Software Lifecycle at CERN and in the HSF

Lukas Heinrich for the HEP Software Foundation

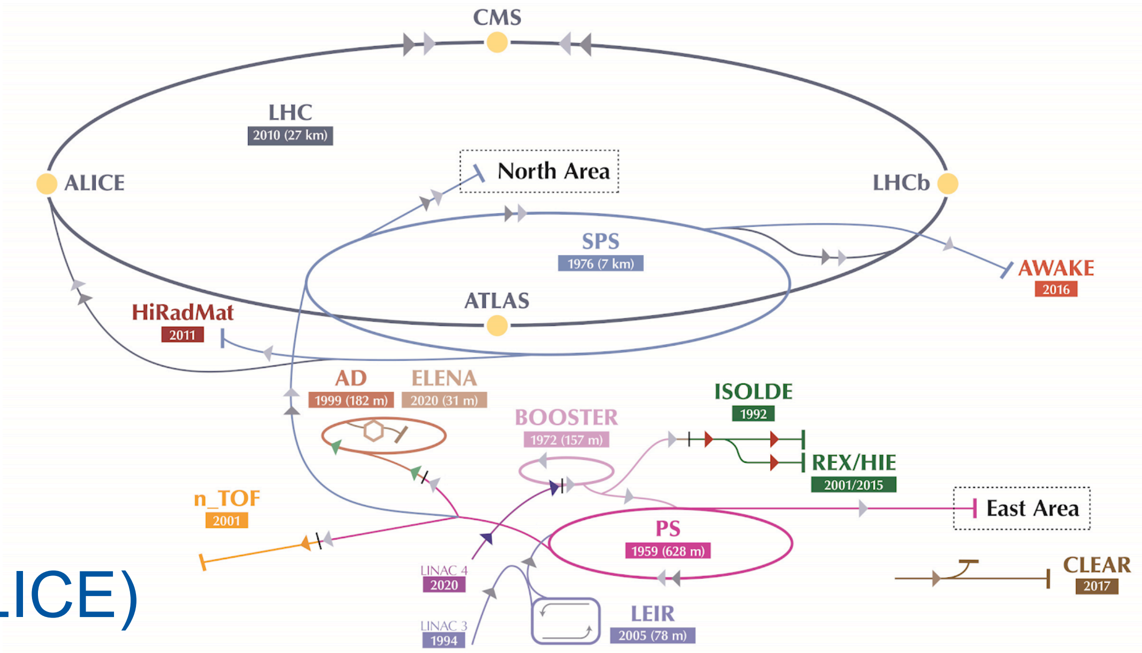
CERN:

Home of some of the biggest scientific experiments:

LHC + its experiments (ATLAS, CMS, LHCb, ALICE)

But also many others smallers ones (TOTEM, ISOLDE, ...)

The Lab is also a central Hub for **High Energy Physics** in general, coordinating many community-wide activities.




Besides massive Hardware...

Software is of course central to everything we do.

Wide range of software: from professional "products" (ROOT, Geant4,SHERPA,...) to collaboration specific million lines-of-code reconstruction frameworks (Athena, CMSSW) to one-off analysis code / shell scripts.

Wide ranging spectrum of "process" of writing and maintaining software.

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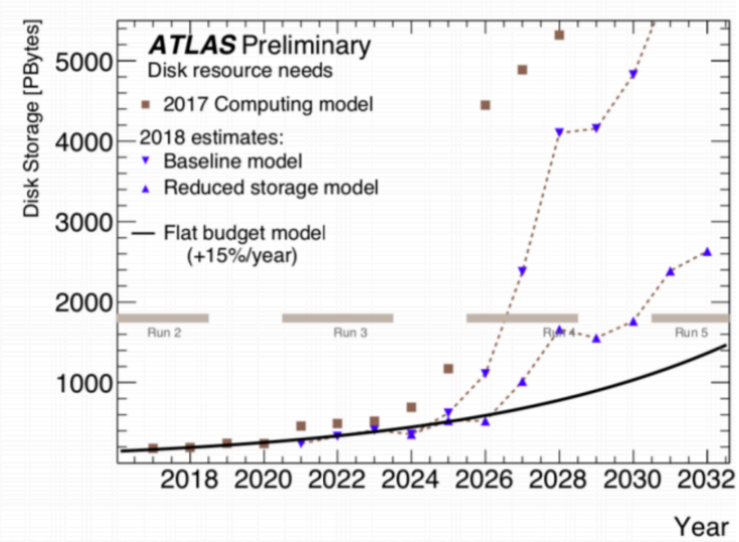
The big challenge ahead of us: HL-LHC



Software needs too rise to the occasion on all levels.
Community needs to be equipped with infrastructure and training to do so.

Software is of course central to everything we do.

HEP Software Foundation

- founded in 2015 to tackle these challenges / to provide a forum for sharing ideas, experience and code between experiments
- Encourage best practice for development
  Both at the algorithmic and tools level
  Most of this work happening in the context of HSF Working Groups

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

HSF
HEP Software Foundation

CERN

Software is of course central to everything we do.

Community White Paper process

- **common document to lay out plans for the next 10 / 20 years in all areas of software & computing.**

Community White Paper Reports

The roadmap summarised reports from fourteen working groups who studied the challenges in their sub-domains. All of the reports produ
during the Community White Paper process are listed below. Working groups are in the process of finalising and uploading their work to ar

Paper	*Report Number*	*Link*
CWP Roadmap	HSF-CWP-2017-01	arXiv
Careers & Training	HSF-CWP-2017-02	arXiv
Conditions Data	HSF-CWP-2017-03	arXiv
Data Organisation, Management and Access	HSF-CWP-2017-04	arXiv
Data Analysis and Interpretation	HSF-CWP-2017-05	arXiv
Data and Software Preservation	HSF-CWP-2017-06	arXiv
Detector Simulation	HSF-CWP-2017-07	arXiv
Event/Data Processing Frameworks	HSF-CWP-2017-08	arXiv
Facilities and Distributed Computing	HSF-CWP-2017-09	Google Doc
Machine Learning	HSF-CWP-2017-10	arXiv
Physics Generators	-	No separate paper, see CWP Roadmap, section 3.1
Security	-	No separate paper, see CWP Roadmap, section 3.13
Software Development, Deployment and Validation	HSF-CWP-2017-13	arXiv
Software Trigger and Event Reconstruction	HSF-CWP-2017-14	arXiv - Executive Summary; arXiv - full document
Visualisation	HSF-CWP-2017-15	arXiv

https://hepsoftwarefoundation.org/organization/cwp.html

HSF-CWP-2017-01
December 15, 2017

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

HEP Software Foundation[1]

Abstract: Particle physics has an ambitious and broad experimental programme for the coming decades. This programme requires large investments in detector hardware, either to build new facilities and experiments, or to upgrade existing ones. Similarly, it requires commensurate investment in the R&D of software to acquire, manage, process, and analyse the shear amounts of data to be recorded. In planning for the HL-LHC in particular, it is critical that all of the collaborating stakeholders agree on the software goals and priorities, and that the efforts complement each other. In this spirit, this white paper describes the R&D activities required to prepare for this software upgrade.

[1] Authors are listed at the end of this report.

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- trend toward integration with standard industry tools
- make our own softwarer more modular / inter-operable

HSF-CWP-2017-01
December 15, 2017

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arXiv:1712.06982v5 [

imental programme
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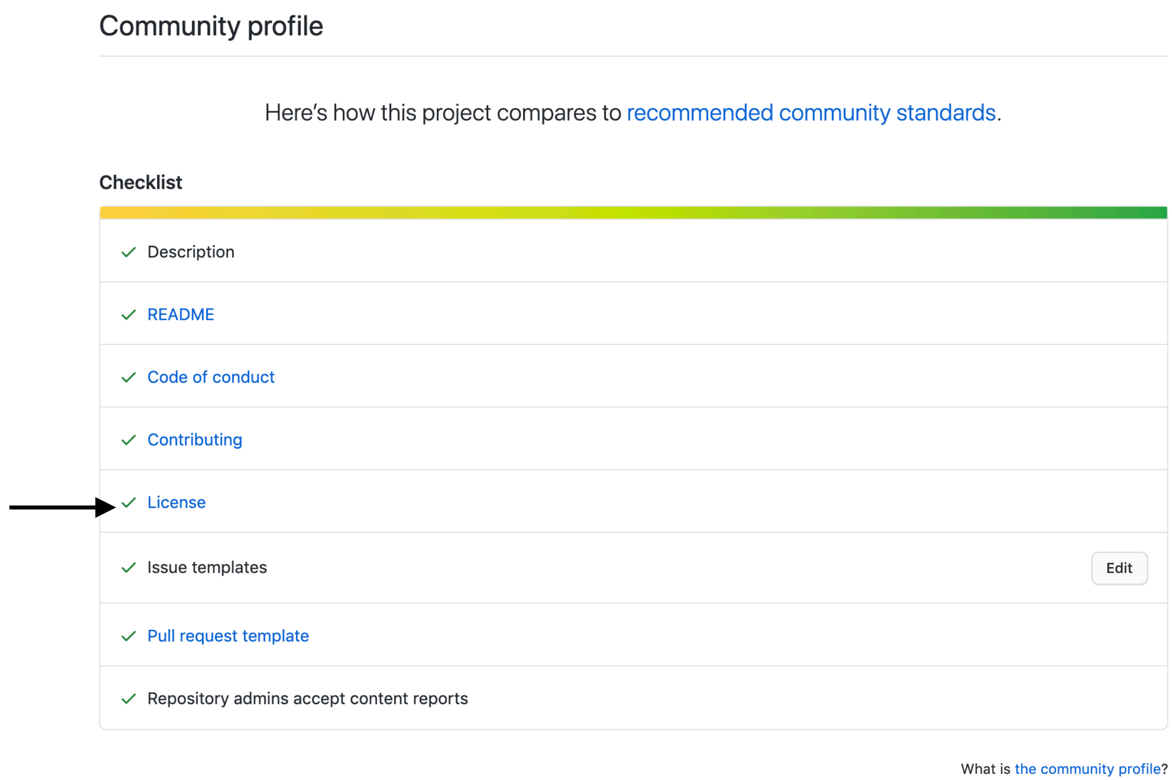
CERN

Preparing your software to be part of a larger community.

CODE

Traditionally has been undervalued in academic s/w (esp personal projects).

- It took a lot of work to correct this situation for the LHC experiments' code
- If it works, getting CERN (or your host lab) to hold copyright for the code works very well (a single copyright holder makes any relicensing easier)
- Collaborations or bodies like HSF cannot hold copyright
- Various Licenses Possible:
    - https://opensource.org/licenses
    - Good idea t ochoose such that your s/w can be easily reused / integrated into other softwaer.



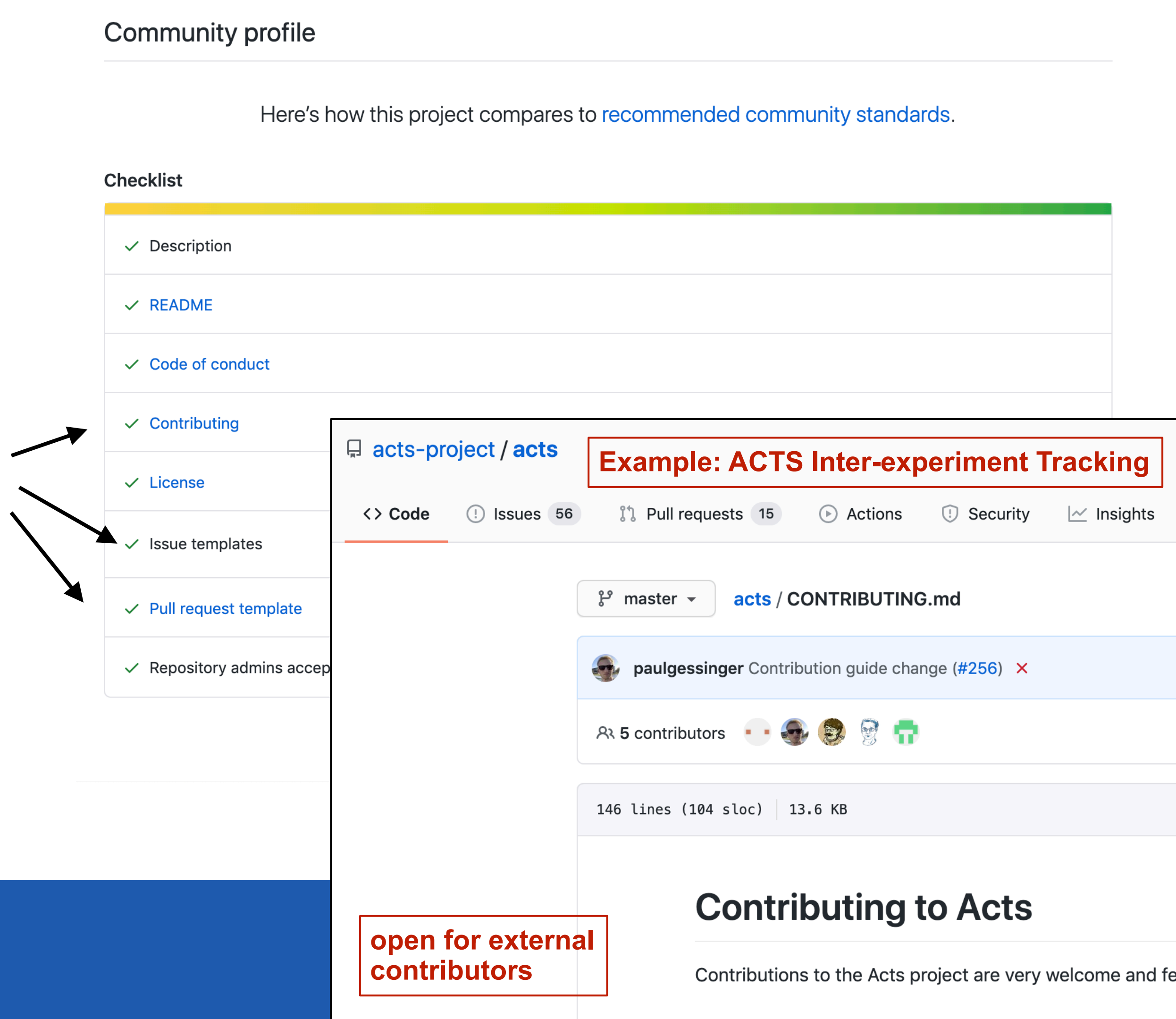
Preparing your software to be part of a larger community.

CONTRIBUTING

Having code "open source" in-name only without expectation / invitation to contribute generally seen as anti-patterrn.

Should provide clear guidelines for new contributors no

- how to raise issues
- develop & test project code
- contribute code (pull requests)



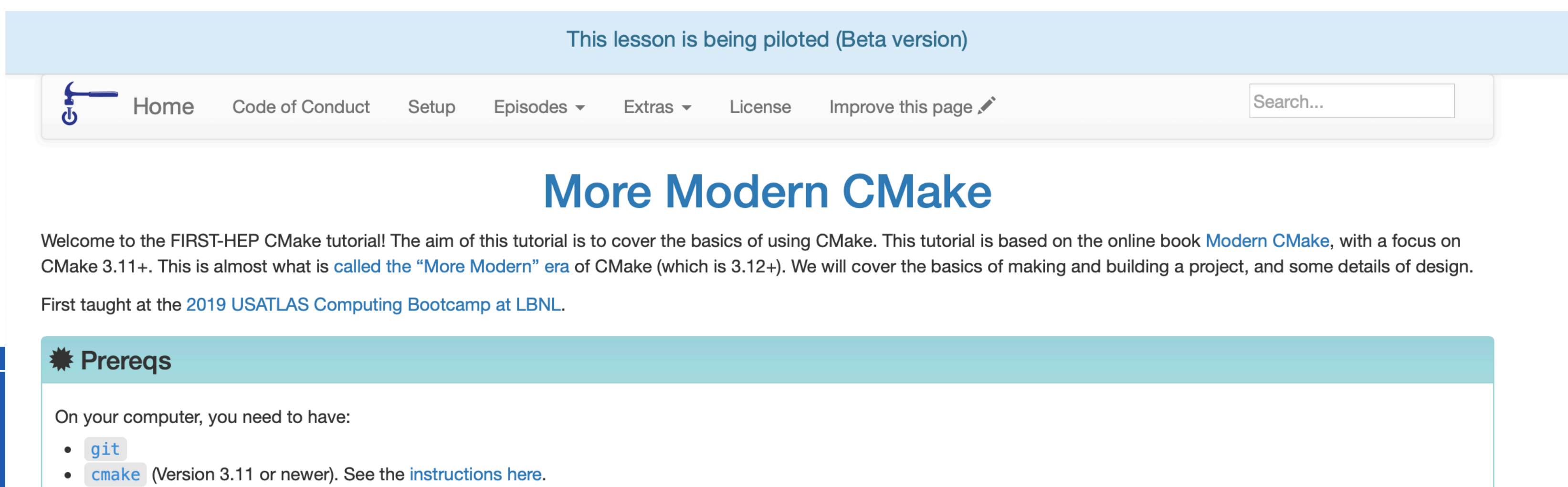
Build Systems

A lot of our code is C++. Traditionally various versions of build systems used:

- in-house developments ("cmt", ..)
- autoconf tools (./configure; make...)

In the meantime CMake has become the dominant build system for C and C++ prrojects. Transitioned huge codebases to it.

Trainings for CMake from HSF/FIRST-HEP



This lesson is being piloted (Beta version)

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More Modern CMake

Welcome to the FIRST-HEP CMake tutorial! The aim of this tutorial is to cover the basics of using CMake. This tutorial is based on the online book Modern CMake, with a focus on CMake 3.11+. This is almost what is called the “More Modern” era of CMake (which is 3.12+). We will cover the basics of making and building a project, and some details of design.

First taught at the 2019 USATLAS Computing Bootcamp at LBNL.

Prereqs

On your computer, you need to have:

- `git`
- `cmake` (Version 3.11 or newer). See the instructions here.

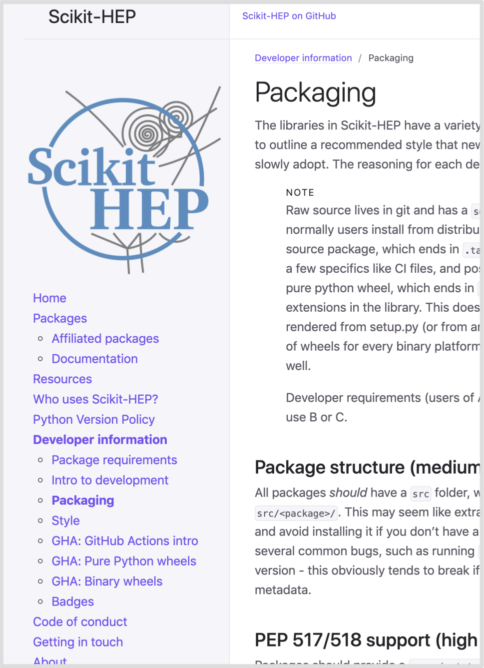
Software Packaging:

Traditionally a lot of "source packaging" but big software projects provide e.g. conda recipes, RPMs, PyPI packages to install software with standard package managers.

```
conda install -c conda-forge root
yum install AnalysisBase
pip install uproot
```

CERN EP-SFT Group evaluated Spack as one of the most promising packaging tools for production use cases

Spack



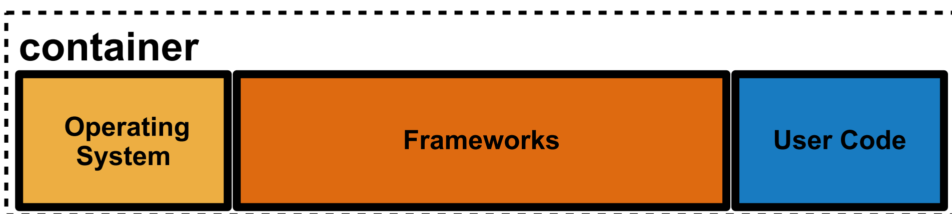
guidelines for python packages from Scikit-HEP

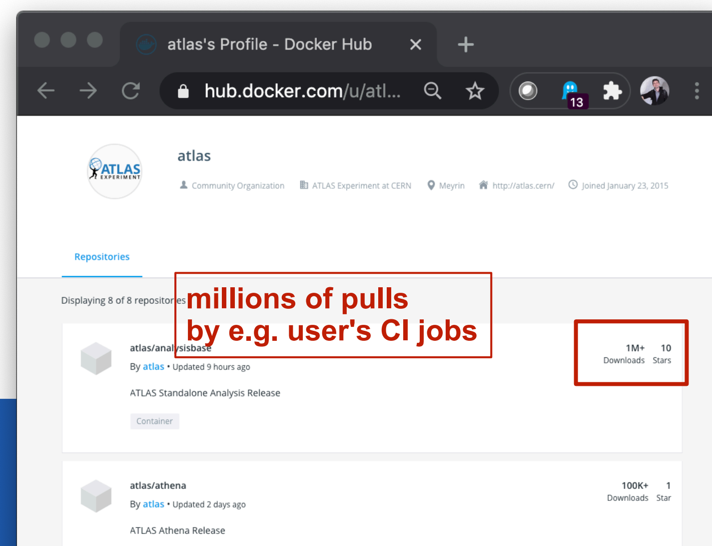
Software Distribution:

Traditional Approach (last 10 years or so):

CVMFS: CERN VM Filesystem:
Model: read-only for most, write for few "publishers"

More recently: Everything is a Container.
- reproducible, portable standard unit
- easy integration into HPC, Cloud, Laptops...
- new development: efficient global distribution of images via cvmfs





Software Distribution:

Integration of Containers into workload mgmt systems

Allows developers increased flexibility to define their "own stack".

- **Particularly useful for Machine Learning Application**

16165474 task: user.lheinric.mlongriddemo.v7/

Task ID	Jobset	Type	Working Group	User	Destination	Task status	Nevents | used	HS06*sec Expected Total done failed	Ninputfiles | finished | failed	Average maxpss	Created	Modified	Cores	Priority	Parent
16165474	3728	analy		Lukas Alexander Heinrich		done	0 | 0 (%)	None 14016 14016	1 | 1 (100%)		2018-11-23 18:41:49	2018-11-23 19:17:29	1	1000	

Prodsys task parameters	
architecture	
cliParams	prun --containerImage docker://lukasheinrich/atlasml:latest --exec "sh -c 'python /btagging/DL1_c_vs_b_slim.py %IN 10 gpu 500'" --inDS user.lheinric:mlongrid.v1 --outDS user.lheinric.mlongriddemo.v7 --noBuild --site ANALY_MANC_GPU_TEST --forceStaged

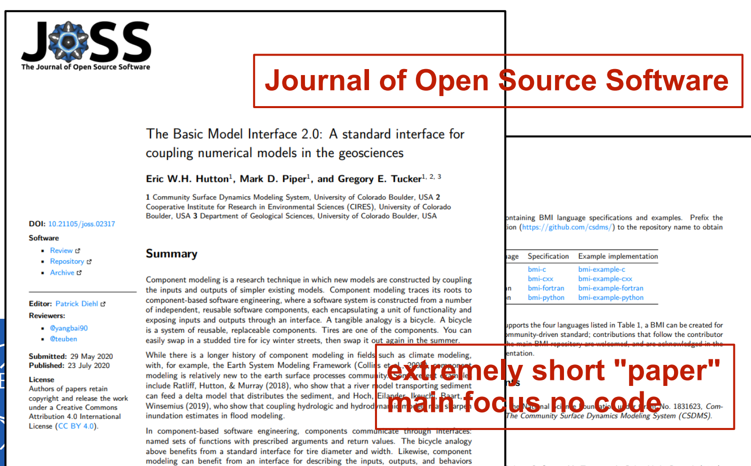
Software Citation:

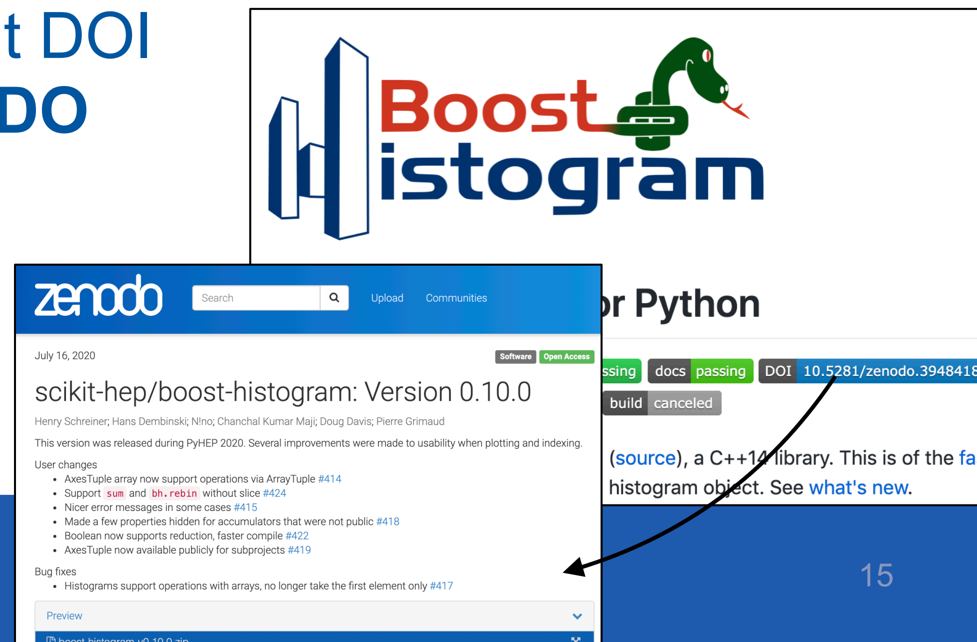
`CITATION`

Software is often the research product itself. Should be treated as part of the scholarly record.

- cite software directly instead of "software papers" to attirbute proper credit
- if you need a paper consider **JOSS**

CERN runs free service to mint DOI deposit code, datasets: **ZENODO**





Example Projects:

generally can implement guidelines on all project scales:

Athena: ATLAS O(M) lines of core Reconstruction Code

https://gitlab.cern.ch/atlas/athena

- on-prem GitLab
- C++
- O(1000) contributors all from same collaboration
- Jenkins CI (moving to GitLab)
- RPM packages
- nightly tests
- docker images
- code linting
- citation available
- IDE integration
- Code Review
- ...

pyhf: statistics code

https://github.com/scikit-hep/pyhf

- GitHub
- 3 core developers with O(10) contibutors
- code linting
- Github Actions CIs
- code auto-forrmatting (black)
- docs auto-generation in CI
- automated PyPI packaging
- O(1000) unit tests
- Test Coverage > 95%
- Code Review

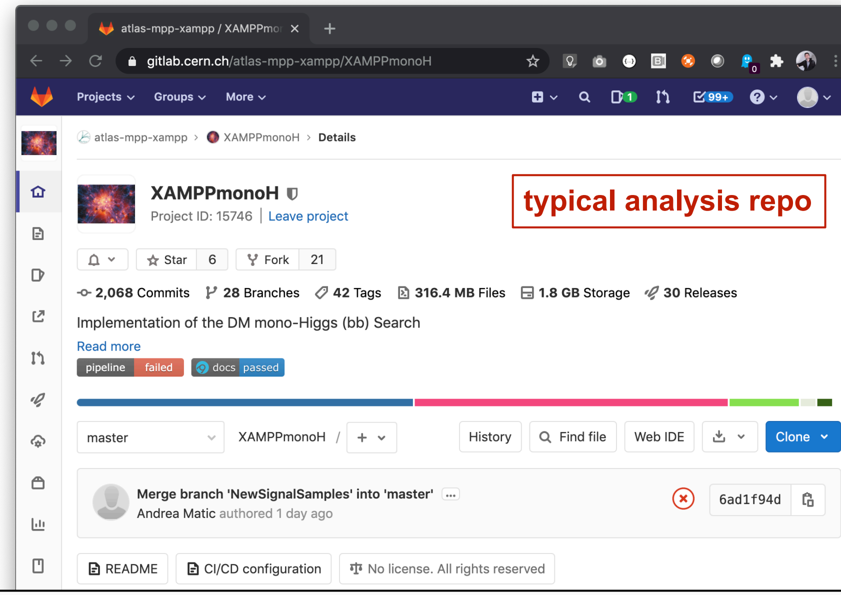
Role of Host Lab / (common entity / EU project) providing **infrastructure is crucial** to enable new developments.

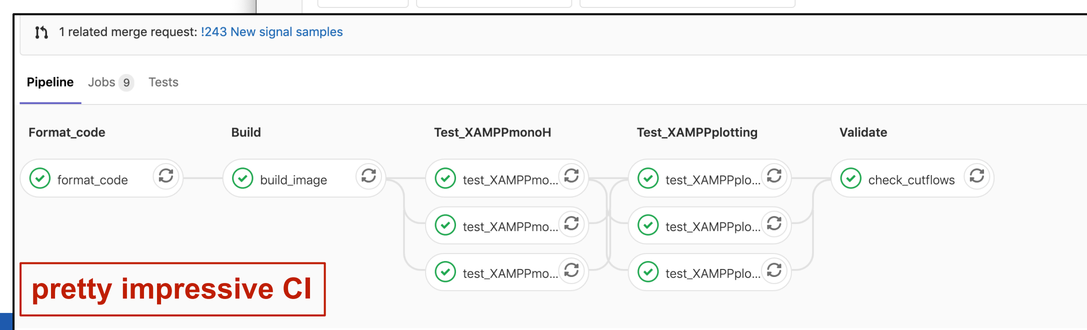
Example 1 (Physical Infrastructure):
GitLab introduced at CERN as new VC System. Analysis Teams required to have code in GitLab

Focus on integrated developer experience, on-prem deployment

Visible Change in attitudes from scientists to improve sofware creation cycle.

If it's easy to use & readily available, people become quite ambitious.





Role of Host Lab / (common entity / EU project) providing **infrastructure is crucial** to enable new developments.

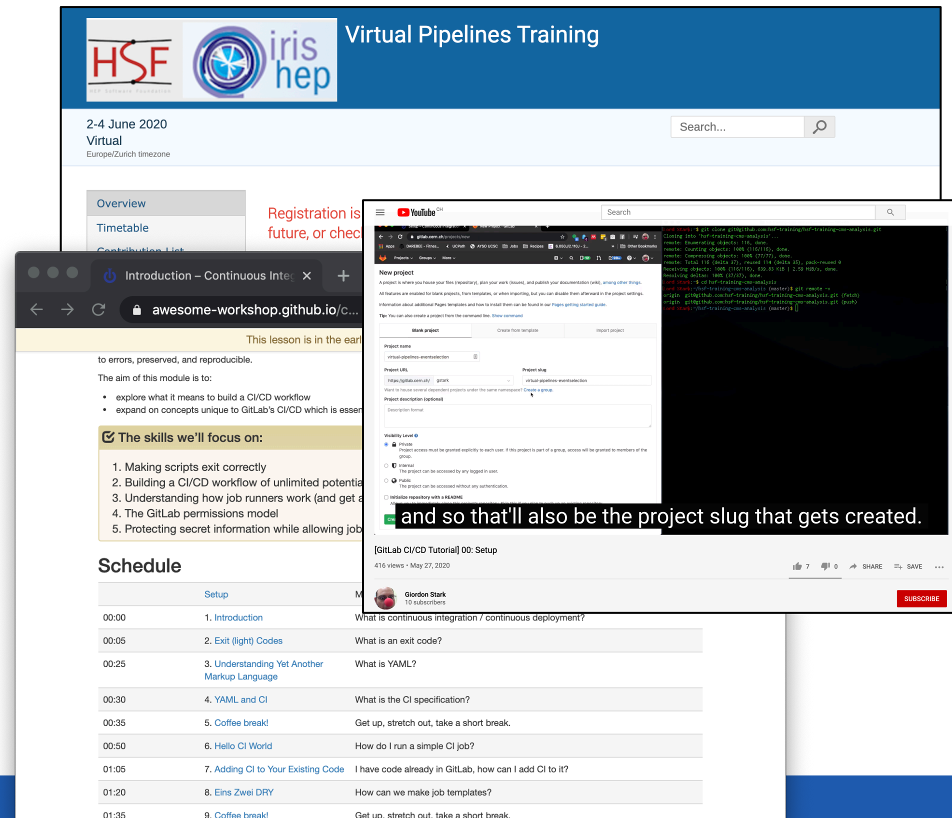
Example 2 (Organizational Infrastructure):
HSF/IRIS-HEP Training on Modern Software Development Tools

Topics: git, cmake,

Format:
- Software Carpentry
- Recorded Lessones (COVID)

Build up a library / catalogue of community-wide training material.

Again: **if you offer it people will come:** 200 sign-ups within days.



Role of Machine Learning:

Clear that ML will play increasing role in our software.

- we won't be driving the core software developments
- hardware increasingly targeted for ML

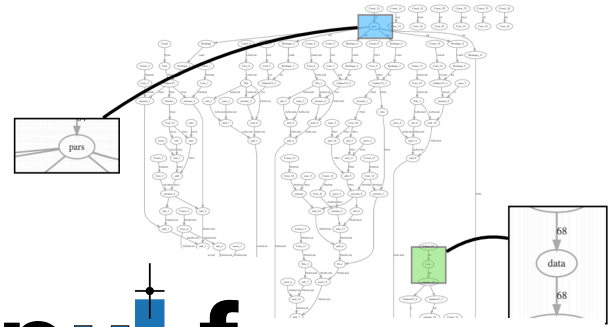
Strategies:

- cast existing problems as ML problems (e.g. tracking in Exa.TrkX)

about TrkX

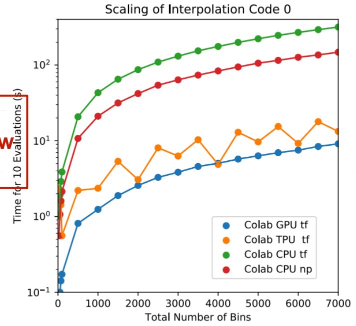
HEP advanced tracking algorithms at the exascale (Project Exa.TrkX)

- instead of replacing our algorithms with ML, use ML foundation (highly vectorized computation + autodiff) for improved implementation (e.g. statistical fits)



pyhf
∂ifferentiable
ℒikelihoods

once implemented on ML tools running on new h/w becomes easy



Role of Quickly Changing Hardware

We're entering a new age of more dynamic hardware platforms.

- **Not only GPU: FPGA, ASIC, Dataflow Engines, ...**
- **can we adapt / rethink our algorithms to match the h/w? ML is one way, but not silver bullet.**
  - **SYCL, Alpaka, etc as underlying libraries for software portability**
- **even if we could, do we have the expertise to implement them? Advanced Training of Experts is crucial**

Examples of Recent GPU initiatives:

- ALICE reco
- LHCb Allen (Trigger)
- CMS Patatrack

	OpenMP Offload	Kokkos	dpc++ / SYCL	HIP	CUDA	Alpaka
NVidia GPU			Intel/codeplay			
AMD GPU		prototype	via hipSYCL			
Intel GPU						very early development
CPU						
Fortran						
FPGA						possibly via SYCL

Supported
Under Development
3rd Party
Not Supported

HSF Frameworks and Reconstruction WGs gathering experience.

End User Software Re-use (Analysis Preservation)

For unique and large datasets such as those in HEP, the end-user software is often the only window to extract insight from a given dataset.

- software defined extraction of interesting data region
- If the software is gone the access to the "region" is gone as well: need to preserve analyses

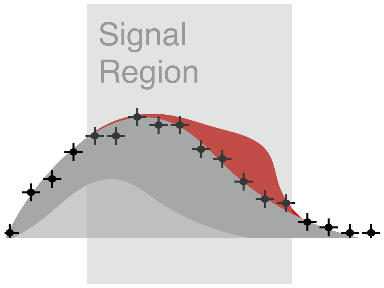
Ideally: continuously maintained code, but more realistically "fixed code" of final published analysis is all we can do

Marquee use-case: RECAST

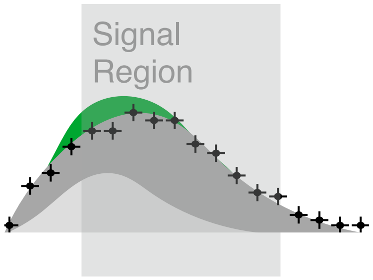
Allow answer simple question: is a given theory already excluded by existing LHC analyses or do we need a dedicated study?

If analysis is preserved & functional: easy to answer

- simulate new model and pass through analysis to get a "reinterpreted result"



original model



alternative model

Simple Software Prerservation is not enough for Analysis Preservation: need the full pipeline

capture software

archive analysis code incl. dependencies

capture commands

what do with the captured software

capture workflow

order of individual steps

data assets

input data needed to run the analysis

Ingredients: Container Images, Workflow Languages

- **similar trends in bioinformatics**

COMMON WORKFLOW LANGUAGE

CERN Working on Cyberinfrastructure to provide Archive of preserved analysis and compute resources to re-execute them (REANA)

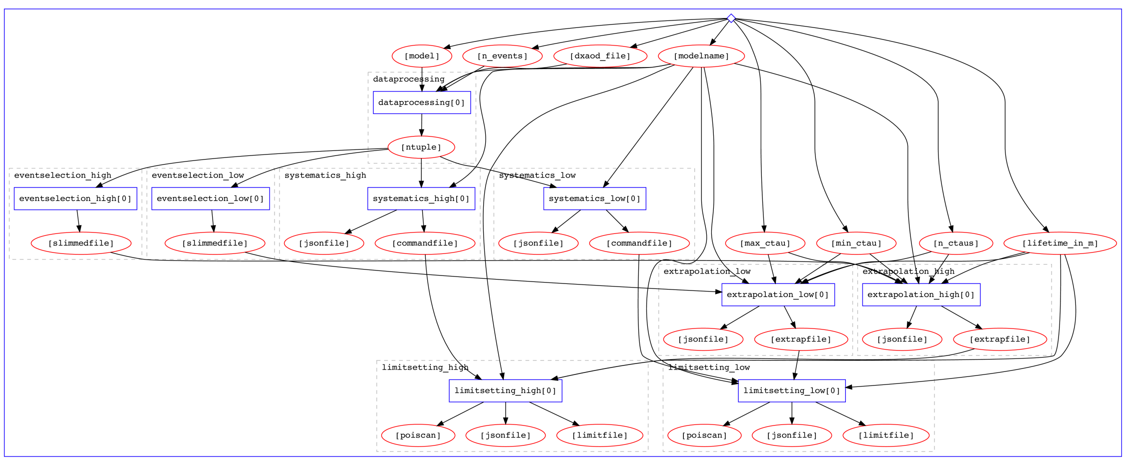
CERN
Analysis Preservation
capture, preserve and reuse physics analyses

reana
Reproducible research data analysis platform

CERN

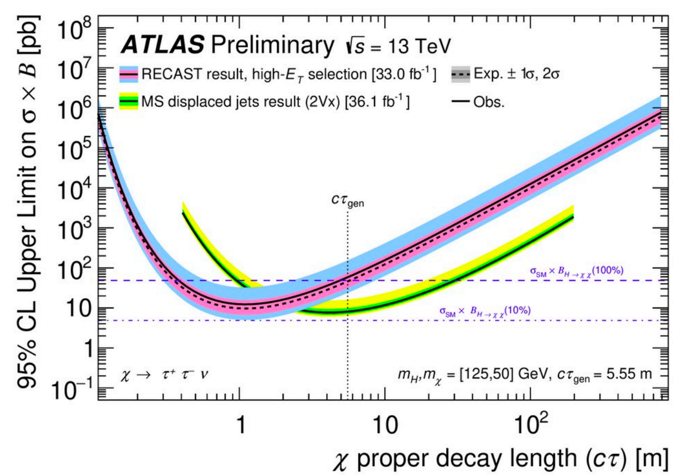
Success Stories: New Science out of Old Code :

- **better scientific exploitation of data at low cost**
- **Examples from ATLAS: <u>requirement</u> on analysis teams to preserve analysis (docker images, workflows) leads to new results**
- **Potentially interesting ESCAPE test science case**



Preserved Workflow (each node a Docker container workload)

ATL-PHYS-PUB-2020-007



New result!

Outlook

HSF founded to provide forum to discuss the big challenges in HEP software & computing (with many trends outside of our direct control: hardware, ML, data-science)

Provide / Develop Strategies and Tools for the full softwaer lifecycle (authoring, build, package, distribute, perserve) to build a sustainable Software Ecosystem for HEP in a changing world.

Training is crucial at all levels: beginners (git, docker, cmake) to experts (accelerator programming, etc). HSF Provides

Given our unique data, the software itself becomes the product: increased attention to preservation, reuse, reproducibility

CERN plays a crucial role as the central Host Lab to provide infrastructure.