A Ceph S3 Object Data Store for HEP

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Abstract.

In CMS, data access and management is organized around the data tier model: a static definition of what subset of event information is available in a particular dataset, realized as a collection of files. We present a novel data management model that obviates the need for data tiers by exploding files into individual event data product objects. The objects are stored and retrieved through Ceph S3 technology, with a layout designed to minimize data and metadata volume while maximizing data processing parallelism. We demonstrate that this object data format shows promise in reducing total storage requirements while allowing more flexible data access patterns. Performance benchmarks of a prototype data processing framework using this object data format and a test Ceph cluster are presented, showing good scaling behavior in a distributed processing task.

1 Introduction

The HL-LHC poses a significant challenge for the CMS experiment's data management model. A combination of higher pile-up and finer detector granularity will result in each collision event of data or simulation requiring considerably larger byte-storage [1]. The overall event rate to storage, currently at approximately 1 kHz, is also anticipated to increase to at least 7.5 kHz [2]. In the early years of Run 4, several new subdetector components will come online, and their low-level data will need to be validated and synthesized into high-level reduced data suitable for analysis. This process will be challenging if the data products pertaining to those detector elements are not easily accessible. Future innovative analysis may necessitate different data reduction strategies. Given these considerations, the amount of data that is regularly accessed by end-user analysts is expected to grow significantly in the coming years.

An inherent limitation in the current CMS data management model is the organization of data around files. File-based organization fundamentally forces certain data products, or collections of related fields (data columns) pertaining to an event to be grouped together with the same data access quality of service (QoS). In the current workflow model, large-scale tasks transform datasets from one set of columns to another more compact set, to afford keeping the latter available with high QoS (i.e., on magnetic disk at several sites.) It is not currently possible to have different subsets of data columns kept at high QoS for different datasets at granularities beyond the *data tier*, a statically defined set of columns. A more flexible data model that keeps only the needed data columns available at high QoS may significantly reduce storage volume risk.

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2 Data-Tier Storage Model

In the current CMS computing model, *data tiers* represent what subset of the detector information per event is stored in a particular *dataset* (e.g. a collection of files). The RAW data tier is the unprocessed output of the CMS detector, and is committed to archival storage (usually tape) while active storage (usually magnetic disk) is dominated by intermediate derived/reduced data formats such as AOD and MiniAOD [3]. For both collider data and simulation, these reduced data tiers are processed by analysis end-users to form data formats with simple data types, *NTuples*. A proliferation of end-user analysis formats has necessitated frequent access of AOD/MiniAOD tiers up to the present day. More universal end-user NTuple formats such as NanoAOD [4] effectively define a new data tier and have helped reduce the need to access upstream data tiers, however they are only expected to meet the needs of a subset (50%) of analysis use cases. An illustration summarizing the data tier model is shown in Fig. 1.



Figure 1. Illustration of the data tier model as used for data management in the CMS experiment.

Attempts at universal formats such as NanoAOD involve a trade-off in that only a subset of information is kept for each event. Innovative physics analyses often require quantities not saved in NanoAOD as they were not considered pertinent at the time the NanoAOD column set was defined. An analysis that requires missing columns will have to run their own derivation over MiniAOD or upstream data tiers to extract the necessary columns and add them to NanoAOD.

Even upstream of NanoAOD formats, the inflexibility of the data tier system leads to a sub-optimal computing model: analysis users cannot access the AOD data tier as it is too large to fit the entire CMS working dataset on disk at that tier. This forces forward-copying certain data products from that tier onward, duplicating information only for the sake of accessibility; and in the case of issues in a data re-processing (e.g. re-MiniAOD), the old and new data may only differ for a small subset of the data columns, yet the remainder have to be re-written so downstream analysis workflows can access it efficiently.

All centrally managed datasets in CMS are concretely a collection of files written in the ROOT [5] format, with an Events *TTree* and extra metadata. In this TTree, each data product is stored as a *TBranch*. Some data product elements are further split into smaller columns for improved compression, but a product is accessed as one unit within the CMS offline software (CMSSW) framework [6]. TBranch objects reference several *TBaskets*, each of

which contain serialized data products for a range of events. In Fig. 2, each TBasket accessed by an example CMSSW workflow reading a MiniAOD file is represented as a rectangle, where the height is the number of events and width is proportional to the compressed bytes. The top 6 largest MiniAOD products represent half of the file size. The second largest data product, LHEEventProduct_externalLHEProducer__GEN., is copied directly from the AOD tier.



Figure 2. Layout of a file in a representative CMS dataset (simulation of semi-leptonic $t\bar{t}$ production), where rows represent event indices, and columns are sized proportional to the average compressed size of a given data product. The labels of the 9 largest data products are shown on the x axis. Unfilled rectangles represent data products that were not accessed.

2.1 Projected Usage

CMS computing plans for the HL-LHC assume that a majority of analyses will utilize centrally produced NanoAOD and that the bulk of intermediate formats currently kept on disk (often with multiple copies) will not be kept on active storage. Even with such assumptions, the disk storage needs of CMS in the first year of Run 4 will exceed one Exabyte across all sites, representing a factor of four increase over the needs in Run 3 (Fig. 3, left) [7]. A plethora of non-NanoAOD data tiers (Fig. 3, right) is expected to be available on disk in 2031 in current projections, and the mixture may well change with detector commissioning needs.



Figure 3. Left: annual disk space requirement estimated for CMS processing and analysis needs. Right: estimated disk space requirements per data tier for 2031, with a total expected usage of 900 PB.

3 Object Stores

Object stores, which operate on a key-value principle, allow for highly-granular access to information via efficient metadata lookup. The evaluation of sub-file or object-based granularity is a key R&D goal for Data Organization Access and Management (DOMA) in the

HEP Software Foundation Community White Paper [8] which was further enforced in the 2021 Snowmass Planning Process [9]. Object stores are widespread in industry and are nearuniversal in cloud storage with the Amazon S3 API emerging as a *de facto* access protocol across them. A central object store can also provide the backbone of a content delivery network (CDN) for end-users and allow for analysis without need for an analysis NTuple format.

To concretely explore the possibilities of object storage for event data in CMS, we developed an object data format, a test cluster using Ceph object store technology, and a S3 input and output module in a prototype event processing framework similar to CMSSW, as discussed in the following subsections.

3.1 An object data format

In our object data format, one index object holds metadata for an entire primary dataset. For each data product, or column of data, a stripe of events is written as an object in an S3 bucket. Each event data product is serialized with standard ROOT IO. The stripe size is chosen on first write, once the compressed output buffer reaches a target stripe size, usually 100k-1MB, and the number of events evenly divides a configurable event batch size. The index object may be replaced by a database, to more easily add and remove products. By forcing the number of events to be a constant even divisor of the event batch size, the metadata volume grows as (N products) + (M events) despite the N*M growth of the number of stripe objects. The data stripes will not exactly meet the target size, but will have a distribution centered very close to the target due to the independent identically-distributed nature of the event data. To handle very small data products which would never reach the target stripe size, we optionally collect them into product groups following a greedy algorithm. This does not inherently prevent independent access of columns in that stripe, as byte-range addressing is available in the S3 protocol. Although this object store system assumes all objects are online-accessible, infrequently used column stripes could be concatenated and offloaded to tape systems based on a caching policy.

Significant improvements in long-term disk storage needs can be realized with this object store scheme. In a mock example (see Table 1), using average per-data-product sizes for a CMS semi-leptonic $t\bar{t}$ production primary dataset, two MiniAOD versions (v1, v2) are produced from the same parent dataset, where the latter is produced to update electron data. In the object store scheme, there is no need to re-produce other (unchanged) data products. In any case, data products such as genParticles would never need to be copied forward in the MiniAOD production.

Data product	kilobytes per event		
	Data tier model	Object store model	
genParticles (upstream)	5.7	5.7	
genParticles (MiniAODv1)	5.7	-	
genParticles (MiniAODv2)	5.7	-	
slimmedElectrons (MiniAODv1)	1.3	1.3	
slimmedElectrons (MiniAODv2)	1.3	1.3	
Other event products (MiniAODv1)	48.7	48.7	
Other event products (MiniAODv2)	48.7	-	
Total	117.1	57	

	Table 1.	Mock	data	usage	exam	ple
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3.2 Test Ceph Cluster

A pilot cluster has been assembled to gain experience in managing a Ceph installation and for evaluation purposes. Nine disk servers, retired from the Fermilab dCache disk pool, provide a total 2 PB of disk drives of vintage 2014-2018, totaling 288 Ceph Object Store Daemons (OSDs). Two servers provide 20 TB of NVMe across 32 OSDs for the metadata pool. All machines have 10 to 100Gbps networking. The cluster supports filesystem access using the xrootd [10] protocol via an edge machine with CephFS mounted, and S3 object access via a RadosGW edge machine. For all performance tests, client machines are accessing the cluster from within the Fermilab network.

For the S3 object access, three buckets are set up with different Ceph pool configurations. In the first configuration, each object is split into 16 kibibyte (KiB) chunks and each chunk is further split into 4 data blocks of 4 KiB and 2 parity blocks using an erasure coding scheme, dubbed EC4+2. The bucket also maintains an index of all objects in it, where each item in the index contains about 300 bytes of metadata such as the last access time and owner. The index is stored in a triply-replicated NVMe pool using Ceph's key-value object type. In a second configuration, the same erasure-coded pool is used but the bucket index is disabled. Without the bucket index, objects can still be read and written, but cannot be listed, so an external metadata database would be necessary to manage object lifecycle properly. In the last configuration, all data is stored a triple-replicated disk pool, dubbed Rep3.

3.3 Prototype Client

The HEP-CCE root_serialization project provides a C++ framework for performance experiments with various I/O packages from within a multi-threaded program [11]. The program mimics behaviors common for HEP data processing frameworks, and uses a Intel Thread Building Blocks (TBB) thread pool to schedule parallel *tasks*. The number of threads in the TBB thread pool is configurable. Within this framework, S3 input and output modules have been developed to read from and write to S3 buckets, respectively. This allows to explore the performance and parallelization behavior of writing to a Ceph S3 service in comparison to local files with ROOT or other formats. The S3 protocol is implemented with libs3 [12]. Requests are performed asynchronously in a separate thread from all other tasks. Network errors are handled with an exponential backoff with retry mechanism.

4 Performance Results

Using the object data format, test cluster, and prototype event processing framework described in Section 3, we evaluated the storage and read/write performance against a baseline of current MiniAOD event size and processing rates. Scaling behavior is probed both in single- and multi-process setting, to understand threading efficiency and client load limits of the cluster, respectively.

4.1 Storage Efficiency

A MiniAOD input dataset is converted into the object data format with various settings of target stripe size (Section 3.1) and stripe compression. The storage efficiency, measured in average kilobytes per event, is shown in Table 2. We find that the object storage format has generally a larger size per event than the input, especially when LZMA compression is not used. Even when LZMA is used, the object format cannot compress as well as MiniAOD due to a limitation in the ROOT object serialization when not used in conjunction with TTree

I/O: the object fields cannot be split further into struct-of-array types, which hinders compressability. A special consideration for Ceph is that small objects incur additional storage overhead (listed in %) due to the minimum object size granularity of 4 KiB. With larger target stripe sizes, as well as with use of product groups, this overhead is reduced. In Fig. 4, the distribution of output stripe sizes is shown for each of the storage configurations shown in Table 2. The amount of small product stripes is significantly reduced with the use of product groups.

Format	Compression	Event batch size	Target stripe size	kB per event
				(granularity overhead)
MiniAOD input	LZMA	-	-	55.7
Object	ZSTD	720	128KiB	71.4 (6.5%)
Object	ZSTD	720	512KiB	70.6 (3.5%)
Object	LZMA	720	512KiB	61.8 (3.7%)
Object (groups)	ZSTD	720	512KiB	70.6 (1.4%)

Table 2. Comparison of data volume with object store scheme and input MiniAOD ROOT file



Figure 4. Distribution of object stripe sizes in the output dataset, for various configurations of the object data format writer.

4.2 Single-client scaling

We performed a set of tests where all data products in the MiniAOD tier are read and written as fast as possible to/from the test object store cluster, using a single executable client process. The executable's thread scaling properties are probed, with the metric being the events processed per second. In the read-write test, events are: read, decompressed, deserialized, serialized, compressed, and written. For the read-only chain, only the first three steps are performed. Tests were run on a 24-core machine with 10Gbps network connection to the Ceph cluster. The tests are performed for two configurations of target stripe size: 128kiB and 512kiB. For each configuration, the source and output modules target one of three S3 buckets with different storage configurations, as described in Section 3.2. Fig. 5 shows good scaling behavior with increased thread count, and negligible performance difference between the storage configurations. As a point of reference, CMS production jobs reading MiniAOD and producing NanoAOD run at a CPU-limited rate of about 10 events/second/thread [13].



Figure 5. Single-client read-only (left) and read-write (right) thread scaling tests.

4.3 Multi-client scaling

We performed a test of converting data in MiniAOD from the ROOT file format to the object format at scale, where the input files are read from Fermilab's dCache disk cluster over xrootd and written to the test cluster via S3. In this test, the conversion processes are single-threaded, and up to 400 simultaneous workers are writing objects with a target size of 512KiB to the EC4+2 bucket. The events per second written to the object store is shown as a function of worker count in Fig. 6, left. A saturation point is observed with approximately 350-400 workers writing 6300 events/s (450 MB/s) to the data pool. In total, 4.5 TB of data was written into 7.4 million objects.

Once the data was written, we performed a read-only test similar to Section 4.2, with 4 threads per worker and several independent worker processes accessing the test cluster in parallel. The results are shown in Fig. 6, right. In this case, there is a larger variation in cluster performance at high worker count, and no apparent saturation is reached. Further tests with additional workers are necessary. In this test, we can directly compare the scaling performance with the single-client scaling results, and they appear consistent.



Figure 6. Scaling Left: multi-client write test. Right: read-only test.

While the scaling tests were in progress, performance profiles of the client application showed that the I/O latency is fully hidden when the S3 server is not heavily utilized, but server saturation can cause the client applications to stall and show poor CPU efficiency. As this is a client application with no CPU-heavy tasks other than decompression and deserialization, we expect that in a realistic processing task, the I/O latency would remain in the shadow of the CPU-bound TBB tasks.

5 Conclusion

In conclusion, the object data format provides novel data management capabilities with respect to a data tier and file-based format. In particular, it shows promise in reducing the total storage requirements as well as providing more flexibility in defining what data are easily accessible to analysis tasks. In a prototype processing framework accessing a Ceph S3 object storage cluster, we find that the data volume is in line with expectations and service scaling is promising, with one Ceph RadosGW node serving 350-400 parallel clients before performance saturation.

To fully realize the possibilities of this object data format, additional software development will be needed. A high priority is to migrate the object I/O modules from the prototype event processing framework to CMS offline software, possibly leveraging the RNtuple integration efforts, as RNtuple also provides an object backend with a very similar design as the one presented here [14]. A new metadata service will be required to track which objects are available, and close integration with the workflow management system will be required.

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