ABSTRACT

OPTIMIZATION OF DERIVATION JOBS AND MODERNIZATION OF I/O INTEGRATION TESTS FOR THE ATLAS EXPERIMENT

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The High-Luminosity LHC (HL-LHC) is a phase of the LHC that is expected to start toward the end of the decade. With this comes an increase in data taken per year that current software and computing infrastructure, including I/O, is being prepared to handle. The ATLAS experiment's Software Performance Optimization Team has areas in development to improve the Athena software framework that is scalable in performance and ready for wide-11 spread HL-LHC era data taking. One area of interest is optimization of derivation production 12 jobs by improving derived object data stored to disk by about 4-5% by eliminating the upper-13 limit on TTree basket buffers, at the expense of an increase in memory usage by about 11%. 14 Athena and the software it depends on are updated frequently, and to synthesize changes 15 cohesively there are scripts, unit tests, that run which test core I/O functionality. This 16 thesis upgrades existing I/O unit tests to now exercise features exclusive to the xAOD Event 17 Data Model (EDM) such as writing and reading object data from the previous EDM using transient and persistent data. These new unit tests also include and omit select dynamic 19 attributes to object data during the component accumulator step.

NORTHERN ILLINOIS UNIVERSITY DE KALB, ILLINOIS

MAY 2025

OPTIMIZATION OF DERIVATION JOBS AND MODERNIZATION OF I/O INTEGRATION TESTS FOR THE ATLAS EXPERIMENT

ВҮ

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A THESIS SUBMITTED TO THE GRADUATE SCHOOL IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE MASTER OF SCIENCE

DEPARTMENT OF PHYSICS

Thesis Director:

Dr. Jahred Adelman

- $_{23}$ Here's where you acknowledge folks who helped. Here's where you acknowledge folks
- ²⁴ who helped. Here's where you acknowledge folks who helped. Here's where you acknowledge
- folks who helped.

DEDICATION

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

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CHAPTER 1

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INTRODUCTION

Particle physics is the branch of physics that studies the fundamental constituents of 137 matter and the forces governing their interactions. The field started as studies in elec-138 tromagnetism, radiation, and further developed with the discovery of the electron. What followed was more experiments to search for new particles, new models to describe the re-140 sults, and new search techniques which demanded more data. The balance in resources for an experiment bottlenecks how much data can be taken, so steps need to be taken to 142 identify interesting interactions and optimize the storage and processing of this data. This 143 thesis investigates software performance optimization of the ATLAS experiment at CERN. 144 Specifically, ways to modernize and optimize areas of the software framework, Athena, to 145 improve input/output (I/O) performance during derivation production and create new tests 146 that catch when specific core I/O functionality is broken. 147

1.1 LHC and The ATLAS Detector

The Large Hadron Collider (LHC), shown in Figure 1.1, is a particle accelerator spanning a 26.7-kilometer ring that crosses between the France-Switzerland border at a depth between 50 and 175 meters underground. [2] The ATLAS experiment, shown in Figure 1.3, is the largest LHC general purpose detector, and the largest detector ever made for particle collision experiments. The detector lies in a cavern 92.5 m underground at a length of 46 m, height and width of 25 m. [3] A quadrant of the detector is shown in Figure 1.2, where η is a measure

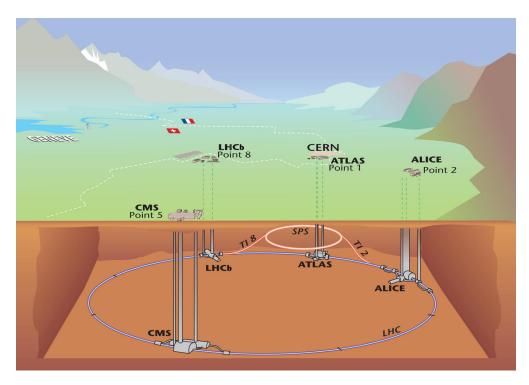


Figure 1.1: Illustration of the LHC experiment sites on the France-Switzerland border.[1]

of the pseudo-rapidity. Pseudo-rapidity is a parameter representing the the angle relative to the beamline and is defined as

$$\eta \equiv -\ln\left[\tan\left(\frac{\theta}{2}\right)\right],\tag{1.1}$$

where if $\theta = 0$ then $\eta = \infty$ and if $\theta = \frac{\pi}{2}$ then $\eta = 0$. Pseudo-rapidity is used, as opposed to traditional Cartesian angles, because it's Lorentz invariant under boosts along the beam axis, making it easier to identify tracks due to symmetry of the collision.

160 Inner Detector

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. Its main function is to measure the track of the charged particles without destroying the particle itself. The first point of contact for particles emerging from *pp*-collisions from the center of the ATLAS detector is the pixel detector.[6]

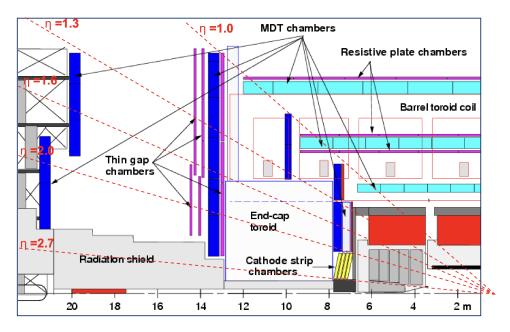


Figure 1.2: One quadrant of the ATLAS detector. The components of the Muon Spectrometer are labelled [4]

It has over 92 million pixels to aid in particle track and vertex reconstruction. Since the 166 pixels are the first point of contact to the incident particles they have to be radiation hard so 167 the electronics may function without fault. When a charged particle passes through a pixel 168 sensor it ionizes the one-sided doped-silicon wafer to produce an excited electron will then 169 occupy the conduction band of the semiconductor producing an electron-hole pair, leaving the valence band empty. [7] This hole in the valence band together with the excited electron in the conduction band is called an electron-hole pair. The electron-hole pair is in the presence 172 of an electric field, which will induce drifting of the electron-hole pair, drifting that will 173 generate the electric current to be measured. 174

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Surrounding the pixel detector is the SemiConductor Tracker (SCT), which uses 4,088 modules of 6 million implanted silicon readout strips. [8] Both the pixel detector and SCT measure the path particles take, called tracks. While the pixel detector has measurement



Figure 1.3: Overview of the ATLAS detectors main components, with two people in figure to scale.[5]

precision up to $10\mu m$ in the $r\phi$ -direction and $70\mu m$ in the z-coordinate direction,[9] the SCT has resolution $17\mu m$ in the $r\phi$ -direction and $580\mu m$ in the z-direction.

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. The TRT's straw walls are made of two $35\mu m$ layers comprised of $6\mu m$ carbon-polymide, $0.20\mu m$ aluminum, and a $25\mu m$ Kapton film reflected back.[10] The straws are filled with a gas mixture of $70\%\text{Xe} + 27\%\text{CO}_2 + 3\%\text{O}_2$. Its measurement precision is around $170\mu m$. Particles with relativistic velocities have higher Lorentz γ -factors,

$$\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}. (1.2)$$

The TRT uses varying materials to discriminate between heavier particles, which have low γ and radiate less, and lighter particles, which have higher γ and radiate more.[11]

Calorimeters

There are two main calorimeters for ATLAS, the Liquid Argon (LAr) calorimeter and the 189 Tile Hadronic calorimeter. The LAr calorimeter surrounds the inner detector and measures 190 the energy deposits of objects that interact via the electromagnetic force. It layers various 191 metals to intercept the incoming particles to produce a shower of lower energy particles. The 192 lower energy particles then ionize the liquid argon that fill the barrier in between the metal 193 layers to produce a current that can be read out. The Tile calorimeter surrounds the LAr 194 calorimeter and is the largest part of the ATLAS detector weighing in around 2900 tons. 195 Particles then traverse through the layers of steel and plastic scintillating tiles. The Tile 196 calorimeter is a hadronic calorimeter, so it interacts with particles via the strong nuclear 197 force. When a particle hits the steel, a cascade of secondary protons, neutrons and other 198 hadrons (quark bound states, with baryons qqq and mesons $q\bar{q}$) is produced with lower 199 energy. Through this mechanism, these decay products will continue until the energy has 200 entirely dissipated. 201

202 Muon Spectrometer (MS)

The MS sits at the end of the ATLAS detector and is designed to identify muon tracks 203 and momentum to high-resolution, its components are shown in Figure 1.2. Monitored Drift 204 Tube (MDT) chambers are used for precision measurement of muon tracks in the principle 205 bending direction of the magnetic fields over a large η . The MDT lie in the endcaps and 206 barrel regions covering the pseudorapidity regions $0 < |\eta| < 2.7$, where the tubes run 207 perpendicular to the beam and in-line with the magnetic field lines. Single cell resolution 208 for these drift tubes can reach $60\mu m.$ [3] The area of highest particle flux is the region of 209 pseudo-rapidity $2 < |\eta| < 2.7$, here is where the cathode strip chambers lie.[12] Cathode 210 strip chambers (CSCs) are layered to determine track vectors and use multi-wire chambers 211 to achieve a resolution up to $50\mu m$. 212

The RPCs are gaseous parallel-plate detectors suited for fast spacetime particle tracking 213 that combines the spatial resolution (around 1 cm) of the wire chambers and the time 214 resolution (around 1 ns) of a scintillation counter. Resistive plate chambers (RPCs) and 215 the Thin gap chambers (TGCs) provide the trigger information for the MDTs and CSCs to 216 then make a precision measurement, so speed takes priority over spatial resolution for the 217 muon trigger system. Though RPCs don't have wires, their design consists of two strips 218 separated by an insulating spacer to create a gap for the gas $(C_2H_2F_4)$ plus some smaller of 219 argon/butane) to occupy. Thin gap chambers (TGCs) exist in the forward region and are thin 220 wire chambers that aide in muon triggering and measurement of the azimuthal coordinate 221 to be used in compliment with MDTs. The time resolution in TCGs help identify bunch-222 crossings and granularity in momentum of the muon that comes within the equipotential 223 of the wires. Since each wire can be given a position in the trigger system, any muon that 224 passes through the TGC can be compared with greater spatial precision with the MDTs and 225 illustrate a track later. The accuracy of identifying the correct bunch crossing with TGCs 226 is 99% and the delivery of bunch crossing identification can be delivered within 25 ns, only 227 a small fraction of bunch crossings arrive later than that window. 228

1.2 ATLAS Trigger/Data Acquisition (TDAQ)

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The LHC produces pp-collisions at a rate of 40 MHz, each collision is an "event". More specifically, around 10^{11} protons are accelerated in one "bunch" with around 2800 bunches per proton beam spaces around 25 ns apart from each other. Each beam is then concentrated to the width of $64\mu m$ at the interaction point where about 20 collisions happen at one bunch crossing, these collisions within one bunch results in "pile-up".

The ATLAS Trigger system is responsible for quickly deciding what events are interesting 235 for physics analysis. The Trigger system is divided into the first- and second-level triggers 236 and when a particle activates a trigger, the trigger makes a decision to tell the DAQ to save 237 the data produced by the detector. The first-level trigger is a hardware trigger that decides, 238 within $2.5\mu s$ after the event, if it's a good event to put into a storage buffer for the second-239 level trigger. The second-level trigger is a software trigger that decides within $200\mu s$ and 240 uses around 40,000 CPU-cores and analyses the event to decide if it is worth keeping. The 241 second-level trigger selects about 1000 events per second to keep and store long-term.[13] 242 The data taken by the TDAQ system is raw and not yet in a state that is ready for analysis, 243 but it is ready for further processing. 244

The amount of data taken at ATLAS is substantial, seeing more than 3 PB of raw data 245 each year and each individual event being around 2 MB.[14] All of the data produced by 246 LHC experiments, especially ATLAS, has to be sent to the Worldwide LHC Computing Grid 247 (WLCG).[15] The WLCG composes of a three-tiered system, CERN serves as the Tier-0 site, 248 there are $\mathcal{O}(20)$ Tier-1 sites, and $\mathcal{O}(200)$ Tier-2 sites. [16] Though, the numbers of each site 249 do change over time. The raw data coming from the TDAQ systems are recorded at the 250 CERN Tier-0 sites where a first-pass at reconstruction will take place and a copy of the raw 251 data is sent to the Tier-1 sites. Multiple 10 Gbps capacity links streamline dataflow from 252 the ATLAS TDAQ to the Tier-0 site. Tier-1 sites offer manage permanent storage of raw and reconstructed data and provide extensive processing capability for analysis that might demand it. Tier-2 sites provide additional computation and storage services that compliment 255 end-user analysis. 256

Athena manages ATLAS production workflows which are involved with simulation of data and event generation, track reconstruction from hits, and derivation production.[17]
Figure 1.4 illustrates the broadstrokes of the entire ATLAS data processing chain for both real detector data and Monte Carlo (MC) simulations. MC simulation starts with the event

generation (EVNT), following simulation of events hitting the detector (HITS) and further simulation of what would be readout of the detector (RDO). The reconstructed Analysis Object Data (AOD) are then processed through derivation production jobs that reduces AODs from $\mathcal{O}(1)$ MB per event to $\mathcal{O}(10)$ kB per event, creating Derived AOD (DAOD). Further discussion on the production of DAOD can be found in Section 2.3.

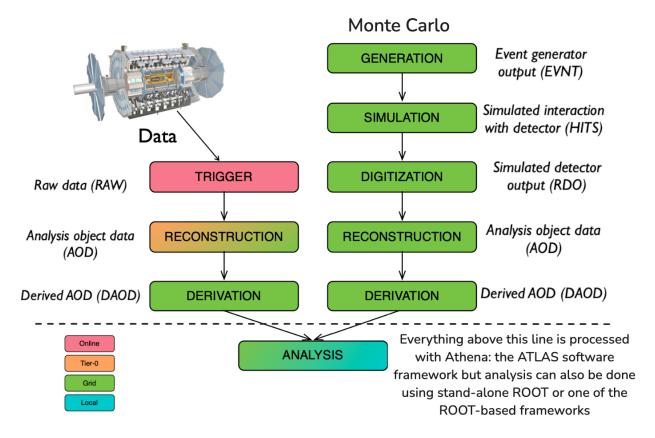


Figure 1.4: ATLAS data chain-processing for data and Monte Carlo simulation. Figure is modified from [18].

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1.3 ATLAS Software and Computing Needs

The High-Luminosity LHC (HL-LHC) is the upgrade to LHC that anticipates more events and more data taken than ever before. The goal is to reach a luminosity of $350fb^{-1}$, which is forecasted to be reached gradually by around 2040.[19] The HL-LHC era will start sooner than that, and it's projected to demand anywhere from 6-10 times data stored per year, so any attempt to save on disk storage should be investigated.[20] Increasing data means more resources from the Grid will be used, so optimization across files and software is an essential part of ensuring scalability of the data taken in by the detector. Figure 1.5 illustrates the projections of the HL-LHC era long-term storage usage for both disk and tape.

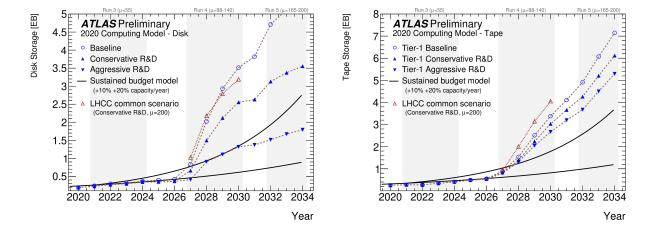


Figure 1.5: HL-LHC computing model projections on the future disk and tape usage compared to the expected budget increases.[21]

One avenue optimization is being investigated is in the method of storing data to file. The traditional method of storing event information for AOD/DAOD is with ROOT TTrees 276 (see Section 2.2). ROOT TTrees (referred to as "TTrees" or "trees") have been the standard 277 data storage format for over two decades, and they provide a clear means of organizing and 278 accessing physics objects for processing and analysis. The development of the ROOT N-Tuple 279 (RNTuple) I/O subsystem updates areas to support multi-thread processing, asynchronous 280 I/O, object stores, and more. It's been shown to outperform the TTree I/O subsystem and 281 other storage formats in file size (by about 15%), throughput, and compression, but still 282 has more development before full implementation into the analysis pipeline. [22] While 283

- 284 RNTuple is in development, there are still insights regarding resource usage optimization
- $_{\mbox{\scriptsize 285}}$ that are found by using TTree in its current state.

CHAPTER 2

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I/O TOOLS

The Trigger/DAQ system sends and saves data from the detector to a persistent data 288 storage solution. It's at this stage where the data isn't yet ready for an effective analysis, so 289 what needs to happen is the data needs to be reconstructed and consolidated into physics objects, or Analysis Object Data (AOD) files. Creating AODs from data requires significant 291 computation power and Athena is the software framework that plays a significant role in this process. This chapter will cover some of the important software tools used by ATLAS 293 to run derivation jobs, as well as introduce data structures that represent event information. 294

Athena and ROOT 2.1

Athena is the open-source software framework for the ATLAS experiment. [24] It is based off the Gaudi project and uses on other software such as ROOT and other software as part of the LCG software stack. It also provides some in-house based analysis tools as well as tools for specifically ROOT based analysis.

An Athena application relies on *components*: Algorithms, Tools, Services and Proper-300 ties. [25] Each component plays a role in executing an Athena application or job, which 301 is written and configured in Python. Specifically, an Algorithm accesses data objects in 302 the event store, as shown with the solid lines in Figure 2.1, but does not own or provide 303 any data itself. Algorithms can "own" Tools, which serve as helpers exclusive to Algorithms or other components that call them. Services are not as exclusive with its access, as they 305

¹ "Ownership" here refers to the components' exclusive access or control of a Tool or Service.

can be used by other components to provide a service such as Athena-ROOT conversion,
random number generators, and others. Properties are able to be called at initialization of
the job configuration and include flag definitions, input and output file names, and other
algorithm specific options. ComponentAccumulator (CA) is a python class that put into
Athena production as a way to prevent extra calls of setting flags during configuration.

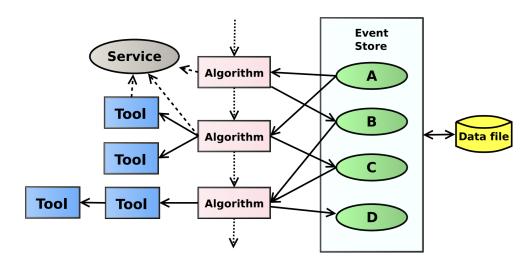


Figure 2.1: An Athena application's general structure. [25]

An important step throughout the development of Athena is to ensure any new changes 311 to the codebase will not overrule the functionality of core features to the present workflows. 312 One of the areas needed to be tested before and upon merging of any new changes to Athena 313 is the I/O functionality, or the performance of reading and writing of stored objects within a 314 broader context of various jobs, i.e. reconstruction or derivation. While CA is a more general 315 mechanism to run any kind of job with Athena, it's within the scope of this thesis where the 316 focus is on testing core I/O functionality of the new event data model. An example Athena 317 job configuration is found in Appendix B. 318

ROOT is an open-source software framework used for high-energy physics analysis at CERN.[26] 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.

ROOT largely revolves around organization and manipulation of TFiles and TTrees into ROOT files. A TTree represents a columnar dataset, and the list of columns are called branches. The branches have memory buffers that are automatically allocated by ROOT. These memory buffers are divided into corresponding baskets, whose size is designated during memory allocation. More detail on branch baskets are explored in Chapter 3 and 4.

CMake and Make are open-source software that is used to build Athena, ROOT, and other software. A sparse build is a way to make changes to an individual package of code without having to recompile the entire framework at once, which saves time and resources.

A user can create a text file identifying the path to the package modified, and the sparse build for Athena will proceed upon issuing the following commands:

```
cmake -DATLAS_PACKAGE_FILTER_FILE=../package_filters.txt ../athena/
Projects/WorkDir/
make -j
```

Where ../package_filters.txt is the text file containing the path to the package modified,
and ../athena/Projects/WorkDir/ is the path to the Athena source.

The POOL framework is part of a larger framework including CORAL and COOL, to-339 gether made up the Persistency Framework (PF). [27] The PF was developed with the intent 340 to be independent of any individual experiment, and the goal was to address data access 341 requirements of LHC experiments in different ways. POOL was in charge of C++ object 342 storage, collection of metadata, and file catalogs by using streaming and relational technolo-343 gies. POOL provided highly scalable object serialization to framework evolving PF files. It 344 was eventually discontinued by other experiments in favor of a newer persistency mecha-345 nism that uses ROOT in a more streamlined way. ATLAS then became the sole supporter 346 of POOL and integrated it within Athena to support persistent navigation of the ROOT storage layer. Now, Athena has both the original PF POOL functionality and a separate modern AthenaPool functionality. AthenaPool resides in the ATLAS I/O framework and controls ROOT TTree and TBranch properties such as compression and basket buffer sizing.

2.1.1 Continuous Integration (CI) and Development

CI is a software development practice where new code is tested and validated upon each

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merge to the main branch of a repository. Every commit to the main branch is automatically
built and tested for specific core features that are required to work with the codebase. This
helps to ensure that the codebase is working as intended and that any new code is compatible
with the existing codebase.

Athena is hosted on GitLab and developed using CI with an instance of Jenkins, called
ATLAS Robot, which builds and tests the new changes within a merge request interface.
ATLAS Robot will then provide a report of the build and test results. If the build or test
fail, ATLAS Robot will provide a report of which steps failed and why. This allows for early

2.2 TTree Object

detection of issues before the nightly build is compiled and tested.

A TTree is a ROOT object that organizes physically distinct types of event data into TBranches, or just branches. Event data could range from information about a specific type of interaction, this includes tracks, position of particles at one point in the detector.

Branches hold data into dedicated contiguous memory buffers, and those memory buffers, upon compression, become baskets. These baskets can have a limited size and a set minimum number of entries. The Athena default basket size at present is 128 kB, and the default minimum number of entries is 10.

Mem Size	Disk Size	Size/Evt	MissZip/Mem	items	(X) Container Name (X=Tree Branch)
108286.649 kb	75465.794 kb 75806.374 kb	0.539 kb 0.541 kb	0.000 0.000	140000	(B) EventInfoAuxDyn.mcEventWeights (B) AntiKt4TruthDressedWZJetsAux.
937529.397 kb	84669.190 kb	0.605 kb	0.000	12816	(T) DataHeaderForm
156560.056 kb 1907707.847 kb	136608.917 kb 447106.466 kb	0.976 kb 3.194 kb	0.000 0.000	140000 140000	(B) InDetTrackParticlesAuxDyn.definingParametersCovMatrixOffD:(B) HLTNav_Summary_DAODSlimmedAuxDyn.decisions

Figure 2.2: A snapshot of the contents of a TTree, TBranches

One function relevant to TTree is Fill(). Fill() will loop over all of the branches in
the TTree and compresses the baskets that make up the branch. This removes the basket
from memory as it is then compressed and written to disk. It makes reading back branches
faster as all of the baskets are stored near each other on the same disk region. [28]

AutoFlush is a function that tells the Fill() function after a designated number of
entries of the branch, in this case vectors, to flush all branch buffers from memory and save
them to disk.

2.3 Derivation Production Jobs

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A derivation production job takes AODs, which comes from the reconstruction step 378 at $\mathcal{O}(1 \text{ MB})$ per event, and creates a derived AOD (DAOD) which sits at $\mathcal{O}(10 \text{ kB})$ per 379 event. Derivation production is a necessary step to make all data accessible for physicists 380 doing analysis as well as reducing the amount of data that needs to be processed. While 381 derivations are reduced AODs, they often contain additional information useful for analysis, 382 such as jet collections and high-level discriminants. [29] The two mainstream output file 383 formats Athena is capable of handling are PHYS and PHYSLITE. Figure 2.3 shows the 384 object composition of a PHYS and PHYSLITE $t\bar{t}$ sample. PHYS output files, at 40.0 kB 385 per event, is predominantly made of jet collections, while PHYSLITE, at 16.1 kB per event, has more trigger and track information. There is ongoing work to reduce the amount of

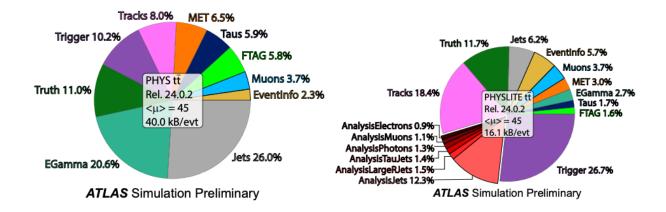


Figure 2.3: Object composition of a PHYS and PHYSLITE $t\bar{t}$ sample from Run 3.

Trigger information in PHYSLITE which would help further reduce the file size saved to
disk. PHYSLITE, being the smallest file of the two, sees the largest effect upon attempts of
optimization. These jobs can demand heavy resource usage on the GRID, so optimization
of the AOD/DAODs for derivation jobs can be vital.

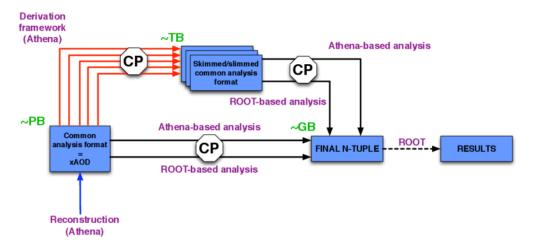


Figure 2.4: Derivation production from Reconstruction to Final N-Tuple[30]

The derivation framework is sequence of steps that are performed on the AODs to create the DAODs. Skimming is the first step in the derivation framework, and it's responsible for removing whole events based on pre-defined criteria. Thinning is the second step, and it removes whole objects based on pre-defined criteria. Lastly slimming removes variables from objects uniformly across events.

2.4 Event Data Models

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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.

2.4.1 Transient/Persistent (T/P) EDM

One of the previous EDM schemas used by ATLAS concerned a dual transient/persistent 406 status of AOD. With this EDM, the AOD was converted into an ntuple based format called 407 D3PDs. While this conversion allowed for fast readability and partial read for efficient analy-408 sis in ROOT, it left the files disconnected from the reconstruction tools found in Athena.[31] 409 When transient data was present in memory, it could have information attached to the ob-410 ject and gain in complexity the more it was used. Transient data needed to be simplified 411 before it could become persistent into long-term storage (sent to disk). ROOT had trouble 412 handling the complex inheritance models that would come up the more developers used this 413 EDM. Before the successor to the T/P EDM was created, ATLAS physicists would convert 414 data samples using the full EDM to a simpler one that would be directly readable by ROOT.

This would lead to duplication of data and made it challenging to develop and maintain the analysis tools to be used on both the full EDM and the reduced ones. Additionally, converting from transient to persistent data was an excessive 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.

2.4.2 xAOD EDM

421

The xAOD EDM is the successor to the T/P EDM and brings a number of improvements.

This EDM, unlike T/P, is usable both on Athena and ROOT. It's easier to pick up for analysis
and reconstruction. The xAOD EDM has the ability to add and remove variables within an

ItemList at runtime, specified in the CA script, these variables are "decorations."

The xAOD EDM use two types of objects handle data, interface objects and payload objects. Interfaces act as an interface for the user to access the object but without its stored data. This differs from T/P where the user would have to load an object into memory to access the object. If the user wanted to delay the loading of data into memory, they could use the interface object to do so. The payload object contains the data for the interface object and is allocating contiguous blocks of memory. Payload classes are often referred to as auxiliary storage.

The specific data structure used by ATLAS is the ROOT TTree, but the EDM is agnostic to the type of data structure used. ATLAS specific libraries are not required to handle files written in the xAOD format since the payload can be read directly from the contiguous allocation of memory, a central tenent of the xAOD EDM. This allows for the separation of ATLAS specific analysis frameworks and the preferred analysis tool of the user. More information on how the xAOD EDM is deployed into unit tests in Section 5.1.

CHAPTER 3

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440

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453

TOY MODEL BRANCH STUDY

Building a toy model for derivation production jobs offers a simplified framework to 441 effectively simulate and analyze the behavior of real and Monte Carlo (MC) data under 442 techniques of optimization aimed to study. One commonality between both data and MC is the data types stored in branches for both is made of a mixture between repeated integer-like data and randomized floating-point data. Integers are easier to compress than floating-point numbers, so adjusting the mixture of each can yield compression ratios closer to real and MC data. Replicating this mixture in a branch give us an effective model that resembles how current derivation jobs act on real and MC simulated data. These toy model mixtures 448 provide an avenue to test opportunities for optimizing the memory and storage demands 449 of the GRID by first looking at limiting basket sizes and their effects on compression of 450 branches. 451

3.1 Toy Model Compression

3.1.1 Random Float Branches

There were a number of iterations to the toy model, but the first was constructed by filling
a TTree with branches that each have vectors with varying number of random floats to write
and read. Vectors are used in this toy model, as opposed to arrays, because vectors are
dynamically allocated and deallocated, which allows for more flexibility when synthesizing
AODs. This original model had four distinct branches, each with a set number of events

(N=1000), and each event having a number of entries, vectors with 1, 10, 100, and 1000 floats each.

The script can be compiled with gcc or g++ and it requires all of the dependencies that come with ROOT. Alternatively, the script can be run directly within ROOT.

The following function VectorTree() is the main function in this code. What is needed 463 first is an output file, which will be called VectorTreeFile.root, and the name of the tree 464 can simply be myTree. The toy model starts variable initialization with the total number of 465 events in the branch, i.e. the number of times a branch is filled with the specified numbers 466 per vectors, N. Additionally the branches have a number of floats per vector, this size will 467 need to be defined as size_vec_0, size_vec_1, etc. The actual vectors that are being stored 468 into each branch need to be defined as well as the temporary placeholder variable for our 469 randomized floats, vec_tenX and float_X, respectively. 470

```
471
      void VectorTree() {
472
473
        const int N = 1e4; // N = 10000, number of events
474
        // Set size of vectors with 10<sup>*</sup> of random floats
475
        int size_vec_0 = 1;
476
        int size_vec_1 = 10;
477
        int size_vec_2 = 100;
478
        int size_vec_3 = 1000;
479
480
        // vectors
481
        std::vector<float> vec_ten0; // 10^0 = 1 entry
482
        std::vector<float> vec_ten1; // 10^1 = 10 entries
483
        std::vector<float> vec_ten2; // 10^2 = 100 entries
484
        std::vector<float> vec_ten3; // 10^3 = 1000 entries
485
486
487.6
        // variables
```

```
float float_0;
float float_1;
float float_2;
float float_3;
...
float float_3;
float float_1;
float float_1;
float float_2;
float float_2;
float float_3;
float float_3;
float float_3;
float float_1;
float float_1;
float float_2;
float float_2;
float float_3;
float_
```

From here, branches are initialized so each one knows where its vector pair resides in memory.

```
497
     void VectorTree() {
498
499
        // Initializing branches
        std::cout << "creating branches" << std::endl;</pre>
501
        tree->Branch("branch_of_vectors_size_one", &vec_ten0);
        tree->Branch("branch_of_vectors_size_ten", &vec_ten1);
503
        tree->Branch("branch_of_vectors_size_hundred", &vec_ten2);
        tree->Branch("branch_of_vectors_size_thousand", &vec_ten3);
505
506
     }
507.0
```

One extra step taken during this phase of testing is the disabling of AutoFlush.

509

Disabling AutoFlush allows for more consistent compression across the various sizes of branch baskets. The toy model needed this consistency more than the later tests as these early tests were solely focused on mimicking data procured by the detector and event simulation. The derivation production jobs tested in Chapter 4 were tested with AutoFlush enabled because

- those tests are not as concerned with compression as they are with memory and disk usage.
- Following branch initialization comes the event loop where data is generated and emplaced into vectors.

```
523
      void VectorTree() {
524
525
        // Events Loop
526
        std::cout << "generating events..." << std::endl;</pre>
527
        for (int j = 0; j < N; j++) {</pre>
528
            // Clearing entries from previous iteration
529
            vec_ten0.clear();
530
            vec_ten1.clear();
531
            vec_ten2.clear();
532
            vec_ten3.clear();
533.0
534
            // Generating vector elements, filling vectors
535
            // Fill vec_ten0
536
            // Contents of the vector:
537.4
                   {float_0}
            11
538
                   Only one float of random value
539.
            float_0 = gRandom->Rndm() * 10; // Create random float value
540
            vec_ten0.emplace_back(float_0); // Emplace float into vector
541
542.9
            // Fill vec_ten1
54320
            // Contents of the vector:
5442
                   {float_1_0, ..., float_1_10}
            11
545
5463
                   Ten floats, each float is random
            for (int n = 0, n < size_vec_1; n++) {</pre>
54724
                 float_1 = gRandom->Rndm() * 10;
5482
                 vec_ten1.emplace_back(float_1);
5496
            }
55027
```

```
5512
               Do the same with vec_ten2 and vec_ten3, except for
5529
                     vectors with size 100 and 1000 respectively.
5533(
5543
            // After all branches are filled, fill the TTree with
55532
                     new branches
5563
            tree->Fill();
5573
        }
558
        // Saving tree and file
5598
        tree->Write();
560%
5618
     }
```

Once the branches were filled, ROOT then will loop over each of the branches in the TTree and at regular intervals will remove the baskets from memory, compress, and write the baskets to disk (flushed), as was discussed in Section 2.2.

As illustrated, the TTree is written to the file which allows for the last steps within this script.

```
void VectorTree() {
570
571
         . . .
572
         // Look in the tree
573
         tree->Scan();
574
         tree->Print();
575
576
         myFile ->Save();
577 8
         myFile ->Close();
578 9
      }
579.0
      int main() {
5812
```

```
VectorTree();

return 0;

$83.4

| return 0;

$84.5

$85
```

Upon reading back the ROOT file, the user can view the original size of the file (Total-586 file-size), the compressed file size (File-size), the ratio between Total-file-size and File-size 587 (Compression Factor), the number of baskets per branch, the basket size, and other infor-588 mation. Filling vectors with entirely random values was believed to yield compression ratios 589 close to real data, but the results in Figure 3.1 show changes needed to be made to bring 590 the branches closer to a compression ratio of $\mathcal{O}(5)$. It is evident that branches containing 591 vectors with purely random floats are more difficult to compress due to the high level of 592 randomization. 593

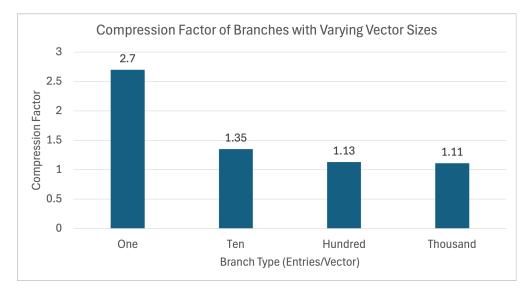


Figure 3.1: Compression factors of N = 1000 entries per branch with random-valued vectors of varying size.

Figure 3.1 shows compression drop-off as the branches with more randomized floats per vector were present. This is the leading indication that there needs to be more compressible data within the branches.

3.1.2 Mixed-Random Float Branches

597

The branches needed to have some balance between compressible and incompressible data to mimic the compression ratio found in real data. How this was achieved was by filling each vector with different ratios of random floats and repeating integers, which will now be described in detail.

The first change was increasing the total number of events per branch from $N = 10^4$ to $N = 10^5$. Mixing of random floats and repeated integer values takes the same script structure as Section 3.1.1 but adjusts the event generation loop.

```
605
      void VectorTree() {
606
607
        // Events Loop
608
        for (int j = 0; j < N; j++) {</pre>
609
            // Clearing entries from previous iteration
610
            vec_ten0.clear();
611 (
            vec_ten1.clear();
612
            vec_ten2.clear();
613
            vec_ten3.clear();
615
            // Generating vector elements, filling vectors
616
            // Generating vec_ten0
617.5
               Contents of the vector:
618
            11
                   {float_0}
619
                   Only one float of random value
620
            // And since there's only one entry, we don't mix the entries.
62116
            float_0 = gRandom->Gaus(0, 1) * gRandom->Rndm();
622
            vec_ten0.emplace_back(float_0);
623
62520
```

```
// Generating vec_ten1
6262
                Contents of the vector:
6272
                    {float_1_0, float_1_1, float_1_2, float_1_3, float_1_4, 1,
6282
       1, 1, 1, 1}
629
             11
                    5 floats of random values, 5 integers of value 1.
6302
             for (int b = 0; b < size_vec_1; b++) {</pre>
6312
                 if (b < size_vec_1 / 2) {</pre>
632
                    float_1 = gRandom->Rndm() * gRandom->Gaus(0, 1);
6332
                    vec_ten1.emplace_back(float_1);
6342
                 } else {
63529
                    float_1 = 1;
636
                    vec_ten1.emplace_back(float_1);
6373
                 }
6383
             }
6393
64084
             // Do the same with vec_ten2 and vec_ten3, except for
64B
                     vectors with size 100 and 1000 respectively.
6428
643/7
64488
             // After all branches are filled, fill the TTree with
6458
                     new branches
6460
             tree->Fill();
647
        }
648
        // Saving tree and file
649
        tree->Write();
650
     }
652l6
653
```

As shown in the if-statements in lines 14, 25, 36 and 47, if the iterator was less than half of the total number of entries in the vector then that entry had a randomized float put in that spot in the vector, otherwise it would be filled with the integer 1. Having a mixture of half random floats and half integer 1 led to the larger branches still seeing poor compression, so a new mixture of 1/4 random data was introduced. Even though $N = 10^5$ had the larger branches closer to the desired compression ratio, testing at $N = 10^6$ events improves the accuracy of the overall file size to more closely resemble real data.

Figure 3.2 shows the difference between compression between the two mixtures at $N = 10^6$ events. When the number of events is increased from $N = 10^5$ to $N = 10^6$, at the 1/2 random-mixture, the branches with more than one entry per vector see their compression factor worsen. Figure 3.3 shows a compression ratio hovering around 3 for the larger branches, whereas Figure 3.2 shows the same branches hovering around 2.

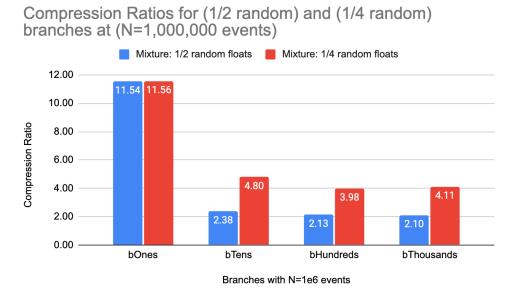


Figure 3.2: Compression Ratios for $(\frac{1}{2} \text{ random})$ and $(\frac{1}{4} \text{ random})$ branches at $(N = 10^6 \text{ events})$

Unlike the mixture of branches having 1/2 random data, the 1/4 mixture does not see
the same compression effect, but with this mixture we see a compression ratio that is in-line
with real data. This is inline with expectation, more repeated integers within the mixture
makes the branch more compressible, and the more random floats in the mixture will make

Compression Ratios for (1/2 random) and (1/4 random) branches at (N=100,000 events)



Figure 3.3: Compression Ratios for $(\frac{1}{2} \text{ random})$ and $(\frac{1}{4} \text{ random})$ branches at $(N=10^5$ events)

the branch more difficult to compress. With these mixtures added to the toy model, we can start looking at varying the basket sizes to see how they affect compression.

Basket-Size Investigation

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673

674

675

Investigating how compression is affected by the basket size requires us to change the basket size, refill the branch and read it out. Changing the basket buffer size was done at the script level with a simple setting after the branch initialization and before the event loop the following code: 676

```
677
        int basketSize = 8192000; // 8 MB
678
        tree->SetBasketSize("*",basketSize);
679
```

This ROOT-level setting was sufficient for the case of the toy model; testing of the basket size 681 setting both at the ROOT- and Athena-level would be done later using derivation production jobs in Section 4.1. The lower bound set for the basket size was 1 kB and the upper bound was 16 MB. The first branch looked at closely was the branch with a thousand vectors with half of them being random floats, see Figure 3.4.

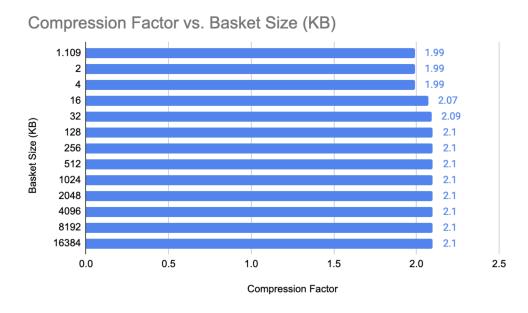


Figure 3.4: Compression Factors vs Branch Size (1000 entries per vector, 1/2 Mixture $N = 10^6$ events)

Figures 3.4 and 3.5 are the first indication that the lower basket sizes are too small to 686 effectively compress the data. For baskets smaller than 16 kB, it is necessary to have as 687 many baskets as events to store all the data effectively. For a mixed-content vector with one thousand entries, containing 500 floats and 500 integers (both are 4 bytes each), its size is 689 approximately 4 kB. ROOT creates baskets of at least the size of the smallest branch entry, 690 in this case the size of a single vector. So even though the basket size was set to 1 or 2 kB, 691 ROOT created baskets of 4 kB. These baskets \leq 4kB have a significantly worse compression 692 than the baskets ≥ 4 kB in size, so the focus was shifted toward baskets. Once the basket 693 size is larger than the size of a single vector, more than one vector can be stored in a single 694 basket and the total number of baskets is reduced. 695

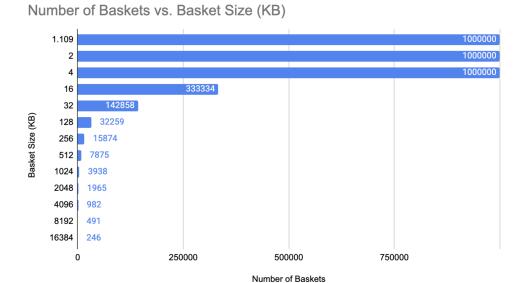


Figure 3.5: Number of Baskets vs Branch Size (1000 entries per vector, 1/2 Mixture $N=10^6$ events)

There were different types of configuration to the toy model investigated by this study.

Looking further into the types of mixtures and how they would affect compression are shown
in Figures 3.6 and 3.7. Here the same mixtures were used but the precision of the floating
point numbers was decreased from the standard 32 floating-point precision to 16 and 8,
making compression easier.

Each of these sets of tests indicate that after a certain basket size, i.e. 128 kB, there is no significant increase in compression. Having an effective compression at 128 kB, it's useful to stick to that basket size to keep memory usage down. Knowing that increasing the basket size beyond 128 kB yields diminishing returns, it's worth moving onto the next phase of testing with actual derivation production jobs.

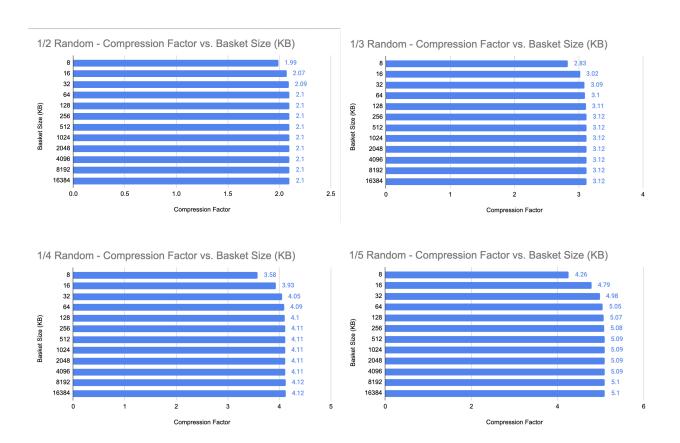


Figure 3.6: Varying Mixtures in 8 point precision - Number of Baskets vs Branch Size $(N=10^6~{\rm events})$

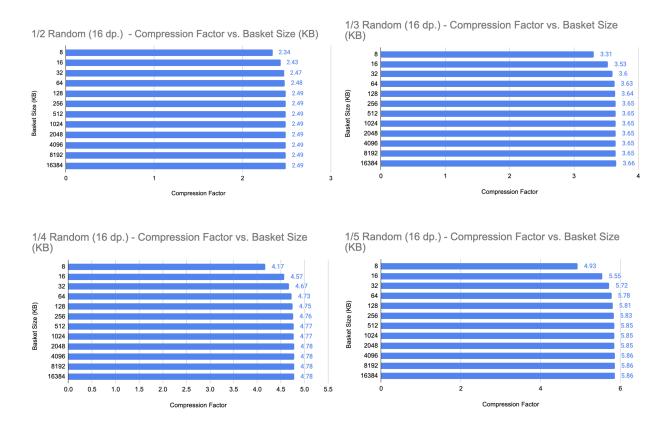


Figure 3.7: Varying Mixtures in 16 point precision - Number of Baskets vs Branch Size $(N=10^6~{\rm events})$

CHAPTER 4

DATA AND MONTE CARLO DERIVATION PRODUCTION

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Derivation production demands high memory usage, and DAODs make up a bulk of disk-708 space usage. DAODs are used in physics analyses and ought to be optimized to alleviate 709 stress on the GRID and to lower disk-space usage. Optimizing both disk-space and memory 710 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 the user will load a larger buffer into 713 memory. This project opted to take is by optimizing for disk-space and memory by testing 714 various basket limits and viewing the effects of the branches on both data and Monte Carlo 715 (MC) simulated analysis object data (AODs). 716

4.1 Basket-size Configuration

As the toy model ruled out, the focus here was on optimizing Athena and not ROOTs contribution for optimization. The initial focus was on the inclusion of a minimum number of entries per buffer and the maximum basket buffer limit. The AthenaPOOL script directly involved with these buffer settings is the PoolWriteConfig.py found in the path athena/Database/AthenaPool/AthenaPoolCnvSvc/python/. As discussed in Section 4.2, further testing opted to keep the minimum number of entries set to its default setting, 10 entries per buffer.

Throughout the duration of this testing, the results of compression or file size are independent of any changes to the release or the nightly version of Athena. The data derivation job comes from a 2022 dataset with four input files and 160,327 events. The MC job comes from a 2023 $t\bar{t}$ standard sample simulation job with six input files and 140,000 events. The datasets are noted in Appendix A.1.

4.1.1 Derivation Job Command

730

To run a derivation job, AODs need to be downloaded by a data-management service, such as Rucio, to a user's local machine. Rucio is the data-management solution used for this project to procure the various AOD input files used for the derivation jobs. The machine running the Rucio client will need to have a valid proxy added for Rucio to run correctly. A sample command would look like:

```
736
737 | rucio download data22_13p6TeV: AOD.31407809._000898.pool.root.1
```

This downloads the AOD file from Rucio and saves it to the user's local directory.

The command used by Athena to run a derivation job takes the form of the following example:

```
ATHENA_CORE_NUMBER=4 Derivation_tf.py \
   --CA True \
744
   --inputAODFile mc23_13p6TeV.601229.PhPy8EG_A14_ttbar_hdamp258p75_SingleLep
       .merge.AOD.e8514_e8528_s4162_s4114_r14622_r14663/AOD.33799166._001224.
746
      pool.root.1 \
   --outputDAODFile art.pool.root \
748
   --formats PHYSLITE \
   --maxEvents 2000 \
750 €
   --sharedWriter True \
751
   --multiprocess True ;
752
753
```

Where Athena allows one to specify the number of cores to use with the ATHENA_CORE_NUMBER environment variable. Derivation_tf.py is a script that runs the derivation job and is part of the Athena release. The --inputAODFile is the input file for the derivation job, in this case an AOD file. The user can specify multiple input files at a time by enclosing the input files in quotes and separating each file with a comma, like the following:

```
759
7601
--inputAODFile="AOD.A.pool.root.1,AOD.B.pool.root.1,AOD.C.pool.root.1,
761
762
AOD.D.pool.root.1"
```

The --outputDAODFile is the output file for the derivation job, in this case a DAOD file.

The --formats PHYSLITE flag allows the job to use the PHYSLITE format for the DAOD.

Here is where the user may choose to include PHYS or PHYSLITE simply by inlusion of one or both. The --maxEvents flag allows one to specify the maximum number of events to run the job on. The --sharedWriter True flag allows the job to utilize SharedWriter. The --multiprocess True flag allows the job to use AthenaMP tools.

The input files for both data and MC jobs were ran with various configurations of Athena by modifying the basket buffer limit. The four configurations tested all kept minimum number of basket buffer entries at 10 and modified the basket limitation in the following ways:

- 1. "default" Athena's default setting, and basket limit of 128 kB
- 2. "256k" Limit basket buffer to 256 kB
- 3. "512k" Limit basket buffer to 512 kB
- 4. "no-lim" Removing the Athena basket limit, the ROOT imposed 1.3 MB limit still remains

778 4.2 Results

4.2.1 Presence of basket-cap and presence of minimum number of entries

The 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 basket buffer entries. PHYSLITE MC derivation production, from Table 4.2, sees a 9.9% increase in output file size when compared to the default Athena configuration. Since this configuration only differs by the omission of the "min-number-entries" requirement, we assume the minimum number of basket buffer entries should be kept at 10 and left alone. Table 4.2 also shows the potential for a PHYSLITE MC DAOD output file size reduction by eliminating our upper basket buffer limit altogether.

Presence of features (Data)	Max PSS (MB) (Δ % default)	PHYS outFS (GB) (Δ %)	PHYSLITE outFS (GB) (Δ %)
basket-cap, min-num-entries (default)	27.1 (+ 0.0 %)	3.22 (+0.0 %)	1.03 (+ 0.0 %)
basket-cap min-num-entries	27.8 (+ 2.5 %)	3.22 (+ 0.2 %)	1.04 (+ 0.2 %)
basket-cap min-num-entries	27.8 (+ 2.5 %)	3.22 (- 0.0 %)	1.03 (- 0.4 %)
basket-cap, min-num-entries	27.3 (+ 0.7 %)	3.22 (+ 0.2 %)	1.04 (+ 0.7 %)

Table 4.1: Comparing the maximum proportional set size (PSS) and PHYS/PHYSLITE output file sizes (outFS) for data jobs while varying the presence of features in Athena PoolWriteConfig.py for 160327 entries.

Presence of features (MC)	Max PSS (MB) ($\Delta\%$ default)	PHYS outFS (GB) (Δ %)	PHYSLITE outFS (GB) (Δ %)
basket-cap, min-num-entries (default)	14.1 (+ 0.0 %)	5.8 (+ 0.0 %)	2.6 (+ 0.0 %)
basket-cap min-num-entries	16.1 (+ 12.1 %)	6.0 (+ 2.9 %)	2.7 (+ 5.1 %)
basket-cap min-num-entries	16.0 (+ 11.5 %)	5.7 (- 2.8 %)	2.5 (- 5.6 %)
basket-cap, min-num-entries	14.2 (+ 0.4 %)	6.2 (+ 5.4 %)	2.9 (+ 9.9 %)

Table 4.2: Comparing the maximum proportional set size (PSS) and PHYS/PHYSLITE output file sizes (outFS) for MC jobs while varying the presence of features in Athena PoolWriteConfig.py for 140000 entries.

779

4.2.2 Comparing different basket sizes

789

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 4.3 through Table 4.4. 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 Configs (Data)	Max PSS (MB) ($\Delta\%$ default)	PHYS outFS (GB) ($\Delta\%$)	PHYSLITE outFS (GB) ($\Delta\%$)
(default)	27.9 (+ 0.0 %)	3.3 (+ 0.0 %)	1.0 (+ 0.0 %)
256k_basket	28.2 (+ 1.3 %)	3.3 (- 0.1 %)	1.0 (- 0.3 %)
512k_basket	28.5 (+ 2.2 %)	3.3 (+ 0.0 %)	1.0 (- 0.3 %)
1.3 MB (ROOT MAX)	28.6 (+ 2.7 %)	3.3 (- 0.1 %)	1.0 (- 0.3 %)

Table 4.3: 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 Configs (Data)	$ $ Max PSS (MB) ($\Delta\%$ default)	PHYS outFS (GB) ($\Delta\%$)	PHYSLITE outFS (GB) ($\Delta\%$)
(default)	15.0 (+ 0.0 %)	5.9 (+ 0.0 %)	2.6 (+0.0 %)
256k_basket	15.3 (+ 1.9 %)	5.8 (- 1.4 %)	2.5 (- 3.1 %)
512k_basket	16.4 (+ 8.6 %)	5.7 (- 2.5 %)	2.5 (- 5.1 %)
1.3 MB (ROOT MAX)	16.9 (+ 11.3 %)	5.7 (- 2.8 %)	2.5 (- 5.6 %)

Table 4.4: Comparing the maximum proportional set size (PSS) and PHYS/PHYSLITE output file sizes (outFS) for MC jobs over various Athena configurations for 140000 entries.

"Max PSS" refers to the maximum proportional set size, which is the maximum memory usage of the job. Table 4.3 tells us that with this $t\bar{t}$ data sample, there are marginal changes in both the memory usage for the job and the output file size of the DAODs. Whereas Table 4.4 shows a much more drastic change, with a 5.6% reduction in output file size for the MC PHYSLITE DAOD when compared to the default Athena configuration. While there's a 5.6% reduction in output file size for the MC PHYSLITE DAOD, there's also a 11.3% increase in memory usage.

4.2.3 Monte Carlo PHYSLITE branch comparison

Derivation production jobs work with initially large, memory-consuming branches, com-

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pressing them to a reduced size. These derivation jobs are memory intensive because they 804 first have to load the uncompressed branches into readily-accessed memory. Once they're 805 loaded, only then are they able to be compressed. The compression factor is the ratio of prederivation branch size (Total-file-size) to post-derivation branch size (Compressed-file-size). 807 The compressed file size is the size of the branch that is permanently saved into the DAOD. 808 Branches with highly repetitive data are better compressed than non-repetitive data, 809 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 811 an opportunity to save memory usage during the derivation job. 812

The following tables look into some highly compressible branches that might lead to areas
where simulation might save some space.

Athena v24.0.16 (default) MC branch	Branch size (kB)	Total-file-size (MB)	Compressed-file-size (MB)	Compression factor
PrimaryVerticesAuxDyn.trackParticleLinks	128	2146.2	24.0	89.4
HardScatterVerticesAuxDyn.incomingParticleLinks	128	118.5	1.7	71.6
HLTNav_Summary_DAODSlimmedAuxDyn.linkColNames	128	784.0	11.9	65.7
HardScatterVerticesAuxDyn.outgoingParticleLinks	128	108.6	1.9	58.7
Truth Bosons With Decay Vertices Aux Dyn. incoming Particle Links	96	31.6	0.7	43.5
HLTNav_Summary_DAODSlimmedAuxDyn.linkColClids	128	390.6	10.7	36.6
AnalysisTauJetsAuxDyn.tauTrackLinks	128	75.0	2.0	36.6
HLTNav_Summary_DAODSlimmedAuxDyn.linkColKeys	128	390.6	11.7	33.4
AnalysisJetsAuxDyn.GhostTrack	128	413.8	13.1	31.5
Truth Bosons With Decay Vertices Aux Dyn. outgoing Particle Links	83.5	27.3	0.9	31.0

Table 4.5: Top 10 branches sorted by compression factor, MC PHYSLITE [Athena v24.0.16 default configuration.]

An immediate observation: with the omission of the Athena basket limit (solely relying on ROOTs 1.3MB basket limit), the compression factor increases. This is inline with
the original expectation that an increased buffer size limit correlate to better compression.

Primary Vertices Aux Dyn. track Particle Links is a branch where, among each configuration of
Athena MC derivation, has the highest compression factor of any branch in this dataset.

Athena v24.0.16 (no-lim) MC branch	Branch size (kB)	Total-file-size (MB)	Compressed-file-size (MB)	Compression factor
Primary Vertices Aux Dyn. track Particle Links	1293.5	2145.5	22.9	93.5
HardScatterVerticesAuxDyn.incomingParticleLinks	693.0	118.5	1.3	90.1
HardScatterVerticesAuxDyn.outgoingParticleLinks	635.5	108.5	1.5	74.0
HLTNav_Summary_DAODSlimmedAuxDyn.linkColNames	1293.5	783.5	11.9	65.8
Truth Bosons With Decay Vertices Aux Dyn. incoming Particle Links	96.0	31.6	0.7	43.5
AnalysisTauJetsAuxDyn.tauTrackLinks	447.0	74.9	1.9	39.2
HLTNav_Summary_DAODSlimmedAuxDyn.linkColClids	1293.5	390.3	11.0	35.5
HLTNav_Summary_DAODSlimmedAuxDyn.linkColKeys	1293.5	390.3	11.3	34.5
AnalysisJetsAuxDyn.GhostTrack	1293.5	413.5	13.0	31.9
Truth Bosons With Decay Vertices Aux Dyn. outgoing Particle Links	83.5	27.3	0.9	31.0

Table 4.6: Top 10 branches sorted by compression factor, MC PHYSLITE [Athena v24.0.16 without limit to the basket buffer.]

Athena v24.0.16 (default) MC branch	Branch size (kB)	Total-file-size (MB)	Compressed-file-size (MB)	Compression factor
Primary Vertices Aux Dyn. track Particle Links	128	2146.2	24.0	89.4
HLTNav_Summary_DAODSlimmedAuxDyn.linkColNames	128	784.0	11.9	65.7
AnalysisJetsAuxDyn.GhostTrack	128	413.8	13.1	31.5
HLTNav_Summary_DAODSlimmedAuxDyn.linkColClids	128	390.6	10.7	36.6
HLTNav_Summary_DAODSlimmedAuxDyn.linkColKeys	128	390.6	11.7	33.4
AnalysisJetsAuxDyn.SumPtChargedPFOPt500	128	148.9	7.3	20.5
AnalysisJetsAuxDyn.NumTrkPt1000	128	148.8	8.7	17.2
AnalysisJetsAuxDyn.NumTrkPt500	128	148.8	11.9	12.5
HardScatterVerticesAuxDyn.incomingParticleLinks	128	118.5	1.7	71.6
AnalysisLargeRJetsAuxDyn.constituentLinks	128	111.5	7.1	15.8

Table 4.7: Top 10 branches sorted by total file size in bytes, MC PHYSLITE [Athena v24.0.16 default configuration.]

Athena v24.0.16 (no-lim) MC branch	Branch size (kB)	Total-file-size (MB)	Compressed-file-size (MB)	Compression factor
Primary Vertices Aux Dyn. track Particle Links	1293.5	2145.5	22.9	93.6
HLTNav_Summary_DAODSlimmedAuxDyn.linkColNames	1293.5	783.5	11.9	65.8
AnalysisJetsAuxDyn.GhostTrack	1293.5	413.5	13.0	31.9
HLTNav_Summary_DAODSlimmedAuxDyn.linkColClids	1293.5	390.3	11.0	35.5
HLTNav_Summary_DAODSlimmedAuxDyn.linkColKeys	1293.5	390.3	11.3	34.5
AnalysisJetsAuxDyn.SumPtChargedPFOPt500	905.5	148.8	6.8	21.9
AnalysisJetsAuxDyn.NumTrkPt1000	905	148.8	8.5	17.6
AnalysisJetsAuxDyn.NumTrkPt500	905	148.8	11.8	12.6
HardScatterVerticesAuxDyn.incomingParticleLinks	693	118.5	1.3	90.2
AnalysisLargeRJetsAuxDyn.constituentLinks	950.5	111.4	6.4	17.4

Table 4.8: Top 10 branches sorted by total file size in bytes, MC PHYSLITE [Athena v24.0.16 without limit to the basket buffer.]

Athena v24.0.16 (default) MC branch	Branch size (kB)	Total-file-size (MB)	Compressed-file-size (MB)	Compression factor
Primary Vertices Aux Dyn. track Particle Links	128	2146.2	24.0	89.4
AnalysisJetsAuxDyn.GhostTrack	128	413.8	13.1	31.5
AnalysisJetsAuxDyn.NumTrkPt500	128	148.8	11.9	12.5
HLTNav_Summary_DAODSlimmedAuxDyn.linkColNames	128	784.0	11.9	65.7
HLTNav_Summary_DAODSlimmedAuxDyn.linkColKeys	128	390.6	11.7	33.4
HLTNav_Summary_DAODSlimmedAuxDyn.linkColClids	128	390.6	10.7	36.6
AnalysisJetsAuxDyn.NumTrkPt1000	128	148.8	8.7	17.2
AnalysisJetsAuxDyn.SumPtChargedPFOPt500	128	148.9	7.3	20.5
AnalysisLargeRJetsAuxDyn.constituentLinks	128	111.5	7.1	15.8
HLTNav_Summary_DAODSlimmedAuxDyn.name	128	80.8	4.4	18.4

Table 4.9: Top 10 branches sorted by compressed file size in bytes, MC PHYSLITE [Athena v24.0.16 default configuration.]

Athena v24.0.16 (no-lim) MC branch	Branch size (kB)	Total-file-size (MB)	Compressed-file-size (MB)	Compression factor
PrimaryVerticesAuxDyn.trackParticleLinks	1293.5	2145.5	22.9	93.5
AnalysisJetsAuxDyn.GhostTrack	1293.5	413.5	13.0	31.9
HLTNav_Summary_DAODSlimmedAuxDyn.linkColNames	1293.5	783.5	11.9	65.8
AnalysisJetsAuxDyn.NumTrkPt500	905	148.8	11.8	12.6
HLTNav_Summary_DAODSlimmedAuxDyn.linkColKeys	1293.5	390.3	11.3	34.5
HLTNav_Summary_DAODSlimmedAuxDyn.linkColClids	1293.5	390.3	11.0	35.5
AnalysisJetsAuxDyn.NumTrkPt1000	905	148.8	8.5	17.6
AnalysisJetsAuxDyn.SumPtChargedPFOPt500	905.5	148.8	6.8	21.9
AnalysisLargeRJetsAuxDyn.constituentLinks	950.5	111.4	6.4	17.4
HLTNav_Summary_DAODSlimmedAuxDyn.name	242	80.8	4.5	18.0

Table 4.10: Top 10 branches sorted by compressed file size in bytes, MC PHYSLITE [Athena v24.0.16 without limit to the basket buffer.]

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 areas of optimization for long term storage and better memory usage during derivation.

4.3 Conclusion to derivation job optimization

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Initially, limiting the basket buffer size looked appealing; after the 128 kB basket buffer size limit was set, the compression ratio would begin to plateau, increasing the memory-usage without saving much in disk-usage. The optimal balance is met with the setting of 128 kB basket buffers for derivation production.

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% increase in memory usage could prove a heavy burden (See Tables 4.2 and 4.4).

By looking at the branches per configuration, specifically in MC PHYSLITE output 836 DAOD, highly compressible branches emerge. The branches inside the MC PHYSLITE 837 DAOD are suboptimal as they do not conserve disk space; instead, they consume mem-838 ory inefficiently. As seen from Table 4.5 through 4.10, we have plenty of branches in MC 839 PHYSLITE that are seemingly empty—as indicated by the compression factor being $\mathcal{O}(10)$. 840 Reviewing and optimizing the branch data could further reduce GRID load during DAOD 841 production by reducing the increased memory-usage while keeping the effects of decreased 842 disk-space. 843

CHAPTER 5

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MODERNIZING I/O CI UNIT-TESTS

Athena uses a number of unit tests during the development lifecycle to ensure core I/O functionality does not break. Many of the I/O tests were originally created for the old EDM and haven't been updated to test the xAOD EDMs core I/O functions. The new software developed in this project takes in track information from a unit test using the T/P EDM, writes the data into an example xAOD object to file and reads it back.

5.1 xAOD Test Object

The object used to employ the new unit test is the xAOD::ExampleElectron object, where 852 the xAOD: is a declaration of the namespace and simply identifies the object as an xAOD 853 object. An individual ExampleElectron object only has a few parameters for sake of testing, 854 its transvese momentum, pt, and its charge, charge. A collection of ExampleElectron 855 objects are stored in the ExampleElectronContainer object, which is just a DataVector of 856 ExampleElectron objects.[32] This DataVector<xAOD::ExampleElectron> acts similar to a 857 std::vector<xAOD::ExampleElectron>, but has additional code to handle the separation 858 of interface and auxiliary data storage. 859

The xAOD EDM uses an abstract interface connecting between the DataVector and the auxiliary data, this is the IAuxStore. The function setStore is responsible for ensuring the auxiliary data store is matched with it's corresponding DataVector. Another feature to the xAOD EDM is the ability to have a dynamic store of auxiliary data. This separates the auxiliary data between static and dynamic data stores. Wheree the static data stores

comprise known variables, the dynamic counterpart stores data of variables not declared but that still might be needed by the user. Figure 5.1 illustrates how a simple setup of storing a 866 DataVector of electrons that hold some specific parameters into one IAuxStore while also 867 having a separate IAuxStore specifically for the dynamic attributes.

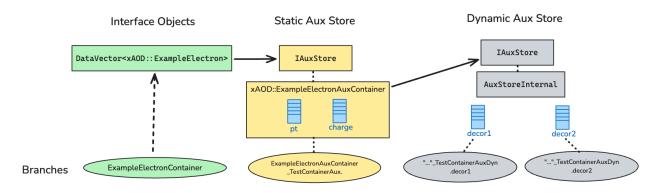


Figure 5.1: The framework between interface objects and the static/dynamic auxiliary data store for a collection of xAOD::ExampleElectrons.

5.2 Unit Tests

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Unit tests are programs that act as a catch during the continuous integration of a codebase 870 and test features that need to remain functional. Athena has a number of unit tests that check every merge request and nightly build for issues in the new code that could break core 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.

Specifically there were no unit tests to handle selection of dynamic attributes, or dec-876 orations, on xAOD objects created during writing and read back. To address this, a new 877 xAOD test object needed to be created and written during a new unit test that fit into the 878 existing unit tests. The list of AthenaPoolExample unit tests that are currently executed 879

during a nightly build can be found in Table 5.1. These tests are executed in this order, as
the objects created in one might be used in proceeding test.

Unit Test	Employed Algorithms
Write	WriteData
ReadWrite	ReadData
Read	ReadData
Copy	None
ReadWriteNext	ReadData, ReWriteData
WritexAODElectron	ReadData, WriteExampleElectron
ReadxAODElectron	ReadExampleElectron

Table 5.1: List of unit tests in the AthenaPoolExample package that are currently executed during a nightly build.

The mechanism for passing a unit test is done automatically by building the framework, running the unit tests, and comparing the diff of the output file to the unit test with a reference file associated with that particular unit test. If the unit test passes, then the diff, a product of the git diff command, will be empty and the unit test will be marked as passing. Conversely, if the unit test fails, then the diff will be non-empty and the unit test will be marked as failing.

5.2.1 WritexAODElectron.py

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The two new tests added to the package were WritexAODElectron and ReadxAODElectron.

During this first unit test, the first algorithm called is to ReadData which reads off all of
the ExampleTrack objects stored in one of the files produced by the ReadWrite unit-test.

Within the python script of the first unit test, the user is able to decide what decorations to
have written to file. This is a part of the OutputStreamCfg parameter, ItemList, wherein
the user specifies the object and its name in the format shown in Figure 5.2.

```
ItemList = [ "ExampleTrackContainer#MyTracks",
    "xAOD::ExampleElectronContainer#TestContainer",
    "xAOD::ExampleElectronAuxContainer#TestContainerAux.-decor2"] )
```

Figure 5.2: WritexAODElectron ItemList for the OutputStreamCfg parameter. Showing how to select dynamic attributes at the CA level.

The header file includes various packages needed by the algorithm, such as data ob-895 jects, Write/ReadHandleKeys, base algorithms that give consistent structure to the algo-896 rithm, and whatever else is required. In the write-algorithm, there are ReadHandleKeys 897 for ExampleTrack objects saved by a prior unit test. For the WriteHandleKeys, there is 898 one for the ExampleElectronContainer and the name given to it is "TestContainer". This 899 "TestContainer" name will be needed for the ReadExampleElectron algorithm as the name 900 is how it's able to refer to the correct ExampleElectronContainer present in the input file. 901 Additionally, a WriteHandleDecorKey for the decoration objects is needed for appending 902 each decoration onto each ExampleElectron object. Figure 5.3 shows the syntax for how 903 these keys would be presently defined.

```
// Read key ExampleTracks
  SG::ReadHandleKey < ExampleTrackContainer > m_exampleTrackKey {
      this, "ExampleTrackKey", "MyTracks"};
  // Write key for the ExampleElectronContainer
  SG::WriteHandleKey <xAOD::ExampleElectronContainer>
      m_exampleElectronContainerKey{this, "ExampleElectronContainerName",
                                   "TestContainer"};
  // Decoration keys
10
  SG::WriteDecorHandleKey < xAOD::ExampleElectronContainer > m_decor1Key {
11
      this, "ExampleElectronContainerDecorKey1", "TestContainer.decor1",
12
      "decorator1 key"};
  SG::WriteDecorHandleKey < xAOD::ExampleElectronContainer > m_decor2Key {
14
      this, "ExampleElectronContainerDecorKey2", "TestContainer.decor2",
      "decorator2 key"};
16
```

Figure 5.3: WriteExampleElectronheader file setup

Then the WriteExampleElectron algorithm is called and takes ExampleTracks, creates an ExampleElectron object and sets the electrons pt to the tracks pt. As shown in Figure

```
auto elecCont = std::make_unique < xAOD::ExampleElectronContainer > ();
auto elecStore = std::make_unique < xAOD::ExampleElectronAuxContainer > ();
elecCont -> setStore(elecStore.get());

SG::ReadHandle < ExampleTrackContainer > trackCont(m_exampleTrackKey, ctx);
elecCont -> push_back(std::make_unique < xAOD::ExampleElectron > ());

for (const ExampleTrack* track : *trackCont) {
    // Take on the pT of the track
    elecCont -> back() -> setPt(track -> getPT());
}

SG::WriteHandle < xAOD::ExampleElectronContainer > objs(
    m_exampleElectronContainerKey, ctx);
ATH_CHECK(objs.record(std::move(elecCont), std::move(elecStore)));
```

Figure 5.4: Algorithm to initialize and write T/P data (ExampleTracks) to an xAOD object container (ExampleElectronContainer).

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5.4, the ExampleElectronContainer and ExampleElectronAuxContainer are created and 907 set to the elecCont and elecStore respectively. The elecCont has an associated aux store, 908 so the setStore function is called with the elecStore pointer. The track container is 909 accessed by using StoreGate's ReadHandle, which associates the m_exampleTrackKey with 910 the ExampleTrackContainer specified in the header file. This is then looped over all elements 911 in the container and the pt of each track is set to the pt of the electron. A WriteHandle, 912 called objs, is then created for the container of ExampleElectrons which is then recorded. 913 Within the same algorithm, the next step is to loop over each of the newly produced 914 ExampleElectrons, accessing the decorations decor1 and decor2, and setting each to an arbitrary float value that are easily identifiable later. Figure 5.5 shows how this is done using two handles for each decoration. Note the difference here using the WriteDecorHandle, 917 where the prior handle type was WriteHandle.

```
SG::WriteDecorHandle < xAOD::ExampleElectronContainer, float > hdl1(
    m_decor1Key,ctx);
SG::WriteDecorHandle < xAOD::ExampleElectronContainer, float > hdl2(
    m_decor2Key,ctx);

for (const xAOD::ExampleElectron* obj : *objs) {
    hdl1(objs) = 123.;
    hdl2(objs) = 456.;
}
```

Figure 5.5: Writing of dynamic variables for each of the ExampleElectron objects.

5.2.2 ReadxAODElectron.py

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The only algorithm called in this test is ReadExampleElectron. The header file for the ReadExampleElectron only creates ReadHandleKey for the container of ExampleElectrons, with the same name from the header of the WriteExampleElectron algorithm header, syntax shown in Figure 5.6. From the source file, we can initialize the ReadHandleKey

```
SG::ReadHandleKey<xAOD::ExampleElectronContainer>
m_exampleElectronContainerKey{this, "ExampleElectronContainerName",
"TestContainer"};
```

Figure 5.6: ReadHandleKey for the container of ExampleElectrons

object by a simple ATH_CHECK(m_exampleElectronContainerKey.initialize()); in the initialize() method. This allows for, when defining the ReadHandle in execute, identifying the correct container defined in the header file. The same can be done for the decoration key, which needs a separate read handle, ReadDecorHandle. Once this is setup, all the read algorithm needs to do is to loop over all the ExampleElectrons in the "TestContainer" and access their p_T and charge.

930 5.3 Results

This project sought to replace existing unit tests that created ExampleHits, T/P EDM objects, to be written and read back. An independent xAOD object, ExampleElectron, was created and implemented into two new unit tests that write and read ExampleElectron objects along with their chosen dynamic attributes. A merge request was created, approved, and merged into the Athena software framework. Future work can be done to fully modernize the package these unit tests reside, AthenaPoolExampleAlgorithms, including unit tests that test core functionality of AthenaMT/AthenaMP, and newer storage formats like RNTuple.

CHAPTER 6

CONCLUSION

The work done for this thesis was primarily motivated to find avenues to optimize resource usage for GRID I/O operations. The toy model testing allowed us to create branches
with data similar compression ratios to real and simulated data, allowing to investigate the
hypothesis that modifying the basket buffer limit had an effect on disk and memory usage.

It led to the conclusion that, upon investigating with real data and real MC simulation, that
there might be an avenue to look at both ROOT and Athena to limit basket sizes.

Modifying the basket buffer sizes at the Athena level shows there was a balance was struck when using the Athena basket buffer size limited to 128 kB between memory-usage and the size of the DAOD to be saved long-term. Removing the basket buffer size limit, the 5.5% saving in PHYSLITE MC disk-usage at the expense of an 11% increase in memory-usage could be a trade-off worth making in some scenarios. A class of potentially unoptimized AOD branches in MC simulated data was also brought to light during this study. The leading indicator to potential optimization is the highly compressible nature of these branches post-derivation. Further work could be done to look into these AOD branches to identify areas where further work can be done to reduce the overall AOD footprint.

The xAOD EDM comes with a number of new additions to bring about optimization the future of analysis work at the ATLAS experiment. Integrating the new features into a few comprehensive unit tests allow for the nightly CI builds to catch any issues that break core I/O functionality as it pertains to the xAOD EDM, which has not been done before. These new unit-tests exercise reading and writing select decorations ontop of the already existing data structures attached to an example object called ExampleElectron.

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APPENDIX A DERIVATION PRODUCTION DATA

A.1 Derivation production datasets

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

```
1065 data22_13p6TeV:data22_13p6TeV.00428855.physics_Main.merge.AOD.

10672 r14190_p5449_tid31407809_00
```

```
was ran with the input files
```

1062

1076

1082

```
1070
1071 1 AOD .31407809 . _000894 . pool . root . 1
1072 2 AOD .31407809 . _000895 . pool . root . 1
1073 3 AOD .31407809 . _000896 . pool . root . 1
1074 4 AOD .31407809 . _000898 . pool . root . 1
```

Similarly, the MC derivation job, comes from the dataset

```
1077

1078 1 mc23_13p6TeV:mc23_13p6TeV.601229.PhPy8EG_A14_ttbar_hdamp258p75_

1079 2 SingleLep.merge.AOD.e8514_e8528_s4162_s4114_r14622_r14663_

1080 3 tid33799166_00
```

was ran with input files

```
1083
1084 1 AOD .33799166._000303.pool.root.1
1085 2 AOD .33799166._000304.pool.root.1
1086 3 AOD .33799166._000305.pool.root.1
1087 4 AOD .33799166._000306.pool.root.1
1088 5 AOD .33799166._000307.pool.root.1
1089 6 AOD .33799166._000308.pool.root.1
```

APPENDIX B

1091

1092

ATHENA CONFIGURATION JOB

A general Athena application using ComponentAccumulator written in pseudocode would take the form:

```
1096
        # Import Packages
1097
        from AthenaConfiguration.AllConfigFlags import initConfigFlags
1098 2
        from AthenaConfiguration.ComponentFactory import CompFactory
1099
        from OutputStreamAthenaPool.OutputStreamConfig import OutputStreamCfg,
1100
         outputStreamName
1101
1102
        outputStreamName = "StreamA"
1103 6
        outputFileName = "output.root"
1104
1105
        # Setup flags
1106 9
        flags = initConfigFlags()
1107.0
1108
        flags.Input.Files = ["input.root"]
        flags.addFlag(f"Output.{streamName}FileName", outputFileName)
1109
        flags.lock()
1110
111114
        # Main Service(s)
1112
        from AthenaConfiguration.MainServicesConfig import MainServicesCfg
1113.6
        acc = MainServicesCfg( flags )
11147
1115.8
        # Add algorithms to the accumulator
1116.9
        acc.addEventAlgo( CompFactory.MyAlgorithm(MyParameters) )
111720
1118
        import sys
11192
        sc = acc.run(flags.Exec.MaxEvents)
1120/3
1121
```

The acc is the ComponentAccumulator, so here the user might have more than one Algorithm it needs to call, but each one would have a separate .addEventAlgo call. When flag.lock() is called, any previously established flags will be set in place and unable to be changed.