pyhf Roadmap for IRIS-HEP Execution Phase

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pyhf core dev team

Lukas Heinrich

CERN

Matthew Feickert

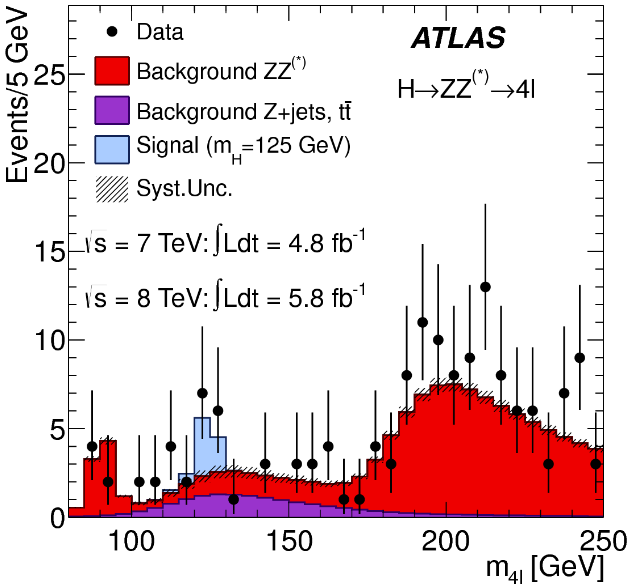
Illinois

IRIS-HEP

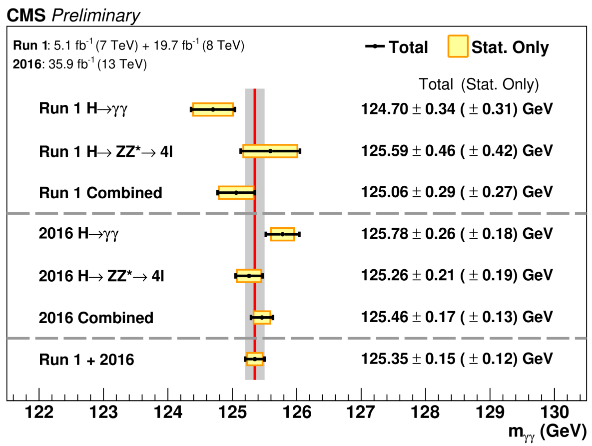
Giordon Stark

UCSC SCIPP

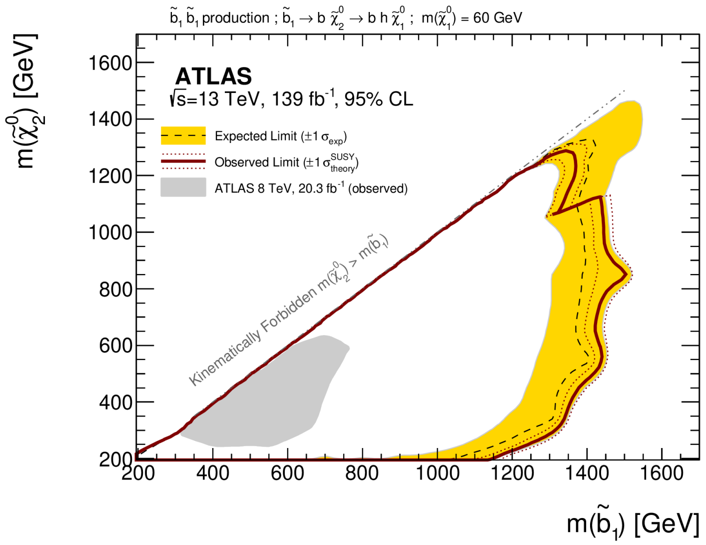
Goals of physics analysis at the LHC



Search for new physics



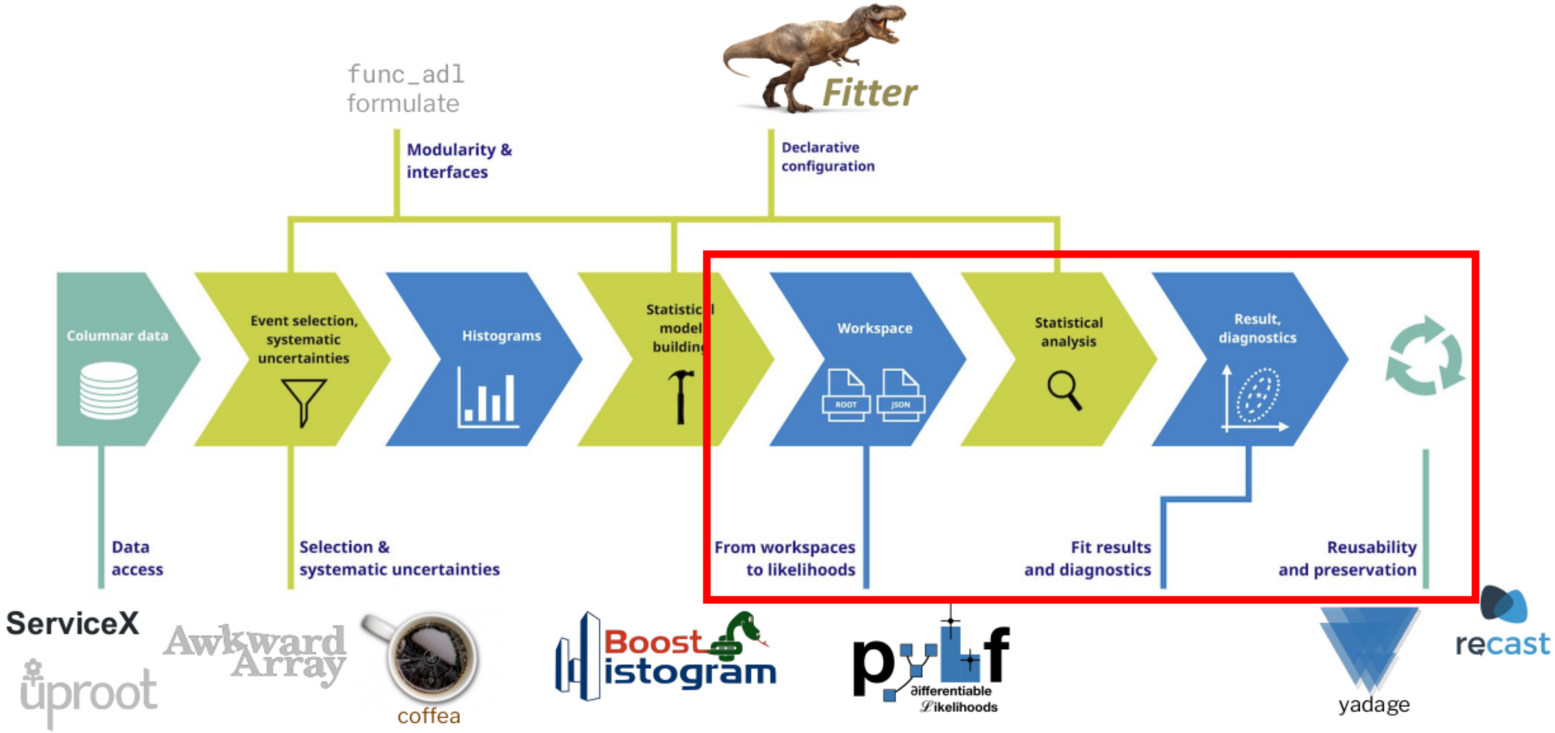
Make precision measurements



Provide constraints on models through setting best limits

- All require **building statistical models** and **fitting models** to data to perform statistical inference
- Model complexity can be huge for complicated searches
- Problem: Time to fit can be **many hours**
- Goal: Empower analysts with fast fits and expressive models

Analysis Systems through the lens of `pyhf`

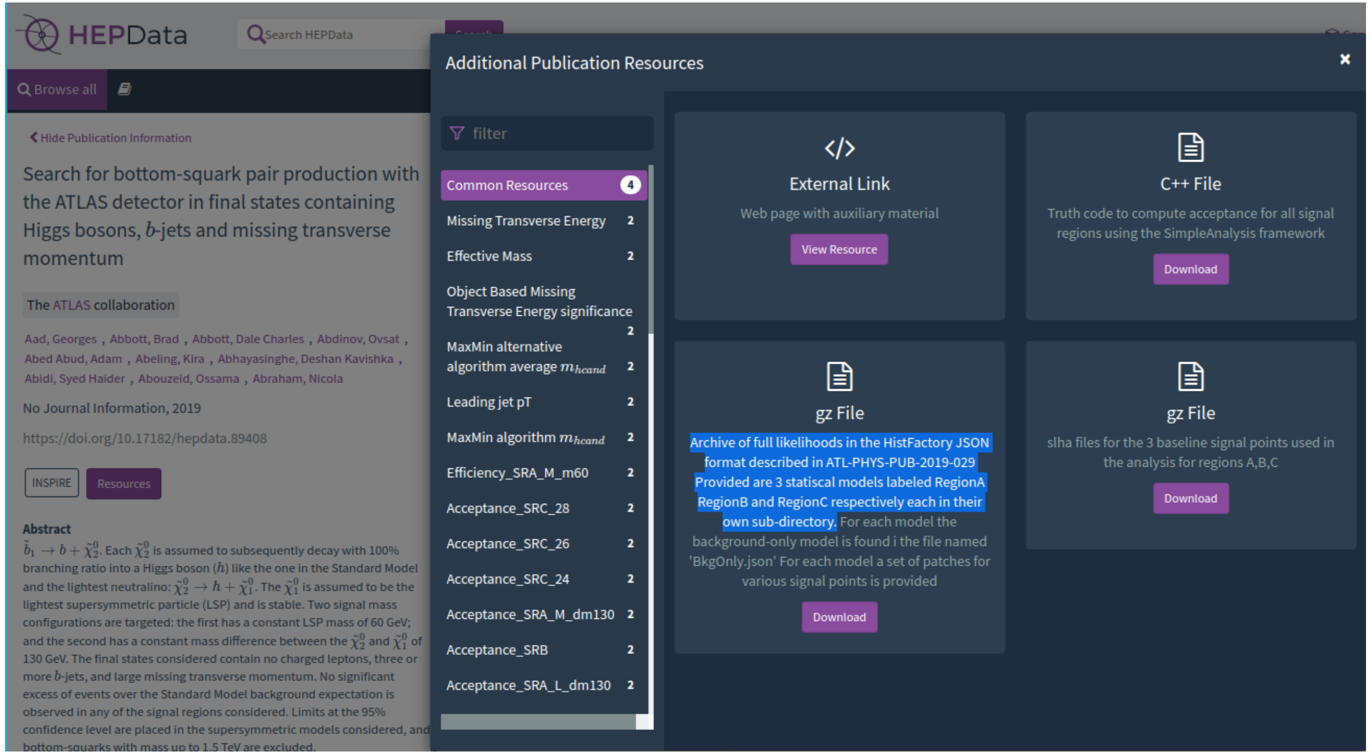


- Accelerating fitting (reducing time to **insight** (statistical inference)!)
- Flexible schema great for open likelihood **preservation**
  - Likelihood serves as high information-density summary of analysis
- An enabling technology for **reinterpretation**

Accomplishments in Year 2

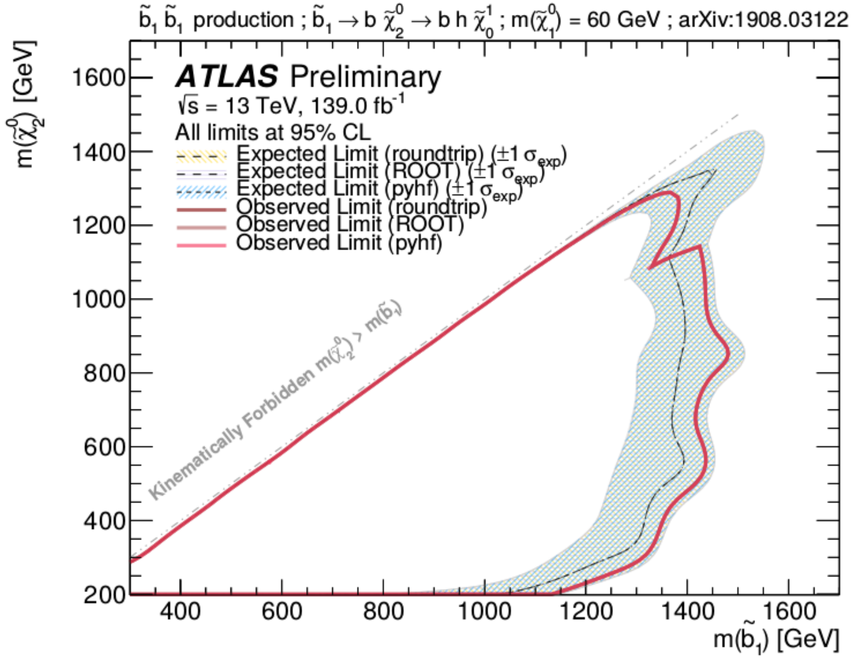
Full likelihoods (3) preserved on HEPData

- Background-only model JSON stored
- Signal models stored as JSON Patch files
- Together are able to fully preserve the full model (with own DOI! DOI 10.17182/hepdata.89408.v1/r2)
- c.f. Matthew's CHEP 2019 talk, Lukas's LHCP 2020 talk



Publications using pyhf

ATLAS Note	
Report number	ATL-PHYS-PUB-2019-029
Title	**Reproducing searches for new physics with the ATLAS experiment through publication of full statistical likelihoods**
Corporate Author(s)	The ATLAS collaboration



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

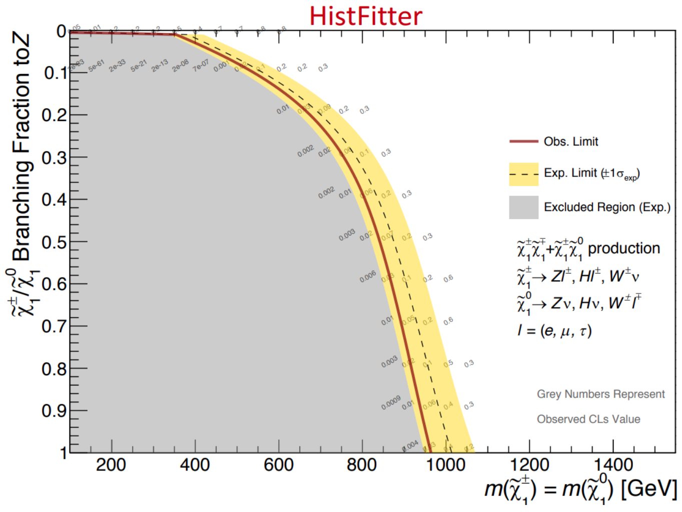
Explore ATLAS open likelihoods on the HEPData platform (Image: CERN)

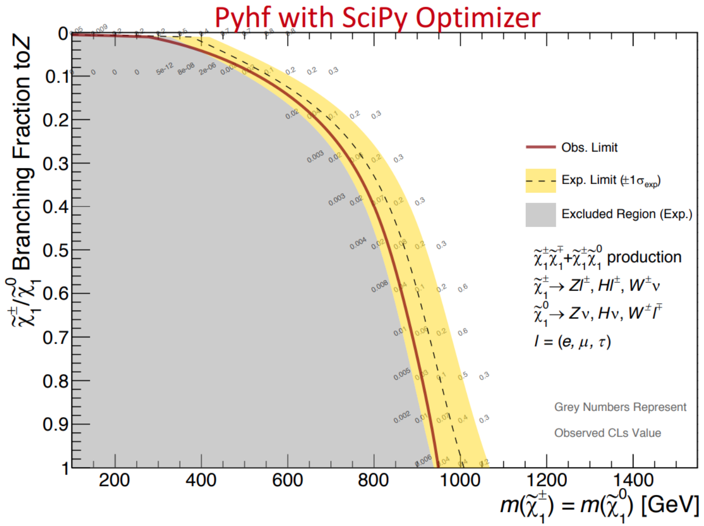
Rapid adoption in ATLAS...

- Impressive appetite for `pyhf` in ATLAS analyses
- Much of SUSY, $HH \to 4b$ limit setting
  - Giordon: SUSY Run-2 Summaries subconvener
  - Lukas: ATLAS Modeling Group convener
- Upcoming: ATLAS Stats Forum recommendation

Thanks for making a tool super easy to use! When I got some [Jupyter] notebooks with this code up and shared with students a lot more of us started including limits in our talks. Before this was a pretty painful step!

— Nicole Hartman (SLAC), ATLAS Ph.D. Student

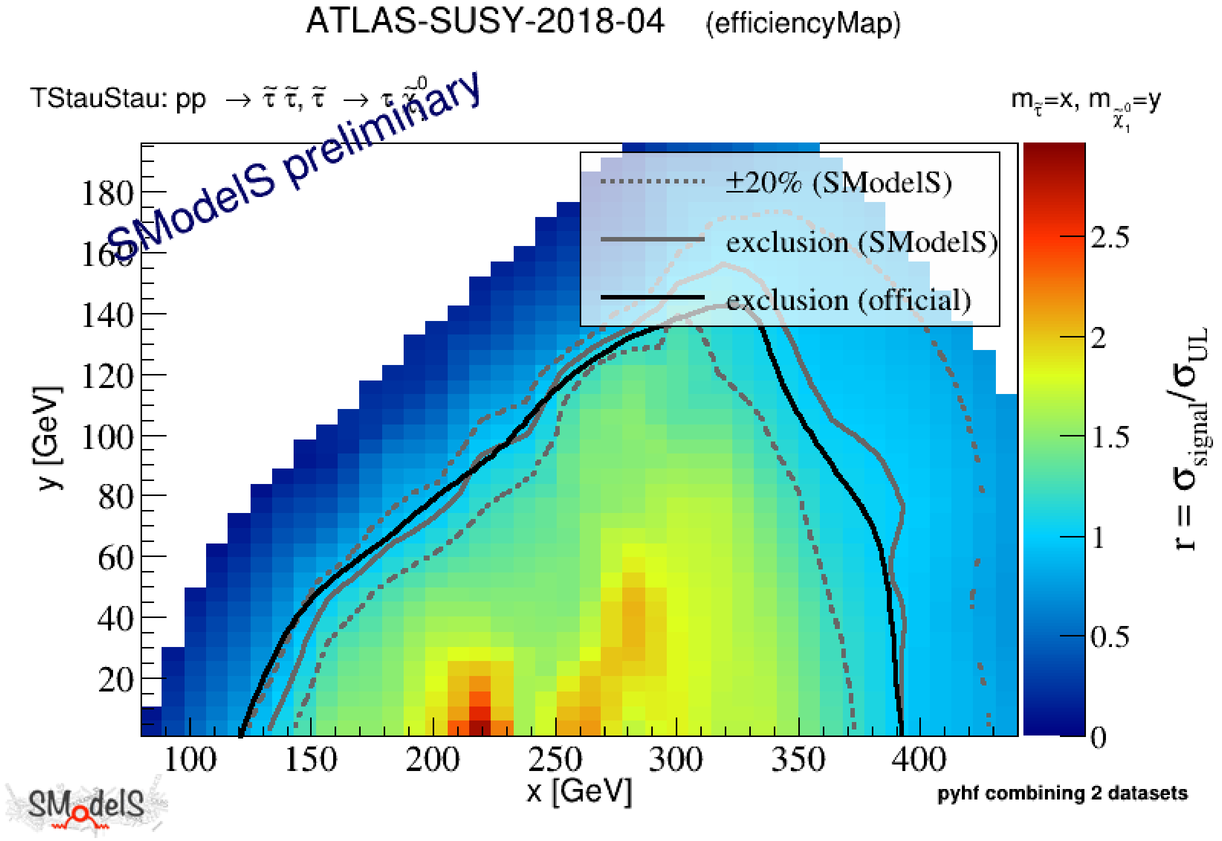




SUSY EWK 3L RPV analysis (ATLAS-CONF-2020-009): Exclusion curves as a function of mass and branching fraction to Z bosons

...and by theory

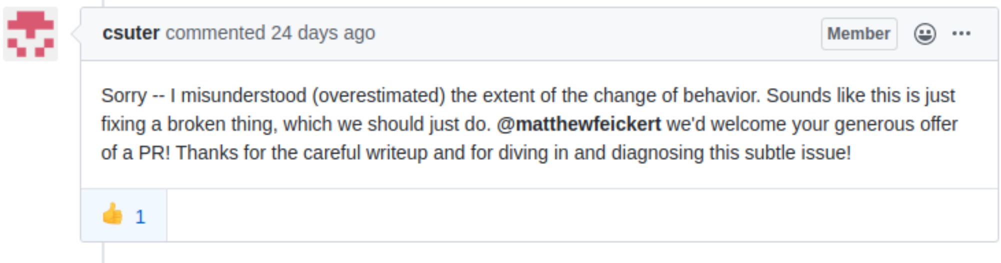
- SModelS team has implemented a `SModelS/pyhf` interface
  - tool for interpreting simplified-model results from the LHC
  - designed to be used by theorists
- Have produced comparison for *Search for direct stau production in events with two hadronic tau leptons in $\sqrt{s}$ = 13 TeV pp collisions with the ATLAS detector* (ATLAS-SUSY-2018-04) published likelihood
  - Compare simplified likelihood (`SModelS`)
  - to full likelihood (`pyhf`)

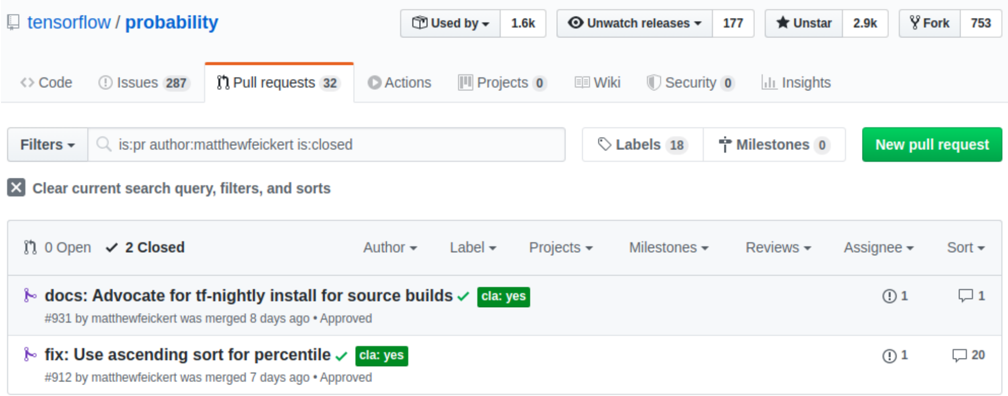


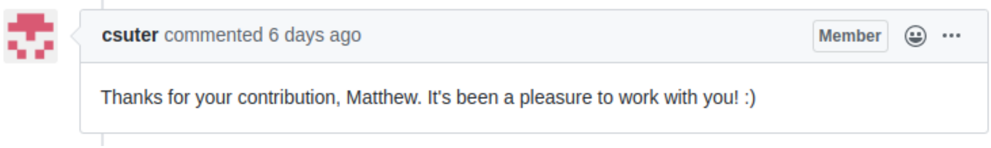
So here is one of our first reasonable validation plots. It's preliminary, the black line is ATLAS-SUSY-2018-04 official exclusion curve. The grey line is SModelS using `pyhf`, running over the published data. — Wolfgang Waltenberger, CMS/SModelS

Broader Impact: Upstream contributions

- In working to add `percentile` method across all backends (as part of toys in `v0.5.0`) discovered discrepancy between NumPy implementation and TensorFlow Probability (TFP)
  - Through research between NumPy and TFP source code found a bug in TFP!
  - Confirmed by dev team in discussion on GitHub Issue
  - Agreed with dev team I would write a PR, which was reviewed and merged in timely manner
- Along with Henry and Jim, now have upstream contributions to open source **directly originating** from IRIS-HEP work
- `pyhf` will **need this bug fix** in the next TFP release, and **thousands** of other projects will benefit
- Bonus: Continuing goodwill development







Roadmap for Year 3 Execution

In a word: Stability

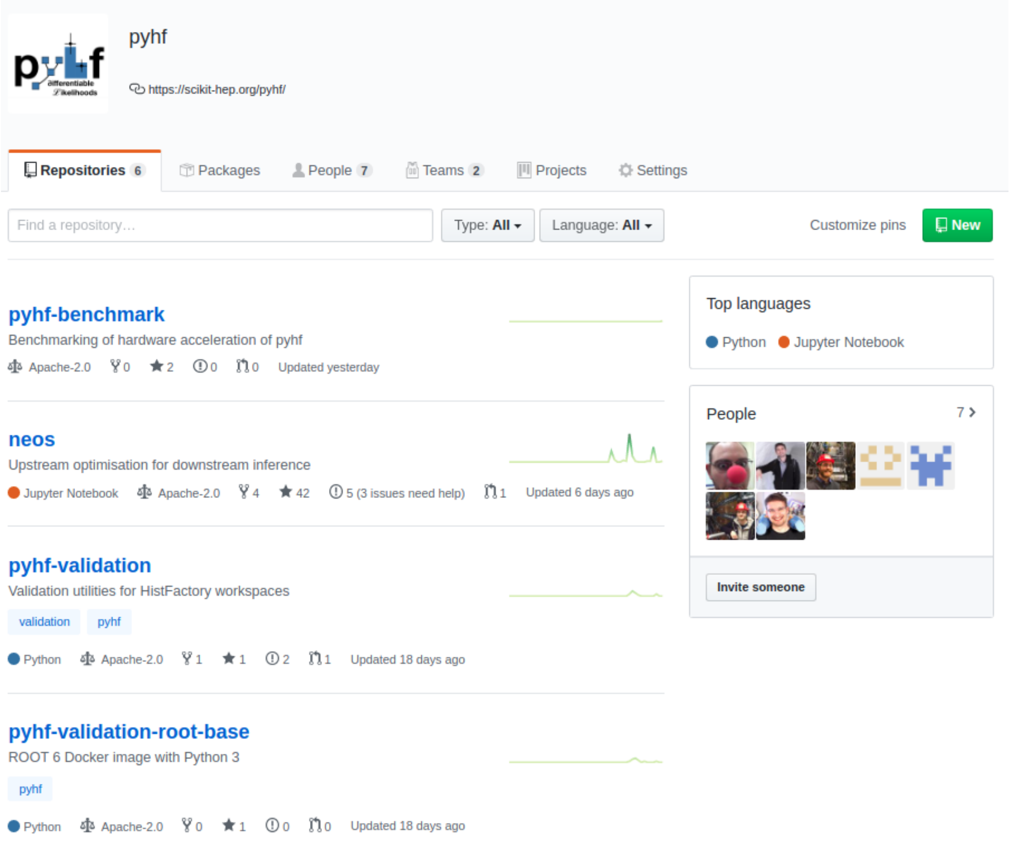
```
$ git diff setup.cfg
diff --git a/setup.cfg b/setup.cfg
index 7d082227..8b7f9b9a 100644
--- a/setup.cfg
+++ b/setup.cfg
@@ -1,6 +1,6 @@
 [metadata]
 name = pyhf
-version = 0.5.1
+version = 1.0.0
 description = (partial) pure Python HistFactory implementation
 long_description = file: README.rst
 long_description_content_type = text/x-rst
@@ -15,7 +15,7 @@ project_urls =
     Source = https://github.com/scikit-hep/pyhf
     Tracker = https://github.com/scikit-hep/pyhf/issues
 classifiers =
-    Development Status :: 4 - Beta
+    Development Status :: 5 - Production/Stable
     License :: OSI Approved :: Apache Software License
     Intended Audience :: Science/Research
     Topic :: Scientific/Engineering
```

Adoption by analyses

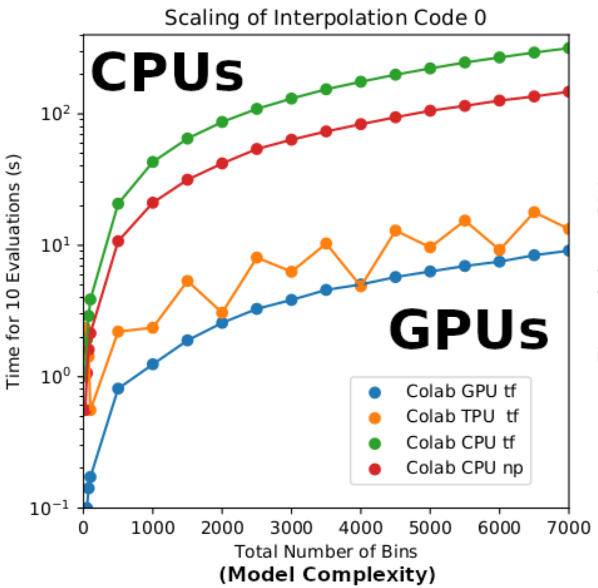
- Any analysis that wants to use `pyhf` for full Run 2 should be able to

Requirements:

- `pyhf` becomes mature in its feature set
  - Stat Config
  - Non-asymptotic calculators (toys in `v0.5.0`)
  - Norm factor expressions
- Validation across all backends against `HistFactory`
  - `pyhf` GitHub org setup to help streamline process
  - Reproduction of published analyses on HEPData
- Documented examples
  - Case studies
  - Public knowledge base (`pyhf` Stack Overflow)
  - Rosetta stone (and what can't be done) between `ROOT HistFactory` and `pyhf`



Benchmarking hardware acceleration



- Preliminary results (old) show hardware acceleration giving **order of magnitude speedup** for some models!
- Improvements over traditional
  - 10 hrs to 30 min; 20 min to 10 sec
- Hardware acceleration benchmarking important to find edges

IRIS-HEP Fellow: Bo Zheng

Fellowship dates: May - August 2020
Home Institution: Rice University

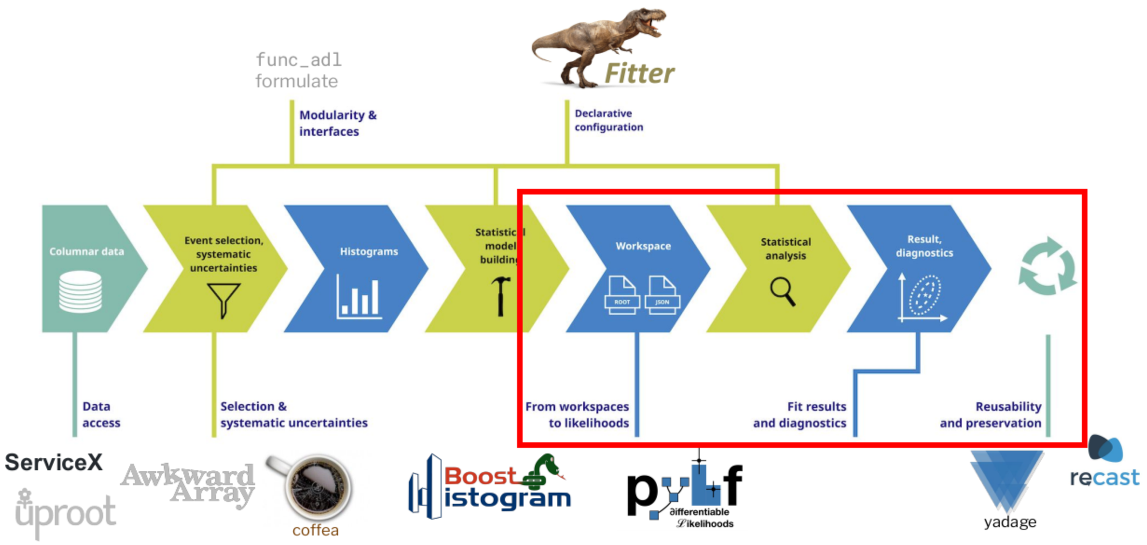
Christopher Tunnell
@AstroTunnell

I am happy to announce that @RiceCompSci student Bo Zheng got an @iris_hep Fellowship to work on benchmarking pyhf. As part of @Rice_D2KLab's RECODE initiative, we found academic internships for those who lost industry internships due to #COVID19. Win win. #interdisciplinary

11:10 AM · May 14, 2020 · Twitter Web App

8 Retweets **18** Likes

Integration into Analysis Ecosystems Pipeline



- Most obvious connections:
  - ServiceX: direct data transform and delivery
    - Illinois team dynamic between Ben and Matthew
  - `cabinetry`: general interfacing to other tools
    - c.f. Alex's poster from 2020 Poster Session for more details

`cabinetry` is a tool to build and steer (profile likelihood) template fits with applications in high energy physics in mind. It acts as an interface to many powerful tools to make it easier for an analyzer to run their statistical inference pipeline. An incomplete list of interesting tools to interface:

- ServiceX for data delivery,
- coffea for histogram processing,
- uproot for reading ROOT files
- for building likelihood functions (captured in so-called workspaces in RooFit) and inference:
  - RooFit to model probability distributions
  - RooStats for statistical tools
  - HistFactory to implement a subset of binned template fits
  - pyhf for a pythonic take on HistFactory,
  - zfit for a pythonic take on RooFit
  - MadMiner for likelihood-free inference techniques

Successful Application: Years 4/5

Reducing time to insight: Fitting as a service

`pyhf` HistFactory model spec is pure JSON: Very natural to use a REST web API for remote fitting!

1. `pyhf` installed on different clusters with GPUs around the world
2. User hits a REST API with JSON `pyhf` workspace as a request
3. `pyhf` fits the workspace on the cluster on demand
4. Returns fit results over REST API to user

```python
import requests
import json

# Send workspace to remote for fitting
request = requests.post(
    "https://www.endpoint.edu/fitting-with-pyhf", json=json.load(open("workspace.json"))
)
request.raise_for_status()

# Remote cluster fits the workspace with pyhf
# and sends user email when done

# User then retreives fit result
response = requests.get(
    "https://www.endpoint.edu/fitresult", json=dict(id=request.json()["id"])
)
response.raise_for_status()
print(json.dumps(response.json(), indent=4, sort_keys=True))
# {
#     "CLs_exp": [
#         0.07807427911686156,
#         0.17472571775474618,
#         0.35998495263681285,
#         0.6343568235898907,
#         0.8809947004472013
#     ],
#     "CLs_obs": 0.3599845631401915
# }
```

Analysis Reuse: `pyhf` JSON native to HEPData

- Growing number of analyses publishing full likelihoods to HEPData
- At the moment each likelihood is the collection of many individual signal patch files
- Introduce concept of "patchsets" to reduce all of this two two files:
  - Background only file
  - Signal patchset file
- Would use `hepdata-validator` to resolve all files to inline JSON
- Allows for entire likelihood to be natively supported in HEPData (no more tarballs required)


```yaml
likelihoods:
- type: histfactory
  name: RegionA
    workspace:
      name: background-only
      description: background-only workspace
      data_file: {$ref: BkgOnly.json}
      data_schema: https://scikit-hep.org/pyhf/schemas/1.0.0/workspace.json
    patchset:
      name: patchsets
      description: sets of signal patches for the background-only workspace
      data_file: {$ref: patchset.json}
      data_schema: https://scikit-hep.org/pyhf/schemas/1.0.0/patchset.json
```

Grand Challenge Integration

Analysis Systems Grand Challenge

Following up on Kyle's presentation yesterday

Grand Analysis Challenge

- End-to-end analysis optimization including systematics on a realistically sized HL-LHC end-user analysis dataset + observed limit & reinterpretation afterburner
    - Focus on vertical slice through tools with game-changing functionality while operating on a realistically sized analysis dataset
    - ~200TB for MC samples [maybe larger, 200TB was only data (see DC2 for details)]
    - Multiple analysis regions, cuts, histogramming specification, and systematic variations declared using cabinetry and func_adl specifications (as in a typical SUSY search for example)
    - ServiceX to perform event selection and deliver histograms for pyhf model
    - Optimize analysis by using automatic differentiation to compute d(Expected limit)/d(analysis parameters), which are back-propagated from from output of stats tool, through pyhf running in fitting service, back to ServiceX running at analysis facility, and through the event selection & histogramming code.
        - Demonstrates forward looking functionality (using autodiff technique that powers deep learning in a physics context and emerging “Differentiable Programing” paradigm) [see grad-hep, neos]
        - Replace “Graduate-student descent” with gradient descent
        - Requires multiple passes over the data (caching)
        - Requires distributed optimization / passing gradients across protocol
    - Once optimized: apply analysis “data” for observed limit and reinterpret efficiently using active learning [excursion]

ServiceX to `pyhf`

ServiceX to perform event selection and deliver histograms for `pyhf` model

- Should be relatively easy to translate from ServiceX output to `pyhf` JSON model, but probably don't want to
- Moving the translation from `pyhf` to `cabinetry` seems like a more robust solution
- `cabinetry` has ability to be a powerful tool, but to `pyhf` translation is most interesting
  - ServiceX to `cabinetry`: data delivery
  - `cabinetry` to `pyhf`: constructing of likelihood
- If useful, Matthew could join contribution efforts
- Alex has pointed out this is even mostly doable now with `TRExFitter`
  - ServiceX feeding histograms to `TRExFitter`
  - Convert XML to JSON with `pyhf xml2json`
  - Fit with `pyhf`

`pyhf`: Fitting as a service

Optimize analysis by using automatic differentiation to compute $d(\text{Expected limit})/d(\text{analysis parameters})$, which are back-propagated from from output of stats tool, through `pyhf` running in fitting service, back to ServiceX running at analysis facility, and through the event selection & histogramming code

- As already covered, fitting with `pyhf` can be scaled up on demand and run almost anywhere
  - Local machine, cluster, AWS
- `pyhf` being built on frameworks that automatically handle gradients allows for this to happen naturally
- Should get taken care of as a natural part of `pyhf` development

Summary

- **Accomplishments**
  - Published and preserved full likelihoods
  - Become hugely popular and adopted inside ATLAS
  - Establishing connections for growth with SModelS and HEPData
- **Year 3 Execution**
  - Reach stable API and `v1.0.0` release
  - Provide analysis support
  - Benchmark and profile hardware acceleration benefits
- **Vision for Year 4/5**
  - Globally deployed and scalable "fitting as a service" using REST web API
  - Have native support in HEPData for analysis preservation
- **Grand Challenge**
  - Integrate with `cabinetry` for ServiceX translation
  - Exploit fitting as a service + gradients for differentiable AS pipeline

Backup

HistFactory Template

$$\mathcal{P}\left(n_c, x_e, a_p | \phi_p, \alpha_p, \gamma_b\right) =$$

$$\prod_{c \in \text{channels}} \left[\text{Pois}\left(n_c | \nu_c\right) \prod_{e=1}^{n_c} f_c\left(x_e | \vec{\alpha}\right)\right] G\left(L_0 | \lambda, \Delta_L\right) \prod_{p \in \mathbb{S}+\Gamma} f_p\left(a_p | \alpha_p\right)$$

Use: Multiple disjoint channels (or regions) of binned distributions with multiple samples contributing to each with additional (possibly shared) systematics between sample estimates

Main pieces:

- Main Poisson p.d.f. for bins observed in all channels
- Constraint p.d.f. (+ data) for "auxiliary measurements"
    - encoding systematic uncertainties (normalization, shape, etc)

References

1. ROOT collaboration, K. Cranmer, G. Lewis, L. Moneta, A. Shibata and W. Verkerke, *HistFactory: A tool for creating statistical models for use with RooFit and RooStats*, 2012.
2. L. Heinrich, H. Schulz, J. Turner and Y. Zhou, *Constraining A_4 Leptonic Flavour Model Parameters at Colliders and Beyond*, 2018.

The end.