



HSF - Python and PyHEP

Eduardo Rodrigues, for the HSF PyHEP WG University of Liverpool



Software & Computing Round Table, 12th January 2021

Python in HEP

I.e., Python in Particle Physics"HEP" is a recognisable acronym

Python (in HEP), you say?

D 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



Why?

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

□ Very large software ecosystem built atop NumPy and SciPy

□ With very large and active community

□ In general, excellent documentation and community support

• ...

Let's roll back a few years ... at the time of the Community White Paper

The HEP Software Foundation

A Roadmap for HEP Software and Computing R&D for the 2020s

Computing and Software for Big Science (2019) 3:7 https://doi.org/10.1007/s41781-018-0018-8

Python had already been identified as a first-class language for Particle Physics back in 2016-17:

"Python has emerged as the language of choice in the data science community, and its use continues to grow within HEP. ... Python could reduce the complexity of analysis code, and therefore contribute to decreasing the "time to insight" for HEP analyses, as well as increasing their sustainability. Increased HEP investment is needed to allow Python to become a first-class supported language."

□ A lot happened in the meantime

- Evolution of (Py)ROOT
- Community-wise

"- Expand support of Python in our ecosystem with a strategy for ensuring long-term maintenance and sustainability. In particular in ROOT, the current Python bindings should evolve to reach the ease of use of native Python modules.."

□ What follows exemplifies the evolution and what helped shape that evolution ...

Why do particle physicists use Python ?



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

Python adoption in HEP – example of a 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 **19400 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





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)
- ROOT from Python is just as used as is from plain C++ !
- Conclusion even stronger if discussing analysis tools independent of ROOT

Which ROOT interface are you using mostly?

multiple answers were possible



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

ROOT & Python

□ (Py)ROOT has evolved enormously over the last few years !

- □ Some sources of material on latest goodies:
 - ICHEP 2020 talk on "Hello RNTuple and friends:

what the new ROOT means for your analysis"

- CHEP 2019 talk on

"A New PyROOT: Modern, Interoperable and more Pythonic" :

□ A game-changer in my opinion –installation via Conda !

- Came largely from the community and not the ROOT team!



	PyROOT : ROOT's automatic Python - C++ bindings				
	Modern	Pythonic			
 New design on top of Cppyy libraries for automatic binding generation https://cppyy.readthedocs.io 		More pythonisations for ROOT classes Make it easier to use ROOT C++ functionality from Python			
PyROC	User API ROOT Pythonisations	 Promote the use of Python syntax 			
Срру	y Automatic Bindings: Proxy Creation, Type Conversion Pythonisations	<pre>myfile.mytree VS myfile.GetObject('mytree')</pre>			
ROOT & C	Cling Reflection Info, ROOT Type Execution System	 Soon: support pythonisations of user classes Lazily executed 			
Support for m	odern C++ syntax	<pre>#pythonization('NyCppClass') def my_pythonizon_function(klass): # Inject new behaviour in the class klassiter =</pre>			
>>> im >>> RO templa int f(>>> RO 3	<pre>port ROT Vorginterpreter.ProcessLine(""" tettypename myTypes); }) (return sizef(myTypes); } DOT.F['int', 'double', 'void+']()</pre>	New Build & Install Support for multi-version builds			
	Interoperable	 Generate PyROOT libraries for multiple Python versions cmake -DPYTHON_EXECUTABLE=/usr/bin/python3.6/root cmake -DPYTHON_EXECUTABLE=/usr/bin/python3.7/root 			
 Integration wit 	th Python data science ecosystem	Switch between Python versions			
PyROOT	Python Scientific	<pre>\$ ROOT_PYTHON_VERSION=3.6 source bin/thisroot.sh \$ ROOT_PYTHON_VERSION=2.7 source bin/thisroot.sh</pre>			
RDataFrame TTree	1 pandas pandas M M M	 Installation on Python directories E.g. /usr/local/lib/pythonX.Y/site-packages No need to set PYTHONPATH! 			
RVec	NumPy	C++ Callables			
std::vector		 Automatically wrap Python callables with C++ callables Uses numba to compile Python callables Usage example: RDataFrame jitted string parameters 			
<pre># Run input pipelin df = ROOT.RDataFram .Filter('pT_j0 .Filter('n_jen .Define('r_j0)</pre>	<pre>ne with C++ performance that can process TBs of data @c('tree', 'file.root') 0 > 30') t >= 2') ', 'sqrt(eta_j0*eta_j0 + phi_j0*phi_j0)')</pre>	<pre>@001.0eclareCppCallable(['flost'], 'flost') def myfunction(/): return x * x</pre>			
<pre># Read out final se col_dict = df.AsNum print(col_dict)</pre>	election with defined variables as NumPy arrays <pre>mpy(['r_j0', 'eta_j0', 'phi_j0'])</pre>	<pre>df = ROOT.RDataFrame('tree', 'file.root') df2 = df.Define('x2', 'CppCallable::myfunction(x)') # New column x2 is calculated by invoking myfunction on column x</pre>			
{'r_j0': ndarray([0 'phi_j0': ndarray([-	0.26,1.,4.45]), 'eta_j@': ndarray(0.1,-1.,2.1), -0.5,0.,0.2])}				
<pre># Wrap data with pu p = pandas.DataFram print(p)</pre>	andas me(col_dict)	New PVROOT in experimental mode			
r_j0 eta_j0 pl 0 0.26 0.1 -0. 1 1.0 -1.0 0. 2 4.45 2.1 0.	h(_j0 .5 .0 .2	To build it: cmake -Deproot_experimental=0N Goal: make new PyROOT the default in 6.22 Mid 2020			
		U			

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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
- General Section 11 (1997) Full likelihoods in all their glory" on <u>HEPData</u>
 - "While ATLAS had published likelihood scans ... those did not expose the full complexity of the measurements"



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 HSF PyHEP – "Python in HEP" Working Group
 PyHEP series of workshops

Community projects towards a HEP Python ecosystem

□ BTW, a lot more information in the back-up slides ...

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

□ 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 last year ☺



Room booking

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

Lots of ways to communicate !

- The main (Gitter) channel now has over 160 people registered

Note: "embraces the broad community". "Broader" is even better © !

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 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
- \Rightarrow strong link with Training WG \odot





Eduardo Rodrigues

□ https://scikit-hep.org/

https://github.com/zfit

https://github.com/CoffeaTeam

https://github.com/FAST-HEP

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 !



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

Software & Computing Round Table, 12th January 2021

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 organise 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)



Eduardo Rodrigues





July 11–13, 2020 — Austin, Texas (USA)

Co-located with SsciPy2020

PyHEP is a series of workshops initiated and supported by the HEP Software Foundation (HSF) to discuss and promote the use of Python in the HEP community.

PyHEP 2020 will be held on the University of Texas at Austin campus, right next door to SciPy 2020, the primary conference for the scientific Python community at large. SciPy 2020 will be held on July 6–12, making it easy to attend both.

The PyHEP workshop will include • keynote from the data science domain • topical sessions • hands-on tutorials • plenty of time for discussion





#PyHEP2020 https://cern.ch/pyhep2020





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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

Surveys

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 stats – diversity and inclusion



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

Gamma 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 and later uploaded to the <u>HSF YouTube channel</u> – dedicated playlist <u>"PyHEP 2020 Workshop"</u>

zoom

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

slido

😪 launch binder

- Used *slido* to crowd-source questions,
- to prioritise the most popular ones upvoted by participants

8 binder

- 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





PyHEP 2020 organisational aspects – agenda (1/2)

Workshop agenda (1/2)

Keynotes

itori

- Rubin Observatory: the software behind the science (Nate Lust)
- **D** 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)
- **D** pyhf: accelerating analyses and preserving likelihoods (Matt Feickert)
- **D** ThickBrick: optimal event selection and categorization in HEP (Prasanth Shyamsundar)

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PyHEP 2020, All@Home, 13 July 2020



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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)

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PyHEP 2020, All@Home, 13 July 2020



7/11

PyHEP 2021 workshop

- □ Pretty clear that we will organise such an event
- □ Likely that we tag along with SciPy again, hence do our workshop just after SciPy, for example SciPy scheduled for July 5-11, undecided if f2f or virtual AFAIK
- □ We plan again a good mix of talks and tutorials. Your engagement/participation is welcome !

PyHEP WG topical meetings

- □ Interest in topical meetings was one of the workshop feedbacks
- Idea came up to follow somewhat the theme of <u>Python 3 Module of the Week</u>, but with a spirit adapted to our needs, hence rather a "Python Module of the Month", presentations with a focus on libraries relevant to data analysis in Particle Physics and why not relevant also to Nuclear Physics?
- □ First tutorial-like presentation will be on Feb. 3rd on Numba, see Indico

Let's collaborate! Your perspective will be enriching

□ <u>HEP Software Foundation (HSF)</u>

- HSF general forum <u>hsf-forum@googlegroups.com</u>

□ <u>HSF PyHEP Working Group</u>

- (main) Gitter channel

- GitHub repository <u>"Python in HEP" resources</u>

Topical meetings and PyHEP 2021

- 1st topical meeting on Feb. 3rd

The HEP Software Foundation (HSF)

• The goal of the <u>HEP Software Foundation (HSF) is to</u>

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. <u>http://doi.org/10.5281/zenodo.3779250</u>, HSF-DOC-2020-01

HED Softward Equadation

HSF - "facilitate coordination and common efforts"



HSF – Gitter channels

All Rooms		8 Rooms	703 People
HSF-GSoC	Discussions about the HEP Software Foundation GSoC program	e 👔 📓 🔘 🔿	317 People
РуНЕР	Discussion of Python in High Energy Physics https://hepsoftwar	🏹 TS 🌉 💐 🐴	165 People
PyHEP-histogramming	Discussions around histogramming	s - 1 💐 🕅 🎘	60 People
PyHEP-newcomers	github.com/hsf-training/PyHEP-resources	n 🎥 🔣 😠 💷	54 People
mpl-hep	Matplotlib proposals related to Particle Physics		36 People
HSF-GSoC-Students		🏶 😪 🛃 👳 🤶	31 People
PyHEP-fitting	Discussions around fitting	A 📓 🔃 👳 🏝	25 People
ADL	Analysis Description Language discussions	(i) 🖽 🕊 🕅 🎆	15 People

PyHEP series of workshops

PyHEP 2019





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**
- **o** Distribution and installation
- 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
- o Lightning talks

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 ⇒ "living workshop proceedings"!
- □ Find out more at <u>mybinder.org</u>







PyHEP @PyHEPConf · 18 Jul

Finally, special thanks to @mybinderteam for ensuring that we had the resources to run all of the talks and tutorials live on the Binder Federation BinderHubs! We really appreciate it and the awesome #Binder team. mybinder.org



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PyHEP 2020 logistics – session attendance & Binder usage



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



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



PyHEP 2020 logistics – Slack for discussion during/after sessions

	Search PyHEP2020	٩	Skip tutorials
PyHEP2020 ~ • Eduardo Rodrigues	#announcements ☆ 発 1 Add a topic		2 97 <u>2</u> + (j
 iii Apps iii Files ↑ Show less • Channels + # announcements # favorite-tools 	group_photo.png •	Today ~	S
 # random session-chairs # talk-question-and-answer # topic-analysis-fundamentals # topic-analysis-platforms-systems # topic-automatic-differentiation # topic-fitting-statistics # topic-hep-ecosystem # topic-performance # tutorial-high-performance-python twitter 	IOrg] Jim Pivarski 4:55 PM Here is mine (Atlantic session). pyhep2020-conference-photo-byjim.png •	A few channels for organisers and session chairs	
zenodo-organisers https://files.slack.com/files-pri/T016PKMCSBD-F0179VI	Ø B I Set <	A	a @ 🙂 🛛 >

PyHEP 2020 logistics – recordings on Parameters



Recordings of all presentations on YouTube, captioned, in dedicated playlist

PyHEP 2020 Workshop

32 videos • 761 views • Last updated on 19 Jul 2020

≡+ \mathcal{X} ...

Talks, tutorials and keynotes from the PyHEP 2020

HEP Software Foundation Workshop, https://indico.cern.ch/e/pyhep2020 230 subscribers Q HOME PLAYLISTS CHANNELS ABOUT VIDEOS DISCUSSION = SORT BY Created playlists 6 11 10 32 13 Ξ, 日本調注 國際的 Ξ, = Ξ, Щ Training: Machine Learning on Training: Intro to Machine Training : Intro to Docker PyHEP 2020 Workshop **Training : Continuous** GPU Learning Integration/Development **VIEW FULL PLAYLIST VIEW FULL PLAYLIST** VIEW FULL PLAYLIST VIEW FULL PLAYLIST VIEW FULL PLAYLIST

@PyHEPConf

<u>#PyHEP2020</u>

← PyHEP 72 Tweets	
HSF	TEXAS
PyHEP 2	2020
$ \begin{array}{c} $	Follow
PyHEP @PyHEPConf	
Workshop for #Python in particle #Physics. #F COVID-19. indico.cern.ch/event/882824/	yHEP2020 is online on Zoom given
S hepsoftwarefoundation.org/workinggroup	os/ 📰 Joined February 2020
101 Following 159 Followers	

A testimony from an astro-particle 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 – background of participants ...



Taken from the pre-workshop survey (408 respondents)

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PyHEP 2020 stats – ... and their hopes



Taken from the pre-workshop survey (408 respondents)

PyHEP 2020 highlights – on workshop topics



(Made with <u>https://www.wordclouds.com/</u> 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"

Phenomenology-HEP





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

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



pyhf.set_backend('jax')



gradHEP

Define the model, fit ... and plot:



PyHEP 2020 organisational aspects – multi-channel advertising is crucial



Taken from the pre-workshop survey (408 respondents)

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



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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
- Open forum to discuss

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



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



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

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

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 ...)

□ 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

□ Simple example:

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







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	<pre>.integrate(limits=(-1,</pre>	<mark>2</mark>))
sample	=	custom_pdf	.sample(n=1000)	
prob	=	custom_pdf	.pdf(sample)	

Eduardo Rodrigues

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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The FAST-HEP project

□ The main product should be the repository

- Talking about contents – publication is another matter ;-)



FAST-HEP

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

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

Your analysis repository is your analysis



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

□ Project towards an Analysis Description Language ...

The FAST implementation



For descriptions: use YAML...

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:



To install this package with conda run one of the following: conda install -c conda-forge uproot

PyROOT – focus of recent developments



The ROOT Team, ACAT 2019

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