

ABSTRACT

RNTUPLE FOR ATLAS ANALYSIS WORKFLOWS

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RNTuple is the new data storage format set to replace TTree at the start of the High-Luminosity LHC. An investigation was conducted to evaluate how analysis workflows for ATLAS researchers will change with RNTuple, using reading speed, writing speed, disk space, and memory consumption as metrics. In this study, improvements in all metrics were observed using converted RNTuple inputs from ATLAS Open Data, compared to their TTree equivalents. Additionally, RNTuples produced with the LZ4 compression algorithm were generated and compared with those produced using ZSTD. Finally, two new versions of the Analysis Grand Challenge (AGC) using ATLAS Open Data were completed for TTree and RNTuple inputs with RDataFrame in Python. This constitutes the first implementation of an end-to-end analysis completed using RNTuple.

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RNTUPLE FOR ATLAS ANALYSIS WORKFLOWS

BY

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DEDICATION

36

Para mis padres, con toda mi gratitud por su amor y apoyo.

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CHAPTER 1

113

INTRODUCTION

114 Our current understanding of the building blocks of our universe is summarized with
115 one model, called the Standard Model (SM) [1]. From the way we power our cities, to the
116 particles that hold them together, the SM explains how the basic building blocks of matter
117 interact, governed by fundamental forces: electromagnetism, the strong force and the weak
118 force. Yet, questions remain about the SM, such as is there a unification theory that includes
119 gravity? Why are there only three generations of fundamental particles? What is the nature
120 of dark matter and dark energy, and how does it fit within the SM? What about the origin of
121 the matter-antimatter asymmetry? Is the SM complete or do other exotic particles exists?
122 Over the years, experimental particle physicists and engineers have built technology to test
123 the SM, either by performing precision measurements of particles and their behaviors, or by
124 colliding particles and measuring their outputs. As a result, we have increased our confidence
125 in the SM theory, but continue to search for answers for these remaining questions through
126 experimental discovery.

127 A Toroidal LHC Apparatus (ATLAS) [2] is a particle physics experiment designed to
128 detect the high-energy particle collisions from the Large Hadron Collider (LHC) [3]. At
129 the LHC, collisions take place at a rate of more than a billion interactions per second,
130 which is a combined data volume of about 60 million megabytes per second [4]. In order to
131 extend its discovery potential, the LHC will have a major upgrade to increase the number
132 of instantaneous collision rate. This upgrade, called the High-Luminosity LHC (HL-LHC)
133 [5], will require a new data storage format that can handle this increase in data.

134 RNTuple [6] is the new ROOT [7] data storage format that will be in use at the start of
135 the HL-LHC [8]. RNTuple takes advantage of modern C++ techniques, which have shown
136 to improve read speed ability and memory usage when compared to its predecessor, TTree,
137 and other data storage formats such as HDF5 and Parquet [9]. RNTuple is currently under
138 heavy development. Its base format has only recently left the experimental stage and many
139 tools and capabilities built around it are still evolving.

140 This thesis investigates the performance of RNTuple for ATLAS analysis workflows. This
141 chapter will provide a more detailed introduction of the SM and physical quantities relevant
142 to this thesis. An introduction to the ATLAS experiment and its detector technology is
143 provided in Chapter 2. In Chapter 3, the ATLAS software and computing system is intro-
144 duced along with an explanation of the RNTuple and TTree format. Performance studies
145 conducted for RNTuple and how they compare with TTree will be presented in Chapter 4.
146 In Chapter 5, the Analysis Grand Challenge (AGC) [10] is presented along with its RNTuple
147 implementation. Finally, conclusions are given in Chapter 6.

148 1.1 Phenomenology at the LHC

149 The SM is a quantum field theory that explains and categorizes all observed funda-
150 mental particles by their properties and interactions. Quantum field theory (QFT) is the
151 main theoretical tool for describing particle interactions by combining special relativity and
152 quantum mechanics. Due to this combination, QFT is a probabilistic theory where each
153 particle has an associated field that permeates all of space; therefore, forces are simply the
154 interactions between these different fields. For example, the electromagnetic force is the
155 interaction between the electromagnetic field and charged matter fields, which fall under
156 quantum electrodynamics (QED). In sum, the SM encompasses all known elementary parti-

157 cle interactions, except for gravity, through a collection of quantum field theories: QED, the
 158 Glashow-Weinberg-Salam theory of electroweak processes, and quantum chromodynamics.

159 The four groups of particles shown in Figure 1.1: quarks, leptons, gauge bosons, and
 160 scalar bosons, can be further categorized as *fermions* or *bosons* because of a fundamental
 161 property called spin. Similar to the Earth, particles carry orbital angular momentum and
 162 spin angular momentum; however, for particles, spin is an intrinsic property. All bosons
 163 carry an integer spin; while, fermions carry half-integer spin.

Standard Model of Elementary Particles

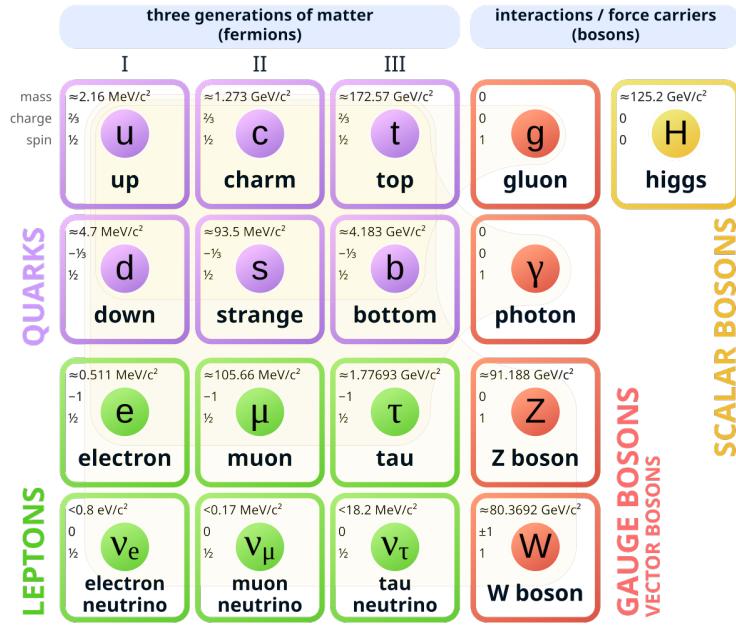


Figure 1.1: Particle content of the Standard Model [11].

164 Fermions are the particles that make up matter. Each fermion has an antiparticle with
 165 the same mass and lifetime as the particle itself, but are oppositely charged. The three
 166 charged leptons (e , μ , τ) are massive, while their corresponding neutrinos (ν_e , ν_μ , ν_τ), are
 167 treated as massless with neutral charge. Quarks combine to form composite particles, such
 168 as protons and neutrons, which are collectively called hadrons. There are six flavors or types

¹⁶⁹ of quarks (up, down, strange, charm, top, and bottom), each of which carries an intrinsic
¹⁷⁰ property called color charge (red, green and blue).

¹⁷¹ Bosons mediate the interactions between fermions. Gluons interact with quarks through
¹⁷² the strong nuclear force. Photons and the $W^\pm Z$ bosons interact with leptons (and quarks),
¹⁷³ giving rise to the electromagnetic and weak nuclear forces. The Higgs boson is separately
¹⁷⁴ categorized as a scalar boson because unlike the spin-1 vector bosons, it has spin 0 and is
¹⁷⁵ responsible for giving other elementary particles their mass.

¹⁷⁶ In sum, there are a total of 12 leptons including their antiparticles, 12 quarks, also
¹⁷⁷ including their antiparticles, 5 vector bosons, and 1 scalar boson, which makes a total of 30
¹⁷⁸ fundamental particles. Together, these particles and their interactions form the complete
¹⁷⁹ framework of the SM of particle physics.

¹⁸⁰ Collider experiments probe the SM by studying the products of collisions between funda-
¹⁸¹ mental particles. In colliders, two particle beams are accelerated to reach high energies and
¹⁸² brought together for collision. Each collision is called an event and specific interactions or
¹⁸³ transformations are called processes. Processes are governed by conservation laws, such as
¹⁸⁴ conservation of energy and charge, which follow the interactions and rules described within
¹⁸⁵ the SM. Around collision points, particle detectors are built to detect the particles produced
¹⁸⁶ from events. These detectors are complex and composed of different parts that allow parti-
¹⁸⁷ cles to interact with by either ionizing material or by depositing energy such that it produces
¹⁸⁸ a signal. The measured signals are then used to reconstruct and classify the particles and
¹⁸⁹ processes. Through QFT, the rate of a process, called cross-sections, can be predicted via
¹⁹⁰ the kinematics of the particles involved, their properties, and the properties of the process.
¹⁹¹ Experimentally, cross-sections can be calculated via Equation 1.1, where N is the number

¹⁹² of events for the process being measured and L is the instantaneous luminosity, defined in
¹⁹³ Equation as 1.2.

$$\sigma = \frac{N}{\int L dt} \quad (1.1)$$

¹⁹⁴

$$L = f \frac{n_1 n_2}{4\pi \sigma_x \sigma_y} \quad (1.2)$$

¹⁹⁵ f is the frequency of collisions, n_1 and n_2 are the number of particles in the colliding bunches.
¹⁹⁶ σ_x and σ_y are the root-mean-squared horizontal and vertical beam sizes. Figure 1.2 displays
¹⁹⁷ the predicted cross-sections for certain processes and the required center of mass energies for
¹⁹⁸ those processes to be observed. Processes with smaller cross-sections are considered rare-
¹⁹⁹ processes because they have a lower probability of being observed. Increasing the probability
²⁰⁰ of these rare-processes would require an increase of energy.

²⁰¹ **1.2 Physics Quantities**

²⁰² This section will cover some relevant physics quantities used in this thesis.

²⁰³ **1.2.1 Invariant Mass**

²⁰⁴ Invariant mass is a quantity that characterizes a system's total energy and momentum
²⁰⁵ independent of the overall motion of the system [13]. Due to special relativity, space and
²⁰⁶ time coordinates are linked, but dependent on a frame of reference. Lorentz transformations
²⁰⁷ are used to convert coordinates from one reference frame to another, and four-vectors are
²⁰⁸ used to simplify these transformations [14]. A four-vector represents a physical quantity
²⁰⁹ in space-time. For example, the position four-vector includes the spatial coordinates (x ,
²¹⁰ y , z) and time, while the four-momentum vector includes the energy and the momentum

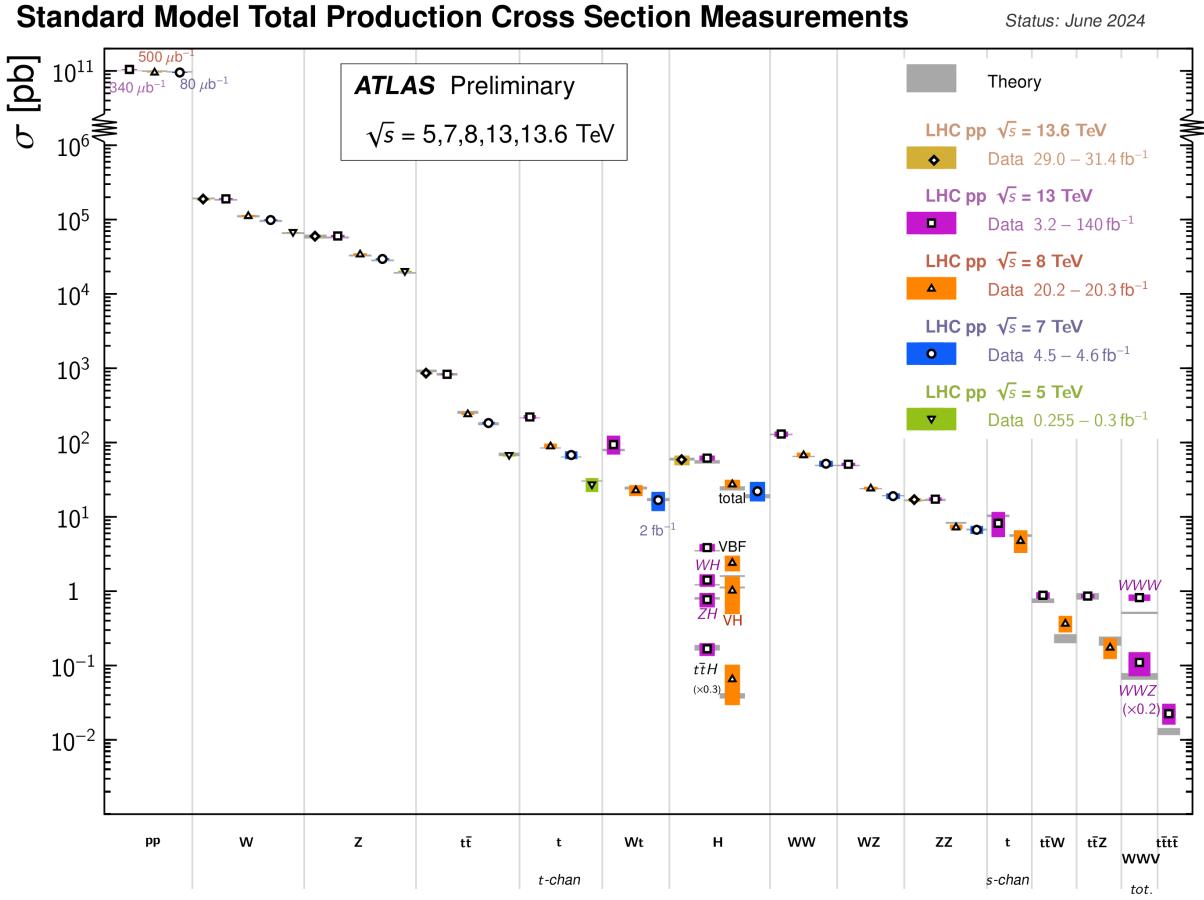


Figure 1.2: Summary of several Standard Model cross-section measurements. The associated references can be found in [12]. The measurements are corrected for branching fractions, compared to the corresponding theoretical expectations.

coordinates in the x, y, and z directions. Four-vectors provide a convenient framework for calculating invariant quantities such as the invariant mass of a resonance that has decayed into other particles.

The invariant mass of oppositely charged muons and electrons is calculated for studies in Chapter 4. A lepton selection with transverse momentum greater than 25 GeV is applied first to suppress background, followed by the pairing of oppositely charged leptons. Their invariant mass is then calculated using Equation 1.3, where p_x , p_y , p_z is momentum in the

218 x, y, z directions and E is energy. The peak of the invariant mass distribution, Figure 1.3,
219 returns the Z boson mass at 75.1338 GeV.

$$m = \sqrt{E^2 - \sum p_x^2 - \sum p_y^2 - \sum p_z^2} \quad (1.3)$$

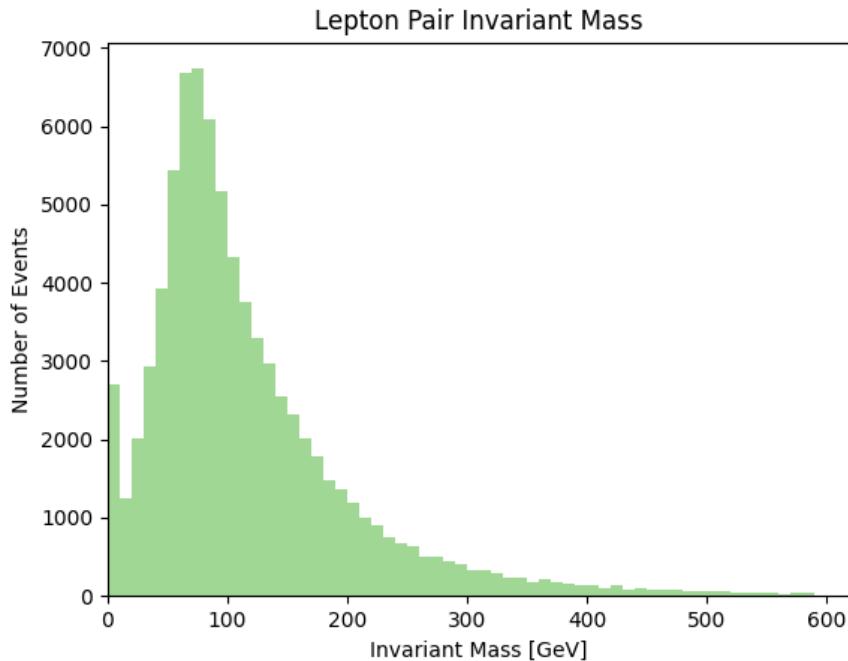


Figure 1.3: Invariant Mass distribution of oppositely charged lepton pairs using data highlighted in Chapter 3.

220

1.2.2 Jets

221 Jets are energy deposits in the detector that are grouped together to represent quarks
222 and gluons, collectively known as partons [15]. Partons cannot be observed in isolation due
223 to their color charge property, causing them to be permanently bound inside hadrons (a
224 composite subatomic particle made of two or more quarks [16]). As a result, jets are used

225 as physical proxies for partons and are reconstructed using various algorithms to different
226 types of objects.

227 In Chapter 5, a selection of b-tagged jets is applied for the AGC. A b-tagged jet is a jet
228 that is identified as being originated by a bottom or anti-bottom quark. B-tagging algorithms
229 use a combination of tracking and vertexing variables that exploit the long lifetime of B-
230 hadrons. In the studies presented in this thesis, a machine learning algorithm based on a
231 deep neural network (DL1) is used. The output of the algorithm are the p_b , p_c , and p_u
232 variables that are combined in Equation 1.4, where f_c is a constant equal to $f_c = 0.018$. The
233 final b-tagging discriminate is defined as D_{DL1} . A jet is considered as b-tagged if D_{DL1} is
234 above the threshold value of 2.456, corresponding to an efficiency of 77% [17].

$$D_{DL1} = \log \left(\frac{p_b}{f_c \times p_c + (1 - f_c) \times p_u} \right) \quad (1.4)$$

235

CHAPTER 2

236

THE ATLAS EXPERIMENT

237 ATLAS was designed to be a general-purpose experiment, optimized to search for the
238 Higgs boson, top quark decays, and supersymmetry. In July 1997, the ATLAS Experiment
239 was approved and by November 2008, ATLAS was the largest detector ever constructed at
240 44 meters long and 25 meters in diameter. By November 2009, ATLAS recorded its first
241 proton-proton collision and by December 2010, ATLAS was first to observed the production
242 of top quark pairs, which are the heaviest known elementary particle with a strong coupling
243 to the Higgs boson. By July 2012, both ATLAS and the Compact Muon Spectrometer
244 (CMS) experiment successfully observed the Higgs boson [18, 19]. ATLAS is projected to
245 continue operation until 2041 to continue searching for standing questions from the SM.

246 This chapter will provide an brief description of the LHC and the Run 2 ATLAS detector,
247 relevant to the data used in the remainder of this study.

248

2.1 The Large Hadron Collider

249 The LHC is a two-ring-superconducting-hadron accelerator and collider built outside of
250 Geneva, Switzerland at the Conseil Europeen pour la Recherche Nucleaire (CERN). It was
251 approved for construction in 1996 to search for beyond the SM physics at energies larger
252 than 10 TeV. Its approval was heavily influenced by the cost-saving idea of reusing the
253 existing 26.5 km tunnels from the Large Electron-Positron (LEP) collider [20]. The LHC
254 has four main collision points that house the ATLAS, CMS, Large Hadron Collider beauty
255 (LHCb) [21], and A Large Ion Collider Experiment (ALICE) [22]. ATLAS and CMS are

256 the two high-energy experiments located at diametrically opposite straight sections. LHCb
 257 is a low luminosity experiment dedicated to investigate the difference between matter and
 258 anti-matter by detecting b quarks. ALICE is an ion experiment dedicated to studying quark-
 259 gluon plasma forms.

260 The LHC is initially supplied with protons from the injector complex, which is a sequence
 261 of accelerators shown in Figure 2.1. The three main components within each of these accel-
 262 erators are magnets, vacuum chambers, and radiofrequency (RF) cavities. Superconducting
 263 magnets are responsible for guiding the beams, and vacuum chambers ensure that particles
 264 do not interact with external residual gas molecules. RF cavities are metallic chambers
 265 located inside the beam vacuum. They are designed to resonate at specific frequencies to
 provide small energy boosts when particles pass through.

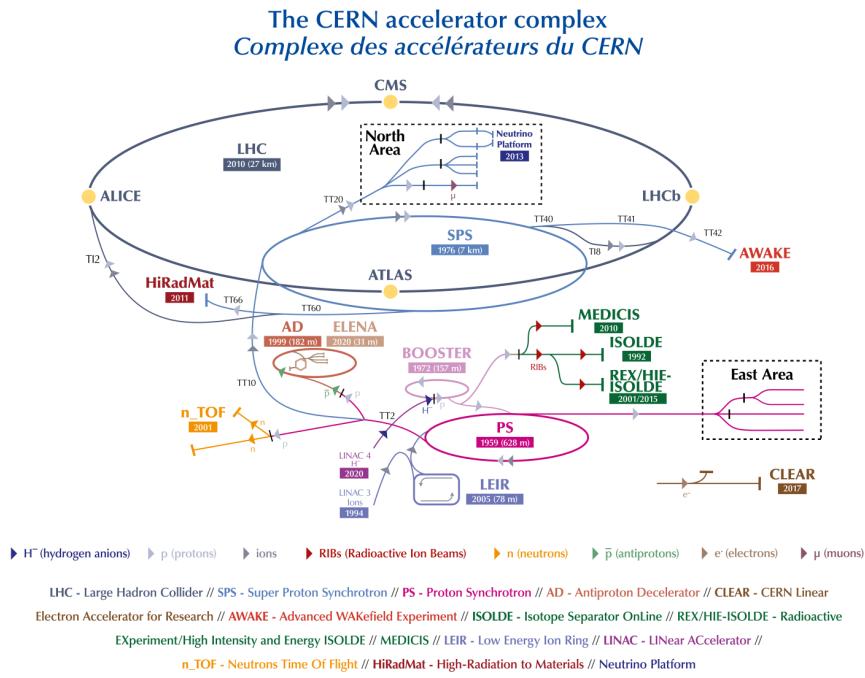


Figure 2.1: The CERN accelerator complex [23].

267 During Run 2, the LHC collided protons at a center of mass energy of $\sqrt{s} = 13$ TeV with
268 a combined integrated luminosity of $L = 140.07 \text{ fb}^{-1}$ [24]. Beams were delivered in bunches
269 with bunch separation of 25 ns, corresponding to a bunch crossing frequency of 40 MHz.

270 2.2 The ATLAS Apparatus

271 The ATLAS detector, shown in Figure 2.2, consists of a collection of subsystems confined
272 in a 46 m long, 25 m in diameter cylinder, 100 m below ground. The first subsystem is the
273 Inner Detector (ID) [25], which is responsible for tracking charged-particles. A calorimeter
274 system follows and measures the energy loss of the particles passing through the detector
275 [26]. The final subsystem is the Muon Spectrometer (MS) [27], which measures the deflection
276 of muons within a magnetic field using a trigger and high precision tracking chambers.
277 Additionally, a first-level and high-level trigger system is implemented to select interesting
278 events and record them to disk [28].

279 ATLAS uses a cylindrical coordinate system (r, η, ϕ) for detector design, reconstruction
280 and data analysis. The polar coordinates, (r, ϕ) , point in the plane towards the center of the
281 LHC ring and upwards. The pseudorapidity, η , is defined in Equation 2.1, where θ is the
282 polar angle and equal to the true rapidity defined in Equation 2.2.

$$\eta = -\ln\left(\tan\frac{\theta}{2}\right) \quad (2.1)$$

$$y = \frac{1}{2} \ln\left(\frac{E + p_z}{E - p_z}\right) \quad (2.2)$$

284 The ID tracks particles in the range $|\eta| < 2.5$, the calorimeter system covers $|\eta| < 4.9$, and
285 the MS detects muon in the $|\eta| < 2.7$ range.

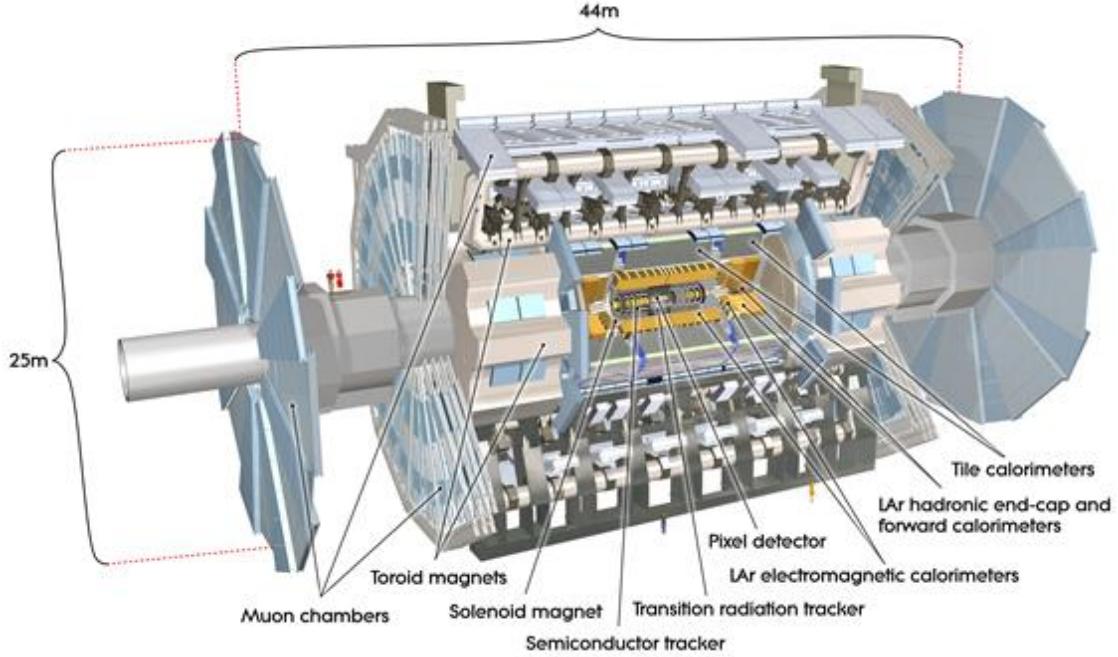


Figure 2.2: Computer generated image of the whole ATLAS detector [29].

286

2.2.1 The Inner Detector

287 The main components of the ID are the Pixel Detector, Semiconductor Tracker (SCT),
 288 and the Transition Radiation Tracker (TRT). This layout is provided in Figure 2.3. The
 289 Pixel Detector is first to pick up the energy deposits of the collisions at a precision of 10
 290 μm . Their signals determine the origin and momentum of the particles. The SCT surrounds
 291 the Pixel Detector, which measures particle tracks with a precision of up to 25 μm . The
 292 TRT is the final layer that provides particle type information, in combination with the other
 293 information gained in the ID.

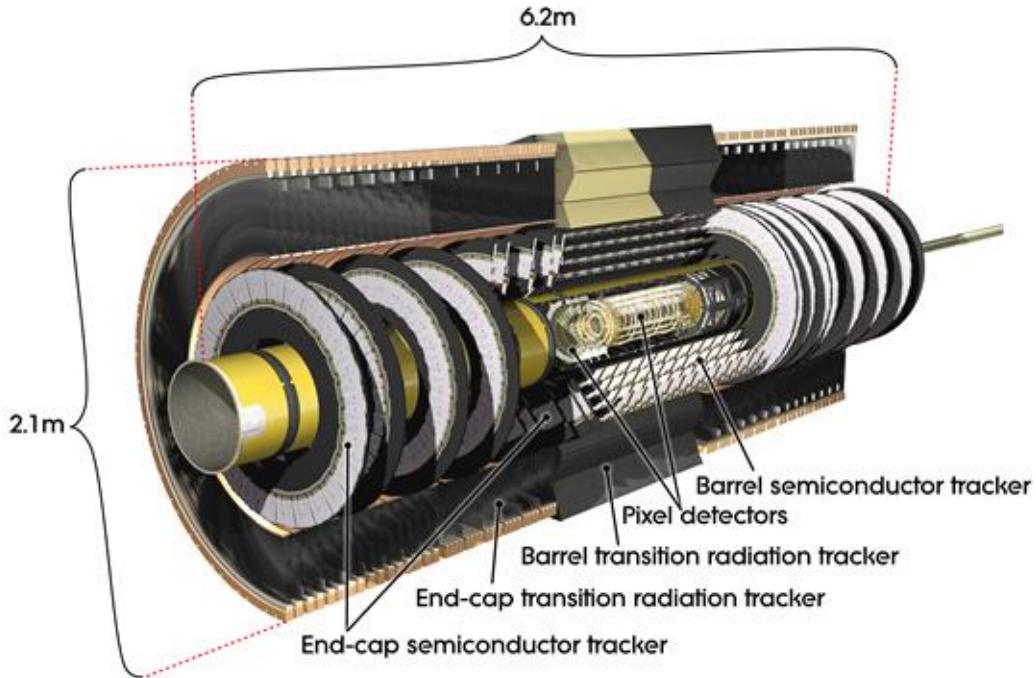


Figure 2.3: Computer generated image of the ATLAS inner detector [29].

294

2.2.2 Calorimeter Systems

295 Calorimeters are detectors that measure the energies and positions of charged and neutral
 296 electromagnetically or strongly interacting particles. They consists of highly-dense materials
 297 that force particles to deposit their energy. That energy is then converted into a measur-
 298 able signal using layers of "active" media. The calorimeter systems consists of two types
 299 of calorimeters as shown in Figure 2.4: electromagnetic and hadronic. Electromagnetic
 300 calorimeters are used to measure charged particles like electrons, positrons, and photons.
 301 Hadronic calorimeters are designed to detect hadrons, such as quarks, protons, and neu-
 302 trons.

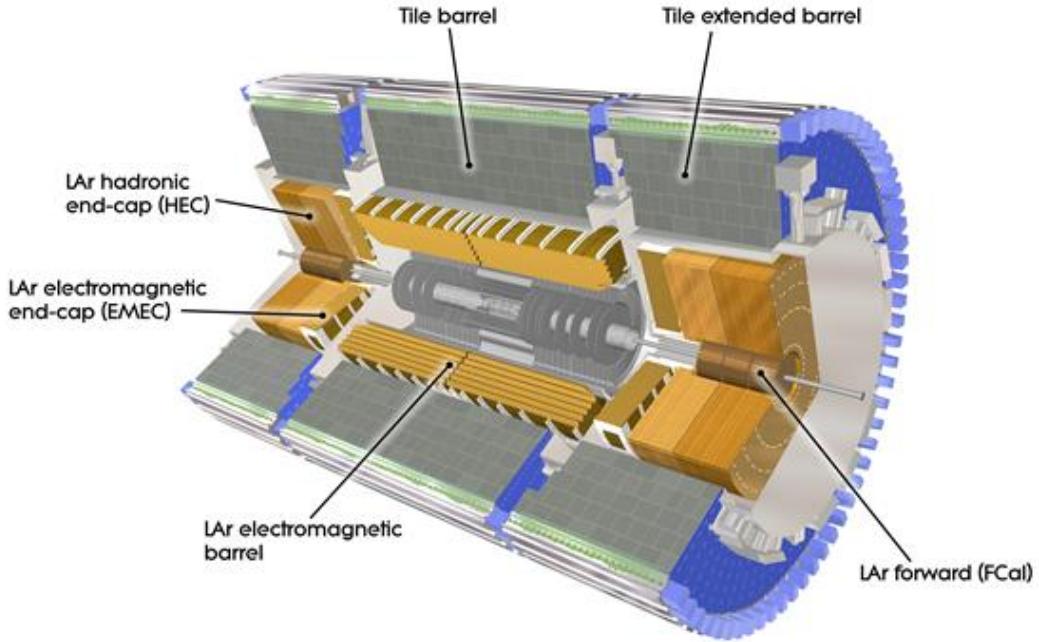


Figure 2.4: Computer generated image of the ATLAS Liquid Argon [29].

303

2.2.3 Muon Spectrometer

304 The muon spectrometer, shown in Figure 2.5, is the outer part of the ATLAS detector,
 305 designed to measuring the momentum of muons. Muons are minimally ionizing particles,
 306 meaning they can travel to the edge and beyond the ATLAS detector. The magnetic field that
 307 bends their directories is generated by superconducting air-core toroidal magnets, located
 308 at the two end caps and one in the center barrel. Three stations of precision chambers,
 309 consisting of layers of Monitored Drift Tubes (MDTs) detect the deflection of the muon
 310 trajectories in the magnetic field. The MDTs allow muons to knock out electrons from gas
 311 when passing through, to produce a signal. Two chambers sit surrounding the central region
 312 and ends of the experiment: the Resistive Plate Chambers (RPCs) and Thin Gap Chambers
 313 (TGCs). They both detect muons when they ionise the gas mixtures to generate signal.

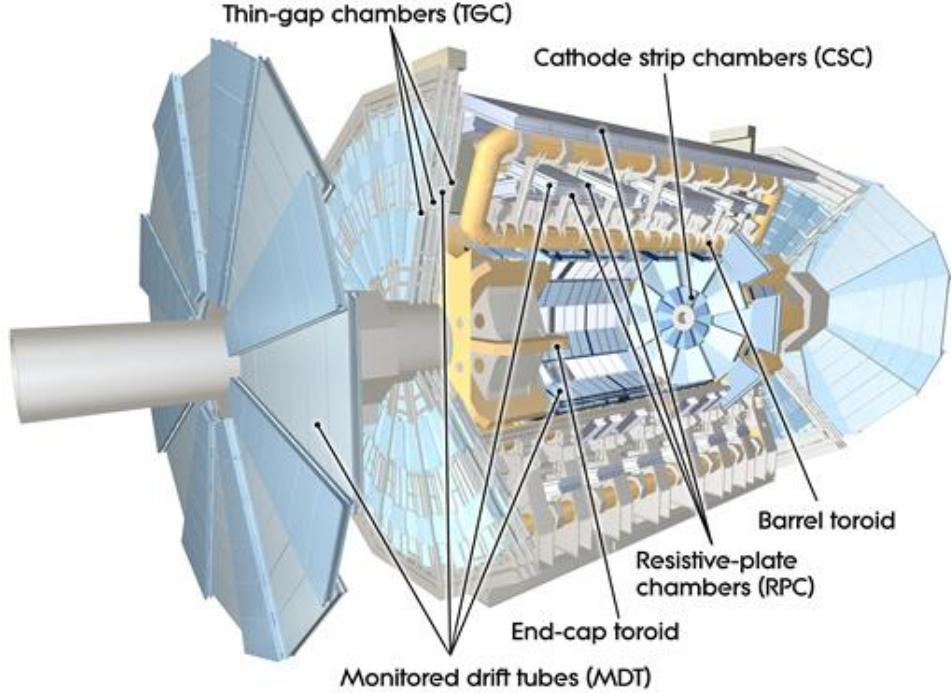


Figure 2.5: Computer generated image of the ATLAS Muons subsystems [29].

314

2.2.4 Magnet System

315 The two main magnet systems are the Central Solenoid Magnet and the Toroid Magnets.
 316 Generally, superconducting magnets are required to bend the directories of charged particles,
 317 allowing for the ATLAS detector to measure their momentum and charge. The Central
 318 Solenoid Magnet provides a 2 Tesla magnetic field surrounding the inner detector. The
 319 Toroid Magnets are located at the ends of the experiment, and a massive toroid magnet
 320 surrounds the center of the experiment. As mentioned in the previous section, the magnets
 321 at the ends of the experiment are to bend muons for the Muon spectrometer.

322 2.2.5 ATLAS Trigger System

323 The ATLAS Trigger system is a collection of electronics that make rapid decisions of
324 saving certain events into disk. There are two trigger subsystems that help selectively read
325 out and store data from interesting physics events. The first level of the trigger system,
326 called the L1 trigger, uses reduced-granularity information from the calorimeters and muon
327 system to search for signatures of these events. The maximum L1 accept rate is 100 kHz,
328 meaning all processing for an event must be completed within that time window. The second
329 level of the trigger system, called the High Level Trigger, which is a software-based system
330 that performs a more thorough reconstruction of the events passed in L1 to then finally pass
331 to a data storage system for offline analysis.

332 2.3 HL-LHC

333 The HL-LHC was proposed in 2010 to extend the discovery potential of the LHC by
334 increasing its instantaneous luminosity (rate of collisions) by a factor of five beyond the
335 original design value and the integrated luminosity (total number of collisions) by a factor
336 ten. Increasing the total number of collisions will increase the probability for ATLAS and
337 CMS to observe rare processes at higher precision [5]. The HL-LHC configuration relies on
338 innovations in accelerator technology such as cutting edge 11 to 12 Tesla superconducting
339 magnets, novel magnet designs, compact superconducting RF cavities for beam rotation
340 with phase control, new technologies and materials for beam collimation, and high-current
341 superconducting links with almost zero energy dissipation.

342 The ATLAS experiment will also require an upgrade following the HL-LHC. New sub-
343 detectors will be installed such as the Inner Tracker [30], the High Granularity Timing

³⁴⁴ Detector [31], and additional Muon chambers [32]. There will also be different electronics
³⁴⁵ upgrades such as the Liquid Argon Calorimeter [33], the Tile Calorimeter [34], the Muon
³⁴⁶ Spectrometer [35], and the Trigger and Data Acquisition (TDAQ) system [36].

349 The data collected from the ATLAS data acquisition system must be compared to a
350 set of simulated data. This dataset aims to mimic the different physics processes: it's
351 production by the colliding beams, the evolution of the collision products within the detector
352 and materials, and the detector's response to ultimately interpret efficiencies and background
353 processes. Except for collision data, the output of all these data processing steps are stored
354 in ROOT files. It starts off with Monte Carlo (MC) simulations, which is a computational
355 technique that uses random sampling to generate events. Given these events, the interactions
356 within the detector and the detector's response is simulated. This reconstructed product is
357 called an Analysis Object Data (AOD), which are then cleaned by compressing the data
358 and cutting any unnecessary events or columns into a finalized product called Derived AOD
359 (DAOD). The products produced at each step are then stored into a compressed binary file,
360 called a ROOT file, and are validated using different software tools. These tools collectively
361 encompass the software framework called Athena [37]. The flow of this process is display in
362 Figure 3.1. This chapter will provide an introduction to ATLAS Open Data [38], ROOT,
363 and its application programming interface (API) for TTree and RNTuple formats.

3.1 ATLAS Open Data

365 ATLAS Open Data is a publicly available dataset produced by the ATLAS collaboration.
366 It's composed of MC simulations of particle collisions within the ATLAS detector and de-
367 tector data measurements. The data used as inputs for the remainder of this study are MC

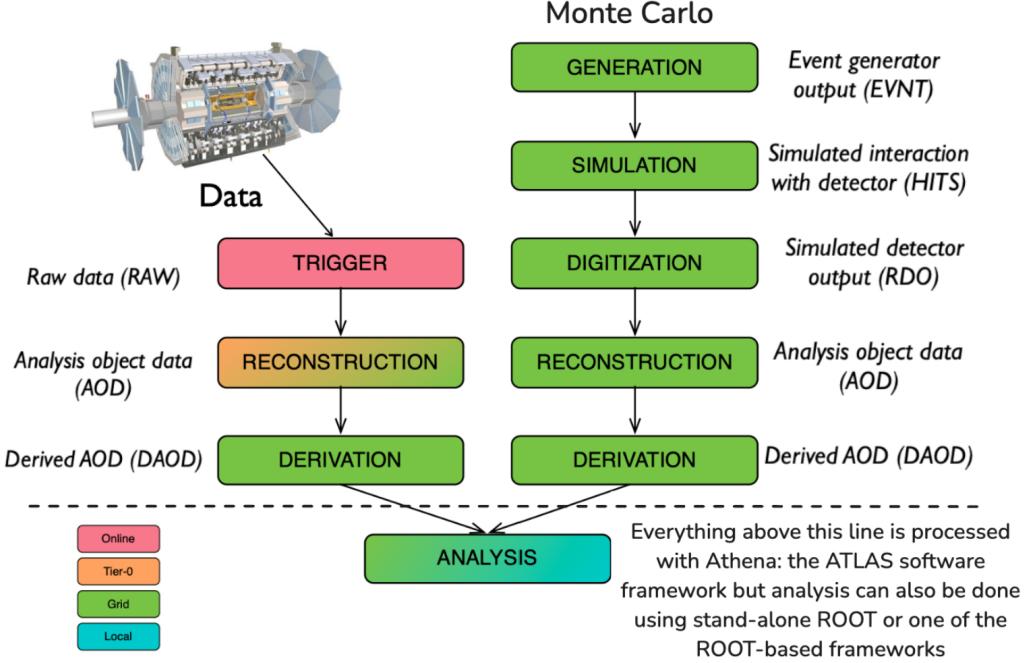


Figure 3.1: ATLAS data chain-processing for data and Monte Carlo simulation [39].

368 simulations of top nominal samples from Run 2 [40, 41]. They are simulated processes that
 369 produce single top quarks, matter-antimatter $t\bar{t}$ pairs, and W boson production in association
 370 with jets. Representative diagrams for these processes are shown in Figure 3.2.

371 The inputs are all provided in PHYSLITE format, which contains already-calibrated
 372 objects directly from an AOD or PHYS product [42]. Those objects include jets, electrons,
 373 muons, photons, taus and their kinematics, such as transverse momentum, mass, charge, eta,
 374 and phi. Each event contains a number of physical objects that depends on the underlying
 375 process, resulting in a multidimensional dataset. A full description of the variables can be
 376 found in [43].

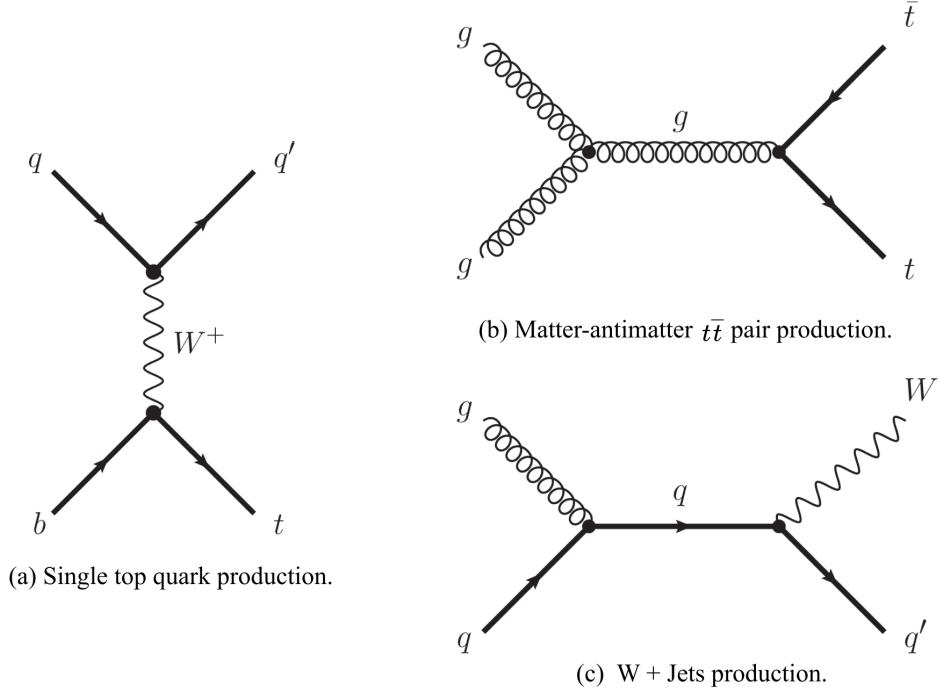


Figure 3.2: The representative diagrams of the processes used in this thesis.

377

3.2 ROOT

378 ROOT is a unified software package developed for processing, analyzing, visualizing and
 379 ultimately storing the massive high-energy physics datasets into ROOT files. Previously,
 380 high-energy experiments used FORTRAN-based libraries; however, an upgrade was needed
 381 to handle the scales and complexities of the data from the LHC. ROOT maintains an object-
 382 oriented structure, meaning it is organized around the data rather than the functions and
 383 logic. Its features include visualization tools such as histogramming, and statistical tools.
 384 ROOT can be used in C++ and python languages. Several sub packages exists for analysis
 385 such as RDataFrame.

386

3.2.1 ROOT Compression Algorithms

387 ROOT offers four different compression algorithms: ZLIB, LZMA, LZ4, and ZSTD [44]. Data
 388 compression allows users to store large files at reduced sizes without losing information from
 389 the original file. It can also increase data reading and writing speeds. There are generally
 390 two types of compression algorithms: lossless and lossy. Lossy algorithms reduce files at
 391 more depth and are irreversible processes. The four compression algorithms from ROOT
 392 are lossless algorithms, meaning they are reversible processes that reduce bits by eliminating
 393 statistical redundancy.

394 There are advantages and disadvantages in each of the four algorithms. LZ4 focuses
 395 on compression and decompression speed, yet provides large files. LZMA provides higher
 396 compression at the cost of significantly slower reading speeds. ZLIB is an older version of
 397 ZSTD. Both provide a balance between compression and reading speeds; however, ZSTD has
 398 been shown to perform better in all metrics in comparison to ZLIB [45]. The input data
 399 applied for this study were all produced with ZSTD. A comparison study between ZSTD and
 400 LZ4 is performed for RNTuple versions of the inputs, shown in Chapter 4.

401

3.2.2 TTree Data Structure

402 ROOT provides a data structure called TTree to store large amounts of columnar data
 403 efficiently. Usually scientific data is stored in what we call row-oriented formats such as
 404 a spreadsheet or CSV table. This format is well organized if one wants to access a single
 405 event, but viewing a single column then becomes inefficient, especially with large datasets.
 406 A TTree is columnar based, meaning it consists of a list of independent columns, called
 407 branches. Examples of branches can be event IDs or particle kinematics such as momentum

408 in the x, y, z coordinates. Branches can hold integers, strings and std::vector data types.
409 Buffers are automatically allocated behind each branch. Buffers are temporary storage areas
410 for the independent binary version of the object. This is done to efficiently handle the
411 writing and reading of the data to and from disk. Each branch has one or more baskets,
412 which manages the in-memory buffer. In other words, a basket holds the values of a branch
413 for a number of consecutive events. When a buffer is full, it is optionally compressed and
414 then the corresponding basket is written to disk, leading to the creation of a new basket
415 to hold the next entries. ROOT allows users to change buffersize parameters of the branch
416 for personalized optimization. Figure 3.3 shows a more detailed flowchart of the TTree data
417 structure.

3.2.3 RNTuple Data Structure

RNTuple is the new columnar data format that will be implemented at the start of the HL-LHC. Its design continues to be columnar based, as its predecessor TTree, but it now uses modern storage technologies for better performance characteristics in data compactness, scalability, and read and write speed. For this reason, RNTuple classes are backwards-incompatible to TTree both on the file format level and API level [47]. Its binary format version follows an *epoch.major.minor.path* scheme, where *epoch* indicates backward-incompatible changes, *major* indicates forward-incompatible changes, *minor* indicates new optional format features, and *patch* indicates backported features from newer format versions. The remainder of this study uses the first public release of RNTuple 1.0.0.0.

RNTuple organizes data using an internal BLOB-based data layout and an external metadata schema. A BLOB (binary large object) is a collection of binary data stored as a single entity. For example, instead of embedding data directly into a database, data can

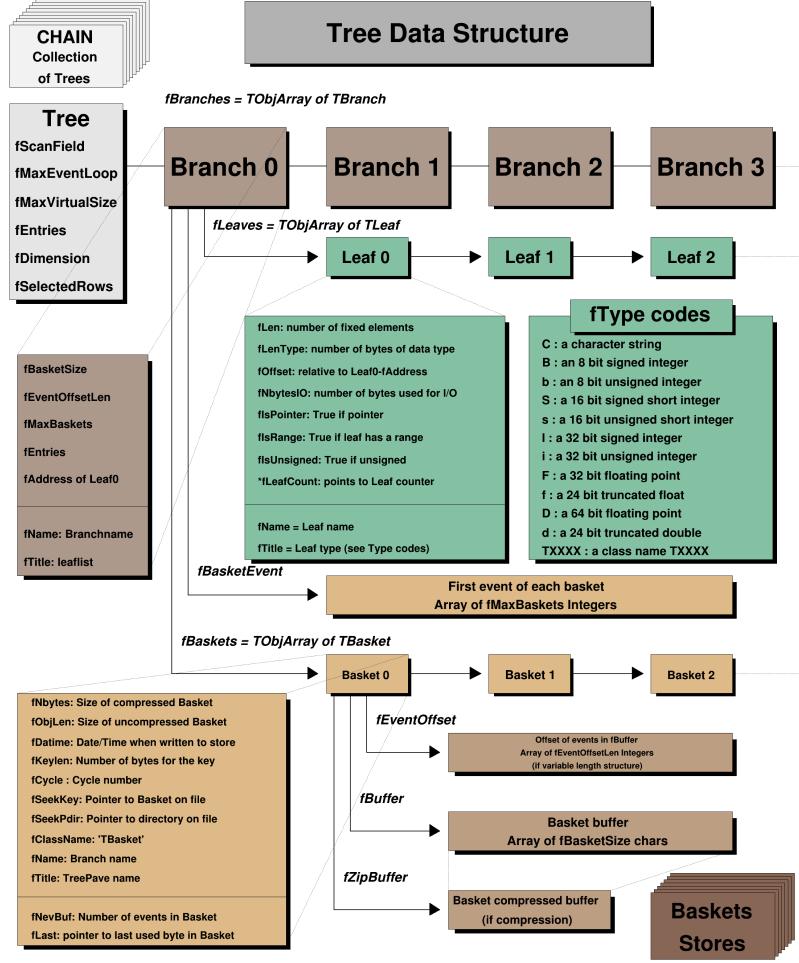


Figure 3.3: Example of the TTree Data Structure [46].

431 be stored as a BLOB along with a unique identifier for later retrieval. This is beneficial for
 432 managing large unstructured data [48]. RNTuple uses a similar approach internally: Data is
 433 organized by columns of a single type and are attached to *fields*, which describes a serialized
 434 C++ type. Columns are partitioned into *pages*. Pages are compressed individually, similar
 435 to TTree baskets. *Clusters* are sets of pages that contain all the data belonging to an entry
 436 range. *Envelopes* are data blocks that contain metadata, such as field and columns types,
 437 cluster descriptions, and page locations. Overall, this structure allows for random-access
 438 of individual events without decompressing the entire dataset and for "fast merging" or

⁴³⁹ concatenating RNTuples. A simplified diagram of the RNTuple structure in comparison to TTree is shown in Figure 3.4.

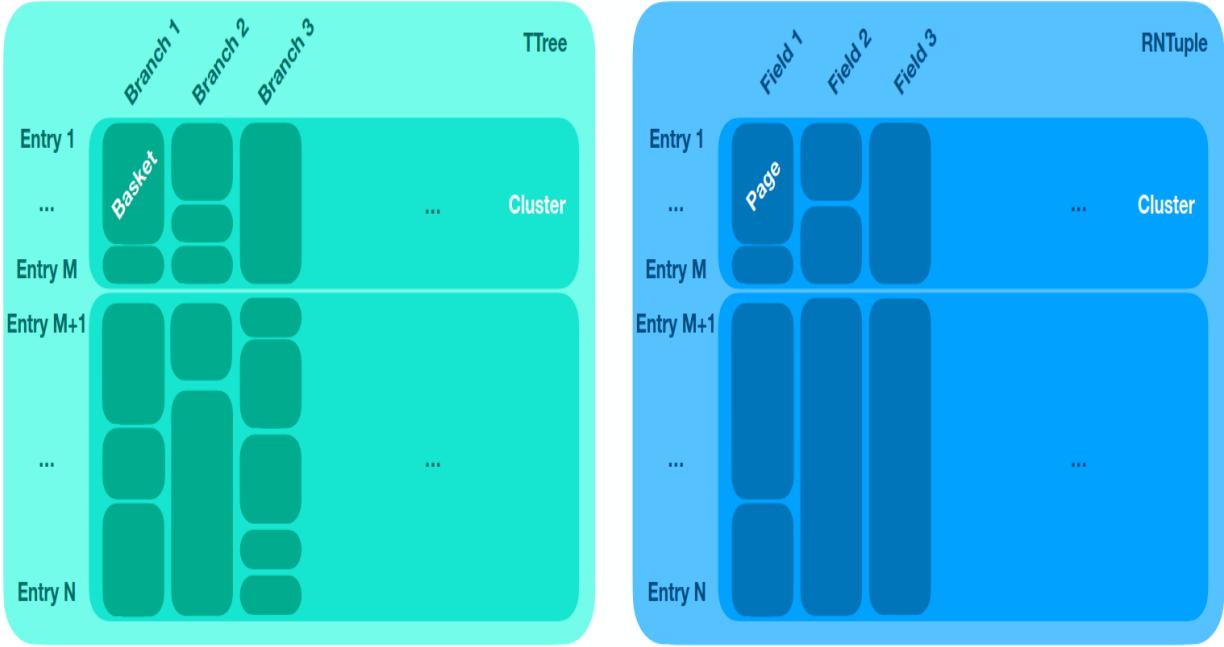


Figure 3.4: TTree Structure vs. RNTuple Structure [49].

⁴⁴⁰

⁴⁴¹

3.3 TTree vs. RNTuple API

⁴⁴² TTree's API is natively compatible with C++, RDataFrame analysis workflows in Python
⁴⁴³ and C++, and the uproot library [50]. At this stage, RNTuple's API is best compatible with
⁴⁴⁴ RDataFrame analysis workflows and hand-written event loops. It currently has limited ca-
⁴⁴⁵ pabilities with the uproot library. For example, functions in uproot that read or concatenate
⁴⁴⁶ multiple RNTuples are still under development, as are the functions for writing RNTuple out-
⁴⁴⁷ puts. As part of this project, an effort was made to test and document the capabilities, usage
⁴⁴⁸ and best practices of RNTuple in a physics analysis context during its development. The

449 corresponding code repository, including the aforementioned documentation can be found in
450 [51]. The sections below will provide examples of RNTuple's API in comparison to TTree's.

451 3.3.1 Native C++ Event Loops

452 Due to the multidimensional nature of particle physics data, event loops are common
453 algorithms used in data analysis workflows. It is a process that continuously iterates through
454 the large datasets to apply specific analysis steps to each event. As seen in Figure 3.5, users
455 must iterate through TTree in order to load branches and define an empty pointer object to
store their entries.



```

// Load ROOT file
std::unique_ptr<TFile> myFile(TFile::Open("DAOD_PHYSLITE.pool.root"));
// Load TTree
auto ttree = myFile->Get<TTree>("CollectionTree");

// Store electron pt data
std::vector<float>* pt=nullptr;
ttree->SetBranchAddress("AnalysisElectronsAuxDyn.pt", &pt);

// Create empty histogram
auto c = new TCanvas("canvas", "Histogram", 800,800);
TH1F* histo = new TH1F("pt", "RNTuple: Electron pt Distribution", ...);

// Iterate through events
for (int i=0; i<ttree->GetEntries(); i++){
    // Load each entry
    ttree->GetEntry(i);
    // Iterate through each value of electron pt
    for (const auto& value: *pt){
        // Fill histogram
        histo->Fill(value/GeV);
    }
}

```

Figure 3.5: Native C++ event loop using TTree. This script loads a PHYSLITE ROOT file containing a TTree titled "CollectionTree", and plots the distribution electron transverse momenta.

457 The RNTuple interface uses smart pointers, which simulates a pointer while providing
 458 automatic memory management [52]. This feature shortens the amount of code necessary to
 459 read and load data by a couple of lines. For example `RNTupleReader::Open` simultaneously
 460 loads the ROOT file and the RNTuple, as seen in Figure 3.6. The function `GetView` also
 simultaneously loads and stores a field.

```
// Load ROOT file and RNTuple
auto rntuple = ROOT::RNTupleReader::Open("EventData", "DAOD_PHYSLITE.pool.root");

// Load and store electron pt data
auto electron_pt = rntuple->GetView<std::vector<float>>("AnalysisElectronsAuxDyn:pt");

// Create empty histogram
auto c = new TCanvas("canvas", "Histogram", 800,800);
TH1F* histo = new TH1F("pt", "RNTuple: Electron pt Distribution", ...);

// Iterate through events
for (int event: rntuple->GetEntryRange()){
    // Iterate through each value of electron pt
    for (int value=0; value < electron_pt(event).size(); value++){
        // Fill histogram
        histo->Fill(electron_pt(event)[value]/GeV);
    }
}
```

Figure 3.6: This is the RNTuple version of Figure 3.5.

461

462 3.3.2 RDataFrame in C++ and Python

463 Analysis done with RDataFrame will mostly remain unmodified with RNTuple, as shown
 464 in Figure 3.7, with the exception of filtering. Due to RNTuple's internal data structure, sub
 465 fields such as "AnalysisElectronsAuxDyn:pt" are separated by their field, "AnalysisElectronsAuxDyn"
 466 by a column, instead of a period. This slight change confuses the filtering function in

⁴⁶⁷ RDataFrame, but can be bypassed by assigning an alias name. Figure 3.8 provides an example of how to read multiple inputs and apply a filter using RDataFrame in C++.

```
filenames = ["DAOD_PHYSLITE_1.pool.root", "DAOD_PHYSLITE_2.pool.root", ...]
df = ROOT.RDataFrame("CollectionTree", filenames)
// ... usual RDataFrame analysis ...
```

(a) Reading multiple TTree inputs.

```
filenames = ["DAOD_PHYSLITE_1.pool.root", "DAOD_PHYSLITE_2.pool.root", ...]
df = ROOT.RDF.FromRNTuple("EventData", filenames)
// ... usual RDataFrame analysis ...
```

(b) Reading multiple RNTuple inputs.

Figure 3.7: Examples of how to load multiple inputs into an RDataFrame in Python.

```
std::vector<std::string> filenames;
ROOT::RDataFrame df("CollectionTree", filenames);
auto filtered_df = new_df.Filter(AnalysisElectronsAuxDyn.pt.size()>=1);
```

(a) Reading multiple TTree inputs.

```
std::vector<std::string> filenames;
auto df = ROOT::RDF::FromRNTuple("EventData", filenames);
auto new_df = df.Alias("electron_charge", "AnalysisElectronsAuxDyn:pt");
auto filtered_df = new_df.Filter(electron_pt.size()>=1);
```

(b) Reading multiple RNTuple inputs.

Figure 3.8: Examples of how to load multiple inputs into an RDataFrame and create a new filtered dataframe in C++.

469

CHAPTER 4

470

RNTUPLE VS. TTREE PERFORMANCE

471 In this chapter, RNTuple performance is analyzed using RDataFrame and compared
472 to TTree. First, 92 TTrees stored in DAOD_PHYSLITE files from ATLAS Open Data were
473 converted to RNTuples using its default compression algorithm setting, ZSTD. An average
474 size reduction of about 47% was observed between the converted RNTuples and the original
475 TTrees, as shown in Figure 4.1. Speed tests were performed for loading and outputting
476 RNTuples in comparison to TTrees using `std::chrono::high_resolution_clock::now()`.
477 Each performance study contains two versions: a TTree version that uses TTree inputs and
478 an RNTuple version that uses RNTuple inputs. A comparison of peak memory consumption
479 was also performed using both sets of inputs. The entirety of this analysis was repeated for
480 RNTuple inputs that were converted with LZ4 compression algorithm.

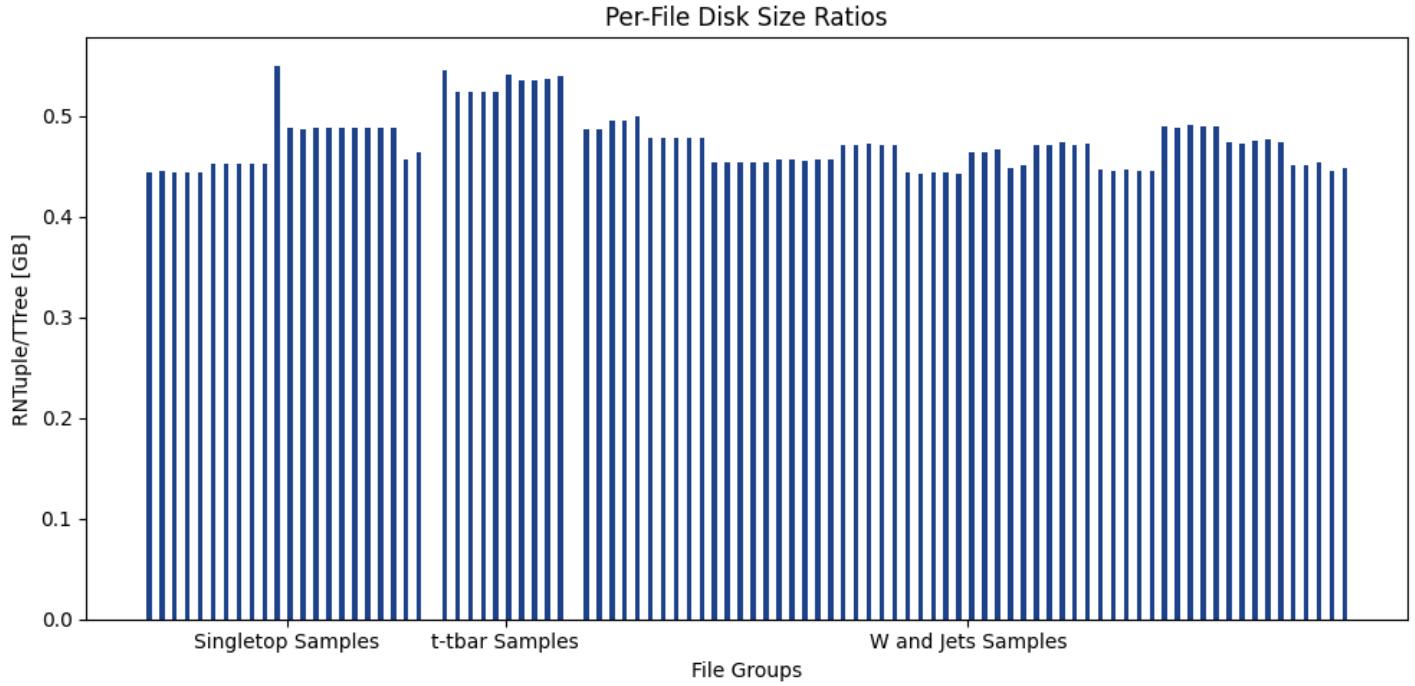


Figure 4.1: The RNTuple:TTree file size ratios over number of events per file.

481

4.1 Readability Speed

482 The total loading times for 92 RNTuples and their TTree equivalence were measured
 483 100 times to ensure consistency. Loading multiple RNTuples in RDataFrame follows an
 484 identical procedure in both TTree and RNTuple versions (seen previously in 3.3.2). The
 485 timer began at the start of the script and was stopped after calculating the sum of the
 486 column "AnalysisElectronsAuxDyn:pt". This was done to ensure that the data was being
 487 loaded and read by RDataFrame. The measured times were recorded onto a text file and
 488 are shown in Figure 4.2. In comparison to TTree, this study finds RNTuple to be 2.38 times
 489 faster at loading a column of data.

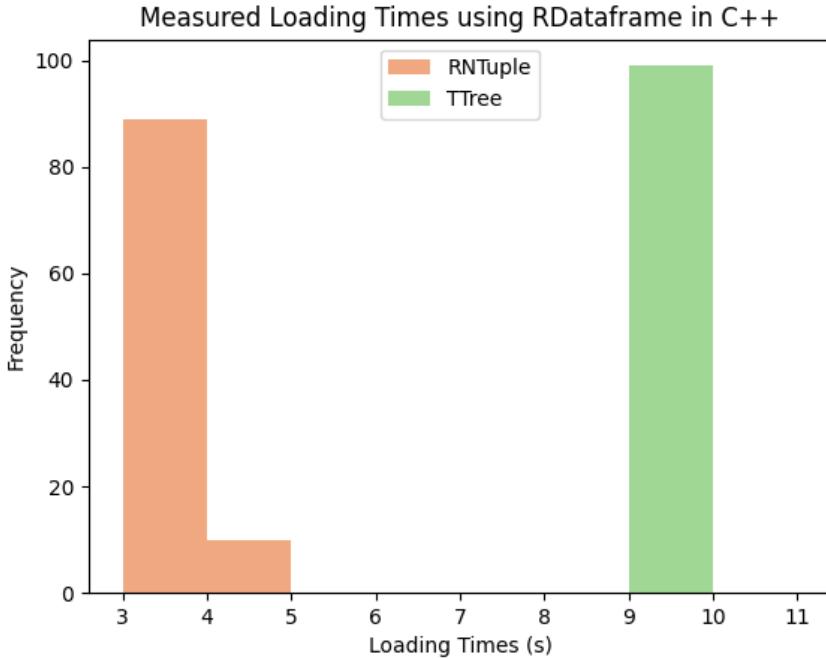


Figure 4.2: Total loading times measured for TTree and RNTuple using RDataFrame in C++.

490

4.2 Writing Speed

491 Writing speed was measured by performing an invariant mass calculation and outputting
 492 a new dataset with two columns: "ElectronPairsInvMass" and "MuonPairsInvMass". The
 493 timer began at the start of an invariant mass calculation and stopped after creating a new
 494 dataset. A TTree was written for the TTree version and an RNTuple was written for the RN-
 495 Tuple version. The quick function that outputs a TTree in RDataFrame, `df.Snapshot(...)`,
 496 is currently not developed to output an RNTuple yet; therefore, for consistency, both ver-
 497 sions of the script uses the RDataFrame function `df.ForEach(...)` to loop through events
 498 and fill in the new columns. This procedure for RNTuple and TTree versions is shown in
 499 Figure 4.3.

```

TFile outFile("tree_invm.root", "RECREATE");
outFile.SetCompressionSettings(ROOT::CompressionSettings(ROOT::RCompressionSetting::EAlgorithm::kZSTD,
5));
// Create a TTree from RDataFrame
TTree *outputTree = new TTree("MyTTree", "MyTree");
// Define variables to hold data
ROOT::VecOps::RVec<float> e_invm, m_invm;
outputTree->Branch("ElectronPairsInvariantMass", &e_invm);
outputTree->Branch("MuonPairsInvariantMass", &m_invm);
// Loop through entries in the RDataFrame to fill output
df_leptons.ForEach([&](const ROOT::VecOps::RVec<float> &e_values, const ROOT::VecOps::RVec<float>
&m_values){
    if (!e_values.empty() || !m_values.empty()){
        e_invm = e_values;
        m_invm = m_values;
        outputTree->Fill();
    }
}, {"invm_electrons", "invm_muons"});
outFile.cd();
outputTree->Write();
outFile.Close();

```

(a) TTree Version.

```

auto model = RNTupleModel::Create();
auto e_invm = model->MakeField<ROOT::VecOps::RVec<float>>("ElectronPairsInvMass");
auto m_invm = model->MakeField<ROOT::VecOps::RVec<float>>("MuonPairsInvMass");
auto ntuple = RNTupleWriter::Recreate(std::move(model), "RNTuple", "rnt_invm.root");
df_leptons.ForEach([&](ROOT::VecOps::RVec<float> &e_vals, ROOT::VecOps::RVec<float> &m_vals){
    *e_invm = e_vals;
    *m_invm = m_vals;
    ntuple->Fill();
}, {"invm_electrons", "invm_muons"});

```

(b) RNTuple Version.

Figure 4.3: TTree vs. RNTuple writing algorithms using the RDataFrame function `df.ForEach(...)` in C++.

500 Although the procedures are the same, the RNTuple version takes up significantly less
 501 code due to the RNTuple API. With TTree, an empty vector has to be created before writing
 502 a branch. With RNTuple, the `ROOT::RNTupleModel` class has the function `MakeField`, which
 503 creates a new field given a name and a corresponding value managed by a shared pointer.
 504 The function `RNTupleWriter::Recreate()` simultaneously creates the RNTuple and the
 505 output ROOT file. In the TTree version, both the TTree and the output file need to be
 506 defined separately.

507 The total output times were measured 100 times and were recorded in a text file. The
 508 results in Figure 4.4 show that writing with RNTuple is 1.51 times faster than with TTrees.

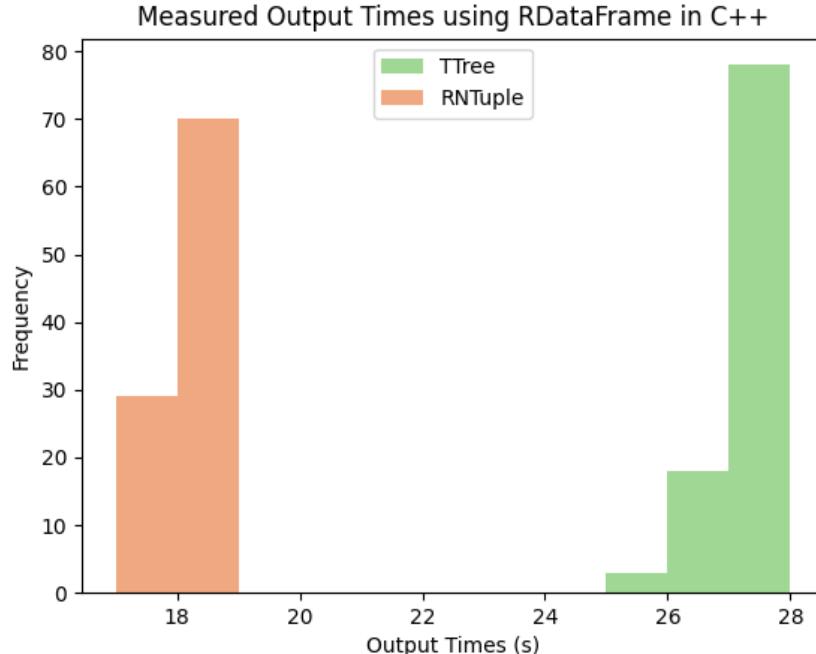


Figure 4.4: Total writing times measured for TTree and RNTuple using RDataFrame in C++.

509

510

4.3 Output Sizes

511 The output file sizes were measured to determine whether RNTuple maintains a consistent
 512 size-reduction behavior at this stage of the analysis. By error, the outputs initially produced
 513 contained empty events; however, this brought some insights on RNTuple when compared to
 514 "cleaned" outputs that filtered out empty events. The results shown in Table 4.1, reveal that
 515 RNTuple provides a 99% event size reduction to TTree when the outputs written include
 516 empty events. This implies that RNTuple is handling repeated bits significantly better than

- ⁵¹⁷ TTree. Table 4.2 reveals a 63% reduction from RNTuple when eliminating the empty events.
- ⁵¹⁸ The latter result is considered more practical or realistic for an analysis; yet, these results open an opportunity to write data and approach analysis workflows differently.

Table 4.1: File size and averaged compressed event size for TTree and RNTuple outputs with empty events. The total number of unfiltered events written is 9,045,000 events.

DataFormat	File Size [bytes]	Average Compressed Event Size [bytes/event]
TTree	48 086 740	5.31
RNTuple	447 414	0.049

⁵¹⁹

Table 4.2: File size and averaged compressed event size for TTree and RNTuple outputs without empty events. The total number of filtered events is 77,411 events.

DataFormat	File Size [bytes]	Average Compressed Event Size [bytes/event]
TTree	791 428	10.23
RNTuple	288 529	3.73

⁵²⁰

4.4 Memory Consumption

- ⁵²¹ Peak memory usage was measured using Python versions of the writing scripts used in
- ⁵²² 4.2. Using the command `usr/bin/time`, memory usage was measured 100 times for both
- ⁵²³ TTree and RNTuple versions. For this test study, results shown in Figure 4.5 demonstrate
- ⁵²⁴ no significant difference between RNTuple and TTree.

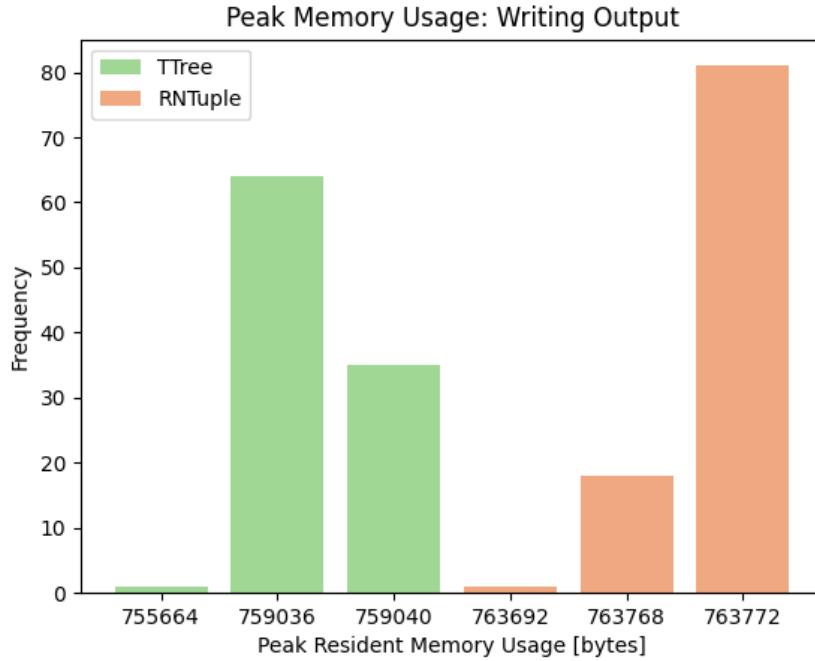


Figure 4.5: Peak memory usage while producing an output with two columns. Measurements were taken 100 times for each version.

525

4.5 LZ4 Compression Algorithm Study

526 Studies have shown that LZ4 improves reading and writing speeds for TTTree, but at
 527 the cost of larger files [44]. This section will investigate if this behavior is consistent with
 528 RNTuple by repeating the loading and writing measurements. The same 92 ATLAS Open
 529 Data files were used to produce RNTuple equivalents with the LZ4 compression algorithm
 530 specified. Time measurements for loading the electron transverse momenta column are shown
 531 in Figure 4.6, and the time measurements for writing an RNTuple output are shown in Figure
 532 4.7. There are no significant differences between reading RNTuples produced from LZ4 or
 533 ZSTD algorithms; however, there is a 2 second difference between writing an RNTuple with
 534 LZ4 versus ZSTD. The ratio of the LZ4 RNTuple sizes over the RNTuples produced with

535 ZSTD are shown in Figure 4.8. They reveal that the LZ4 algorithm increases the RNTuple
536 file sizes by an average of 14% from ZSTD.

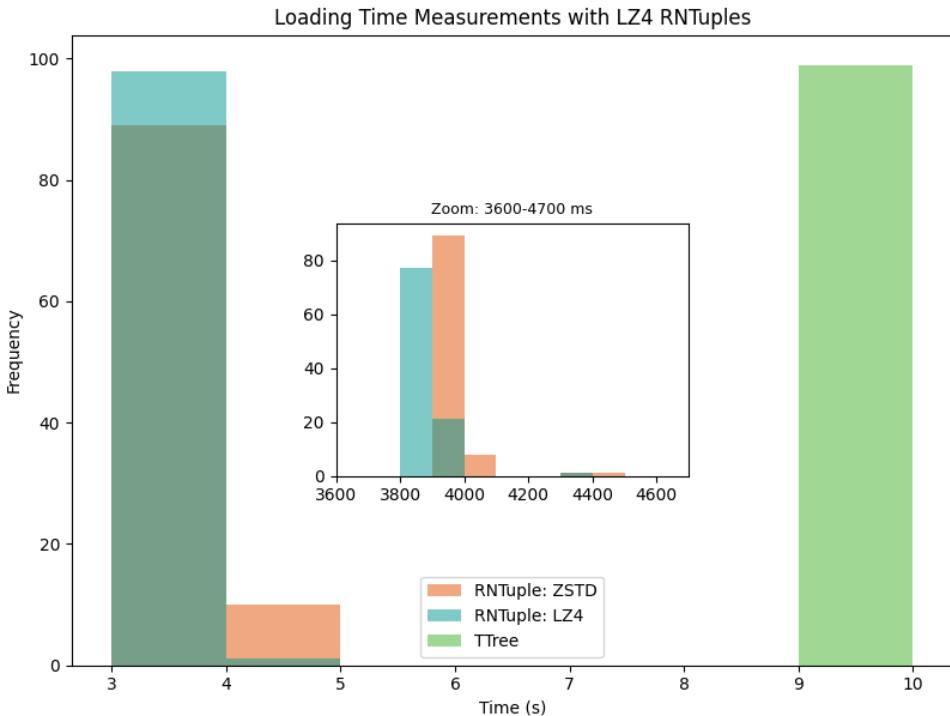


Figure 4.6: Loading time measurements for RNTuples produced by the LZ4 and ZSTD algorithms, and for TTree. The RNTuples composed with ZSTD and LZ4 only differ by a couple of milliseconds.

537

4.6 Performance Discussion

538 Common analysis steps used in RDataFrame workflows have improved with RNTuple
539 compared to its TTree predecessor. Converting TTree to RNTuple showed immediate re-
540 ductions in file size on disk. Reading and writing speeds increased without any significant
541 cost to memory usage. Additionally, the RNTuple API reduces lines of code, making it more
542 user-friendly than the TTree API.

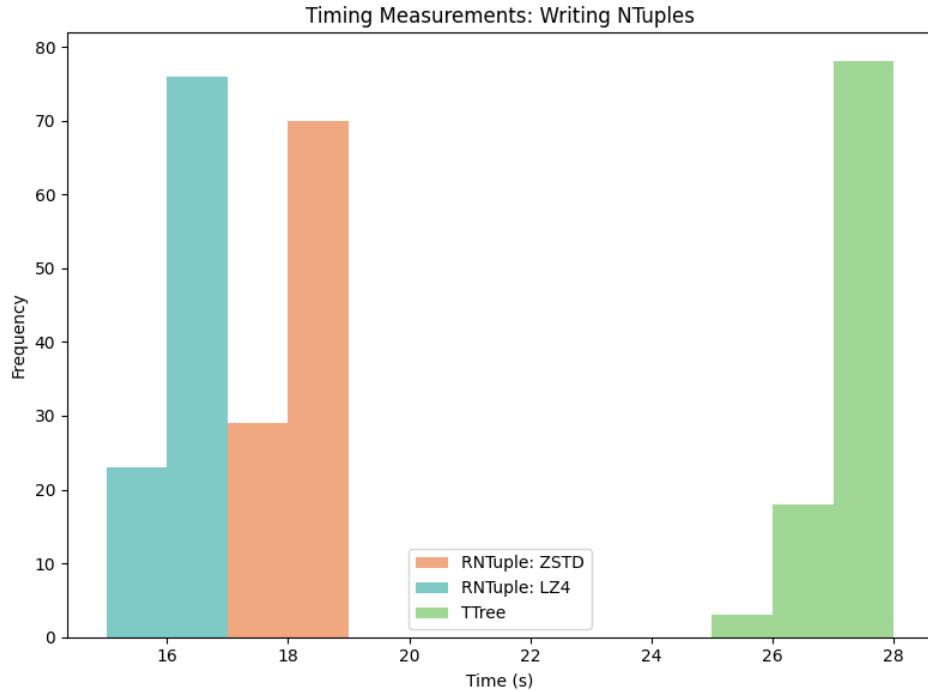


Figure 4.7: Writing time measurements for RNTuples produced by the LZ4 and ZSTD algorithms, and TTree.

543 The comparisons between RNTuples produced with LZ4 versus ZSTD provide a first
 544 look at how RNTuple behaves with different compression algorithms. RNTuples produced
 545 with LZ4 show improved reading and writing speeds, though not at significant levels and
 546 at the cost of increased disk size. Given this study, producing RNTuples with ZSTD is
 547 recommended.

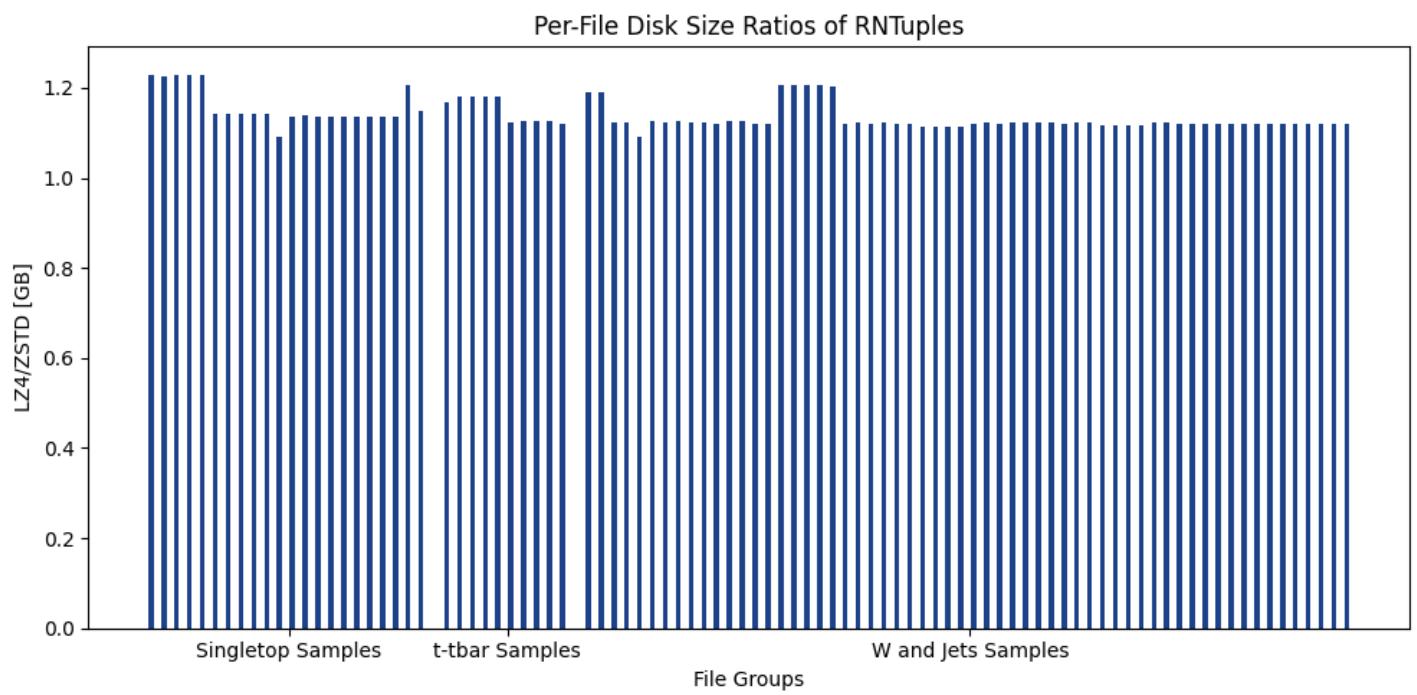


Figure 4.8: Per-file compression ratios of LZ4:ZSTD over total number of events.

ANALYSIS GRAND CHALLENGE: RNTUPLE VS. TTREE

550 The Analysis Grand Challenge (AGC) is an analysis on top quark production meant to
551 showcase an end-to-end analysis pipeline. Developed and organized by Iris-HEP, the AGC
552 has several versions that showcase different cyber infrastructure and workflows, making it a
553 great benchmark to test RNTuple. This section will describe the development of two new
554 AGC versions that use ATLAS Open Data and RDataFrame: TTree and RNTuple versions.
555 These versions were heavily influenced on the existing RDataFrame AGC repository that
556 applies CMS open data and the uproot AGC repository that uses ATLAS Open Data. The
557 full implementations of the AGC can be found in [53].

5.1 RDataFrame Analysis Workflow

559 The AGC is divided into two parts: an analysis script and a statistical script, both
560 written in Python. The analysis scripts uses RDataFrame to apply preselections and output
561 histograms of the top quark mass and the scalar sum of the transverse momenta, H_T , into
562 a ROOT file. The statistical script performs a simple statistical analysis using the output
563 ROOT file from the analysis script.

564 The inputs used for the AGC are the same 92 ROOT file from ATLAS Open Data, as
565 described in 3.1. Specifically, there are 22 single top samples, 10 $t\bar{t}$ samples, and 60 W+jets
566 samples.

567

5.1.1 Event Selections

568 To reconstruct the top quark mass, events are selected from top quark pair production
 569 with final states that include a single charged lepton corresponding to the signature of
 570 semileptonic $t\bar{t}$ events, as shown in Figure 5.1. The leptons must have p_t larger than 30 GeV
 571 and $|\eta|$ less than 2.1 events must include four jets, with two of the four being b-tagged. The
 572 other two jets are from the W boson decay. The top mass observable is then reconstructed
 573 by taking the invariant mass of the trijet with the largest transverse momentum, p_t . To plot
 574 the H_T observable, the selected events must have at least one b-tagged jet among the four
 jets and exactly one lepton.

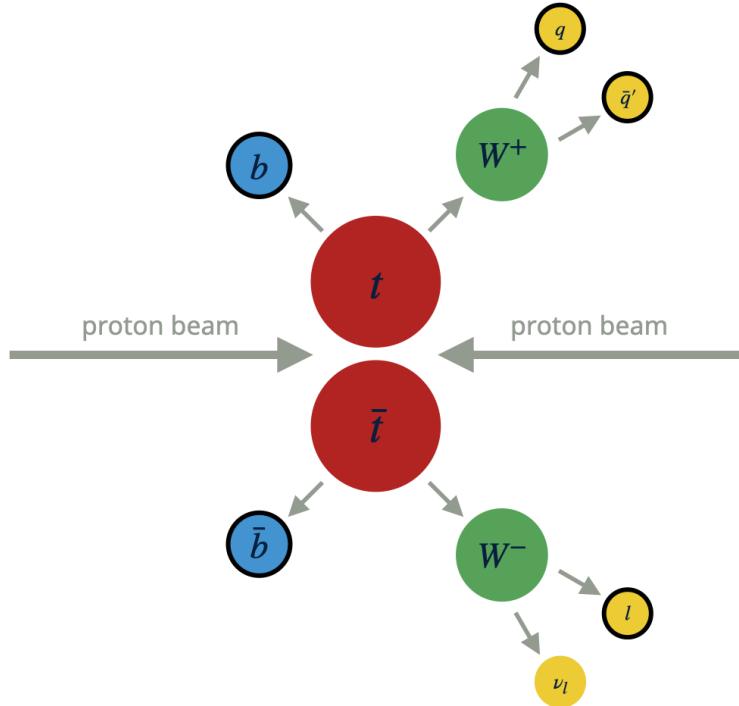


Figure 5.1: The schematic view of a top and anti-top quark collision [54]

575

576 The results of the newly developed AGC using ATLAS Open Data are shown in Figures
 577 5.2 and 5.3. Both the RNTuple and TTTree versions produced the same output, confirming

578 that analysis performed in RDataFrame using RNTuple will remain largely unmodified. As
 579 previously mentioned, RNTuple only changes the structure of variable field names; therefore,
 alias variable names were applied to both TTree and RNTuple versions for consistency.

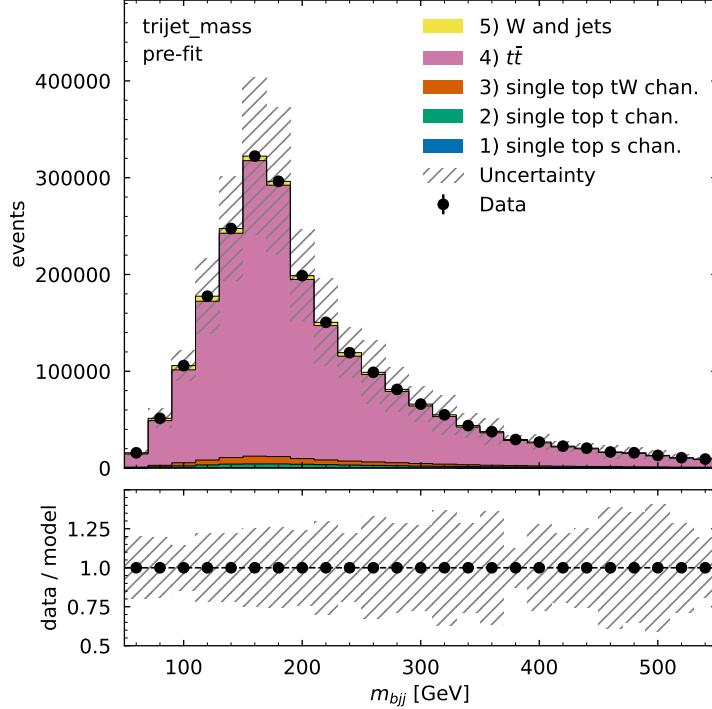


Figure 5.2: The trijet mass prefit. This result is the same for both RNTuple and TTree versions of the AGC.

580

581

5.2 AGC Performance Studies

582 A performance study evaluating execution speed and memory usage was conducted for
 583 both TTree and RNTuple versions of the AGC. Total execution times were measured 100
 584 times for each version using the Python *time* library. Both versions used inputs produced
 585 with the ZSTD compression algorithm. As shown in Figure 5.4, RNTuple averaged 47.58
 586 seconds to produce the top quark mass and H_T histograms into a ROOT file, while TTree
 587 averaged 71.75 seconds. RNTuple was approximately 1.51 times faster, consistent with

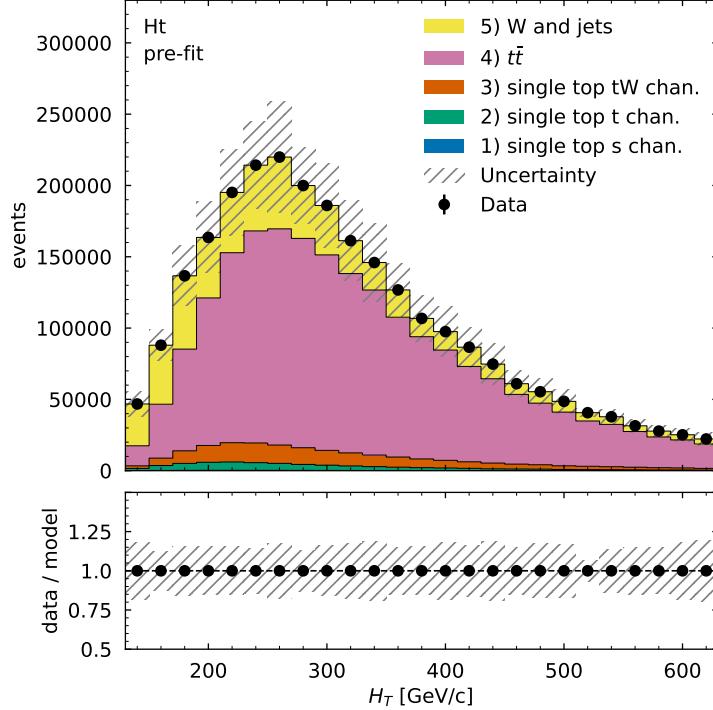


Figure 5.3: The H_T observable prefit. This result is the same for both RNTuple and TTree versions of the AGC.

588 previous time measurements shown in Chapter 4. The execution times were then remeasured
 589 using RNTuples produced with the LZ4 compression algorithm. As shown in Figure 5.5,
 590 LZ4 yields a slight improvement on the order of a few seconds, which is also consistent with
 591 previous results. Peak memory usage was measured using the inputs produces with ZSTD
 592 and with `/usr/bin/time`. As shown in Figure 5.6, RNTuple consumes slightly less memory
 593 usage than TTree when executing the AGC analysis script.

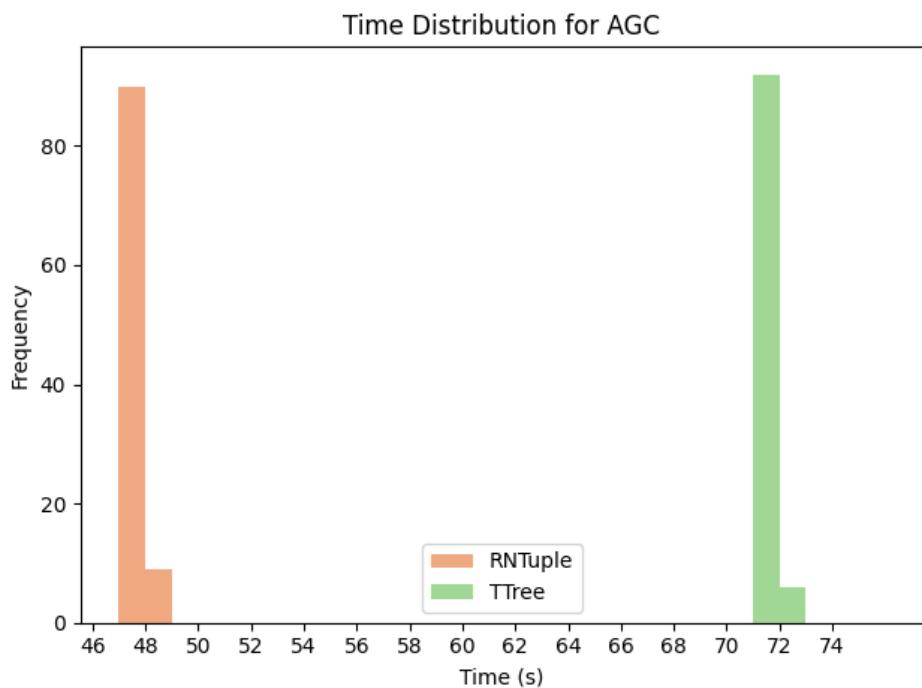


Figure 5.4: The total execution times of the AGC measured 100 times for TTree and RNTuple versions.

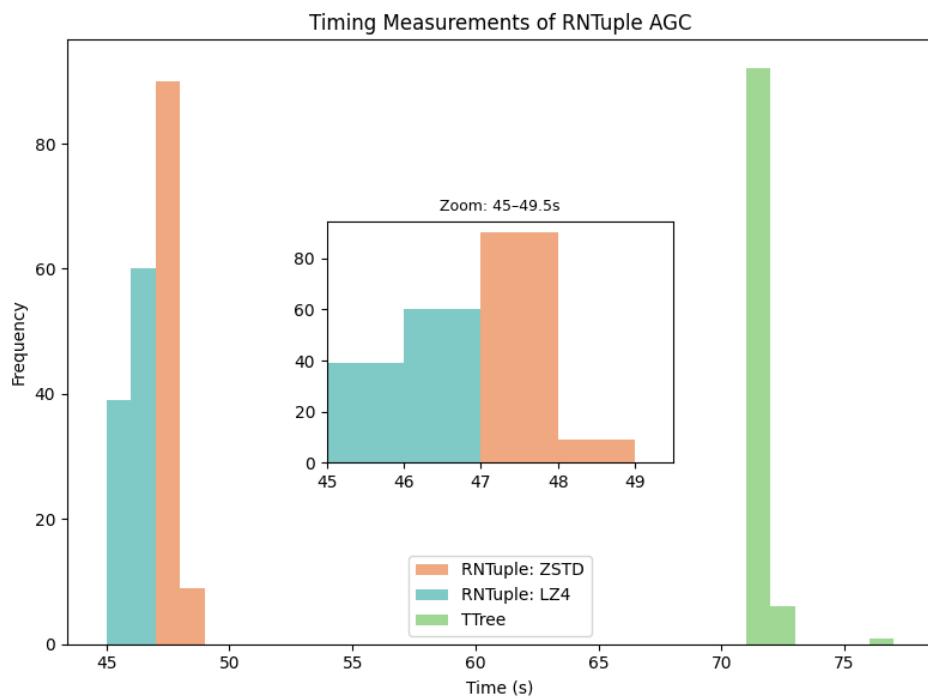


Figure 5.5: The total execution times of the AGC measured 100 times with RNTuples produced with the LZ4 compression algorithm.

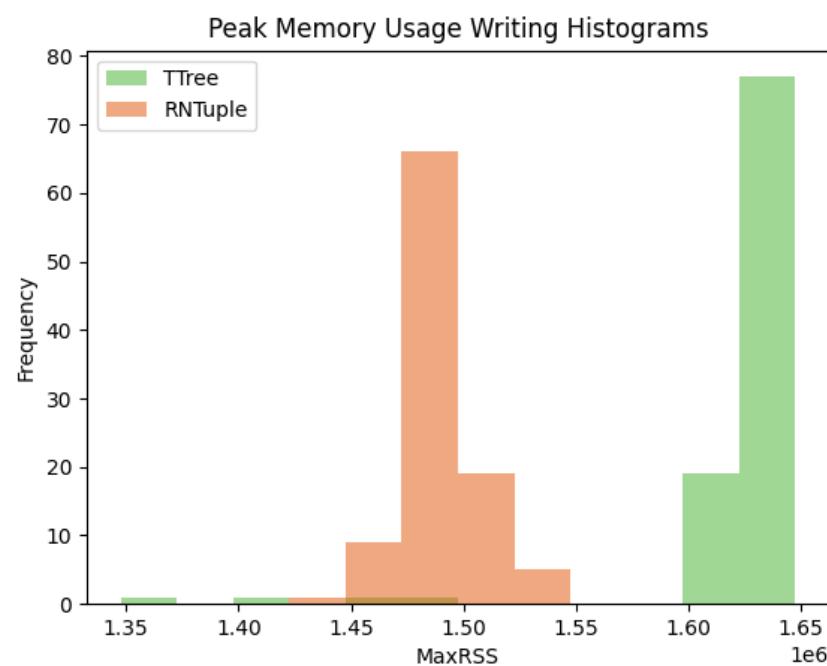


Figure 5.6: The peak memory usage when executing the AGC.

596 RNTuple performance meets expectations, demonstrating improvements in reading and
597 writing speed and disk space usage, with little variance on memory consumption. An average
598 size reduction of 47% was observed when converting the TTree inputs to RNTuples using
599 ZSTD compression algorithm. Using RDataFrame in C++, the average time execution
600 for loading one column of data was found to be 2.4 times faster using RNTuple inputs
601 versus TTree. The average time execution for writing a set with two columns was about 1.5
602 times faster for RNTuple than TTree. The peak memory usage measured while writing the
603 two column output also improved by an average of 4,767 bytes. These improvements were
604 achieved while preserving the RDataFrame workflow in C++ and requiring only minimal
605 code changes, demonstrating a seamless transition from TTree to RNTuple.

606 An initial evaluation of RNTuple behavior using the ZSTD and LZ4 compression algo-
607 rithms was conducted. Performance tests repeated with RNTuple inputs produced using the
608 LZ4 compression algorithm show a 14% file size increase with no significant improvements
609 in reading or writing speeds. Inputs produced with LZ4 exhibited only millisecond-level im-
610 provements when loading a field compared to RNTuple inputs produced with ZSTD. Writing
611 speed also improved slightly, by about two seconds when using LZ4-produced RNTuple in-
612 puts versus those produced with ZSTD inputs. These minimal improvements in reading and
613 writing speeds occur at the cost of larger file sizes. Given these result, the ZSTD compression
614 algorithm is recommended when producing RNTuples.

615 The first implementations of the AGC using ATLAS Open Data were completed for
616 both TTree and RNTuple inputs. The RNTuple version represents the first full end-to-end

617 implementation of a physics analysis using RNTuple and demonstrates the feasibility and
618 improvements of the format. The analysis script for the RNTuple AGC version remained
619 largely unchanged from the TTree version, indicating a smooth analysis workflow transition
620 within RDataFrame. For completeness, performance studies were repeated using the AGC
621 and demonstrate consistent RNTuple performance. The total execution times for reading the
622 91 ATLAS Open Data inputs and writing the top mass and H_T histograms were improved
623 by an average of about 24.17 seconds using RNTuple inputs; hence, the RNTuple version
624 was 1.5 times faster than the TTree version. No significant improvements in speed were
625 observed when executing the AGC with RNTuple inputs produced with LZ4. Overall, these
626 consistent improvements in RNTuple performance reaffirm it as a promising data storage
627 format for ATLAS at start of the HL-LHC.

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