

# The First Release of ATLAS Open Data for Research



CHEP 2024

21 October 2024

Zach Marshall (LBNL) on behalf of the ATLAS Collaboration

ATLAS Open Data for Research - CHEP 2024 - 21 Oct 2024 - Zach Marshall





# **Open Data for Research**



# **Open Data for Research** Public, licensed, Can be used for documented, FAIR scientific publications Understandable, light, useful format





This talk: what we're doing, when, why, how, and a bunch of fun facts

# A Brief Introduction to Open Data

• The Data Preservation for HEP (DPHEP) Collaboration <u>defined four levels</u> of open data

Preservation Model	Use case
1. Provide additional documentation	Publication-related information search
2. Preserve the data in a simplified format	Outreach, simple training analyses
3. Preserve the analysis level software	Full scientific analysis based on existing
and data format	reconstruction
4. Preserve the reconstruction and simulation software and basic level data	Full potential of the experimental data

- 1. Yep, we do that all the time! <u>Plot records</u>, <u>HepData</u>, <u>Rivet analyses</u>...
- 2. We've been doing that for years as well! Previous open data (<u>8 TeV</u>, <u>13 TeV</u>) <u>widely used</u> <u>for education and outreach</u>: <u>more in Giovanni's talk</u>
- 3. This is what we're talking about today
- 4. Being preserved, but will not be released. 50 PB/year in Run 3 in a complex format, huge resources required for processing not useful to the public (even expert public).

## **Open Data for Research**



- We have lots of **bespoke datasets** for **targeted research applications** 
  - Top jet tagging, Fast Simulation training, BSM BDT training, ...  $\bigcirc$
  - Kaggle Challenges: Higgs boson ML Challenge, TrackML Challenge Ο
- Four large LHC experiments agreed to release data for **general research use**
- ATLAS Schedule:



# What's the Goal?



- All the goals of Outreach and Education open data
  - Democratic access, education and inspiration of future scientists
- These Open Data meet research standards can be used for scientific papers
- Would love for excited researchers to use this as a step towards collaboration
  - Particularly if they want access to the **full dataset**
- This is also a step towards **data preservation** 
  - Open data represents the **minimum** level of long-term support for data
  - If in 2040 we can no longer reconstruct Run 2 data, at least we have open data

# **Open Data**

### Definition

Gen research data refers to the publishing of the data underpinning scientific research results so that they have no restrictions on their access and usage. Openly sharing data opens it up to inspection and re-use, forms the basis for research verification and reproducibility, and opens up a path to broader collaboration.

"

More on the web

UNESCO Open research data definition

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Open question: is this realistic?	"
<u>UNESCO</u> Open research data d	efinition
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# What did we Release?



### ATLAS DAOD\_PHYSLITE format Run 2 2016 proton-proton collision data

ATLAS collaboration

Nore on the web Cite as: ATLAS collaboration (2024). ATLAS DAOD PHYSLITE format Run 2 2016 proton-proton collision data. CERN Op DOI:10.7483/OPENDATA.ATLAS.4ZES.DJHA

#### Dataset characteristics

#### 5383448881 events, 45571 files, 35.4 TiB in total



#### Documentation on PHYSLITE Variables for ATLAS Open Data

Page generated from sample: mc20\_13TeV.410471.PhPv8EG\_A14\_ttbar\_hdamp258p75\_allhad.deriv.DAOD\_PHYSLITE.e6337\_s3681\_r13167\_p563'

#### List of Containers:

AnalysisElectrons AnalysisJets AnalysisLargeRJets AnalysisMuons AnalysisPhotons AnalysisTauJets AnalysisTrigMatch AntiKt10TruthSoftDropBeta100Zcut10Jets AntiKt4TruthDressedWZJets BTagging AntiKt4EMPFlow CombinedMuonTrackParticles egammaClusters EventInfo ExtrapolatedMuonTrackParticles GSFConversionVertices GSFTrackParticles HardScatterParticles HardScatterVertices InDetTrackParticles Kt4EMPFlowEventShape MET\_Core\_AnalysisMET MET\_Truth MuonSpectrometerTrackParticles PrimaryVertices TauTracks TruthBoson TruthBosonsWithDecayParticles TruthBosonsWithDecayVertices TruthBottom TruthElectron TruthEvents TruthForwardProtons TruthMuons TruthNeutrinos TruthPhotons TruthPrimaryVertices TruthTaus TruthTop

#### AnalysisElectrons[back to top]

Variable Name	Туре	Description
ambiguityLink	vector <elementlink<datavector<xaod::egamma_v1> &gt; &gt;</elementlink<datavector<xaod::egamma_v1>	Links Photon<-> Electron when ambiguous
ambiguityType	vector <unsigned char=""></unsigned>	Ambiguity (almost surely electron 0 or photon 7/0 rel22/rel21) or ambiguous 1-6/5, (>= rel22/
author	vector <unsigned short=""></unsigned>	Electron, Photon, Ambiguous, Forward
caloClusterLinks	vector <vector<elementlink<datavector<xaod::caloclu ster_v1&gt; &gt; &gt;</vector<elementlink<datavector<xaod::caloclu 	Photon/electron -> Cluster
charge	vector <float></float>	Electron charge
DFCommonElectronsECIDS	vector <char></char>	Charge s of signment)
DFCommonElectronsECIDSResult	vector <double></double>	BD NOTE The charge
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DFCommonElectronsLHLooseBL	vector <char></char>	Like Cation decision

#### 2015+2016 Run 2 pp collision data

- 45 TB of data, 6.3 kB/event, 7.1B events, Ο 55k files in ~300 runs
- 20 TB of MC, ~10 kB/event, 2B events, 16k files in ~300 MC datasets

### Explanation of our nomenclature

- Giant tables of metadata
  - Cross sections, k-factors, filters / Ο efficiencies, processes, how to combine samples, configurations, ...
- PHYSLITE (ROOT-based) format
  - Already columnar Uproot friendly
  - Used for our own papers too
- Pre-calibrated (first for ATLAS)
  - Just draw a plot!
- Extensive effort to document variables
- Useful documentation for us as well!

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# What is the Right License?

- We want our Open Data to be usable for everyone
- We want people to cite us when they use our Open Data
- What's the right License to choose?

© © CC0 1.0 CCO 1.0 UNIVERSAL Deed	© ① CC BY 4.0 ATTRIBUTION 4.0 INTERNATIONAL Deed		
Canonical URL : <a href="https://creativecommons.org/publicdomain/zero/1.0/">https://creativecommons.org/publicdomain/zero/1.0/</a>	Canonical URL : https://creativecommons.org/licenses/by/4.0/		
No Copyright  The person who associated a work with this deed has <b>dedicated</b> the work to the public domain by waiving all of his or her rights to the work worldwide under copyright law, including all related and neighboring rights, to the extent allowed by law.	You are free to: Share — copy and redistribute the material in any medium or format for any purpose, even commercially. Adapt — remix, transform, and build upon the material for any purpose, even commercially.		
You can copy, modify, distribute and perform the work, even for commercial purposes, all without asking permission. See <b>Other Information</b> below.	The licensor cannot revoke these freedoms as long as you follow the license terms.		



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under copyright law, including all related and neighboring rights, to the extent allowed by law.

You can copy, modify, distribute and perform the work, even for commercial purposes, all without asking permission. See Other Information below.



### **Citing ATLAS**

The public datasets are accessible on the CERN Open Data portal, under Creative Commons CC0 license.

Any paper published using these data should cite the corresponding DOI of the datasets. The citation should be similar to this:

ATLAS Collaboration (2020). ATLAS simulated samples collection for jet reconstruction training, as part of the 2020 Open Data release, CERN Open Data Portal, DOI:10.7483/OPENDATA.ATLAS.L806.5CKU

A few additional useful papers for citation are provided below. Please ensure that the ATLAS Collaboration is acknowledged as well. Our preferred acknowledgement is:

"We acknowledge the work of the ATLAS Collaboration to record or simulate, reconstruct, and distribute the Open Data used in this paper, and to develop and support the software with which it was analysed."

For citing the ATLAS Detector:

More on the web ATLAS Collaboration. "The ATLAS Experiment at the CERN Large Hadron Collider." JINST 3 (2008) SC DOI:10.1088/1748-0221/3/08/S08003.

#### Disclaimer

Neither ATLAS nor CERN endorse any works, scientific or otherwise, produced

# Software to Use Them



- <u>Athena</u> is already open-source
- cymfs distributions available
  - Great for folks who know what this is  $\bigcirc$
- Containers are available
  - Great for tutorials, already in use  $\bigcirc$
  - For some applications these are **huge** Ο
  - Through cvmfs we currently distribute Ο 138 GB of PDFs for event generation

### For **notebooks**, lots of resources

- Also binder and so on to run on Ο
- Making public an **ntuple maker** 
  - Based on our analysis tutorial  $\bigcirc$
  - Exactly the example used to create the Ο education and outreach open data
- Analysis code is ~never public (!)
  - All examples are custom no real code 0 has been shared to date
  - (It is preserved, sometimes well Ο

### ATLAS releases new open software

20 November 2020 | By Mariana Velho, Katarina Anthony

The ATLAS Collaboration has just released a collection of 200 software packages that make up the Trigger and Data Acquisition System (TDAQ). With this new More on the web release, most ATLAS software is now open - reinforcing the Collaboration ongoing commitment to open science.

ATLAS' first major step into open software was the release of Atb Athena (available here) is a collision-event processing softwa for event reconstruction, detector simulation, and other key tas ed for data



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### **Event Displays**



- With <u>Phoenix</u> we have an in-browser interactive event display
  - Detector geometry exploration too!

• Providing lots of examples for users to play with (SM and BSM, MC and real)

- Light python script to go from PHYSLITE or education ntuple to Phoenix input
  - Users can make event displays out of any event they wish!
  - Minimal infrastructure don't need any ATLAS software or containers

♠ > Tutorials for Research > Phoenix for Event Visualisation

### **Phoenix for Event Visualisation**

Visualizing an event inside the detector opens a path to a deeper understanding of the physical processes resulting from a collision. One commonly used tool for event visualisation is Phoenix, a framework that allows 3D visualisation of collision events inside the detector.



### **Documentation!**



• We've constructed "paths" through the Open Data for different kinds of users



## **Documentation!**



Statistics

- We've constructed "paths" through the Open Data for different kinds of users
- The eventual goal is to have a **web** of paths that satisfy many users and interests
  - Independent modules for specific learning objectives (hours months)
  - **Chains** for folks that want to go 'end to end'
  - Connections for folks who want to go 'one step deeper'



# **Documentation: How to Write an Analysis**

- Jupyter Notebooks are **fantastic** for fast-uptake documentation and examples
- Once they want something sufficiently complex, there's no (easy) option:
  - We send users to our real analysis software tutorial  $\bigcirc$
- Have not yet found a great way to bridge these two worlds
  - Perhaps this will happen naturally if our analyses evolve to be more notebook-like?  $\bigcirc$

#### How to use a PHYSLITE file

For the ATLAS Open Data for Research, we have released hundreds of datasets in PHYSLITE format. In this notebook we are going to show you how to access the event and variables, and how to do a basic analysis using uproot and awkward arrays.

#### # Import basic libraries

import copy # copy variables import os # manage paths

#### import uproot # use of root files

import awkward as ak # nested, variable sized data import vector # lorentz vectors vector.register awkward() import matplotlib.pvplot as plt # plotting import tqdm # progress bars

#### In this notebook we are using a dataset from

mc20\_13TeV.410470.PhPy8EG\_A14\_ttbar\_hdamp258p75\_nonallhad.deriv.DA0D\_PHYSLITE.e6337\_s3681\_r13167\_p5855 To run this notebook locally, please download a dataset from this container and substitute the file and path in the filename variable below.

# mc20 13TeV.410470.PhPy8EG A14 ttbar hdamp258p75 nonallhad.deriv.DAOD PHYSLITE.e6337 s3681 r13167 p5855 filename = "DAOD PHYSLITE.34865537. 000312.pool.root.1"

#### Read PHYSLITE with uproot

More on the web We can open a TFile using uproot, open. To check the Ttree objects in the file we use the .kevs() methods

#### print('TTree objects inside the ROOT file:') for ii in uproot.open(filename).keys(): print('-',ii)

TTree objects inside the ROOT file: - ##Params;3

### **ATLAS Analysis Software Tutorial**



Welcome to the ATLAS Analysis Software Tutorial pages.

This is the portal to the ATLAS analysis software tutorial held multiple times throughout the year.

This tutorial is aimed at (new and old) members of the ATLAS collaboration interested in learning the basics of ATLAS software and the latest physics analysis tools. There are several introductory lectures aimed at introducing the topics.

### **Tutorial Week**

More on the web Follow a week-long analysis software tutorial with lectures and hands-on exercises. The new tutorial forma November 2022) is designed to be done in small groups and to follow an example ATLAS analysis from end. The introductory material and hands-on exercises are kept available online, so if you cannot week, you can still work through the material.

The curriculum, recorded lectures (for self-guided/asynchronous study), and links

**Tutorial material** 

# **Documentation: The Really Hard Part**



### **Setting Uncertainties**

One of the most important parts of any data analysis is the inclusion of proper uncertainties. Uncertanties help quantify the reliability and precision of a conclusion obtained from data.

When comparing detector data to simulations, you can see a difference that might seem significant. However, whether that difference is interesting or important requires understanding uncertainties. Agreement within uncertainties implies that the observed and predicted values are consistent. If a number is measured to be 1000 and it was predicted to be 2000±1000, then the measurement and prediction agree. Despite the measurement appearing far from the prediction, the large uncertainty range indicates that the prediction is not very precise, allowing for agreement

Similarly, it is important not to misinterpret agreement that is better than the uncertainty suggests. If a number is measured to be 1000 and the prediction was 1000±500, that does not mean that the true value will be 1000. A more precise model might give a prediction of 600±100, which would be in consistent with the original prediction, but would no longer agree with the measurement.

A key part of scientific training is understanding when a difference between a prediction and an observation is meaningful and significant, and that comes down to understanding uncertainties.

#### Why Consider Uncertainties?

In ATLAS analyses we consider uncertainties for several reasons:

- More on the web 1. Accurate Parameter Estimation: To get reliable estimates of the parameters of interest (PO boson couplings or the top guark mass, we need to account for all sources of uncertainty uncertainties can lead to biased estimates and incorrect conclusions
- 2. Robust Hypothesis Testing: In testing theoretical models against ensure that discrepancies between the observed data and theor new physics or phenomena, instead that they are correctly identif experimental or theoretical setup.



The **hardest part** of an analysis is understanding and calculating systematic uncertainties Explaining how to do this in an approachable way is extraordinarily difficult and important

### **Evergreen documentation** of concepts

- Useful for our students as well!  $\bigcirc$
- Can be integrated into our tutorials

### Technical documentation for code

- Momentarily matches internal documentation until Ο we move on (except CERN-specifics, Grid use...)
- Needs to be **fool proof** to avoid science problems Ο
- Good examples are a **huge** help here Ο
- Related documentation we haven't written yet: what you **cannot** do
  - Things our systematics don't cover
  - Things our datasets / simplification don't permit Ο

# Resources for Open Data



#### Resources

Downloading all the available Open Data requires significant resources. For those who wish to tinker, but might not have the computing resources to hand, there are a few options.

- There is a cluster at the University of Nebraska-Lincoln on which an account can be requested. It's possible to authenticate with Google, for example (no institutional affiliation is required)
- · Google offers cloud resources, with free credit for new users.

On these resources, we recommend installing dependencies via a terminal

More on the we pip3 install --user jupyterlab matplotlib tqdm xrootd zstandard uproot==5.1.2 awkward==2.5.0 vec client[xrootd]







- Who pays for resources?
- CERN's Open Data Portal, storage, support provided by CERN IT
  - Is this a 'host lab responsibility'? Long-term?
- CERN only providing open storage
  - CFRN users have access to standard resources (notebooks, etc)
  - Security and abuse concerns with providing Ο CPU to 'any' user
- CPU is *critical* to **equitable** open data
  - We cannot expect people to have network, Ο local storage, local CPU, ...
  - Notebooks with a web interface might work?
- A few sites are trying to provide CPU
  - UNL has done a great job Ο
- Trying to provide instructions for commercial cloud resources (second copy of data too?)

# How are Users Finding Us?

- How many entry points do we have?
  - o ATLAS news articles
  - CERN news articles
  - YouTube videos, Tweets, Reels, ...
  - ATLAS Open Data website
  - Individual Open Data records
  - 0 ...
- Documentation that can't be found is wasted effort!
  - Duplicate documentation is painful and risks inconsistencies and other major problems...
- Single Open Data Portal 'entry' record
- Everything redirecting to the <u>ATLAS Open</u> <u>Data Website</u>



rted with ATLAS Open Data

Subscribe



# User Support

### • Open Data Forum at CERN

- Social media login allowed
- Harder to track who's there to help (who is tracking the relevant issues)
- Issues / Pull Requests on GitHub
  - GitLab requires CERN account
- Several egroups dedicated to help
  - Within ATLAS and within CERN
  - Harder to track answers Did we cc an expert? Did something get answered off-list?
- Asking expert users to come to our meetings and give feedback
  - IRIS-HEP summer students, e.g.
- Have to meet the users where they are!
  - If someone asks for help on Reddit, we should find it and answer

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categories →         Latest         New         Unread (1)         Hot         Categories			New Topic
£Ξ Topic	Replies	Views	Activity
Welcome to the CERN Open Data forum!     News     Welcome to the CERN Open Data discussion forum! The CERN Open Data portal     manages several petabytes of open data from particle physics. The data are released by LHC collaborations in periodic batches after a certain em read more	0	2.3k	Dec 2019
Unable to use open data over URL via TFile 2 5 2	3	2	3d
Embed the OD forum in the ATLAS Open Data website	1	17	13d
Empty ElementLinks in ATLAS PHYSLITE Open Data	1	25	23d
Broken Link to PHYSLITE Data Format Info	2	13	the web
Using Scikit-Learn to classify signal using Secondary vertex characteristics	3	More	n - S Aug

÷	🞯 r/CERN -1 day ago Legal-Bar-3719 ATLAS open data Higgs to ZZ Binder	r/CERN Joined CERN: the European Organization for Nuclear Research		
	Hi there! I'm trying to open the Higgs to ZZ Open Data Jupyter notebook from: https://opendata.atlas.cern/docs/13TeVDoc/13tutorial#Higgs-to-%CE%B3%CE%B3-analysis but Binder loads forever and crashes in the end. Did this ever haopen to anone here? Thanks!	News and discussion about CERN, home o the Large Hadron Collider and birthplace o the World Wide Web.		ut CERN, home of and birthplace of
	◆ 3 ↔ 🖓 🖓 4 😞 🎓 Share	45K Members	4 Online	<b>Top 3%</b> Rank by size 더

# Advanced User Support

- Significant discussion in the collaboration about effort for support "What Ifs"
  - What if someone requests an SM sample?
  - What if someone wants to run their own (BSM?) MC?
  - What if someone needs help with a tool?
  - What if someone publishes a paper that requires a response?
- Agreed on 'best effort' volunteer support
- Point of concern to be watched
  - Need to ensure that we don't need Sherpas to guide all Open Data users
  - Shouldn't *waste* significant effort, but it's ok to *spend* effort that helps us too
- Hoping to connect with expert users via <u>Short Term Associations</u>
  - Become 'insiders' for specific projects







# Tracking Open Data Usage: Key Performance Indicators





opendata

### Research output KPIs

- Now tracking citations via DOI and URL
- Indications this is not well reported (tools?)

### Repository / code tracking KPIs

• Watches / forks / stars

### Website KPIs

• Clicks, website search results

### • Direct Data KPIs

- Downloads, remote reads, reads from eos
- These require pretty good infrastructure monitoring
- Useful to know how many people are using the <u>opendata client</u> software

### • 'Experience' KPIs

Surveys for usage and satisfaction, user feedback forms, attendance at events

### • Some day: CPU KPIs

- Integrating CPU monitoring from 'friendly' sites to understand CPU used for open data
- Must track **educational** usage as well!

# A Playground for Future-Proofing

- Who will store the data in 2050?
  - Does this scale for the lifetime of the experiment?
  - What about the software? Websites? Documentation? Examples?
- Where physically are they stored?
  - **All** of them? Even the little example mini-formats?
- Who has rights to the repos?
  - Ownership? At CERN? Outside?
  - What about **after** the experiment?
- Can we reproduce them? Add to them?
  - If someone wants "just one more" MC dataset?
     15 years from now?
- How do we release **more** data?
  - New format... new release of everything? Keep what's there?
  - Update examples? Abandon them? Delete them?
- Are old tutorials / recordings useful? Watched?
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**HI, I'M TROY MCCLURE** 

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# What's Next



- Monitoring and watching
  - Users will let us know what they think of our open data in comparison to other offerings
- Heavy Ion open data coming soon
  - Required by / following the Open Data Policy
  - Different format that supports different analyses
- Filling in more parts of the documentation chain
- More examples, integrating **your** examples
  - We would love to build a library in the style of Rivet with examples developed in projects around the world
  - Maybe also **our own** analysis? (TBD)
- Beginning to plan a workshop / hackathon

♠ > Tutorials for Research > Community Contributions

### **Community Contributions**

Here we gather various projects and analyses created using our open data for research. We believe in the power of collaboration and the insights that can emerge from diverse perspectives. If you've used our open data for something cool, we would love to hear about it! Please share your work with us through the contact us form. Your contributions can inspire others and help to show the potential of open data.

A full list of uses of ATLAS Open Data can be found on INSPIRE-HEP.

### Notebooks



### ATLAS Open Data



### High Energy Physics data for everyone.

#### For Education

To provide data and tools to high school, undergraduate and graduate students, as well as teachers and lecturers, to help educate them and exercise in physics analysis techniques used in experimental particle physics.

#### For Research

To provide researchers with high-quality data recorded by the ATLAS detector, enabling them to conduct state of the art analyses in particle physics.

GET STARTED







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# Extra Notes on Open Data Release



- Publications will not be reviewed by, endorsed by, or marked as ATLAS
  - We will, however, provide instructions for how to cite and acknowledge our work
- "ATLAS expects its members to publish as part of the collaboration but does not forbid them from publishing on open data"
- Composed an "appropriate set of MC samples" in PHYSLITE format
  - Including both baseline and variation samples for systematics, and some signals
  - Luminosity of ~2x the data to start (rounding to the nearest file)