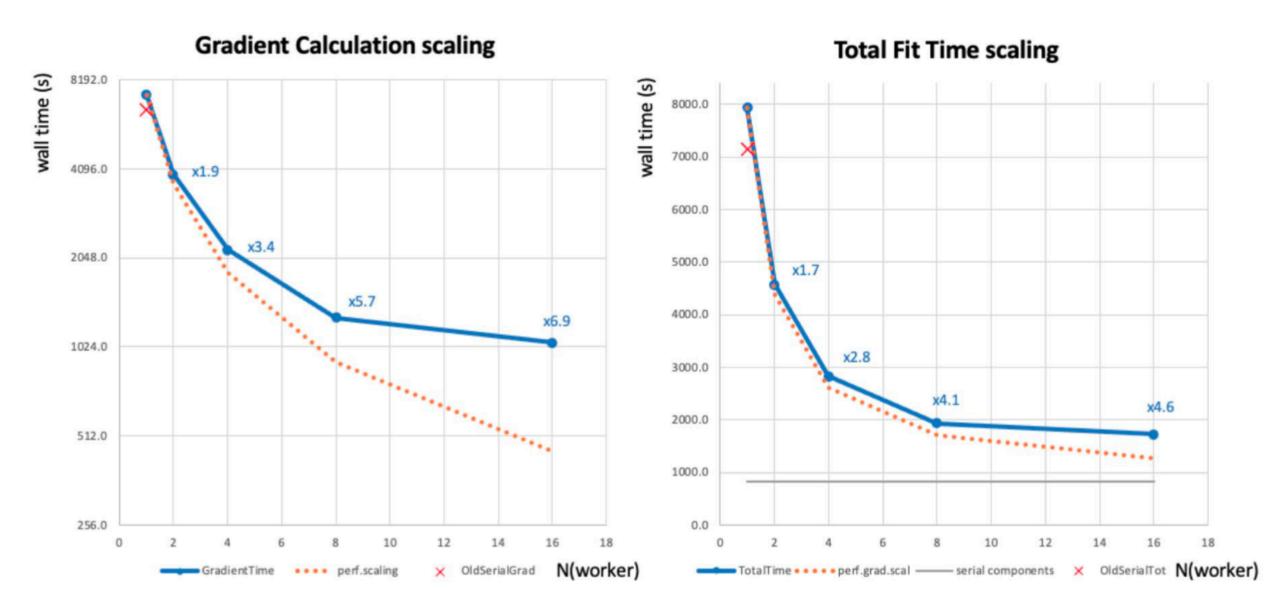
# Gradient parallelization





- Parallelize at gradient calculation level
  - N parameters: ~O(2N) function evaluations for computing numerical derivatives
  - Line search: serial part ~O(3) function evaluation
- Dynamic load balancing over workers through random work stealing algorithm
  - complexity of derivative calculation varies
- Designed to have maximum speed impact of complex fits with many parameters

- Wall time decrease in Higgs combination fit:
  - from 2h12m26s → 28m52s
     (~4/5 times faster)
- Result validated: all parameters agreed with serial fit within 1% of their uncertainties!



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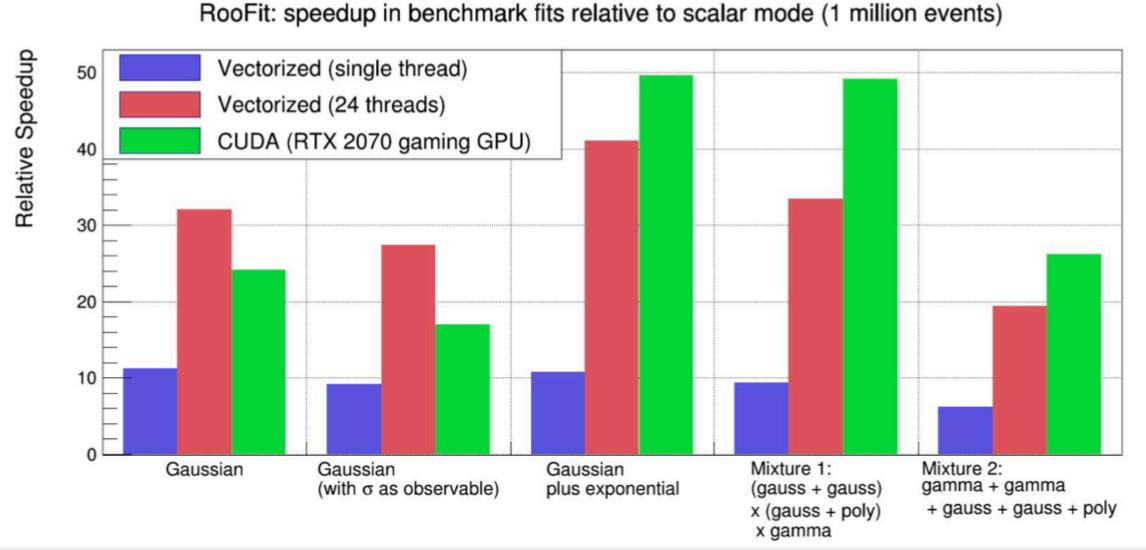


## Vectorisation and GPU Computation

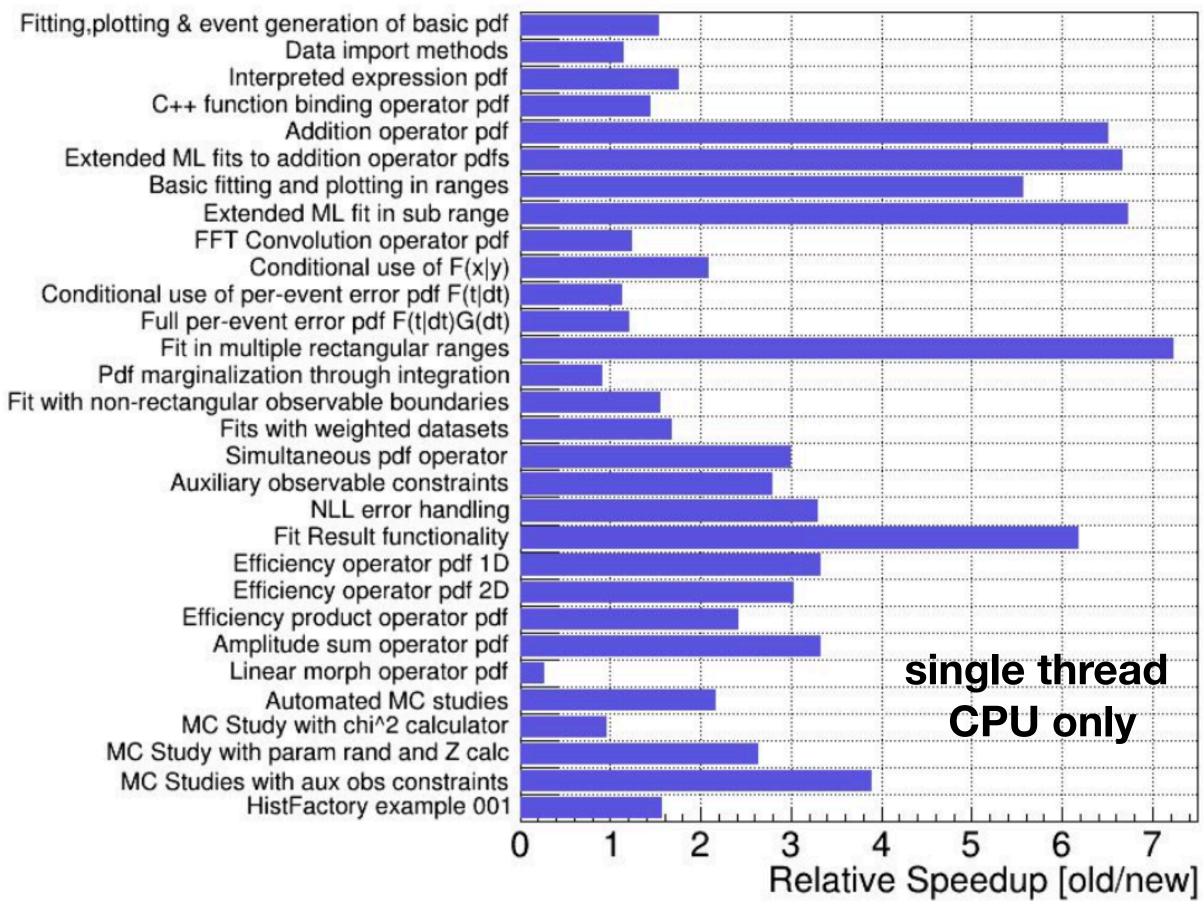


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- Batch evaluation of RooFit models:
  - allow code vectorisation
  - optionally allow multi-threading or GPU computation (with CUDA)
- possible due to a re-structure of RooFit computational graph.
  - from event-by event to batch node evaluation



RooFit/HistFactory stress tests: speedup of NLL minimization by using BatchMode



Additional speed-up obtained in Batch mode by better CPU caching and vectorisation!

from J. Rembser@PPP meeting

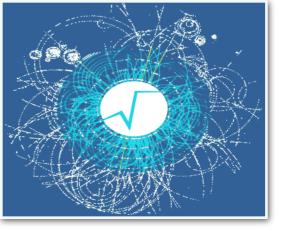


# RooFit Pythonizations



- RooFit is more pythonic in latest ROOT (6.26):
  - use Python keyword arguments instead of RooFit command arguments
  - pass around Python sets or lists or dictionaries instead of RooFit collections
  - converters from/to Numpy/Pandas and RooFit data classes
- All Pythonizations are documented in the reference guide

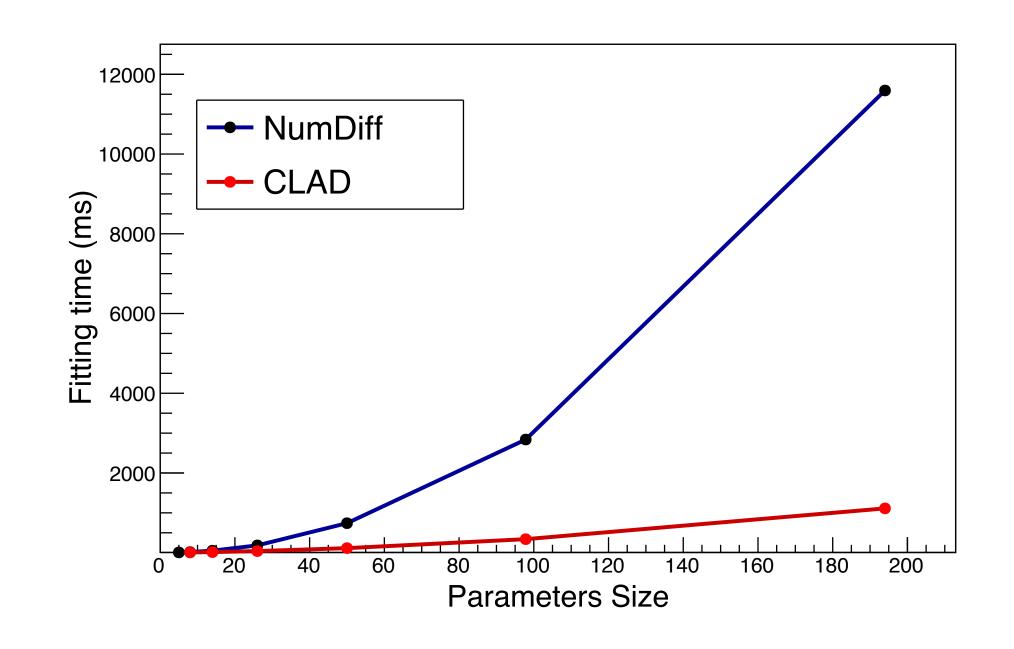
#### Example code from a RooFit tutorial

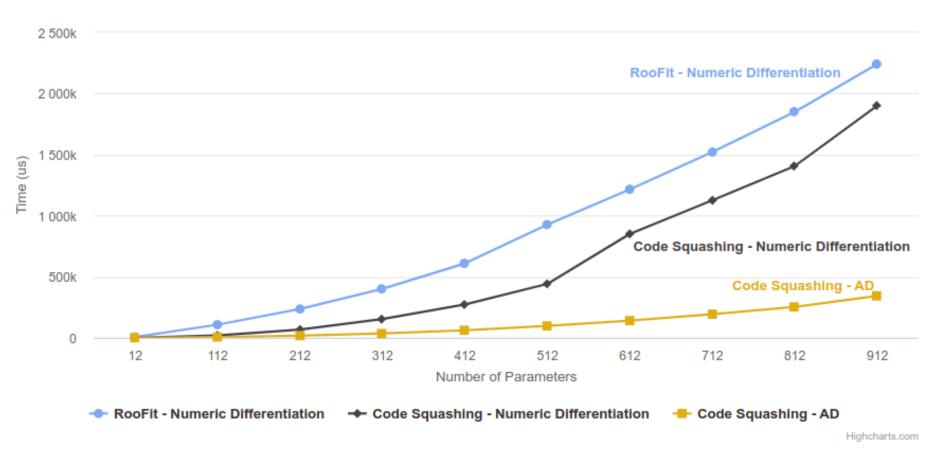


# Auto-differentiation (AD)



- AD available in ROOT TFormula class for fitting
- Large speedup can be obtained with respect to using numerical differentiation in case of large number of parameters
  - ~ 10x speedup for 100 parameters fit
- Also AD for Hessian (covariance matrix)
  - working in adding support in Minuit
- Integrating AD in RooFit
  - started with HistFactory models (binned likelihood fits, many parameters, few integrals): ~ 5x speedup







# Summary



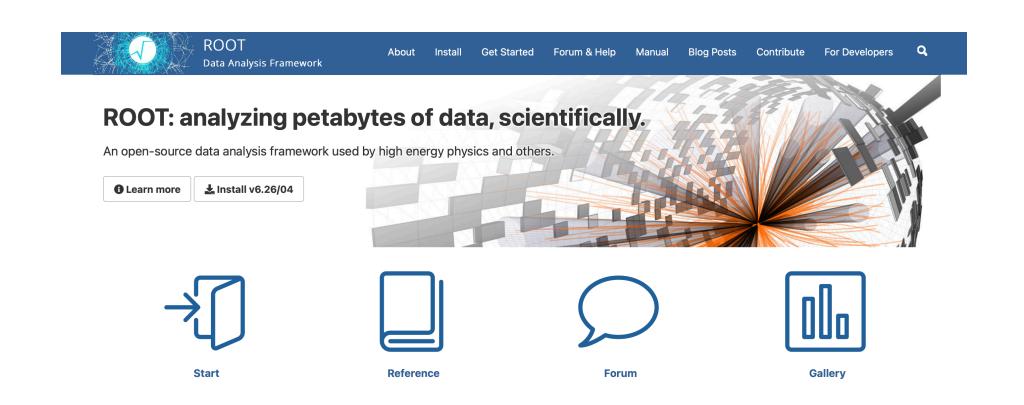
- Future analyses in HEP and Nuclear Physics will use larger data sets and be more complex (e.g. larger parameter spaces)
- Analysis tools for physicists will need to be
  - efficient and performant
  - with simple interfaces
  - robust, reliable and supported
  - allow interoperability (e.g. with Python ecosystem)
- ROOT is rapidly evolving in all its components to fulfil these requirements
  - thanks to a large effort from all the team and user contributions
- Need your help for continuous feedback and support



## References



- root.cern
- https://cern.ch/forum
- https://github.com/root-project



- For more information of current developments see presentations at latest <u>ROOT Users Workshop</u>
- see also the ICHEP 22 presentations in the <u>Computing session</u>





# Backup Slides



## RDF Benchmarks



Fully compiled C++ RDataFrame

Coffea 0.7.12 (using chunksize=2\*\*19)

query, 1x data (s), 10x data (s)			query, 1x	query, 1x data (s), 10x data (s)		
Q1	0.37	1.50	Q1	1.40	4.24	
Q2	0.46	3.70	Q2	1.51	5.76	
Q3	0.73	6.23	Q3	1.81	7.96	
Q4	0.65	5.92	Q4	1.65	6.58	
Q5	0.84	7.45	Q5	2.41	12.43	
Q6	3.08	27.99	Q6	13.89	124.59	
Q7	2.56	22.27	Q7	4.19	29.12	
Q8	1.17	10.22	Q8	3.27	17.70	

- note that these benchmarks are not representative of large analysis workloads
- see also this ACAT talk by Nick Smith

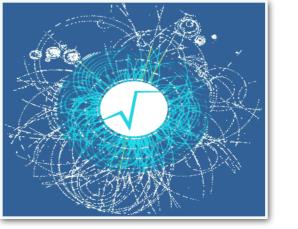
Benchmark from <u>github.com/nsmith-/coffea-benchmarks</u> Setup: AMD EPYC 7702P, using 48 physical cores, data read from filesystem cache



# Coming Soon in RDF



- Performance improvements (e.g. bulk processing, ROOT PoW 2022)
- Collection aggregations (muon\_{pt,eta,phi} → muons) being discussed
- Simpler Pythonic interfaces (less C++ strings in Python code), PoW 2022
- Allow default values for missing branches, PoW 2022, GitHub issue



## RooFit Interoperability with NumPy



- New converters between NumPy arrays/ Pandas dataframes and RooDataSet/ RooDataHist:
  - RooDataSet.from\_numpy()
  - RooDataSet.to\_numpy()
  - RooDataSet.from\_pandas()
  - RooDataSet.to\_pandas()
  - RooDataHist.from\_numpy()
  - RooDataHist.to\_numpy()
- New RooRealVar.bins() function to get RooFit bin boundaries as NumPy array

```
from ROOT import RooRealVar, RooCategory, RooGaussian
x = RooRealVar("x", "x", 0, 10)
cat = RooCategory("cat", "cat",
                   {"minus": -1, "plus": +1})
mean = RooRealVar("mean", "mean",
                   5, 0, 10)
sigma = RooRealVar("sigma", "sigma",
                    2, 0.1, 10)
gauss = RooGaussian("gauss", "gauss",
                     x, mean, sigma)
                                                      x cat
                                               0 6.997865
data = gauss.generate((x, cat), 100)
                                               1 7.211196 -
df = data.to pandas()
                                               2 3.198248
                                               3 5.015824
                                               4 7.782388
                                              95 6.878027
                                                0.475900
                                              97 4.451101 -1
                                              98 3.481015 -1
                                              99 4.010105 -1
```

100 rows x 2 columns