

CHEP 2024







ROOT RNTuple & EOS A holistic approach to data analysis

Chapter 1: ROOT RNTuple - Next Generation Event Data I/O for HENP Chapter 2: Exploring Client-Server Scalability with RNTuple & EOS

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https://root.cern

Part of the work presented is formalized in a two years joint project between the EP-SFT and IT-ST group at CERN:

Large-scale validation and optimisation of RNTuple, the HL-LHC event data format

March 2023 | J. Biomer (EP-SFT), J. T. Mościcki (IT-SD)

Large-scale validation and optimisation of RNTuple, the HL-LHC event data format

Purpose (Why?)

The ROOT RNTuple project is the HL-LHC I/O upgrade of the TTree event data file format and access API [1]. More than 1 EB of data of LHC Runs 1-3 are stored workholde in the TTree format. The RNTuple format is expected to store in the order of 10 EB Run 4-6 data comprising all the experiment event data modes (EDMs) stored in TTree bday.

Compared to TTree, RNTuple stores the same content in 10% to 20% smaller files and it provides 3x-5x better single-core performance for typical analysis-level EDMs and analysis tasks [2, 3].

The RVTLedge project a coppion PAGN in the ROOT term. It is supported by the LHC experiments and the FRAID programmer. The ROOT term will share the RVTLedge that backmark-compatible drugge. As a preventies the RVTLedge the flowmark will be included the drugge. As a preventies if for production on the discontenties. RVTLege to flow an week to be validated with the most common experiment EDMs on large, that and drugge poors. This prior the Selem enriced by the LHCC drugge that and drugge poors. This prior the Selem enriced by the LHCC drugge that pools (summark prior the 23 Mach methods).

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Scope (What?)

The scope of this initiative is to launch a testbed and performance study for RNTuple on large EOS/XRootD disk pools. We propose a joint R&D project between EP-SFT and IT-SD from mid 2023 to 2025 in order

¹ RNTuple can read and write the listed EDMs and existing TTree files can be converted into RNTuple files. Full ATLAS and CMS transwork integration hinges on the support for modifying the data model during writing of files. This functionality is currently being added to RNTuple.

This activity is part of the **RCS-IT** Research and Computing Sector & CERN IT Engagement



Scope & Approach

RNTuple work in progress in ROOT :: Experimental

LS 2					LHC Run 3			LS 3		Run 4	-6 (HL-LHC)
2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	

RNTuple goes production, adoption phase



• Local IO optimizations

- End-user analysis
- Data conversion tools
- Parallel Writing

• Remote IO optimizations

- Scale-out for Analysis
- Facility Usage

• Data Format optimizations

- Compression schemes
- IO sizes

• Final Validation

• Data Challenge

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Chapter 1

ROOT RNTuple

RNTuple: redesigned columnar I/O for HENP



RBrowser showing RNTuple data

- Building on 25+ years of TTree experience, modern & 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 (2040+)

HENP I/O Challenge: Rich Event Data Models

Type Class	ype Class Types			EDM Coverage			
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			Full AOD / ESD / RECO	Available			
User-defined collections Non-associative collection proxy					Available		
<pre>std::pair, std::tuple, std::bitset, stdlib types std::(unordered_)(multi)set, std::(unordered_)(multi)map</pre>					Available		
Alternating types std::variant, std::unique_ptr, std::optional					Available		
Streamer I/O All ROOT streamable objects (stored as byte array)					Available		
Low-precision	Double32_t, f16				Available		
floating points	Custom precision / range (bfloat16, TensorFloat-32, other AI formats)	Optimiza	Available				

HENP I/O Challenge: Rich Event Data Models

Type Class	Types		EDM Coverag	RNTuple Status	
PoD	<pre>bool, char, std::byte, (u)int[8,16,32,64]_t, float, double</pre>				Available
Records Limit of H (Nested) vectors	ecords Limit of HDF5 and Big Data formats (e.g., Parquet) Iested) vectors C-style fixed-size arrays				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
std::pair, std::tuple, std::bitset,stdlib typesstd::(unordered_) (multi) set,std::(unordered) (multi)map					Available
Alternating types std::variant, std::unique_ptr, std::optional					Available
Streamer I/O	All ROOT streamable objects (stored as byte array)				Available
Low-precision	Double32_t, f16			Available	
floating points	Custom precision / range (bfloat16, TensorFloat-32, other AI formats)	Optimiza	tion benefitting	Available	

HENP I/O has unique requirements and challenges

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, <u>foins</u>
- 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
 - Schema extension during writing
 - Availability in the Python & C++ analysis ecosystem, e.g. in ROOT RDataFrame
- 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

Event data model, very simplified

struct Hit { float x, y, z; 5 struct Particle { float fE; 8 std::vector<Hit> fHits; 9 10 11 12 struct Event { int fEventNo; 13 14 std::vector<Particle> fParticles; 15 3;

> In reality: >1000 data classes >10k properties billions of events decades of retention

Due to ROOT's C++ interpreter: classes *are* the schema

- For maximum optimization opportunities, RNTuple introduces a new on-disk format and a new API
- At the same time, RNTuple is **smoothly integrated** with the established ROOT/HENP ecosystem.
 - RNTuple data stored in **ROOT files**
 - Consistent tooling
 - **RBrowser** support
 - **TFileMerger** & hadd support
 - Disk-to-disk converter TTree → RNTuple [1]
 - RNTuple adopts TTree's I/O customization and schema evolution system
 - For **RDataFrame** code: no change required
 - Based on the specification: 3rd party readers available, e.g. for <u>dr Julia</u>
- For frameworks and power users, RNTuple provides a modern API for (multi-threaded) writing and reading

Brookhaven

- Follows C++ core guidelines
- e.g., smart pointers, runtime errors signaled by exceptions
- Reviewed by <u>HEP-CCE</u>





root [1] .ls	
TFile** /da	ata/gg_data.root
TFile* /da	ata/gg_data.root
KEY: TTree mir	ni;55 mini [current cycle]
KEY: TTree mir	ni;54 mini [backup cycle]
KEY: ROOT::RNTup]	<pre>le mini_imported;1 object title</pre>
root [2]	
TTree and an RNTup	le in the same ROOT file. In this exam
be DNIT: up la slave la s	. Is a sub-state of the state o

A TTree and an RNTuple in the same ROOT file. In this example, the RNTuple data has been converted from the tree using the RNTupleImporter.

RNTuple in Practice

- For maximum optimization opportunities, RNTuple introduces a new on-disk format and a new API
- At the same time, RNTuple is **smoothly integrated** with the established ROOT/HENP ecosystem.
 - RNTuple data stored in **ROOT files** 0
 - Consistent tooling 0
 - **RBrowser** support
 - **TFileMerger & hadd** support
 - Disk-to-disk converter TTree → RNTuple [1]
 - RNTuple adopts TTree's I/O customization and schema evolution system Ο
 - For **RDataFrame** code: no change required 0
 - Based on the specification: 3rd party readers available, e.g. for <u>*t*</u> 0
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 - Follows C++ core guidelines 0
 - e.g., smart pointers, runtime errors signaled by exceptions 0
 - Reviewed by HEP-CCE Ο







TFile**

TFile*



RNTuple Performance: Data Volume



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

Also: new default settings, e.g. **zstd** compression algorithm

More performance studies

- 🛛 👉 LHCb
- <u>f Comparison with HDF5 & Parquet</u> (ACAT 21)

RNTuple Performance: Throughput Examples

Higher single-core RDataFrame read throughput across various final-stage ntuple types and data access modes.



- 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 RDataFrame I/O scheduler







Single core end-to-end throughput with RDataFrame

Beyond Files: Support for Object Stores

- Object store (S3) is the primary storage technology in the cloud
- A storage option for HPC, too (e.g., DAOS on Aurora)
- RNTuple is built such that its data blocks can be directly mapped to an object store.
- **Pre-production implementation for DAOS**
 - Prototype implementation for S3
- RNTuple design gives access to native performance of object stores

Native RNTuple object store support reaches 2GB/s/client. The file system emulation layer peaks at 250MB/s/client.

<u>FRNTuple on DAOS</u>



Example of mapping onto S3 objects

Chapter 1 - Status & Outlook

RNTuple is a HENP I/O system for the HL-LHC era



\succ	RNTuple is transitioning into production
	 Major milestone after 6 years of R&D
	Final first version of on-disk format for ROOT 6.34 (November 2024)
	 Future ROOT versions will be backwards-compatible
	 First production API: ROOT 6.36 (H1 / 2025)
	 Will incorporate the HEP-CCE API review suggestions
\succ	Start of first exploitation phase in 2025
\succ	RNTuple provides a solid basis for future I/O R&D
A A	 First production API: ROOT 6.36 (HT/2025) Will incorporate the HEP-CCE API review suggestions Start of first exploitation phase in 2025 RNTuple provides a solid basis for future I/O R&D

Chapter 2 RNTuple with Remote Storage





See also Next-Gen Storage Infrastructure for ALICE https://indico.cern.ch/event/1338689/contributions/6010773/



- We set up a bare-metal computing environment, EO²C, with 70 nodes on 100GE for a large-scale validation study and benchmarked it using three different storage backends.
- The performance studies used an Analysis Grand Challenge example using RDataFrame
 - In all measurements, the dataset is **uncached** both in the back-end and, where applicable, in the client cache.



EO²C Analysis Facility



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Test cases: CMS Analysis Grand Challenge

https://github.com/iris-hep/analysis-grand-challenge/tree/main/analyses/cms-open-data-ttbar







 Six datasets were used as input for the benchmarks, based on CMS OpenData *ttbar*, including **three generations** of **AGC RNTuple** files

Name	Format	Comp	Size	#Files
	TTree	ZLIB	1.94 TB	787
	TTree	ZSTD	1.59 TB	787
AGC ¹	RNTuple	ZSTD	1.04 TB	787
AGC ²	RNTuple 2xcondensed Cluster Size 200M	ZSTD	1.04 TB	396
AGC ³	RNTuple Cluster Size 100M Adaptive Pagesize	ZSTD	965 GB	787
AGC ^{100 20} 0	RNTuple 100x inflated AGC^{1 2}	ZSTD	104 TB	39600

→ The runtime of *ttbar* AGC is relatively short, making it unsuitable for running with distributed Dask and large-scale parallelism, *runtime* < *init.time* (> 100 workers ...)

→ We created a 100x inflated Dataset adding each data file 100x into the 104 TB AGC^{100|200} dataset



• The CMS OpenData ttbar analysis poses a **challenging use-case** for a *spinning-disk-based* infrastructure because ...

offset

- → the analysis reads only 6.4% of the full data set as input
 - sparse scattered forward reading
 - not really HDD friendly

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1800						a,					
1600					······································						
1400	ici, findalada Antonio Antonio										
1200											
1000										·····	
800											
600									, <u>en e</u> e		
400										5 - <u>5</u> -	-
200						· · · · · · · · · · · · · · · · · · ·		===			2 2 1 4 4 4
0	10	20	30	40	50	6	60	70	80	90	100 tst

AGC¹ ttbar read pattern may 2024 - x:timestamp y:file - offset

AGC RNTuple Size



Size Reduction from TTree to RNTuple



Advantage of using RNTuple: the identical contents is stored using less disk space

	TTRee ZLIB	TTree ZSTD	RNTuple
AGC	1'946'631'920'767	1'594'321'501'163	964082593461000

- → For a fair comparison, we rewrote the data using the ZSTD TTree format and compared the resulting size to RNTuple, achieving a 39% reduction in volume for AGC³
- → How do Realtime & CPU when running the *mt* AGC¹ ttbar analysis?

Realtime Meas. March 2024: **TTree ZSTD** : 250s **RNTuple AGC¹** : 240s "Something is wrong ..."

AGC mt

multi-threaded

The AGC *mt* **RNTuple Journey** 2024 in short 240s→ 70s



AGC dask-local

multi-process



The AGC **RNTuple Journey** 2024 - *mt* vs *dask*

Figure: Runtime dask-local AGC³





Processing Time



- *Green computing: dask-local* uses ~30% more CPU than *mt* for the identical **AGC**³ job
 - \circ startup phase \rightarrow

- *But:* dask allows **scale out** over multiple nodes
 - startup phase low impact for longer running jobs

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AGC dask-scale-out

multi-node/process



AGC **RNTuple** - IO scalability

 When scaling AGC¹⁰⁰ to few nodes with *dask-ssh* it was able to saturate the EOSPILOT and even the EOSALICEO² Instances ... not limited by bandwidth ...





AGC **RNTuple** - Format Improvements

Introducing modified RNTuple format for AGC²⁰⁰ with EOSPILOT



PILOT

AGC **RNTuple -** Format Improvements - fewer **IOPS**

Introducing modified RNTuple format for AGC²⁰⁰ with EOSALICEO²



the



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AGC **RNTuple** Backend Traffic

Average Backend Traffic GB/s

 Average and peak output rates for 2x condensed RNTuple format for AGC²⁰⁰ with EOSALICEO² Virtual IO rates: scaling traffic from 6.4% of the accessed data to the entire data - sparseness defines instance output [0.345 - 5 TBit /s]



Peak Backend Traffic GB/s

"Can we use a high-performance shared filesystem as a distributed cache and still gain performance?"

AGC Optimized Caching





JCache - why journaling?



By default **CephFS** creates **4x** read amplification

- A 22.5 GB/s
 Filesystem delivers
 5.6 GB/s of data you need
- After disabling read-ahead still
 +30% amplification
- **JCache** avoids read amplification and space overhead in the cache
 - Works well with default read-head
 - 22.5 GB/s used for the requested IO by applications



JCache - deployment model



client-side JCache deployment

simplification: no need for credential delegation/forwarding



LAN/WAN SERVER





JCache - embedded IO benchmarking

#				#	
#	JCache : 2024 CERN.EOS - Andreas-	Jo	achim Peters	#	
# # # # #	JCache : cache combined hit rate JCache : cache read hit rate JCache : cache readv hit rate	:	100.00 % 100.00 % 100.00 %	#	
# # #	JCache : total bytes read JCache : total bytes readv	:	8976091232 53958826610	#	
: # # #	JCache : total iops read JCache : total iops readv JCache : total iops readvread	: : :	34056 10707 93611	#	
# # #	JCache : avg. bytes read JCache : avg. bytes readv	:	263568.00 5039584.00	#	
# # #	JCache : open files read JCache : open unique f. read JCache : time to open files (s)	: : :	1050 796 0.000	#	
+ + + + + + + + + + + + + + + + + + +	JCache : total unique files bytes JCache : total unique files size JCache : percentage dataset read	:	976614396598 976.61 GB 6.44 %	#	
# # # # # #	JCache : app user time JCache : app real time JCache : app sys time JCache : app acceleration JCache : app readrate	:	3329.07 s 72.48 s 41.17 s 45.93x 868.35 MB/s [peak (1s) 1.94 GB/s]	Ħ	
#				#	11



- JCache provides easy insight into application IO including bandwidth profiling
- JCache is maintaining 100% async IO and allows disconnected operation

#	IO Timeprofile		
#			
#	1670.00 MB/s		
#	1484.44	** *	
#	1298.89	** **	
#	1113.33	* ** ** ***	
#	927.78	* * * * *	
#	742.22	* ** ** *	
#	556.67	* * *	
#	371.11		
#	185.56	*	
#	0.00	****	
#			
#		0 10 20 30 40 50 60 70 80 90 [100 % = 72.48s]	
#			



AGC²⁰⁰ - Backend Performance Comparisons



AGC with SWAN&HTCondor* *A Pilot Analysis Facility at CERN dask-remote



CERN Analysis Facility Pilot - SWAN + HTCondor





CERN Analysis Facility Pilot - SWAN + HTCondor

Extensive Monitoring Abilities

New Jupyter Lab Interface with HTCondor Plug-in





CERN Analysis Facility Pilot - Results

• Positive

- **Works** with similar runtime assuming a similar performance environment for Dask workers operating in batch
- Simple access in a web browser
- Integration of EOS/CERNBox Sharing
- Access to hundreds of thousands of cores in batch farm

Room for Improvements

- Long time to initialize setup for an interactive system
 - can take few minutes
- HTCondor cluster interface can get disconnected
- Dask initialization time correlated to number of workers
 - User needs to understand how many workers are useful for a given task
- The **setup is not yet fully automated** and requires few manual steps

AGC cms ttbar benchmark



More about the SWAN+HTCondor analysis pilot this afternoon see https://indico.cern.ch/event/1338689/contributions/6010680/

Summaries



Chapter 2 - Summary Holistic Approach RNTuple + EOS

- **Detailed benchmarking** has allowed for **substantial improvements** in RNTuple for remote access from EOS (AGC example)
 - for remote access from EOS (AGC example)
 - Excavated several issues which don't appear in local environments
 - Achieved >3x less run-time for TTree \rightarrow RNTuple
 - Achieved **-39%** size reduction for TTree \rightarrow RNTuple
 - Achieved **-40%** size reduction for moving from Replication \rightarrow EC(10+2) in EOS
 - Achieved running extreme case of sparse CMS AGC analysis at **345 GBit/s** during processing (HDD storage)

• Optimized caching plug-in R&D JCache

- Suitable to use high-performance shared file systems as shared cache with low overhead
- Provides out of the box IO summaries and profiles
- Allows to optimize AGC benchmark to lowest run-time performance eliminating read overhead
- Suitable to run on end-user devices
- These results can provide valuable input for the architecture of future analysis facilities
 - NVME and HDDs Shared File System combined with Remote Accessible Storage
 - Baremetal approach and/or SWAN+HTCondor
 - Usability and savings with EOS erasure coded storage for analysis

Final Summary & Future Outlook

A special thanks to all the teams from the IT and EP group who have helped advancing this project.

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- **RNTuple** is transitioning to production
- Solid basis for future IO R&D
- Local and remote access **optimizations** with significant improvements
 - used a worst-case test case validating NVME and HDD storage backends
- For the final part of this activity we **count on participation from experiments** to
 - optimize specific data formats
 - validate them in a large scale data challenge

Thank You For Your Attention!

Appendix



Storage & Compute Hardware

Storage EOSPILOT/ALICEO2

- 2x AMD EPYC 7302 and 7313 16-Core Processor
- DDR4 3200 MT/s 16x16 GB 256 GB
- Intel® Ethernet Network Adapter E810 1x100GE
- Filesystems
 - / EXT4 2 TB NVME
 - /data01..96 XFS 18TB HDD



Compute EO²C

- 2x AMD EPYC 7302 and 7313 16-Core Processor
- DDR4 3200 MT/s 16x16 GB 256 GB
- Intel® Ethernet Network Adapter E810 1x100GE
- Filesystems
 - I EXT4 2 TB NVME
 - /cvmfs CvmFS filesystem
 - /shared CephFS home directory
 - /jcache CephFS cache directory





Observation: when you repeat a measurement twice reading initially uncached data from remote you see a significant reduction in run-time with the second run. This is due to a client side bottleneck!

Connection Demultiplexing eliminates this bottleneck.



- Reported last year at CHEP in the context of **XCache benchmarking**
- If your storage is made of **more servers than threads used** in your application, multiplexing does not play a role (e.g. large CERN instances like EOSATLAS/CMS/PUBLIC)
- For **EOSPILOT** it still plays a role.
- XRootD team identified problem in parallel-socket implementation when this is fixed enabling parallel sockets should eliminate this problem without the need for *manual multiplexing*



Can we use an NVME based shared filesystem as a distributed cache and gain performance?

yes! *R&D project*



• XCache

- well established in HEP as a block based XRootD based cache server
 - If data is only partially accessed block chunking introduces moderate to significant space overhead of the payload vs cached data contents e.g. 128k blocksize +123%
 - there is also a visible real time overhead when reading cold data through XCache in a LAN environment with not saturated infrastructure (2x 5x).
 - Implemented as a server-side plug-in in XRootd

• JCache

- JCache is using **journaling** to cache file contents not blocks (code derived from **eosxd**)
 - Stores only payload 0% size overhead 15% real-time overhead for cold AGC case in LAN
 - Implemented as a client plug-in which can be deployed client and server-side



JCache - caching into shared filesystems - CephFS

- Using file locking for cache journals allows to use a shared file system as a distributed cache on many clients
 - we used CephFS with 8 NVME nodes (see before) and double replication
- One drawback of using a shared file system is the impact of automatic read-ahead and object block sizes defined
 - With default mount options **CephFS inflates** the required **traffic** on the wire **>4x** due to the automatic read-ahead algorithm
 - With **ra=64k or ra=0k** this creates still **1.3x more traffic** than required
 - We used a default block size of 4M, tried also 1M no change in behaviour
- When running AGC²⁰⁰ on 30 nodes using dask-ssh the run-time is defined by the maximal bandwidth of the CephFS backend and the read overhead
 - The CephFS back-end saturates at around **22.5 GB/s**
 - Run-time is 550s 50% longer than on EOSPILOT (due to bandwidth limit + read overhead)
 - Origin is that our CephFS cluster has only 25GE on each storage node!