Fair Universe 2024: HiggsML Uncertainty Challenge

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Background on Fair Universe Project

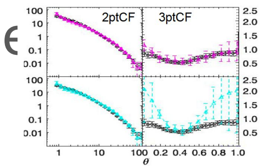
- 3 year US Dept. of Energy, AI for HEP project. Aims to:
  - Provide an open, **large-compute-scale AI ecosystem** for sharing datasets, training large models, fine-tuning those models, and **hosting challenges and benchmarks.**
  - **Organize a challenge series**, progressively rolling in tasks of increasing difficulty, based on novel datasets.
  - Tasks will focus on **measuring and minimizing the effects of systematic uncertainties** in HEP (particle physics and cosmology).
- Broad team in HEP, ML and computing involved in several previous challenges and benchmarks for HEP (e.g. HiggsML and TrackML, LHC Olympics, Fast Calorimeter Simulation Challenge) and wider (e.g NeurIPS competition track, MLPerf HPC); as well as Uncertainty aware learning in HEP

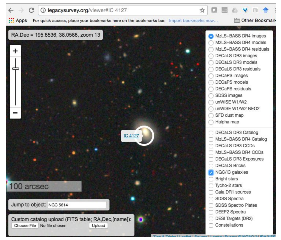
Measuring and minimizing the effects of systematic uncertainties in HEP

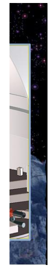
Bias and uncertainty in the fundamental sciences

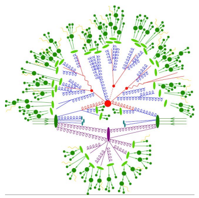
Theory into Simulations

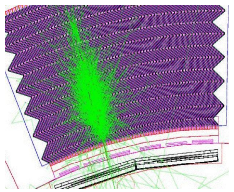
- Estimate Systematic Uncertaintie

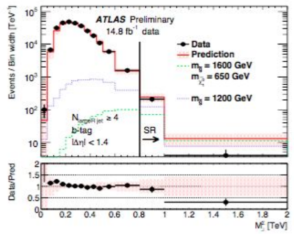


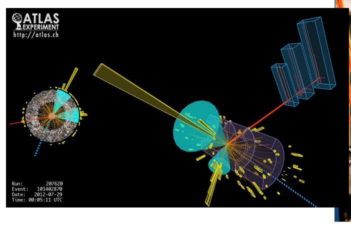


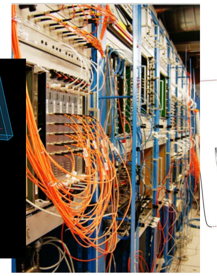


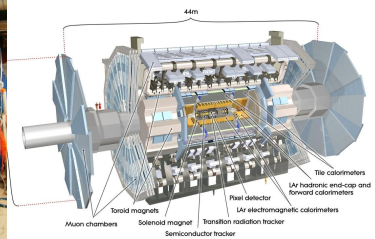










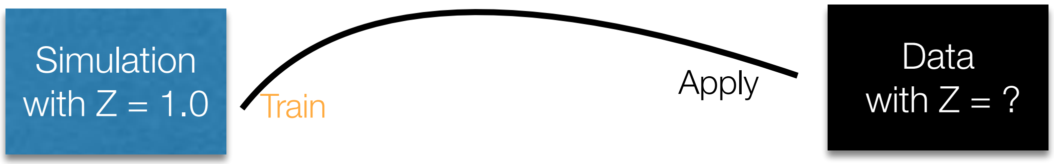


Exp/Obs reconstruction

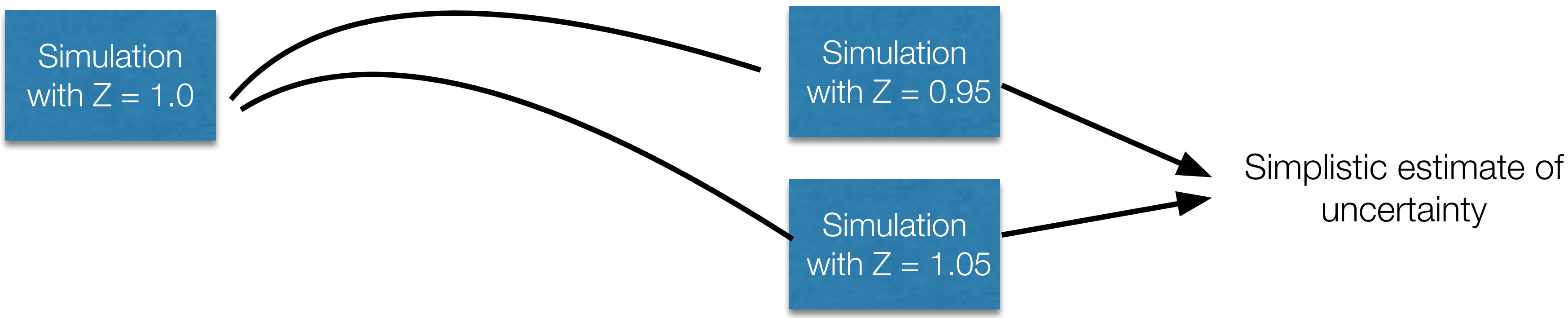
Differences between simulation and data can bias measurements

Bias and uncertainty in ML in the fundamental sciences

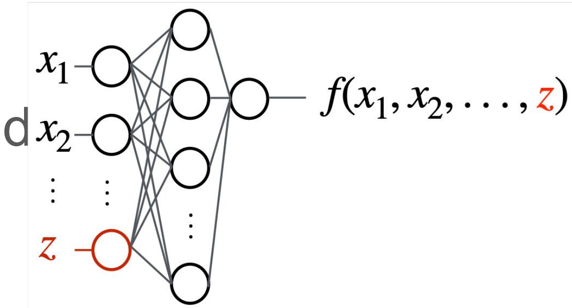
- ML methods in HEP are often trained based on simulation which has estimated systematic uncertainties (“Z”)
- These are then applied in data with the different detector state Z=?



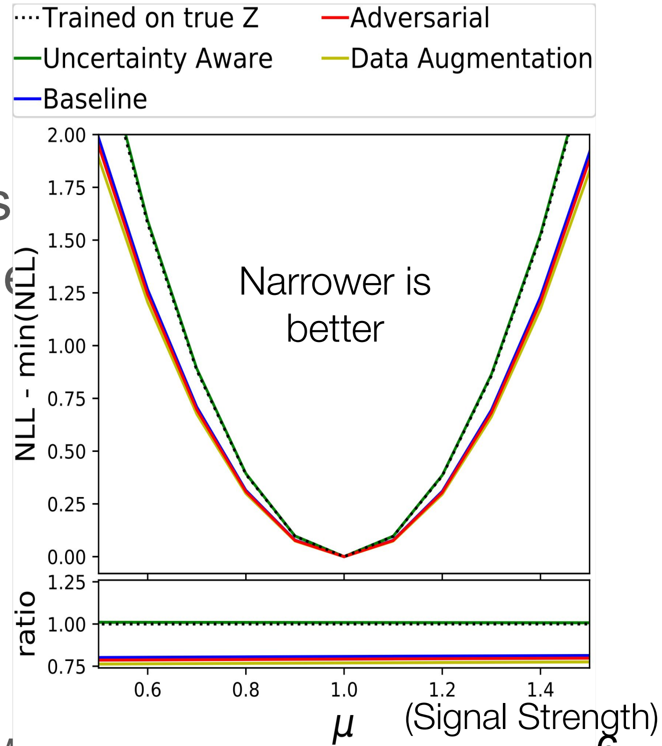
- Common baseline approach: Train classifier on nominal data (e.g. Z=1) and estimate uncertainties with alternate simulations. Shift Z and look at impact or perform full profile likelihood



Increasingly sophisticated approaches

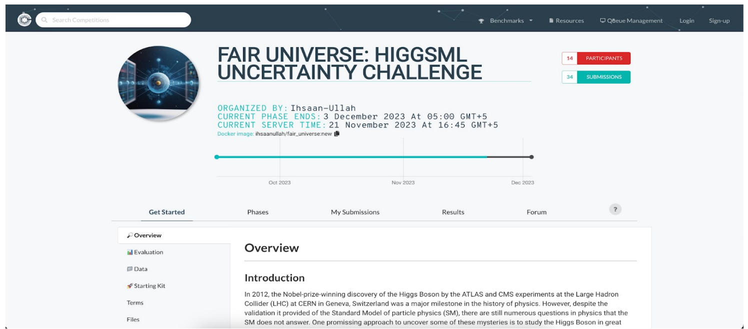


- Several focussed on decorrelation, e.g. augmentation; ad… tangent propagation etc.
- "pivot" Louppe, Kagan, Cranmer : arXiv:1611.01046
- "Uncertainty-aware" approach of Ghosh, Nachman, Whiteson PhysRevD.104.056026
  - Parameterize classifier using Z
  - Measured on "Toy" 2D Gaussian Dataset and datas… *Challenge* modified to include systematic on tau-ene…
  - Performs as well as classifier trained on true Z
- Other novel approaches e.g. (not comprehensive)
  - Inferno: arxiv:1806.04743
  - Direct profile-likelihood: e.g. arxiv:2203.13079



Progress requires new datasets, metrics, and platform

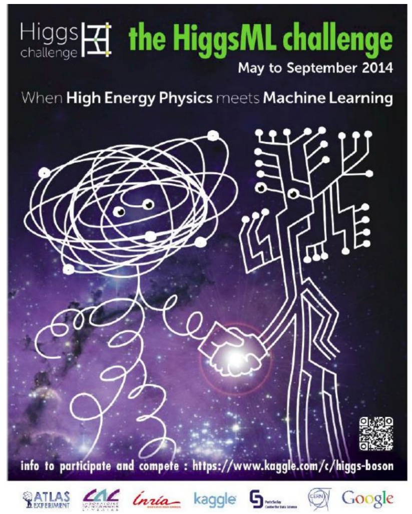
- Uncertainty-aware papers demonstrated on single systematic uncertainty, with limited data
- Original HiggsML dataset too small for ambitious approaches (systematic uncertainty small compared to statistical uncertainty)
- How to scale methods to many values of Z? (training difficulty increases, profiling approach used is expensive)
- Can faster methods allow for directly evaluating profile likelihood?
- Need for novel metrics to evaluate uncertainty determination for such methods



Organize a challenge series, progressively rolling in tasks of increasing difficulty, based on novel datasets

Fair Universe: HiggsML Uncertainty Challenge

- Extension of previous HiggsML challenge from 2014 (a classification problem for Higgs decaying to Tau leptons based on final state 3-momenta and derived quantities):
  - 30 features : l,h,MissingET,up to 2 jets, and high level quantities like transverse masses
- Dataset : HiggsML 2014 data set on CERN Open Data portal doi:10.7483/OPENDATA.ATLAS.ZBP2.M5T8
- ⇒new Fair Universe dataset, with following improvements
  - Instead of ATLAS G4 simulation, use Pythia LO + Delphes
  - Numbers of events 800.000⇒ >50 millions
  - Parametrised systematics (Nuisance Parameters) :
    - Tau Energy Scale : on had Tau Pt (and correlated MET)
    - Jet Energy Scale (and correlated MET impact)
    - additional randomised Soft MEt
    - background normalisation
    - W background normalisation (a subdominant poorly constrained BKG)



- Task : given a pseudo-experiment with given signal strength (==amount of signal), provide a Confidence Interval on signal strength

Pseudo-experiments

Test Dataset

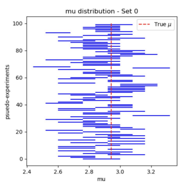
$\{\mathbf{x}, \mathbf{w}\}$

Create pseudo experiments for each test cases

$\{\mathbf{x}, \mathbf{w_1}\}$, w_1 = Pois (w)

Case 1

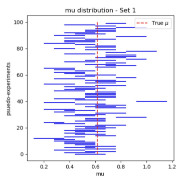
$\{NP\}=\{NP\}_1$ $\mu = \mu_1$



$\{\mathbf{x}, \mathbf{w_2}\}$, , w_2 = Pois (w)

Case 2

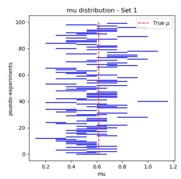
$\{NP\}=\{NP\}_2$ $\mu = \mu_2$



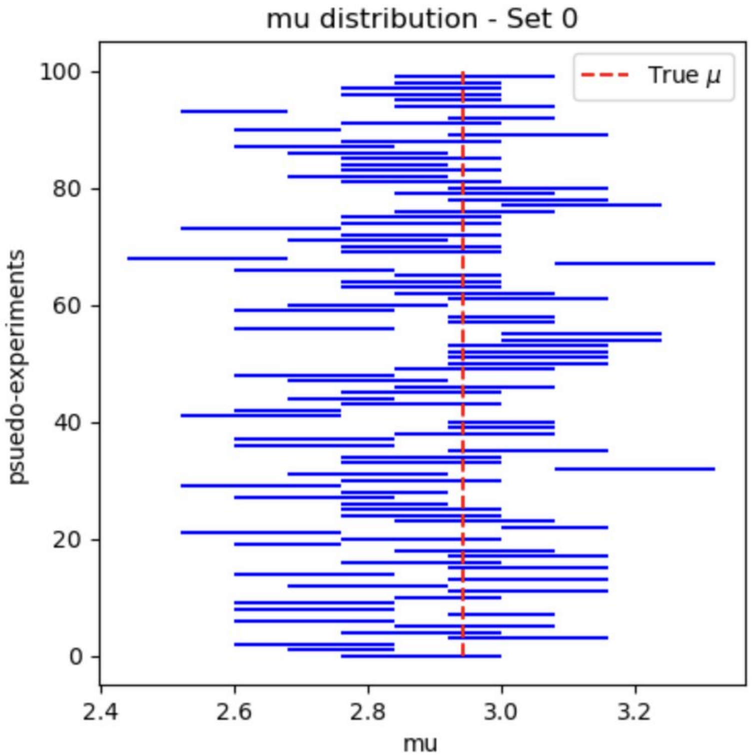
$\{\mathbf{x}, \mathbf{w_N}\}$, , w_N = Pois (w)

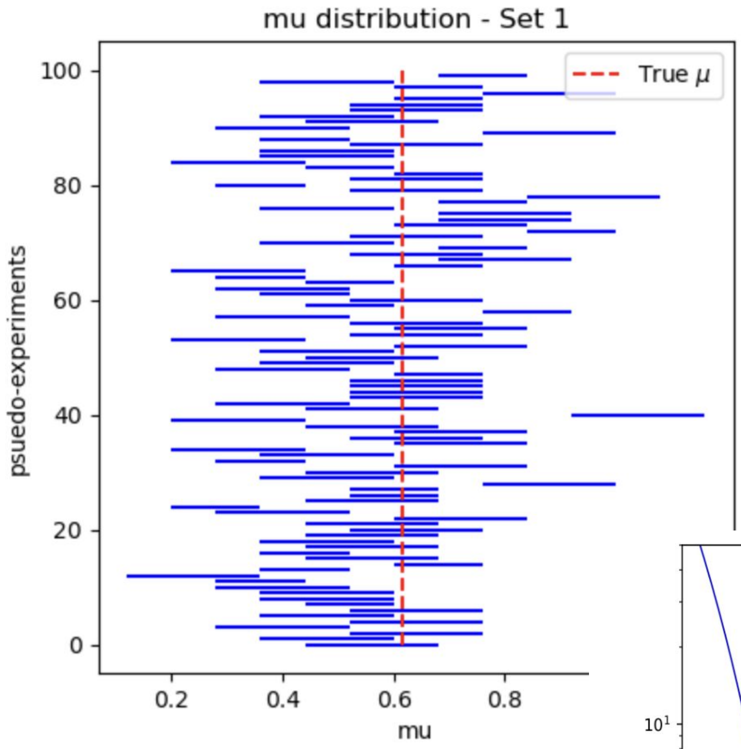
Case N

$\{NP\}=\{NP\}_N$ $\mu = \mu_N$

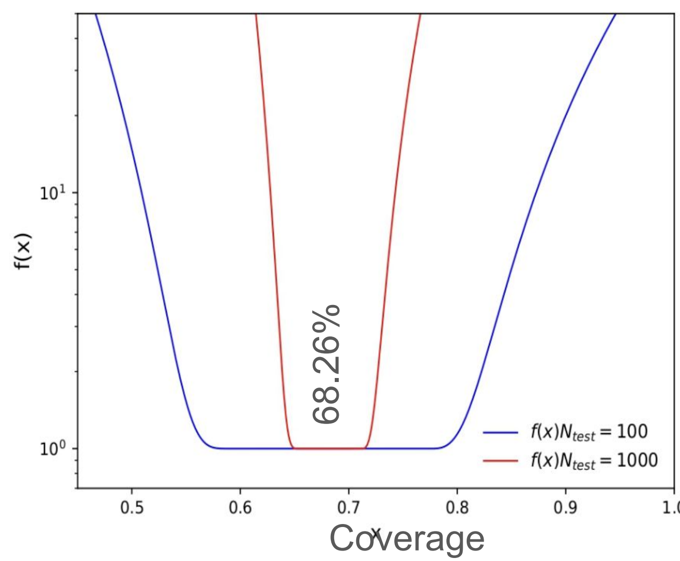


Coverage evaluation





Coverage penalisation function



score : <CI length> x coverage penalisation

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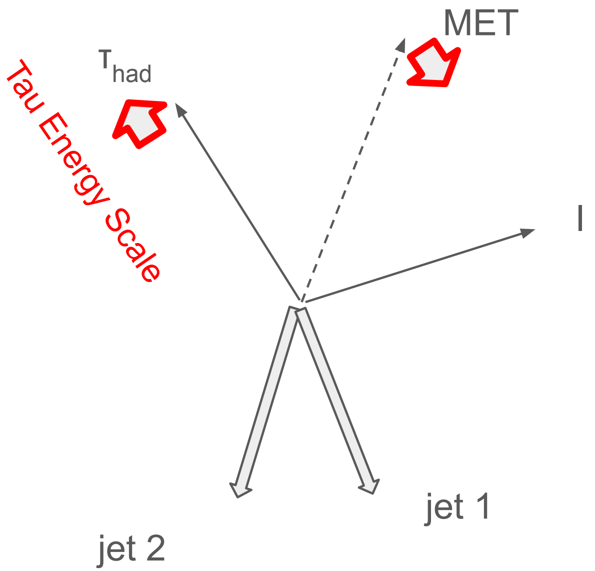
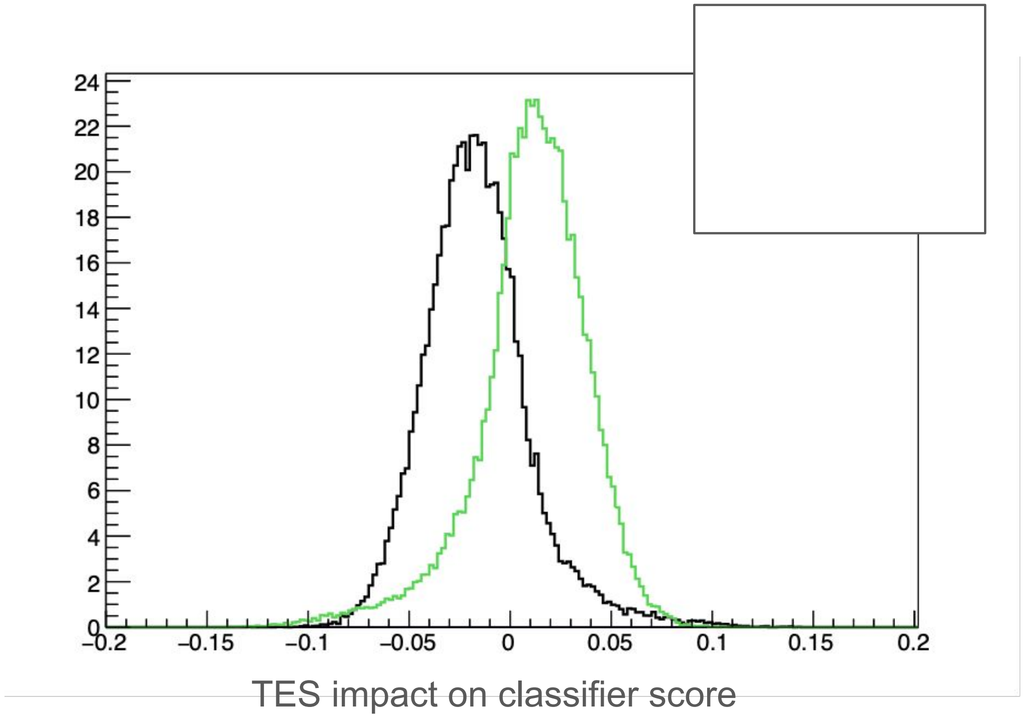
Task:				Fact Sheet Answers	Higgs Uncertainty Challenge			
#	Participant	Entries	Date of last entry	Method Name	Quantile Score	Interval	Coverage	Detailed Results
1	ragansu	30	2024-01-22	Histogram_10	**1.45**	0.226	0.57	
2	ragansu	30	2024-01-22	One_bin NLL	**1.07**	0.333	0.57	
3	laurensslu	20	2023-12-01	cheat7	**0.68**	0.504	0.63	
4	laurensslu	20	2023-12-01	cheat7	**0.61**	0.544	0.68	
5	laurensslu	20	2023-12-01	cheat4	**0.31**	0.732	0.61	
6	laurensslu	20	2023-12-01	cheat4	**0.16**	0.852	0.71	
7	laurensslu	20	2023-12-01	Cheat2	**-0.44**	1.55	0.62	
8	laurensslu	20	2023-12-01	Cheat2	**-0.74**	1.375	0.55	
9	ragansu	30	2024-01-22	tes_finder	**-0.95**	1.124	0.54	
10	laurensslu	20	2023-12-01	Cheat2	**-1.59**	1.325	0.53	
11	Ihsan Ullah	4	2024-01-18	Sascha sys aware 8	**-2.69**	0.329	0.47	
12	Rafał Masełek	10	2023-12-01	1binNLL	**-2.9**	1.233	0.5	
13	ihsanchalearn	16	2023-12-18	1 bin NLL	**-2.9**	1.233	0.5	
14	Rafał Masełek	10	2023-12-01	1binNLL	**-2.9**	1.233	0.5	
15	ihsanchalearn	16	2023-12-18	Sascha sys aware 8	**-3.01**	0.33	0.46	

Systematic parameterisation

Systematic parameterisation

- provide to participant a systematic parameterisation script
- recompute all features and weight consistently
- e.g. for Tau Energy Scale

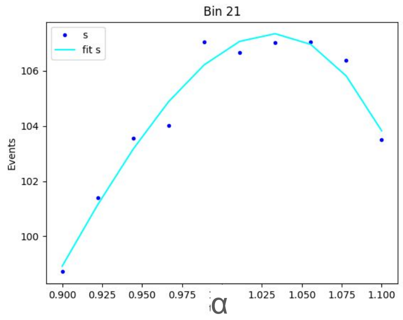




A simple Baseline Model

…to get people started

Baseline Model

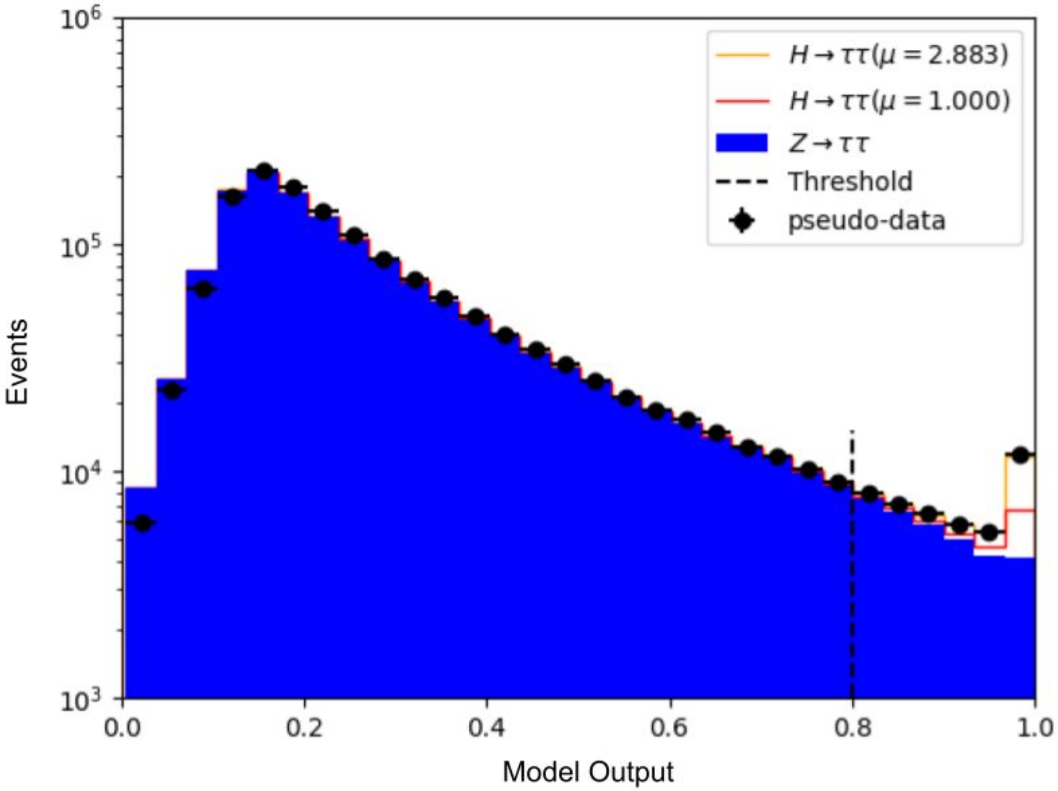


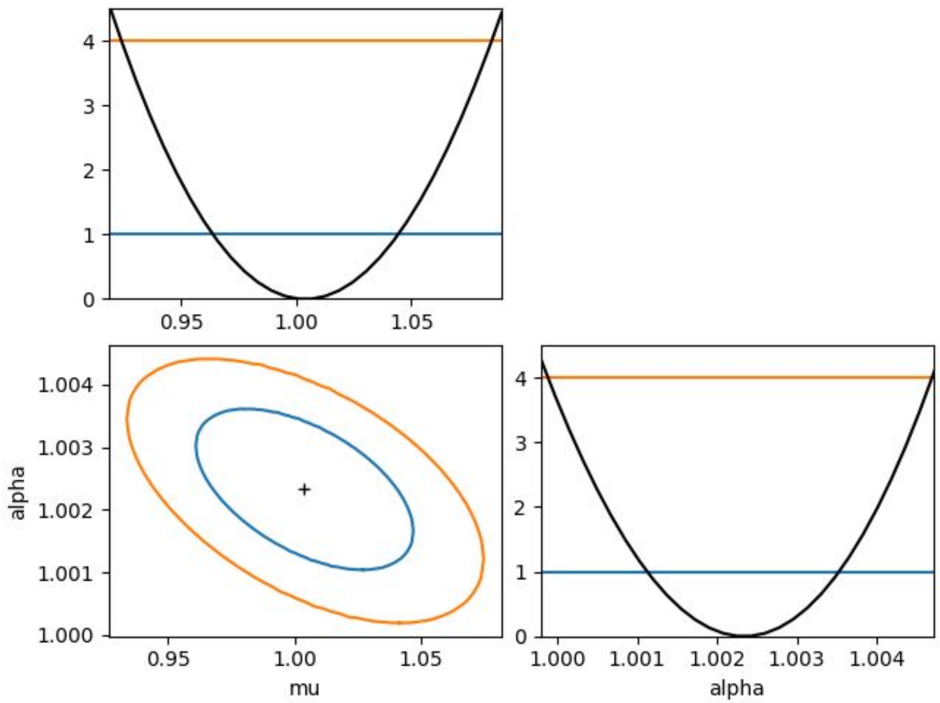
- Train a simple classifier (dense NN, BDT,...)
- Bin the score for Background and Signal : B_i, S_i
- Parameterise as a function of nuisance parameter α $B_i(\alpha)$, $S_i(\alpha)$:
- Binned Negative Log Likelihood function as function of NP and mu ⇒
- For Each pseudo experiment
  a. compute score distribution
  b. NLL regress mu (and α but throw it away)
  c. Returns mu 68% confidence interval

- works nicely for 1 NP, breaks down for more

- …people can take it from there with the more sophisticated uncertainty-aware approaches mentioned earlier

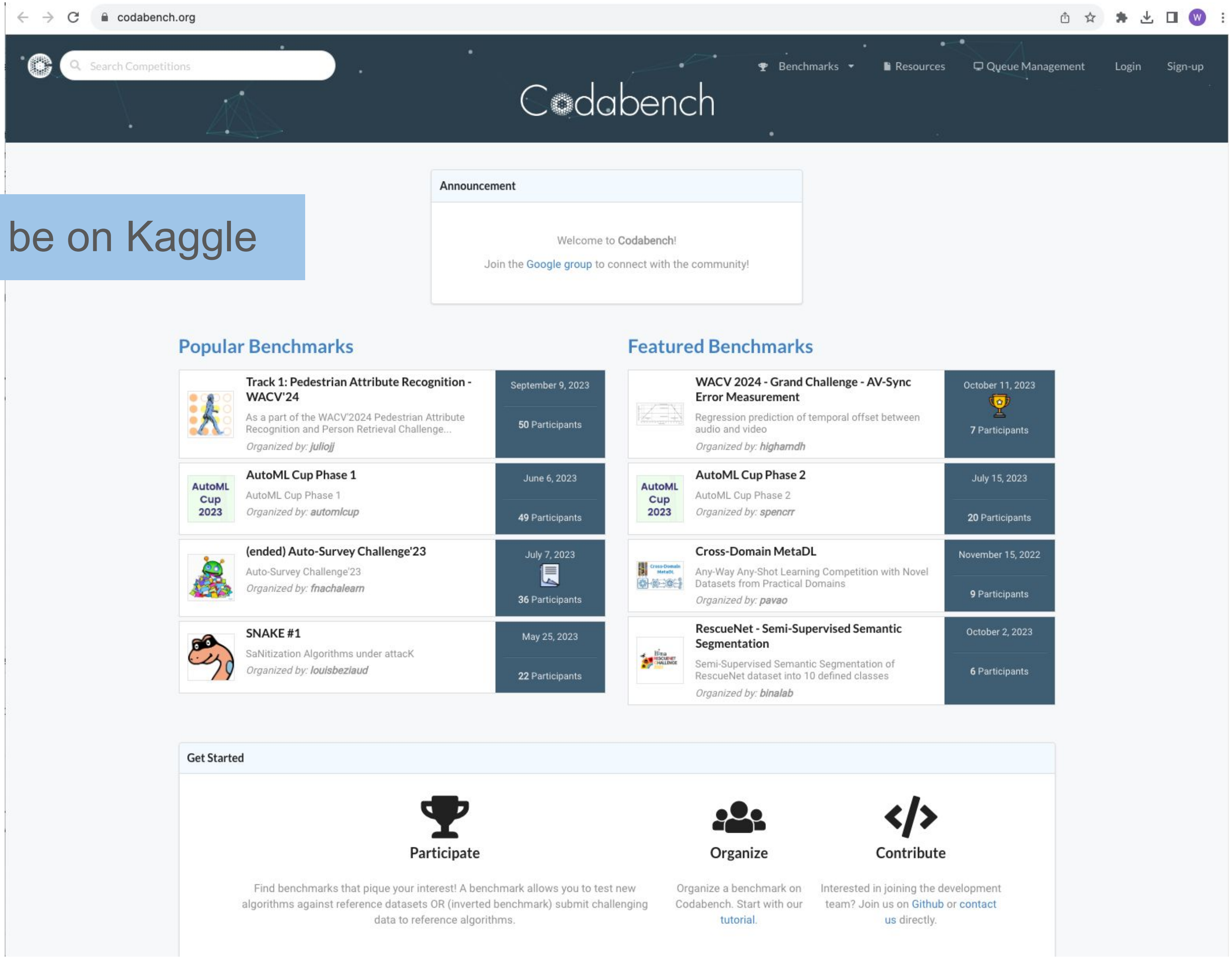
Fit on one pseudo experiment





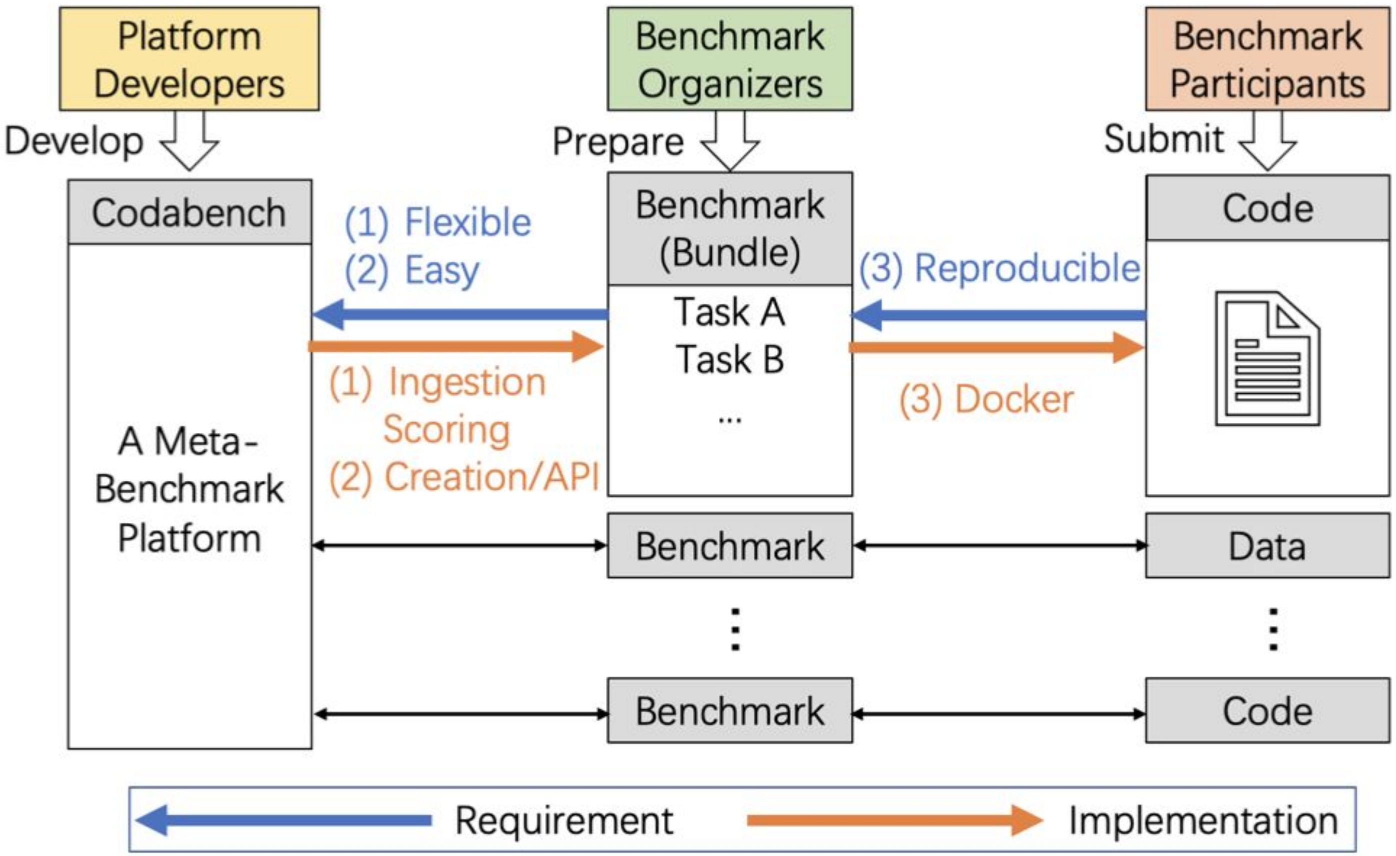
Large-compute-scale AI ecosystem … hosting challenges and benchmarks.

We’ll not be on Kaggle

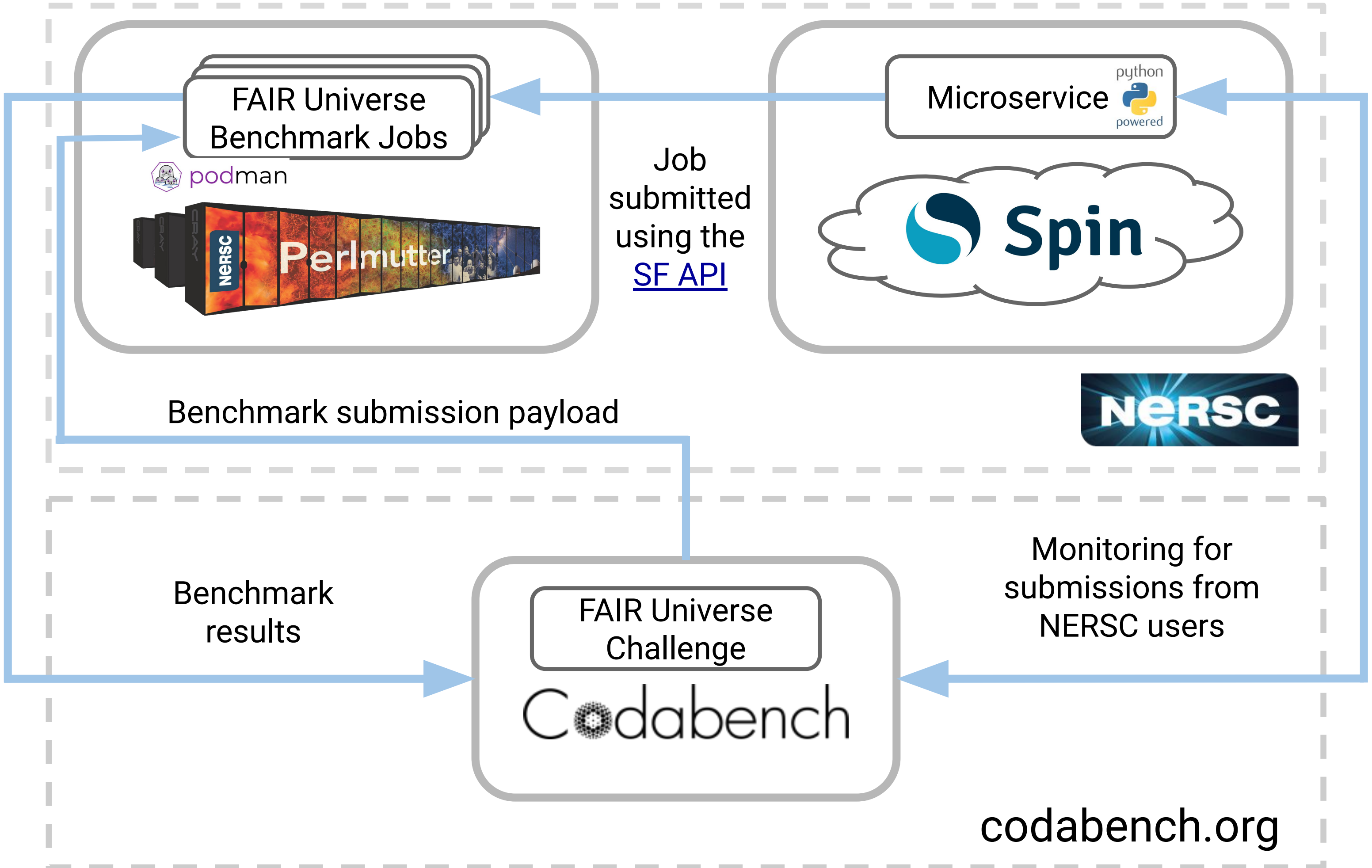


Codabench/“Fair Universe” Platform

Evolution of Codalab
https://www.codabench.org/



Fair Universe Platform: Current Codabench/NERSC integration



Conclusion

- a major new scientific competition on measuring Higgs cross-section,
  - taking into account/minimizing impact from modelisation systematics
  - winner to provide a narrow confidence interval with good coverage
- on Codabench platform with NERSC back-end for precise evaluation of submissions
- early prototype run as part of Paris AI uncertainties workshop in Nov 2023 and ACAT 2024
- to run June-Sep 2024
- submitted to NeurIPS 2024 competition track
- will be announced on : lhc-machinelearning-wg@cern.ch

- A cosmology challenge (weak-lensing) is also in the pipeline