

ABSTRACT

1 OPTIMIZATION OF DERIVATION JOBS AND MODERNIZATION OF NIGHTLY CI 2 BUILD I/O TESTS FOR THE ATLAS EXPERIMENT

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7 High-Luminosity LHC (HL-LHC) is a phase of the LHC that is expected to run toward
8 the end of the decade. With this comes an increase in data taken per year that current
9 software and computing infrastructure, including I/O, is not prepared to handle. The ATLAS
10 experiment's Software Performance Optimization Team has efforts in developing the Athena
11 software framework that is scalable in performance and ready for wide-spread use during
12 Run-3 and HL-LHC data ready to be used for Run-4. It's been shown that the storage bias
13 for TTree's during derivation production jobs can be improved upon compression and stored
14 to disk by about 4-5% by eliminating the basket capping, with a simultaneous increase in
15 memory usage by about 11%. Additionally, job configuration allows opportunity to improve
16 many facets of the ATLAS I/O framework.

17 Athena and software it depends on are updated frequently, and to synthesize changes
18 cohesively there are scripts, unit tests, that run which test core I/O functionality. This
19 thesis also addresses a project to add a handful of I/O unit tests that exercise features
20 exclusive to the new xAOD Event Data Model (EDM) such as writing and reading object
21 data from the previous EDM using transient and persistent data. These new unit tests also
22 include and omit select dynamic attributes to object data.

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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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25 Here's where you acknowledge folks who helped. Here's where you acknowledge folks
26 who helped. Here's where you acknowledge folks who helped. Here's where you acknowledge
27 folks who helped.

DEDICATION

28

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 explores the fundamental constituents of matter and the forces governing their interactions. The field started as studies in electromagnetism, 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 results, 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 identify interesting interactions and optimize the storage and processing of this data. This thesis investigates software performance optimization of the ATLAS experiment at CERN. Specifically, ways to modernize and optimize areas of the software framework, Athena, to improve input/output (I/O) during derivation production and create new tests that catch when specific core I/O functionality is broken.

1.2 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.[13] The ATLAS experiment, shown in Figure 1.2, 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.[15] The ATLAS

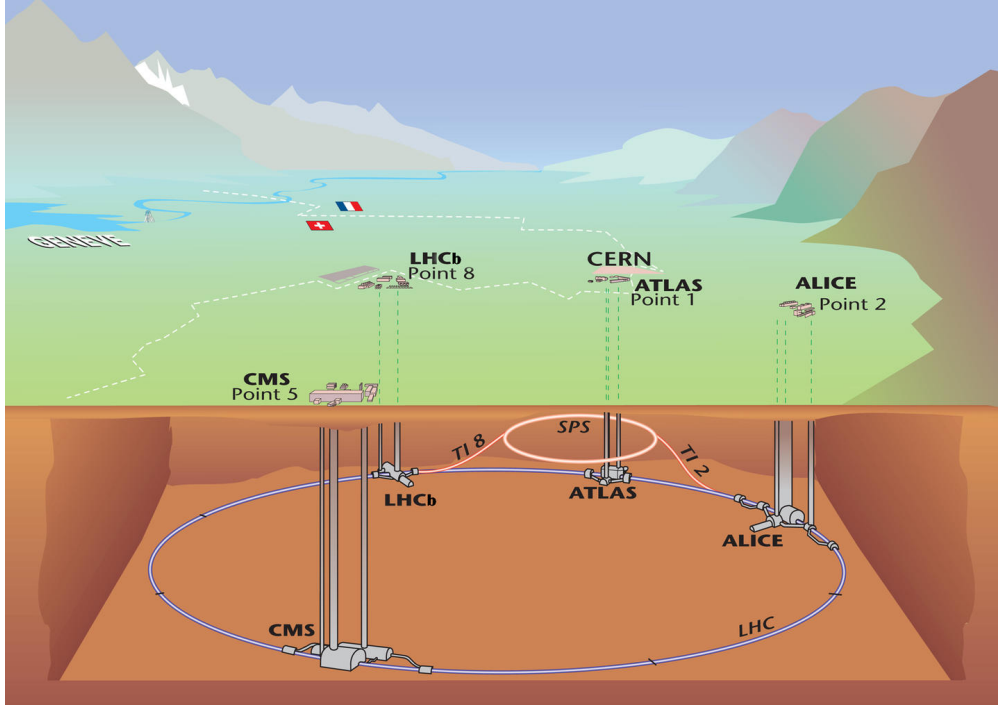


Figure 1.1: Illustration of the LHC experiment sites on the France-Switzerland border. [5]

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.[1] It has over 92 million pixels and is radiation hard to aid in particle track and vertex reconstruction. When charged particles pass through a pixel sensor, it ionizes the one-sided doped-silicon wafer to produce an excited electron which will then occupy the conduction band of the semiconductor producing an electron-hole pair, leaving the valence band empty.[10] 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 of an electric field, which will induce drifting of the electron-hole pair, drifting that will generate the electric current to be measured.

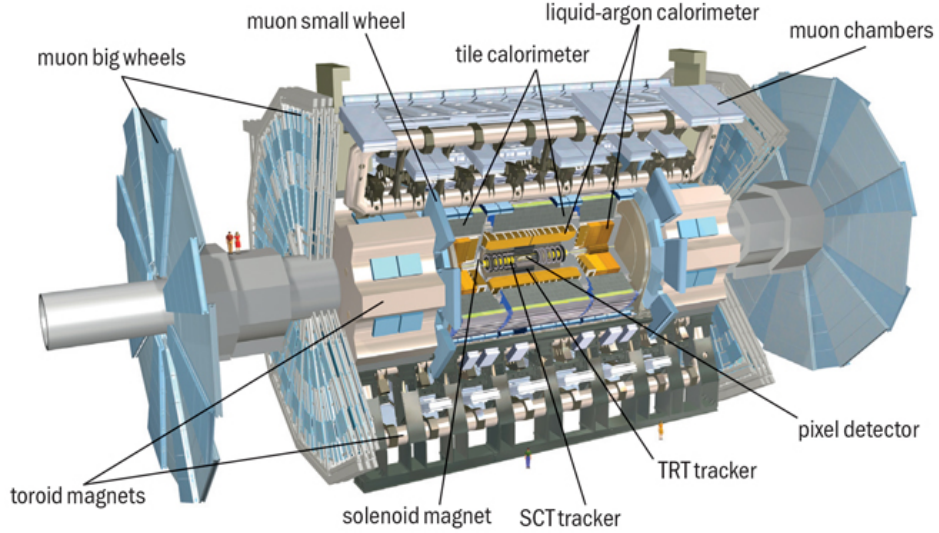


Figure 1.2: Overview of the ATLAS detectors main components. [7]

Surrounding the pixel detector is the SemiConductor Tracker (SCT), which uses 4,088 modules of 6 million implanted silicon readout strips.[2] Both the pixel detector and SCT measure the path particles take, called tracks. While the pixel detector has measurement precision up to $10\mu m$, the SCT has 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. 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.[6] The straws are filled with a gas mixture of $70\%Xe + 27\%CO_2 + 3\%O_2$. Its measurement precision is around $170\mu m$. Particles with relativistic velocities have higher Lorentz γ -factors (see Eq. (1.1)). 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. [14]

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

There are two main calorimeters for ATLAS, the Liquid Argon (LAr) calorimeter and the Tile Hadronic calorimeter. The LAr calorimeter surrounds the inner detector and measures the energy deposits of electrons, photons and hadrons (quark bound states, such as baryons qqq and mesons $q\bar{q}$). It layers various metals to intercept the incoming particles to produce a shower of lower energy particles. The lower energy particles then ionize the liquid argon that fill the barrier in between the metal layers to produce a current that can be read out. The Tile calorimeter surrounds the LAr calorimeter and is the largest part of the ATLAS detector weighing in around 2900 tons. Particles then traverse through the layers of steel and plastic scintillating tiles. When a particle hits the steel, a cascade of secondary particles is generated, and the plastic scintillators will produce photons whose current can be measured.

1.3 ATLAS Trigger and Data Acquisition

The LHC produces pp -collisions at a rate of 40 MHz, each collision is an “event”. The ATLAS Trigger system is responsible for quickly deciding what events are interesting for physics analysis. The Trigger system is divided into the first- and second-level triggers and when a particle activates a trigger, the trigger makes a decision to tell the Data Acquisition System (DAQ) to save the data produced by the detector. The first-level trigger is a hardware trigger that decides, within $2.5\mu s$ after the event, if it’s a good event to put into a storage buffer for the second-level trigger. The second-level trigger is a software trigger that decides within $200\mu s$ and uses around 40,000 CPU-cores and analyses the event to decide if it is worth keeping. The second-level trigger selects about 1000 events per second to keep and store long-term. [4] The data taken by this Trigger/DAQ system is raw and not yet in a state that is ready for analysis, but it is ready for the reconstruction stage.

171 The amount of data taken at ATLAS is substantial. ATLAS sees more than 3.2 PB of
172 raw data each year, each individual event being around 1.6 MB. [15] All of the data produced
173 by LHC experiments, especially ATLAS, has to be sent to the LHC Computing Grid (LCG).
174 The increase in data means more resources from the Grid will be needed, so optimization is
175 an essential part of ensuring scalability of the data able to be taken in by the experiment.
176 Reconstructed AOD are then processed through derivation jobs that reduced AODs from
177 $\mathcal{O}(1)$ MB per event to $\mathcal{O}(10)$ kB per event, creating Derived AOD (DAOD).

CHAPTER 2

I/O TOOLS

The Trigger/DAQ system sends and saves data from the detector to a persistent data storage solution. It's at this stage where the data isn't yet ready for an effective analysis, so 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 computation power and Athena is the software framework that plays a significant role in this process. This chapter will cover the software tools used by ATLAS

2.1 Athena and ROOT

Athena is the open-source software framework for the ATLAS experiment.[8] It uses 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.[9] It also provides some in-house based analysis tools as well as tools for specifically ROOT based analysis.

ROOT is an open-source software framework used for high-energy physics analysis at CERN.[17] 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.

2.1.1 Continuous Integration (CI) and Development

CI is a software development practice where new code is tested and validated upon each 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 the new code is compatible with the existing codebase.

Athena is developed with CI by using an instance of Jenkins, called ATLAS Robot, to build and test 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 detection of issues before the nightly build is compiled and tested.

2.2 TTree Object

A TTree is a ROOT object that organizes physically distinct types of event data into branches. 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.

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. [18]

`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

A derivation production job takes AODs, which comes from the reconstruction step at $\mathcal{O}(1 \text{ MB})$ per event, and creates a derived AOD (DAOD) which sits at $\mathcal{O}(10 \text{ kB})$ per event. Derivation production is a necessary step to make all data accessible and useful for physicists doing analysis. While derivations are reduced AODs, they often contain additional information useful for analysis, such as jet collections and high-level discriminants.[16] Athena provides two types of output files from a derivation job, PHYS and PHYSLITE. 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.

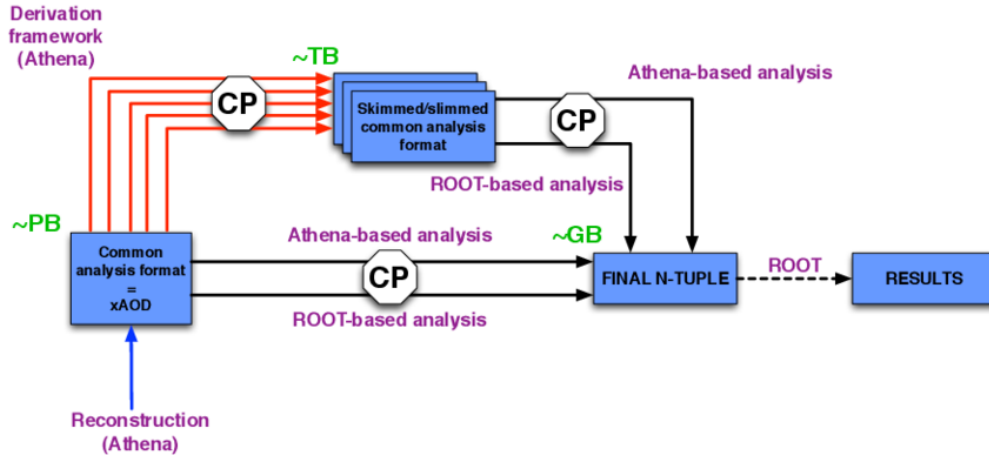


Figure 2.1: Derivation production from Reconstruction to Final N-Tuple[12]

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

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 nature of AOD. The AOD at this point was converted into an ntuple based format called D3PDs. While this conversion allowed for fast readability and partial read for efficient analysis in ROOT, it left the files disconnected from the reconstruction tools found in Athena.[3] 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. Before the successor to the T/P EDM was created, ATLAS physicists would convert

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

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. xAOD EDM has the ability to add and remove variables at runtime, these variables are called “decorations.”

CHAPTER 3

TOY MODEL BRANCHES

Building a toy model for derivation production jobs offers a simplified framework to effectively simulate and analyze the behavior of real and Monte Carlo (MC) data under 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 will yield compression ratios closer to real and MC data. Replicating this mixture in a branch give us an effective model that resemble how current derivation jobs act on real and MC simulated data. These toy model mixtures provide an avenue to test opportunities for optimizing the memory and storage demands of the GRID by first looking at limiting basket sizes and their effects on compression of branches.

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 AOD. This original model had four distinct branches, each with a set number of events

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

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

289 The following function `VectorTree()` is the main function in this code. What is needed
 290 first is an output file, which will be called `VectorTreeFile.root`, and the name of the tree
 291 can simply be `myTree`. Initializing variables start with the total number of events in the
 292 branch, i.e. the number of times a branch is filled with the specified numbers per vectors,
 293 N. Additionally the branches have a number of floats per vector, this size will need to be
 294 defined as `size_vec_0`, `size_vec_1`, etc. The actual vectors that are being stored into each
 295 branch need to be defined as well as the temporary placeholder variable for our randomized
 296 floats, `vec_tenX` and `float_X` respectively.

```

297 1  void VectorTree() {
298 2      ...
299 3      const int N = 1e4; // N = 10000, number of events
300 4      // Set size of vectors with 10^# of random floats
301 5      int size_vec_0 = 1;
302 6      int size_vec_1 = 10;
303 7      int size_vec_2 = 100;
304 8      int size_vec_3 = 1000;
305 9
306 0      // vectors
307 1      std::vector<float> vec_ten0; // 10^0 = 1 entry
308 2      std::vector<float> vec_ten1; // 10^1 = 10 entries
309 3      std::vector<float> vec_ten2; // 10^2 = 100 entries
310 4      std::vector<float> vec_ten3; // 10^3 = 1000 entries
311 5
312 6      // variables

```

```

313 7     float float_0;
314 8     float float_1;
315 9     float float_2;
316 0     float float_3;
317 1     ...
318 2 }

```

319 From here, initialize the branches so each one knows where its vector pair resides in
320 memory.

```

321 1 void VectorTree() {
322 2     ...
323 3     // Initializing branches
324 4     std::cout << "creating branches" << std::endl;
325 5     tree->Branch("branch_of_vectors_size_one", &vec_ten0);
326 6     tree->Branch("branch_of_vectors_size_ten", &vec_ten1);
327 7     tree->Branch("branch_of_vectors_size_hundred", &vec_ten2);
328 8     tree->Branch("branch_of_vectors_size_thousand", &vec_ten3);
329 9     ...
330 0 }

```

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

```

332 1 void VectorTree() {
333 2     ...
334 3     tree->SetAutoFlush(0);
335 4     ...

```

336 Disabling `AutoFlush` allows for more consistent compression across the various sizes of branch
337 baskets. The toy model needed this consistency more than the later tests as these early tests
338 were solely focused on mimicking data procured by the detector and event simulation. The
339 derivation production jobs tested in Chapter 4 were tested with `AutoFlush` enabled because
340 those tests are not as concerned with compression as they are with memory and disk usage.

341 Following branch initialization comes the event loop where data is generated and emplaced
 342 into vectors.

```

343 1  void VectorTree() {
344 2      ...
345 3      // Events Loop
346 4      std::cout << "generating events..." << std::endl;
347 5      for (int j = 0; j < N; j++) {
348 6          // Clearing entries from previous iteration
349 7          vec_ten0.clear();
350 8          vec_ten1.clear();
351 9          vec_ten2.clear();
352 0          vec_ten3.clear();
353 1
354 2          // Generating vector elements, filling vectors
355 3          // Fill vec_ten0
356 4          // Contents of the vector:
357 5          //     {float_0}
358 6          //     Only one float of random value
359 7          float_0 = gRandom->Rndm() * 10; // Create random float value
360 8          vec_ten0.emplace_back(float_0); // Emplace float into vector
361 9
362 0          // Fill vec_ten1
363 1          // Contents of the vector:
364 2          //     {float_1_0, ... , float_1_10}
365 3          //     Ten floats, each float is random
366 4          for (int n = 0, n < size_vec_1; n++) {
367 5              float_1 = gRandom->Rndm() * 10;
368 6              vec_ten1.emplace_back(float_1);
369 7          }
370 8

```

```

3719 // Fill vec_ten2
3720 // Contents of the vector:
3731 // {float_2_0, ... , float_2_99}
3742 // Hundred floats, each float is random
3753 for (int a = 0, a < size_vec_2; a++) {
3764     float_2 = gRandom->Rndm() * 10;
3775     vec_ten2.emplace_back(float_2);
3786 }
3797
3808 // Fill vec_ten3
3819 // Contents of the vector:
3820 // {float_3_0, ... , float_3_999}
3831 // Thousand floats, each float is random
3842 for (int b = 0, b < size_vec_3; b++) {
3853     float_3 = gRandom->Rndm() * 10;
3864     vec_ten3.emplace_back(float_3);
3875 }
3886 tree->Fill(); // Fill our TTree with all the new branches
3897 }
3908 // Saving tree and file
3919 tree->Write();
3920 ...
3931 }

```

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

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

```

399 1 void VectorTree() {

```

```

400 2      ...
401 3
402 4      // Look in the tree
403 5      tree->Scan();
404 6      tree->Print();
405 7
406 8      myFile->Save();
407 9      myFile->Close();
408 0  }
409 1
410 2  int main() {
411 3      VectorTree();
412 4      return 0;
413 5  }

```

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

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

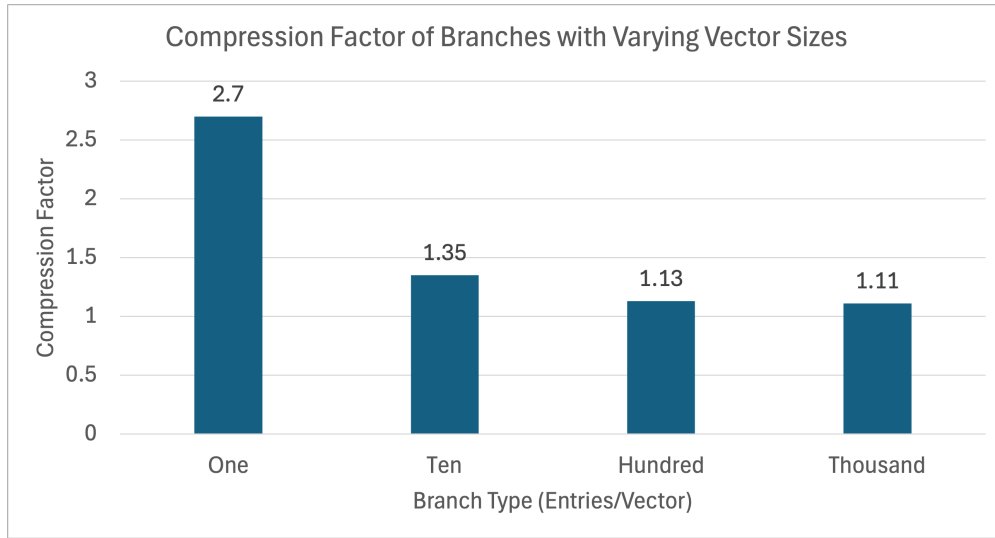


Figure 3.1: Compression factors of $N = 1000$ entries per branch with random-valued vectors of varying size.

3.1.2 Mixed-Random Float Branches

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 $N = 10^5$, or from 10,000 to 100,000. Mixing of random floats and repeated integer values takes the same script structure as Section § 3.1.1 but adjusts the event generation loop.

```

433 1 void VectorTree() {
434 2     ...
435 3     // Events Loop
436 4     for (int j = 0; j < N; j++) {
437 5         // Clearing entries from previous iteration
438 6         vec_ten0.clear();

```

```

439 7     vec_ten1.clear();
440 8     vec_ten2.clear();
441 9     vec_ten3.clear();
442 0
443 1     // Generating vector elements, filling vectors
444 2     // Generating vec_ten0
445 3     // Contents of the vector:
446 4     //     {float_0}
447 5     //     Only one float of random value
448 6     // And since there's only one entry, we don't mix the entries.
449 7     float_0 = gRandom->Gaus(0, 1) * gRandom->Rndm();
450 8     vec_ten0.emplace_back(float_0);
451 9
452 0
453 1     // Generating vec_ten1
454 2     // Contents of the vector:
455 3     //     {float_1_0, float_1_1, float_1_2, float_1_3, float_1_4, 1,
456 4     1, 1, 1, 1}
457 5     //     5 floats of random values, 5 integers of value 1.
458 6     for (int b = 0; b < size_vec_1; b++) {
459 7         if (b < size_vec_1 / 2) {
460 8             float_1 = gRandom->Rndm() * gRandom->Gaus(0, 1);
461 9             vec_ten1.emplace_back(float_1);
462 0         } else {
463 1             float_1 = 1;
464 2             vec_ten1.emplace_back(float_1);
465 3         }
466 4     }
467 5
468 6     // Generating vec_ten2
469 7     // Contents of the vector:

```

```

470:7 // {float_2_0, ... ,float_2_49, 1, ... , 1}
471:8 // 50 floats of random values, 50 integers of value 1.
472:9 for (int c = 0; c < size_vec_2; c++) {
473:0     if (c < size_vec_2 / 2) {
474:1         float_2 = gRandom->Rndm() * gRandom->Gaus(0, 1);
475:2         vec_ten2.emplace_back(float_2);
476:3     } else {
477:4         float_2 = 1;
478:5         vec_ten2.emplace_back(float_2);
479:6     }
480:7 }
481:8
482:9 // Generating vec_ten3
483:0 // Contents of the vector:
484:1 // {float_3_0, ... , float_3_499, 1, ... , 1}
485:2 // 500 entries are floats of random values,
486:3 // 500 entries are integers of value 1.
487:4 for (int d = 0; d < size_vec_3; d++) {
488:5     if (d < size_vec_3 / 2) {
489:6         float_3 = gRandom->Rndm() * gRandom->Gaus(0, 1);
490:7         vec_ten3.emplace_back(float_3);
491:8     } else {
492:9         float_3 = 1;
493:0         vec_ten3.emplace_back(float_3);
494:1     }
495:2 }
496:3 tree->Fill(); // Fill our TTree with all the new branches
497:4 }
498:5 // Saving tree and file
499:6 tree->Write();
500:7 ...

```

5018 }

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

509 Figure 3.2 shows the difference between compression between the two mixtures. When
 510 the number of events is increased from $N = 10^5$ to $N = 10^6$, branches where only half of the
 511 mixture is random data become larger and the branches with more vectors per entry become
 512 more difficult to compress. Figure 3.3 shows a compression ratio hovering around 3 for the
 513 larger branches, whereas Figure 3.2 shows the same branches hovering around 2.

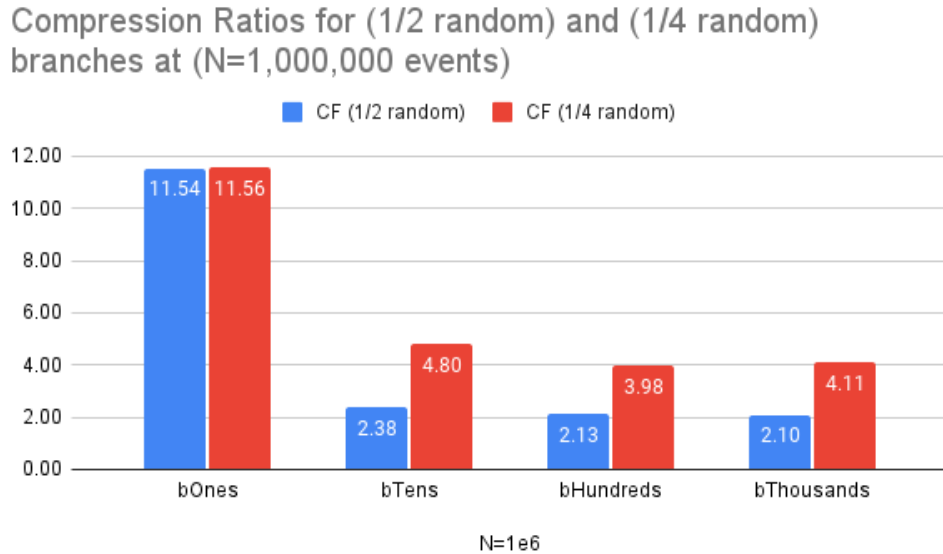


Figure 3.2: Compression Ratios for ($\frac{1}{2}$ random) and ($\frac{1}{4}$ random) branches at ($N = 10^6$ events)

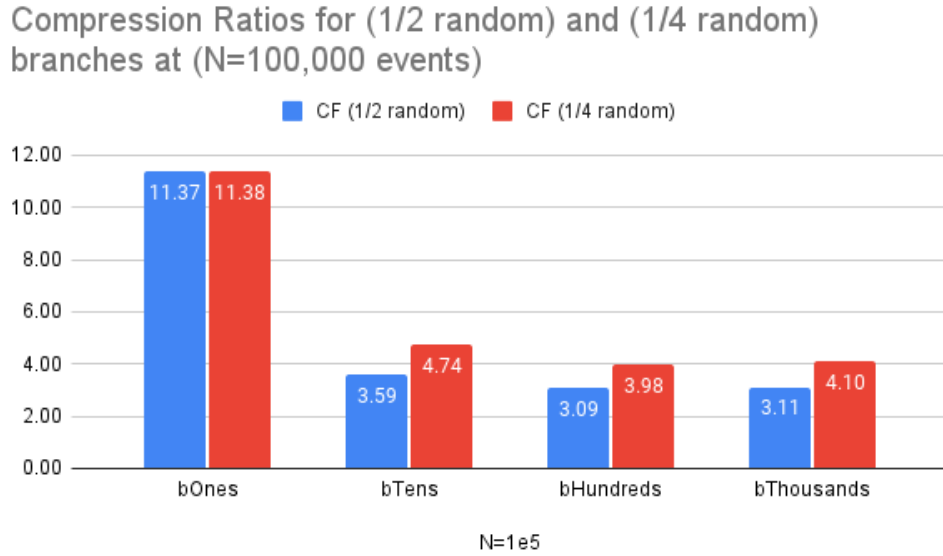


Figure 3.3: Compression Ratios for ($\frac{1}{2}$ random) and ($\frac{1}{4}$ random) branches at ($N = 10^5$ events)

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. Here is where tuning the basket size can begin to start.

3.2 Basket-Size Investigation

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 sizes was done at the script level with a simple setting after the branch initialization and before the event loop the following code:

```
int basketSize = 8192000;
tree->SetBasketSize(" ", basketSize);
```

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

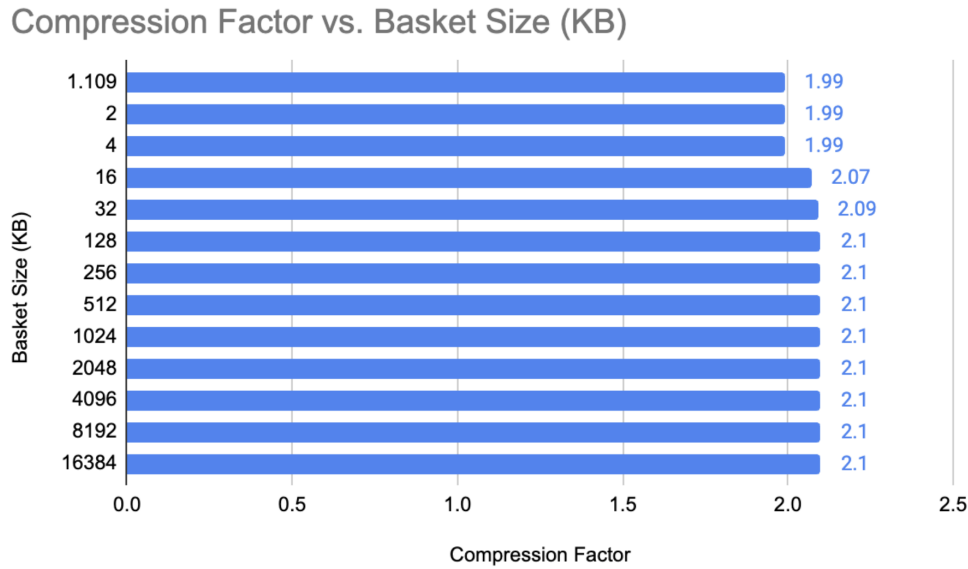


Figure 3.4: Compression Factors vs Branch Size (1/2 Mixture $N = 10^6$ events)

529 Figure 3.4 and Figure 3.5 is the first indication that the lower basket sizes are too small
 530 to effectively compress the data. For baskets smaller than 16 kB, it is necessary to have as
 531 many baskets as events to store all the data effectively. For a mixed-content vector with one
 532 thousand entries, containing 500 floats and 500 integers (both are 4 bytes each), its size is
 533 approximately 4 kB. ROOT creates baskets of at least the size of the smallest branch entry,
 534 in this case the size of a single vector. So even though the basket size was set to 1 or 2 kB,
 535 ROOT created baskets of 4 kB. These baskets ≤ 4 kB have a significantly worse compression
 536 than the baskets ≥ 4 kB in size, so the focus was shifted toward baskets. Once the basket

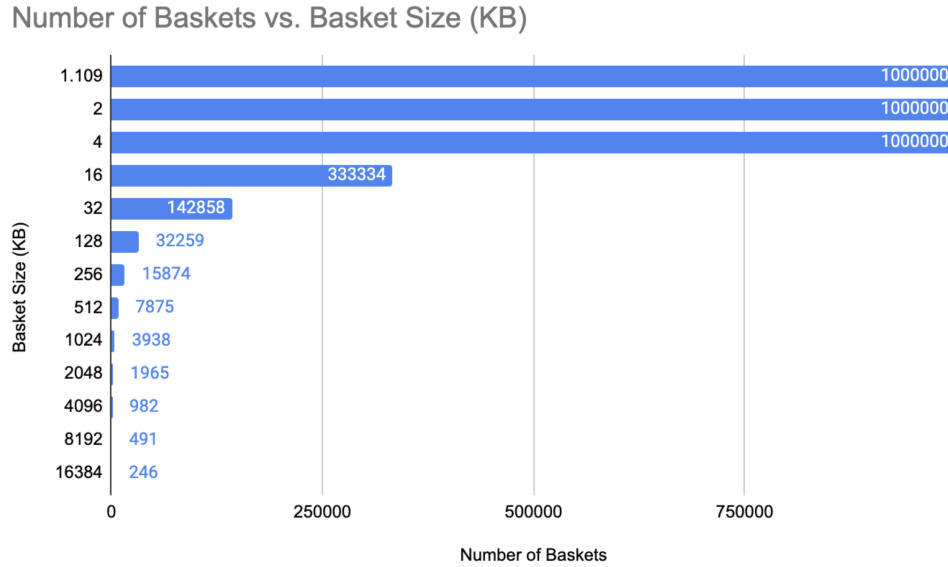


Figure 3.5: Number of Baskets vs Branch Size (1/2 Mixture $N = 10^6$ events)

size is larger than the size of a single vector, more than one vector can be stored in a single basket and the total number of baskets is reduced.

There were more variations in the data that were looked at. For instance, looking further into the types of mixtures and how those mixtures would affect compression are shown in Figure 3.6. Another instance looked into the same mixtures but decreasing the precision of the floating point values that we used from the standard 32 floating-point precision to 16 and 8 which made 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.

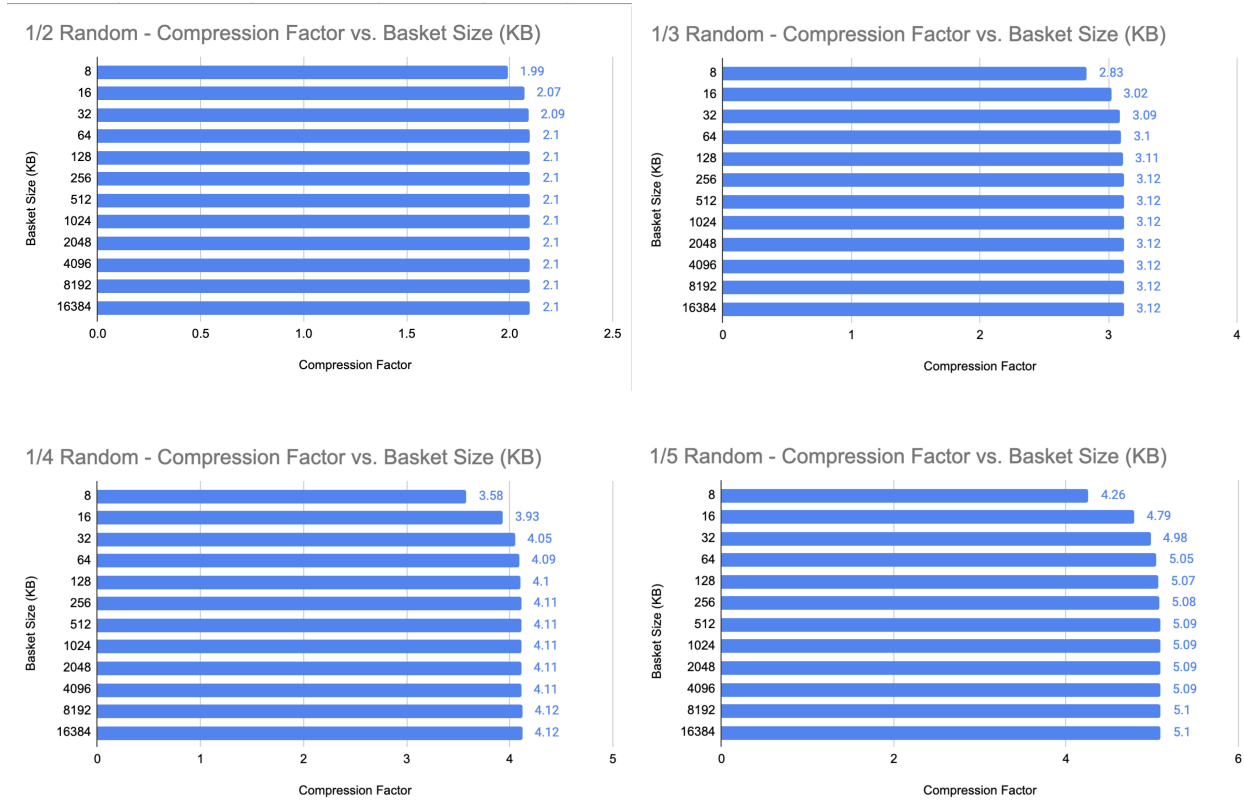


Figure 3.6: Varying Mixtures in 8 point precision - Number of Baskets vs Branch Size ($N = 10^6$ events)

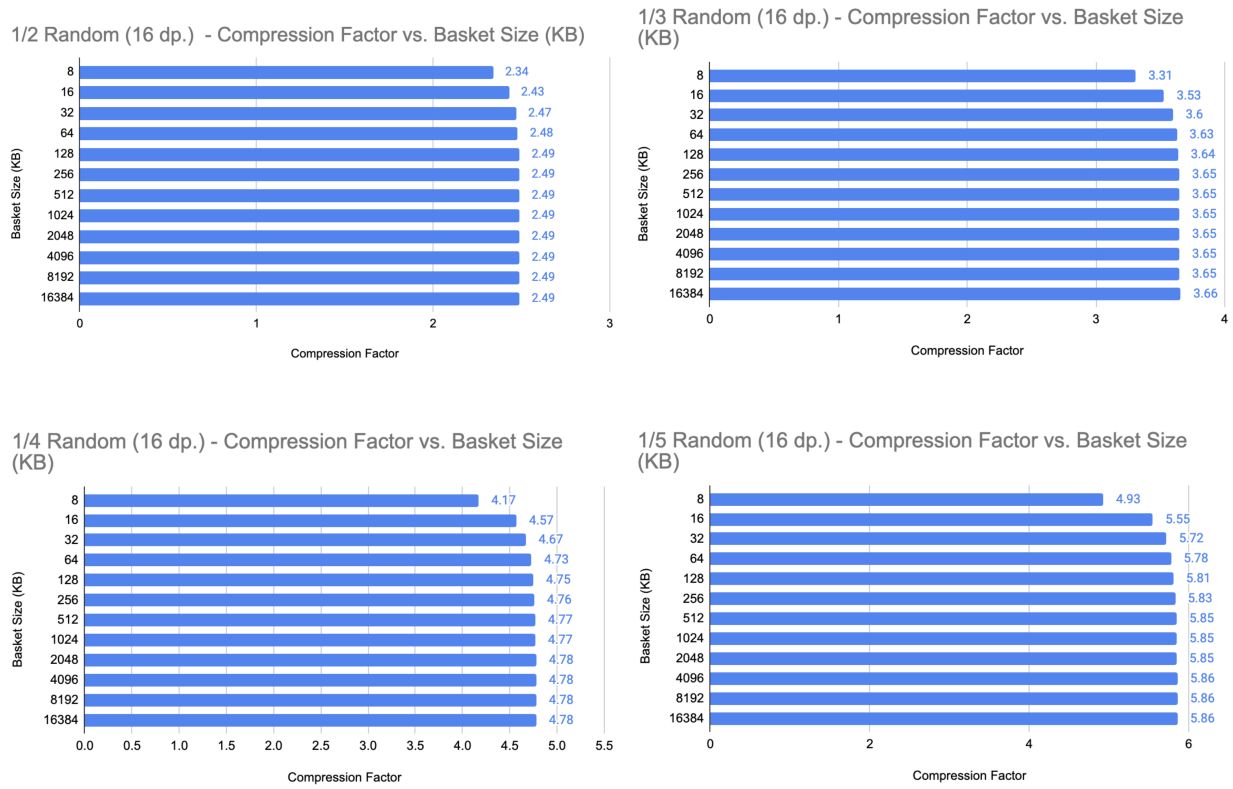


Figure 3.7: Varying Mixtures in 16 point precision - Number of Baskets vs Branch Size ($N = 10^6$ events)

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 Section §4.3, 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 128×1024 bytes
2. “*no-lim*” - Removing the Athena basket limit, the ROOT imposed 1.3 MB limit still remains
3. “*256k*” - Limit basket buffer to 256×1024 bytes
4. “*512k*” - Limit basket buffer to 512×1024 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. [11]

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 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 elimination of the “min-number-entries” we assume the

minimum number of entries per branch should be kept at 10 and left alone. Table 4.2 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 4.3 through Table 4.10. 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 configurations (Data) | Max PSS (MB) ($\Delta\%$ default) | PHYS outFS (GB) ($\Delta\%$) | PHYSLITE outFS (GB) ($\Delta\%$) |
|------------------------------|------------------------------------|--------------------------------|------------------------------------|
| (default) | 27.8591 (+ 0.00 %) | 3.2571 (+ 0.00 %) | 1.0334 (+ 0.00 %) |
| no_limit | 28.6432 (+ 2.74 %) | 3.2552 (- 0.06 %) | 1.0302 (- 0.31 %) |
| 256k_basket | 28.2166 (+ 1.27 %) | 3.2553 (- 0.05 %) | 1.0303 (- 0.30 %) |
| 512k_basket | 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.

| Athena configurations (Data) | Max PSS (MB) ($\Delta\%$ default) | PHYS outFS (GB) ($\Delta\%$) | PHYSLITE outFS (GB) ($\Delta\%$) |
|------------------------------|------------------------------------|--------------------------------|------------------------------------|
| (default) | 15.00 (+ 0.00 %) | 5.88 (+ 0.00 %) | 2.59 (+ 0.00 %) |
| no_limit | 16.90 (+ 11.27 %) | 5.72 (- 2.80 %) | 2.45 (- 5.55 %) |
| 256k_basket | 15.28 (+ 1.87 %) | 5.80 (- 1.35 %) | 2.51 (- 3.11 %) |
| 512k_basket | 16.41 (+ 8.60 %) | 5.74 (- 2.46 %) | 2.46 (- 5.11 %) |

Table 4.4: Athena v24.0.16: Comparing the maximum proportional set size (PSS) and PHYS/PHYSLITE output file sizes (outFS) for MC jobs over various Athena configurations for 140000 entries.

4.3.3 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?)

| 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 |
| TruthBosonsWithDecayVerticesAuxDyn.incomingParticleLinks | 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 |
| TruthBosonsWithDecayVerticesAuxDyn.outgoingParticleLinks | 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.]

| 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 |
| 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 |
| TruthBosonsWithDecayVerticesAuxDyn.incomingParticleLinks | 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 |
| TruthBosonsWithDecayVerticesAuxDyn.outgoingParticleLinks | 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 |
|---|------------------|----------------------|---------------------------|--------------------|
| PrimaryVerticesAuxDyn.trackParticleLinks | 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.SumPtChargedPFOp500 | 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 |
|---|------------------|----------------------|---------------------------|--------------------|
| PrimaryVerticesAuxDyn.trackParticleLinks | 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.SumPtChargedPFOp500 | 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 |
|---|------------------|----------------------|---------------------------|--------------------|
| PrimaryVerticesAuxDyn.trackParticleLinks | 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.]

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. *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 of derivation jobs.

4.3.4 Conclusion to derivation job optimization

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 2 and 4).

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 $\mathcal{O}(10)$. 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.

CHAPTER 6

CONCLUSION

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 struck

This study also illuminated the possibility at a class of unoptimized branches in MC simulated data, from which it was not clear

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 on top of the already existing data structures attached to an example object called `ExampleElectron`.

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714

APPENDIX

715

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

```
data22_13p6TeV:data22_13p6TeV.00428855.physics_Main.merge.AOD.
r14190_p5449_tid31407809_00
```

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.PyPy8EG_A14_ttbar_hdamp258p75_
SingleLep.merge.AOD.e8514_e8528_s4162_s4114_r14622_r14663_
tid33799166_00
```

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
```