University of CINCINNATI
ARTS AND SCIENCES

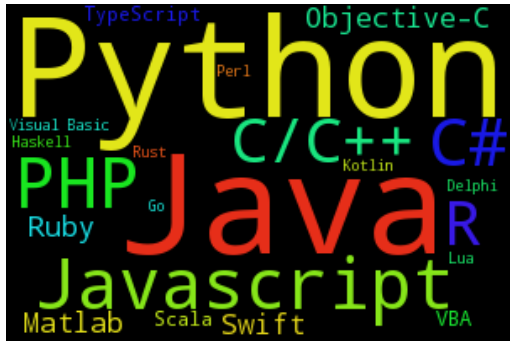
Python in HEP

first workshop, community activities

Eduardo Rodrigues
University of Cincinnati

LHCb Tuesday Meeting, CERN, 19th Sep. 2018

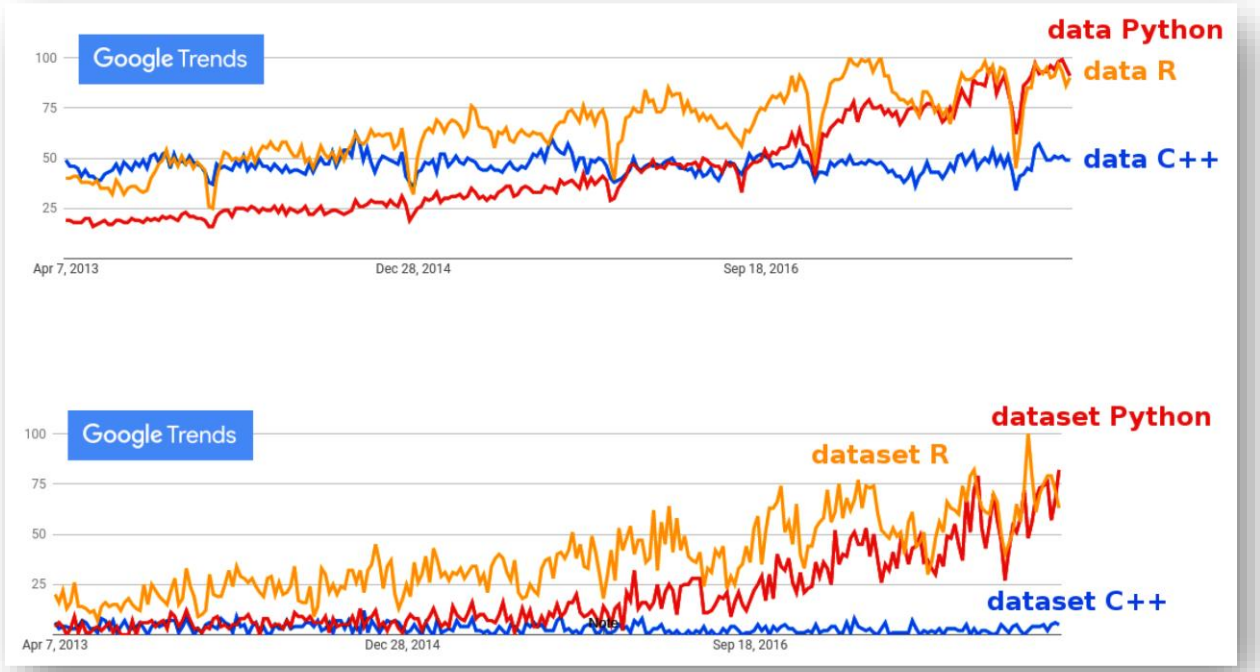
Popularity of
Programming Language
http://pypl.github.io/PYPL.html

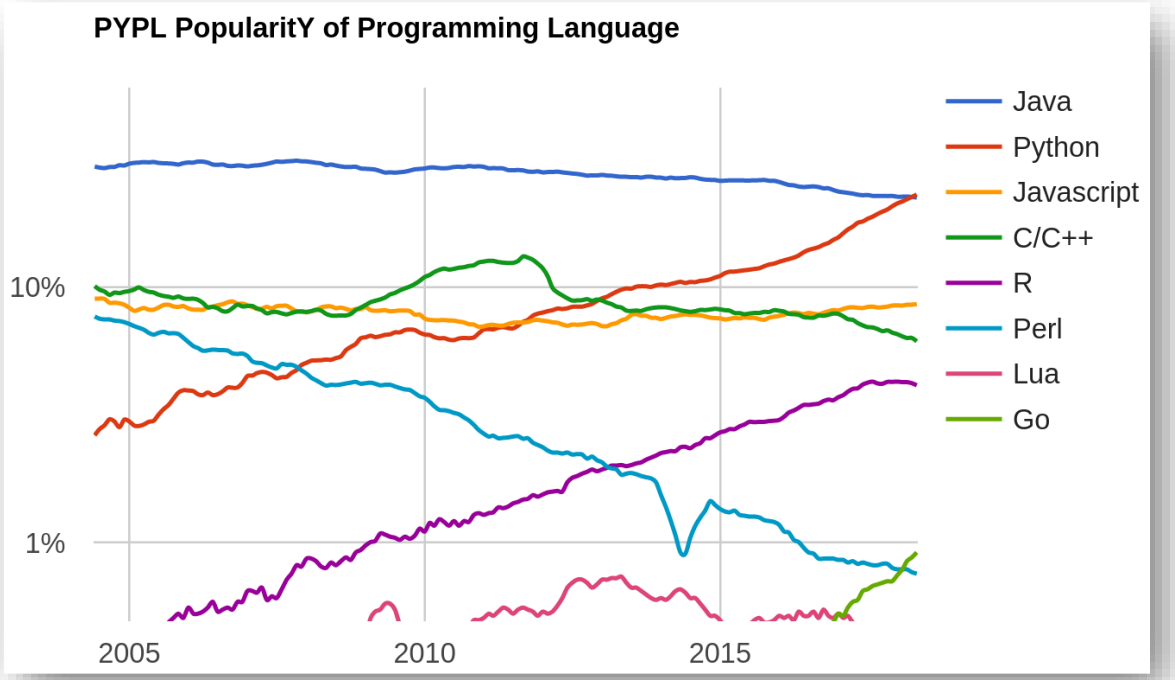


Python, you say ?

- Taken from opening talk at PyHEP 2018 workshop, 7-8 July, Sofia, Bulgaria

  Pivarski, Jim. (2018, July). The Python Scientific Software Ecosystem: Past, Present and Future. Zenodo. http://doi.org/10.5281/zenodo.1410167





Source: http://pypl.github.io/PYPL.html

- Starts to illustrate why I organised a first workshop to look at the role of Python in HEP … See later …

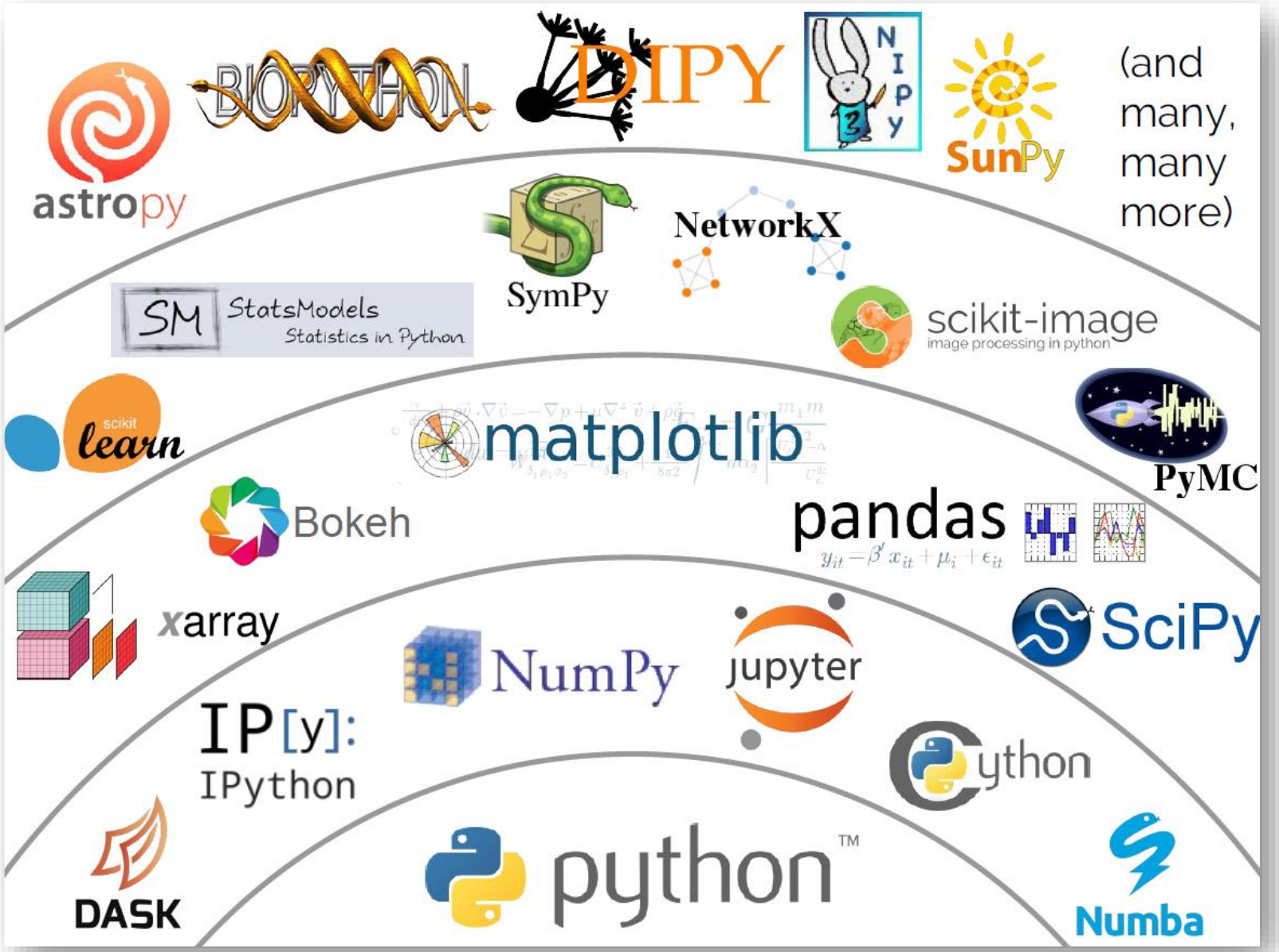
How's the Python scientific ecosystem like, outside HEP?

Domain-specific

Python's

Scientific

stack

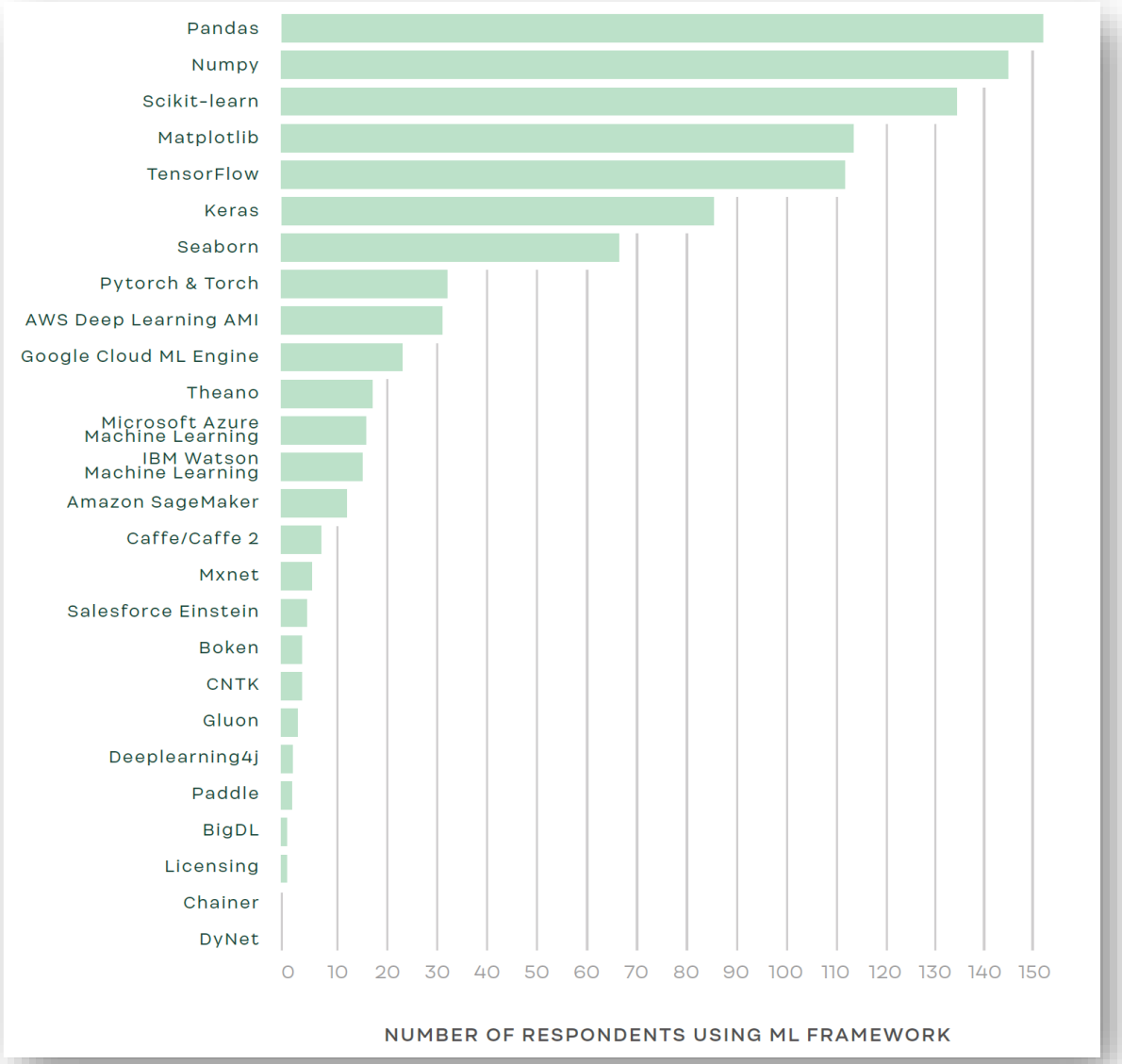


See the Scikit-HEP project GitHub for a HEP domain-specific community effort …

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

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)

Python – in and out of HEP

Outside HEP

- Has become the lingua franca for data science and machine learning
- Traditionally, emphasis on developer productivity over code runtime
- Steering high performance backends gives excellent performance for the right problems

HEP

- Python is a first-class language in HEP
- Very popular in analysis and job configuration
- HEP exploits this route to some extent, but much more to/can be done

- See also discussions on need for adequate Python support in the HSF Community White Paper (CWP)
  "A Roadmap for HEP Software and Computing R&D for the 2020s", HSF-CWP-2017-01, arXiv:1712.06982 [physics.comp-ph]
  and the supporting paper from the CWP Analysis & Interpretation WG,
  HSF-CWP-2017-05, arXiv:1804.03983 [physics.comp-ph]

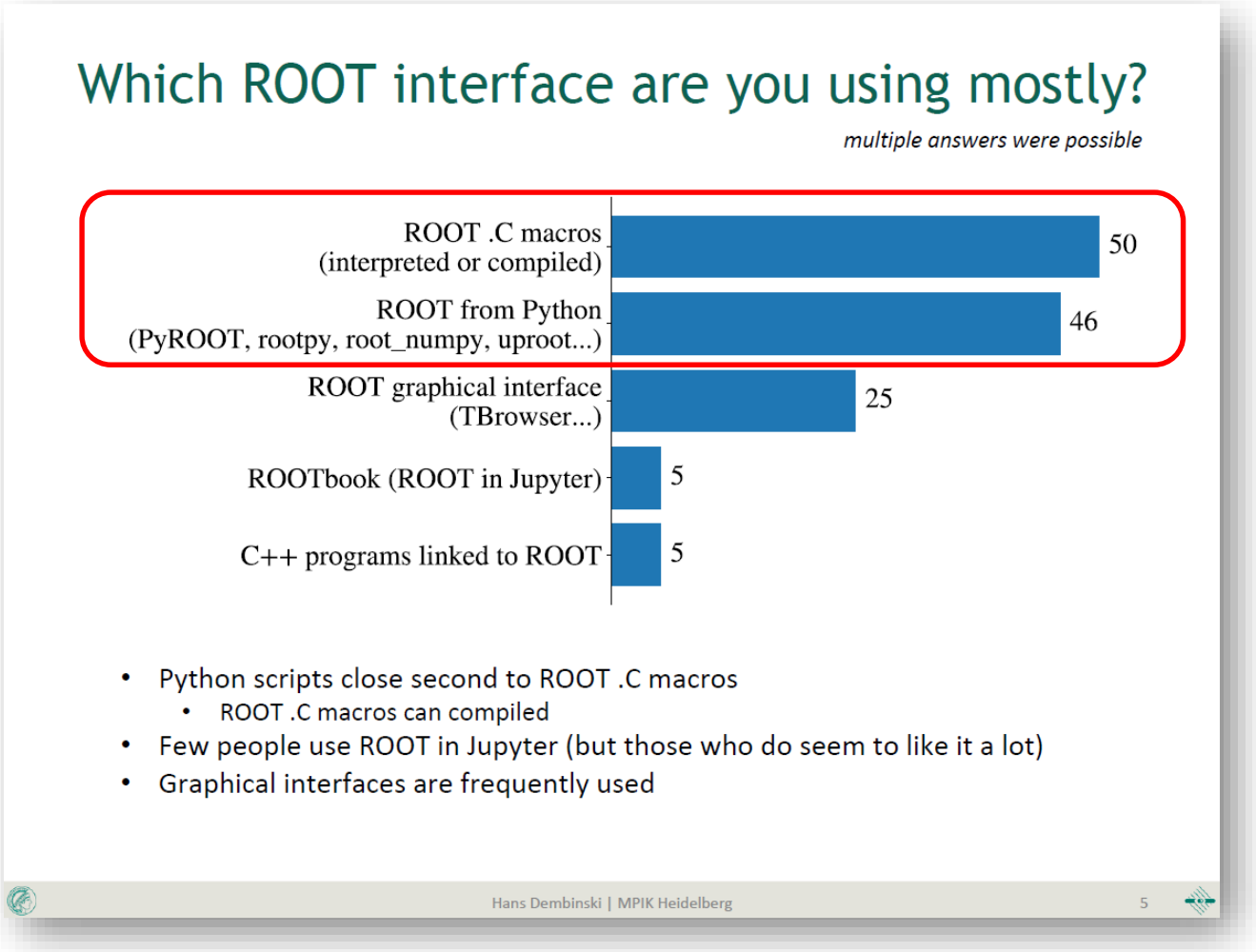
ROOT from Python in LHCb

Remember:
Hans Dembinski conducted recently an online ROOT survey among LHCb analysts

- Use of ROOT software
- Primary sources for learning and debugging
- Positive and negative experiences with ROOT
- Free comments

⇒ 74 responses received

❑ **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

PyHEP 2018 Workshop

PyHEP 2018 Workshop

Workshop link

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 2018 Workshop – overview

- 1.5 day workshop
- Pre-CHEP2018 event @ Sofia, Bulgaria

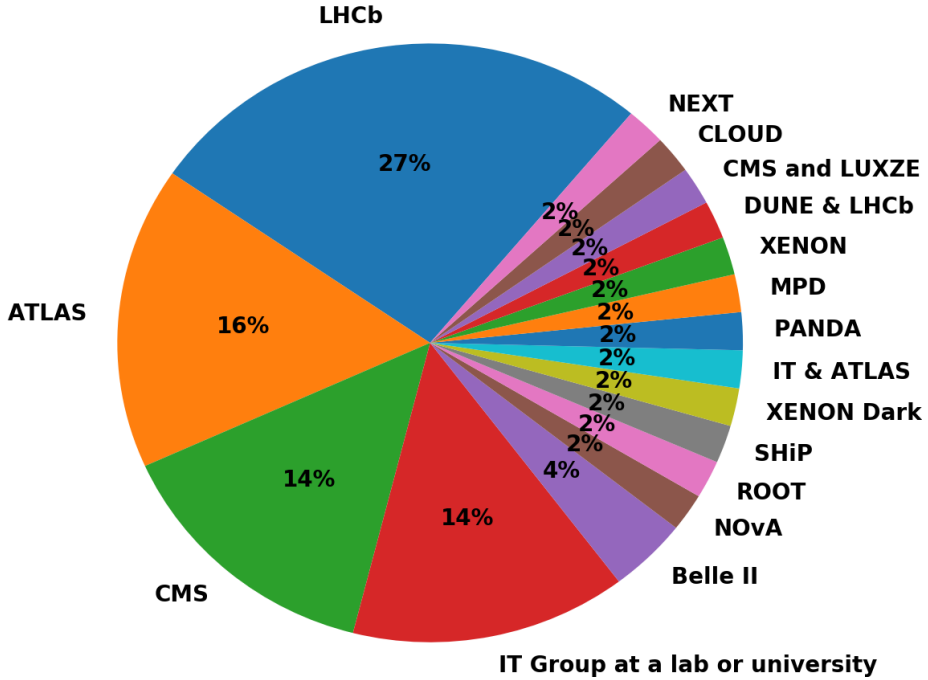
- Indico agenda – for all details
- 70 participants

- Kind sponsorship from

python SOFTWARE FOUNDATION

Nikhef

- We had a very diverse set of participants
  - BTW, excellent contingent from LHCb 🎖 !



(Taken from the pre-workshop questionnaire)

PyHEP 2018 Workshop – overview

❑ **Organisation not totally standard – worked really well**

1. **Pre-workshop questionnaire**
   - To understand the background, interests and concerns of those coming to the workshop
   - We hoped it would guide the topics we addressed, and we think it has validated what we put on the agenda
   - And could stimulate some discussion…

2. **Workshop**
   - Presentation and discussion of results of pre-workshop questionnaire at 1st session "Historical perspective / overview"
   - 7 Sessions, all plenary, including an open discussion on education and training
   - Live notes taken during the sessions, which provided plenty of food for thought

3. **Post-workshop survey**

Workshop topics / sessions:

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

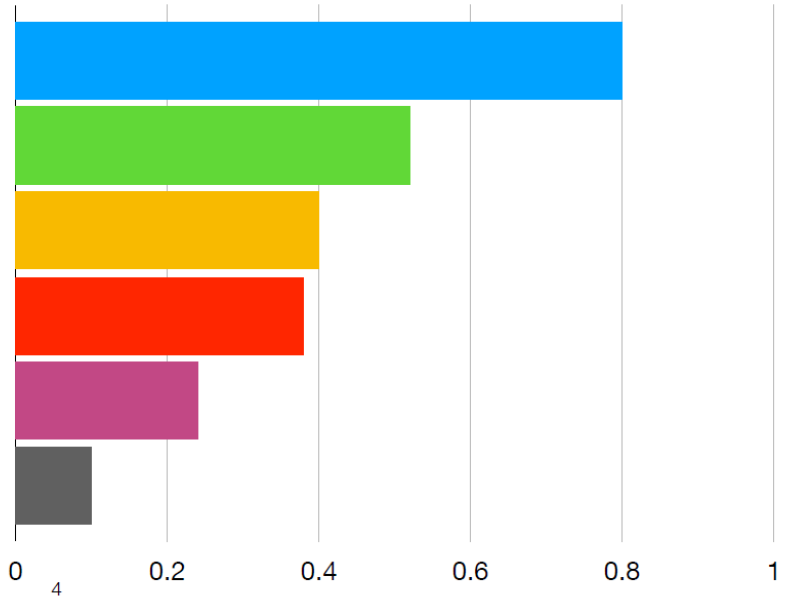
PyHEP 2018 Workshop – pre-workshop questionnaire

- 71% of workshop participants responded
- See details in

  Stewart, Graeme. (2018, July). PyHEP - Questionnaire and Discussion. Zenodo. http://doi.org/10.5281/zenodo.1419157

Motivation to use Python

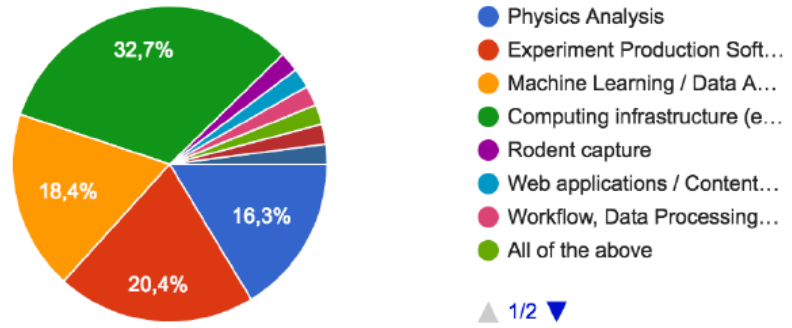
Motivation	Important to	%age
Development speed and efficiency	40	80%
Availability of other software packages	26	52%
Interface language	20	40%
Machine learning packages	19	38%
I just like it	12	24%
They make me do it…	5	10%



What are we using Python for?

How would you characterise your principle use of Python?

49 réponses



- Lots of physics (no surprise)
  - ML, Experiment Production, Physics Analysis
- More infrastructure use than we expected
  - But plays to Python's strengths, of course

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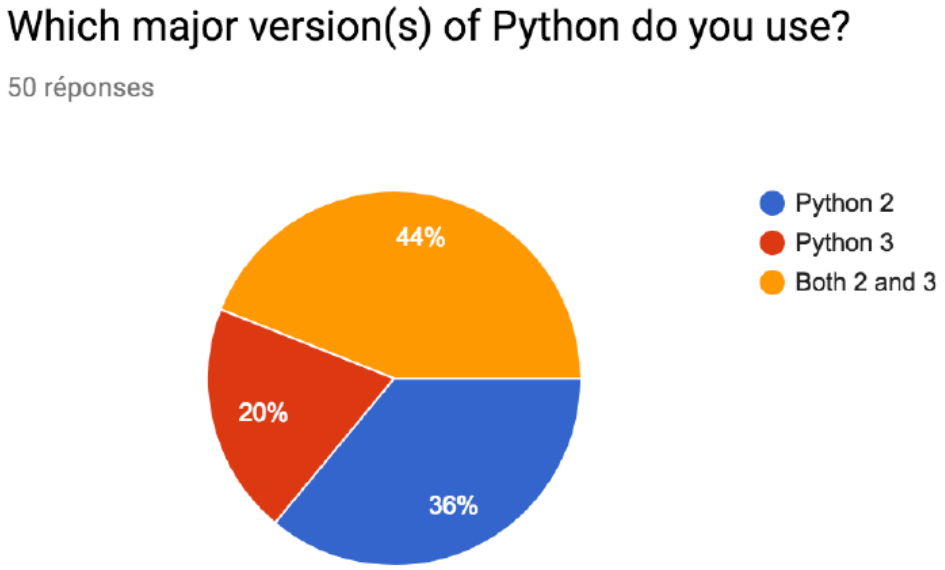
PyHEP 2018 Workshop – pre-workshop questionnaire

2, 3, 2.5?

- Amongst us there is a very healthy use of Python 3
  - Both 2 and 3 we interpret as “3 when I can, 2 if I have to”
  - Migration to Python 3 is a big concern for the community as we’ll see later



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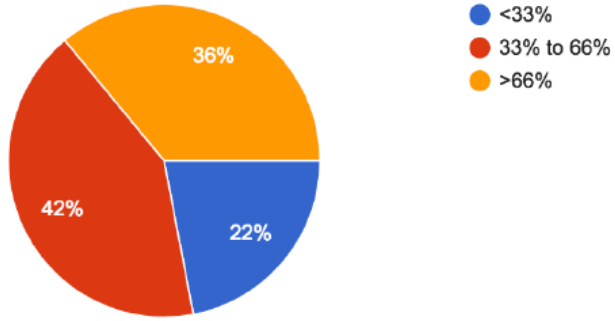
PyHEP 2018 Workshop – pre-workshop questionnaire

Use and Evolution

What fraction of your programming is done in Python?

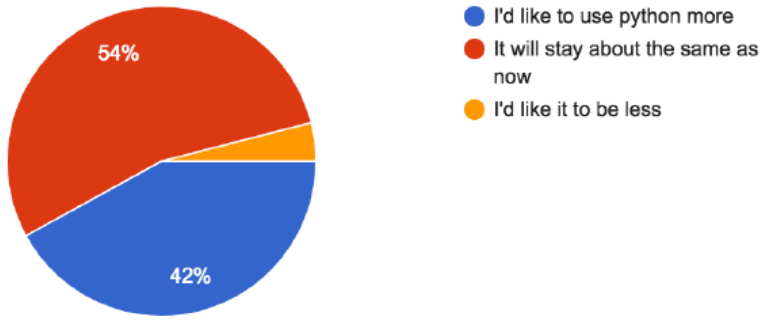
50 réponses



- We do use Python a lot (selection bias!)

In the future, how would you like your use of Python to evolve (as a fraction of your programming time)?

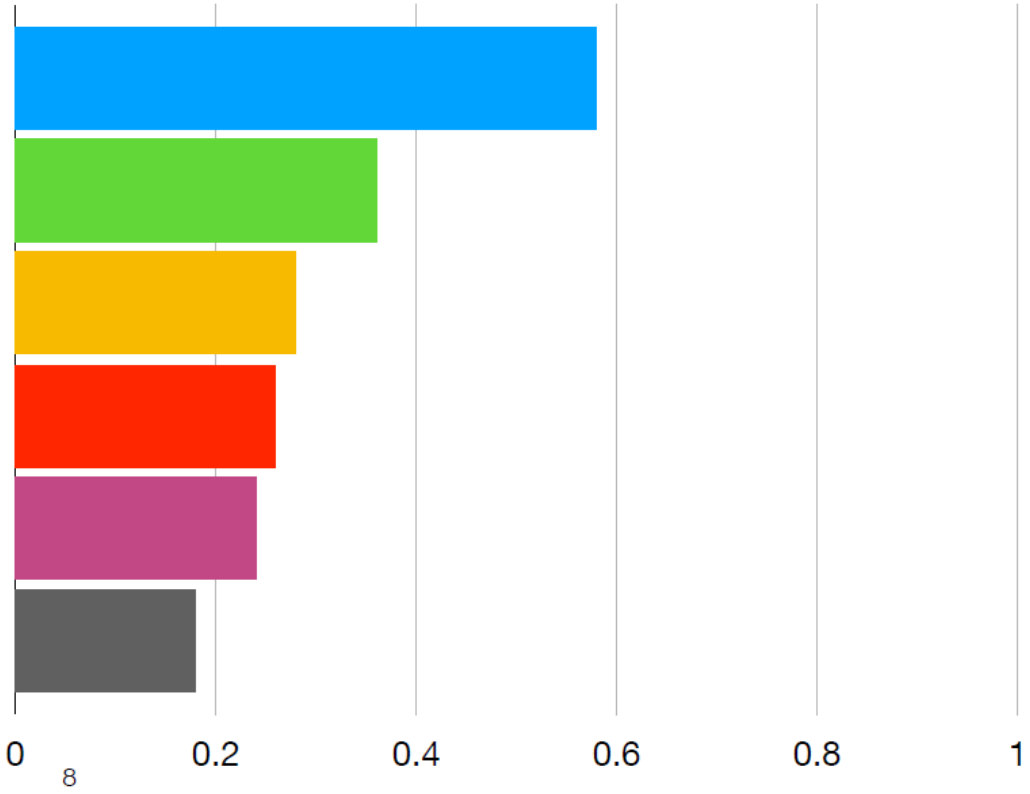
50 réponses



- Anticipating that will stay the same or increase

HEP Investments for the future?

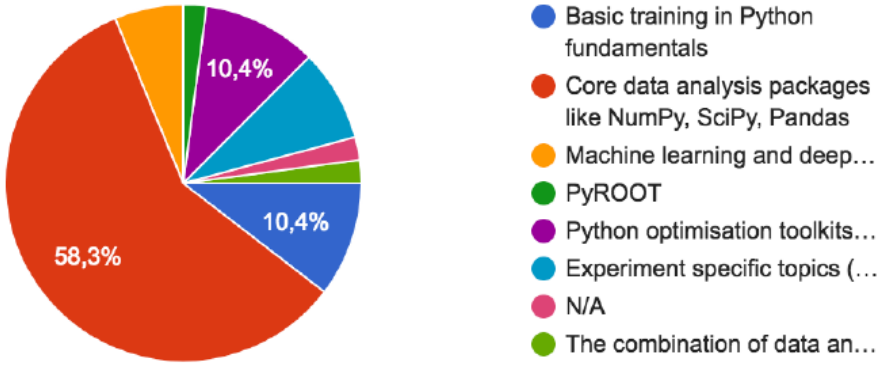
Important Development / Investment for HEP	Important to	%age
Migration from Python 2 to 3	29	58%
Better ROOT integration	18	36%
Better experiment software integration	14	28%
Better development tooling	13	26%
Improved training	12	24%
Runtime speed improvements	9	18%



Training Needs

For training, what do you think is the most urgent training to develop and give in HEP?

48 réponses



- Very strong interest in Python data analysis ecosystem
  - Open question is what is the role of HEP in this sort of training?
    - In particular what's the boundary between HEP specific topics and generic ones?

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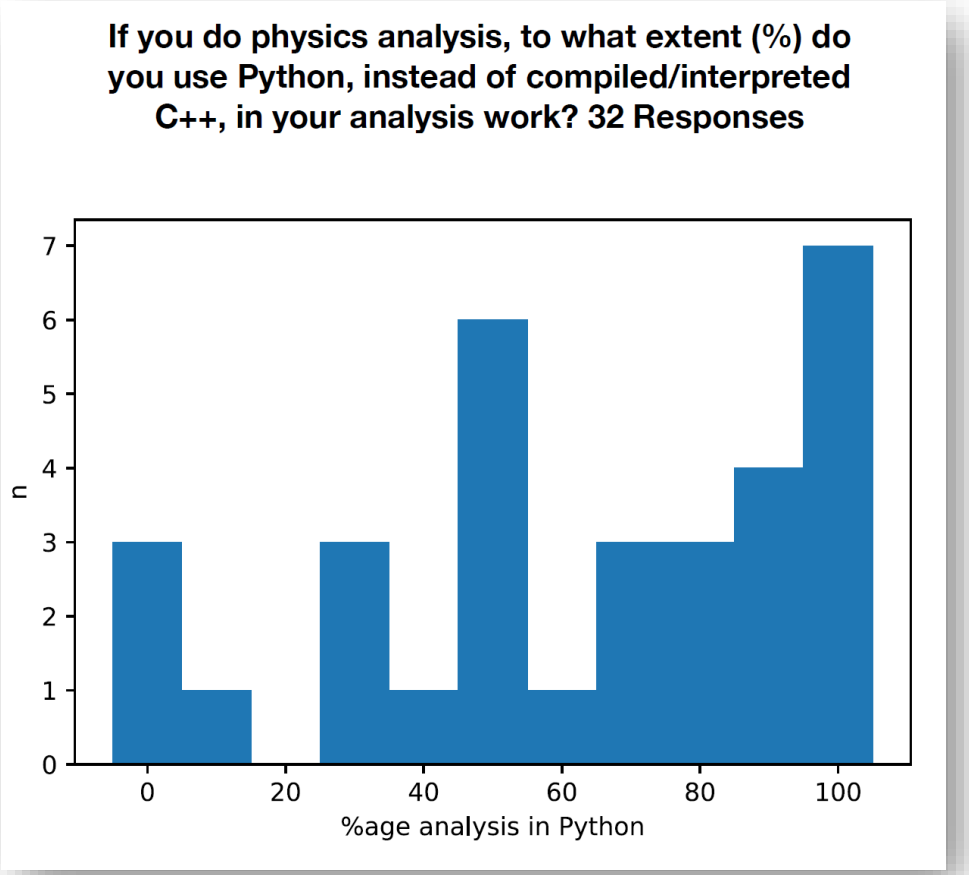
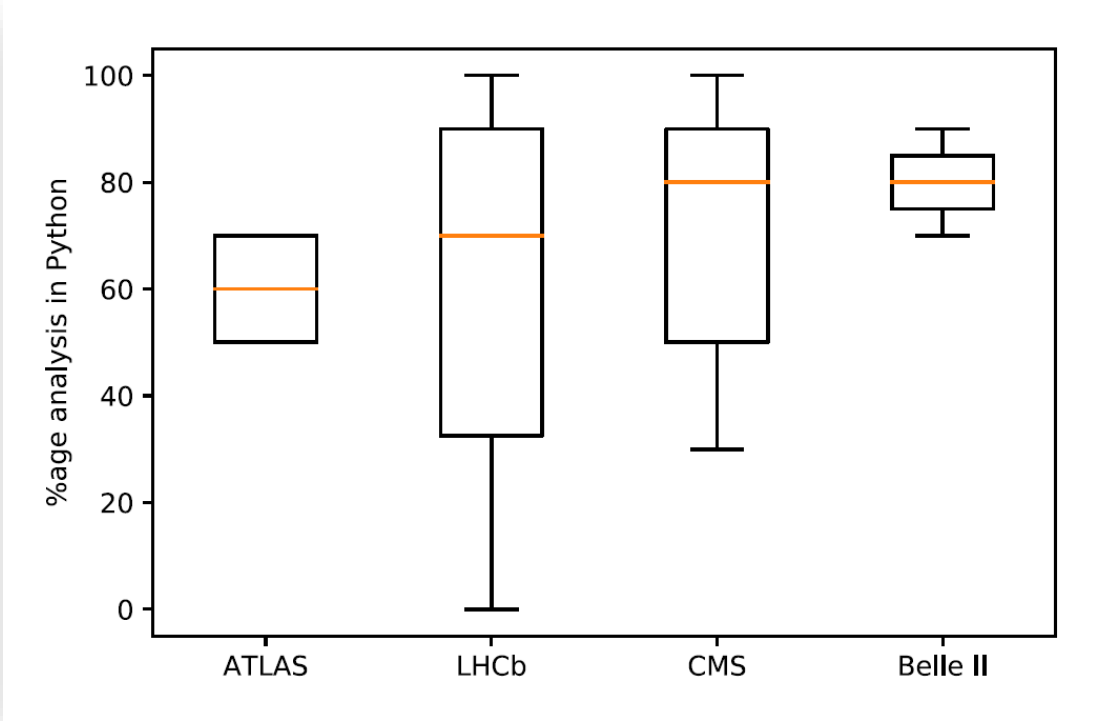
PyHEP 2018 Workshop – pre-workshop questionnaire

- Significant use of Python for a significant fraction of analyses



- Surprisingly little correlation with experiment (caveat for this one question: small statistics)



PyHEP 2018 Workshop – summary and outcomes

"Summary and outcomes" taken from:
Rodrigues, Eduardo, & Stewart, Graeme. (2018, July). PyHEP Workshop Summary and Outcomes. Zenodo. http://doi.org/10.5281/zenodo.1419148

Overview

- Python is on an upward trajectory
  - Data science, Machine learning providing strong drivers
- HEP usage is increasing too
  - Coupled to expansion of Python ecosystem, but also building on Python's traditional strengths
- Notebooks are a huge hit
  - Many thanks to Vidar for the JupyterLab talk
- Pre-workshop questionnaire
  - Training
  - Plotting
    - Galleries are really useful to find examples, didactic too!
  - Installation

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PyHEP 2018 Workshop – summary and outcomes

Inventory

- Even we did not know what useful packages are available
- Inventory of tools appropriate to HEP would be great
  - With notebooks and galleries to show how to use them
- Orphaned packages, but still useful?
  - Way to look for a maintainer
  - Scikit-HEP has handed over packages between maintainers
- Repository of expertise in the PyHEP community
  - Ties well with hot topic of education and training across the field

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PyHEP 2018 Workshop – summary and outcomes

Experiment and Analysis Directions

- Python is a language that can be used for all the computing
  - End to end
  - Flexible
  - Naturally modular
- The Belle II analysis/training jupyter cluster looks great
- Extensions to full analysis clusters?
  - Need good integration with storage
  - SWAN as an integrated, stable and reproducible environment

This looks like a key direction, aligned with Community White Paper Roadmap

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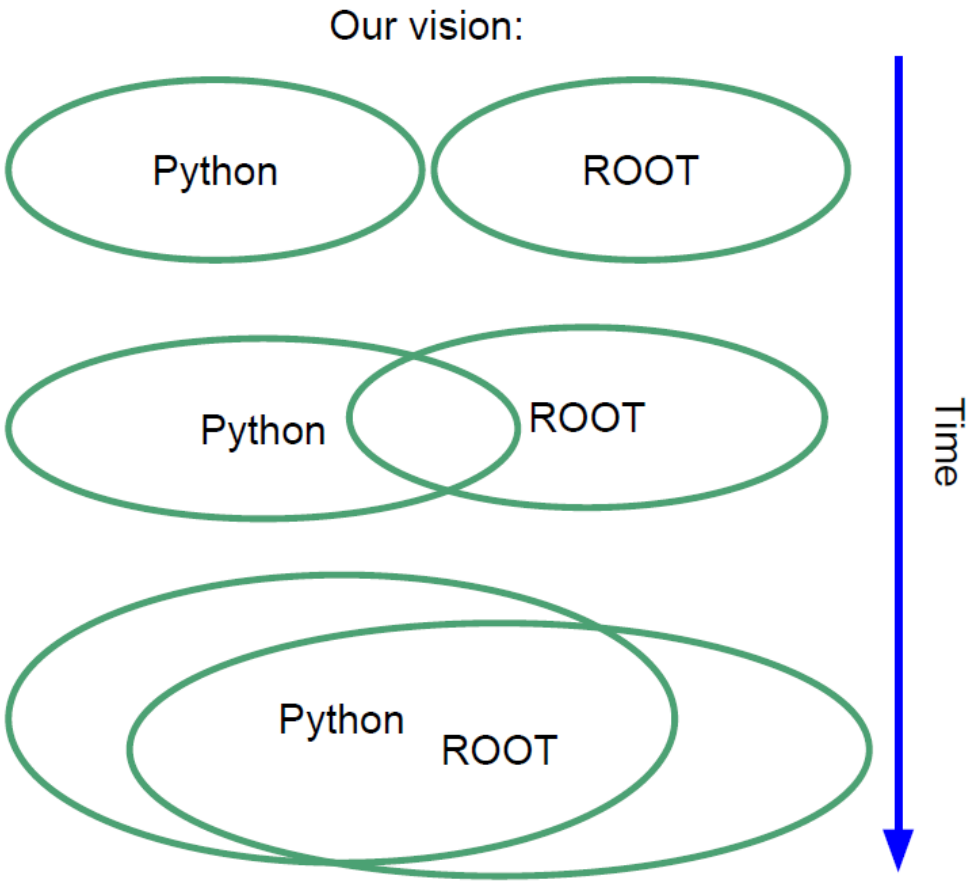
PyHEP 2018 Workshop – summary and outcomes

ROOT

- Data model ideal for HEP
- Fitting, histograms best in class
- Heavy component
  - Too burdensome for some small experiments it seems
  - Modularity would help
- Easier ways to install
  - NLeSC effort was greatly appreciated
- cppyy is a contribution that is far less well known than it should be
- PyROOT developments exciting
  - Particularly adding pythonisation, to make things natural



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PyHEP 2018 Workshop – summary and outcomes

Training

- The Belle II analysis jupyter cluster looks great
- Extensions to analysis clusters?
  - Need good integration with storage
  - Cf. SWAN
- Using standard Python libraries to achieve HEP workflows is a concern for *our community*
- Training session discussion was brilliant, right!
  - (What do you mean you forgot already what was said?)

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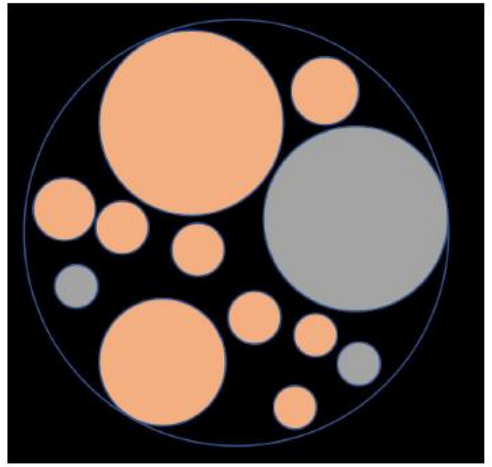
PyHEP 2018 Workshop – summary and outcomes

Distribute and Install



- Can we be as standard as possible?
  - CMS using pip + PyPI
- Distributing whole HEP stack is a difficult problem
  - Worse than Python, multidimensional
- Distinguish experiment stack from analysis
  - Toolboxes, not frameworks
  - SWAN encapsulates things really well
  - Daring view: ubiquitous network access + browser...
- Modularity and flexibility of the solution vital
  - HSF Packaging Group should pay more attention to this

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PyHEP 2018 Workshop – summary and outcomes

Figure 1-1. Guido van Rossum's PyCon 2014 keynote address (photo credit: David Lesieur 2014, CC-BY-SA)

To Python 3

Python 2.7 will retire in...

1	5	23	13	10	20
Year	Months	Days	Hours	Minutes	Seconds

Enable Guido Mode Huh?

- Will be painful for the large pieces, but we just have to do this
  - LS2 project for LHC experiments - having to get to the end of Run 3 with an unsupported Python would be uncomfortable
  - An increasing gap between legacy Python 2 and Python 3 would hurt

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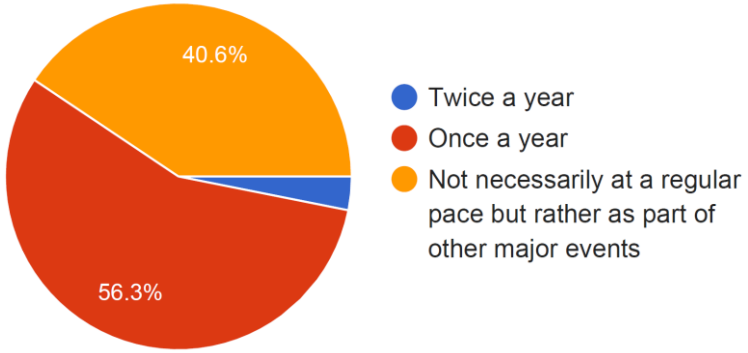
PyHEP 2018 Workshop – post-workshop survey

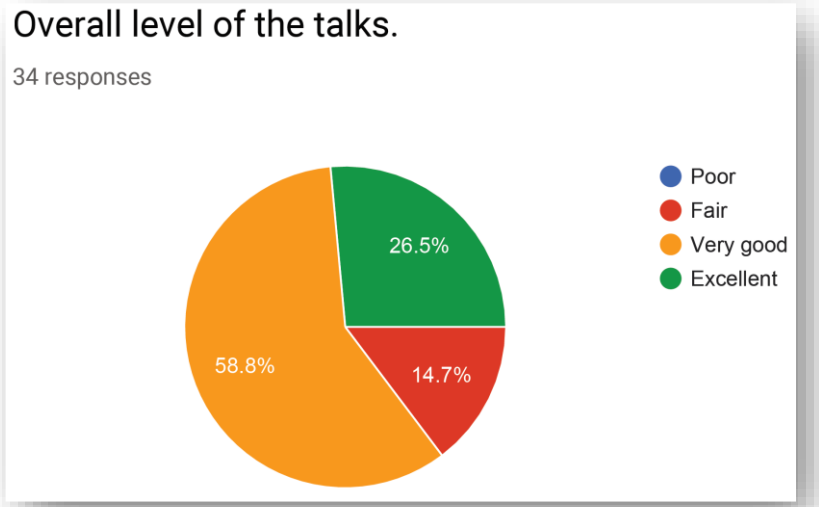
- Stardard survey to assess level of satisfaction of participants

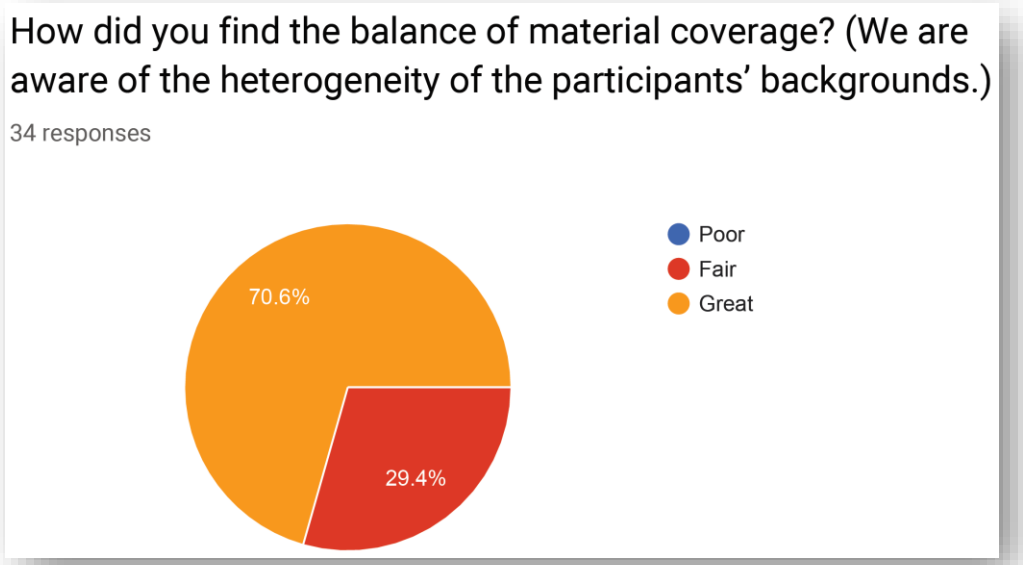
Main conclusions

- Participants largely happy
- Interest in having more PyHEP workshops



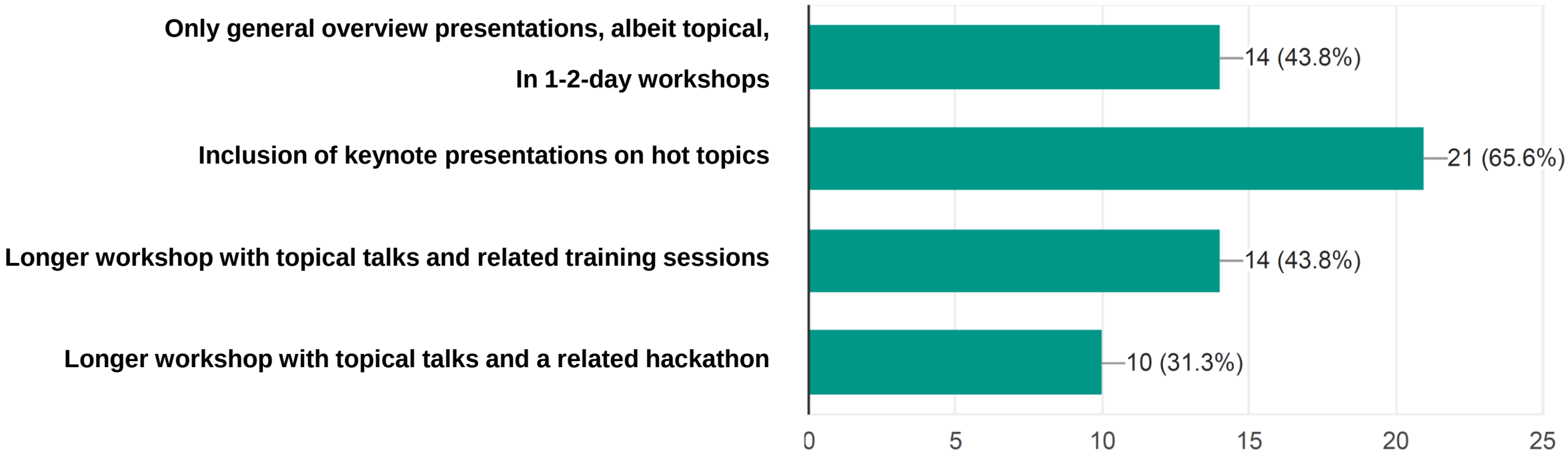
- Mild interest in occasional 1-hour PyHEP meetings organized by the HSF





PyHEP 2018 Workshop – post-workshop survey

❑ **Format of future PyHEP workshops (participants picked 2 preferred options)**



“Python in HEP” community

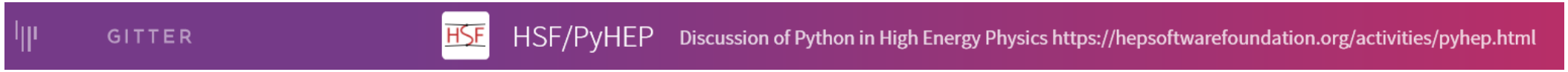
Building a community - communication

Community "start-up"

- ❑ Obvious interest from PyHEP 2018 workshop participants in building a community of developers and users
- ❑ Created a (non-formal) coordination team to push activities forward
  - Careful selection of team, to embrace Particle Physics at large
  - So far: Eduardo (LHCb & DIANA-HEP), Graeme Stewart (ATLAS & HSF), Jeff Templon (Nikhef & Grid computing), Chris Tunnell (XENON1T). Person from neutrino community to join soon.
- ❑ Fully in line with the HSF activities & interests, with HSF support

Actions, please !

- ❑ Need a low entry-level and informal way to communicate and exchange ideas, material, etc.
- ❑ We created a "Python in HEP" Gitter channel



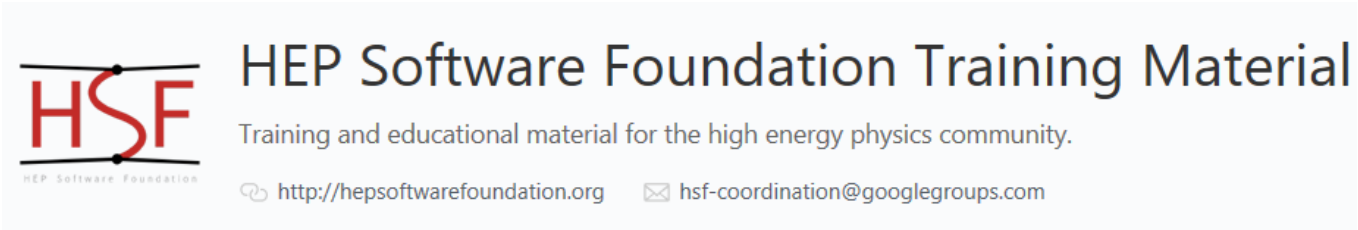
- ❑ Well over 100 messages exchanged already, on a diverse set of topics, from general to technical !
- ❑ Free and trivial sign-in … (e.g. with a GitHub or GitLab account)

Building a community – training & education

- Seen as a very important topic
- General interest in sharing material and knowledge, organise events across experiment boundaries

Actions, please !

- We created an HSF organisation on GitHub for training and education material: https://github.com/hsf-training



- 2 repositories exist as of today:
  - Good-old LHCb "analysis essentials" course moved to this HSF organisation, see https://github.com/hsf-training/analysis-essentials, to push on a community-wide effort around training and education
  - New repository for "Python in HEP" resources: https://github.com/hsf-training/PyHEP-resources

Software – recognition and citations

Recognition of work in software & computing

- ❑ Recurrent topic, even more following the preparation and release of the HSF Community White Paper
- ❑ Still a long way to go for software work to be on the same recognition level as analysis and hardware work !

Actions, please !

- ❑ Please cite software-related publications and software packages you use!
- ❑ As far as the PyHEP 2018 workshop goes:
  - We created a PyHEP2018 community on Zenodo, to collect all talks (there are no proceedings)
  - Each uploaded presentation gets attributed a DOI, for standard citation - nice and easy

In short

- Feeling the urge to connect and contribute?

- We are a community ⇒ everybody welcome !
- Easy, just join and start contributing … much to take in and give out !

Links

- Gitter channel HSF/PyHEP
- GitHub repository "Python in HEP" resources

Mailing lists

- HSF general forum hsf-forum@googlegroups.com
- PyHEP coordination team: hsf-pyhep-organisation@googlegroups.com

Thank you