HEP data analysis in Python ecosystem and community efforts

Eduardo Rodrigues
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Outline

Data analysis in High Energy Physics (HEP) has evolved considerably in recent years. In particular, the role of Python has been gaining much momentum, sharing at present the show with C++ as a language of choice.
To support and enhance the usage of Python across the community, the HEP Software Foundation created a PyHEP - "Python in HEP" - working group and has been organising PyHEP workshops since 2018. Moreover, many projects and analysis packages have seen the light, which are now providing interesting, modern and alternative ways to perform analysis, in Python. In short, a global community effort is only getting stronger. I have been intimately involved in all these endeavours, and will provide an overview of the landscape. I will also detail the Scikit-HEP project I started in late 2016 with a few colleagues from various backgrounds and domains of expertise. Scikit-HEP is a community-driven and community-oriented project with the aim of providing Particle Physics at large with an ecosystem for data analysis in Python. It has developed considerably in the past year and is now part of the official software stack of experiments such as Belle II and KM3NeT.

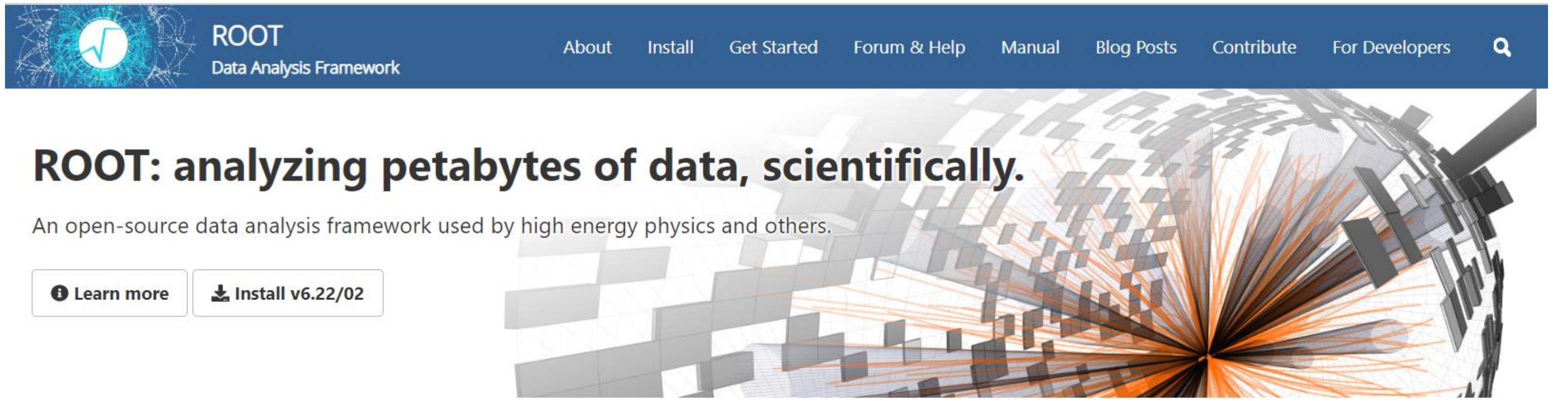
- ❑ **Particle Physics and Big Data**
- ❑ **The reign of Python**
- ❑ **Community efforts – HSF, PyHEP**
- ❑ **The PyHEP 2020 workshop**
- ❑ **The Scikit-HEP project**
- ❑ **Community software projects**
- ❑ **Final remarks**

Particle Physics and Big Data
Some "random" thoughts

- ❑ **"Big Data" projects**
- ❑ **Setting the scene**

Particle Physics and Big Data

- A lot of what has happened in the HEP Python ecosystem (recent years) can be thought of as trying to bridge the Particle Physics & Big Data worlds
  and profit from what the Data Science scientific software stack has to offer
- We will come back to software, but what about the data itself? Is that "Big Data"?
- The CERN ROOT team advertises that of the order of 1 EB of data exists right now in the *.root* format:



- Impressive. We are already in the exascale era!

Particle Physics and Big Data – on the CERN Data Centre storage

- For the record, the CERN Data Centre had accumulated more than 200 PB of data back in 2017 already!
  - CERN news, July 6, 2017

- And in just an extra 1.5 years, 50% more data got saved in CERN's Data Centre

- Citing the CERN news, March 1, 2019:

> *"The CERN Advanced Storage system (CASTOR), which relies on a tape-based backend for permanent data archiving, reached 330 PB of data (equivalent to 330 million gigabytes) stored on tape, an equivalent of over 2000 years of 24/7 HD video recording. In November 2018 alone, a record-breaking 15.8 PB of data were recorded on tape, a remarkable achievement given that it corresponds to more than what was recorded during the first year of the LHC's Run 1."*

- In fact, in 2018, over 115 PB of data in total (including about 88 PB of LHC data) were recorded on tape

CERN Data Centre passes the 200-petabyte milestone

The CERN Data Centre passed a major milestone on 29 June 2017 with more than 200 petabytes of data now archived on tape

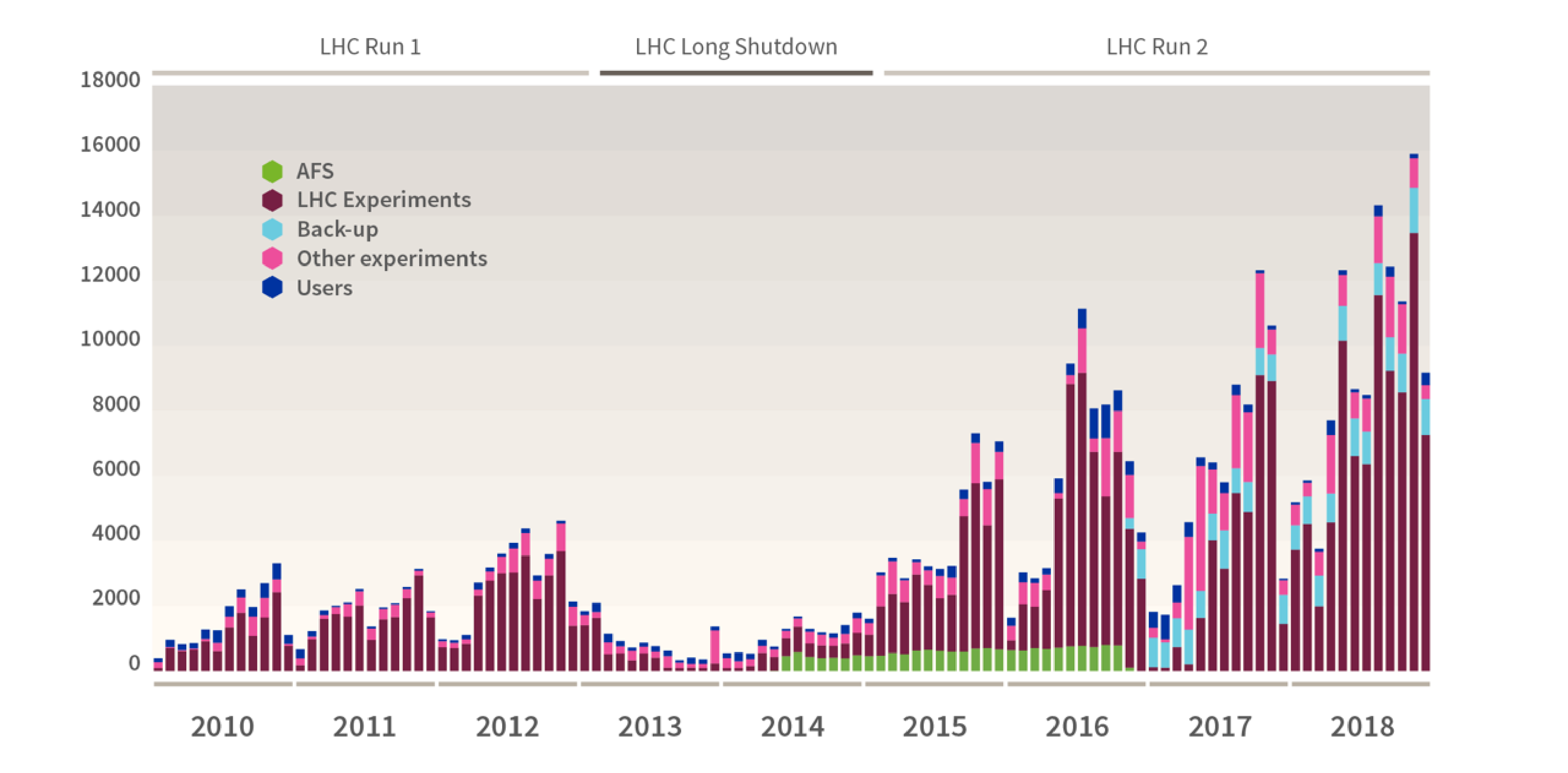
6 JULY, 2017 | By Mélissa Gaillard

CERN's Data Centre (Image: Robert Hradil, Monika Majer/ProStudio22.ch)

On 29 June 2017, the CERN DC passed the milestone of 200 petabytes of data permanently archived in its tape libraries. Where do these data come from? Particles collide in the Large Hadron Collider (LHC) detectors approximately 1 billion times per second, generating about one petabyte of collision data per second. However,

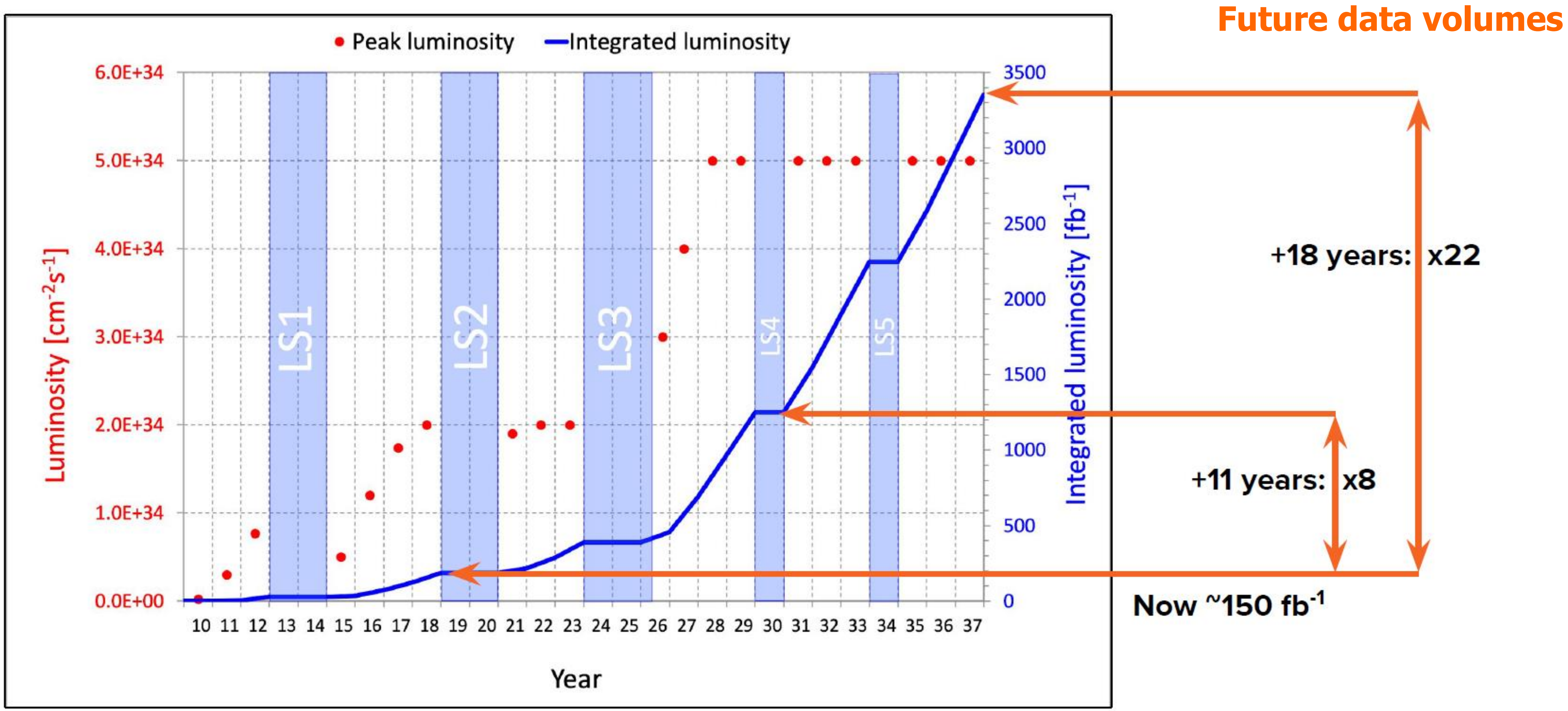
Particle Physics and Big Data – on the CERN Data Centre storage

- The accumulation of data generated by the LHC experiments alone, over a decade-ish, speaks for itself, as seen by this graph on CERN computing:
  data (in terabytes) recorded on tapes at CERN month-by-month (2010–2018)



Taken from CERN CDS.

A "Big Data project" – HL-LHC (High Luminosity LHC)



Beautification of https://lhc-commissioning.web.cern.ch/lhc-commissioning/schedule/images/optimistic-nominal-19.png taken from Ben Krikler

Another "Big Data project" – SKA

SQUARE KILOMETRE ARRAY
Exploring the Universe with the world's largest radio telescope

Square Kilometer Array

Minh Huynh, CHEP 2019
The Square Kilometre Array Computing

SDP headline design numbers*

- **Input**
  - ~800 GByte/s INGEST (in total), from Central Signal Processor
- **Temporarily store**
  - Data set up to 15 PBytes
  - 100PBytes total distributed buffer
- **Process**
  - 250 PFLOPS total peak
    - 10% efficiency assumed
- **Preserve and ship**
  - (up to) 2 PetaByte per day of Science Data Products

*all numbers subject to change (Totals for both SKA-Low and SKA-Mid SDP)

> 600 PB per year for around 50 years
⇒ 30 Exabytes of data
⇒ "Exascale computing"

7

Slide taken from Ben Krikler

Particle Physics and Big Data – and what about the outside world?

- Let's look at Amazon for the sake of argument:

> *"AWS Snowmobile is an Exabyte-scale data transfer service used to move extremely large amounts of data to AWS. You can transfer up to 100PB per Snowmobile, a 45-foot long ruggedized shipping container, pulled by a semi-trailer truck."*

Taken from Amazon page.

> *"Each Snowmobile includes a network cable connected to a high-speed switch capable of supporting 1Tbps of data transfer spread across multiple 40Gbps connections."*

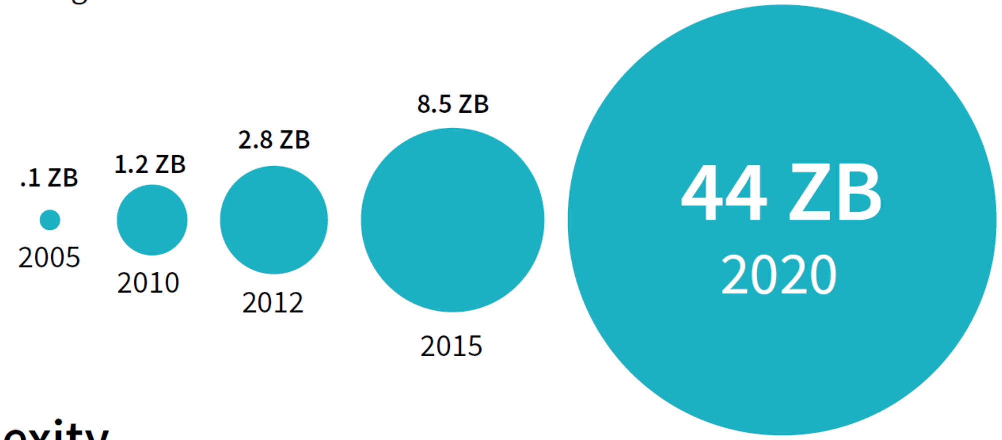
- To be compared with the throughput of 1-2 Tbps the LHCb experiment's first high-level trigger HLT1 (partial reconstruction on GPUs) will put to buffer while the real-time calibration and alignment is run, which is needed to digest the data in the HLT2 (full reconstruction) !

Particle Physics and Big Data – data is growing big, and fast!

- These solutions are necessary to massage the shear amounts of data being produced, and going to be produced, worldwide

Data Growth

Data, and how it is put to use, are key to any business success. At issue is that data volumes are increasing in an almost vertical trajectory, are becoming highly distributed, and can come in a variety of formats. According to IDC, global data generation will reach 180 zettabytes by 2025 — up from close to 10 zettabytes today.[1] Capitalizing on the promise of big data to fuel the next phase of innovation is an incredible challenge for any organization. Exploring data at scale and building models in real-time requires on-demand compute power and elastic infrastructure that is built for big data.

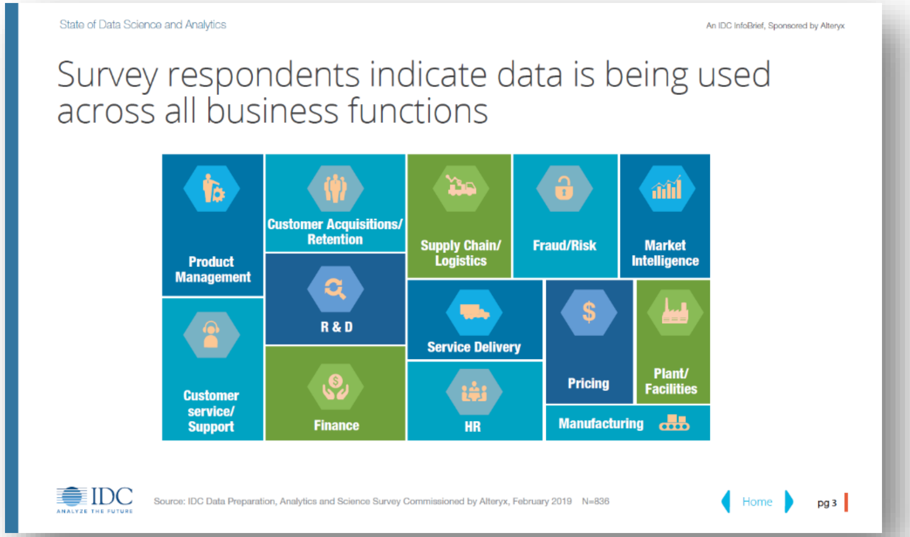


Infrastructure Complexity

Taken from this report.

Is it relevant and useful to learn non-HEP tools? Mostly Python, BTW!

- We've just quickly recalled that data requirements for Particle Physics match those of the Big Data world
- Huge amounts of data are in fact used by companies worldwide for just about any business, see for example the report "State of Data Science and Analytics, IDC InfoBrief, April 2019":

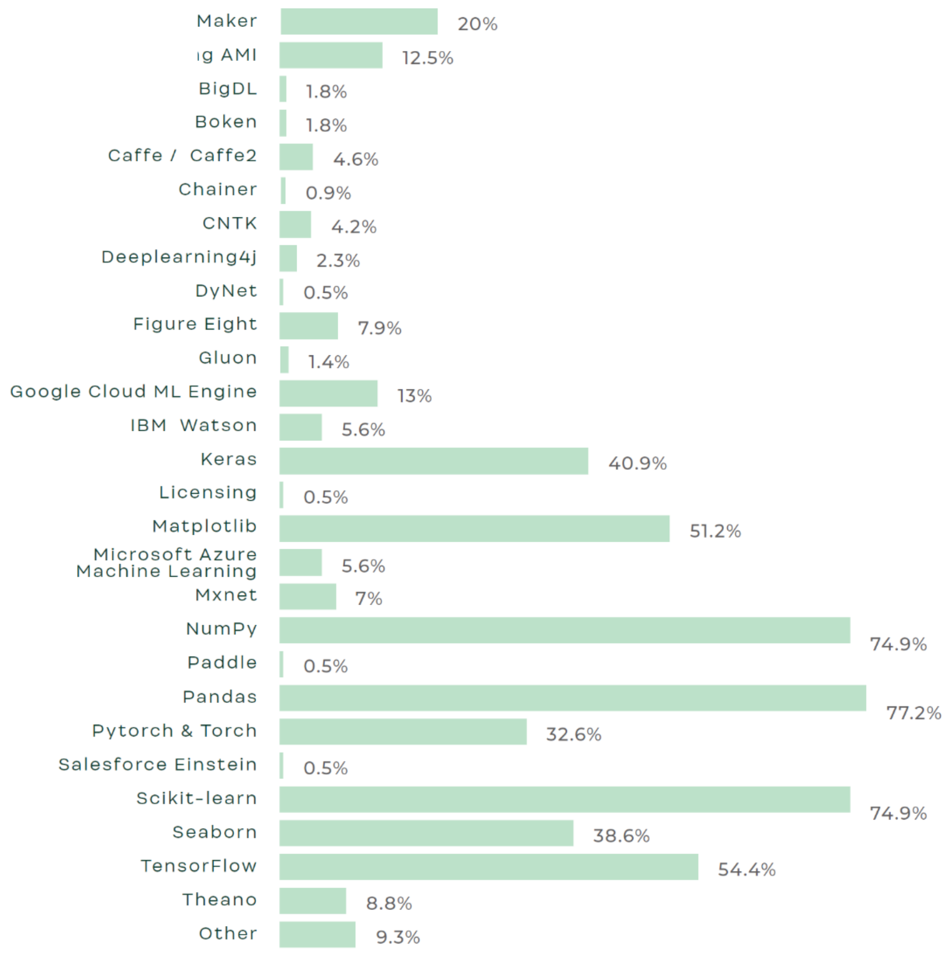


- International surveys indicate over 50M data workers worldwide!
- Can we really compete in terms of tools for data analysis?... Or should we rather try and profit from, and even contribute to, the huge ecosystem available to do Data Science?
- Anyway, what are data scientists, data engineers, etc., using for their daily work? That largely involves to some (larger and larger) extent Machine Learning, statistics, and even AI. International surveys give a hint ... the tools are dominated by Python tools ...!

Is it relevant and useful to learn non-HEP tools? Mostly Python, BTW!

- **From the 2019 Figure Eight report "The State of AI and Machine Learning":**

> *"Some popular frameworks and tools technical practitioners prefer in different stages of the ML pipeline are:*
> *Numpy and Pandas for loading data; Matplotlib for visualization;*
> *Scikit-learn and TensorFlow (including Keras) for ML models.":*



(Figure 17: Machine learning frameworks used by AI technical practitioners)

Tackling the challenges for (offline) data analysis – possible routes

Take aways

- Particle Physics and Data Science deal with Big Data and share requirements.
- The Data Science world has over the years built an extensive, powerful, well maintained and documented software ecosystem.
- It would be real shame for Particle Physics not to profit from it, as user but potentially also as a contributor.
- Python is the programming language of choice.

❑ **Lots of data?**
⇒ **Look at what the Big Data community is doing**

❑ **Evolution of computing resources won't be enough to digest all data**
⇒ **Use resources as efficiently as possible**

❑ **Physicists want to minimise the "time to insight". But coding takes a fair share of one's time, and is error-prone.**
⇒ **Adopt open-source best practices, popular and easy languages**

⇒ ***This talk will focus on offline data analysis tools, hence post trigger processing***

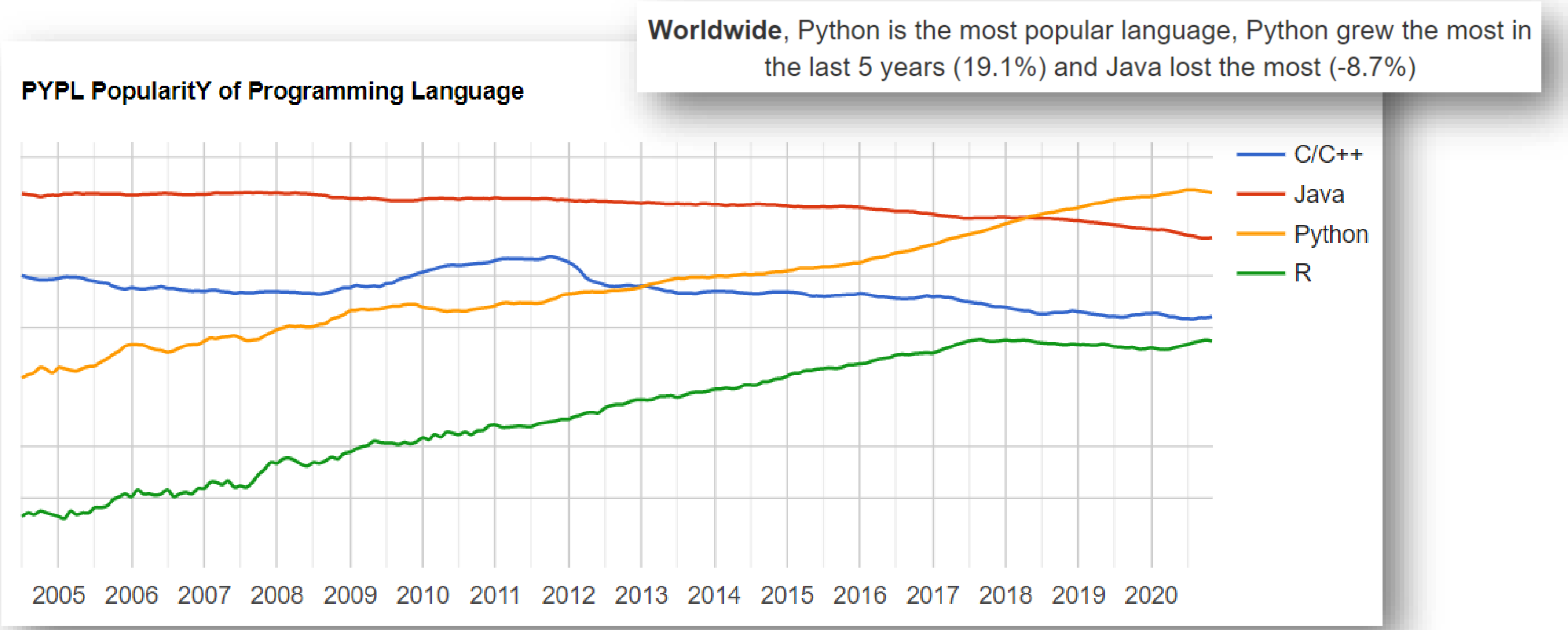
(it will not discuss ROOT either)

The reign of Python

- Popularity has never been so high
  - in Data Science
  - in Particle Physics

Python (in HEP), you say?

- ❑ PopularitY of Programming Languages (PYPL) – Python is the big winner!
- ❑ Popularity based on how often language tutorials are searched for
  - Data from Google Trends
  - Log scale!
- ❑ Same conclusion for popularity of languages for ML



[Taken from http://pypl.github.io/PYPL.html]

Why?

- ❑ Very large software ecosystem built atop NumPy and SciPy
- ❑ With very large and active community
- ❑ In general, excellent documentation and community support

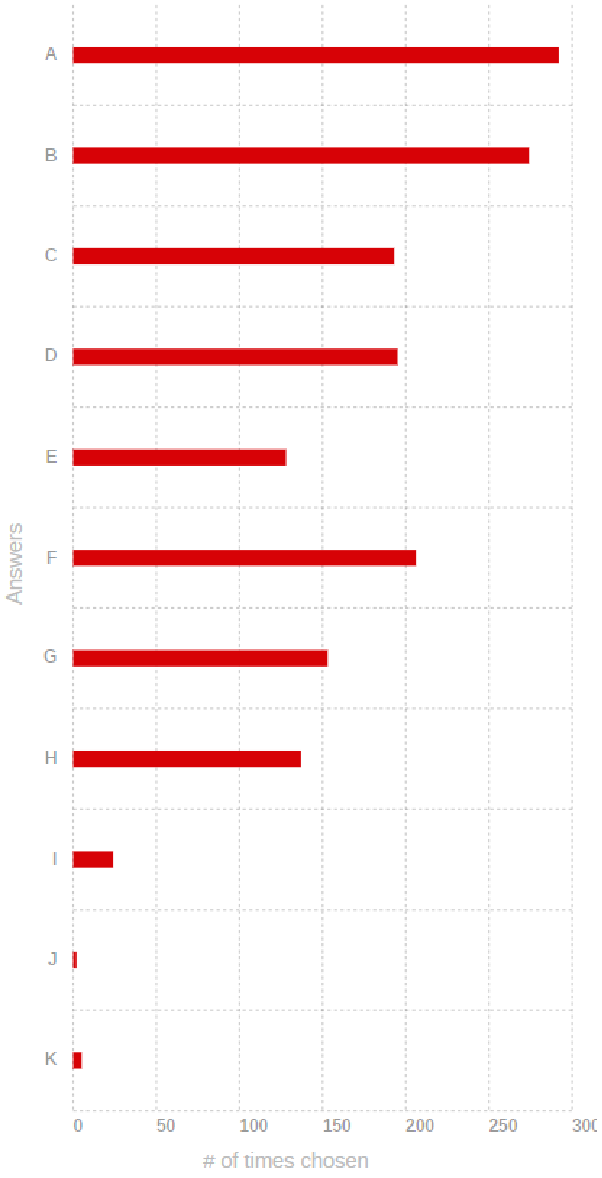
(All Open Source – FOSS has proven its worth!)

- ❑ …

Why do particle physicists use Python ?

What are your main reasons for using Python? — **Answered:** *405*

- **A. Availability of general-purpose data analysis toolkits**: 292 (18.15%)
- **B. Availability of machine learning/deep learning toolkits**: 274 (17.03%)
- **C. Availability of particle physics analysis tools (other than ROOT)**: 193 (12.00%)
- **D. Availability of ROOT through PyROOT**: 195 (12.12%)
- **E. Availability of collaboration-specific software in Python**: 128 (7.96%)
- **F. Development speed and efficiency**: 206 (12.80%)
- **G. Ability to use Python as an interface to other software**: 153 (9.51%)
- **H. Just because I like Python**: 137 (8.51%)
- **I. Not a choice: requirement comes from other constraints**: 24 (1.49%)
- **J. I don't use Python**: 2 (0.12%)
- **K. Other reasons, not listed above**: 5 (0.31%)



Taken from the PyHEP 2020 pre-workshop survey (408 respondents)

Python adoption in HEP – CMS study

Direct method: look at their code!

GitHub API lets us query users and repositories (URL → JSON).

Can we identify "physicist" users?

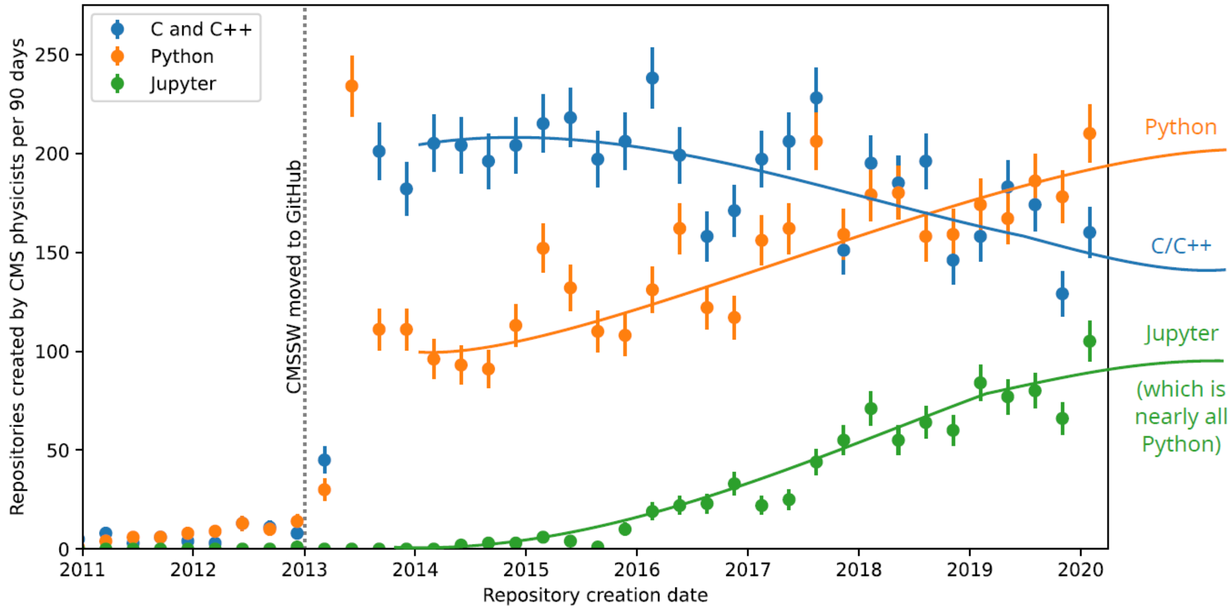
- CMSSW has been on GitHub since 2013.
- Assumption: most users who fork CMSSW are CMS physicists.
- Then examine their **non-fork** repositories.

Why GitHub/CMS? Until recently, all (free) GitHub repos were public, making them searchable by the API.

Large dataset: **3100 users** with **19 400 non-fork repos** spanning **7 years**.

- **Study by Jim Pivarski**
  [presentation @ Snowmass 2021, Aug. 11th]
- **Not from survey but rather directly using GitHub API to measure software adoption**

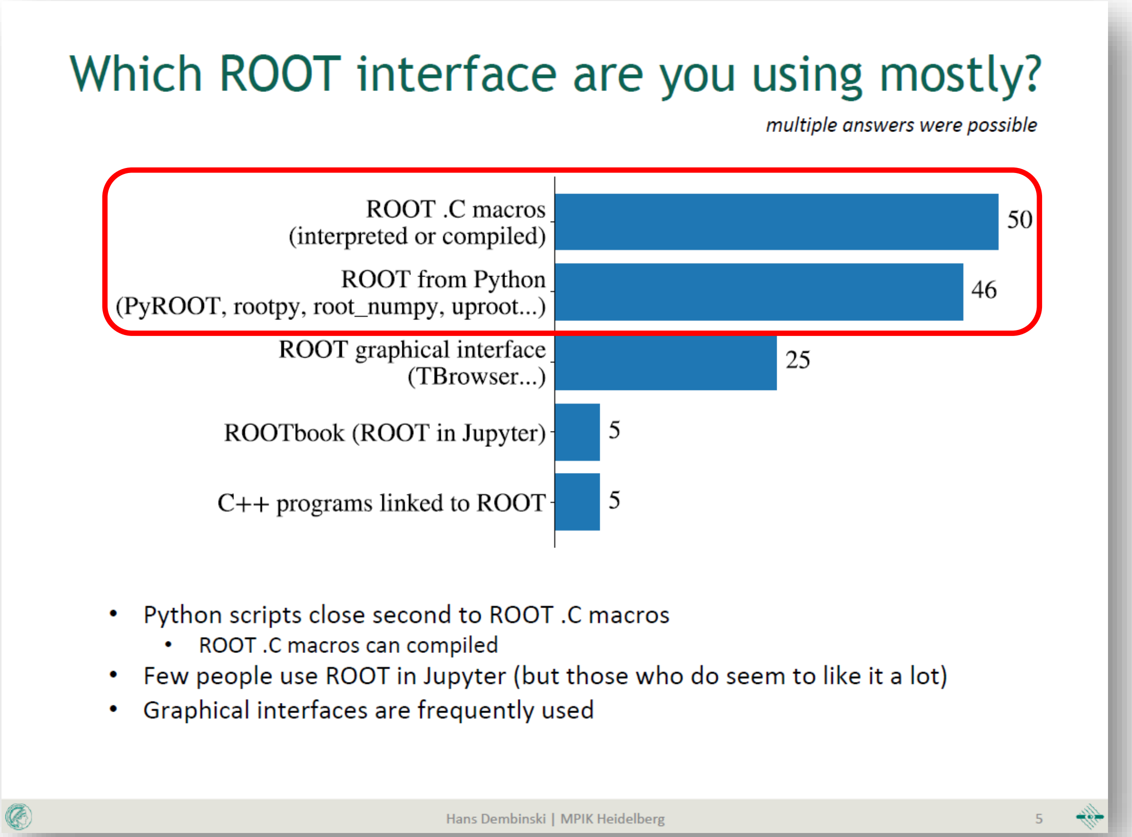
Language of repos created by CMS physicists



Python adoption in HEP – ROOT from Python in LHCb

Surveys from the LHCb experiment

- ❑ Python and C++ equally used among analysts
  - Trend seen in our LHCb survey for the ROOT User's Workshop in 2018
  - And in the LHCb 2018 Analysis Survey Report (by Eduardo Rodrigues)
- ❑ ROOT from Python is just as used as is from plain C++ !
- ❑ Conclusion even stronger if discussing analysis tools independent of ROOT



Taken from
Hans Dembinski, *User Feedback from LHCb*, ROOT Users' workshop, Sarajevo, Sep. 2018

Community efforts

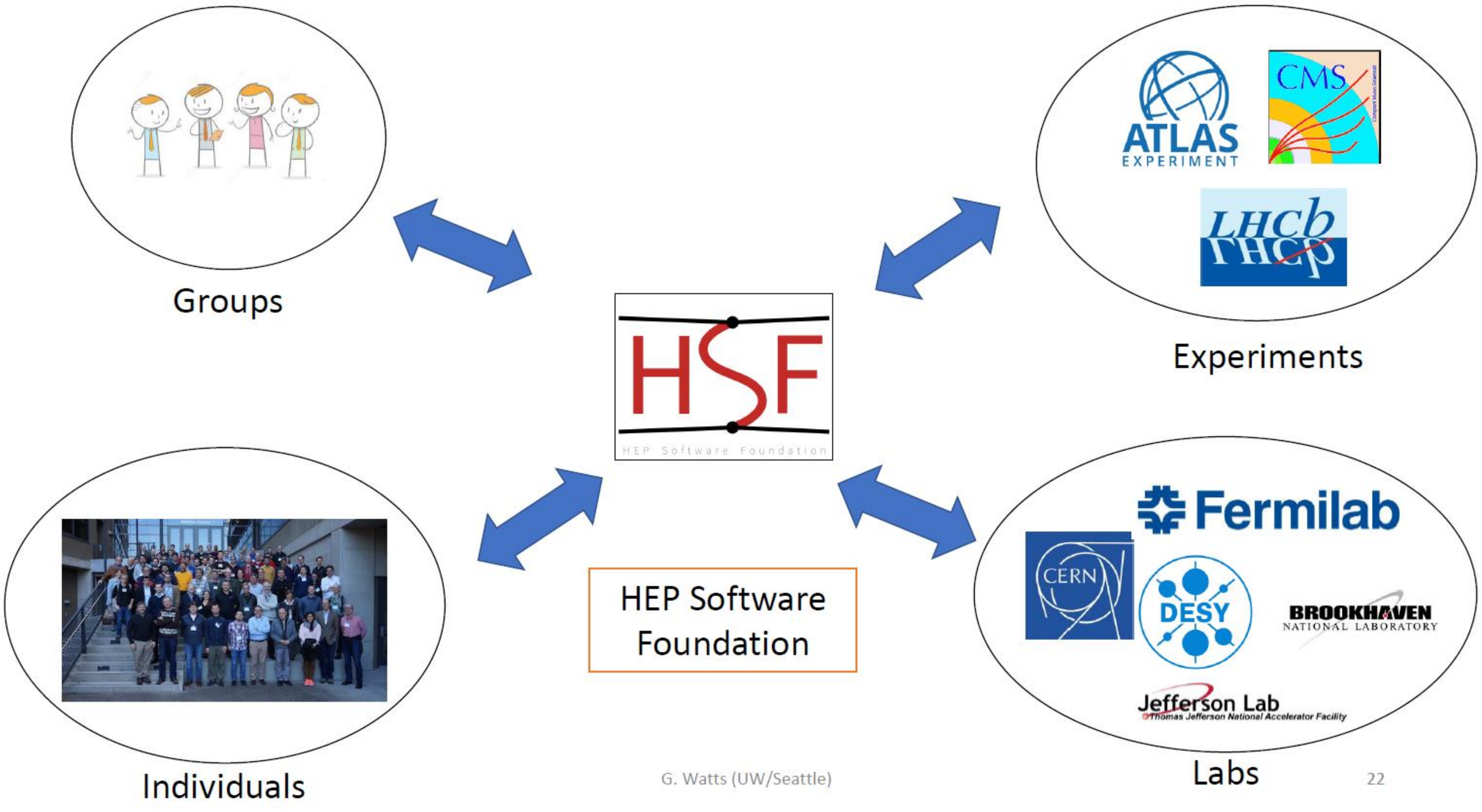
- The HEP Software Foundation (HSF)
- HSF PyHEP – “Python in HEP” Working Group
- PyHEP series of workshops
- Community projects towards a HEP Python ecosystem

The HEP Software Foundation (HSF)

- The goal of the HEP Software Foundation (HSF) is to facilitate coordination and common efforts in software and computing across HEP in general
  - Our philosophy is bottom up, a.k.a. *Do-ocracy*
  - Also work in common with like-minded organisations in other science disciplines
- Founded in 2014, explicitly to address current and future computing & software challenges in common
- Finalised in Dec. 2017 a Community White Paper (CWP) "A Roadmap for HEP Software and Computing R&D for the 2020s"
  - Almost all major domains of HEP Software and Computing covered
  - Large support for the document from the community (> 300 authors from >120 institutions)
  - Comput Softw Big Sci (2019) 3, 7; arXiv:1712.06982
- The CWP was a major accomplishment made by the community, with HSF "coordination"
- But it was a milestone, not a final step
- HSF activities post-CWP are very diverse …
- 2020: new community document "HL-LHC Computing Review: Common Tools and Community Software", Stewart, Graeme Andrew *et al*. (2020, May 1). Zenodo. http://doi.org/10.5281/zenodo.3779250, HSF-DOC-2020-01

HSF - "facilitate coordination and common efforts"

Gordon Watts, ACAT 2019



HSF – PyHEP ("Python in HEP") Working Group

HSF
HEP Software Foundation

- **The "Python in HEP" WG effectively started in early 2018 as an activity group**
  - **I put it forward with the proposal of the 1st workshop, held as a pre-CHEP 2018 event**
- **It became "formally" a WG this year ☺**

Activities ▾ | Working Groups ▾

Differentiable Computing
Season of Docs
Google Summer of Code
Licensing
Quantum Computing
Reviews
Software Forum
Visualisation

Data Analysis
Detector Simulation
Frameworks
Physics Generators
PyHEP - Python in HEP
Reconstruction and Software Triggers
Software Developer Tools and Packaging
Training

indico
Home | Create event ▾ | Room booking
Home » Projects » HEP Software Foundation
HEP Software Foundation

Weekly meetings
HSF workshops and events
Working groups
Software Forum
Training

HSF – PyHEP ("Python in HEP") Working Group

- Lots of ways to communicate !
  - The main (Gitter) channel now has over ~160 people registered

The PyHEP working group brings together a community of developers and users of Python in Particle Physics, with the aim of improving the sharing of knowledge and expertise. It embraces the broad community, from HEP to the Astroparticle and Intensity Frontier communities.

The group is currently coordinated by Ben Krikler (CMS, LZ), Eduardo Rodrigues (LHCb) and Jim Pivarski (CMS). All coordinators can be reached via hsf-pyhep-organisation@googlegroups.com.

Getting Involved

Everyone is welcome to join the community and participate by means of the following:

- Gitter channel PyHEP for any informal exchanges.
- GitHub repository of resources, e.g., Python libraries of interest to Particle Physics.
- Twitter Handle: #PyHEP

Extra Gitter channels have been created by and for the benefit of the community:

- PyHEP-newcomers for newcomers support (very low entry threshold).
- PyHEP-histogramming for discussions around histogramming.
- mpl-hep for Matplotlib proposals related to Particle Physics.

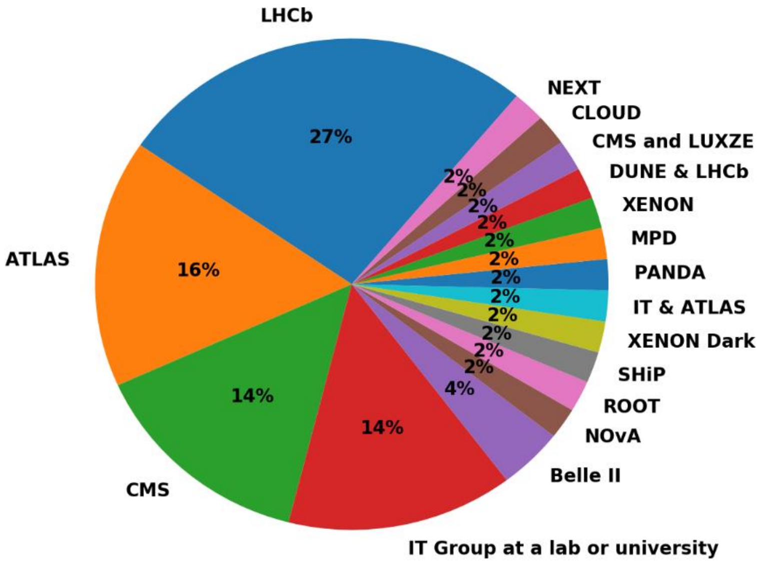
PyHEP Series of Workshops

PyHEP workshops – a (not so) new series of workshops

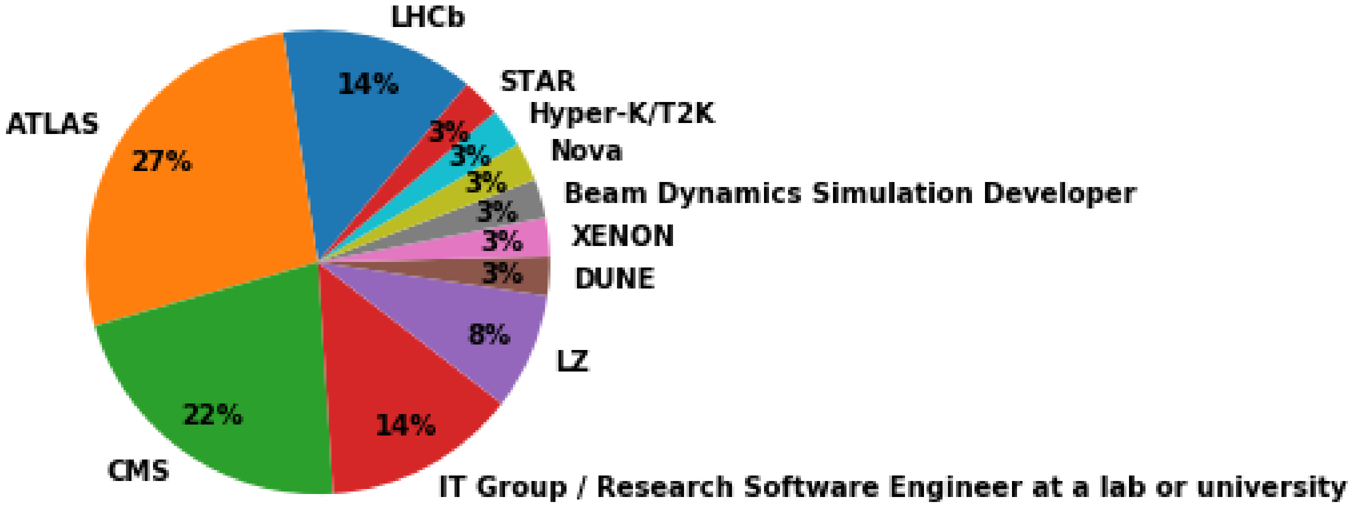
The **PyHEP workshops** are a series of workshops initiated and supported by the HEP Software Foundation (HSF) with the aim to provide an environment to discuss and promote the usage of Python in the HEP community at large. Further information is given on the PyHEP WG website.

- **Community diversity is paramount – great to see such a very diverse set of participants !**

PyHEP 2018
Sofia, Bulgaria



PyHEP 2019
Abingdon, U.K.



(Both pie charts taken from the pre-workshop questionnaires)

PyHEP workshops – a (not so) new series of workshops

Workshop raison d'être and goals, in brief

- **Step back and review evolution of Python in the HEP community at large**
  - There are certainly HEP conferences & workshops discussing computing & software but none really devoted to this critical language in analysis
- **Python clearly identified as first-class language during the Community White Paper process**
- **Need to consolidate this consensus and plan the future directions**
  - Where we are going, want to go, need to improve
  - Tools usage, needs and developments, training and education, which Python, etc.
- **Bring together users and developers from a wide audience**
- **Educative, not just informative, workshop, with lively discussions in the many free and dedicated time slots we foresaw**

Eduardo Rodrigues PyHEP 2018, Sofia, Bulgaria, 7 July 2018 2/6

Community projects towards a HEP Python ecosystem for data analysis

- Citing Gordon Watts (ACAT 2019) – how can we tackle the following issues?
  - Increased LHC dataset sizes and CPU requirements
  - Flat budgets & stable or decreasing staffing
  - New software tools and communities inside and outside HEP
  - High turn-over inside HEP
  - Educational responsibility

Tackle them as a community !

(Note that much of this is not HEP specific ;-))

- PyHEP WG serves as a forum for discussion, means to exchange experiences and material
- Our workshops present many of these packages and provide educative material

⇒ strong link with Training WG ☺

Various projects have seen the light:

- Coffea
- FAST-HEP
- Scikit-HEP (1st one of the gang)
- zfit

- https://github.com/CoffeaTeam
- https://github.com/FAST-HEP
- https://github.com/root-project/
- https://scikit-hep.org/
- https://github.com/zfit

PyHEP 2020 Workshop

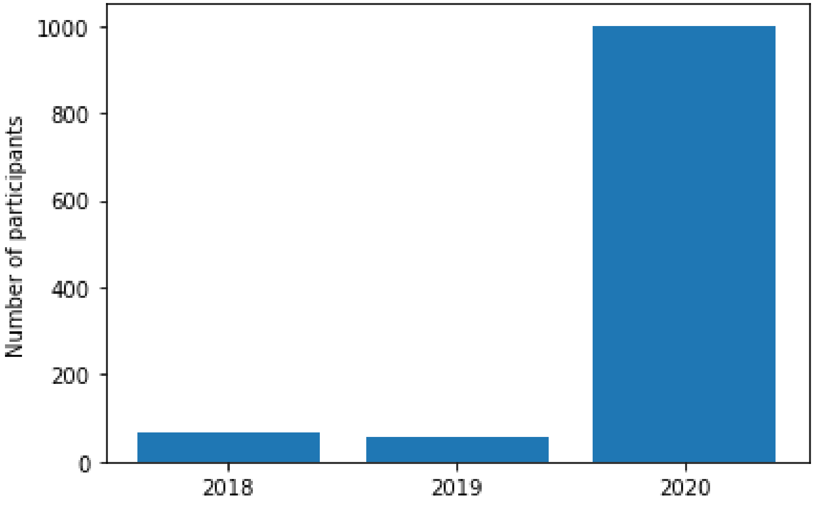
We now even have a logo ☺ !

- ❑ A special cuvée
- ❑ On organisational aspects
- ❑ Highlights

- ❑ BTW, *a lot more information* in the back-up slides …

PyHEP 2020, a special cuvée

- 3rd edition was meant to be in the US for the first time, co-locating with the important SciPy 2020 conference
  - We even had a nice poster ;-)!
- We engaged with this very large scientific community
  - Had several talks from HEP colleagues @ SciPy 2020
- But we both had to materialise as a virtual event given the worldwide situation with COVID-19
- Truly global event with participants from all over the world (benefit from running virtual)
  - Impressive level of interest with 1000 registrations (limited to) (72, 55 in previous years)



PyHEP 2020 – Indico page, organising team, sponsors

PyHEP 2020 (virtual) Workshop

13-17 July 2020
US/Central timezone

- Overview
- Call for Abstracts
- Timetable
- Registration
- Participant List
- Poster
- Code of conduct
- EDI statement
- Workshop photos

Contact us

pyhep2020-organisation...

Organising Committee

Eduardo Rodrigues - University of Liverpool (Chair)
Ben Krikler - University of Bristol (Co-chair)
Jim Pivarski - Princeton University (Co-chair)
Matthew Feickert - University of Illinois at Urbana-Champaign

Local organisation

Chris Tunnell - Rice University
Peter Onyisi - The University of Texas at Austin

Sponsors

The event is kindly sponsored by

iris hep – Institute for Research & Innovation in Software for High Energy Physics
University of Liverpool
python Software Foundation
Software Sustainability Institute
Fermilab

- **Great list of kind sponsors is a proof of workshops being relevant and attracting attention – my personal opinion ;-)**

PyHEP 2020 organisational aspects – overview

- **Zoom video conferencing system**
  - With capacity for 1000 participants
  - Public room but PIN provided via email

- **Slack channels**
  - Various channels:
    - By topic, mapping to sessions, discussions encouraged here
    - Announcements, for actual announcements
    - Random, used to encourage community spirit and add social context

- **Questions & answers with slido**
  - Used *slido* to crowd-source questions, to prioritise the most popular ones upvoted by participants
  - Session chair shares link to questions at end of presentation
  - Most popular ones get answered/discussed
  - At end of Q&A all questions are copied to Slack in the appropriate topical channel
    $\Rightarrow$ participants can continue to discuss and exchange
  - A few polls also run via slido

- **Communication also on**

- **Sessions & presentations**
  - Spread in sessions for "Atlantic"- and "Pacific"-friendly time zones
  - We strongly encouraged notebook presentations, available in public Github repositories with a Binder launch button
  - All presentational material posted on workshop agenda and later given a DOI with Zenodo, in a dedicated "pyhep2020 community" – formal citation, replaces proceedings
  - All talks got recorded, captioned and later uploaded to the HSF YouTube channel – dedicated playlist "PyHEP 2020 Workshop"

PyHEP 2020 organisational aspects – agenda (1/2)

Workshop agenda (1/2)

Keynotes

- Rubin Observatory: the software behind the science (Nate Lust)
- Python & HEP: a perfect match, in theory (David Straub)

Tutorials

- Uproot & Awkward Arrays (Jim Pivarski)
- Jagged physics analysis with Numba, Awkward, and Uproot on a GPU (Joosep Pata)
- Ganga: flexible virtualization for user-based large computations (Ulrik Egede)
- A prototype U.S. CMS analysis facility (Oksana Shadura)
- Columnar analysis at scale with Coffea (Mat Adamec)
- Introduction to automatic differentiation (Lukas Heinrich)
- High-performance Python (Henry Schreiner)
- Model-building & statistical inference with zfit and hepstats (Jonas Eschle)
- pyhf: accelerating analyses and preserving likelihoods (Matt Feickert)
- ThickBrick: optimal event selection and categorization in HEP (Prasanth Shyamsundar)

Typically 45 minutes

Eduardo Rodrigues PyHEP 2020, All@Home, 13 July 2020 6/11

PyHEP 2020 organisational aspects – agenda (2/2)

Workshop agenda (2/2)

Talks

- NanoEvents object (Nick Smith)
- TITANIA: how to structure dector monitoring (Jakub Kowalski, Maciej Witold Majewski)
- A new PyROOT for ROOT 6.22 (Enric Tejedor Saavedra)
- Resample: bootstrap and jackknife from Python (Hans Dembinski)
- Design pattern for analysis automation using Luigi (Marcel Rieger)
- ServiceX: on-demand data transformation & delivery (Kyungeon Choi)
- Integrating Coffea and WorkQueue (Cami Carballo)
- High granularity calorimeter (HGCAL) test beam analysis using Jupyter (Matteo Bonanomi)
- neos: physics analysis as a differentiable program (Nate Simpson)
- SModelS: a tool for interpreting simplified-model results (Wolfgang Waltenberger)
- TensorFlow-based maximum likelihood fits for high-precision Standard Model measurements at CMS (Josh Bendavid)
- Error computation in iminuit and MINUIT: how HESSE and MINOS work (Hans Dembinski)
- zfit with TensorFlow 2.0: dynamic and compiled HPC (Jonas Eschle)
- Machine learning for signal-background separation of nuclear interaction vertices in CMS (Anna Kropivnitskaya)
- The boost-histogram package (Henry Schreiner)
- Providing Python bindings for complex and feature-rich C and C++ libraries (Martin Schwinzerl)
- Integrating GPU libraries for fun and profit (Adrian Oeftiger)
- mplhep: bridging Matplotlib and HEP (Andrzej Novak)
- ROOT preprocessing pipeline for machine learning with TensorFlow (Matthias Komm)
- Integrated data acquisition in Python (Charles Burton)

Typically
20+10 minutes

Eduardo Rodrigues PyHEP 2020, All@Home, 13 July 2020 7/11

PyHEP 2020 logistics – Jupyter notebook talks / tutorials with Binder

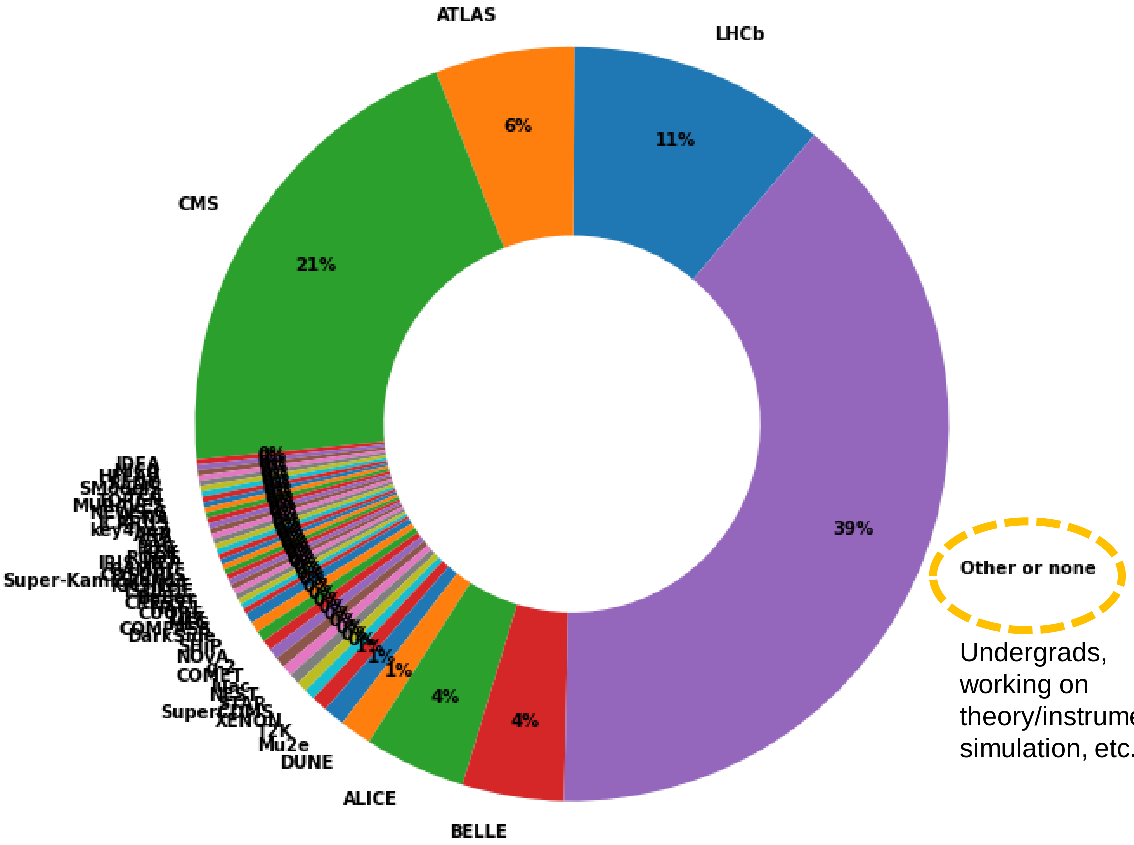
- We relied on **Binder to have interactive computing experiences for all Jupyter notebook presentations**
- Speakers with notebooks were requested to have a "launch binder" badge in their talk repositories
- Binder:
  - Free open-source project and service from the Jupyter team
  - Runs on donated compute resources from the Binder Federation
- We used both **Binder Federation and CERN Binder Hub resources** (for those with CERN accounts)
  - Got in touch with Binder team to have **resources allocated to talk repositories at the relevant time !**
  - It worked very well – thank you MyBinderTeam
  - Binder was a leitmotif during the workshop:
- With Zenodo + Binder, all code from the workshop should be reproducible into the future
  $\Rightarrow$ **"living workshop proceedings"!**
- Find out more at mybinder.org

binder | launch binder

From PyHEPConf Twitter account

PyHEP 2020 stats – diversity and inclusion

PyHEP 2020
Virtual event



Undergrads, working on theory/instrumentation/ simulation, etc.

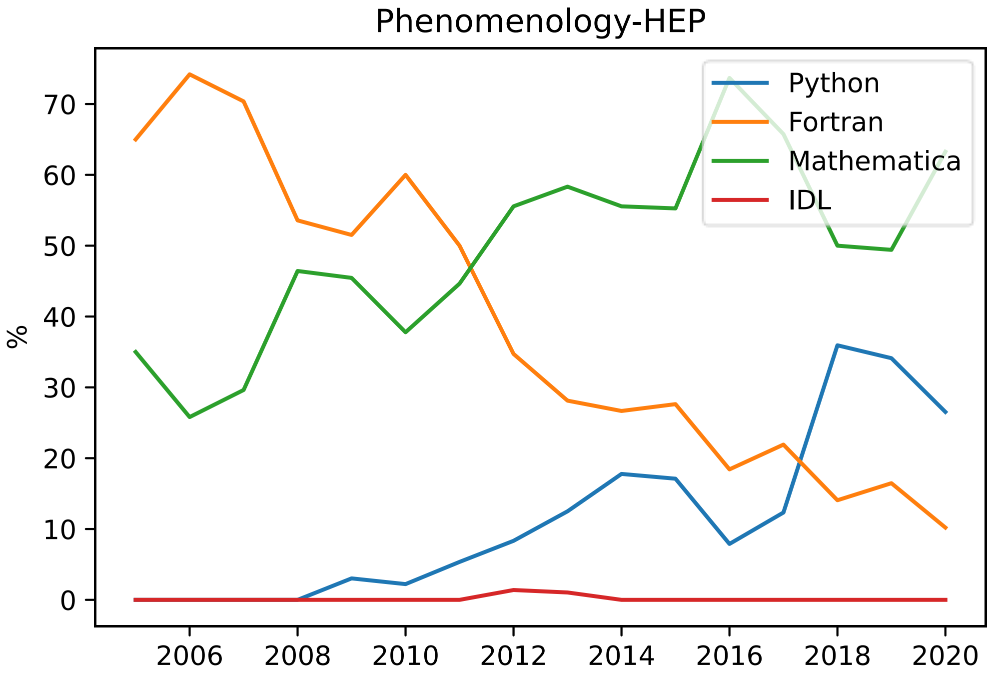
- Great to see such a diverse set of participants !

(Pie chart and "logo art" with information taken from the pre-workshop questionnaire)

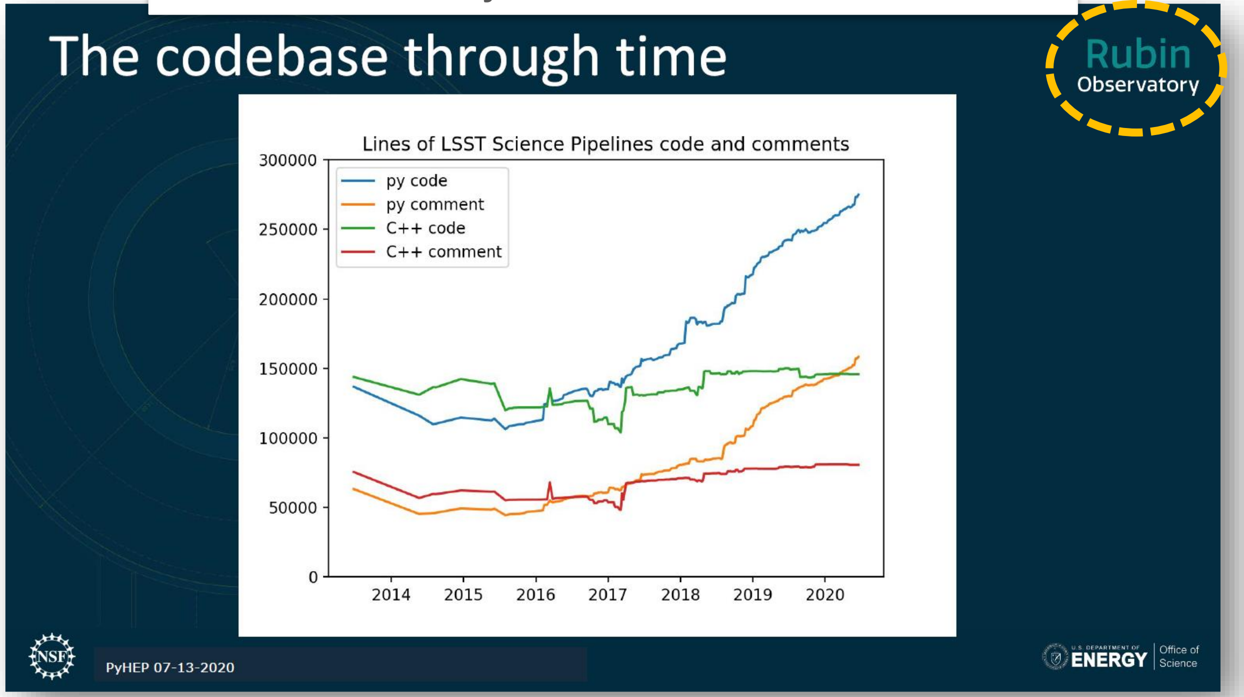
PyHEP 2020 highlights – keynote presentations

- ❑ **Python on the rise not just in experimental particle physics**

David Straub (flavour phenomenologist)
“Python & HEP: a perfect match, in theory”



Nate Lust (astronomy)
“Rubin Observatory: The software behind the science”



Challenges for Python in HEP-Ph

Python's full potential is harnessed when embracing the **open source paradigm**:

- Open source code
- Transparency (development, decision making, bugs!)
- Release early and often (software is **not** a paper!)
- Community

In HEP-Ph, there are very few open source projects in this sense, only "public codes".

PyHEP 2020 highlights – on trends

" Automatic differentiation is a method to compute exact derivatives of functions implements as **programs**. It's a widely applicable method and famously is used in many Machine learning optimization problems."

- **Auto-differentiation, specifically in the context of differentiable analysis, came out as an unforeseen "theme" and a new direction**
  - 1 tutorial and 1 talk on the subject

- Introduction to automatic differentiation (TUTORIAL)
- neos: physics analysis as a differentiable program

In HEP

Of course we can use automatic differentiation for neural networks. But other things in HEP also can make use of gradients. A prime example where this is the case is statistical analysis

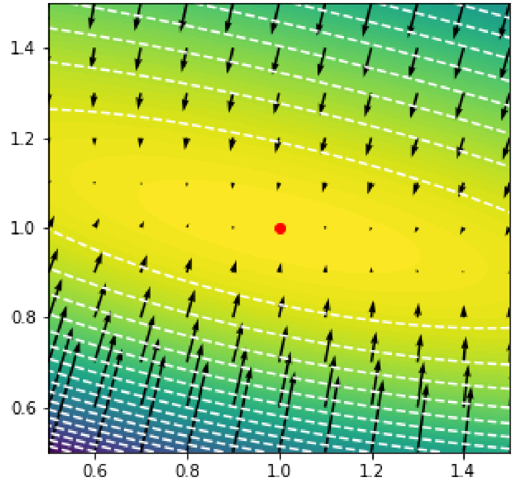
For a maximum likelihood fit we want to minimize the log likelihood

$\theta^* = \mathrm{argmin}_\theta(\log L)$

```
import jax
import jax.numpy as jnp
import numpy as np
import pyhf
import matplotlib.pyplot as plt
```

```
pyhf.set_backend('jax')
```

Define the model, fit … and plot:



(Taken from the tutorial)

gradHEP is an effort to consolidate differentiable building blocks for analysis into a set of common tools, and apply them.

See the 'Differentiable computing' HSF activity to find ways to get involved -- all are welcome at this very early stage! :)

gradHEP

The Scikit-HEP project

- ❑ **Motivation for such a community project**
- ❑ **Whirlwind tour of packages**

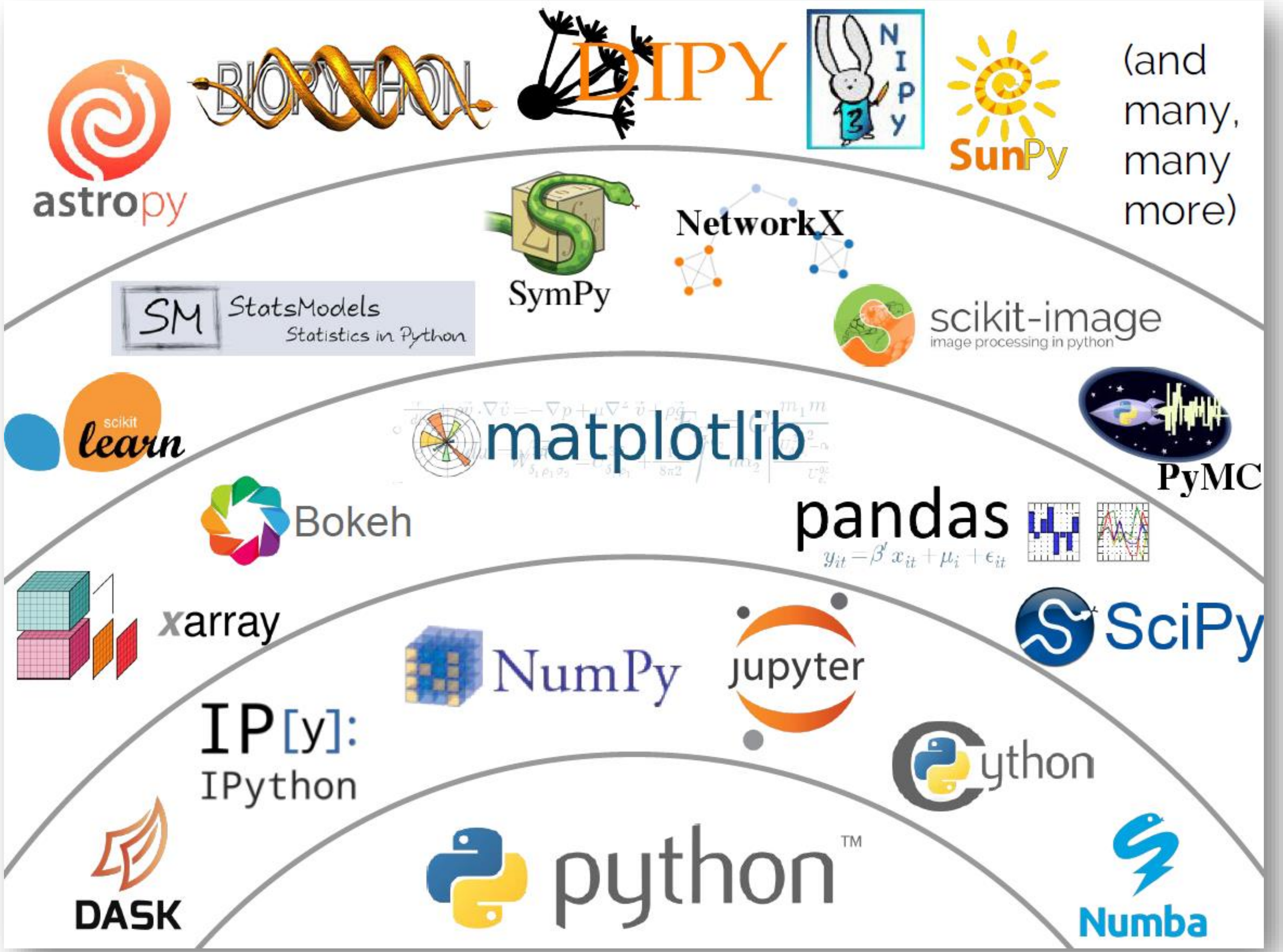
How’s the Python scientific ecosystem like, outside HEP?

Domain-specific

Python’s

Scientific

stack



What about HEP …?

Community projects towards HEP domain-specific Python tools ⇒ ecosystem

Jake VanderPlas,
The Unexpected Effectiveness of Python in Science,
PyCon 2017

Scikit-HEP project – the grand picture

- ❑ Create an ecosystem for particle physics data analysis in Python
- ❑ Initiative to improve the interoperability between HEP tools and the scientific ecosystem in Python
  - Expand the typical ~~toolkit~~ toolset for particle physicists
  - Set common APIs and definitions to ease “cross-talk”
- ❑ Promote high-standards, well documented and easily installable packages
- ❑ Initiative to build a community of developers and users
  - Community-driven and community-oriented project
  - Open forum to discuss
- ❑ Effort to improve discoverability of (domain-specific) relevant tools

Scikit-HEP project – overview of most popular and/or used packages

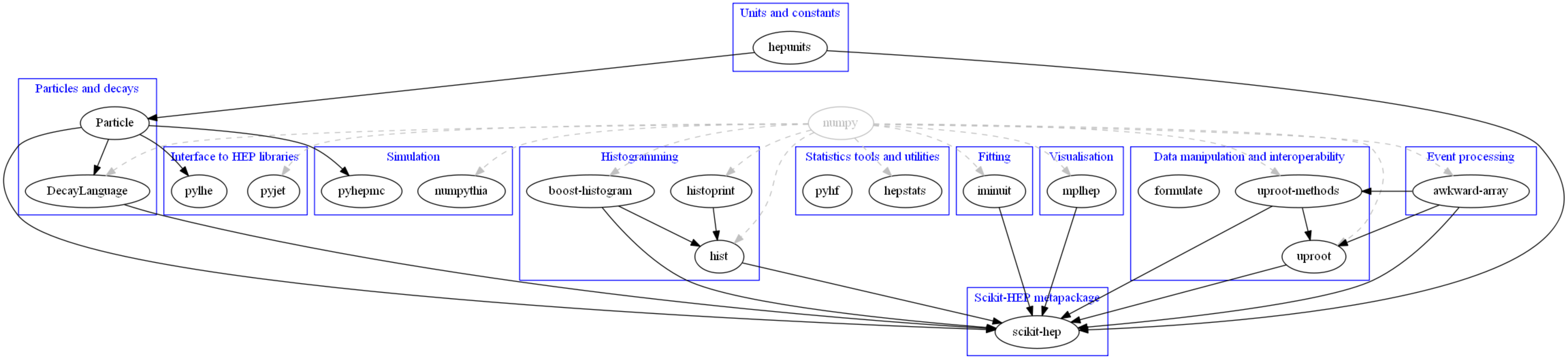
uproot
Awkward Array
iminuit
Boost-histogram
Scikit-HEP
pyhf
differentiable Likelihoods
hepstats
mplhep
hist
hepunits
histoprint
Particle
DecayLanguage
pylhe

[Not the full set of Scikit-HEP packages.]

Scikit-HEP project – packages and dependencies

- Pattern of inter-package dependencies nicely "explains" why the project is a *toolset* and not a toolkit !

https://scikit-hep.org/



Not a comprehensive list. There are other packages: test data, tutorials, org stats, etc.
(and some which tend to now be superseded, hence deprecated …)

Who uses (some of) Scikit-HEP ?

- Groups, other projects, HEP experiments
- Links are important, especially if they strengthen the overall ecosystem
- Good community adoption ⇔ we're on the right path ;-)
- Rewarding to collaborate / work with / interact with many communities
  - Responsibility and importance of sustainability …

Experiment collaborations

BelleII - the Belle II experiment at KEK, Japan.

CMS - the Compact Muon Solenoid experiment at CERN, Switzerland.

KM3NeT - the Kilometre Cube Neutrino Telescope, an Astroparticle Physics European research infrastructure located in the Mediterranean Sea.

Phenomenology projects

flavio - flavour physics phenomenology in the Standard Model and beyond.

Software projects

Coffea - a prototype Analysis System incorporating Scikit-HEP packages to provide a lightweight, scalable, portable, and user-friendly interface for columnar analysis of HEP data. Some of the sub-packages of Coffea may become Scikit-HEP packages as development continues.

The zfit project - it provides a model fitting library based on TensorFlow and optimised for simple and direct manipulation of probability density functions.

Data manipulation and interoperability – `uproot` "suite of packages"

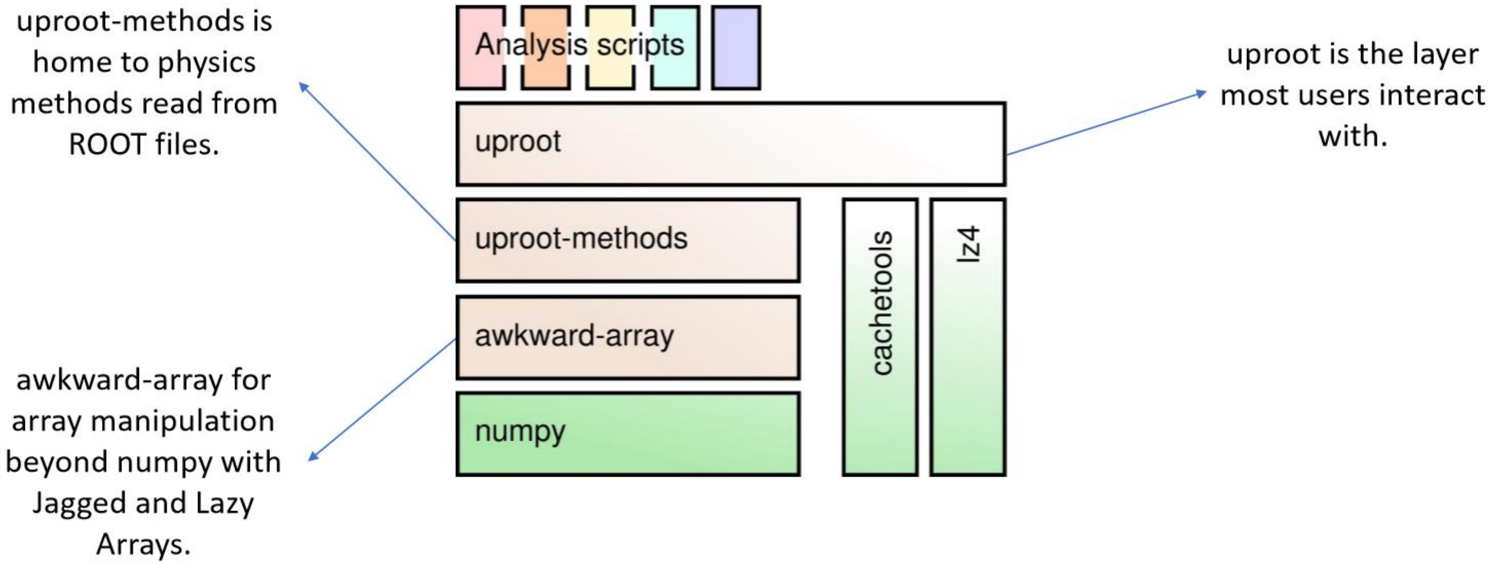
- (Does it still need an intro ;-)?)
- Trivially and Python-ically read ROOT files
- Need only NumPy, no ROOT, using this pure I/O library!
- Design and dependencies:

uproot

ROOT I/O
in pure Python and Numpy

uproot-methods

Pythonic mix-ins
for non-I/O ROOT classes



- Write ROOT files: newest development, limited scope = write Ttree, histograms and a couple more classes only
  - See talk at PyHEP 2019 workshop

Event processing – awkward-array package

- Provide a way to analyse nestes, variable-sized data in Python, by extending NumPy's idioms from flat arrays to arrays of data structures

Awkward Array

Manipulate arrays of complex data structures as easily as NumPy

- Pure Python+NumPy library for manipulating complex data structures even if they
  - Contain variable-length lists (jagged/ragged)
  - Are deeply nested (record structure)
  - Have different data types in the same list (heterogeneous)
  - Are not contiguous in memory
  - Etc.
- This is all very relevant and important for HEP applications !

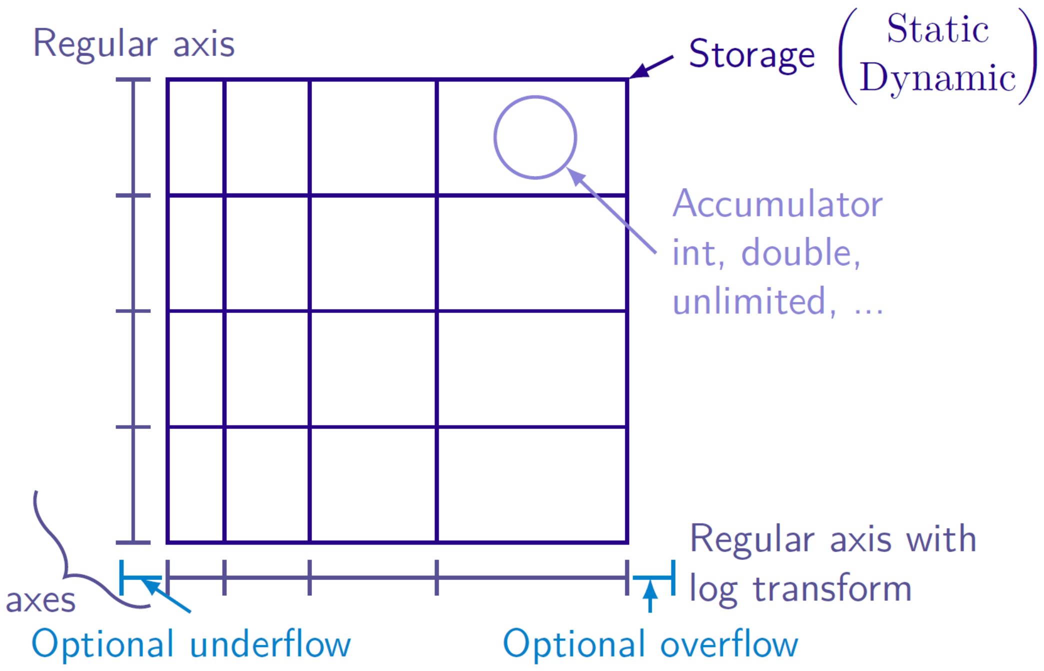
```
pip install awkward                  # maybe with sudo or --user, or in virtualenv
pip install awkward-numba            # optional: integration with and optimization by Numba
```

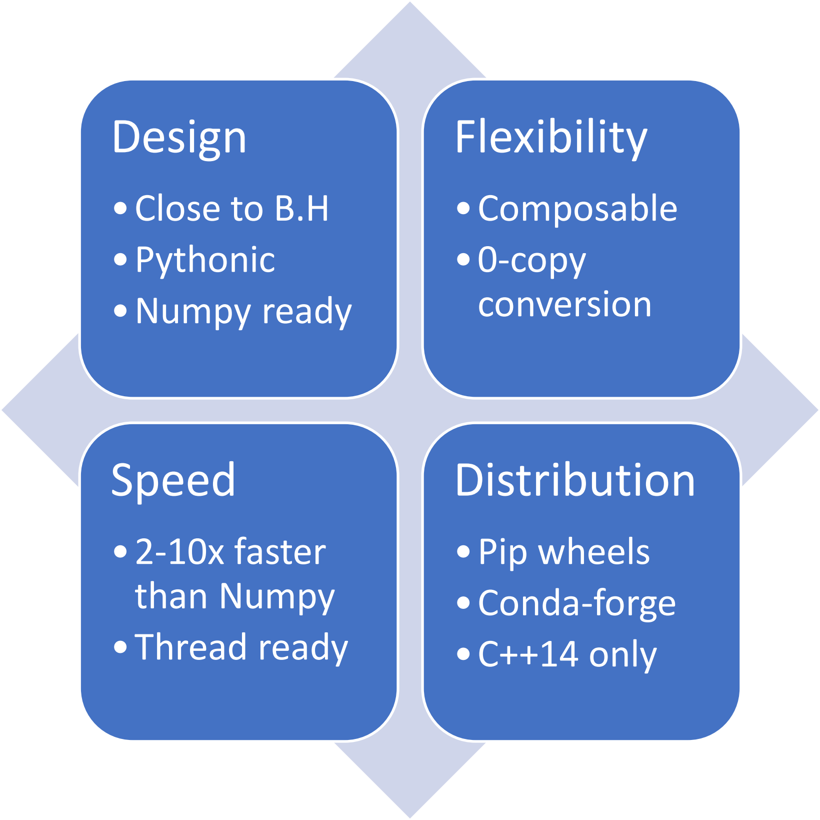
- Package re-implemented in C++, with a simpler interface and less limitations
  - Major endeavour
  - See https://github.com/scikit-hep/awkward-1.0 ...
- BTW, uproot 4 is re-engined based on awkward-1.0

P.S.: Uproot and awkward-arraw would need a talk on their own ! Go and explore …

Histogramming – `boost-histogram` package

- (pybind11) Python bindings for the C++14 Boost.Histogram library
  (multi-dimensional templated header-only, designed by Hans Dembinski)
- A histogram is seen as collection of Axis objects and a storage
  - Several types available, e.g. regular, circular, category





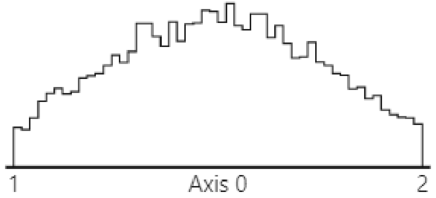
Histogramming & visualisation – build atop `boost-histogram` `Hist`

- Trivial creation and display in notebooks !

```python
import hist
from hist import Hist
import numpy as np
```

1. Cool representations in notebooks

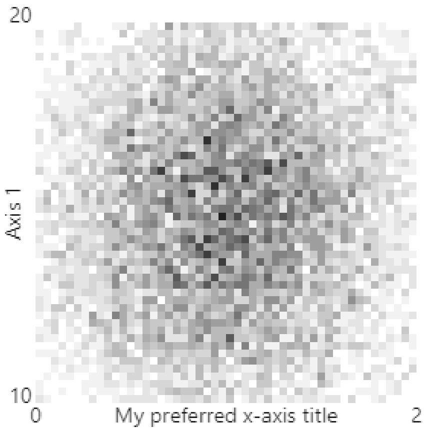
```python
Hist.new.Reg(50, 1, 2).Double().fill(np.random.normal(1.5, 0.3, 10_000))
```



Regular(50, 1, 2, label='Axis 0')

Double() Σ=8984.0 *(10000.0 with flow)*

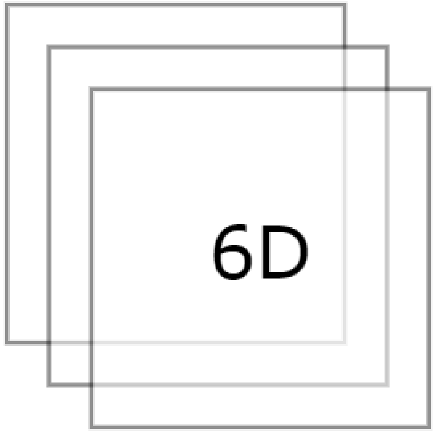
```python
h2 = Hist.new.Reg(50, 0, 2, name='My preferred x-axis title').Reg(50, 10, 20).Double().fill(
    np.random.normal(1, 0.5, 10_000), np.random.normal(15, 3, 10_000)
)
h2
```



Regular(50, 0, 2, name='My preferred x-axis title', label='My preferred x-axis title')
Regular(50, 10, 20, label='Axis 1')

Double() Σ=8638.0 *(10000.0 with flow)*

```python
# Add the axes using the shortcut method
h = (
    Hist.new.Reg(10, -5, 5, overflow=False, underflow=False, name="A")
    .Bool(name="B")
    .Var(range(10), name="C")
    .Int(-5, 5, overflow=False, underflow=False, name="D")
    .IntCat(range(10), name="E")
    .StrCat(["T", "F"], name="F")
    .Double()
)
h
```



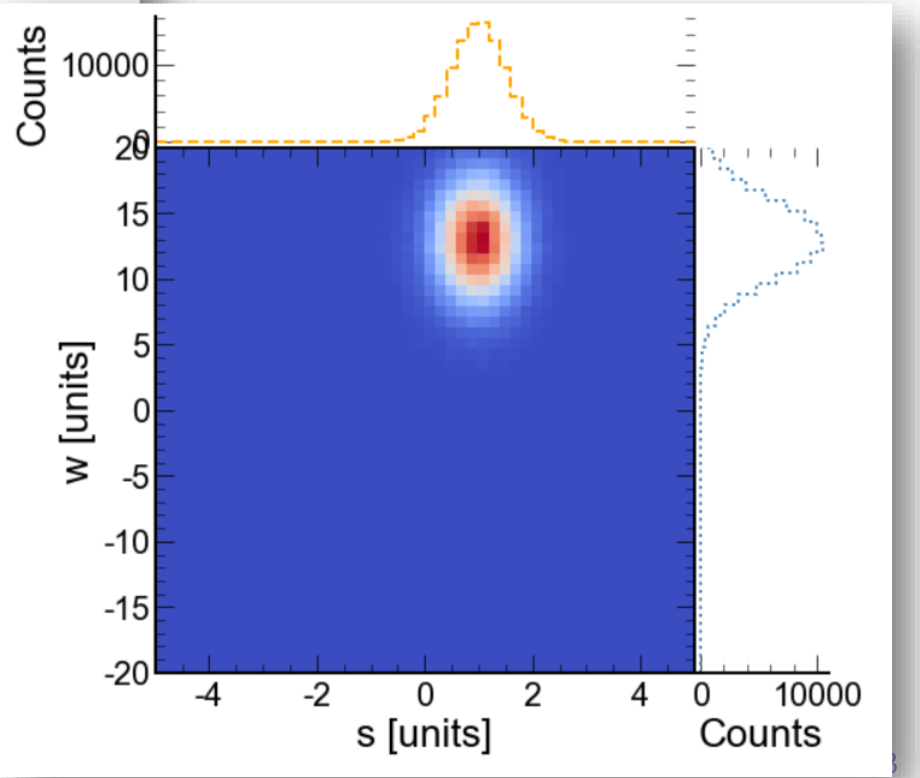
Regular(10, -5, 5, underflow=False, overflow=False, name='A', label='A')
Boolean(, name='B', label='B')
Variable([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
Integer(-5, 5, underflow=False, overflow=False)
IntCategory([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
StrCategory(['T', 'F'])

Double() Σ=0.0

- Several types of axis available

Histogramming & visualisation – build atop `boost-histogram`


```python
h = Hist(
    hist.axis.Regular(50, -5, 5, name="S", label="s [units]", flow=False),
    hist.axis.Regular(50, -5, 5, name="W", label="w [units]", flow=False),
)

import numpy as np

s_data = np.random.normal(size=10_000) + np.ones(10_000)
w_data = np.random.normal(size=10_000)
s_data = np.random.normal(1, 0.5, 100_000)
w_data = np.random.normal(13, 3, 100_000)

# normal fill
#h.fill(s_data, w_data)
#h = Hist.new.Reg(50, 0, 2, name="S", label="s [units]", flow=False).Reg(50, 10, 20, name="W", label="s [units]", flow=False).Double().fill(
#    np.random.normal(1, 0.5, 100_000), np.random.normal(15, 0.5, 100_000)
#)
h = Hist.new.Reg(50, -5, 5, name="S", label="s [units]", flow=False).Reg(50, -20, 20, name="W", label="w [units]", flow=False).Double().fill(
    s_data, w_data)

# plot2d_full
plt.figure(figsize=(8, 8))

h.plot2d_full(
    main_cmap="coolwarm",
    top_ls="--",
    top_color="orange",
    top_lw=2,
    side_ls=":",
    side_lw=2,
    side_color="steelblue",
)

plt.show()
```



Fitting – `iminuit` package

- Provides Python interface to the MINUIT2 C++ package (built on Cython)
  - Version 2.0 about to be out uses PyBind11 instead – much better
- Minimises arbitrary functions and computes standard errors
  - Uses HESSE (inverse of Hesse matrix) or MINOS (profile likelihood method)
- Used as backend in many other HEP (e.g. zfit) and non-HEP (e.g. astroparticle) packages
- Binary wheels for all major platforms, supports for all Python versions; availability via conda-forge
- Used interactively (Jupyter-friendly displays) to do advanced fits or for learning

iminuit

Python interface
to the Minuit2 C++ package

- Example usage:

```
from iminuit import Minuit

def f(x, y, z):
    return (x - 2) ** 2 + (y - 3) ** 2 + (z - 4) ** 2

m = Minuit(f)

m.migrad()   # run optimiser
print(m.values)   # {'x': 2,'y': 3,'z': 4}

m.hesse()    # run covariance estimator
print(m.errors)   # {'x': 1,'y': 1,'z': 1}
```

FCN = 1.624E-22			Ncalls = 36 (36 total)	
EDM = 1.62E-22 (Goal: 1E-05)			up = 1.0	
Valid Min.	Valid Param.	Above EDM	Reached call limit	
True	True	False	False	
Hesse failed	Has cov.	Accurate	Pos. def.	Forced
False	True	True	True	False

	Name	Value	Hesse Error	Minos Error-	Minos Error+	Limit-	Limit+	Fixed
0	x	2.0	1.0					
1	y	3.0	1.0					
2	z	4.0	1.0					

Particles and decays – `Particle` package

- Pythonic interface to the Particle Data Group (PDG) particle data table and MC particle identification codes
- With many extra goodies
- Simple and natural APIs

- Main classes for queries and look-ups:
  - Particle
  - `PDGID`
  - Command-line queries also available
- Powerful and flexible searches as 1-liners, e.g.

```
from particle import Particle, PDGID

pid = PDGID(211)
pid
```

```
<PDGID: 211>
```

```
pid.is_meson
```

```
True
```

```
Particle.from_pdgid(415)
```

$D_2^*(2460)^+$

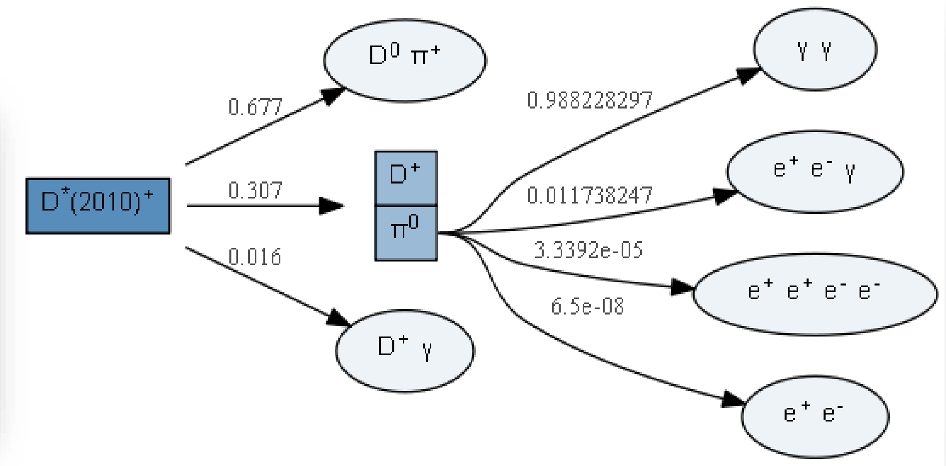
```
In [7]: from particle import Particle, SpinType

        Particle.findall(lambda p: p.pdgid.is_meson and p.pdgid.has_charm and p.spin_type==SpinType.PseudoScalar)

Out[7]: [<Particle: name="D+", pdgid=411, mass=1869.65 ± 0.05 MeV>,
         <Particle: name="D-", pdgid=-411, mass=1869.65 ± 0.05 MeV>,
         <Particle: name="D0", pdgid=421, mass=1864.83 ± 0.05 MeV>,
         <Particle: name="D~0", pdgid=-421, mass=1864.83 ± 0.05 MeV>,
         <Particle: name="D(s)+", pdgid=431, mass=1968.34 ± 0.07 MeV>,
         <Particle: name="D(s)-", pdgid=-431, mass=1968.34 ± 0.07 MeV>,
         <Particle: name="eta(c)(1S)", pdgid=441, mass=2983.9 ± 0.5 MeV>,
         <Particle: name="B(c)+", pdgid=541, mass=6274.9 ± 0.8 MeV>,
         <Particle: name="B(c)-", pdgid=-541, mass=6274.9 ± 0.8 MeV>,
         <Particle: name="eta(c)(2S)", pdgid=100441, mass=3637.6 ± 1.2 MeV>]
```

Particles and decays – DecayLanguage package

- Tools to parse decay files (aka .dec files) and programmatically manipulate them, query, display information
- Universal representation of particle decay chains
- Tools to translate decay amplitude models from AmpGen to GooFit, and manipulate them

- Parse, extract information and visualise a decay chain:

```
from decaylanguage import DecFileParser, DecayChainViewer

dfp = DecFileParser('Dst.dec')
dfp.parse()

chain = dfp.build_decay_chains('D*+', stable_particles=['D+', 'D0'])
DecayChainViewer(chain)
```



- Represent a complex decay chain:

```
dm1 = DecayMode(0.0124, 'K_S0 pi0', model='PHSP')
dm2 = DecayMode(0.692, 'pi+ pi-')
dm3 = DecayMode(0.98823, 'gamma gamma')
dc = DecayChain('D0', {'D0':dm1, 'K_S0':dm2, 'pi0':dm3})
```

Statistics tools and utilities – `pyhf` package

- ❑ **Pure Python implementation of ROOT's HistFactory, widely used for *binned* measurements and searches**
- ❑ **Benefit that can on CPUs and GPUs, transparently**
- ❑ **JSON specification that *fully* describes the HistFactory model**
- ❑ **Used for re-interpretation**

Declarative binned likelihoods

$$f(\boldsymbol{n},\boldsymbol{a}\,|\,\boldsymbol{\phi},\boldsymbol{\chi}) = \underbrace{\prod_{c\in\text{channels}}\prod_{b\in\text{bins}_c}\text{Pois}\left(n_{cb}\,|\,\nu_{cb}\left(\boldsymbol{\eta},\boldsymbol{\chi}\right)\right)}_{\text{Simultaneous measurement of multiple channels}} \underbrace{\prod_{\chi\in\mathcal{X}} c_\chi(a_\chi|\,\chi)}_{\text{constraint terms for ``auxiliary measurements''}}$$

Primary Measurement:

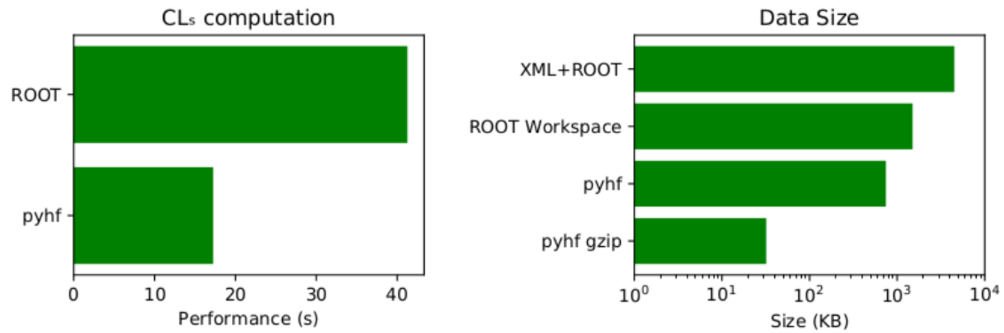
- Multiple disjoint "channels" (e.g. event observables) each with multiple bins of data
- Example parameter of interest: strength of physics signal, μ

Auxiliary Measurements:

- Nuisance parameters (e.g. in-situ measurements of background samples)
- Systematic uncertainties (e.g. normalization, shape, luminosity)

Performance

Efficient use of tensor computation makes pyhf fast



Competitive with traditional C++ implementation — often faster

(Taken from M. Feickert's CHEP 2019 poster)

A metapackage for Scikit-HEP – `scikit-hep` package

- The project now has a special package,

scikit-hep

A metapackage

- Unlike all others, which target specific topics, this metapackage simply provides an easy way to have a compatible set of project packages installed via a simple `pip install scikit-hep` (soon will also be available via Conda)

  - Benefit especially for stacks for experiments, since tags define compatible releases of the whole toolset
  - Stable stacks installable in a simple way
  - Helps in analysis preservation matters

- Trivial to check the versions available
  - Example of my laptop:

```
import skhep
skhep.show_versions()
```

```
System:
    python: 3.8.5 (default, Sep  3 2020, 21:29:08) [MSC v.1916 64 bit (AMD64)]
executable: C:\home\sw\Anaconda3\python.exe
   machine: Windows-10-10.0.19041-SP0

Python dependencies:
       pip: 20.2.4
setuptools: 50.3.2
     numpy: 1.19.2
     scipy: 1.5.2
    pandas: 1.1.3
matplotlib: 3.3.2

Scikit-HEP package version and dependencies:
        awkward: 0.14.0
       awkward1: 0.4.3
boost_histogram: 0.11.0
  decaylanguage: 0.9.1
       hepstats: 0.3.0
       hepunits: 2.0.1
           hist: 2.0.1
     histoprint: 1.5.2
        iminuit: 1.5.2
         mplhep: 0.2.7
       particle: 0.13.1
          skhep: 1.2.0
 uproot_methods: 0.8.0
         uproot: 3.13.0
        uproot4: 0.1.0
```

Other community projects

Other community projects

- Other groups are working toward the same goal,
  i.e. a Python(ic) ecosystem for data analysis in Particle Physics,
  which is community-driven and community-oriented

- Interested? Get involved, become a user *and* a developer !

- https://github.com/CoffeaTeam
- https://github.com/FAST-HEP
- https://github.com/root-project/
- https://scikit-hep.org/
- https://github.com/zfit

(Not a comprehensive list!)

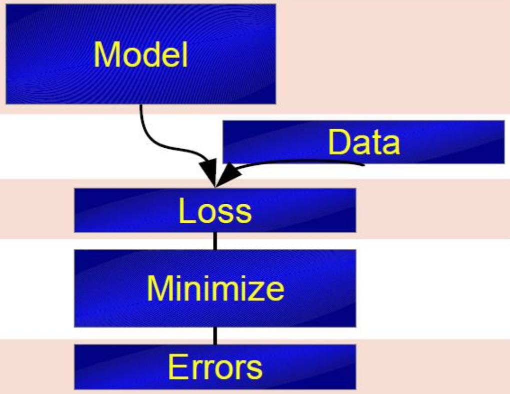
The `zfit` project and package

- Project: provide a stable fitting ecosystem, in close collaboration with the community
- `zfit` package:
  - Scalable, Pythonic, HEP specific features
  - Pure Python, no ROOT dependency, performant (TensorFlow as main backend)
  - Highly customisable and extendable
  - Depends on iminuit

affiliated

- Simple example:

```
obs = zfit.Space("x", limits=(-2, 3))

mu = zfit.Parameter("mu", 1.2, -4, 6)
sigma = zfit.Parameter("sigma", 1.3, 0.1, 10)
gauss = zfit.pdf.Gauss(mu=mu, sigma=sigma, obs=obs)

data = zfit.Data.from_numpy(obs=obs, array=normal_np)

nll = zfit.loss.UnbinnedNLL(model=gauss, data=data)

minimizer = zfit.minimize.Minuit()
result = minimizer.minimize(nll)

param_errors = result.error()
```



implement custom function

```
from zfit import ztf

class CustomPDF(zfit.pdf.ZPDF):
    _PARAMS = ['alpha']

    def _unnormalized_pdf(self, x):
        data = x.unstack_x()
        alpha = self.params['alpha']

        return ztf.exp(alpha * data)

custom_pdf = CustomPDF(obs=obs, alpha=0.2)

integral  = custom_pdf.integrate(limits=(-1, 2))
sample    = custom_pdf.sample(n=1000)
prob      = custom_pdf.pdf(sample)
```

The `coffea` project

Coffea - Column Object Framework for Effective Analysis

Fermilab project to build an analysis framework on top of awkward array and uproot

Separation of "user code" and "executors"

- User writes a Processor to do the analysis
- Executor runs this on different distributed job systems, e.g.:
  - Local multiprocessing, Parsl or Dask (batch systems), Spark cluster

Coffea ***achieved 1 to 3 MHz*** event processing rates

- Using Spark cluster on same site as data at Fermilab

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Slide taken from Ben Krikler

The FAST–HEP project

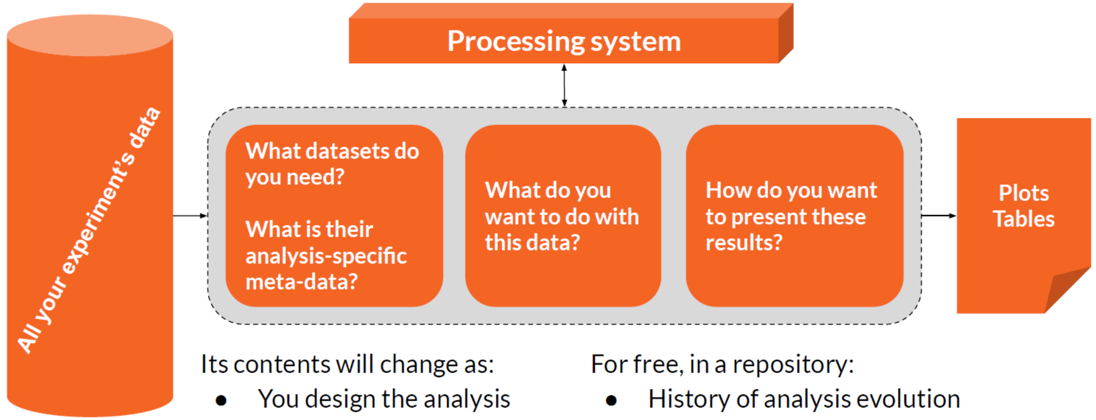
FAST-HEP

Toolkit to help high-level analyses, in particular, within particle physics

http://fast-hep.web.cern.ch   fast-hep@cern.ch

- ❑ **The main product should be the repository**
  - **- Talking about contents – publication is another matter ;-)**

Your analysis repository *is* your analysis



Its contents will change as:
- You design the analysis
- You get new / updated data

For free, in a repository:
- History of analysis evolution
- Continuous integration and validation

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The FAST implementation

For tools:
use Python

NumPy
uproot
Awkward Array
NumExpr
at (☕)

For data:
use Pandas
Demoed at CHEP 2018

pandas

For descriptions:
use YAML...

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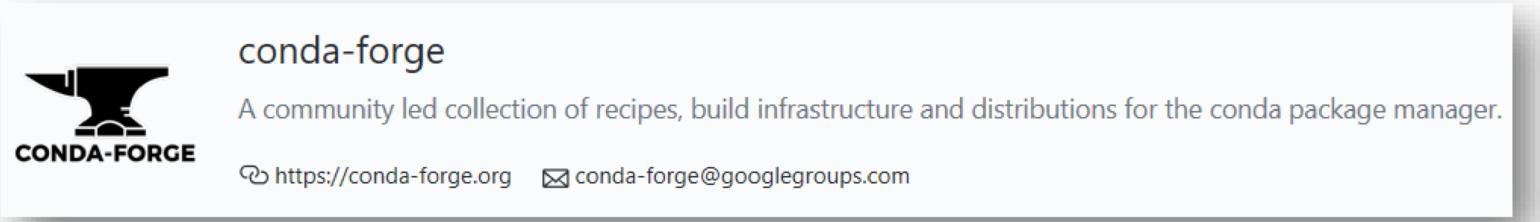
- ❑ **Use a declarative programming approach:**
  User sys WHAT, interpretation decides HOW

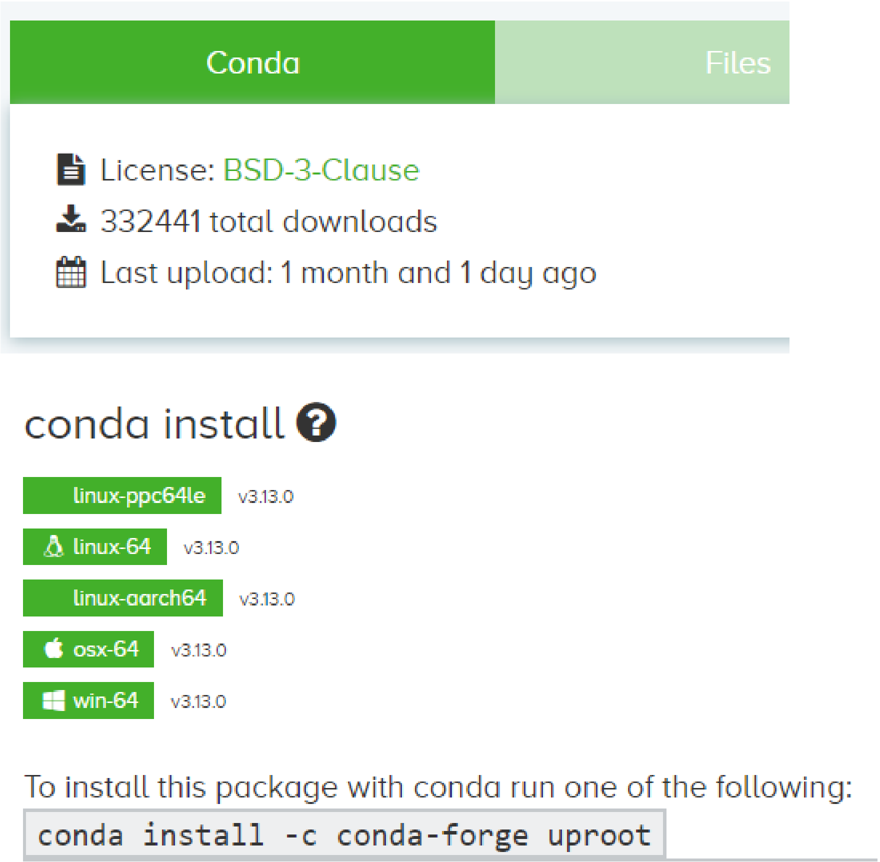
- ❑ **Project towards an Analysis Description Language …**

Material taken from Ben Krikler

Conda-forge – making it easy for users



- Easy / trivial installation in many environments is a must !
- Much work has been done in 2019 to provide binary "wheels" on PyPI, and conda-forge packages for many of these new packages
- Example of `uproot`:



Let's step back a second
Some final remarks

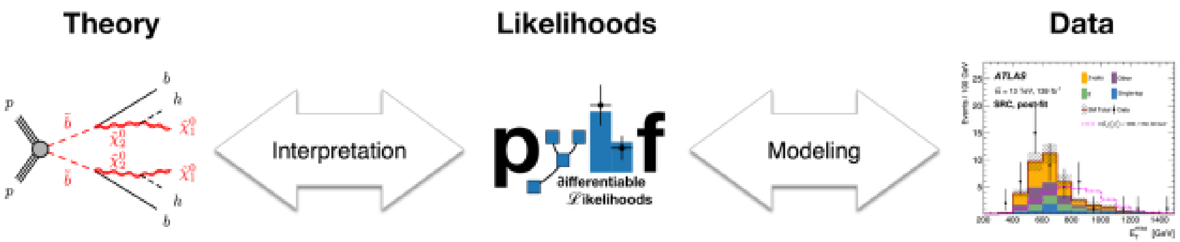
- Is "Python in HEP" making an impact? Examples …
- Towards a
  Big Data Python ecosystem for HEP (analysis)!

Python increasingly present in analysis tools used in publications

Full analysis likelihoods published on HEPData

- ❑ Test theory against LHC data
- ❑ All that's needed captured in a convenient format

- ❑ "Full likelihoods in all their glory" on HEPData
  - "While ATLAS had published likelihood scans …
    those did not expose the full complexity of the measurements"



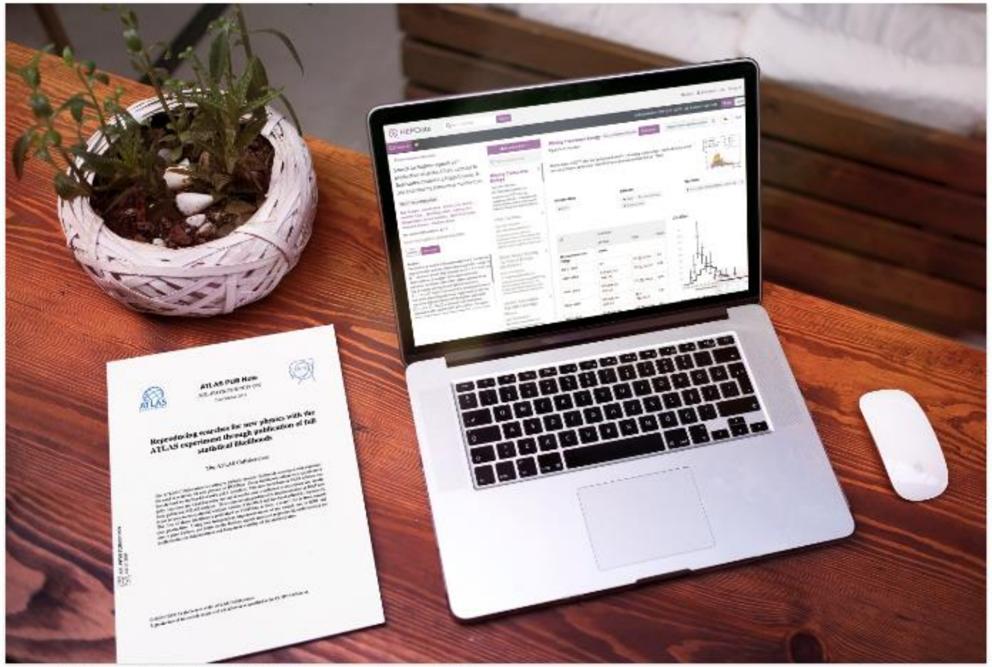
Work done with

- ❑ `RooStats` (C++)
- ❑ `pyhf` (Python)

New open release allows theorists to explore LHC data in a new way

The ATLAS collaboration releases full analysis likelihoods, a first for an LHC experiment

9 JANUARY, 2020 | By Katarina Anthony



Explore ATLAS open likelihoods on the HEPData platform (Image: CERN)

What if you could test a new theory against LHC data? Better yet, what if the expert knowledge needed to do this was captured in a convenient format? This tall order is now on its way from the ATLAS collaboration, with the first open release of full analysis likelihoods from an LHC experiment.

Taken from https://home.cern/news/news/knowledge-sharing/new-open-release-allows-theorists-explore-lhc-data-new-way

LHCC referees now also get software reports in parallel to collab. reports

Snapshop of PyHEP WG report in Graeme Stewart's presentation on November 17th 2020:

PyHEP WG

- 3rd PyHEP workshop, PyHEP 2020, held on July 13-17
  - Was to be co-located with SciPy 2020 in Austin TX, but both became virtual due to COVID-19
  - PyHEP 2020 agenda organised in 2 time zones to accommodate Asia, Europe and Americas
  - Remarkable level of interest - *we limited at 1000 registrations!*
  - 2 keynote talks and ~30 hands-on tutorials and "notebook-talks"
  - Various tools and procedures tried, with very positive feedback from participants
    - Topical Slack channels for communication, Slido for after-talk Q&A sessions, notebook talks launchable online with Binder (dedicated resources), recordings *captioned* and uploaded to dedicated YouTube playlist, all presented materials given a DOI via Zenodo
- Topical meetings being planned for 2021
  - Interest from a growing community, with several experiment-agnostic projects

Coffea, Scikit-HEP, ROOT, FAST-HEP, SWAN, zfit

- https://github.com/CoffeaTeam
- https://github.com/FAST-HEP
- https://github.com/root-project/
- https://scikit-hep.org/
- https://github.com/zfit

10

Scikit-HEP made it to the PDG !

11.2 Particle Physics software

General purpose software packages

- FastJet: This is a software package for jet finding in pp<math xmlns="http://www.w3.org/1998/Math/MathML"><mi>p</mi><mi>p</mi></math> and e^+e^-<math xmlns="http://www.w3.org/1998/Math/MathML"><msup><mi>e</mi><mo>+</mo></msup><msup><mi>e</mi><mo>-</mo></msup></math> collisions. It includes fast native implementations of many sequential recombination clustering algorithms, plugins for access to a range of cone jet finders and tools for advanced jet manipulation.

- GAMBIT: A global fitting code for generic Beyond the Standard Model theories, designed to allow fast and easy definition of new models, observables, likelihoods, scanners and backend physics codes.

- Geant4: This is a toolkit for the simulation of the passage of particles through matter. Its areas of application include high-energy, nuclear and accelerator physics, as well as studies in medical and space science.

- LHAPDF: HEP community standard library for parton distribution function interpolation, including official collection of PDF data sets.

- QUDA: Library for performing calculations in lattice QCD on GPUs using NVIDIA's CUDA platform. The current release includes optimized solvers for Wilson, Clover-improved Wilson,Twisted mass, Staggered, Improved staggered, Domain wall and Mobius fermion actions.

- Rivet: The Rivet toolkit, a system for validation of Monte Carlo event generators, provides a large set of experimental analyses useful for MC generator development, validation, and tuning.

- ROOT: This framework for data processing in high-energy physics, born at CERN, offers applications to store, access, process, analyze and represent data or perform simulations.

- Scikit-HEP: This is a community-driven and community-oriented project with the aim of providing Particle Physics at large with an ecosystem for data analysis in Python. The project started in Autumn 2016 and is under active development. It focuses on providing core and common tools for the community but also on improving the interoperability between HEP tools and the scientific ecosystem in Python as well as the discoverability of utility packages and projects.

Taken from Online Particle Physics Information (see PDG)

Thank you for listening

- HEP Software Foundation (HSF)
  - HSF general forum hsf-forum@googlegroups.com
- HSF PyHEP Working Group
  - (main) Gitter channel
  - GitHub repository “Python in HEP” resources
- PyHEP 2020 workshop
- Scikit-HEP project
  - Get in touch

HSF – Gitter channels

All Rooms — 8 Rooms — 630 People

HSF-GSoC	Discussions about the HEP Software Foundation GSoC program	260 People
PyHEP	Discussion of Python in High Energy Physics https://hepsoftwar…	159 People
PyHEP-histogramming	Discussions around histogramming	57 People
PyHEP-newcomers	github.com/hsf-training/PyHEP-resources	49 People
mpl-hep	Matplotlib proposals related to Particle Physics	36 People
HSF-GSoC-Students		30 People
PyHEP-fitting	Discussions around fitting	25 People
ADL	Analysis Description Language discussions	14 People

PyHEP series of workshops

PyHEP 2019

Abingdon, U.K.

PyHEP 2018

Sofia, Bulgaria

PyHEP 2020

- *Was meant to be held in Austin (Texas), U.S.A., in July 11-13*
- *Next to SciPy 2020 conference, to enhance cross-community exchange*
- *Run as a virtual event, as most conferences this year*

PyHEP workshops – diverse topics presented/discussed

PyHEP 2018
Sofia, Bulgaria

- Historical perspective / overview
- HEP python software ecosystem
- Analysis & HEP frameworks
- PyROOT and Python bindings
- Distribution and installation
- Python 2 to 3
- Open discussion on education and training

+

Keynote presentation on JupyterLab

PyHEP 2019
Abingdon, U.K.

- Accelerators-enabled code
- Analysis platforms
- Analysis fundamentals
- HEP Python software ecosystem
- High-level analysis tools
- Histogramming
- Packaging, distribution, CI
- PyROOT
- Research software
- Statistics
- Visualisation
- Lightning talks

- ❑ Organisation:
  - Topical sessions, all plenary
  - 1/3 of time devoted to discussions rather than presentations
- ❑ Pre- and post-workshop surveys
- ❑ Live notes taken during the sessions

PyHEP 2020 – on workshop topics

Word cloud of abstracts

(Made with https://www.wordclouds.com/
removing author names, institutes and some other trivial words.)

- ❑ Many topics
- ❑ Too much content to adequately review here!

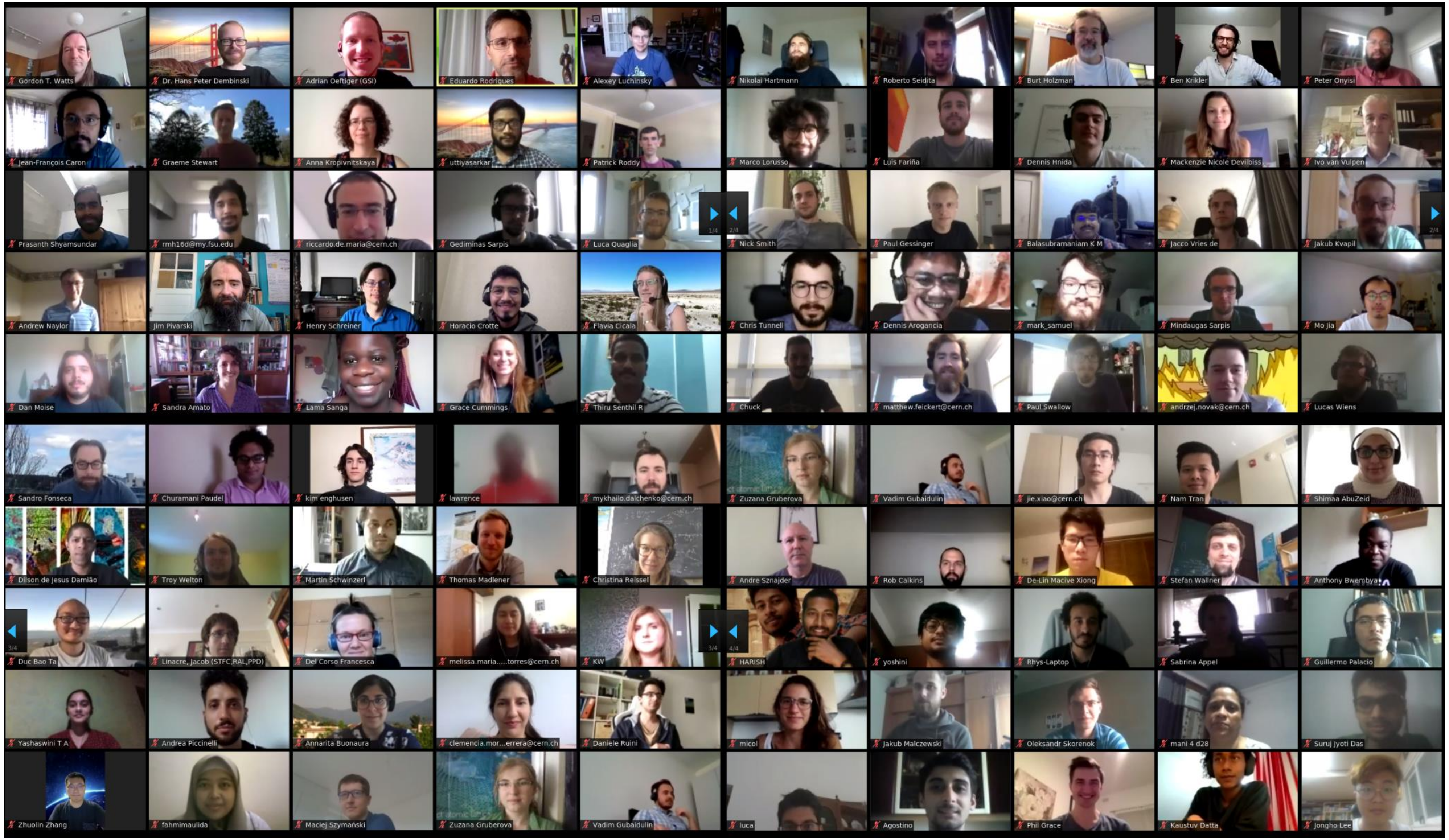
- ○ Analysis fundamentals
- ○ Analysis platforms & systems
- ○ Automatic differentiation
- ○ Performance
- ○ Fitting & statistics
- ○ HEP analysis ecosystem

+

2 keynote presentations (astronomy & pheno.)

- ❑ Organisation:
  - Topical sessions, all plenary
  - Tutorials and standard talks
  - Much time devoted to discussions
- ❑ Pre- and post-workshop surveys

PyHEP 2020 – "workshop photo" @ end of last Atlantic session

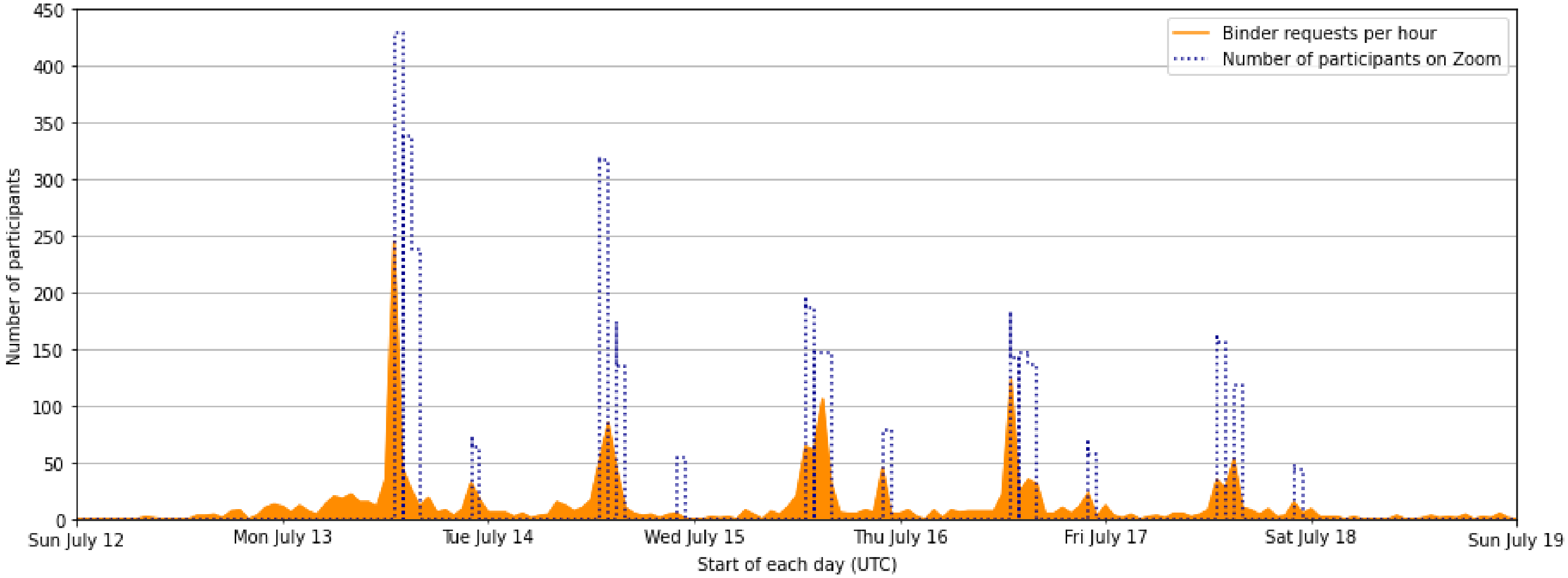


PyHEP 2020 – "workshop photo" @ end of last Pacific session

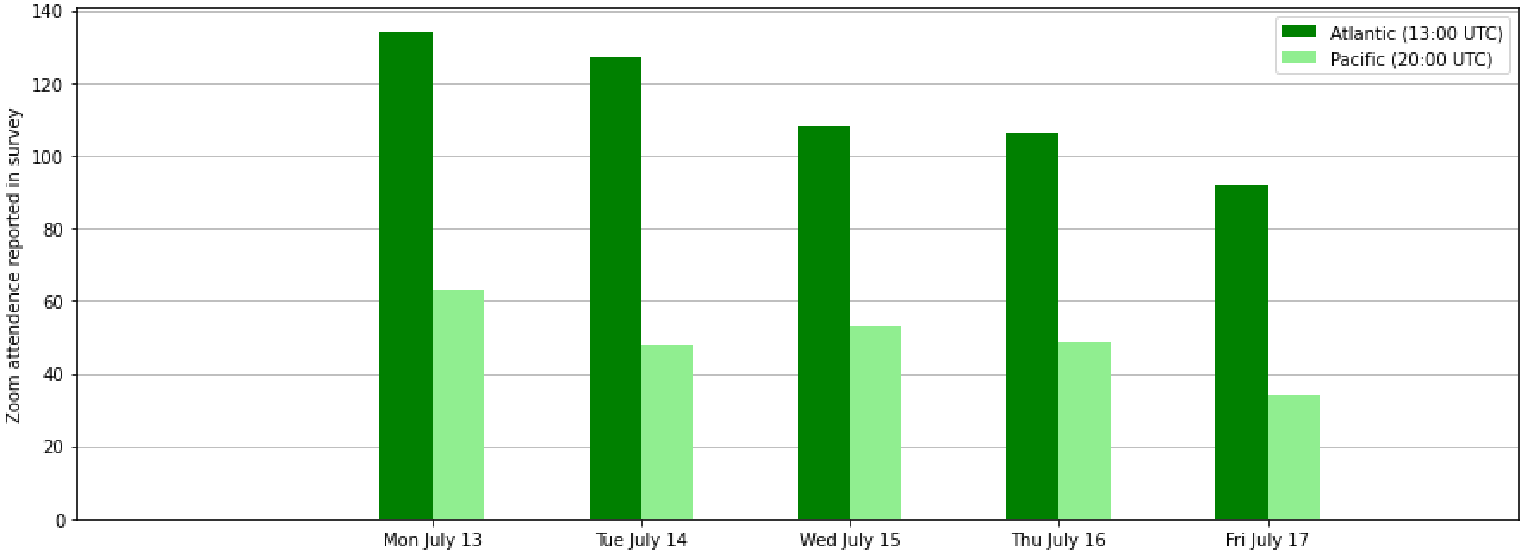
PyHEP 2020 logistics – session attendance & Binder usage

- Session participants
- Binder requests during sessions

⇒ Clear correlation !



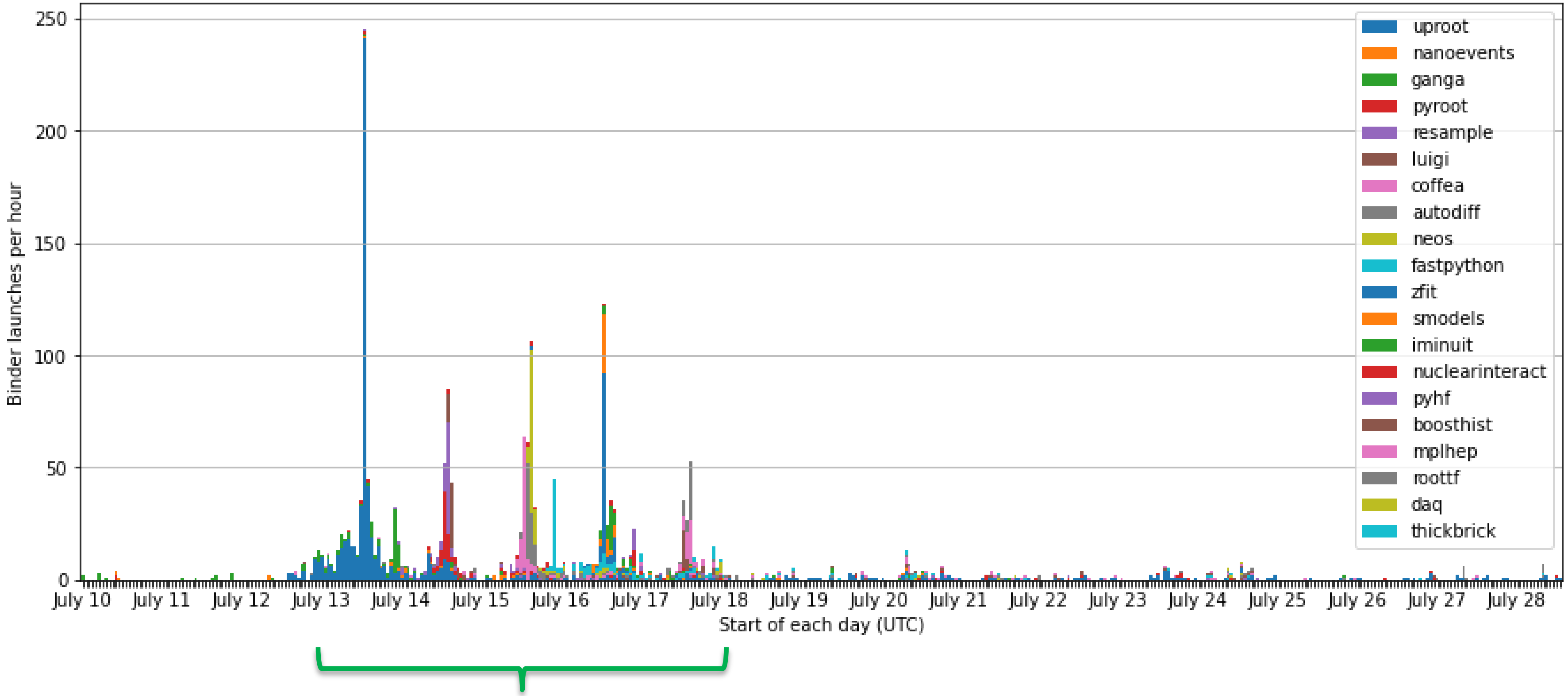
- Number of participants per day & time zone, *as reported by those who filled in the post-workshop survey*
  - "Atlantic" time zone suited most



Study by Jim Pivarski

PyHEP 2020 stats – Jupyter notebook presentations & Binder usage

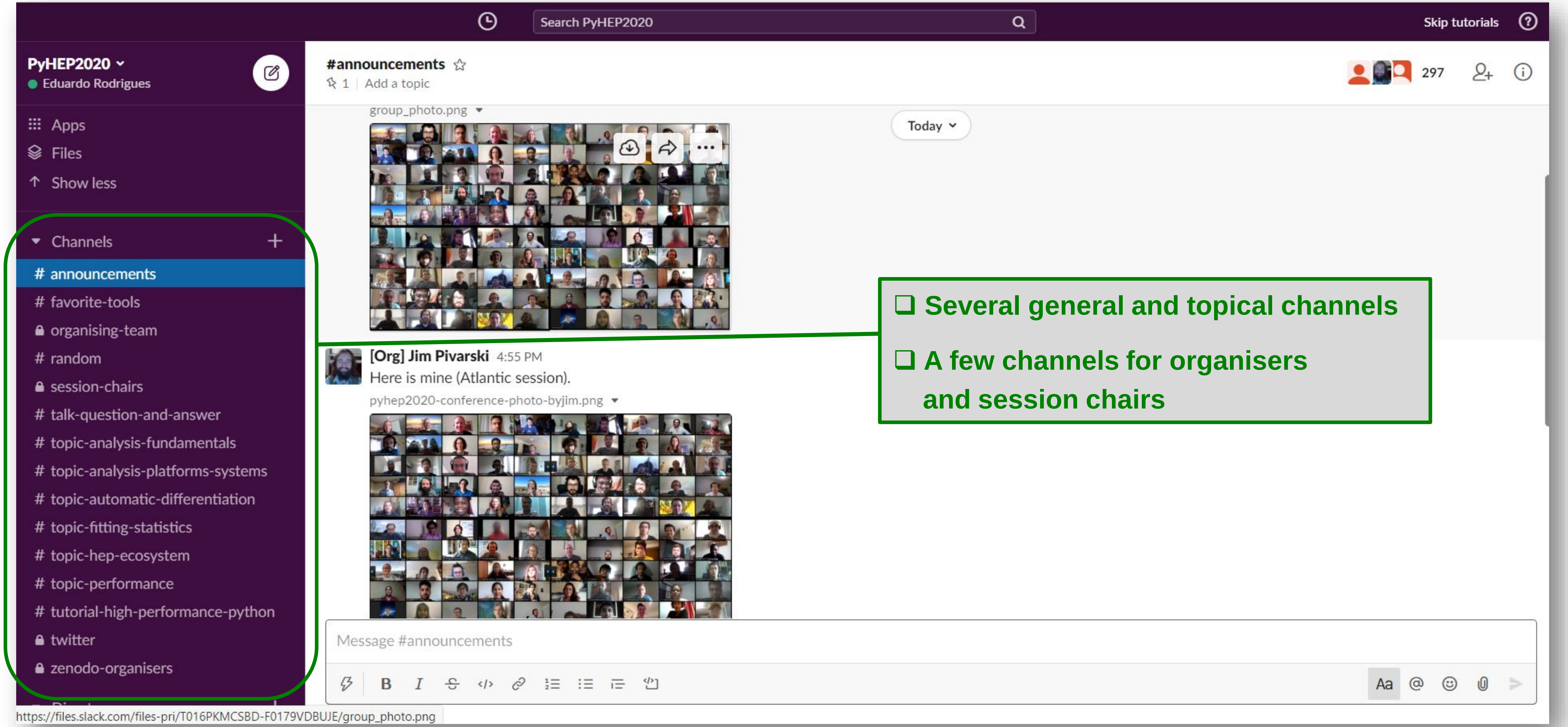
Binder launches per hour



PyHEP 2020 workshop time frame

Study by Jim Pivarski

PyHEP 2020 logistics – Slack for discussion during/after sessions



- ❑ Several general and topical channels
- ❑ A few channels for organisers and session chairs

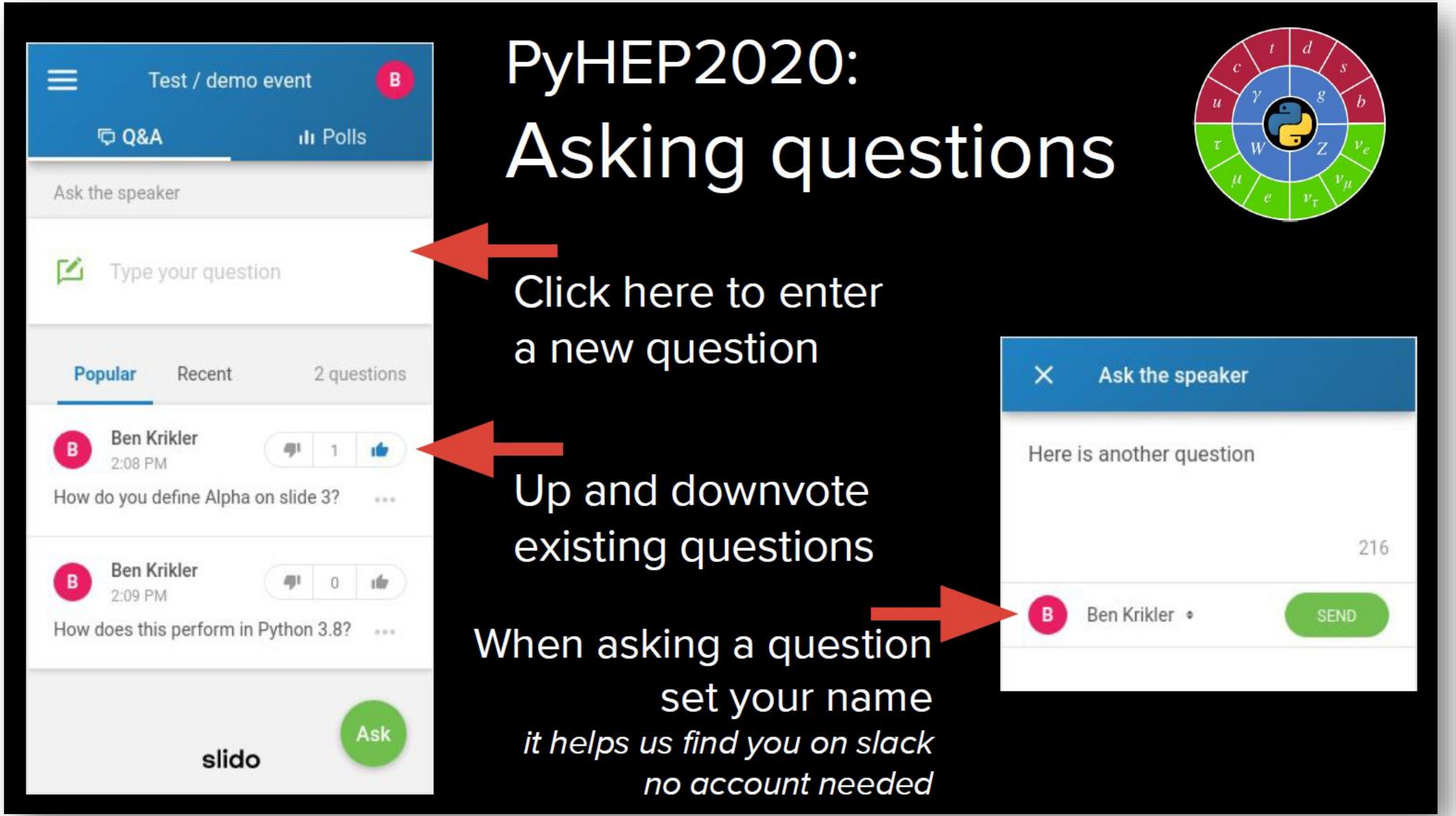
PyHEP 2020 logistics – slido at work for Q&As and polls

As actually seen by participants

PyHEP 2020 logistics – how does slido work for Q&As

slido

Easy to use · Works with your live video · No app downloads



PyHEP 2020 logistics – slido for Q&A post-talk sessions

Was slido a success? Yes !

slido

Event summary report
PyHEP2020

Active users	181
Engagement score	978
Engagement per user	5.4

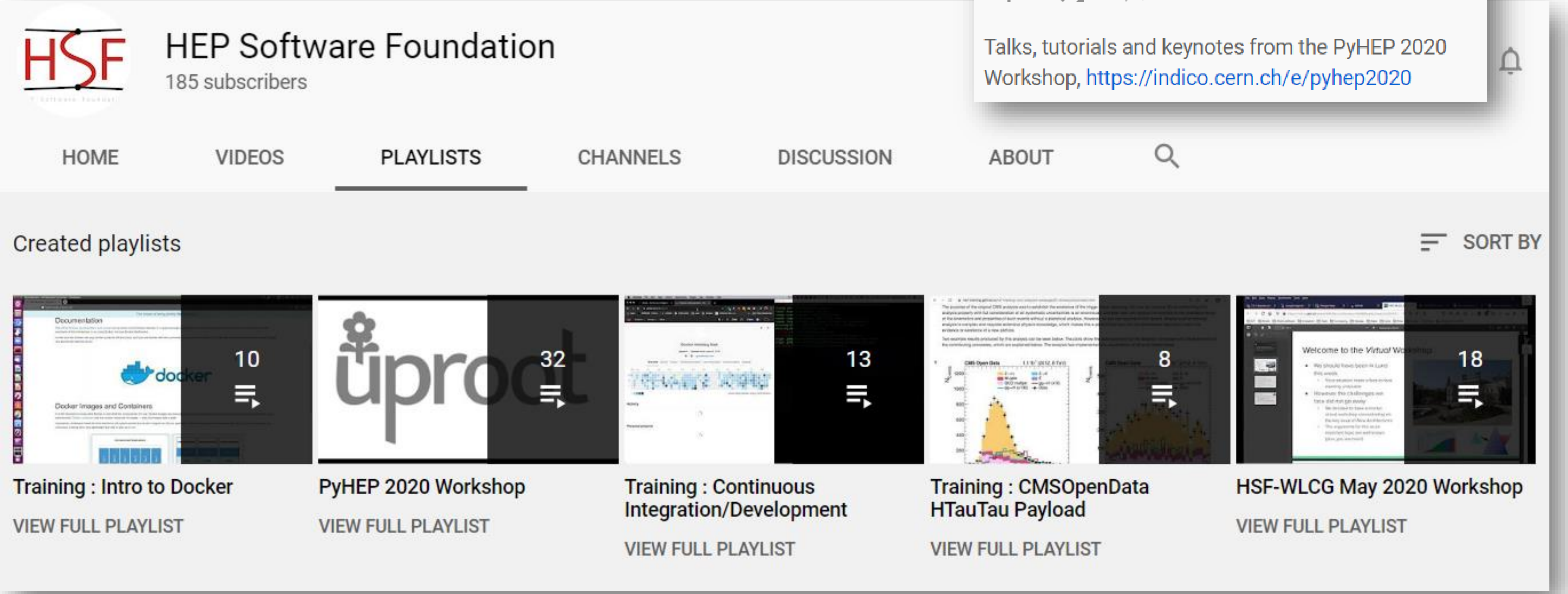
Questions	182
Likes / dislikes	483 / -54
Anonymous rate	34%

Poll votes	195
Polls created	5
Votes per poll	39

With 413 joined participants in total

PyHEP 2020 logistics – recordings on YouTube

- ❑ **HSF has its own channel, with several playlists**
- ❑ **PyHEP 2020 recordings of presentations on YouTube, captioned, in dedicated playlist**

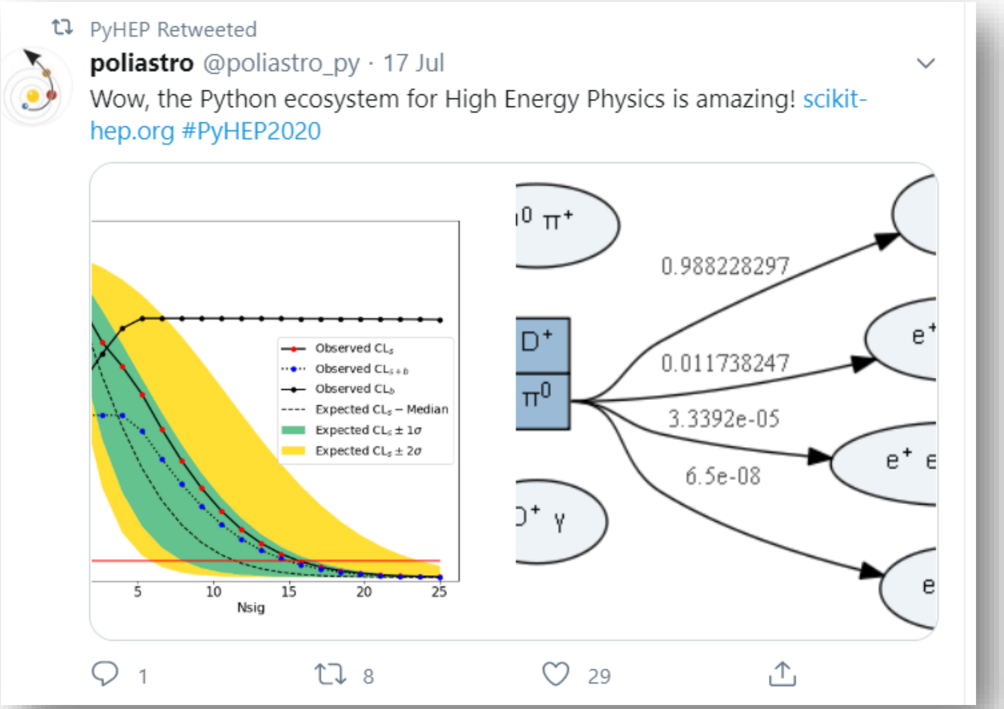


PyHEP 2020 logistics – we are even on

@PyHEPConf

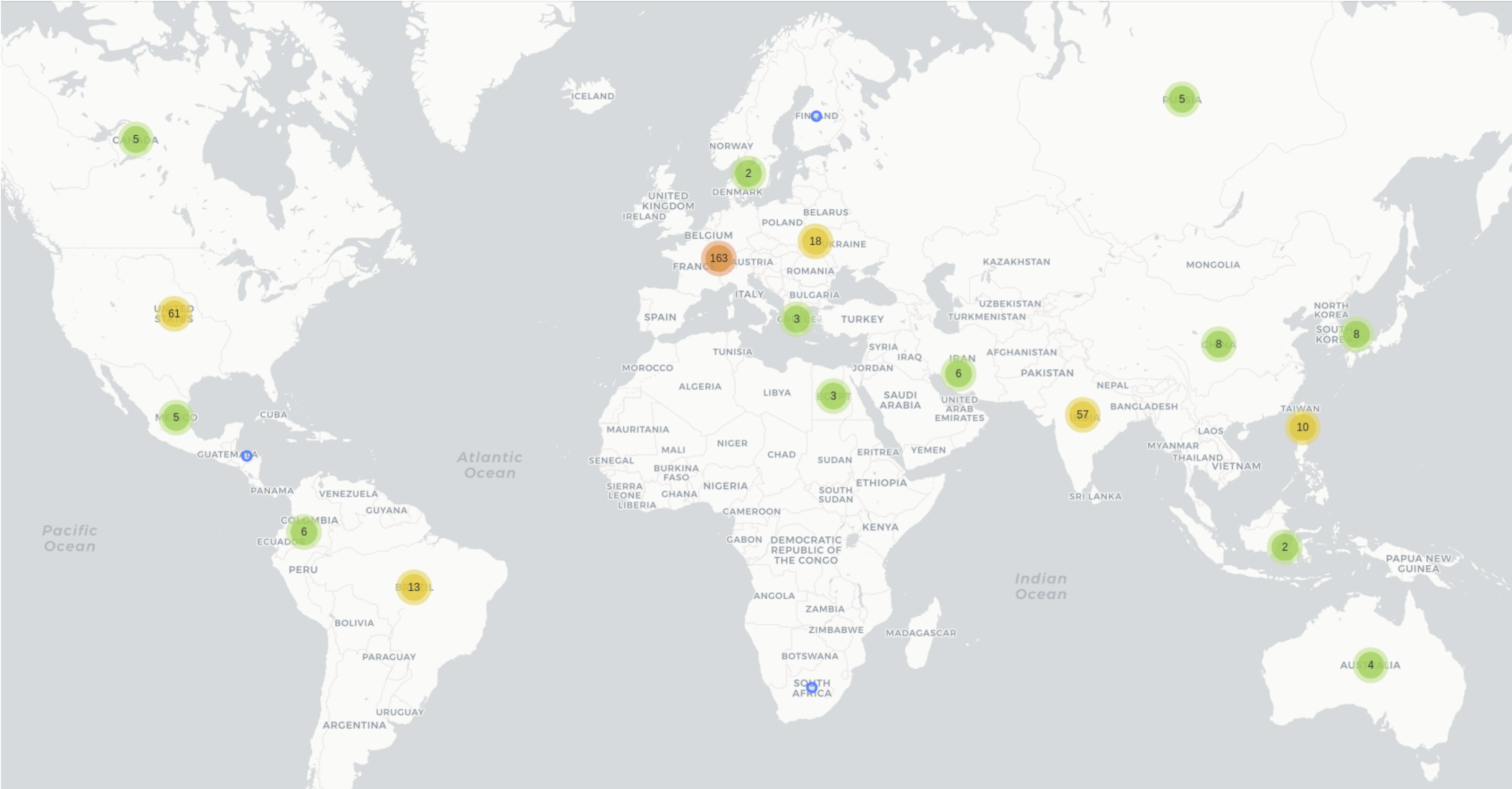
#PyHEP2020

A testimony from an astroparticle colleague …



PyHEP 2020 stats – diversity and inclusion

- Diverse participation from all over the world !



Plot by Jim Pivarski

- Information taken from the 408/1000 responses received from the pre-workshop survey

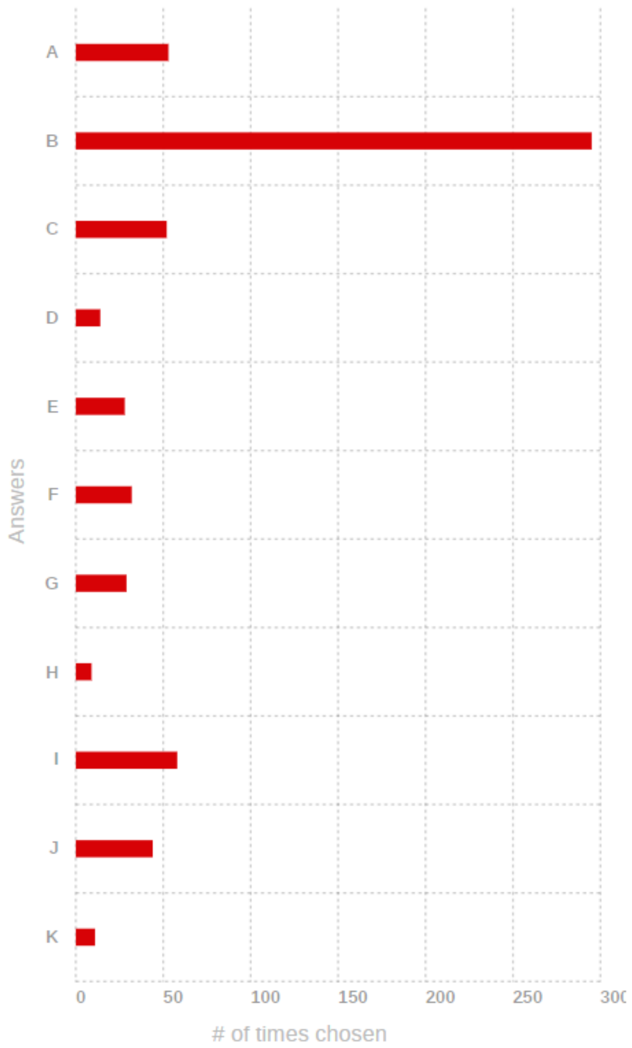
PyHEP 2020 stats – background of participants …

If you're involved in physics, what area(s) do you study?

Answered : *405*

You can answer this AND the area of computing (below) or only one, depending on what you do.

- **A. General physics (student)**: 53 (8.48%)
- **B. High-energy collider physics**: 295 (47.20%)
- **C. Neutrino physics**: 52 (8.32%)
- **D. Physics of nuclei or exotic atoms**: 14 (2.24%)
- **E. Precision frontier**: 28 (4.48%)
- **F. Direct dark matter searches**: 32 (5.12%)
- **G. Astroparticle physics**: 29 (4.64%)
- **H. Astronomy**: 9 (1.44%)
- **I. Theory/simulations**: 58 (9.28%)
- **J. Instrumentation**: 44 (7.04%)
- **K. Other, not listed above**: 11 (1.76%)

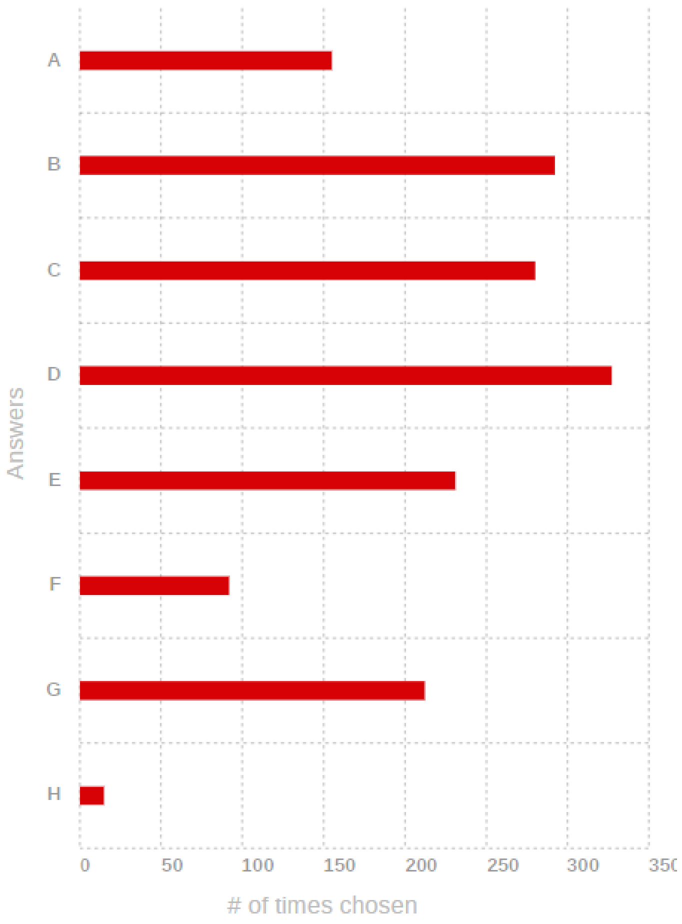


Taken from the pre-workshop survey (408 respondents)

PyHEP 2020 stats – … and their hopes

What are you hoping to learn from this workshop? Answered: 405

- **A. Python fundamentals (how to program in Python)**: 155 (9.66%)
- **B. General-purpose data analysis toolkits**: 292 (18.20%)
- **C. Machine learning/deep learning toolkits**: 280 (17.46%)
- **D. Particle physics analysis tools (other than ROOT)**: 327 (20.39%)
- **E. ROOT and PyROOT**: 231 (14.40%)
- **F. Collaboration-specific topics**: 92 (5.74%)
- **G. Software engineering skills (beyond the fundamentals)**: 212 (13.22%)
- **H. Other**: 15 (0.94%)



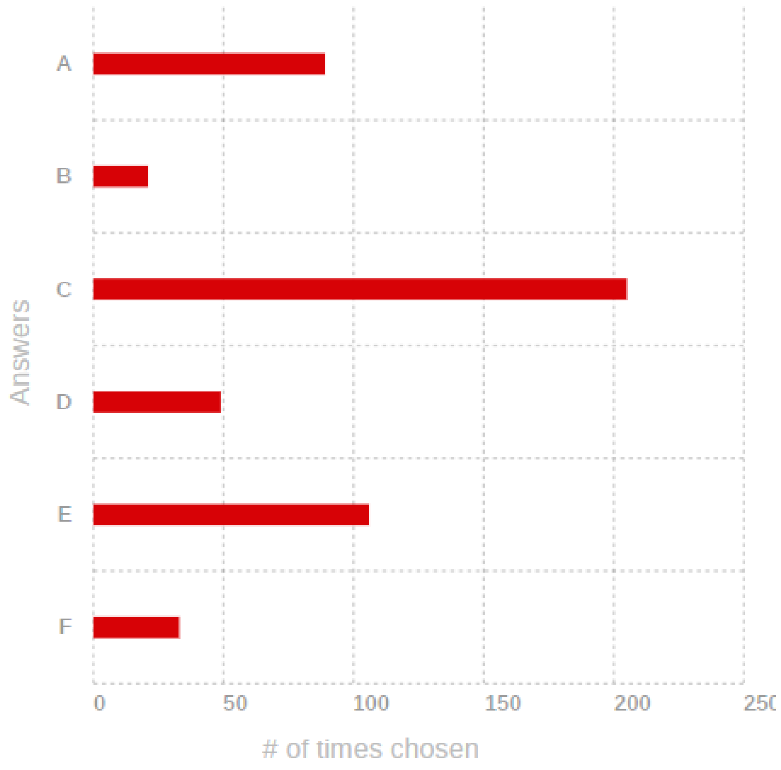
Taken from the pre-workshop survey (408 respondents)

PyHEP 2020 organisational aspects – multi-channel advertising is crucial

How did you hear about this workshop?

Answered: *405*

- **A. HSF mailing lists or announcements**: 89 (17.69%)
- **B. HSF/PyHEP Twitter**: 21 (4.17%)
- **C. My physics collaboration's mailing list(s)**: 205 (40.76%)
- **D. Laboratory or university posting (physical or electronic)**: 49 (9.74%)
- **E. Word of mouth (in person, personal email, chat...)**: 106 (21.07%)
- **F. Other**: 33 (6.56%)



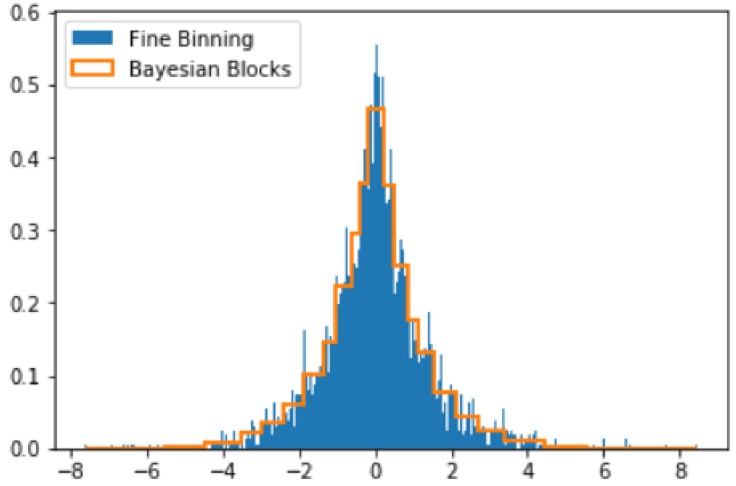
Taken from the pre-workshop survey (408 respondents)

Statistics tools and utilities – `hepstats` package

- Statistical tools and utilities in Python, under development

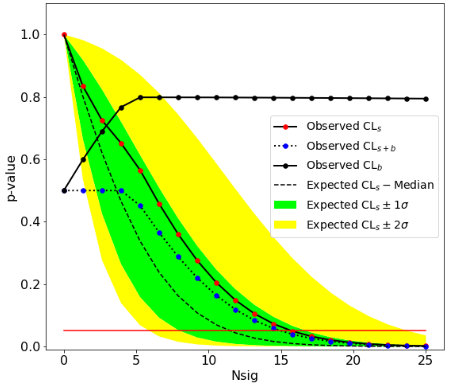
- Currently implements two submodules:
  - Modeling with the Bayesian block algorithm – improved binning determination, robust to statistical fluctuations

```
>>> import numpy as np
>>> import matplotlib.pyplot as plt
>>> from hepstats.modeling import bayesian_blocks

>>> data = np.random.laplace(size=10000)
>>> blocks = bayesian_blocks(data)

>>> plt.hist(data, bins=1000, label='Fine Binning', density=True, alpha=0.6)
>>> plt.hist(data, bins=blocks, label='Bayesian Blocks', histtype='step', density=True, linewidth=2)
>>> plt.legend(loc=2)
```

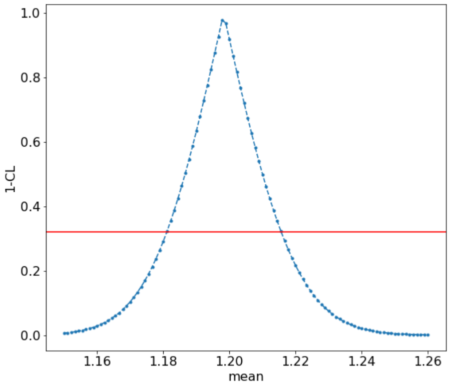


  - Likelihood-based hypothesis tests, upper limit and confidence interval calculations
    - Works with a fitting library providing models, likelihood, etc.
    - Built on a common interface, used by zfit, and does not depend on a fitting backend

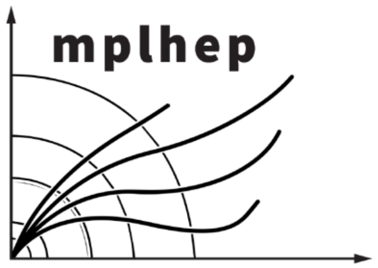
Upper limit on signal yield:



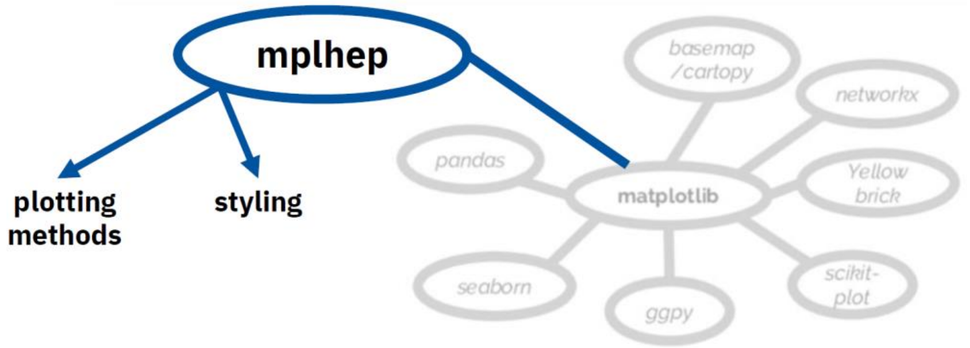
1-CL plot for the mean of a peak:



mplhep package – helper visualisation tool for HEP atop Matplotlib

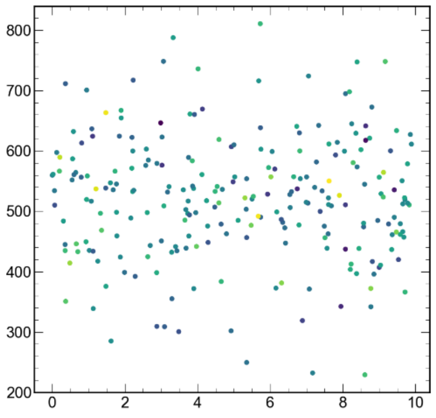


- ❑ Matplotlib is a key tool for visualisation in the data science domain
- ❑ But it not provide all that HEP wants
  - Requires a lot of tinkering
- ❑ mplhep idea:
  - Keep matplotlib as a versatile and well-tested backend
  - Provide a new domain-specific API



Minimal Example

```
import numpy as np
import matplotlib.pyplot as plt
+ import mplhep as hep

x = np.random.uniform(0, 10, 240)
y = np.random.normal(512, 112, 240)
z = np.random.normal(0.5, 0.1, 240)

+ plt.style.use(hep.style.ROOT)
f, ax = plt.subplots()
ax.scatter(x,y, c=z);
```



Visualisation – VegaScope package

- **Minimal viewer of Vega & Vega-Lite graphics on the browser from local or remote Python processes**
  - Vega = declarative "visualisation grammar", see [GitHub org]
  - The Python process generating the graphics does not need to be on the same machine as the web browser viewing them
- **0 dependencies - can be installed as single file, used as a Python library or as a shell command, watching a file or stdin**
- **Example:**

```
import vegascope
canvas = vegascope.LocalCanvas()
canvas("https://vega.github.io/vega/examples/stacked-bar-chart.vg.json")
```

- **`Altair` can use `VegaScope` as a renderer:**

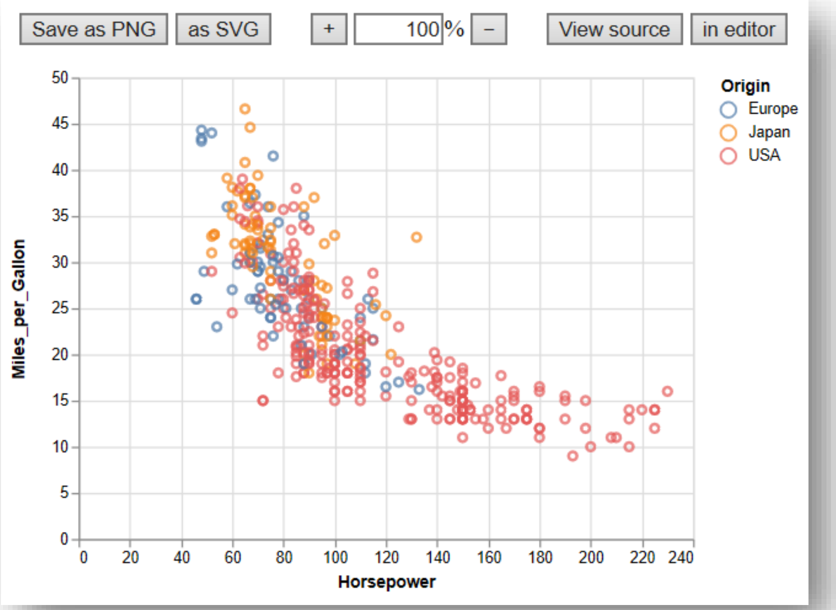
```
import vegascope
canvas = vegascope.LocalCanvas()
canvas("https://vega.github.io/vega/examples/stacked-bar-chart.vg.json")
```

```
import altair as alt
alt.renderers.enable('vegascope')
```

```
RendererRegistry.enable('vegascope')
```

```
from vega_datasets import data
cars = data.cars()
alt.Chart(cars).mark_point().encode(x='Horsepower',
                                    y='Miles_per_Gallon',
                                    color='Origin'
                                   ).interactive()
```

```
Rendered at http://localhost:56574
```



Simulation & jet clustering – `numpythia` and `pyjet` packages

- Generate events with Pythia and pipe them into NumPy arrays

```python
from numpythia import Pythia, hepmc_write, hepmc_read
from numpythia import STATUS, HAS_END_VERTEX, ABS_PDG_ID

params = {"Beams:eCM": 13000, "WeakSingleBoson:ffbar2gmZ": "on",
          "23:onMode": "off" ,"23:onIfAny": "13", "WeakZ0:gmZmode": 2}

pythia = Pythia(params=params)
selection = ((STATUS == 1) & ~HAS_END_VERTEX)

for event in pythia(events=100):
    array = event.all(selection)
    muplus  =  array[array["pdgid"] == 13]
```

numpythia

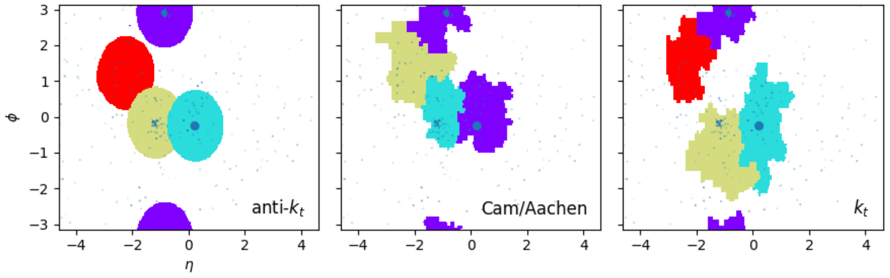
Interface between PYTHIA and NumPy

- Possible to feed those events into FastJet using `pyjet`

```python
from pyjet import cluster
from pyjet.testdata import get_event

vectors = get_event()
sequence = cluster(vectors, R=1.0, p=-1)
jets = sequence.inclusive_jets()  # list of PseudoJets
```

pyjet

Interface between FastJet and NumPy



Units and constants in the HEP system of units – hepunits package

- **Units and constants in the HEP system of units**
  - Not the same as the SI system of units
- **Trivial package, but handy**
- **Typical usage:**

```
from hepunits.constants import c_light
from hepunits.units     import picosecond, micrometer

tau_Bs = 1.5 * picosecond    # a particle lifetime, say the Bs meson's
ctau_Bs = c_light * tau_Bs   # ctau of the particle, ~450 microns
print(ctau_Bs)               # result in HEP units, so mm
```

```
0.44968868700000003
```

```
print(ctau_Bs / micrometer)  # result in micrometers
```

```
449.688687
```

Quantity	Name	Unit
Length	millimeter	mm
Time	nanosecond	ns
Energy	Mega electron Volt	MeV
Positron charge	eplus	
Temperature	kelvin	K
Amount of substance	mole	mol
Luminous intensity	candela	cd
Plane angle	radian	rad
Solid angle	steradian	sr

- **More "advanced":**

```
from hepunits import c_light, GeV, meter, ps
from math import sqrt

def ToF(m, p, l):
    """Time-of-Flight = particle path length l / (c * beta)"""
    one_over_beta = sqrt(1 + m*m/(p*p))
    return (l * one_over_beta /c_light)
```

```
from particle.particle.literals import pi_plus, K_plus  # particle name literals
```

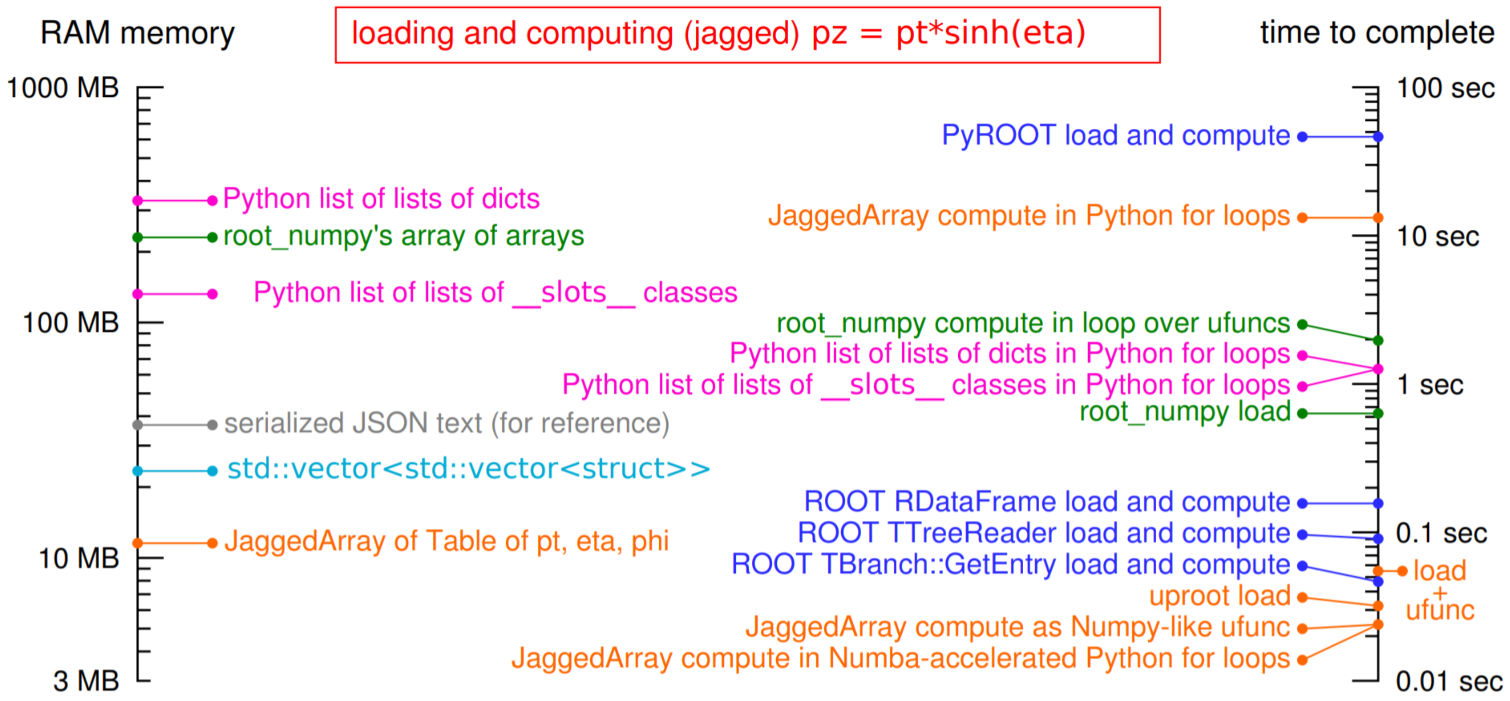
```
delta = ( ToF(K_plus.mass, 10*GeV, 10*meter) - ToF(pi_plus.mass, 10*GeV, 10*meter) ) / ps
print("At 10 GeV, Delta-TOF(K-pi) over 10 meters = {:.5} ps".format(delta))
```

```
At 10 GeV, Delta-TOF(K-pi) over 10 meters = 37.374 ps
```

Intermezzo – wait, it's Python, it must be slow!

- **NOPE !**

"The lack of per-event processing is why reading in uproot and processing data with awkward-array can be fast, despite being written in Python."



See https://github.com/scikit-hep/uproot#jagged-array-performance

Intermezzo – wait, it's Python, it must be slow!

- Much is thanks to building atop NumPy: