



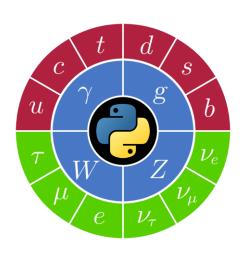




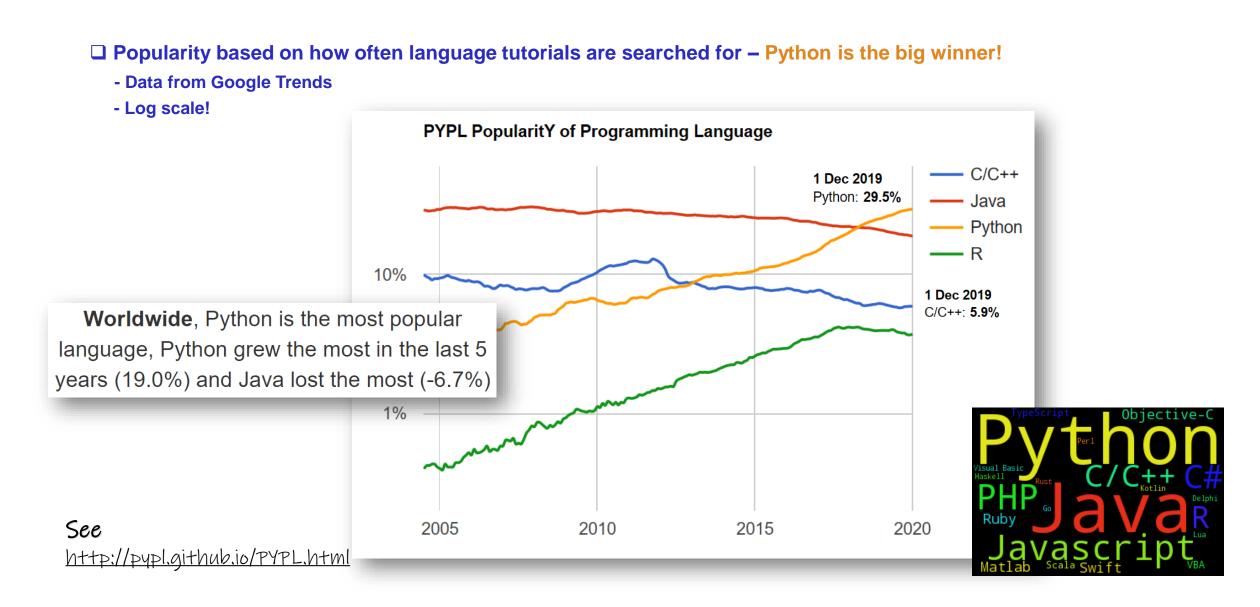
# HSF PyHEP WG and the PyHEP 2020 workshop

**Eduardo Rodrigues**University of Liverpool

# Python, you say?

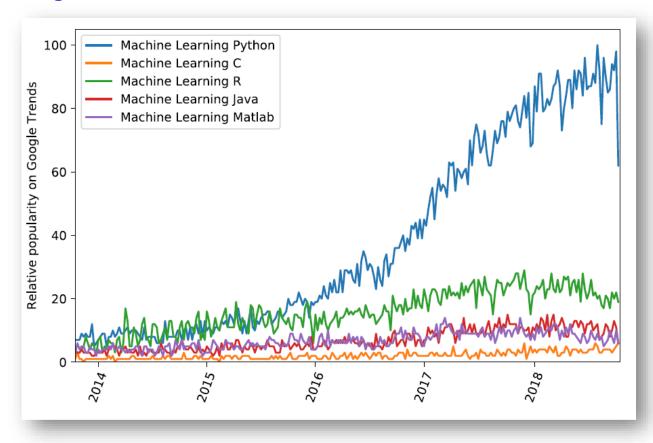


# **PopularitY of Programming Languages (PyPL)**



# PopularitY of Programming Languages for Machine Learning

#### ☐ Popularity again from Google Trends data

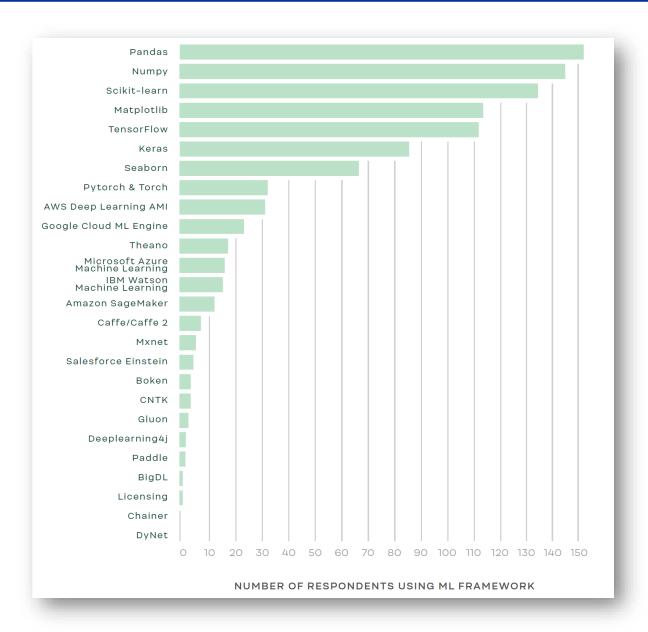


Starts to illustrate why "Python in HEP" was meant to be relevant ...

#### Python ML package usage among data scientists

- □ The Python scientific stack really is important, even more if you are thinking about a career outside HEP ...
- □ And since we talk a lot on how to help young people, training on (at least some of) these tools should be seen as very relevant

Taken from:
figure eight,
Data Scientist Report 2018
(full report)



# Why Python for scientific research?

Adapted from Jake Vander Plas'

<u>The unexpected effectiveness</u>

of Python in Scientific Research

- ☐ Ecosystem built atop NumPy and SciPy
- ☐ Open source FOSS has proven its worth!
- ☐ Very popular, with large and active community

#### Interoperability with other languages

- o Bindings to C++, fortran, etc
- We can continue using existing tools (if wanted)

#### Perfect for exploratory work

- No compiling
- Little boilerplate code
- E.g. Jupyter notebooks (though this is no longer python-only)

#### Package ecosystem

- "Batteries included" so standard library provides many functions: argparse, globbing, regular expressions, URL requests, math
- Package manager gives access to huge community-driven ecosystem
- "Open-source" by default

16

# Python adoption in HEP – CMS study

#### Direct method: look at their code!



GitHub API lets us query users and repositories (URL  $\rightarrow$  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.

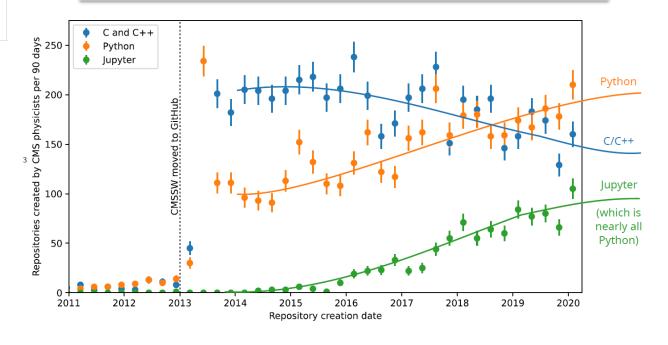
Why GitHub/CMS? Until recently, all (free) GitHub repos were public, making them searchable by the API.

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

- ☐ Study by Jim Pivarski

  [presentation @ Snowmass 2021, Aug. 11<sup>th</sup>]
- Not from survey but rather directly using GitHub API to measure software adoption

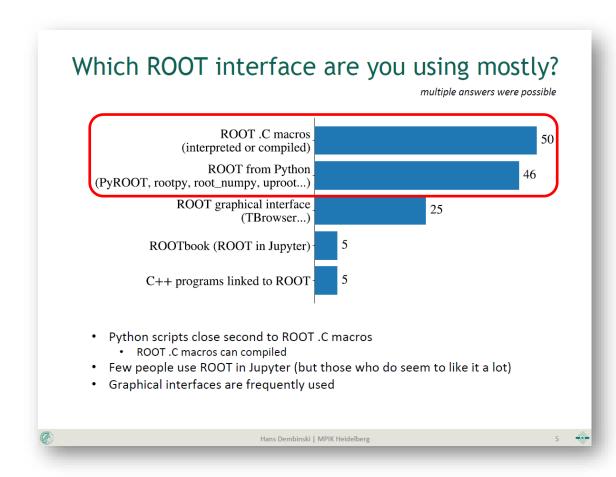
#### Language of repos created by CMS physicists



# Python adoption in HEP – ROOT from Python in LHCb

#### Surveys from the LHCb experiment

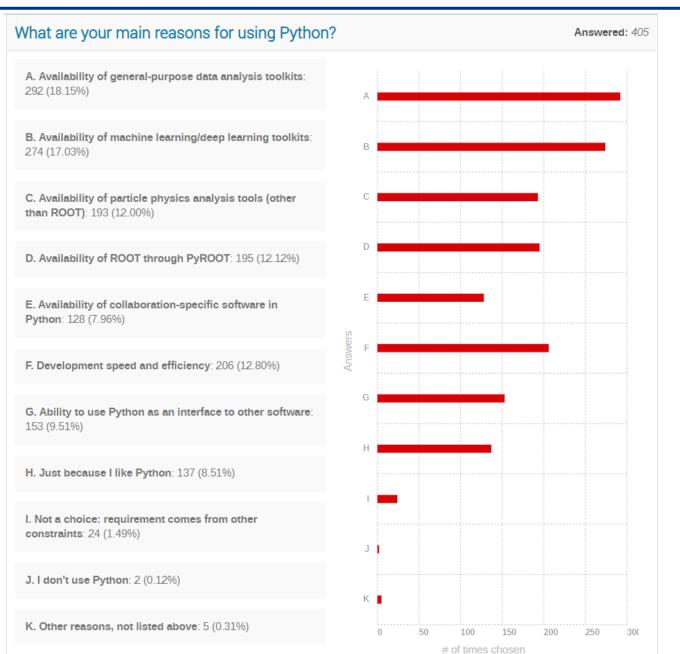
- **□** Python and C++ equally used among analysts
  - Trend seen in our <u>LHCb survey</u>
     for the ROOT User's Workshop in 2018
  - And in the LHCb 2018 Analysis Survey Report (by Eduardo Rodrigues)
- □ Conclusion clearly even stronger if discussing analysis tools independent of ROOT
- ROOT from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



#### Taken from

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

# Why do particle physicists use Python?



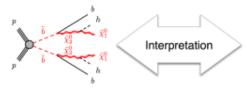
Taken from the PyHEP 2020 pre-workshop survey (408 respondents)

# 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"

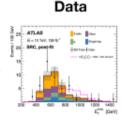
#### Theory



#### Likelihoods







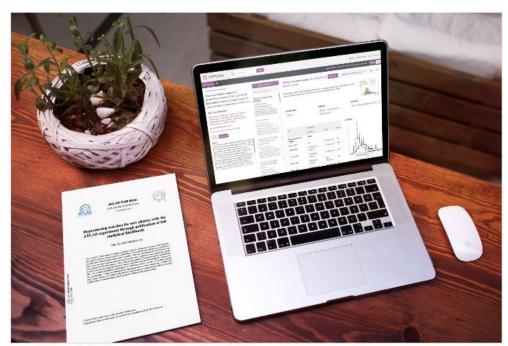
#### Work done with

- □ 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.

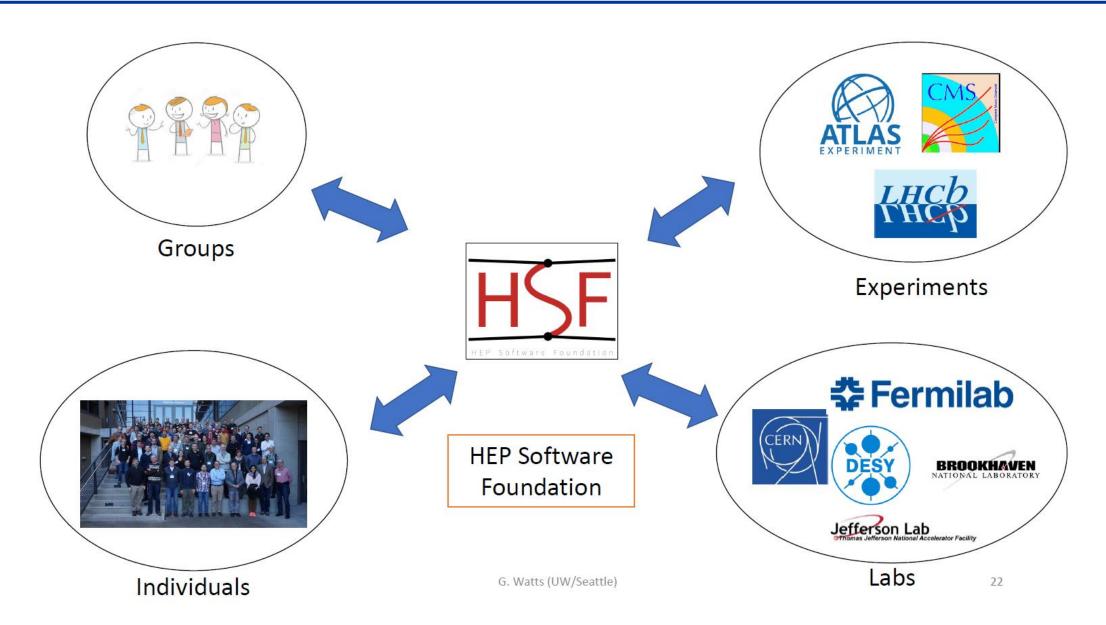
Taken from https://home.cern/news/news/knowledge-sharing/new-open-release-allows-theorists-explore-lhc-data-new-way

# **HSF & PyHEP**

- ☐ 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 <u>HEP Software Foundation</u> (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. <a href="http://doi.org/10.5281/zenodo.3779250">http://doi.org/10.5281/zenodo.3779250</a>, HSF-DOC-2020-01



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

- □ The "Python in HEP" WG effectively started in early 2018 as an activity group, which I put forward with the proposal of the 1<sup>st</sup> workshop, held as a pre-CHEP 2018 event
- ☐ It became "formally" a WG this year ⑤



Differentiable Computing

Season of Docs

Google Summer of Code

Licensing

**Quantum Computing** 

Reviews

Software Forum

Visualisation

Data Analysis

**Detector Simulation** 

Frameworks

Physics Generators

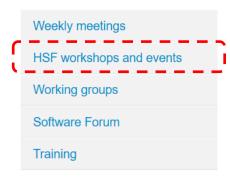
PyHEP - Python in HEP

Reconstruction and Software Triggers

Software Developer Tools and Packaging

Training





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

- ☐ Lots of ways to communicate!
  - The main channel now has just over 150 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

#### Community projects towards a HEP Python ecosystem for data analysis

- ☐ Citing Gordon Watts (ACAT 2019) how can we tackle these 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 <sup>©</sup>

- □ https://github.com/CoffeaTeam
- □ <a href="https://github.com/FAST-HEP">https://github.com/FAST-HEP</a>
- □ <a href="https://github.com/root-project/">https://github.com/root-project/</a>
- □ https://scikit-hep.org/
- □ https://github.com/zfit

Various projects have seen the light:

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



#### How's the Python scientific ecosystem like, outside HEP?

(and many, **Domain-specific** many astropy more) NetworkX SymPy StatsModels scikit-image Statistics in Python matplotlib learn Python's Bokeh Scientific SciPy xarray jupyter NumPy **IP**[y]: stack ython **IPython** DASK Numba

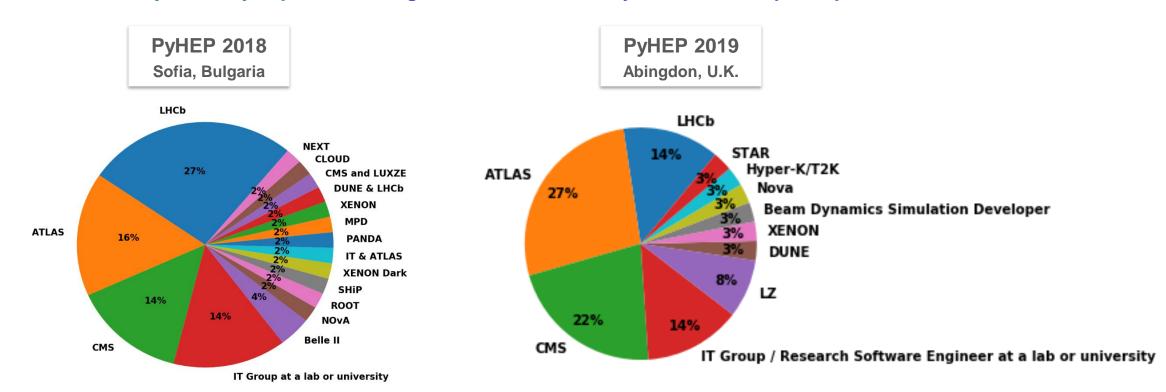
Community
projects towards
HEP domain-specific
Python tools
⇒ ecosystem

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

# PyHEP workshops – a 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!



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

#### PyHEP workshops – a 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

#### 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
- o Python 2 to 3
- Open discussion on education and training

+

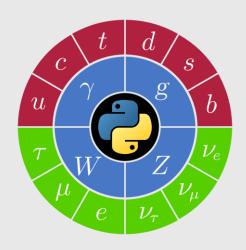
**Keynote presentation on JupyterLab** 

- **□** 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 2019 Abingdon, U.K.

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

# PyHEP 2020 Workshop



☐ A special cuvée

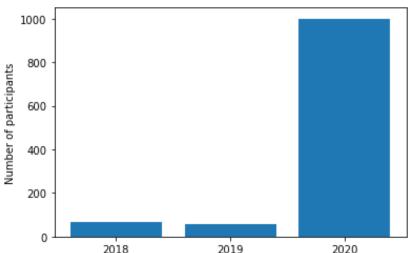
**☐** On organisational aspects

**☐** Highlights

We now even have a logo ⊚!

# PyHEP 2020, a special cuvée

- □ 3<sup>rd</sup> 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)





Eduardo Rodrigues 2018 2019 2020 lly@JLab, 26th August 2020 22/39

# PyHEP 2020 – Indico page, organising team, sponsors

#### PyHEP 2020 (virtual) Workshop

#### 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











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

# PyHEP 2020 organisational aspects – overview

zoom

- 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

#### slido

- 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
  - ⇒ participants can continue to discuss and exchange
- A few polls also run via slido

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 <u>"pyhep2020 community"</u> formal citation, replaces proceedings
- All talks got recorded, captioned YouTube
  and later uploaded to the HSF YouTube channel dedicated playlist "PyHEP 2020 Workshop"

# PyHEP 2020 organisational aspects – agenda (1/2)

# Workshop agenda (1/2)



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



- □ 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)

Eduardo Rodrigues

PyHEP 2020, All@Home, 13 July 2020

Typically
45 minutes

6/11

# PyHEP 2020 organisational aspects – agenda (2/2)

# Workshop agenda (2/2)



# From PyHEPConf Twitter account

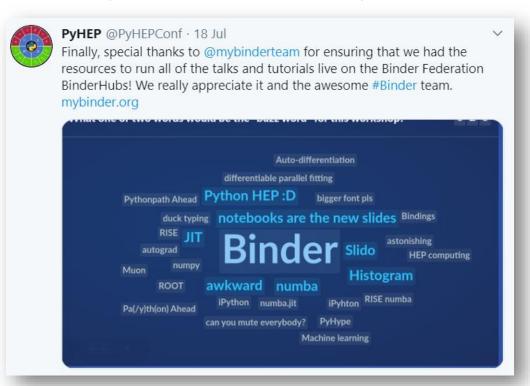
#### PyHEP 2020 logistics – Jupyter notebook talks / tutorials with Binder

- **☐** 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:

☐ Find out more at <u>mybinder.org</u>







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



# PyHEP 2020 logistics – recordings on VouTube

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



#### HEP Software Foundation

185 subscribers

HOME

VIDEOS

**PLAYLISTS** 

CHANNELS

DISCUSSION

#### PyHEP 2020 Workshop

32 videos · 622 views · Last updated on 19 Jul 2020







Talks, tutorials and keynotes from the PyHEP 2020 Workshop, https://indico.cern.ch/e/pyhep2020

SORT BY

ABOUT



#### Created playlists



Training: Intro to Docker

VIEW FULL PLAYLIST



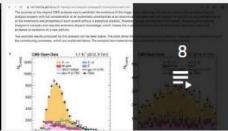
PyHEP 2020 Workshop

VIEW FULL PLAYLIST



Training: Continuous Integration/Development

VIEW FULL PLAYLIST



Training: CMSOpenData HTauTau Payload

VIEW FULL PLAYLIST



HSF-WLCG May 2020 Workshop

VIEW FULL PLAYLIST

#### PyHEP 2020 logistics – we are even on

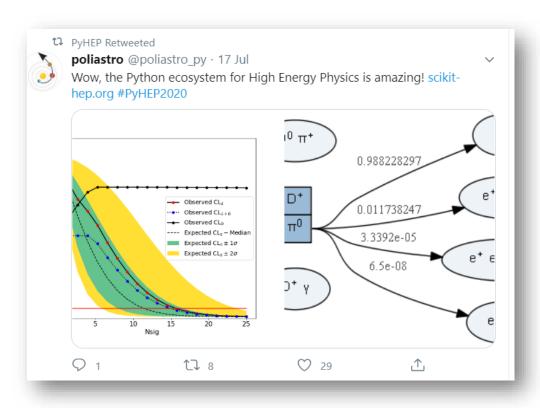


@PyHEPConf

**#PyHEP2020** 



#### A testimony from an astroparticle colleague ...



# PyHEP 2020 stats – diversity and inclusion

Diverse participation from all over the world!



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

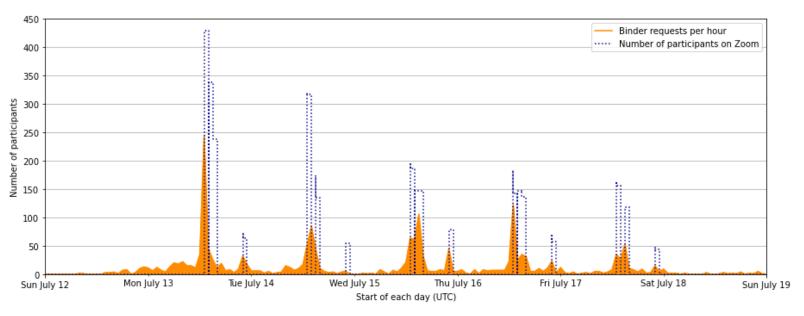
# PyHEP 2020 stats – diversity and inclusion

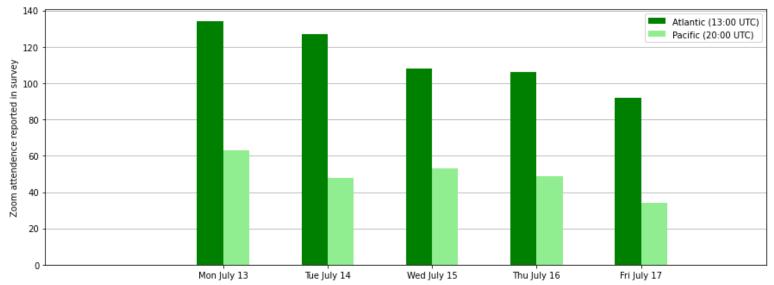
- □ Great to see such a diverse set of participants!
- □ "Logo art" with information on collaborations taken from the pre-workshop survey



- Session participants
- Binder requests during sessions
  - ⇒ Clear correlation!

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

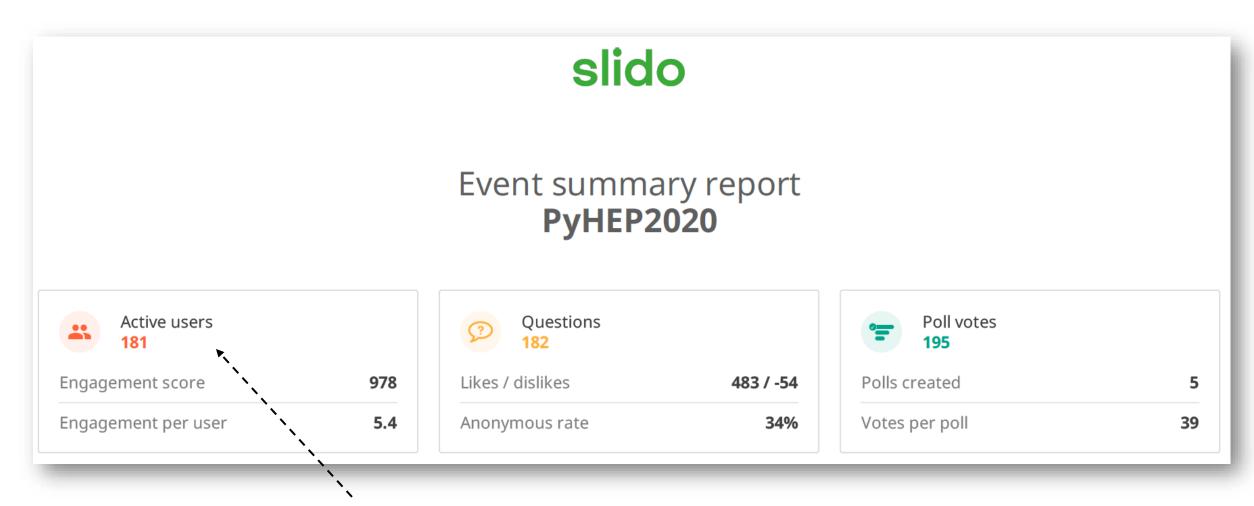




Study by Jim Pivarski

# PyHEP 2020 stats - slido for Q&A post-talk sessions

Was slido a success? Yes!



With 413 joined participants in total

# PyHEP 2020 highlights – on workshop topics

#### Word cloud of abstracts



(Made with <a href="https://www.wordclouds.com/">https://www.wordclouds.com/</a> 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

+

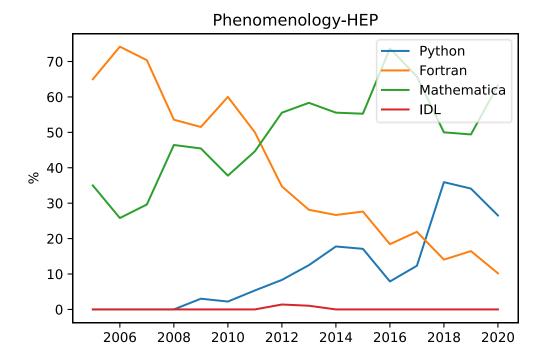
2 keynote presentations (astronomy & pheno.)

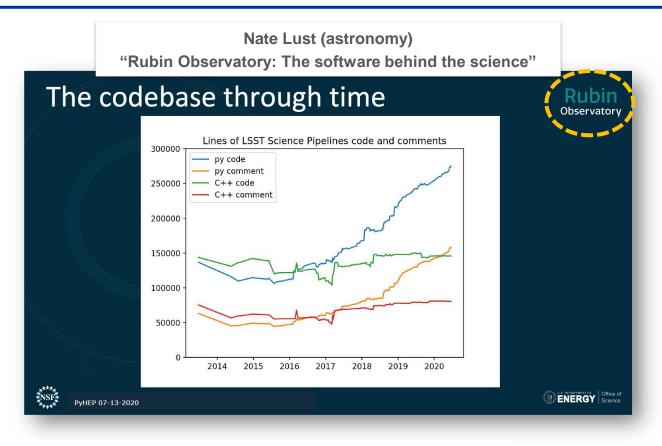
- **□** Organisation:
  - Topical sessions, all plenary
  - Tutorials and standard talks
  - Much time devoted to discussions
- ☐ Pre- and post-workshop surveys

# PyHEP 2020 highlights – keynote presentations

□ Python on the rise not just in experimental particle physics

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





#### 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".

"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

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

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

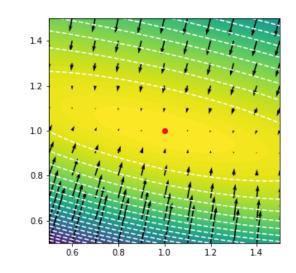
```
pyhf.set backend('jax')
```

#### Define the model, fit ... and plot:

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

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





Taken from the tutorial)

#### Wrapping up – "Python in HEP" brought to official instances ...

#### **Graeme A Stewart, HSF report to CERN Scientific Policy Committee, 10/12/2019**

# PyHEP ("Python in HEP") and New Approaches

- Python is ever more popular in Particle Physics
- Impressive developments of a Python scientific ecosystem for HEP in the last 2 years
- With strong links to the general scientific ecosystem
  - Interest in *data science* tools and *machine learning* is significant for this growing community
- Inspiring new approaches for data analysis
  - Exploiting modern approaches declarative programming, heterogeneous resources, etc.
  - This is an ecosystem into which HEP can, and does, contribute
  - Knowledge transfer goes both ways
  - Various projects under development, inter-communicating
- Yearly PyHEP workshops have been a success
  - Next year hoping to co-locate with SciPy 2020



19

# Thank you for listening

- **□** HEP Software Foundation (HSF)
  - HSF general forum <a href="mailto:hsf-forum@googlegroups.com">hsf-forum@googlegroups.com</a>
- **☐** HSF PyHEP Working Group
  - (main) Gitter channel
  - GitHub repository <u>"Python in HEP" resources</u>
- □ PyHEP 2020 workshop

Abingdon, U.K.



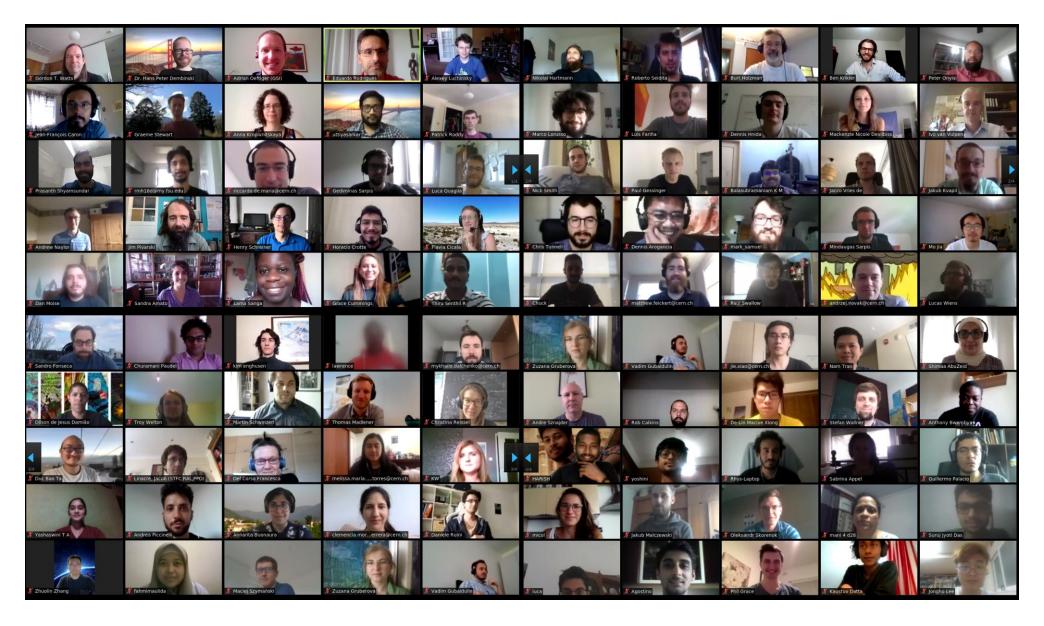




#### **PyHEP 2020**

- 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

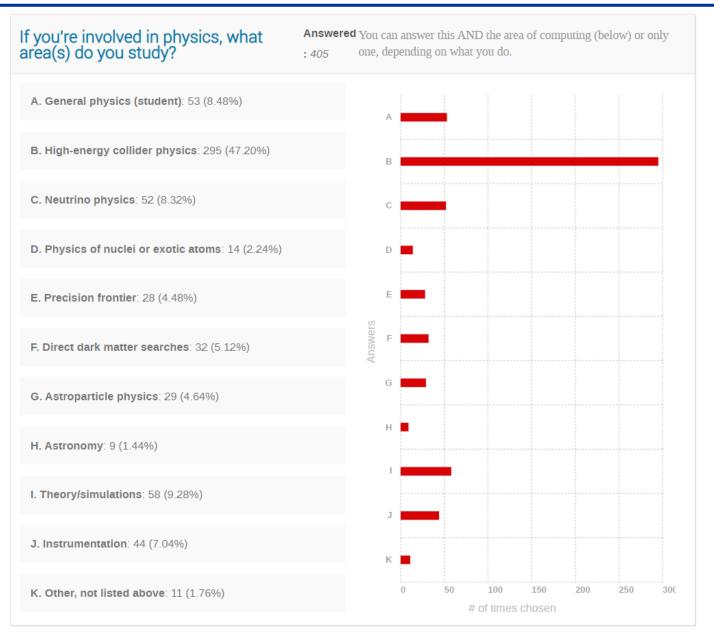
### PyHEP 2020 – "workshop photo" @ end of last Atlantic session



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

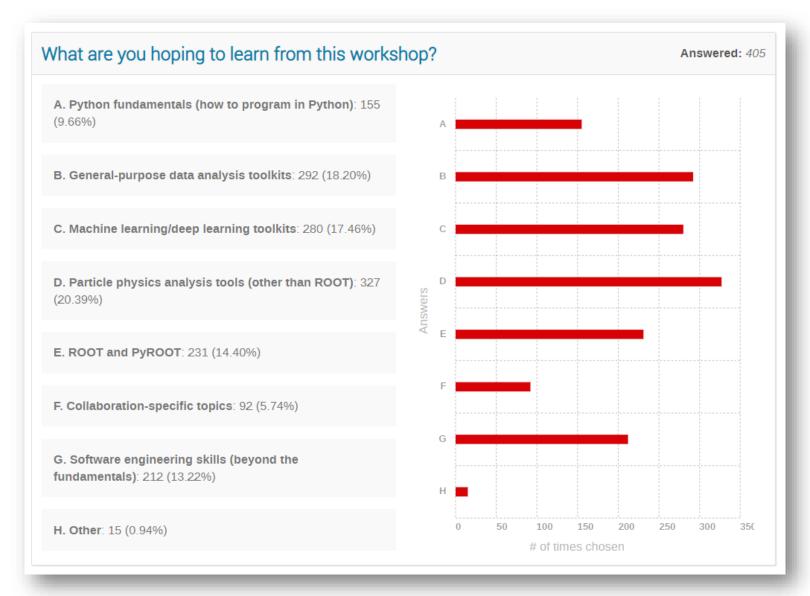


### PyHEP 2020 stats – background of participants ...



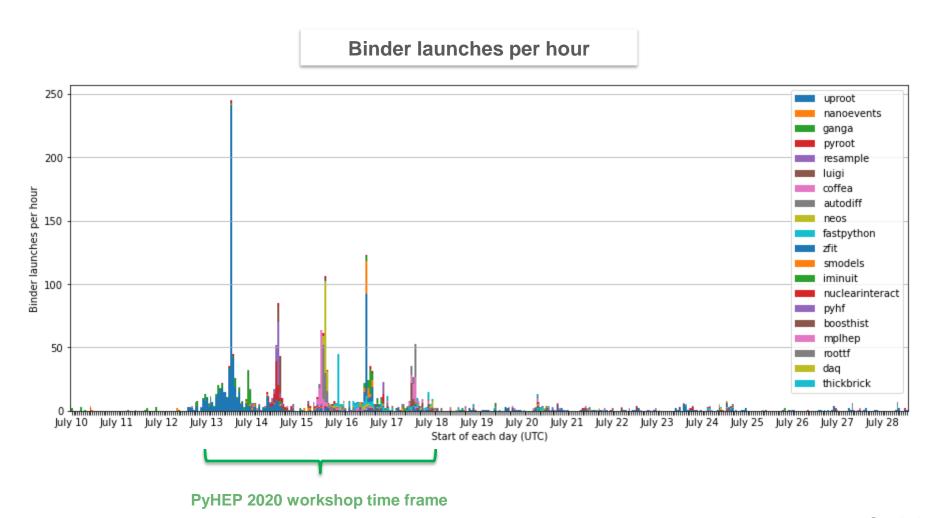
Taken from the pre-workshop survey (408 respondents)

#### PyHEP 2020 stats – ... and their hopes



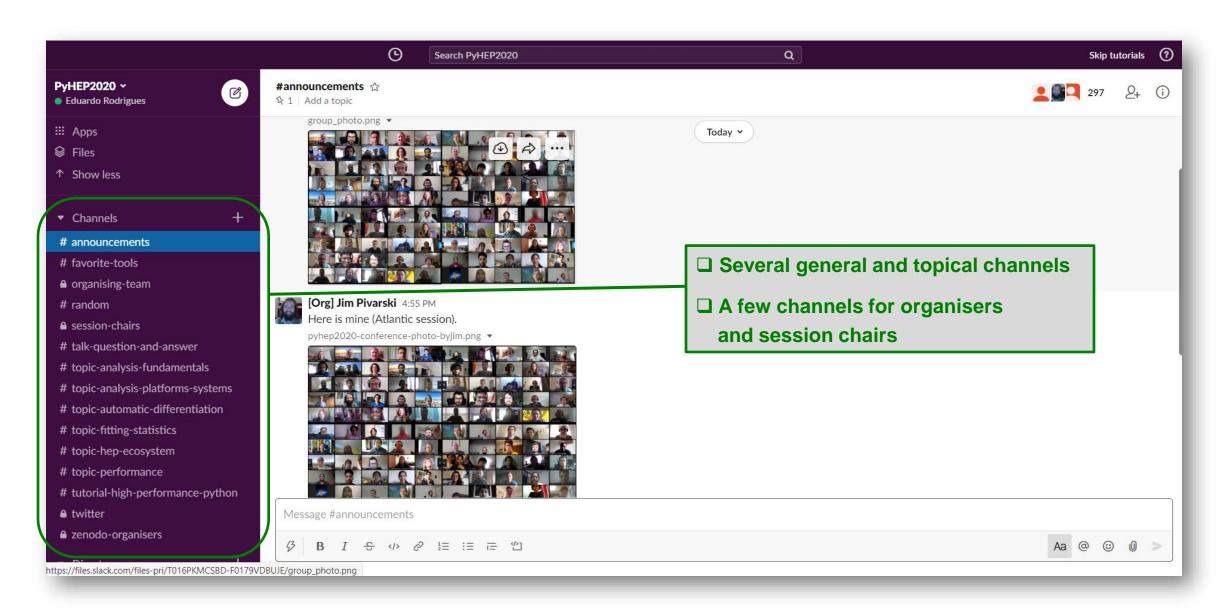
Taken from the pre-workshop survey (408 respondents)

### PyHEP 2020 stats – Jupyter notebook presentations & Binder usage

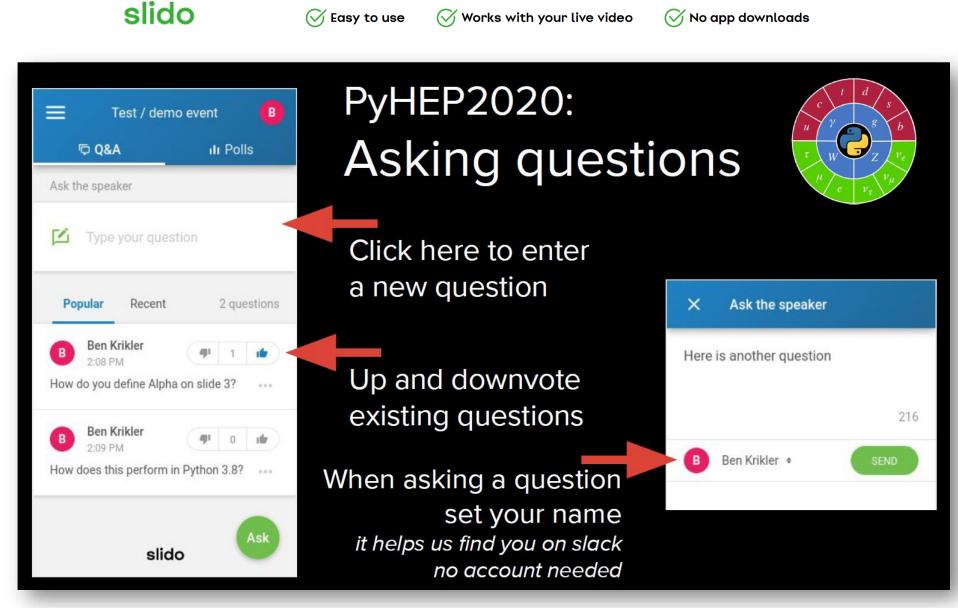


Study by Jim Pivarski

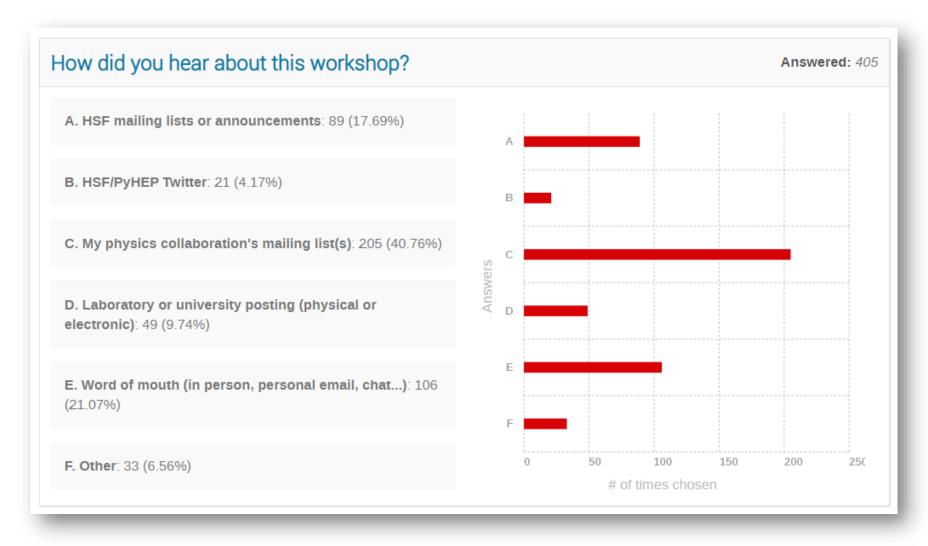
#### PyHEP 2020 logistics – Slack for discussion during/after sessions



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

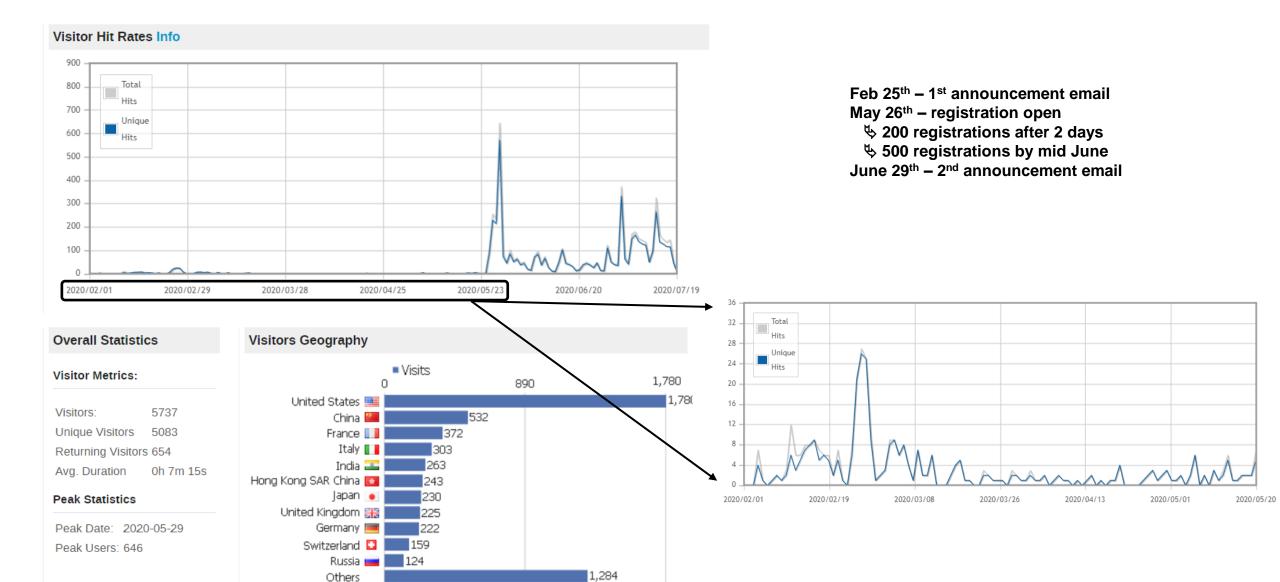


### PyHEP 2020 organisational aspects – multi-channel advertising is crucial

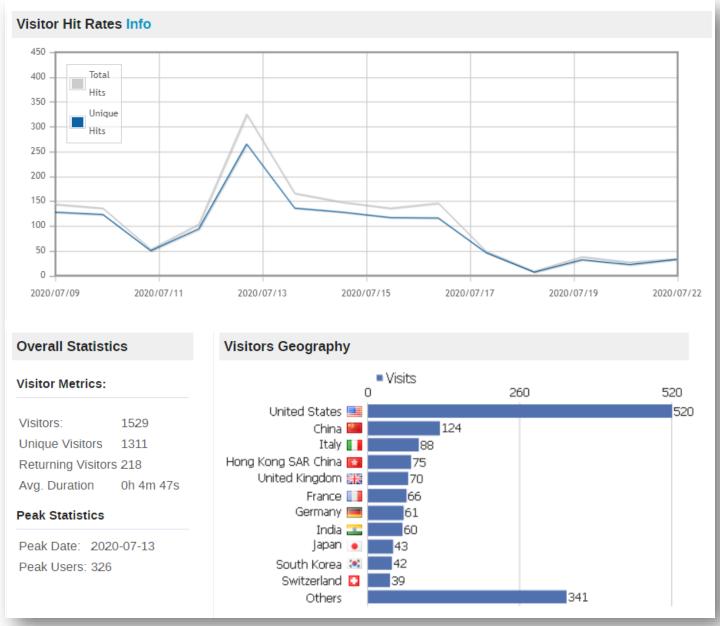


Taken from the pre-workshop survey (408 respondents)

#### PyHEP 2020 organisational aspects – Indico visits prior to start



### PyHEP 2020 organisational aspects – Indico visits during workshop



#### 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 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
- ☐ Effort to improve discoverability of (domain-specific) relevant tools





Reproducibility



Interoperability

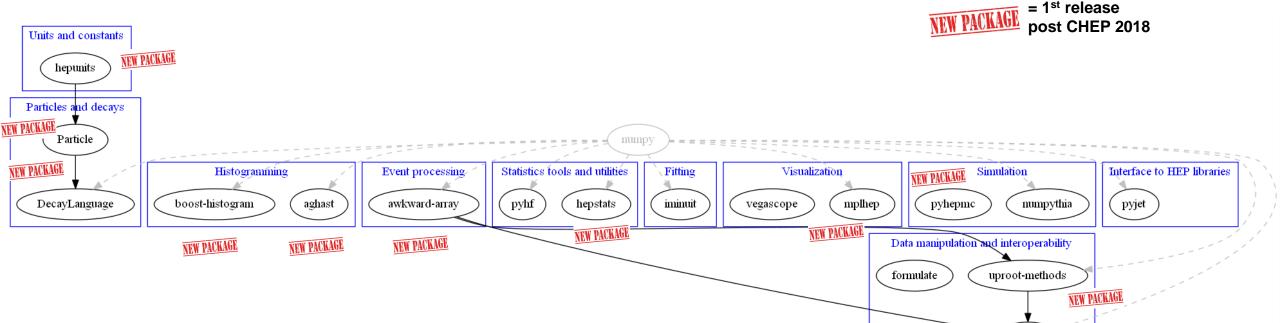


**Sustainability** 

#### Scikit-HEP project – overview of (most of the) packages

#### https://scikit-hep.org/

uproot



 $\Rightarrow$ 

There are other packages: test data, tutorials, org stats, etc. (and some which tend to now be superseded, hence deprecated ...)