# HEP in the Cloud Computing and Open Science Era

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**Our job: extract as much information from experimental data** 

what we want

 $p(\text{theory}|\text{data}) = \frac{p(\text{data}|\text{theory})}{p(\text{data})}p(\text{theory})$ 

hep-ex

hep-ph/hep-th

### **Big Picture Goals**







**Our job: extract as much information from experimental data** 

what we want

- What's the best way to do this in our Big Science setting?
- How can we collaborate best across theory-experiment divide?

 $p(\text{theory}|\text{data}) = \frac{p(\text{data}|\text{theory})}{p(\text{data})}p(\text{theory})$ hep-ex hep-ph/hep-th

- **1.** The data is large:
- At a project level:

LHC: 1 EB today, O(30) EB HL-LHC (?) LSST: O(1) EB SKA: O(0.5) EB/year

At an analysis level:

routinely O(100) TB that analysis teams process as a small group - will be O(PB) how do we maintain explorative research?



[LHC Projections]

### 2. The data is unique:

### There is only one LHC / LSST / SKA / ...

- What data products are released to the public?
- How do we ensure rigorous analysis if public?





Square Kilometer Array

Robin Observatory / LSST

### / ... to the public? sis if public?



LHC

### 3. The data is complex:

### In HEP:

- complex generative history across many energy scales
- heterogeneous detectors (not a single 100Mpx sensor / image)





$$p(x|\theta, \theta_{\text{nuis}}) = \iiint dz_d dz_h dz_p p(x|z_d, \theta_{\text{set}})$$

high-dimensional integrals: needs MC





ensor)  $p(z_d|z_h, \theta_{geom}) p(z_h|z_p, \theta_{pQCD}) p(z_p|\theta)$ 



- 3. The data is complex:
- analysis heavily simulation-driven
- heavy reconstruction from raw  $\rightarrow$  physics data
- exceeds data volume & resources of actual data
- extremely software-reliant (O(M) LoC)

- can we prioritize human time over computing?  $\rightarrow$  interactive analysis



### Analyzing any part of the data is very expensive human resources-wise:

• if we invest so much?  $\rightarrow$  how do we exploit these analyses maximally?





### **Technical:**

### 1. Machine Learning

- powerful & creeps into every aspect of scientific workflow
- 2. Cloud Computing & Heterogeneous Future Present
  - anybody can get access to vast amounts of compute

### can we use these to create new ways to push our science forward?

# raises questions of how analysis details are disseminated (th $\leftrightarrow$ ex)

# new requirements on hardware / software (GPU, CPU, TPU, Dataflow,...)





### **Political:**

### 1. Open & FAIR Data

publicly funded research must be accessible

### 2. Reproducibility

Uniqueness of data & analysis → special responsibility

### But how does this work at Big Science scale? usually not focus of those discussions. are there useful ways to interpret these buzzwords?

### (Open) Data Analysis at LHC Scale

### **Open Data**

### **Significant Development in HEP**

### **All LHC Experiments agree to** release data publicly.

including software to analyze rigorously

• (e.g. systematic uncertainties)

### Intent:

 foster more interdisciplinary collaboration (e.g. ML, Theory, cross-experiment R&D, ...)



### **Open Data: a growing Ecosystem**

New paradigm for HEP, we're learning.

### **CERN:**

 develop supporting cyberinfrastructure (Open Data Portal, Zenodo)

### **Experiments:**

how to release data to outsiders

### **Theorists:**

- develop data analysis expertise
- own ecosystem of tools

**Can you scale to realistic analysis?** 





### ZEOCO

**Docs** » Documentation » Datasets

+

### **CMS Open Data and the MOD HDF5 Format**

Starting in 2014, the CMS Collaboration began to release research-grade recorded and simulation datasets on the CERN Open Data Portal. These fantastic resources provide a unique opportun researchers with diverse connections to experimental particle phylics world to engage with cu edge particle physics by developing tools and testing novel strategies on actual LHC data. Our making portions of the CMS Open Data available in a reprocessed format is to ease as best as possible the technical complications that have thus far been present when attempting to use O Data (see also recent efforts by the CMS Collaboration to make the data more accessible).

To facilitate access to Open Data, we have developed a format utilizing the widespread HDF5 format that stores essential information for some particle physics analyses. This "MOD HDF5 Format" is currently optimized for studies based on jets, but may be updated in the future to su other types of analyses.

To further the goals of Open Data, we have made our reprocessed samples available on the Zer

Docs » Home

### Welcome to EnergyFlow





EnergyFlow is a Python package containing a suite of particle physics tools:

### [CMS OD] / [Thaler et al.]

[ATLAS OD]

### **Benchmark Example: CMS Open Data Higgs → 4I Analysis**

### **Anatomy:**

- 70TB / 25k files
- **Data, Background + Signal Simulation**





 C++ based data analysis (CMSSW) (event selection + feature comp)

The physics is there: but requires large-scale compute

**Question: How quickly can we analyze the data?** 



[A. Geiser, N. Jomhari]



### **Benchmark Example: CMS Open Data Higgs** $\rightarrow$ 4I Analysis

Fast enough to do 70TB analysis in real-time.

 Open Data as a tool for R&D to develop interactive analysis systems @ HL-LHC



In [2]:		json matplotlib.pyplot as p plotting.plotnb as plo	
In [3]:	figure	≈ plotnb.setup_figure	0
		Figure	1
		0.0 fb <sup>-1</sup> (7 TeV), 0.0 f	b <sup>-1</sup> (8 TeV)
	25 25 20 20 15	CMS Open Data	$\begin{array}{c} \longrightarrow \\ \text{Data} \\ \hline m_{\text{H}} = 125 \\ \hline ZZ \rightarrow 4I \\ \hline ZY^* + X \\ \hline t \\ \hline t \\ \end{array}$
	10		
	0 <sup>1</sup> 11:2	80 100 120 5:11	) 140 160 m <sub>4l</sub> Re

(slightly sped-up version) <sup>15</sup>

### [KubeCon 2019]

# Answer: 5 minutes with cloud computing techniques $\rightarrow$ >1Tbps throughput



[R. Rocha (CERN IT), LH (ATLAS), C. Lange (CMS)]

CERN



### 25k files $\rightarrow$ 25k cores across 10 clusters

Uses Kubernetes to schedule work

- cluster system originated in Google
- can handle service, batch, interactive work
- containers: easy to deploy HEP s/w

### **Cloud characteristic: only CPUh matters** 25k CPU @ 5 minutes = 8 CPU @ 10d

(not true for physicist-hours, try to minimize time to do physics)

### individual user can get this on-demand (as long as you can pay)



### Storage 70 TB (S3)



### **Cloud-native Clusters (25k cores)**





### **Interactive Visualization (Jupyter)**





### **Bringing the technology to HEP**

- push to go beyond standard batch/grid picture
- crucial for maintaining physics-driven/explorative data analysis at next phase of physics experiments: technology choices matter.



# → Analysis Facilities / Science Platforms (cf: PUNCH4NFDI / IRIS-HEP)



### **Bringing the technology to HEP**

### In production:

- Grid-scale ML on GPUs (ATLAS)
- WLCG for volunteer computing (folding@home, 50k cores)

### Key: Containers allowing user-defined s/w environment





<b>Rank</b> Overall		<b>Users</b> Active	<b>Users</b> Total	Change 24hr	Change 7days	<b>Points</b> 24hr Avg	<b>Points</b> Update	<b>Points</b> Today	
1		1,200	2,000			14,868,491,388	1,629,724,245	4,966,192,700	33,501,103,7
2		26,910	105,550				595,799,121	1,704,651,305	
3			23,837			1,209,843,224	154,586,434	445,858,938	2,809,558,2
4	PC Master Race - PCMR	7 746	48 847		+2 ▲	1 056 141 646	114 336 343	329 271 240	2 302 740 3
5	CERN & LHC Computing	145	214	+1 🔺	+7 🔺	794,993,726	103,003,621	301,591,243	1,862,010,9
6	NVIDIA Corp	46	74		+6 🔺	943,008,120	83,172,296	236,982,978	1,861,543,4
7	folding@evga	1,003	19,610			644,096,447	78,377,970	230,860,571	1,477,464,8
8	VMware	769	1,696		+2 🔺	450,549,575	56,778,849	172,933,812	1,081,783,0



### Is dumping PB of data open enough?

### **Beyond Open Data**

**Open Data: with great freedom comes great responsibility** 

- allows looking at uncovered corners of the dataset (comp. feasible)
- but: cost of developing an analysis in full rigour is enormous

Are there other ways data can be "open"? → instead of the source data, release the result data

What should we release?

many types of results

**Event Counts, post-fit parameters p-value scans, ....** 

### es great responsibility ers of the dataset (comp. feasible) s *in full rigour* is enormous



### **Remember:**



### **Likelihood Principle:** Full experimental information captured in the likelihood $p(x \mid \theta)$ !

- all analysis details are reflected in it
- most other types of results are derived from it.

Best, almost lossless summary of the measurements performed by a data analysis

 $p(\text{theory}|\text{data}) = \frac{p(\text{data}|\text{theory})}{p(\text{data})}p(\text{theory})$ 



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### **1st PHYSTAT workshop:**

ORGANISATION EUROPÉENNE POUR LA RECHERCHE NUCLÉAIRE CERN EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH

## preserve the likelihood! universal concept applicable to a broad set of experiments (also beyond HEP)

WORKSHOP ON CONFIDENCE LIMITS

CERN, Geneva, Switzerland 17–18 January 2000



**PROCEEDINGS** Editors: F. James, L. L

### **Massimo Corradi**

CERN 2000–005 30 May 2000

Sur 2000 26

It seems to me that there is a general consensus that what is really meaningful for an experiment is *likelihood*, and almost everybody would agree on the prescription that experiments should give their likelihood function for these kinds of results. Does everybody agree on this statement, to publish likelihoods?

### Louis Lyons

Any disagreement ? Carried unanimously. That's actually quite an achievement for this Workshop.

GENEVA 2000

### Likelihoods

### How do we archive likelihoods?

### Not straightforward: $p(x \mid \theta)$ could by anything! (Open World)

**Obvious Candidate: RooFit workspaces** 

- Key development in early LHC stats
- designed as "sharable data product"

### But:

- opaque, binary format
- tied to specific data analysis tool



### What goes in a Workspace



The workspace stores the full probability model and any data necessary to evaluate the likelihood function

- it is the code necessary to evaluate the likelihood function at an arbitrary point in the parameter space. It is not a big table of likelihood values!
- we are using the same ROOT technology that the LHC experiments are using to save their data
- well supported, and supports "schema evolution" / backwards compatibility
- the probability model also allows you to generate toy data for any given parameter point
  - necessary for frequentist methods, goodness of fit, coverage)
- PDFs and functions can be extended by the user (source stored in workspace)

I will show some visualization of real-life LHC probability models. Let's start with a simple example:



[K. Cranmer @ DESY 2010]



### Likelihoods

 $p(x \mid \theta)$  could by anything... but in reality they're not!

### For LHC a very large fraction of analyses use standardized binned likelihood functions built from data counts + simulation-derived templates

SUSY

**ATLAS: HistFactory CMS: HiggsCombine**   $f(\boldsymbol{n}, \boldsymbol{a} \mid \boldsymbol{\eta}, \boldsymbol{\chi}) =$  $c \in \text{channels } b \in \text{bins}_c$ 





SM

**Exotics** 

700 800



### **HistFactory**

# Fixed Template (Closed World) simplifies likelihood problem:

- archive template ingredients (pure tabular data)
- template math defined independent of implementation - not tied to s/w



25

### pyhf - fast, pythonic HistFactory

Statistics tool with likelihoods as vectorized computation based on ML libraries

- run on heterogenous hardware (TPU, GPU)
- automatic differentiation for exact  $\nabla_{\theta} p(x \mid \theta)$

### **Full suite of HEP inference algorithms** Profile Likelihood, Asymptotics & Toys







[LH, Feickert, Stark]

### pyhf - fast, pythonic HistFactory

### Nice:

- adoption across theory-experiment divide
- developed at LHC, but used in larger range of settings

Chargeo	Lepton Flavor Violation at the EIC	arXiv: 2102.06176
incenzo Ci 1d Bin Yan	rigliano, Kaori Fuyuto, Christopher Lee, Emanuele Mereghetti,	
Theoretical : E-mail: c	Division, Los Alamos National Laboratory, Los Alamos, NM 87545, U.S.A. acceptance, obtained from the yields of the two validation regions gi	ven in Ref. [63]. We
emereghe	then used signal and background events in a likelihood analysis using	
	$BR(t \to qe\tau) \le 2.2 \cdot 10^{-4}.$	(6.10)
	ity of Future Hadron Colliders to Leptoquark Pair tion in the Di-Muon Di-Jets Channel	arXiv: 1911.04455 <b>FCC</b>
B. C. Allana	${ m ach}^1,  { m Tyler}   { m Corbett}^2,  { m Maeve}   { m Madigan}^{{ m a},1}$	
<sup>1</sup> DAMTP, Univ	$r_{\rm r}$ fixed $\mu$ . The upper limit at	95% CL on $\mu$ is then give

### nt divide ger range of settings



Rodolfo Capdevilla,<sup>a,b</sup> Fede

diction in  $SR_{1t}^{\gamma}$  has been reduced to 10%. The discovery significance is evaluated from the expected discovery *p*-value, while limits are set at 95% CL using the CLs method [91] with the pyhf software package [92, 93]. Additional lines show the sensitivity of the conservative scenario inflating the background estimates by an order of magnitude. The sensitivity is

### pyhf byproduct: JSON serialization

### **Plain-text format for HEP Workspaces**

(for those using HistFactory template)

### **Ubiquitous format: JSON**

- readable in any language
- independent of s/w implementation

### Ideal for long-term archival of likelihoods $\rightarrow$ as promised in 2000

### **Expected Bkg** observed ... Signal Nominal **Systematic Variations**

```
"channels": [
     { "name": "singlechannel",
       "samples":
        { "name": "signal",
          "data": [7.0, 2.0],
          "modifiers": [ { "name": "mu", "type": "normfactor", "data": null} ]
        { "name": "background",
          "data": [50.0, 60.0],
          "modifiers": [ {"name": "uncorr_bkguncrt", "type": "shapesys", "data": [5.0,12.0]} ]
],
"data": {
    "singlechannel": [50, 60]
},
"measurements": [
    { "name": "Measurement", "config": {"poi": "mu", "parameters": []} }
```

[LH, Feickert, Stark]



### Likelihood Preservation in ATLAS

### **ATLAS first experiment to publish full likelihood** stored on public archive as citable data product: HepData DOI continuation of long-term effort (cf. simplified l'hoods in CMS) best information we have even within experiment full set of systematics → global fits / combinations / ...



[N. Wardle et al]



9 JANUARY, 2020 | By Katarina A



With full likelihood functions, theorists can calculate how well their theories fit the data collected by the detector "at a completely different level of reliability and precision," says Kraml.

To understand just how much more sophisticated and complex the analysis becomes, she says, consider the difference between a simple song and a full orchestral symphony.









### DOI 10.17182/hepdata.90607.v3





DOI 10.17182/hepdata.91214.v3

### DOI 10.17182/hepdata.98796.v2











### Let's reproduce this result! **Two separate measurements:**

### 1. 3 Signal region + 6 Control regions 59 source of system. uncertainties **8 Source of Background events**

2. 4 Signal region + 5 Control regions 66 source of system. uncertainties 8 Source of Background events

### Theory: 130 SUSY models

### **Measurements overlap:** take most sensitive result

### **Demo: reproduce full contour (260 CLs)** for simplified SUSY model using cloud APIs auto-scaling, distributed statistics



**User Session** 

 $L(\theta, \theta_{\text{nuis}}) = p(x_{\text{obs}} | \mu s(\theta) + b(\theta_{\text{nuis}}))$ 

send likelihood

get results

$$CL_{s}(\theta)$$



**Cloud Fitting Service** 



# Demo





(Cost: 0.05\$)

### pyhf - with functions as a service

### As with Higgs example:

- can offload heavy computation to cloud cost only per CPUh scale to hundreds of (private) cores within seconds
- Here: "Fitting-as-a-service": user only needs a URL can optimize hardware for stat. analysis.

### **Related: ML-as-service**

 Investigated for fast FPGA-based inference (Trigger, Reco, ...)

# Open Data provides access to LHC data: but now a more refined product.



[J.Ngadiuba, D. Rankin]





### Hold on, why so restrictive?

(just reproducing things is boring)
### Reinterpretation

## Did we over-correct from Open Data? Open Likelihood is great for

- reproducing results
- $\rightarrow$  but not enough to study new theories

combination with other measurements wrt. to same theory ("global fits")

# Main Concern creating new analyses internally & externally (w/ Open Data)

### Human resources for

- analysis design
- background estimation
- systematic analysis

### Can we maybe reuse the analysis we already have?





### Reinterpretation

## Increasing coverage of data space as LHC progresses.

It's likely that a analysis already did all the hard work for us

Not optimized for new theory but can be quite sensitive





### Reinterpretation





### "Original Likelihood"







• remove old signal • compute new signal • inject into likelihood • run stat. analysis



### "Likelihood Patch" from RECAST

"Recasted Likelihood"



Simple/Obvious Idea: whats the problem?

- Need to be able to compute new signal component
- Need an archived, but operational version of the analysis
  - ready to be re-run if needed
- "reuse" much more powerful than "reproducibility"









### **Analysis Preservation**

capture software capture scripts templates how to use package software the software itself in system-indep format (all dep.)

In ATLAS, we provide common infrastructure to make this easy

- automation for software archiving via containers
- workflow language to capture physics logic
- requirement now for across BSM program

Similar efforts across many data-intensive sciences:



capture workflow

correct sequence of steps for analysis pipeline







which will be automatically deployed to any execution environment.

### From Cartoon to reality:







### Used in cross-cutting summary analyses w/ multiple analyses

- Dark Matter models at the LHC
  SUSY reinterpretations
  - RPC-RPV Combination:  $\tilde{g} \rightarrow tt \tilde{\chi}_{..}^{"}(\rightarrow tbs) / \tilde{g} \rightarrow tbs, m(\tilde{\chi}_{..}^{"})=200 \text{ GeV}, bino-like \tilde{\chi}_{..}^{"}$ 3000 m(g) [GeV] **ATLAS** Preliminary 2800 — RPC ≥ 3 b-jets √s=13 TeV, 36.1 fb<sup>-1</sup> — RPC 0L 7-11j 2600 **RPV 1L** -⊙- Expected **2400** Observed 95% CL limits 2200⊢ -0-2000⊢ 1800⊢ **1600**∃ 1400⊢ **1200** ⊢ 1000<sup>t</sup> RPC  $10^{-3}$ 10<sup>-2</sup> 10<sup>-1</sup> ^<sub>323</sub>  $10^2$  10 1  $\tilde{\chi}_1^0$  lifetime [ns]  $10^{-1}$   $10^{-2}$  0.1 0.3 0.7 0.9  $\text{BR}(\widetilde{g} \to \text{tbs})$

**RPV SUSY** 



### **Institutional Support**

# **CERN** investing in infrastructure to systematically archive and re-run analyses on using cloud technologies



Archive



Re-run



### **Once we gain experience: Open Data at a higher abstraction level** allow external researches to query LHC wrt. to new theories





### Theory space is large, LHC is not sensitive everywhere. With streamlined reinterpretation, use ML to identify interesting models



### Now being tested in ATLAS - stay tuned! [P. Rieck, P. Gadow, J. v. Ahnen, I. Espejo +]

### Outlook

## HEP & other big science have unique challenges due to scale

### **Recent trends in IT, Data Science, ML bring us new tools** possibility to fundamentally rethink how we approach analysis foundation of HL-LHC analysis & computing is defined now (join!)

- $\rightarrow$  PB-scale interactive analysis?
- Technology can drive physics reach

### **Open Data, Reproducibility: How can we fill the buzzwords with life?** LHC-wide policy: growing community & ecosystem of external tools **Open Likelihoods: release the best info we have**

- **RECAST:** reuse vs just reproduce