HSF PyHEP WG
and the PyHEP 2020 workshop

Eduardo Rodrigues
University of Liverpool
Python, you say?
PopularitY of Programming Languages (PyPL)

- Popularity based on how often language tutorials are searched for – **Python is the big winner!**
  - Data from Google Trends
  - Log scale!

Worldwide, Python is the most popular language, Python grew the most in the last 5 years (19.0%) and Java lost the most (-6.7%).

See [http://pypl.github.io/PYPL.html](http://pypl.github.io/PYPL.html)
Popularity again from Google Trends data

Starts to illustrate why “Python in HEP” was meant to be relevant …
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' *The unexpected effectiveness 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
  - 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

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Eduardo Rodrigues
EIC Software Seminar, virtually@JLab, 26th August 2020
Python adoption in HEP – CMS study

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

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 19400 non-fork repos spanning 7 years.

Language of repos created by CMS physicists

![Diagram showing the language of repos created by CMS physicists over time.]
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)

- 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?

What are your main reasons for using Python?

- 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: 126 (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 (8.50%)
- 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 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)

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 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

  - Almost all major domains of HEP Software and Computing covered
  - Large support for the document from the community (> 300 authors from >120 institutions)

- 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 ...

HSF - "facilitate coordination and common efforts"

Groups

HEP Software Foundation

Experiments

Individuals

Labs

G. Watts (UW/Seattle)
The “Python in HEP” WG effectively started in early 2018 as an activity group, which I put forward with the proposal of the 1st workshop, held as a pre-CHEP 2018 event.

It became “formally” a WG this year 😊
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 😊

Various projects have seen the light:

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

(PyHEP WG serves as a forum for discussion, means to exchange experiences and material)

- https://github.com/CoffeaTeam
- https://github.com/FAST-HEP
- https://github.com/root-project/
- https://scikit-hep.org/
- https://github.com/zfit
How’s the Python scientific ecosystem like, outside HEP?

Python’s Scientific stack

Domain-specific

Community projects towards HEP domain-specific Python tools ⇒ ecosystem

Eduardo Rodrigues
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

- Educatve, not just informative, workshop,
  with lively discussions in the many free and dedicated time slots we foresaw
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 Workshop

- A special cuvée
- On organisational aspects
- Highlights

We now even have a logo 😄!
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 conference poster](image-url)
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
  - ⇒ 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 “pyhep2020 community” – formal citation, replaces proceedings
  - All talks got recorded, captioned and later uploaded to the **HSF YouTube channel** – dedicated playlist “**PyHEP 2020 Workshop**”
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)
Workshop agenda (2/2)

- NanoEvents object (Nick Smith)
- TITANIA: how to structure detector 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 (Kyungeun Choi)
- Integrating Coffea and WorkQueue (Cami Carballo)
- High granularity calorimeter (HGCAL) test beam analysis using Jupyter (Matteo Bonanomi)
- neoos: physics analysis as a differentiable program (Nate Simpson)
- SModelS: a tool for interpreting simplified-model results (Wolfgang Walterberger)
- 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 Oefinger)
- mplhep: bridging Matplotlib and HEP (Andrzej Novak)
- ROOT preprocessing pipeline for machine learning with TensorFlow (Matthias Komm)
- Integrated data acquisition in Python (Charles Burton)
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 mybinder.org
PyHEP 2020 logistics – slido at work for Q&As and polls

As actually seen by participants
- HSF has its own channel, with several playlists
- PyHEP 2020 recordings of presentations on YouTube, captioned, in dedicated playlist

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](https://indico.cern.ch/e/pyhep2020)

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 Twitter

@PyHEPConf

#PyHEP2020

A testimony from an astroparticle colleague …
- 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
PyHEP 2020 stats – 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
Was slido a success? Yes!

<table>
<thead>
<tr>
<th>Active users</th>
<th>181</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engagement score</td>
<td>978</td>
</tr>
<tr>
<td>Engagement per user</td>
<td>5.4</td>
</tr>
<tr>
<td>Questions</td>
<td>182</td>
</tr>
<tr>
<td>Likes / dislikes</td>
<td>483 / -54</td>
</tr>
<tr>
<td>Anonymous rate</td>
<td>34%</td>
</tr>
<tr>
<td>Poll votes</td>
<td>195</td>
</tr>
<tr>
<td>Polls created</td>
<td>5</td>
</tr>
<tr>
<td>Votes per poll</td>
<td>39</td>
</tr>
</tbody>
</table>

With 413 joined participants in total
PyHEP 2020 highlights – on workshop topics

- 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

(Made with https://www.wordclouds.com/ removing author names, institutes and some other trivial words.)
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". 
PyHEP 2020 highlights – on trends

- 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

\[ \theta^* = \text{argmin}_\theta (\log L) \]

```
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:
Wrapping up – "Python in HEP" brought to official instances …

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
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
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 2020 stats – background of participants ...

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

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

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

Taken from the pre-workshop survey (408 respondents)
PyHEP 2020 stats – … and their hopes

What are you hoping to learn from this workshop?

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%)

Answered: 405

Taken from the pre-workshop survey (408 respondents)
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 – how does slido work for Q&As

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

PyHEP2020: Asking questions

Click here to enter a new question

Up and downvote existing questions

When asking a question, set your name. It helps us find you on slack. No account needed.
PyHEP 2020 organisational aspects – multi-channel advertising is crucial

How did you hear about this workshop?

- 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)
Eduardo Rodrigues

PyHEP 2020 organisational aspects – Indico visits prior to start

Feb 25th – 1st announcement email
May 26th – registration open
％ 200 registrations after 2 days
％ 500 registrations by mid June
June 29th – 2nd announcement email
PyHEP 2020 organisational aspects – Indico visits during workshop

Visitor Hit Rates

Overall Statistics

Visitor Metrics:
- Visitors: 1529
- Unique Visitors: 1311
- Returning Visitors: 218
- Avg. Duration: 0h 4m 47s

Peak Statistics:
- Peak Date: 2020-07-13
- Peak Users: 326

Visitors Geography

- United States: 520 visits
- China: 124 visits
- Italy: 88 visits
- Hong Kong SAR, China: 75 visits
- United Kingdom: 70 visits
- France: 66 visits
- Germany: 61 visits
- India: 60 visits
- Japan: 43 visits
- South Korea: 42 visits
- Switzerland: 39 visits
- Others: 341 visits

Eduardo Rodrigues
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
- Effort to improve discoverability of (domain-specific) relevant tools

Collaboration  Reproducibility  Interoperability  Sustainability
Scikit-HEP project – overview of (most of the) packages

https://scikit-hep.org/

= 1st release post CHEP 2018

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