

## ABSTRACT

### OPTIMIZATION OF DERIVATION JOBS AND MODERNIZATION OF NIGHTLY CI BUILD I/O TESTS FOR THE ATLAS EXPERIMENT

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The ATLAS experiment's Software Performance Optimization Team has efforts in developing the Athena software framework that is scalable in performance and ready for widespread use during Run-3 and HL-LHC data ready to be used for Run-4. It's been shown that the storage bias for TTree's during derivation production jobs can be improved upon compression and stored to disk by about 4-5% by eliminating the basket capping, with a simultaneous increase in memory usage by about 11%. Additionally, job configuration allows opportunity to improve many facets of the ATLAS I/O framework.

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OPTIMIZATION OF DERIVATION JOBS AND MODERNIZATION OF NIGHTLY CI  
BUILD I/O TESTS FOR THE ATLAS EXPERIMENT

BY

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## DEDICATION

To all of the fluffy kitties. To all of the fluffy kitties. To all of the fluffy kitties. To all of  
the fluffy kitties.

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# CHAPTER 1

## INTRODUCTION

### 1.1 Particle Physics and the Large Hadron Collider

Particle physics is the branch of physics that seeks out the origins of the universe by probing the smallest interactions at high energies. It has roots in electromagnetism, with the discovery of the electron and other particles, and quantum mechanics, that include descriptions of atoms, particles, and their interactions both relativistic and non-relativistic speeds. There have been many efforts in experimentally probing for unique interactions, and the Large Hadron Collider (LHC) at CERN has been at the forefront in revealing new insights. The LHC is a 26.7-kilometer ring that crosses between the France-Switzerland border at a depth between 50 and 175 meters underground.[6]

#### 1.1.1 The ATLAS Experiment

The ATLAS experiment is the largest LHC general purpose detector, and the largest detector ever made for particle collision experiments. It's 46 meters long, 25 meters high and 25 meters wide.[8] The ATLAS detector is comprised of three main sections, the inner detector, calorimeters and the muon detector system.

The inner detector measures the direction, momentum and charge of electrically charged particles. The first point of contact for ATLAS is the pixel detector. It has over 92 million pixels to help determine the origin and momentum of the particle. Surrounding the pixel detector is the semiconductor tracker, which uses 4,088 modules of 6 million implanted



silicon readout strips. The semiconductor tracker helps measure the path particles take, called tracks, with precision up to  $25\mu m$ . The final layer of the inner detector is the transition radiation tracker (TRT). The TRT is made of a collection of tubes made with many layers of different materials with varying indices of refraction. Particles with relativistic velocities have higher Lorentz  $\gamma$ -factors, see Eq. (1.1), the TRT uses varying materials to discriminate between heavier particles (with low  $\gamma$  and radiate less) and lighter particles (higher  $\gamma$  and radiate more). [7]

$$\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} \quad (1.1)$$

## CHAPTER 2

### ATLAS I/O

At any given time, code changes to Athena or the LCG stack could break various core I/O functionality. [1] A measure often taken to ensure stability and security of essential code functionality is the involvement of unit testing during continuous integration of new software. [3] It's not always the case that new core I/O functionality is integrated into Athena with new unit tests.

#### 2.1 Athena and ROOT

Athena is the open-source software framework for the ATLAS experiment.[2] It relies on other software such as ROOT, Geant4 and other software as part of the LCG software stack. Athena manages ATLAS production workflows which include event generation, simulation of data, reconstruction from hits, and derivation of reconstructed hits.[4]

ROOT is an open-source software framework used for high-energy physics analysis at CERN.[9] It uses C++ objects to save, access, and process data brought in by the various experiments based at the LHC, the ATLAS experiment uses it in conjunction with Athena.

One of the ways Athena works with ROOT is by taking and manipulating ROOT files in such a way to make them smaller.

### 2.1.1 TTree

### 2.1.2 Derivation Production Jobs

A derivation job is that process that takes Analysis Object Data (AODs), which comes from the reconstruction step at  $\mathcal{O}(1 \text{ MB})$  per event, and creates a Derived Analysis Object Data (DAOD) which sits at  $\mathcal{O}(10 \text{ kB})$  per event.

## 2.2 Event Data Models

An Event Data Model (EDM) is a collection of classes and their relationships to each other that provide a representation of an event detected with the goal of making it easier to use and manipulate by developers. An EDM is how particles and jets are represented in memory, stored to disk, and manipulated in analysis. It's useful to have an EDM because it brings a commonality to the code, which is useful when developers reside in different groups with various backgrounds. An EDM allows those developers to more easily debug and communicate issues when they arise.

### 2.2.1 Transient/Persistent EDM

One of the previous EDMs used by ATLAS concerned a dual transient/persistent nature of data. The transient data was present in memory and could have information attached to the object, this data could gain complexity the more it was used. Persistent data needed to be simplified before it could be persisted into long-term storage (sent to disk). ROOT had trouble handling the complex inheritance models that would come up the more developers

used this EDM. Additionally, converting from transient to persistent data was an extraneous step which was eventually removed by the adoption of using an EDM that blends the two stages of data together, this was dubbed the xAOD EDM.

## CHAPTER 3

### TOY MODEL DERIVATION PRODUCTION

Building a toy model for derivation production jobs provides a schema by which it makes using real data and Monte Carlo simulated data much simpler. One general principle about both data and Monte Carlo is the branch data within both is made up a mixture of randomized floats and repeated integer-like data. If we test the ideas behind limiting basket sizes to see how it affects compression, effects should be evident.

#### 3.1 Building the Toy Model

The first toy model example that was investigated was filling up a TTree

#### 3.2 Toy Model Derivation Production

## CHAPTER 4

### DATA AND MONTE CARLO DERIVATION PRODUCTION

#### 4.1 Current Derivation Framework

Derivation production jobs suffer from high memory usage, and DAODs make up a bulk of disk-space usage. DAODs are used in physics analyses and ought to be optimized to alleviate stress on the GRID and to lower disk-space usage. Optimizing both disk-space and memory usage is a tricky balance as they are typically at odds with one another. For example, increasing memory output memory buffers results in lower disk-space usage due to better compression but the memory usage will increase since one will have to load a larger buffer into memory. The route we opted to take is by optimizing for disk-space and memory by testing various basket limits and viewing the effects of the branches on both data and Monte Carlo (MC) simulated analysis object data (AODs)

#### 4.2 Performance Metrics and Benchmarking

Our initial focus was on the inclusion of a minimum number of entries per buffer and the maximum basket buffer limit. As we'll see in the following section, we then opted to keep the minimum number of entries set to its default setting (10 entries per buffer).

For both the nightly and the release testing, the data derivation job comes from a 2022 dataset with four input files 160327 events. The MC job comes from a 2023  $t\bar{t}$  standard sample simulation job with six input files with 140k events. The specific datasets for both are noted in Appendix A.1.

The corresponding input files for both data and MC jobs were ran with various configurations of Athena (version 24.0.16) and its specified basket buffer limit. The four configurations tested all kept minimum 10 entries per basket and modified the basket limitation in the following ways:

1. “*default*” - Athena’s default setting, and basket limit of  $128 \times 1024$  bytes
2. “*no-lim*” - Removing the Athena basket limit, the ROOT imposed 1.3 MB limit still remains
3. “*256k*” - Limit basket buffer to  $256 \times 1024$  bytes
4. “*512k*” - Limit basket buffer to  $512 \times 1024$  bytes

Interesting results come from the comparison of “no-lim” and “default” configuration. The “256k” and “512k” configurations were included for completeness and provided to be a helpful sanity check throughout. Building and running these configurations of Athena are illustrated in a GitHub repository. [5]

## 4.3 Results

### 4.3.1 Presence of basket-cap and presence of minimum number of entries

First batch testing was for data and MC simulation derivation production jobs with and without presence of an upper limit to the basket size and presence of the minimum number of entries per branch. PHYSLITE MC derivation production, from Table 2, sees a 9.9% increase in output file size when compared to the default Athena configuration. Since this configuration only differs by the elimination of the “min-number-entries” we assume the

minimum number of entries per branch should be kept at 10 and left alone. Table 4.3 also shows the potential for a PHYSLITE MC DAOD output file size reduction by eliminating our upper basket buffer limit altogether.

Athena v22.0.16 configurations (Data)	Max PSS (MB) ( $\Delta\%$ default)	PHYS outFS (GB) ( $\Delta\%$ default)	PHYSLITE outFS (GB) ( $\Delta\%$ default)
With basket-cap and min-num-entries (default)	27.109 ( + 0.00 %)	3.216 ( + 0.00 %)	1.034 ( + 0.00 %)
Without both basket-cap and min-num-entries	27.813 ( + 2.53 %)	3.222 ( + 0.20 %)	1.036 ( + 0.21 %)
Without basket-cap but with min-num-entries	27.814 ( + 2.53 %)	3.216 ( - 0.00 %)	1.030 ( - 0.39 %)
With basket-cap but without min-num-entries	27.298 ( + 0.69 %)	3.221 ( + 0.15 %)	1.042 ( + 0.71 %)

Table 4.1: Athena v22.0.16: Comparing the maximum proportional set size (PSS) and PHYS/PHYSLITE output file sizes (outFS) for data jobs over various Athena configurations for 160327 entries.

Athena v22.0.16 configurations (MC)	Max PSS (MB) ( $\Delta\%$ default)	PHYS outFS (GB) ( $\Delta\%$ default)	PHYSLITE outFS (GB) ( $\Delta\%$ default)
With basket-cap and min-num-entries (default)	14.13 ( + 0.00 %)	5.83 ( + 0.00 %)	2.59 ( + 0.00 %)
Without both basket-cap and min-num-entries	16.08 ( + 12.13 %)	6.00 ( + 2.93 %)	2.72 ( + 5.06 %)
Without basket-cap but with min-num-entries	15.97 ( + 11.51 %)	5.67 ( - 2.80 %)	2.45 ( - 5.58 %)
With basket-cap but without min-num-entries	14.19 ( + 0.42 %)	6.16 ( + 5.35 %)	2.87 ( + 9.90 %)

Table 4.2: Athena v22.0.16: Comparing the maximum proportional set size (PSS) and PHYS/PHYSLITE output file sizes (outFS) for MC jobs over various Athena configurations for 140000 entries.

#### 4.3.2 Comparing different basket sizes

Pre-existing derivation jobs were ran for data and MC simulations to compare between configurations of differing basket sizes limits. The results for this set of testing are found from Table 3 through Table 10. The following tables are the DAOD output-file sizes of the various Athena configurations for PHYS/PHYSLITE over their respective data/MC AOD input files.



Athena v24.0.16 configurations (Data)	Max PSS (MB) ( $\Delta\%$ default)	PHYS outFS (GB) ( $\Delta\%$ default)	PHYSLITE outFS (GB) ( $\Delta\%$ default)
With basket-cap and min-num-entries (default)	27.8591 ( + 0.00 %)	3.2571 ( + 0.00 %)	1.0334 ( + 0.00 %)
Without both basket-cap and min-num-entries	28.6432 ( + 2.74 %)	3.2552 ( - 0.06 %)	1.0302 ( - 0.31 %)
Without basket-cap but with min-num-entries	28.2166 ( + 1.27 %)	3.2553 ( - 0.05 %)	1.0303 ( - 0.30 %)
With basket-cap but without min-num-entries	28.4852 ( + 2.20 %)	3.2571 ( + 0.00 %)	1.0307 ( - 0.26 %)

Table 4.3: Athena v24.0.16: Comparing the maximum proportional set size (PSS) and PHYS/PHYSLITE output file sizes (outFS) for Data jobs over various Athena configurations for 160327 entries.

### 4.3.3 Monte Carlo PHYSLITE branch comparison

Derivation production jobs work with initially large, memory-consuming branches, compressing them to a reduced size. These derivation jobs are memory intensive because they first have to load the uncompressed branches into readily-accessed memory. Once they're loaded, only then are they able to be compressed. The compression factor is the ratio of pre-derivation branch size (Total-file-size) to post-derivation branch size (Compressed-file-size). The compressed file size is the size of the branch that is permanently saved into the DAOD.

Branches with highly repetitive data are better compressed than non-repetitive data, leading to high compression factors—the initial size of the branch contains more data than it needs pre-derivation. If pre-derivation branches are larger than necessary, there should be an opportunity to save memory usage during the derivation job.

The following tables look into some highly compressible branches and might lead to areas where simulation might save some space. (AOD pre compression?)

[Table 5 from the int note]

An immediate observation: with the omission of the Athena basket limit (solely relying on ROOTs 1.3 MB basket limit), the compression factor increases. This is inline with the original expectation that an increased buffer size limit correlate to better compression. \*PrimaryVerticesAuxDyn.trackParticleLinks\* is a branch where, among each configuration of Athena MC derivation, has the highest compression factor of any branch in this dataset.

Some branches, like `*HLTNav Summary DAODSlimmedAuxDyn.linkColNames*` show highly compressible behavior and are consistent with the other job configurations (data, MC, PHYS, and PHYSLITE). Further work could investigate these branches for further optimization

#### 4.3.4 Conclusion to derivation job optimization

Initially, limiting the basket buffer size looked appealing; after 128kB basket buffer size the compression ratio would begin to plateau, increasing the memory-usage without saving much in disk-usage. The optimal balance could be the basket buffer limit of 128 kB.

Instead, by removing the upper limit of the basket size, a greater decrease in DAOD output file size is achieved. The largest decrease in file size came from the PHYSLITE MC derivation jobs without setting an upper limit to the basket buffer size. While similar decreases in file size appear for derivation jobs using data, it is not as apparent for data as it is for MC jobs. With the removal of an upper-limit to the basket size, ATLAS stands to gain a 5% decrease for PHYSLITE MC DAOD output file sizes, but an 11 - 12

By looking at the branches per configuration, specifically in MC PHYSLITE output DAOD, highly compressible branches emerge. The branches inside the MC PHYSLITE DAOD are suboptimal as they do not conserve disk space; instead, they consume memory inefficiently. As seen from (Table 5) through (Table 10), we have plenty of branches in MC PHYSLITE that are seemingly empty—as indicated by the compression factor being  $O(10)$ . Reviewing and optimizing the branch data could further reduce GRID load during DAOD production by reducing the increased memory-usage while keeping the effects of decreased disk-space.

## CHAPTER 5

### MODERNIZING I/O CI UNIT-TESTS

#### 5.1 Continuous integration unit tests

Unit tests are programs that act as a catch during the continuous integration of a codebase and exhaust features that need to remain functional. Athena has a number of unit tests which check every new merge request and nightly build for issues in the new code that could break core I/O functionality, either at the level of Athena, ROOT, or any other software in the LCG stack. With the adoption of the xAOD EDM, there were no unit tests to cover core I/O functionality related to this new EDM.

## BIBLIOGRAPHY

- [1] ATLAS Collaboration. *Software and computing for Run 3 of the ATLAS experiment at the LHC*. 2024. arXiv: 2404.06335 [hep-ex]. URL: <https://arxiv.org/abs/2404.06335>.
- [2] ATLAS software group. *Athena*. URL: <https://doi.org/10.5281/zenodo.2641997>.
- [3] ATLAS software group. *Athena Continuous Integration*. URL: <https://atlassoftwaredocs.web.cern.ch/athena/git/continuous-integration/>.
- [4] ATLAS software group. *Athena Software Documentation*. URL: <https://atlassoftwaredocs.web.cern.ch/athena/>.
- [5] A.C. Kraus. *GitHub Repository: building-athena*. <https://github.com/arthurkraus3/building-athena.git>. 2023.
- [6] Ana Lopes and Melissa Loyse Perry. *FAQ-LHC The guide*. 2022. URL: <https://home.cern/resources/brochure/knowledge-sharing/lhc-facts-and-figures>.
- [7] Bartosz Mindur. *ATLAS Transition Radiation Tracker (TRT): Straw tubes for tracking and particle identification at the Large Hadron Collider*. Geneva, 2017. DOI: 10.1016/j.nima.2016.04.026. URL: <https://cds.cern.ch/record/2139567>.
- [8] ATLAS Outreach. “ATLAS Fact Sheet : To raise awareness of the ATLAS detector and collaboration on the LHC”. 2010. DOI: 10.17181/CERN.1LN2.J772. URL: <https://cds.cern.ch/record/1457044>.
- [9] ROOT Team. *ROOT, About*. URL: <https://root.cern/about/>.

APPENDIX  
APPENDIX ONE

## A.1 Derivation production datasets

For both the nightly and the release testing, the data derivation job, which comes from the dataset

`data22_13p6TeV: data22_13p6TeV.00428855.physics_Main.merge.AOD.r14190_p5449_ti`

was ran with the input files

`AOD.31407809._000894.pool.root.1`

`AOD.31407809._000895.pool.root.1`

`AOD.31407809._000896.pool.root.1`

`AOD.31407809._000898.pool.root.1`

Similarly, the MC derivation job, comes from the dataset

`mc23_13p6TeV: mc23_13p6TeV.601229.PhPy8EG_A14_ttbar_hdamp258p75_SingleLep.merge`

was ran with input files

`AOD.33799166._000303.pool.root.1`

`AOD.33799166._000304.pool.root.1`

`AOD.33799166._000305.pool.root.1`

`AOD.33799166._000306.pool.root.1`

`AOD.33799166._000307.pool.root.1`

`AOD.33799166._000308.pool.root.1`