Scikit-HEP project status

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Why Scikit-HEP ? (A bit o a recap)

❑ Python usage over time:
simple scripting tasks → daily tasks → an analysis framework

HEP, ROOT-based

❑ ROOT for almost everything

❑ Toolkit for modeling / fitting: RooFit

❑ Statistics: RooStats

❑ Machine learning: TMVA

❑ Etc.

Scientific Computing in Python

❑ The father of them all: SciPy

❑ Data manipulation: NumPy, Pandas

❑ Plotting: matplotlib, seaborn, Bokeh

❑ Machine learning: scikit-learn, TensorFlow

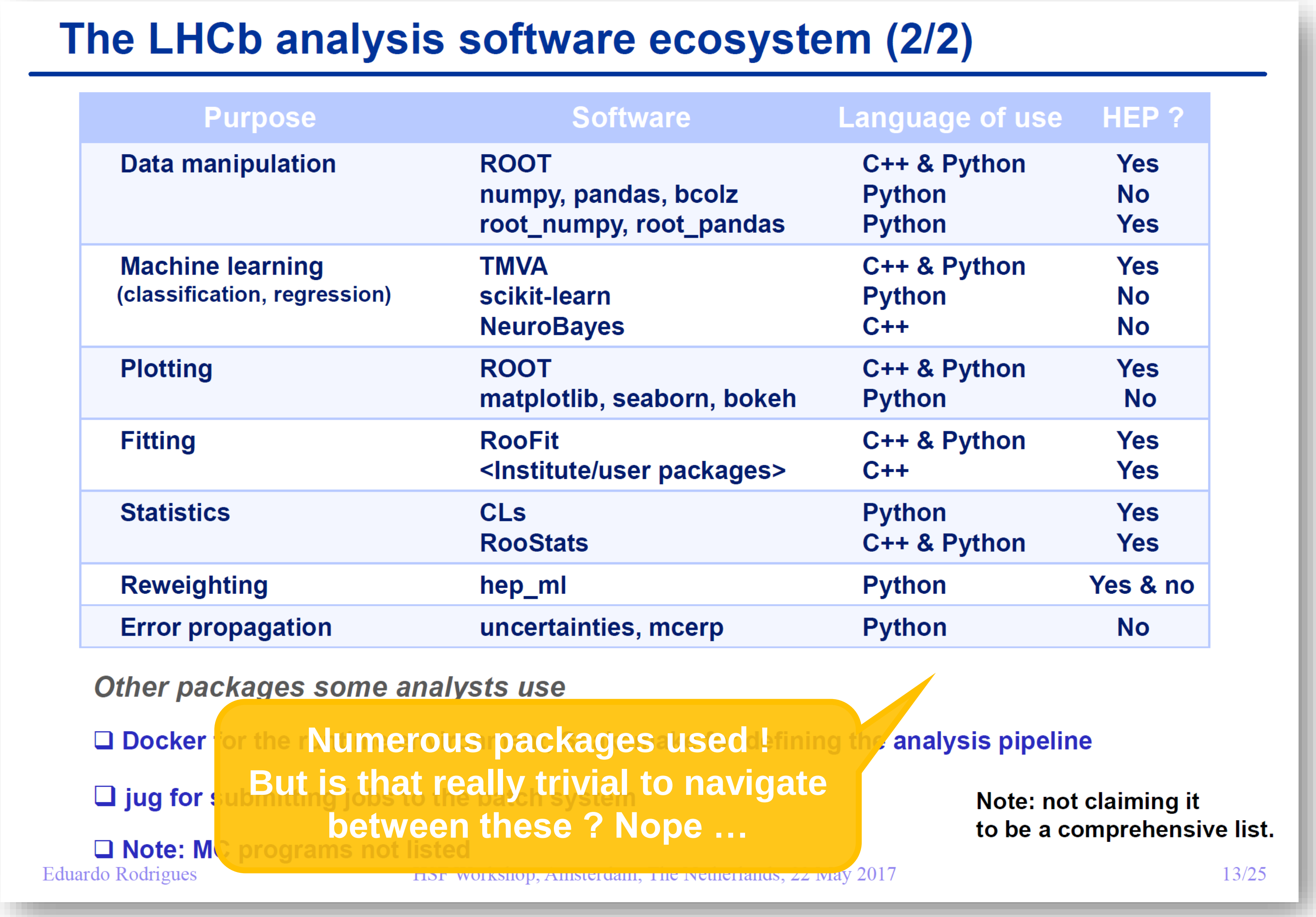
❑ Etc.

❑ + dedicated projects built atop the above:
Astropy, biopython, etc.

➡

- This is where we start to strongly link with the scientific computing community
- We need ways to bridge between ROOT and the Python scientific ecosystem, and more
- Scope / need for a general(ised) effort
- A toolset rather than a toolkit seems the way forward (IMHO)

Why Scikit-HEP ? Example from LHCb practises …



The LHCb analysis software ecosystem (2/2)

Purpose	Software	Language of use	HEP ?
Data manipulation	ROOT numpy, pandas, bcolz root_numpy, root_pandas	C++ & Python Python Python	Yes No Yes
Machine learning (classification, regression)	TMVA scikit-learn NeuroBayes	C++ & Python Python C++	Yes No No
Plotting	ROOT matplotlib, seaborn, bokeh	C++ & Python Python	Yes No
Fitting	RooFit <Institute/user packages>	C++ & Python C++	Yes Yes
Statistics	CLs RooStats	Python C++ & Python	Yes Yes
Reweighting	hep_ml	Python	Yes & no
Error propagation	uncertainties, mcerp	Python	No

Other packages some analysts use

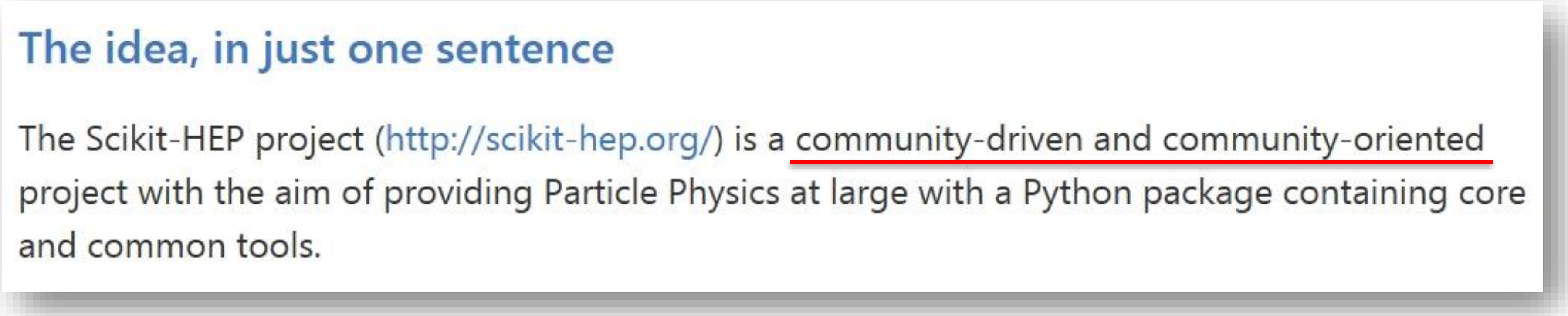
- ❑ Docker for the r[illegible] defining the analysis pipeline
- ❑ jug for submitting jobs to the batch system
- ❑ Note: MC programs not listed

Note: not claiming it
to be a comprehensive list.

Eduardo Rodrigues HSF Workshop, Amsterdam, The Netherlands, 22 May 2017 13/25

Numerous packages used !
But is that really trivial to navigate
between these ? Nope …

The Scikit-HEP project



The idea, in just one sentence

The Scikit-HEP project (http://scikit-hep.org/) is a community-driven and community-oriented project with the aim of providing Particle Physics at large with a Python package containing core and common tools.

What it is NOT …

❑ **A replacement for ROOT**

❑ **A replacement for the Python ecosystem based on NumPy, scikit-learn & co.**

… and what IT IS

❑ **A non-monolithic Python toolset, a clearinghouse for doing HEP analysis in Python**

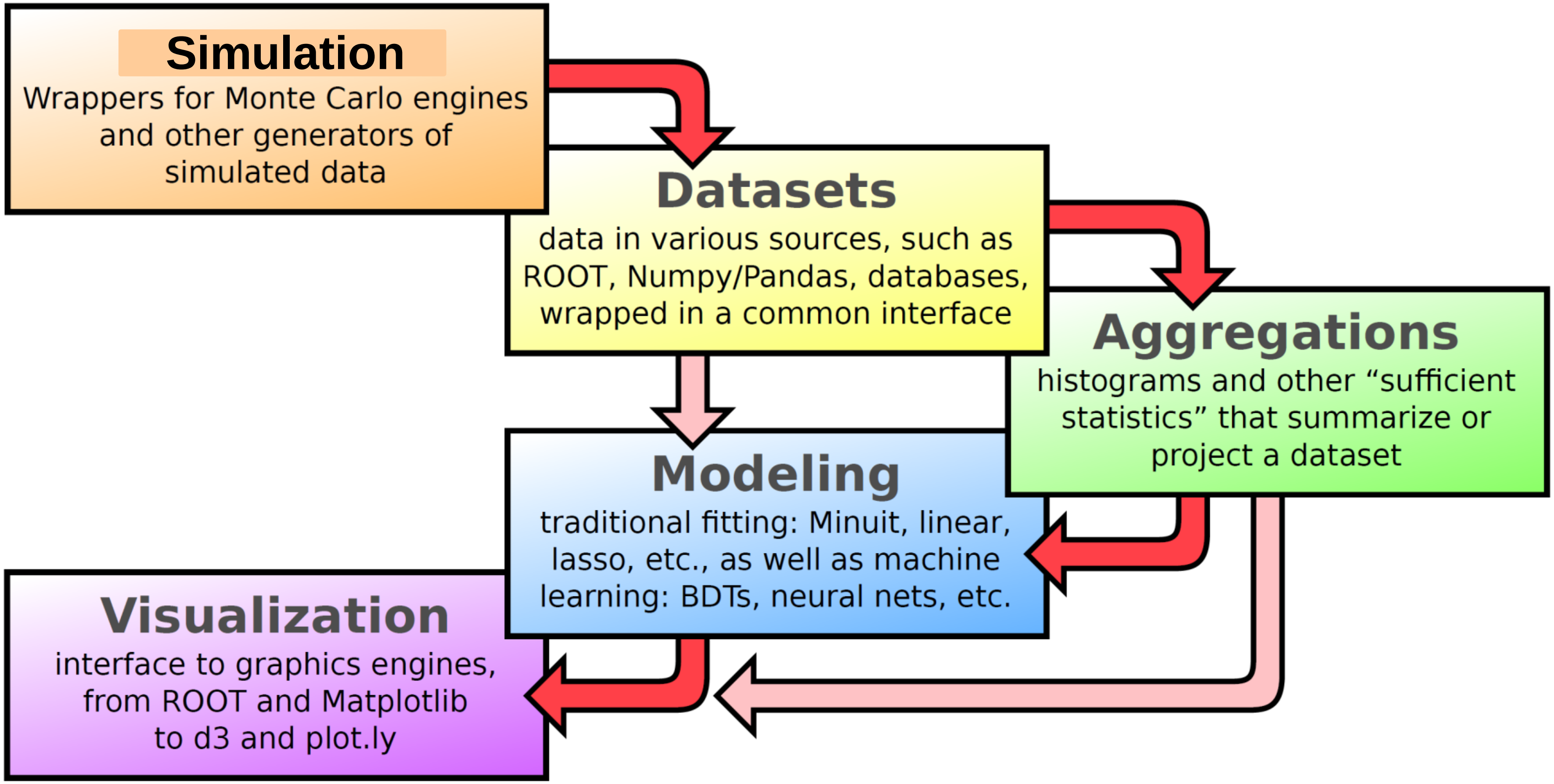
❑ **Emulate Scikit-Learn's unified interface with Astropy's embrace of third-party packages**

❑ **Bridge/glue between the ROOT-based and the Python scientific ecosystem**

❑ **We are building a community, engaging with (future) collaborators in various experiments**

❑ **Effort to improve discoverability of relevant tools**

The Scikit-HEP project – 5 « pillars »



Simulation
Wrappers for Monte Carlo engines and other generators of simulated data

Datasets
data in various sources, such as ROOT, Numpy/Pandas, databases, wrapped in a common interface

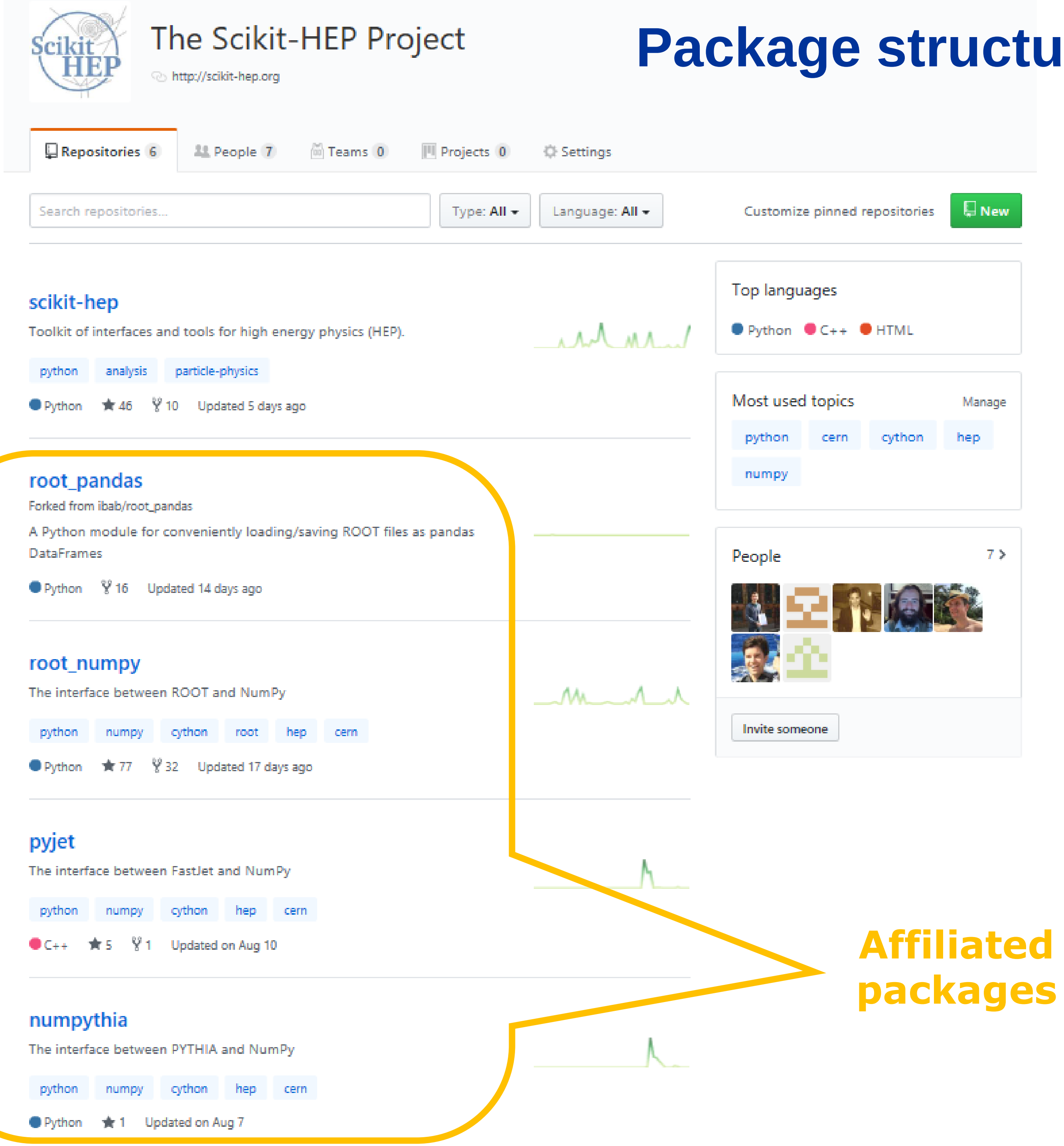
Aggregations
histograms and other “sufficient statistics” that summarize or project a dataset

Modeling
traditional fitting: Minuit, linear, lasso, etc., as well as machine learning: BDTs, neural nets, etc.

Visualization
interface to graphics engines, from ROOT and Matplotlib to d3 and plot.ly

➡ **They cover all grand topics … !**

Package structure on GitHub



The Scikit-HEP Project

http://scikit-hep.org

Repositories 6 | People 7 | Teams 0 | Projects 0 | Settings

Search repositories... | Type: All ▾ | Language: All ▾ | Customize pinned repositories | New

scikit-hep

Toolkit of interfaces and tools for high energy physics (HEP).

python | analysis | particle-physics

● Python ★ 46 10 Updated 5 days ago

root_pandas

Forked from ibab/root_pandas

A Python module for conveniently loading/saving ROOT files as pandas DataFrames

● Python 16 Updated 14 days ago

root_numpy

The interface between ROOT and NumPy

python | numpy | cython | root | hep | cern

● Python ★ 77 32 Updated 17 days ago

pyjet

The interface between FastJet and NumPy

python | numpy | cython | hep | cern

● C++ ★ 5 1 Updated on Aug 10

numpythia

The interface between PYTHIA and NumPy

python | numpy | cython | hep | cern

● Python ★ 1 Updated on Aug 7

Top languages

● Python ● C++ ● HTML

Most used topics Manage

python | cern | cython | hep | numpy

People 7 >

Invite someone

Affiliated packages

Interoperability

Collaboration

Reproducibility

Core package versus affiliated packages

scikit-hep

❑ Provides general “core” functionality (see next slide for examples)

❑ Does so with a unified interface

❑ Builds atop the affiliated packages providing bridges where relevant

Affiliated packages

❑ (Take good concept from Astropy of an affiliated package)

❑ Package not part of core scikit-hep but related to, and seen as part of, the community & project

❑ Bring-in functionality specific to certain topics/areas not of the widest community interest
- Package can have a life of its own

❑ But the usage within the Scikit-HEP project should be profitable,
since ability to interoperate more easily

scikit-hep core package (non-exhaustive list)

□ Dataset

- Common interface for data from/to various sources
- Dealing with ROOT Ttree, Numpy arrays, etc.

□ Aggregation

- Summarise or project a dataset
- Typically data aggregation = histogram

□ Modeling

- Data models and fitting utilities

□ Visualization

- Interface to graphics engines such as ROOT and matplotlib, among others

□ Simulation

- utilities, wrappers for Monte Carlo engines and other generators of simulated data

□ Modules for units and constants

□ Maths and statistics tools

Some modules
are much more
advanced than others

Affiliated packages

Part of Scikit-HEP

- ❑ root_numpy & root_pandas – ROOT-NumPy and ROOT-pandas interfaces
- ❑ numpythia – Pythia-NumPy interface
- ❑ pyjet – FastJet-NumPy interface

} To be presented at the DIANA/HEP meeting on Oct. 23rd

Planned and/or worth trying to get

- ❑ Histogrammar – histogramming in a more functional programming way (http://histogrammar.org/)
- ❑ hep_ml package a ML library with miscellaneous tools for HEP (https://arogozhnikov.github.io/hep_ml/)
- ❑ Linking module to Hydra(.Python), a library for data analysis in massively parallel platforms (https://github.com/multithreadCorner/Hydra)
  - See the 2 following presentations!
- ❑ (There's for sure more)

Some of the achievements so far

- ❑ The project has been defined as community-driven and community-oriented
  ⇒ the concept of a community is central !
- ❑ Community bonding work is time- and effort-consuming
- ❑ We do now have various contact persons in various experiments (Belle-II, CMS, DUNE, LHCb)

- ❑ We have a site page for a forum of project ideas … (needs to be updated BTW ;-))
- ❑ You are most welcome to bring your own ideas too !

- ❑ The scikit-hep package has numerous modules mostly ready for release

- ❑ Most of the affiliated packages are mature

- ❑ We had a Google Summer of Code project with outcome of relevance to this project (see next talks)

Planning

Next steps

❑ Finalise a few bits and pieces and make sure the code feels as uniform as possible

❑ Provide examples of how to perform typical simple-ish tasks, to lower threshold for users

❑ Bring test suite up to speed

❑ Test a distribution within LHCb for “guinea pigs”

❑ Development release end of October

❑ Further engage with Particle Physics community at large

- Project presentations & tutorials

Releases

❑ End of October: development release

❑ End of 2017: 1st official release

Interested?

Links

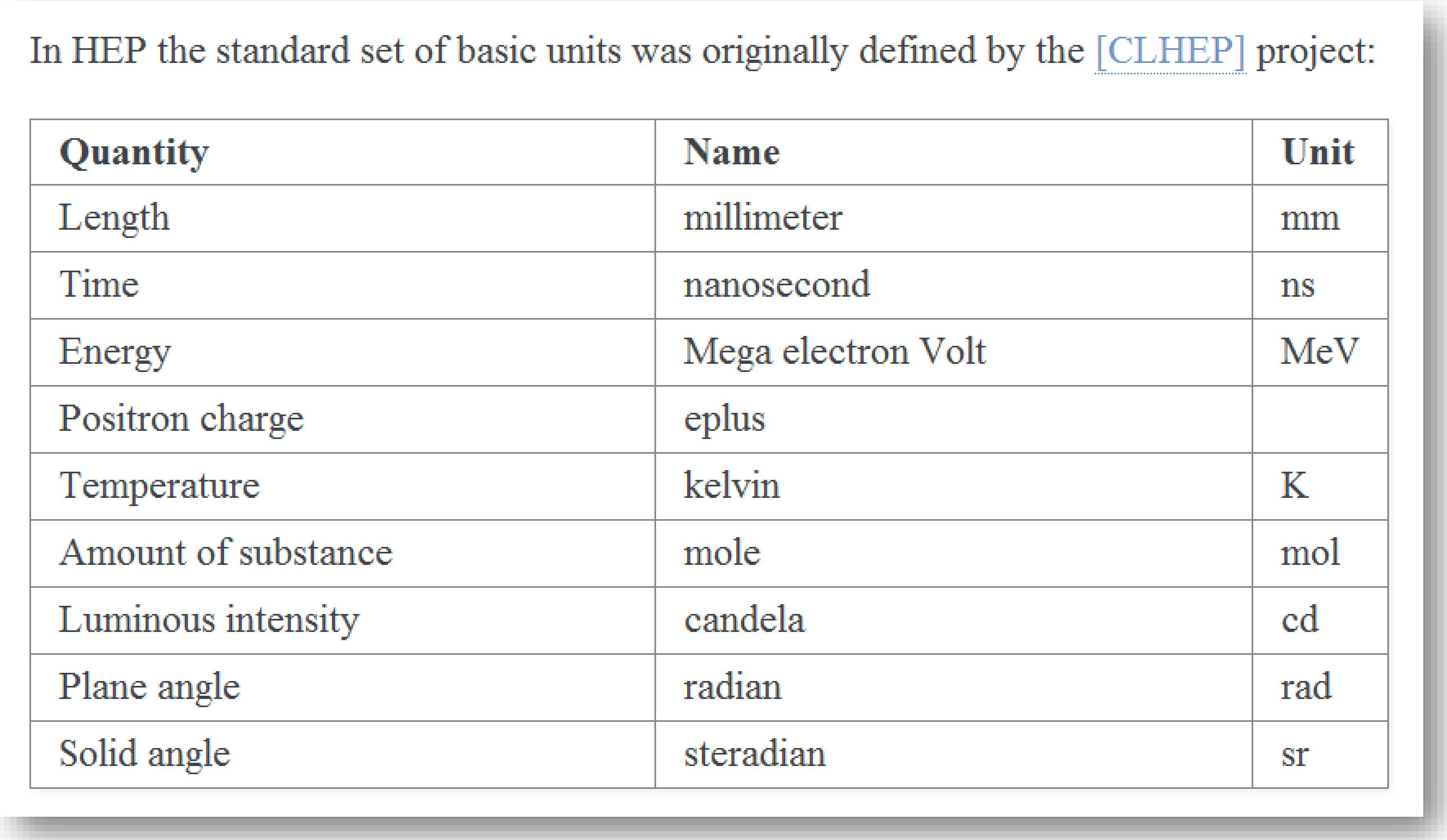
- **GitHub:** https://github.com/scikit-hep/
- **Website:** http://scikit-hep.org/

Mailing lists

- **Get in touch with the team “privately”:** scikit-hep-admins@googlegroups.com
- **Forum for anyone:** scikit-hep-forum@googlegroups.com

Thank you

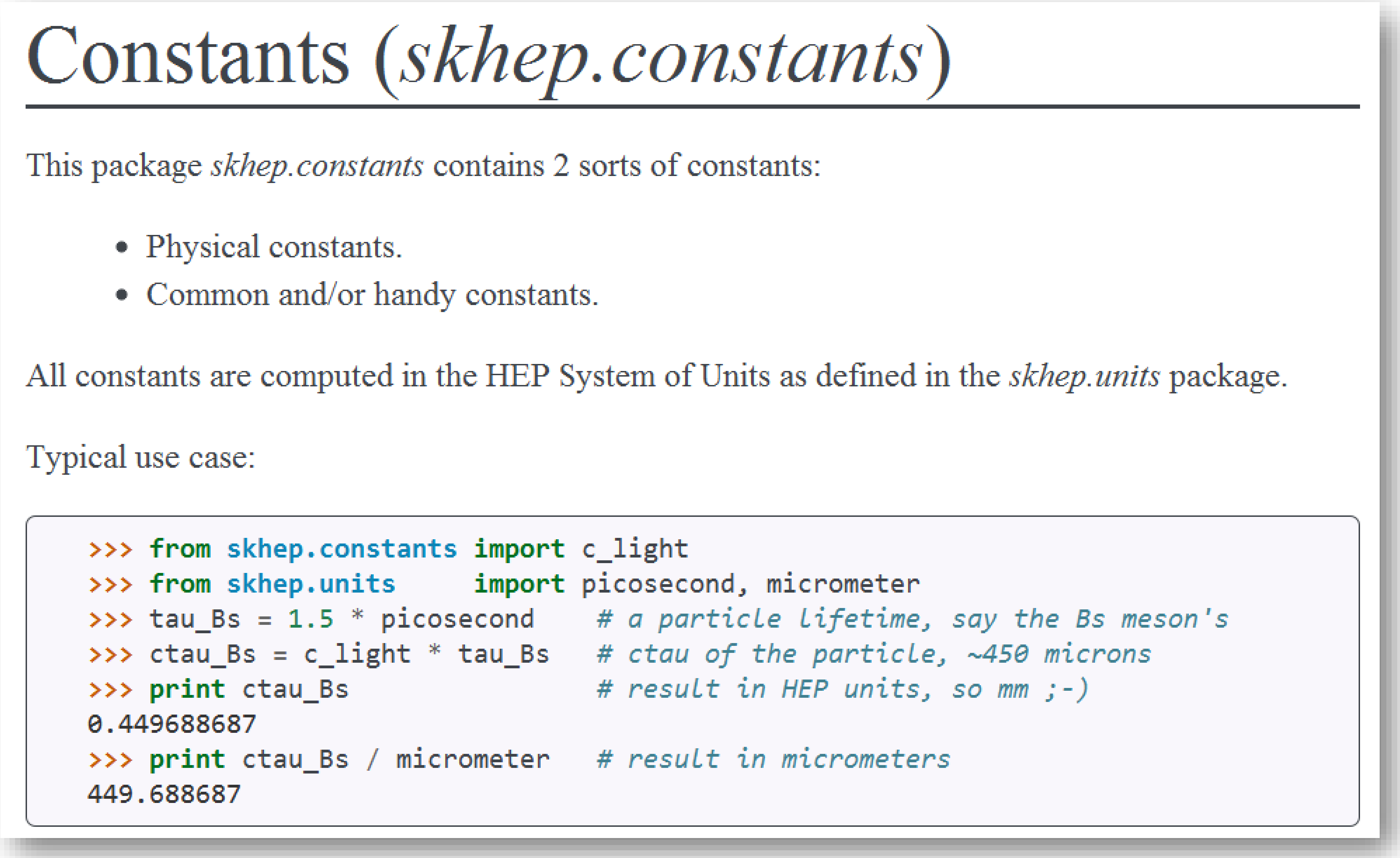
Module examples – HEP units



In HEP the standard set of basic units was originally defined by the [CLHEP] project:

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

Module examples – constants



Constants (*skhep.constants*)

This package *skhep.constants* contains 2 sorts of constants:

- Physical constants.
- Common and/or handy constants.

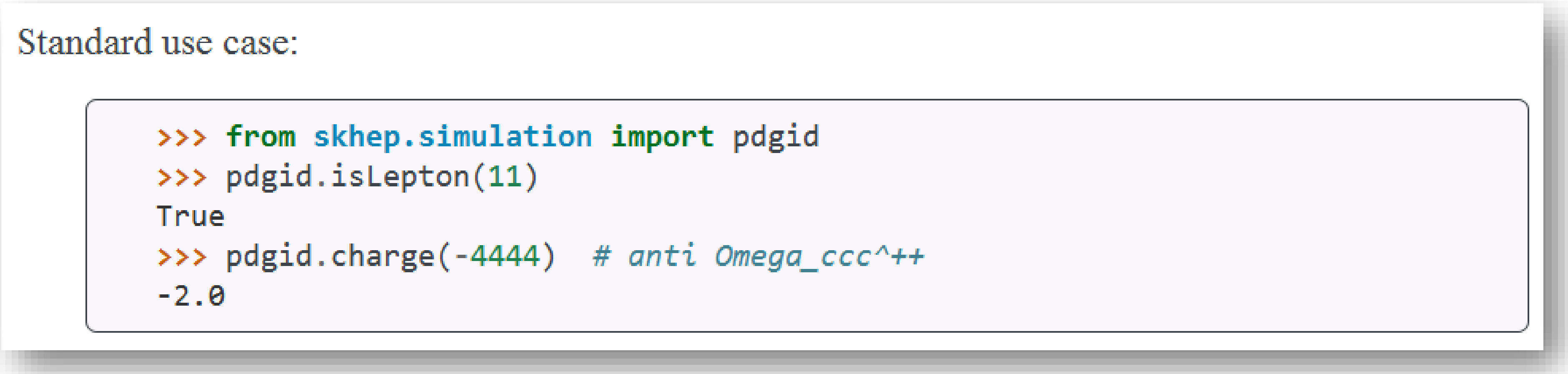
All constants are computed in the HEP System of Units as defined in the *skhep.units* package.

Typical use case:

```
>>> from skhep.constants import c_light
>>> from skhep.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 ;-)
0.449688687
>>> print ctau_Bs / micrometer   # result in micrometers
449.688687
```

Module examples – simulation

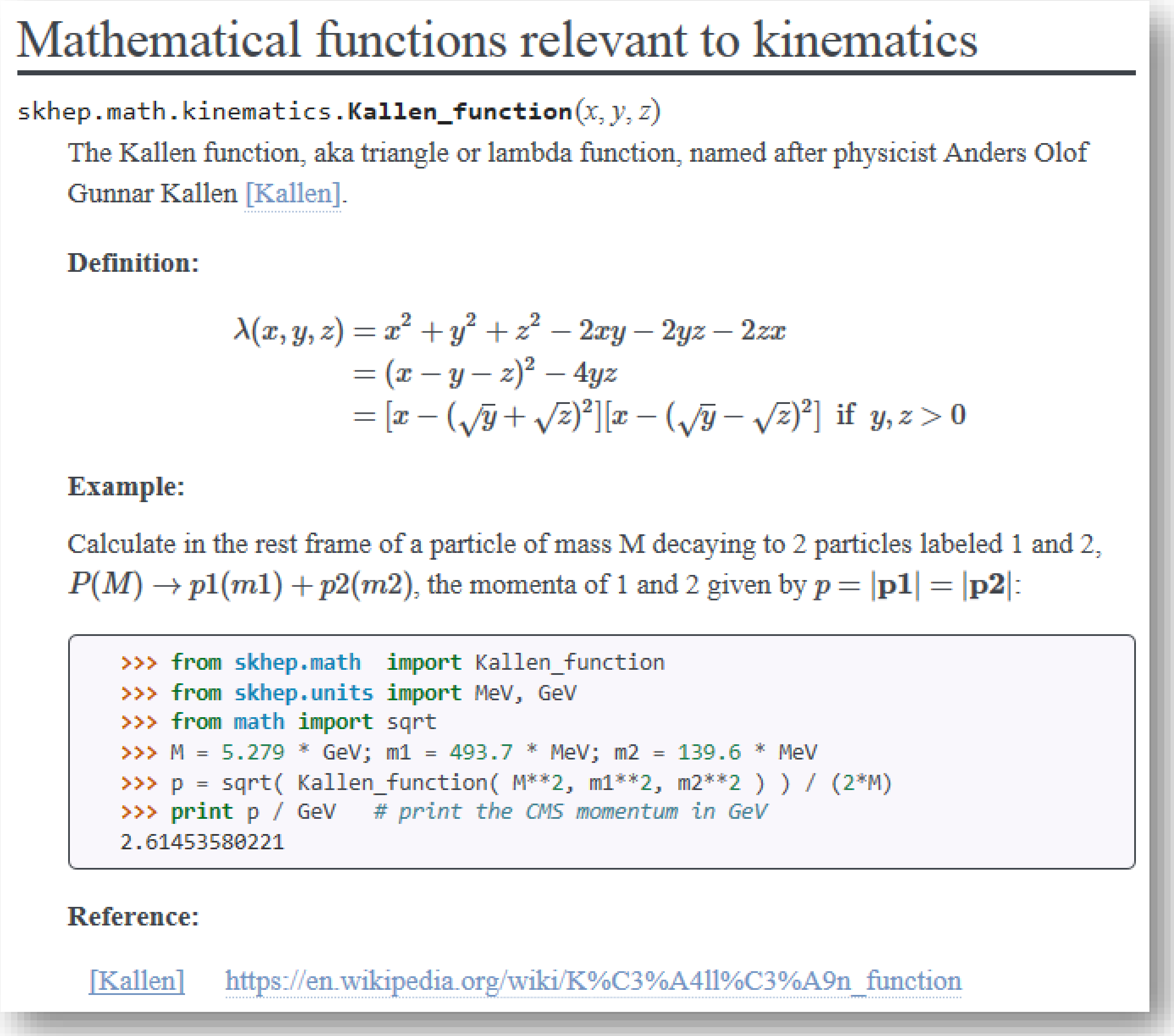
- ❑ **Trivial wrapper for the HepPID C++ library, using PyPDT**
- ❑**(More is coming on this front)**



Standard use case:

```
>>> from skhep.simulation import pdgid
>>> pdgid.isLepton(11)
True
>>> pdgid.charge(-4444)  # anti Omega_ccc^++
-2.0
```

Documentation – online version



Mathematical functions relevant to kinematics

`skhep.math.kinematics.`**`Kallen_function`**(x, y, z)

The Kallen function, aka triangle or lambda function, named after physicist Anders Olof Gunnar Kallen [Kallen].

Definition:

$$\begin{aligned}\lambda(x,y,z) &= x^2 + y^2 + z^2 - 2xy - 2yz - 2zx \\ &= (x-y-z)^2 - 4yz \\ &= [x - (\sqrt{y}+\sqrt{z})^2][x - (\sqrt{y}-\sqrt{z})^2] \;\text{ if }\; y,z > 0\end{aligned}$$

Example:

Calculate in the rest frame of a particle of mass M decaying to 2 particles labeled 1 and 2, $P(M) \to p1(m1) + p2(m2)$, the momenta of 1 and 2 given by $p = |\mathbf{p1}| = |\mathbf{p2}|$:

```
>>> from skhep.math  import Kallen_function
>>> from skhep.units import MeV, GeV
>>> from math import sqrt
>>> M = 5.279 * GeV; m1 = 493.7 * MeV; m2 = 139.6 * MeV
>>> p = sqrt( Kallen_function( M**2, m1**2, m2**2 ) ) / (2*M)
>>> print p / GeV   # print the CMS momentum in GeV
2.61453580221
```

Reference:

[Kallen] https://en.wikipedia.org/wiki/K%C3%A4ll%C3%A9n_function