Introduction to the Scikit-HEP project

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HEP Seminar, DESY, 3rd March 2020

Outline

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

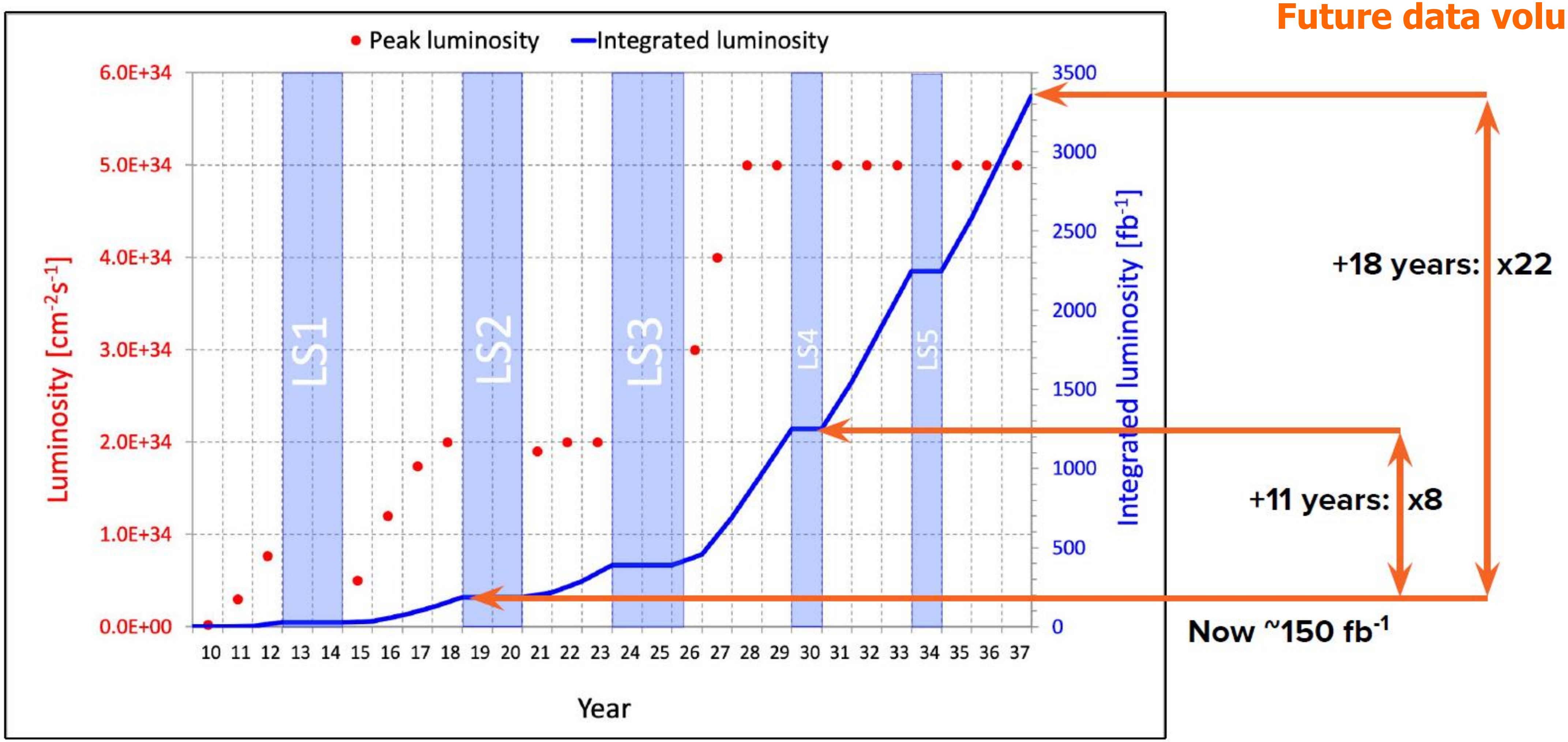
- **Challenges in data analysis in High Energy Physics (HEP)**
- **The reign of Python**
- **Community efforts – HSF, PyHEP**
- **The Scikit-HEP project**
- **Other community software projects**
- **Final remarks**

Challenges in data analysis in High Energy Physics

- ❑ “Big Data” projects
- ❑ Computing & software challenges

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

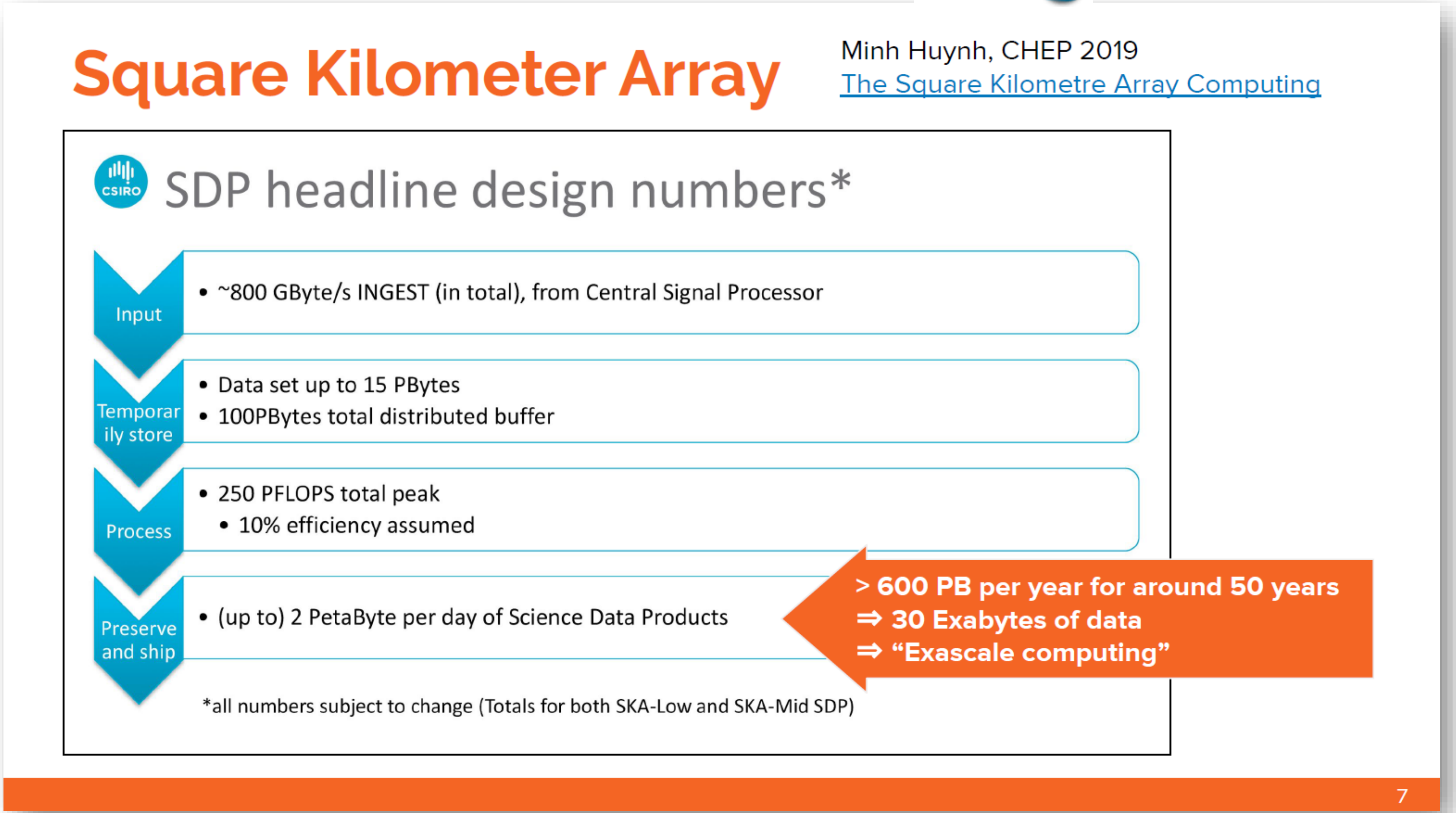
Future data volumes



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

Another "Big Data project" – SKA

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



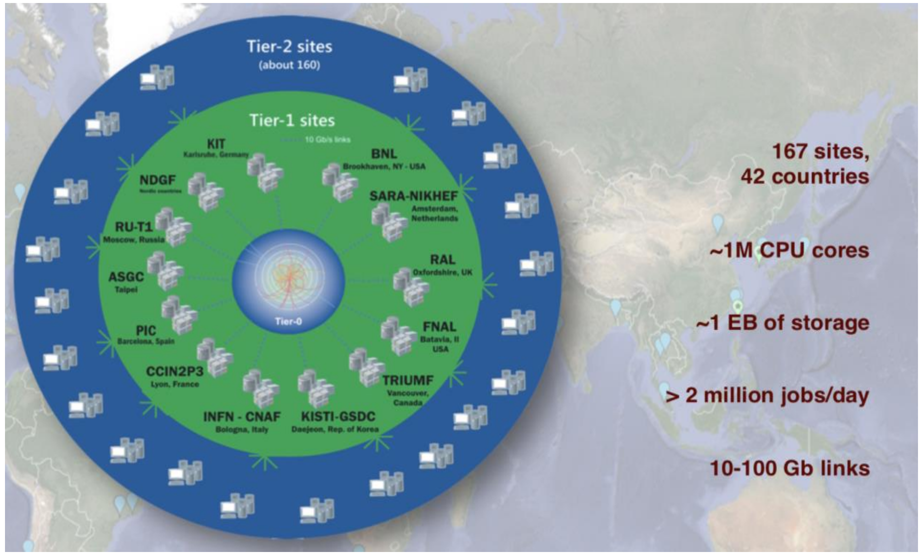
Slide taken from Ben Krikler

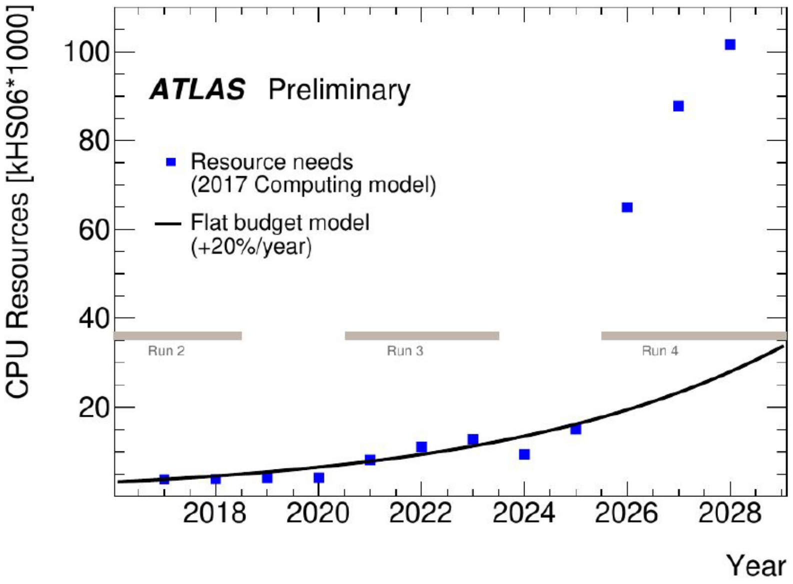
Computing & software challenges

- ❑ **HEP has made a vast investment in software**
  - Estimated to be around 50M lines of C++
  - It would cost $500M to develop commercially
- ❑ **This software is a critical part of our physics production pipeline**
- ❑ **LHC experiments use about 1M CPU cores per hour per day: about 1 TB of data with 100 PB of data transfers per year**
  - We are in the Exabyte era already
- ❑ **Future physics programmes pose significant challenges**
  - Factor of 10-100 more computing resources needed in the HL-LHC

WLCG: the international collaboration to distribute and analyse LHC data

WLCG
Worldwide LHC Computing Grid





Technology evolution

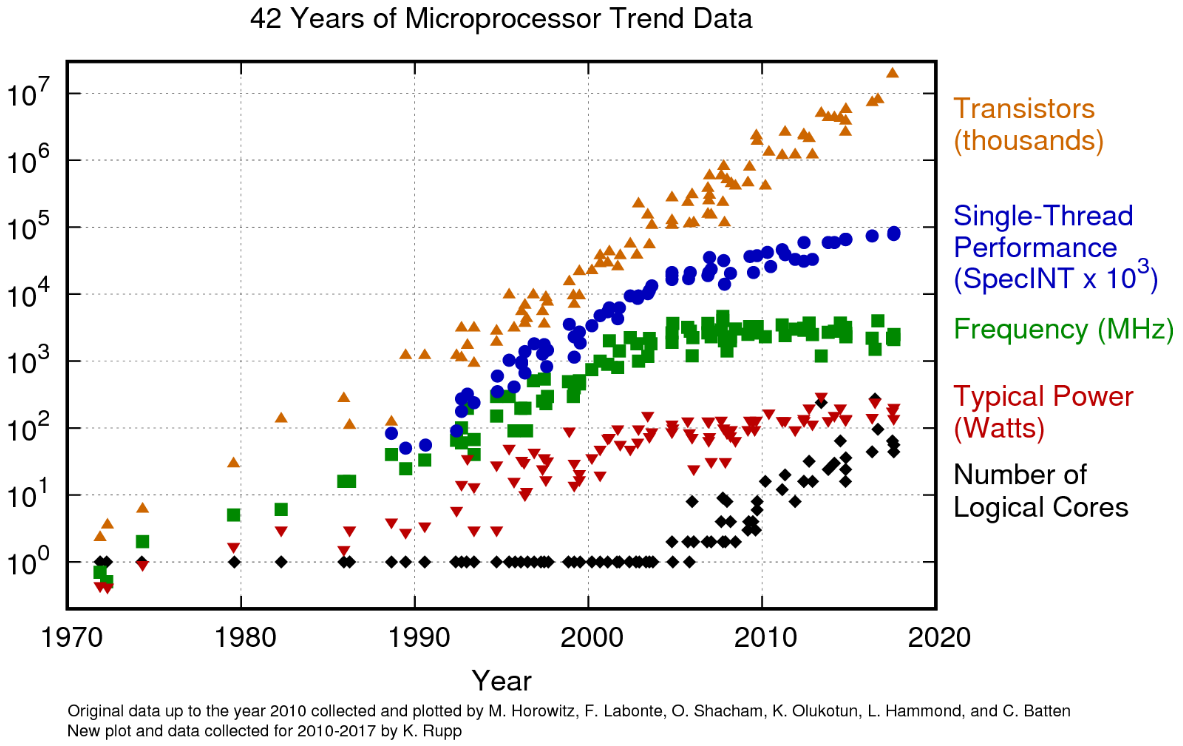
❑ Moore's law continues but doubling time is lengthening
(is the observation that the number of transistors in a dense integrated circuit doubles about every two year)

❑ Clock speed scaling failed around 2006

❑ Memory access times are now ~100s of clock cycles
Poor data layouts are catastrophic for software performance

❑ HEP also needs to deal with non-CPU architectures
- GPUs, FPGAs, TPUs

❑ This makes it more complex to write (efficient) code



https://www.karlrupp.net/2018/02/42-years-of-microprocessor-trend-data/

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

Words from an LHCb 2018 Analysis Survey Report

- ❑ **Lots of data?**
  - ⇒ **Look at what the Big Data community is doing**
- ❑ **Evolution of computing resources won't be enough to digest all data**
  - ⇒ **Use resources as efficiently as possible**
- ❑ **Physicists want to minimise the "time to insight". But coding takes a fair share of one's time, and is error-prone.**
  - ⇒ **Adopt open-source best practices, popular and easy languages**

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

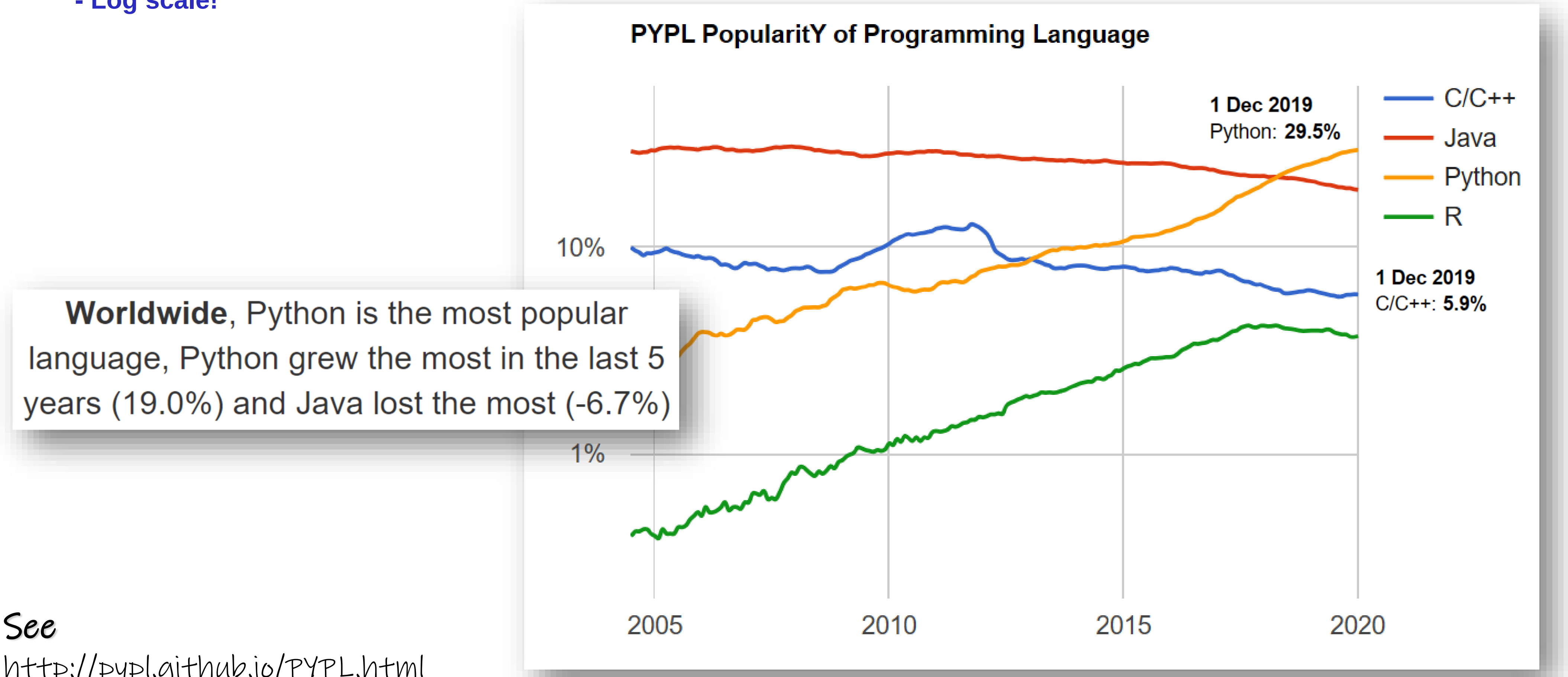
(it will not discuss ROOT either)

The reign of Python

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

PopularitY of Programming Languages (PyPL)

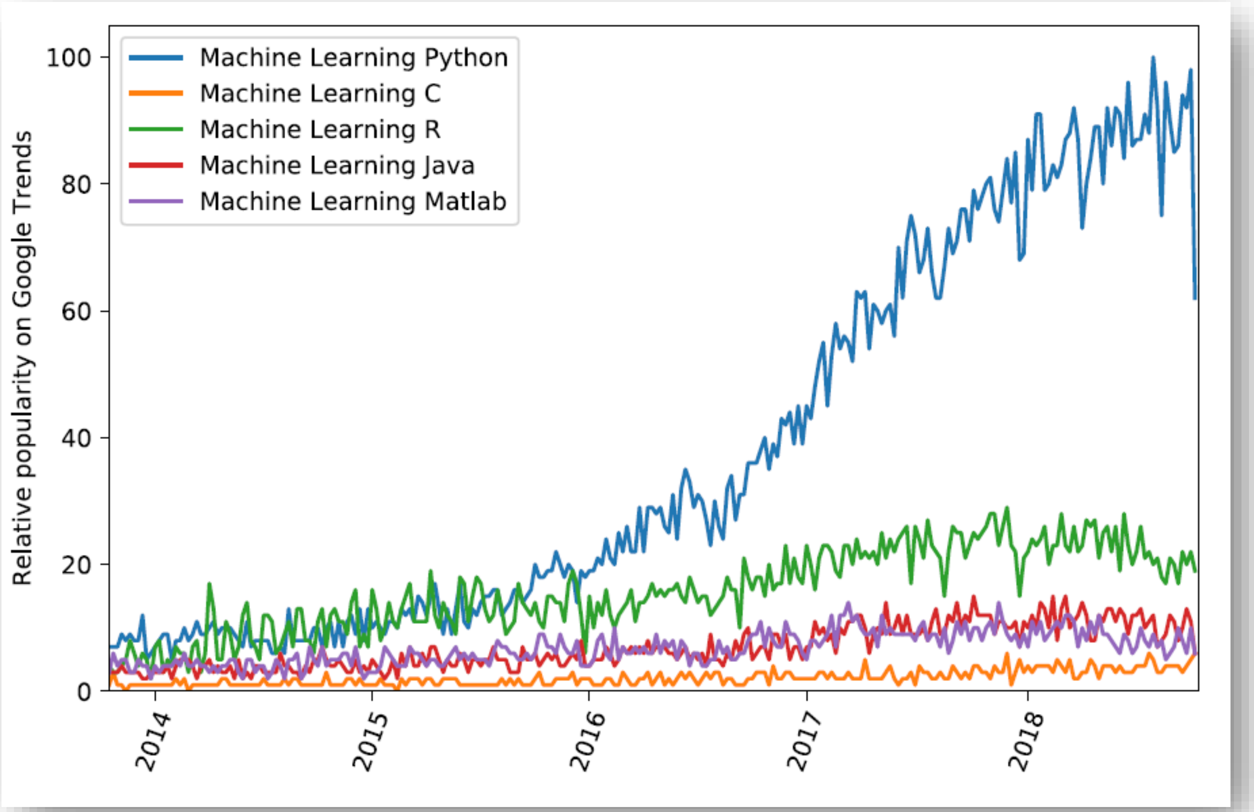
- Popularity based on how often language tutorials are searched for – Python is the big winner!
  - Data from Google Trends
  - Log scale!



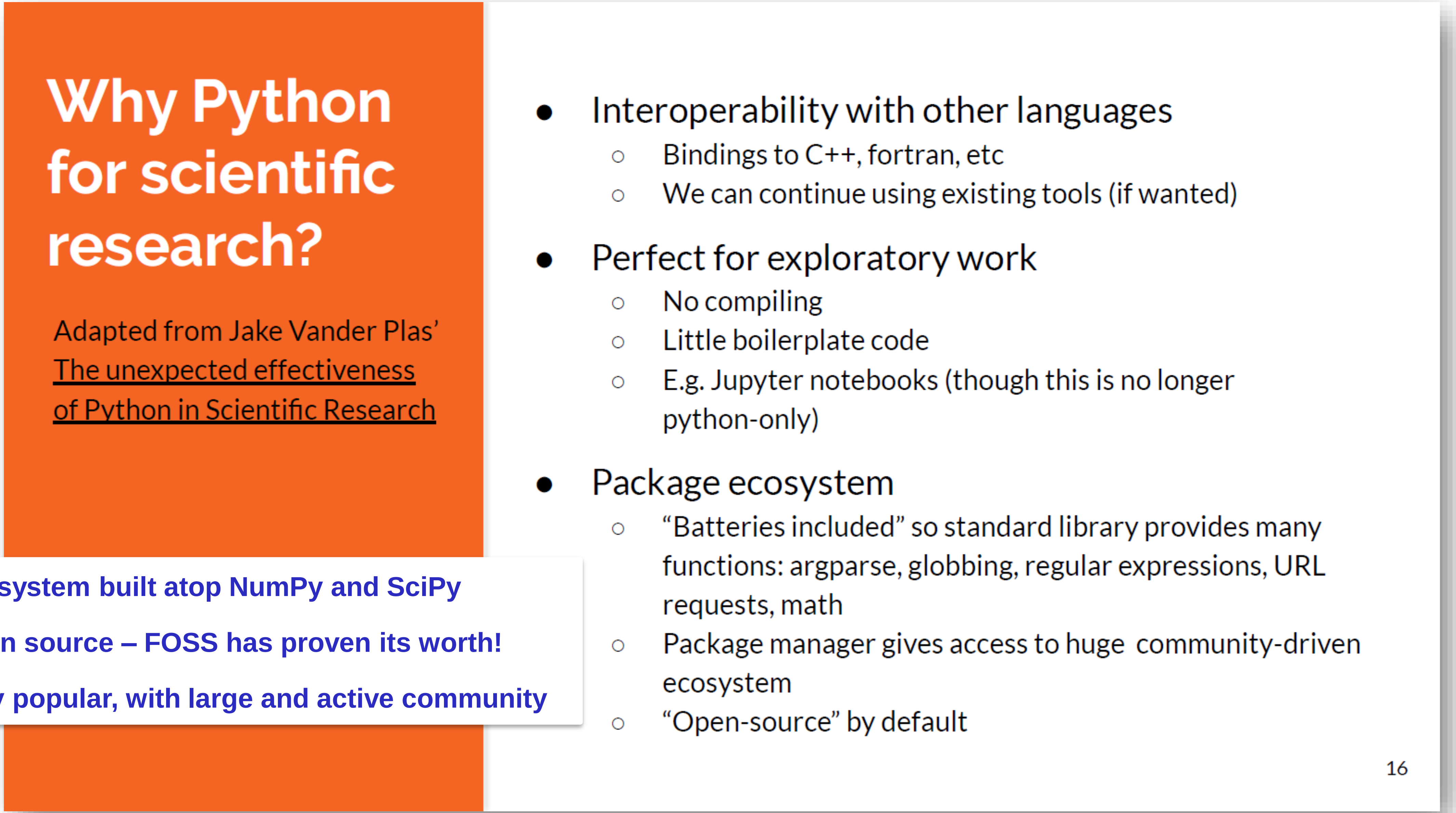
See
http://pypl.github.io/PYPL.html

PopularitY of Programming Languages for Machine Learning

- ❑ **Popularity again from Google Trends data**



Why Python for scientific research ?



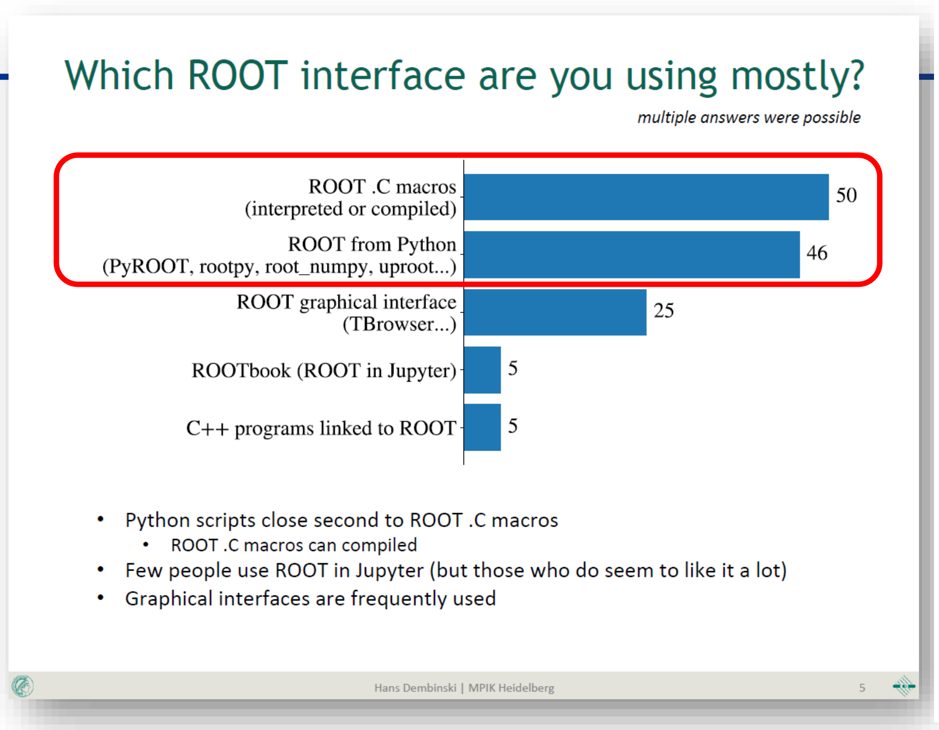
- ❑ **Ecosystem built atop NumPy and SciPy**
- ❑ **Open source – FOSS has proven its worth!**
- ❑ **Very popular, with large and active community**

Slide taken from Ben Krikler

HEP data analysis … in C++ or Python ?

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
- ❑ **Conclusion clearly even stronger if discussing analysis tools independent of ROOT**

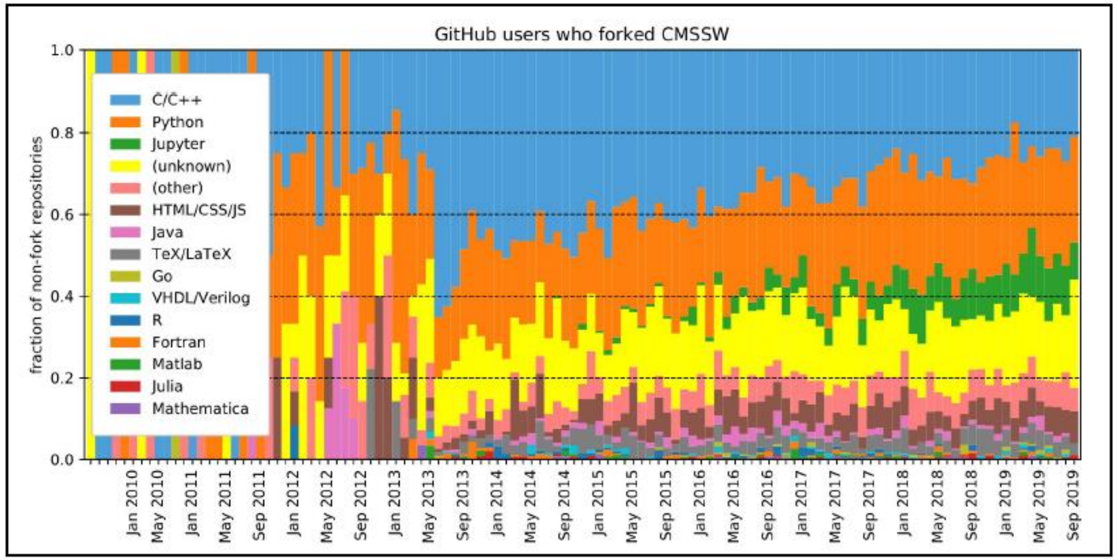


Taken from
Hans Dembinski, *User Feedback from LHCb*,
ROOT Users' workshop, Sarajevo, Sep. 2018

CMS study

- ❑ **Most users code outside of CMSSW(*) is now Python**
  - Python has been eating the share of C/C++

(*) CMS software framework



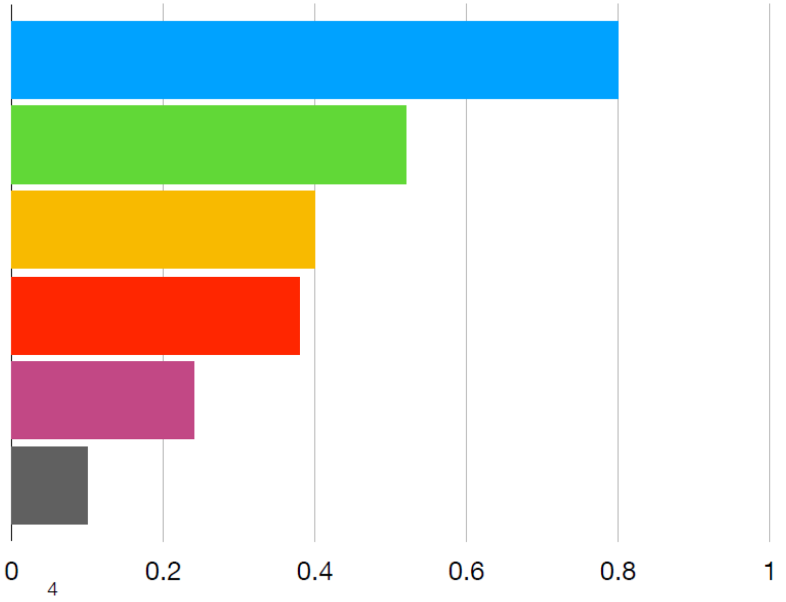
Analysis by Jim Pivarski

Why do particle physicists use Python ?

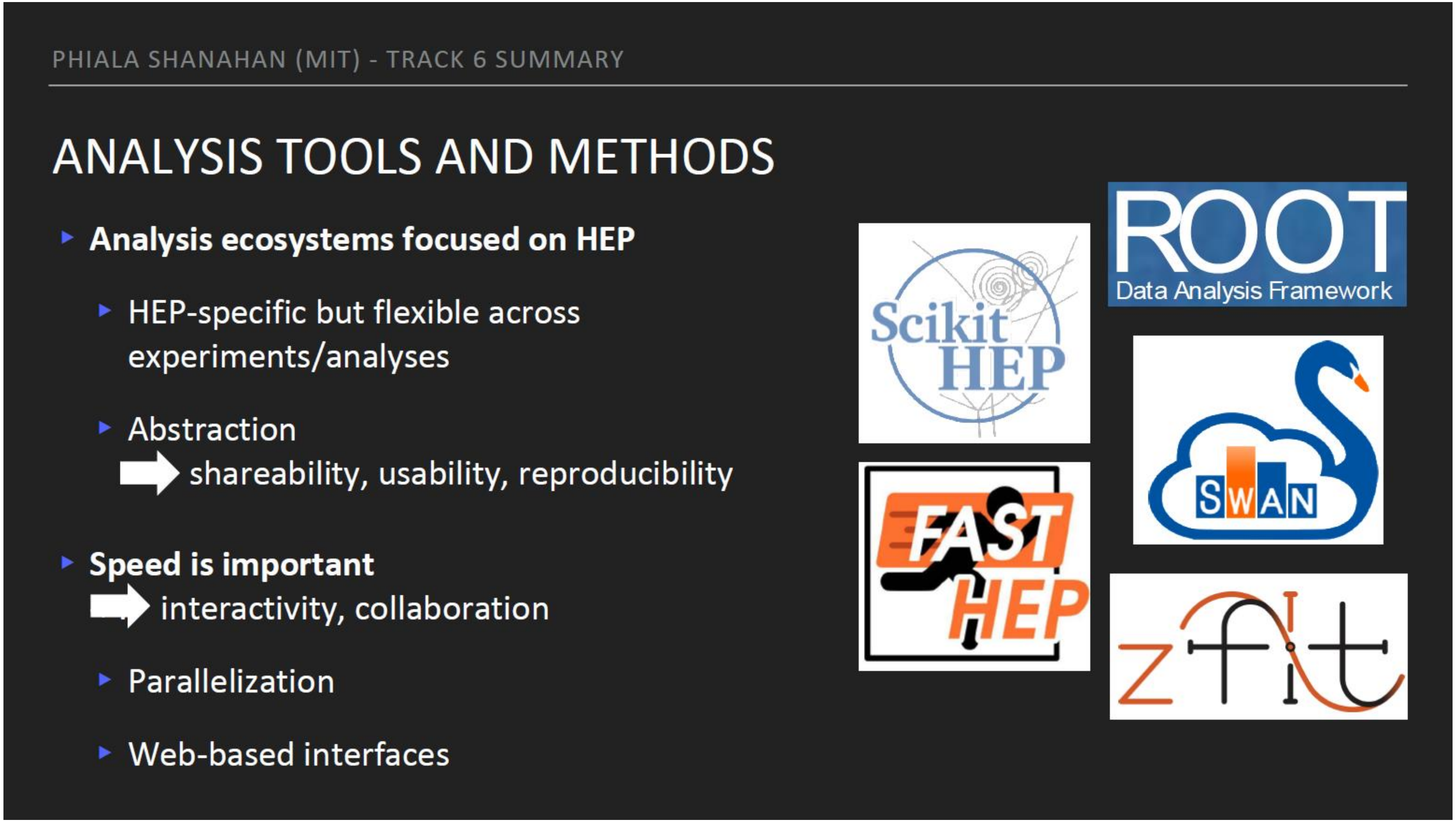
- Result of PyHEP 2018 pre-workshop questionnaire
  Stewart, Graeme. (2018, July). PyHEP - Questionnaire and Discussion. Zenodo. http://doi.org/10.5281/zenodo.1419157

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%

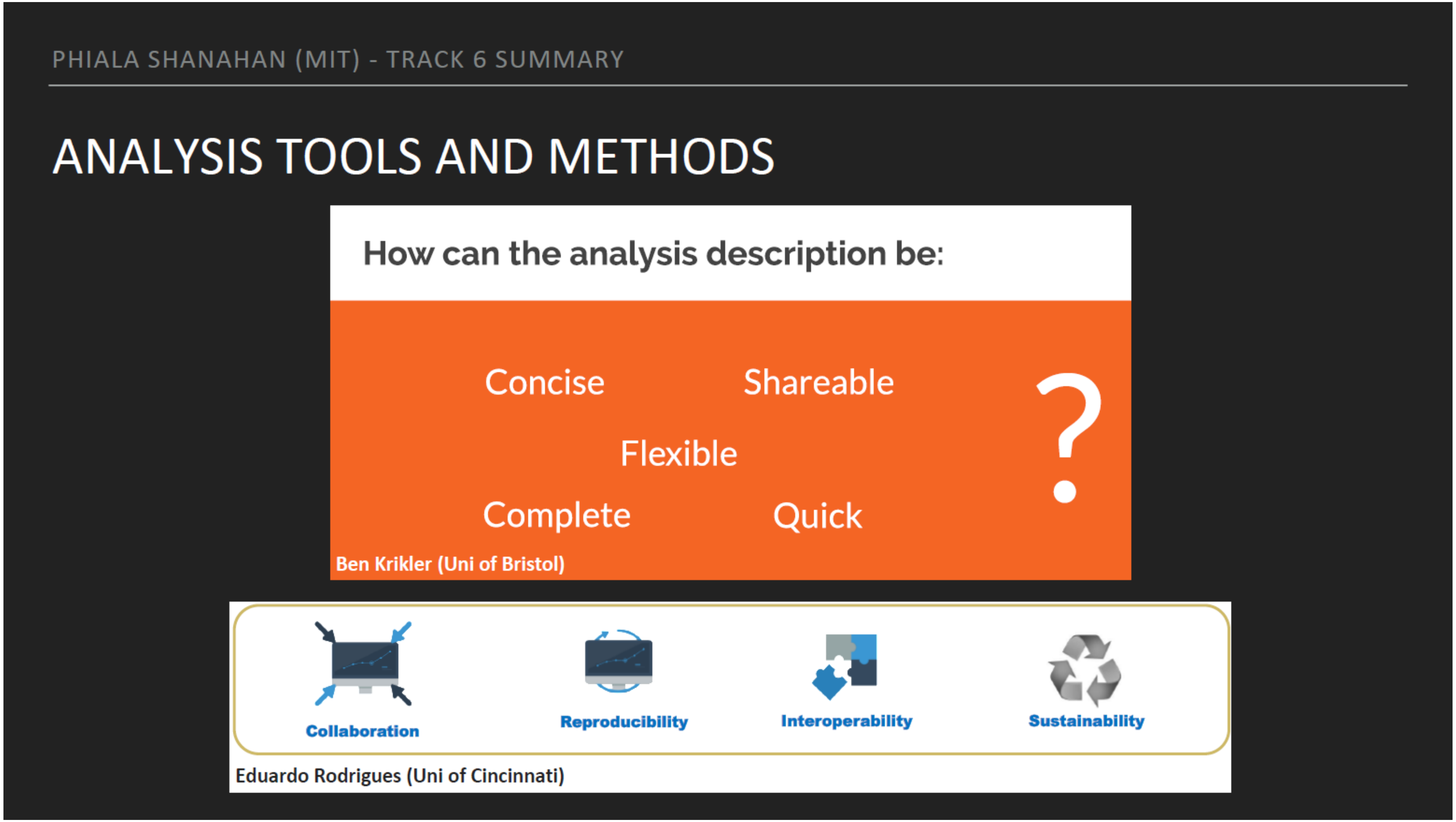


Focus of this talk – (offline) analysis software in Python



Taken from
Phiala Shanahan, "Track 6 highlights - Physics Analysis",
CHEP 2019 Conference, Adelaide, Australia, 4-8 Nov. 2019

Focus of this talk – (offline) analysis software in Python



Taken from
Phiala Shanahan, "Track 6 highlights - Physics Analysis",
CHEP 2019 Conference, Adelaide, Australia, 4-8 Nov. 2019

Community efforts

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

The HEP Software Foundation (HSF)

- The goal of the HEP Software Foundation (HSF) is to facilitate coordination and common efforts in software and computing across HEP in general
  - Our philosophy is bottom up, a.k.a. *Do-ocracy*
  - Also work in common with like-minded organisations in other science disciplines

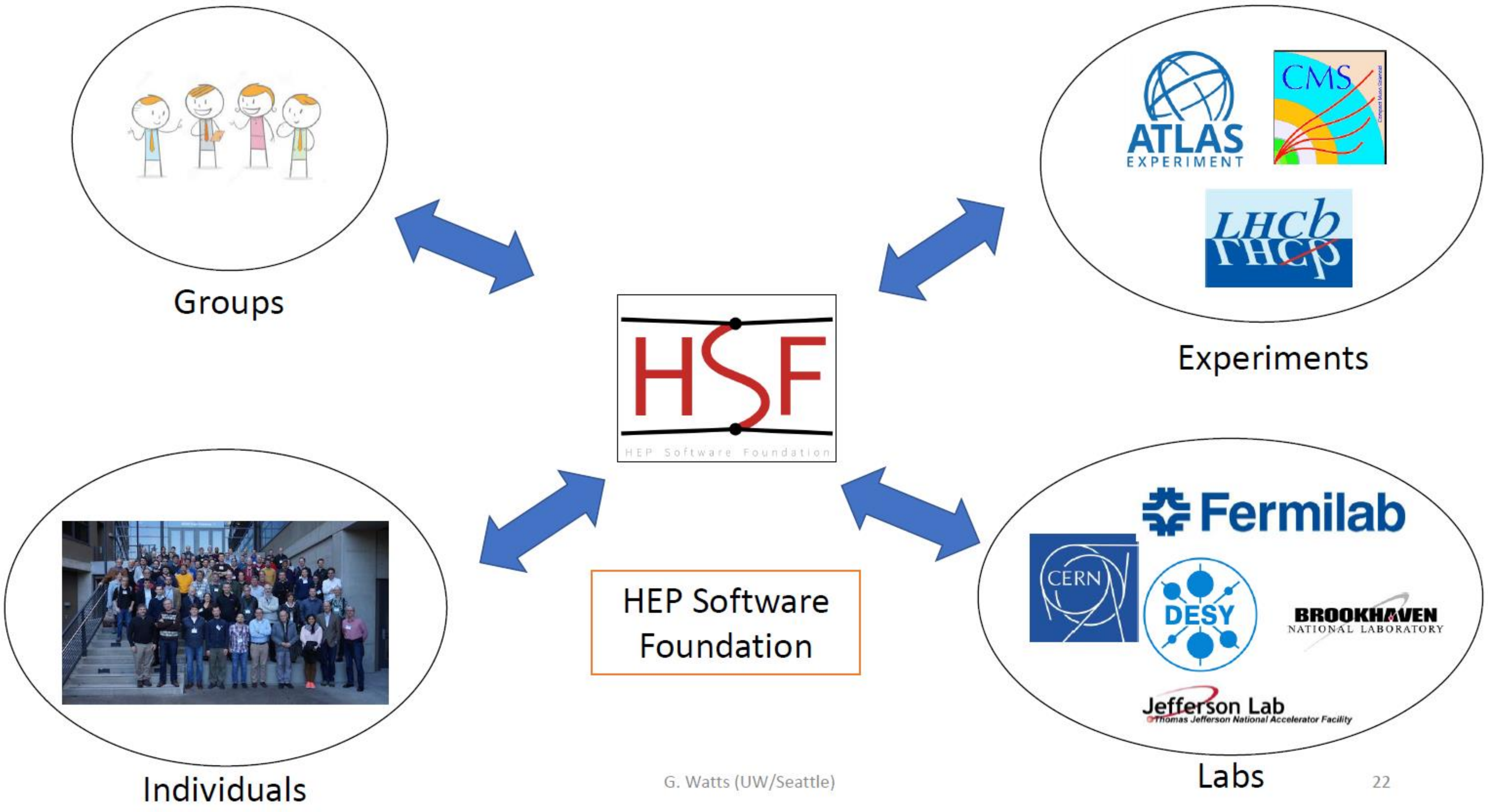
- Founded in 2014, explicitly to address current and future computing & software challenges in common

- Finalised in Dec. 2017 a Community White Paper (CWP) "A Roadmap for HEP Software and Computing R&D for the 2020s"
  - Almost all major domains of HEP Software and Computing covered
  - Large support for the document from the community (> 300 authors from >120 institutions)
  - Comput Softw Big Sci (2019) 3, 7; arXiv:1712.06982

- The CWP was a major accomplishment made by the community, with HSF "coordination"
- But it was a milestone, not a final step
- HSF activities post-CWP are very diverse …

HSF - "facilitate coordination and common efforts"

Gordon Watts, ACAT 2019



HSF – working groups, activities & events

Activities | **Working Groups**

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

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

indico

Home | Create event | Room booking

Home » Projects » HEP Software Foundation

HEP Software Foundation

- Weekly meetings
- HSF workshops and events
- Working groups
- Software Forum
- Training

❑ **The HSF also acts as an umbrella organisation for participation in the Google Summer of Code programme**

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

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

If you still need a motivation ;-) :

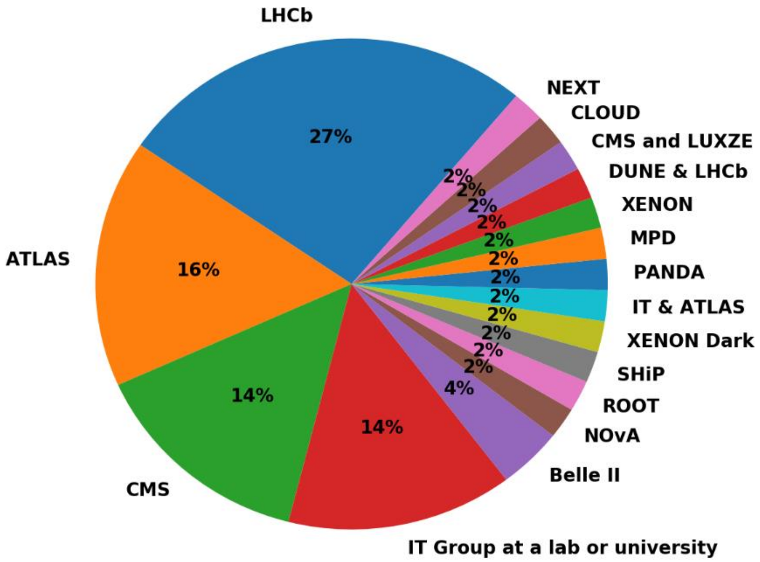
- ❑ **Python has become a first-class language in HEP**
- ❑ **And is the lingua franca for data science and machine learning**

PyHEP workshops – a new series of workshops

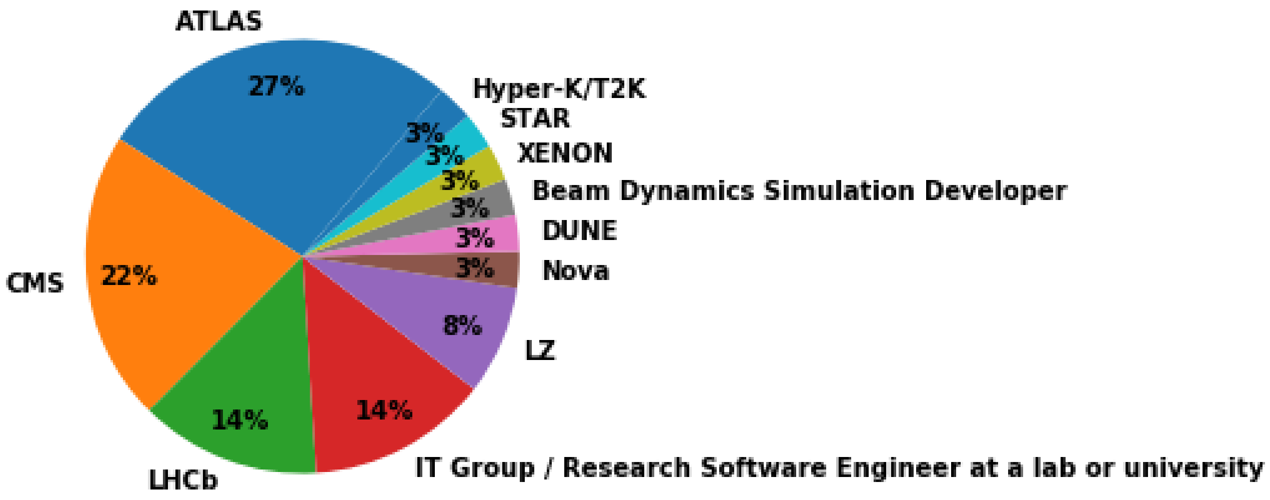
The **PyHEP workshops** are a series of workshops initiated and supported by the HEP Software Foundation (HSF) with the aim to provide an environment to discuss and promote the usage of Python in the HEP community at large. Further information is given on the PyHEP WG website.

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

PyHEP 2018



PyHEP 2019



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

PyHEP series of workshops

PyHEP 2018

Sofia, Bulgaria

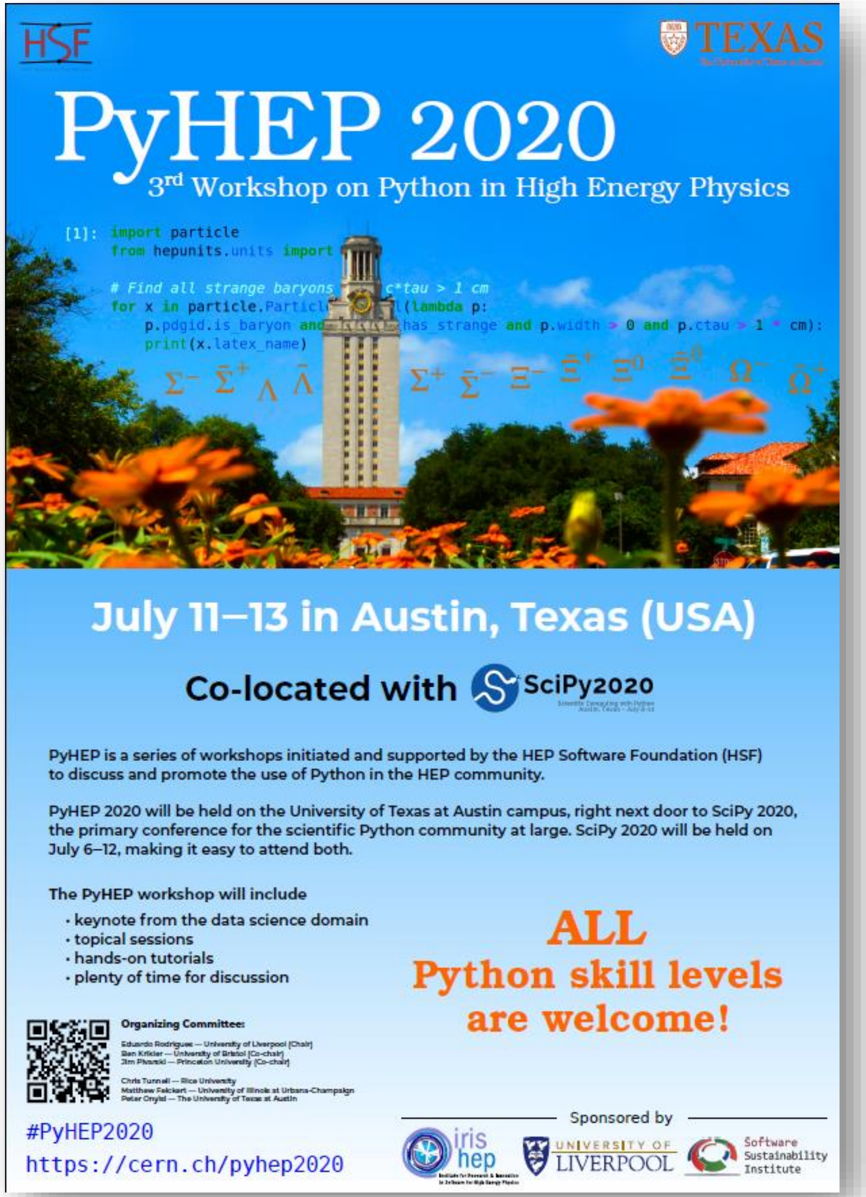
PyHEP 2019

Abingdon, U.K.

PyHEP series of workshops – PyHEP 2020

PyHEP 2020

- To be held in Austin (Texas), U.S.A., in July 11-13
- Next to SciPy 2020 conference, to enhance cross-community exchange
- First official announcement email sent out on Feb. 25th
- See also Indico agenda



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 ;-))

Various projects have seen the light:

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

The Scikit-HEP project

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

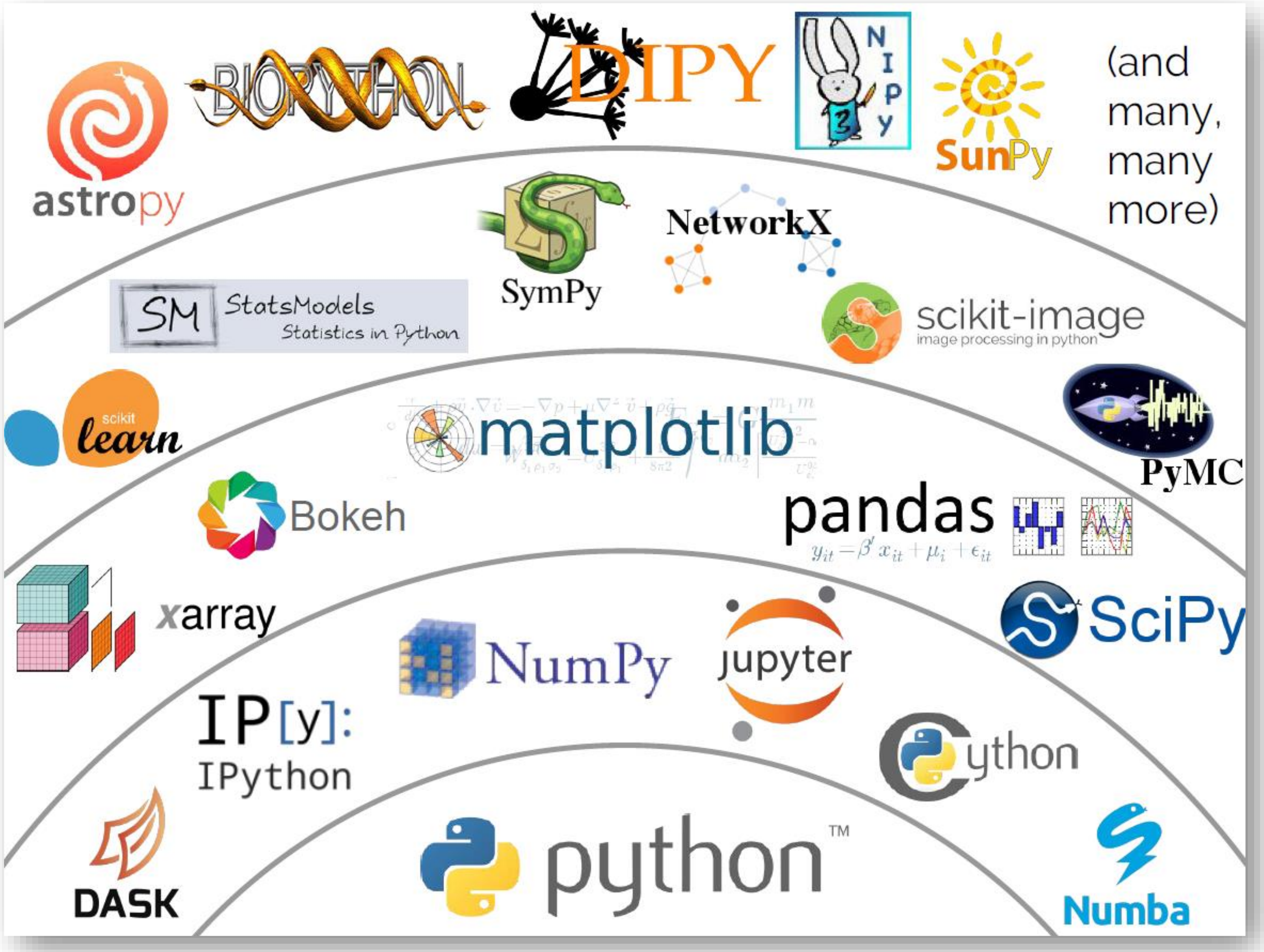
How’s the Python scientific ecosystem like, outside HEP?

Domain-specific

Python’s

Scientific

stack



What about HEP …?

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

Scikit-HEP project – the grand picture

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

Scikit-HEP project – 5 grand "pillars" embracing all major topics

Scikit-HEP

Scikit-HEP on GitHub

Home

Getting in touch

Documentation

Who uses Scikit-HEP?

Affiliated packages

Miscellaneous resources

FAQ

Funding

Supported Python Versions

This site uses Just the Docs, a documentation theme for Jekyll.

Scikit-HEP project - welcome!

The Scikit-HEP project is a community-driven and community-oriented project with the aim of providing Particle Physics at large with an ecosystem for data analysis in Python. The project started in Autumn 2016 and is in full swing.

It is not just about providing core and common tools for the community. It is also about improving the interoperability between HEP tools and the scientific ecosystem in Python, and about improving on discoverability of utility packages and projects.

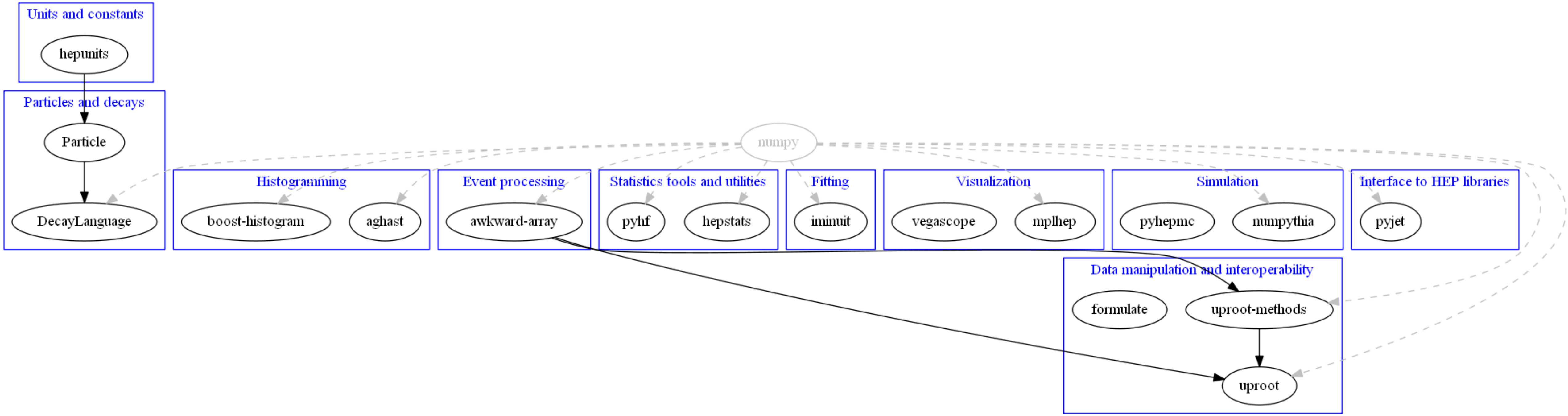
For what concerns the project grand structure, it should be seen as a *toolset* rather than a *toolkit*. The project defines a set of five *pillars*, which are seen to embrace all major topics involved in a physicist's work. These are:

- **Datasets**: data in various sources, such as ROOT, Numpy/Pandas, databases, wrapped in a common interface.
- **Aggregations**: e.g. histograms that summarize or project a dataset.
- **Modeling**: data models and fitting utilities.
- **Simulation**: wrappers for Monte Carlo engines and other generators of simulated data.
- **Visualization**: interface to graphics engines, from ROOT and Matplotlib to even beyond.

Toolset packages

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

https://scikit-hep.org/

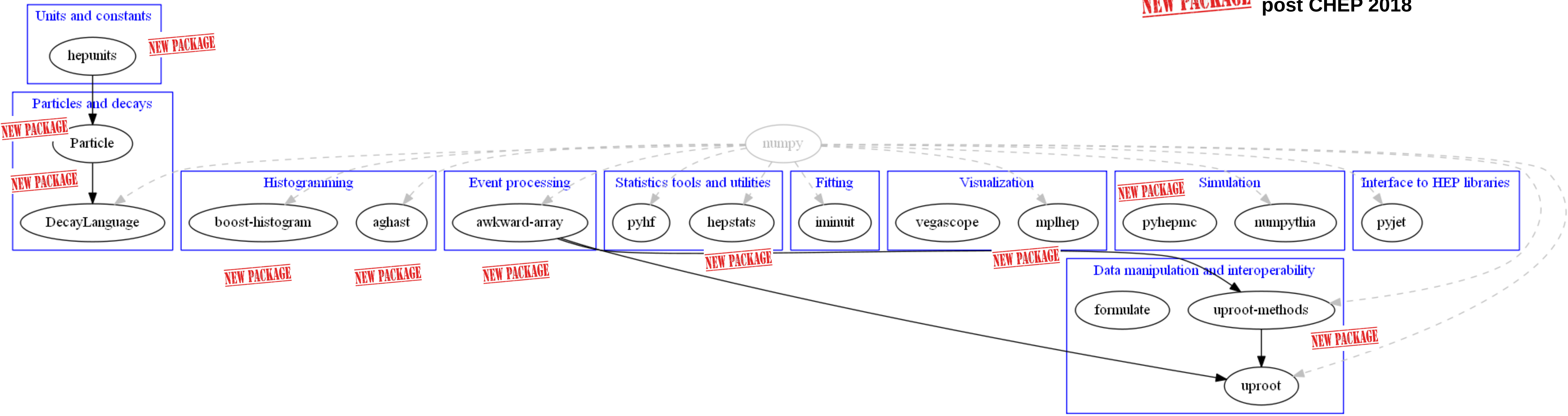


There are other packages: test data, tutorials, org stats, etc.
(and some which tend to now be superseded, hence deprecated …)

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

https://scikit-hep.org/

NEW PACKAGE = 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 …)

Who uses (some of) Scikit-HEP ?

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

Software projects

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

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

Experiment collaborations

BelleII - the Belle II experiment at KEK, Japan.

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

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

Phenomenology projects

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

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

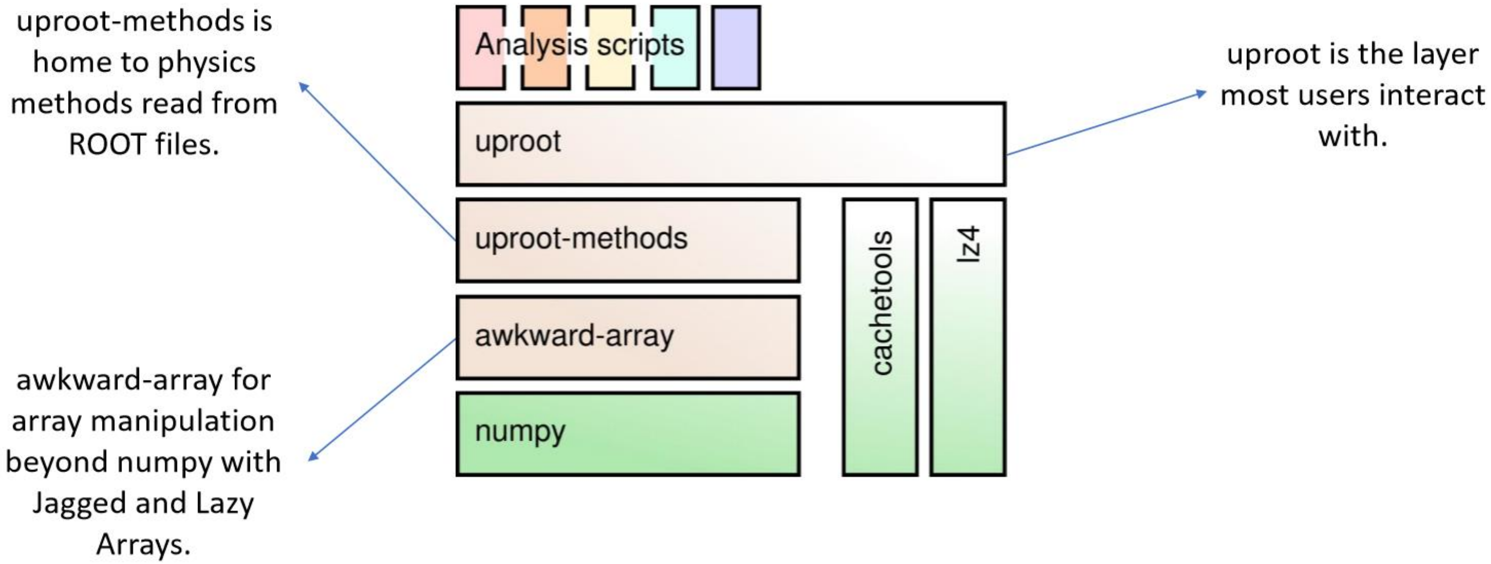
- (Does it still need an intro ;-)?)
- Trivially and Python-ically read ROOT files
- Need only NumPy, <u>no ROOT</u>, using this pure I/O library!
- Design and dependencies:

uproot

ROOT I/O
in pure Python and Numpy

uproot-methods

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

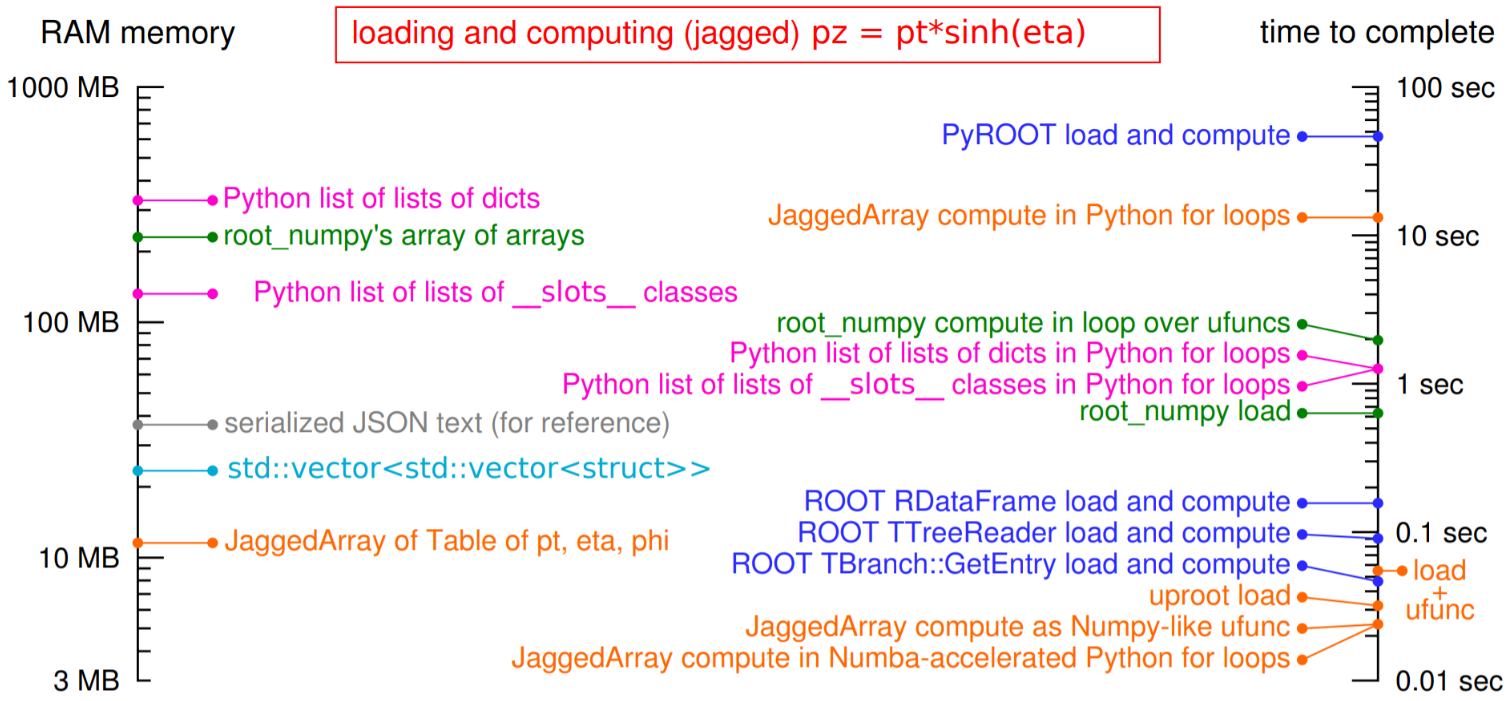


- Write ROOT files: newest development, limited scope = write Ttree, histograms and a couple more classes only
  - See <u>talk</u> at <u>PyHEP 2019 workshop</u>

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

- NOPE !

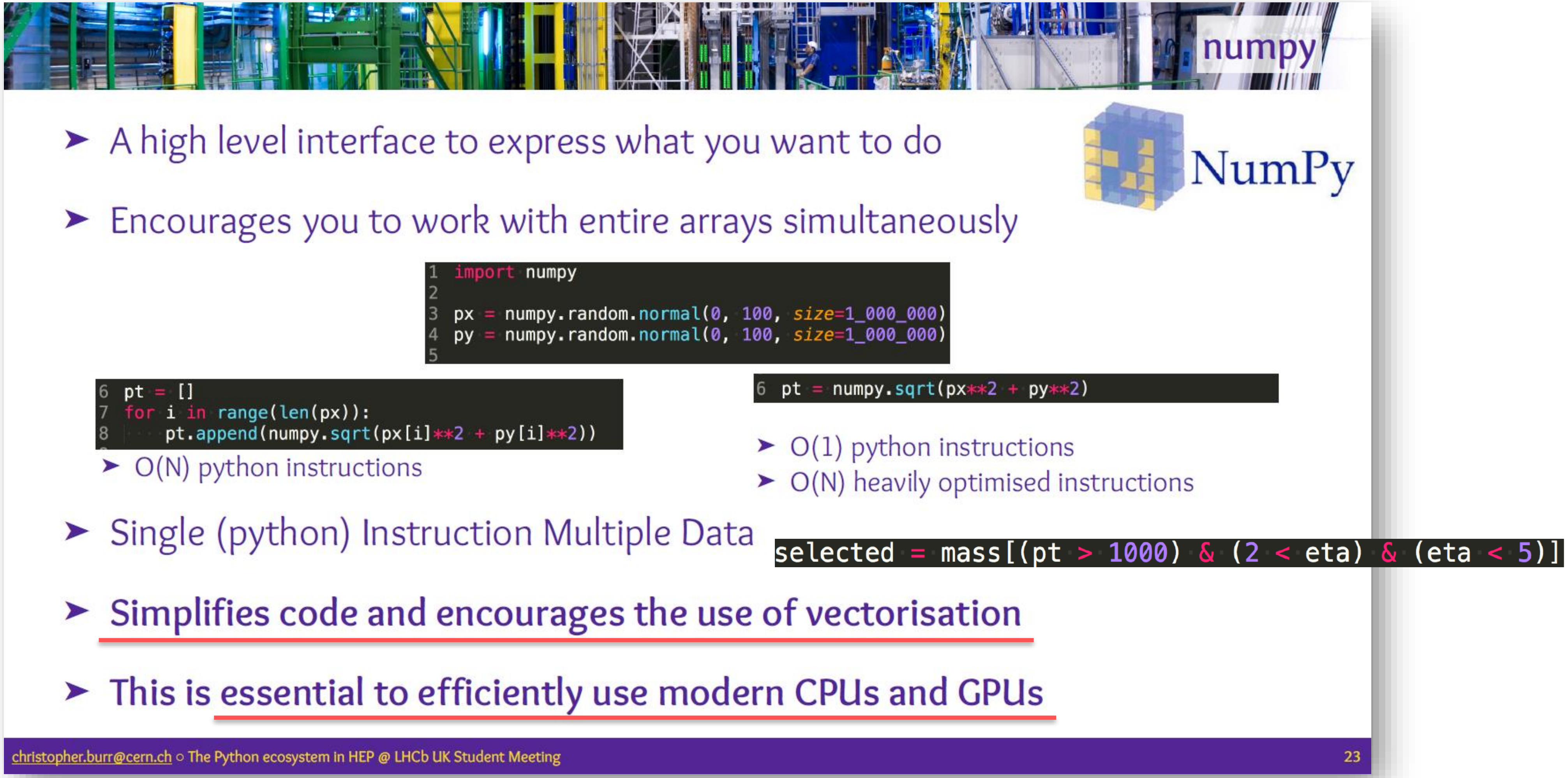
"The lack of per-event processing is why reading in uproot and processing data with awkward-array can be fast, despite being written in Python."



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

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

- **Much is thanks to building atop NumPy:**



Event processing – `awkward-array` package

Awkward Array

Manipulate arrays
of complex data structures
as easily as NumPy

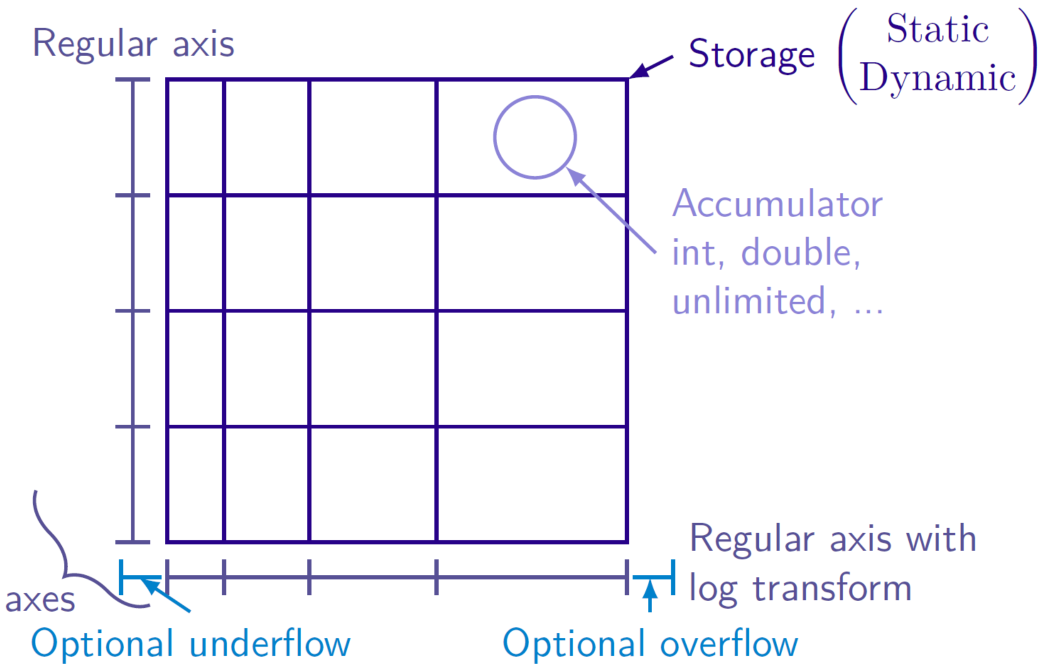
- Provide a way to analyse variable-length and tree-like data in Python, by extending NumPy's idioms from flat arrays to arrays of data structures
- Pure Python+NumPy library for manipulating complex data structures even if they
  - Contain variable-length lists (jagged/ragged)
  - Are deeply nested (record structure)
  - Have different data types in the same list (heterogeneous)
  - Are not contiguous in memory
  - Etc.
- This is all very relevant and important for HEP applications !

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

- Package being re-implemented in C++, with a simpler interface and less limitations
  - Major endeavour
- Work-in-progress, see https://github.com/scikit-hep/awkward-1.0 ...
- BTW, uproot 4 will be re-engine based on awkward-1.0

Histogramming – `boost-histogram` package

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



Design
- Close to B.H
- Pythonic
- Numpy ready

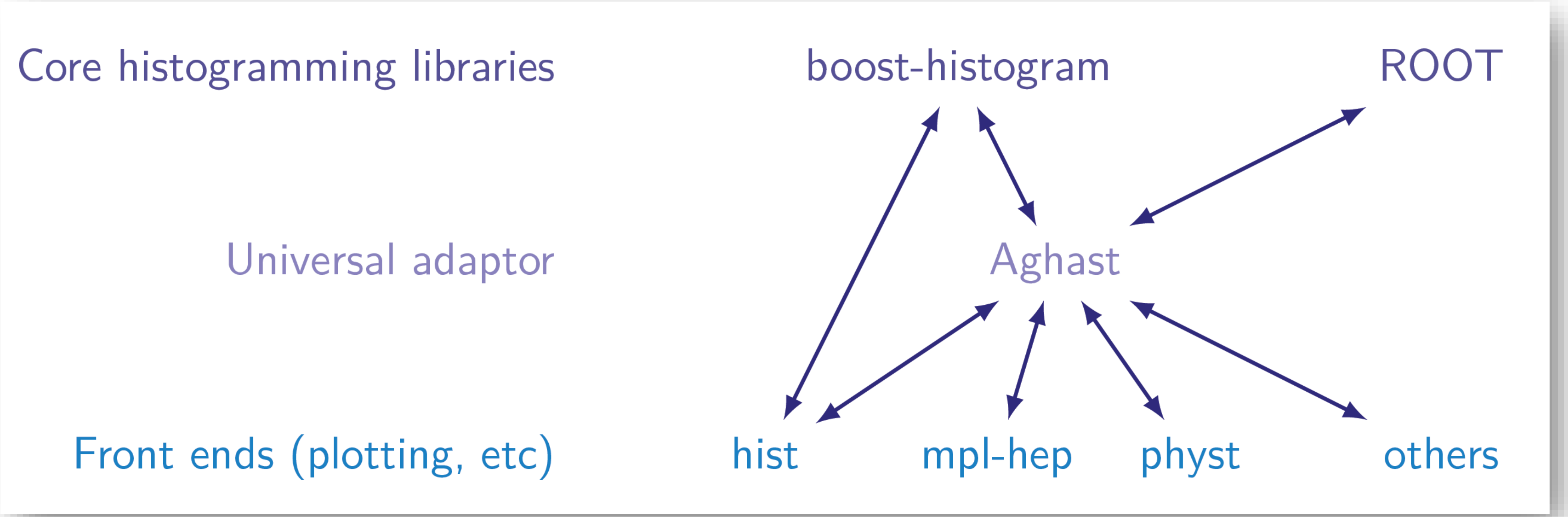
Flexibility
- Composable
- 0-copy conversion

Speed
- 2-10x faster than Numpy
- Thread ready

Distribution
- Pip wheels
- Conda-forge
- C++14 only

Histogramming – looking ahead

- A fair amount of interest in the (HEP) community to develop a histogramming sub-ecosystem that meets our requirements
- Involves packages for core functionality such as filling, plotting, serialisation, and interoperability
- Interaction with popular fitting packages is also paramount



Taken from Henry Schreiner, IRIS-HEP talks

Fitting – `iminuit` package

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

iminuit

Python interface to the MINUIT2 C++ package

- Example usage:

```python
from iminuit import Minuit

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

m = Minuit(f)

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

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

FCN = 1.624E-22	Ncalls = 36 (36 total)
EDM = 1.62E-22 (Goal: 1E-05)	up = 1.0

Valid Min.	Valid Param.	Above EDM	Reached call limit
True	True	False	False

Hesse failed	Has cov.	Accurate	Pos. def.	Forced
False	True	True	True	False

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

Particles and decays – `Particle` package

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

```
from particle import Particle, PDGID

pid = PDGID(211)
pid
```

```
<PDGID: 211>
```

```
pid.is_meson
```

```
True
```

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

$D_2^*(2460)^+$

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

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

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

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

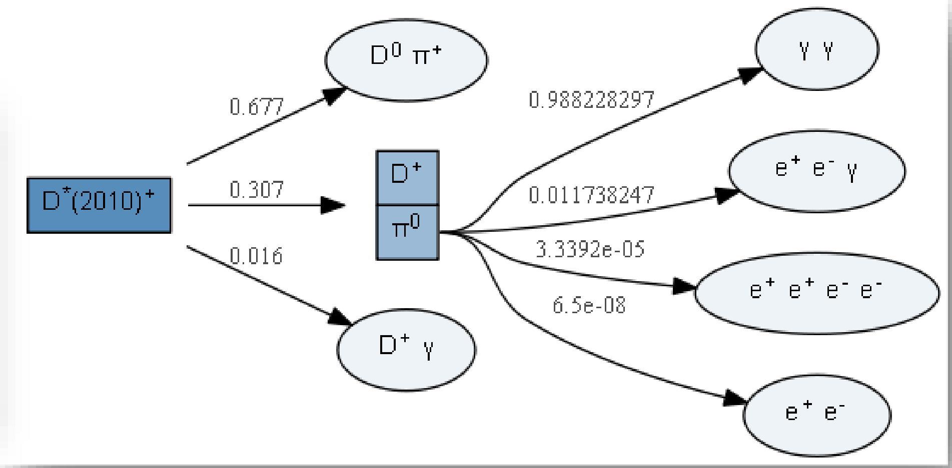
Particles and decays – `DecayLanguage` package

DecayLanguage

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

- Parse, extract information and visualise a decay chain:

```python
from decaylanguage import DecFileParser, DecayChainViewer

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

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



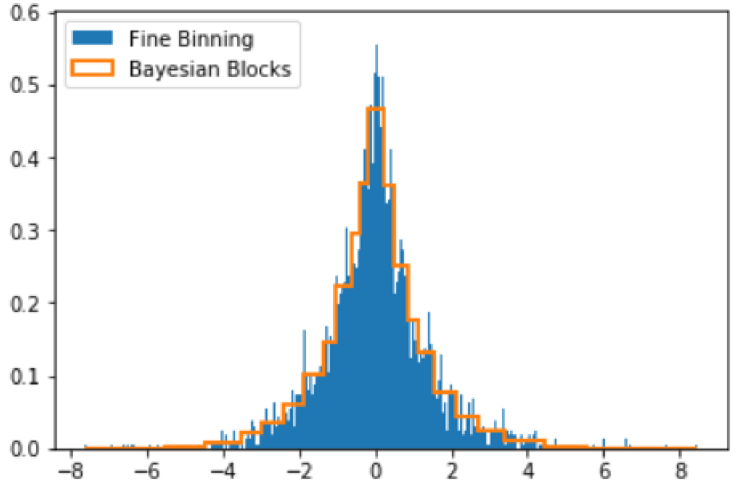
- Represent a complex decay chain:

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

Statistics tools and utilities – `hepstats` package

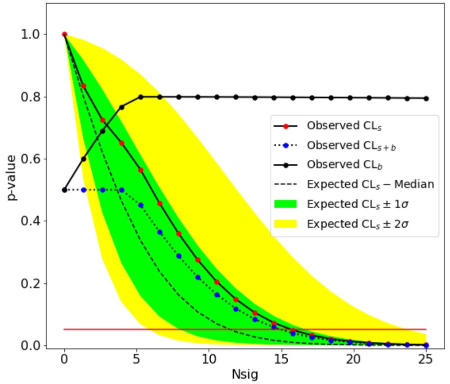
- **Statistical tools and utilities in Python, under development**
- **Currently implements two submodules:**
  - **Modeling with the Bayesian block algorithm – improved binning determination, robust to statistical fluctuations**

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

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

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

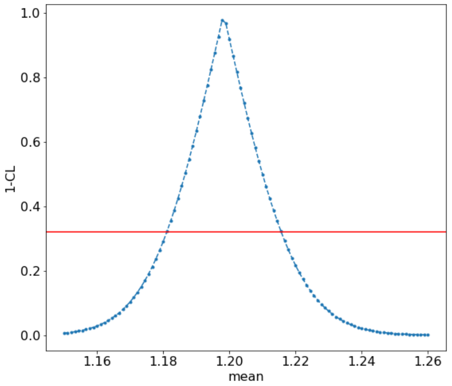


- **Likelihood-based hypothesis tests, upper limit and confidence interval calculations**
  - **Works with a fitting library providing models, likelihood, etc.**
  - **Built on a common interface, used by zfit, and does not depend on a fitting backend**

Upper limit on signal yield:



1-CL plot for the mean of a peak:



Statistics tools and utilities – `pyhf` package

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

Declarative binned likelihoods

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

Primary Measurement:

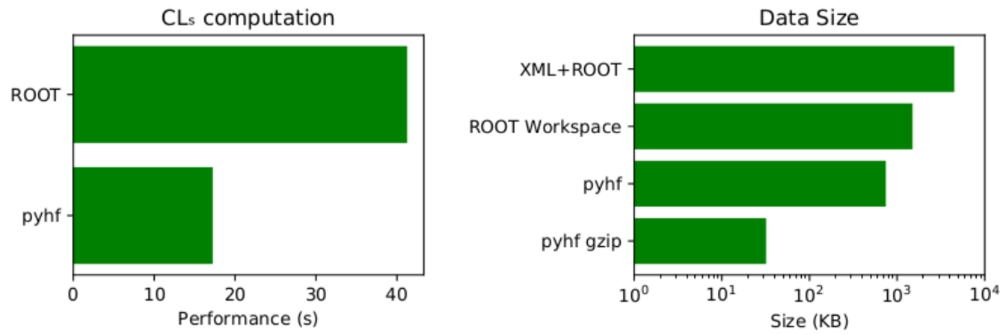
- Multiple disjoint "channels" (e.g. event observables) each with multiple bins of data
- Example parameter of interest: strength of physics signal, μ

Auxiliary Measurements:

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

Performance

Efficient use of tensor computation makes pyhf fast



Competitive with traditional C++ implementation — often faster

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

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"

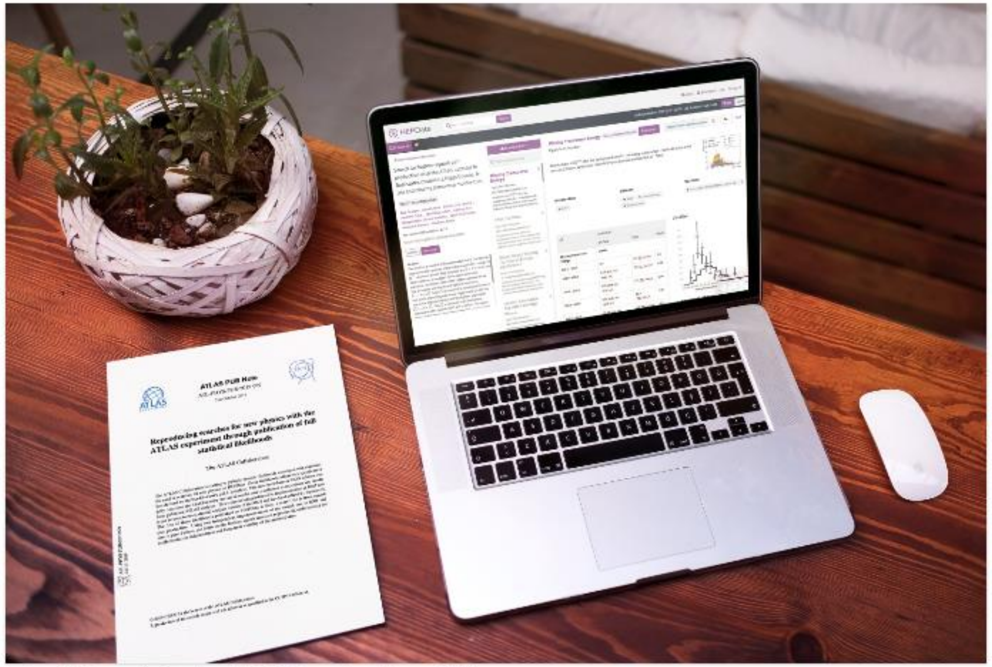
Work done with

- ❑ RooStats
- ❑ pyhf

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

Simulation – pyhepmc packages

- HepMC3: a new rewrite of the C++ HepMC event record for MC generators

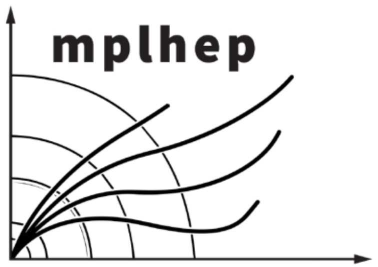
pyhepmc

Python wrapper for the HepMC3 C++ library

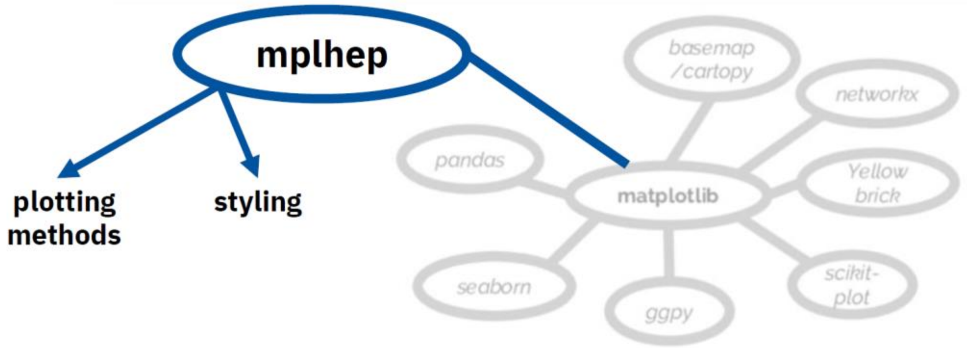
- pyhepmc: Python wrapper for the HepMC3 C++ library
- Bindings built on pybind11
- Supports all Python versions
- On PyPI as source distribution

- Development done with exchanges with the HepMC3 team
  - Idea is to provide pyhepmc as the official bindings, included in the HepMC3 distribution

mplhep package – helper visualisation tool for HEP atop Matplotlib

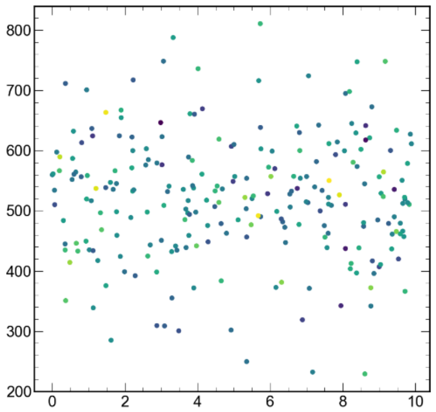


- ❑ Matplotlib is a key tool for visualisation in the data science domain
- ❑ But it not provide all that HEP wants
  - Requires a lot of tinkering
- ❑ mplhep idea:
  - Keep matplotlib as a versatile and well-tested backend
  - Provide a new domain-specific API



Minimal Example

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

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

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



Visualisation – VegaScope package

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

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

- ❑ Altair can use VegaScope as a renderer:

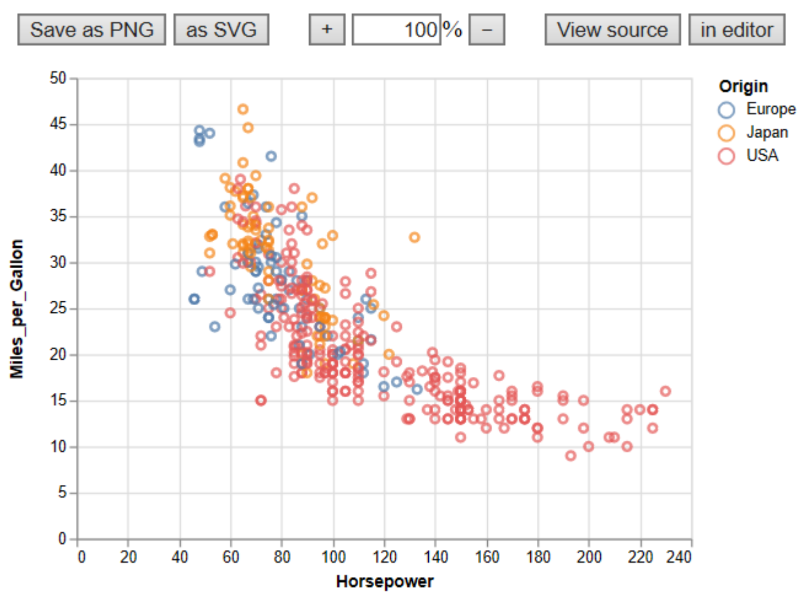
```
import vegascope
canvas = vegascope.LocalCanvas()
canvas("https://vega.github.io/vega/examples/stacked-bar-chart.vg.json")
```

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

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

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

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



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

- Generate events with Pythia and pipe them into NumPy arrays

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

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

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

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

numpythia

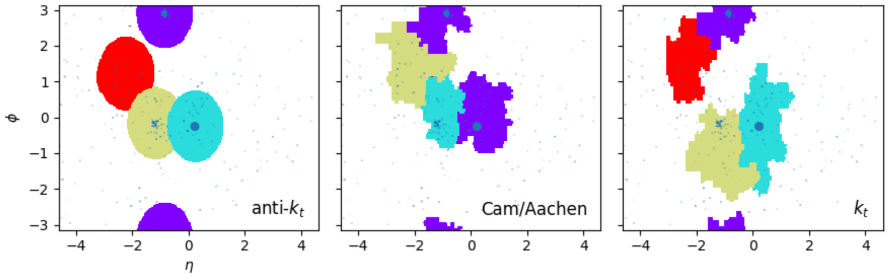
Interface between PYTHIA and NumPy

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

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

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

pyjet

Interface between FastJet and NumPy



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

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

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

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

```
0.44968868700000003
```

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

```
449.688687
```

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

- **More "advanced":**

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

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

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

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

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

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

scikit-hep

A metapackage
(WIP, near future)

- The `scikit-hep` package has historically contained a variety of things:
  - Kinematics and geometry classes for HEP
  - Modelling module
  - Visualisation utilities
  - Etc.
- The Scikit-HEP project has evolved and a different route has emerged as more adequate …

- Vision for the future: have the scikit-hep package become a metapackage for the Scikit-HEP project
- Benefit especially for stacks for experiments: `scikit-hep` tags defining compatible releases of the whole toolset
  - Clear what "scikit-hep version 1.0.0" is
  - Stable stacks installable in a simple way
  - Having a well-defined stack also helps in analysis preservation matters, widely discussed at present
- This is (still) work-in-progress …
- "vector": example of future package taken out, which will provide awkward-/numpy-array based vector classes, and more

Other community projects

- zfit - fitting
- Coffea - Columnar Object Framework For Effective Analysis
- FAST-HEP – Analysis Description Language oriented toolkit
- Package availability via conda-forge, not just pip

Other community projects

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

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

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

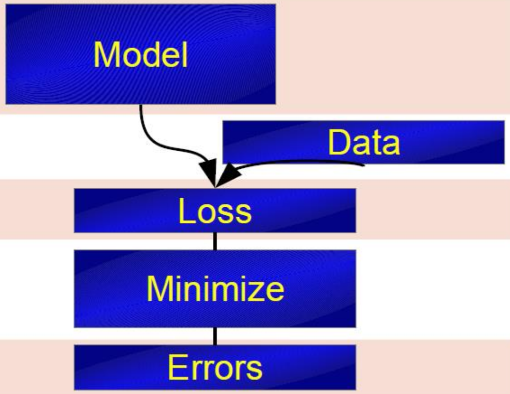
The `zfit` project and package

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

affiliated

- Simple example:

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

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

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

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

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

param_errors = result.error()
```



implement custom function

```
from zfit import ztf


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

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

        return ztf.exp(alpha * data)


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

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

The `coffea` project

Coffea - Column Object Framework for Effective Analysis

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

Separation of "user code" and "executors"

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

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

- Using Spark cluster on same site as data at Fermilab

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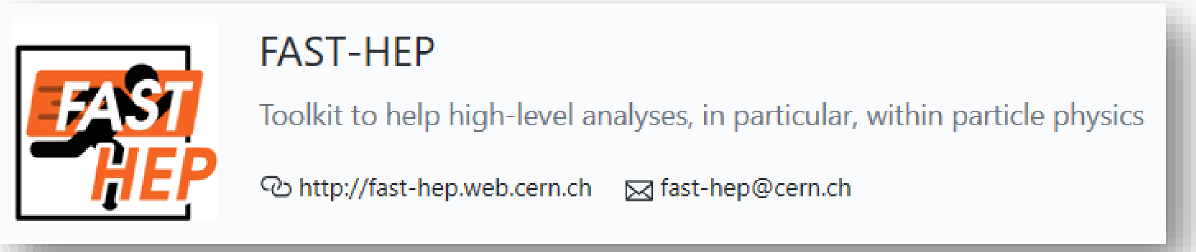
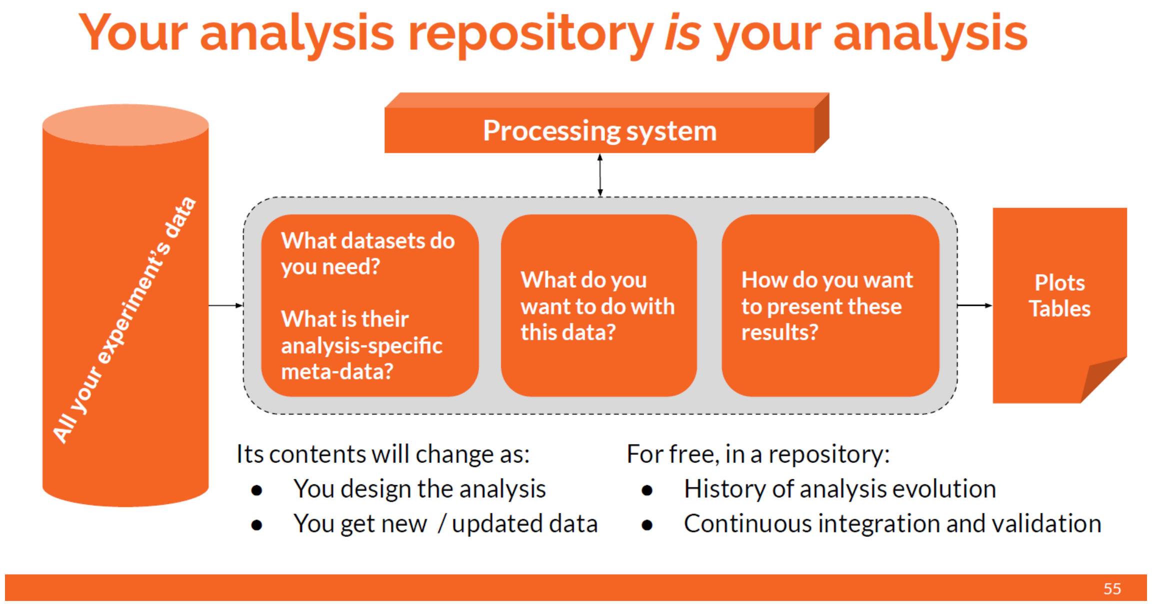
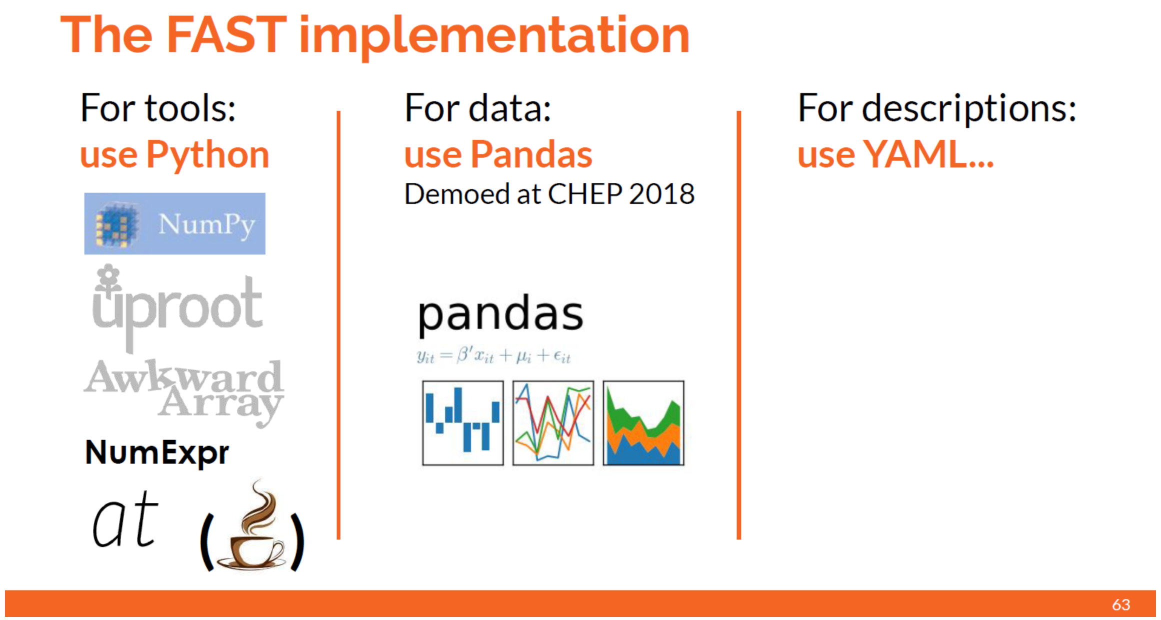
Slide taken from Ben Krikler

The FAST-HEP project



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



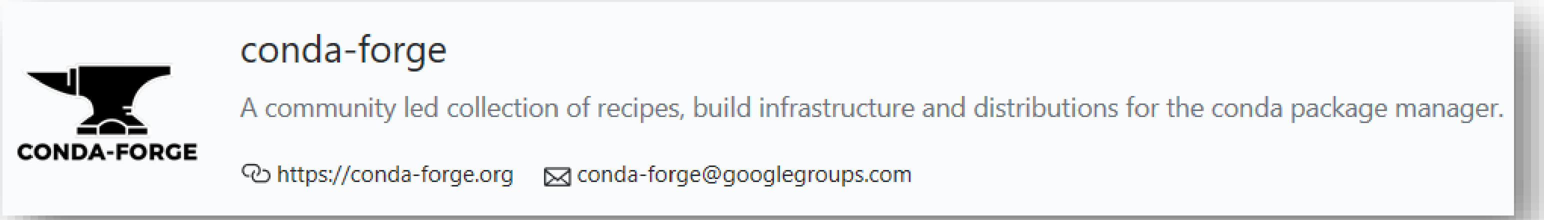


- Use a declarative programming approach:
  User sys WHAT, interpretation decides HOW

- Project towards an Analysis Description Language …

Material taken from Ben Krikler

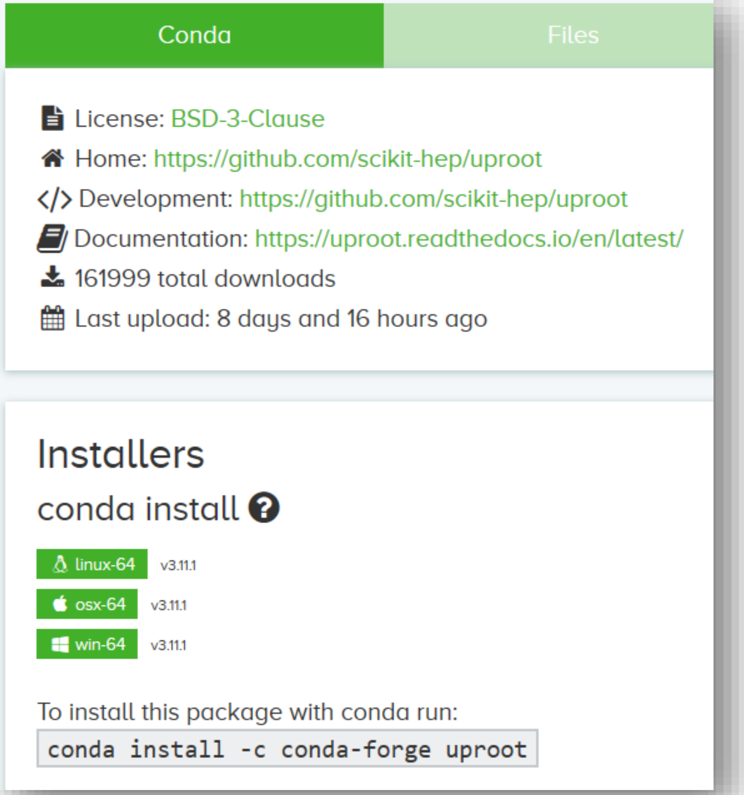
Conda-forge – making it easy for users



- ❑ **Easy / trivial installation in many environments is a must !**

- ❑ **Much work has been done in 2019 to provide binary “wheels” on PyPI, and conda-forge packages for many of these new packages**

- ❑ **Example of `uproot`:**



Wrapping up

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

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Thank you for listening

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