FAIR Universe

# Fair Universe

## Unbiased Data Benchmark Ecosystem for Physics
## HiggsML Uncertainty Challenge


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https://fair-universe.lbl.gov/

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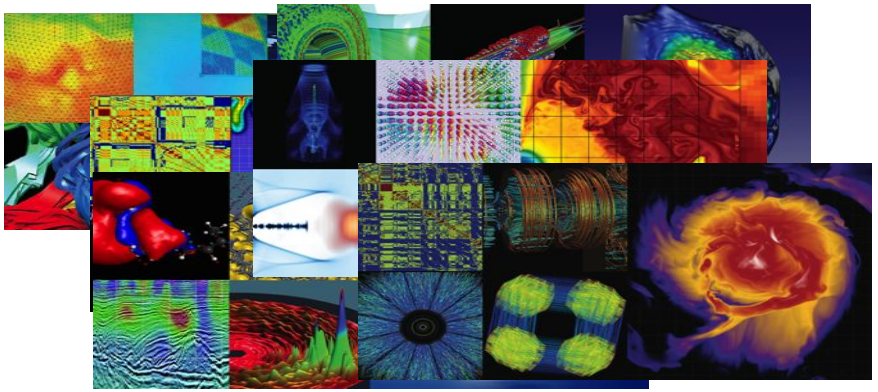
# Fair Universe:
# Unbiased Data Benchmark Ecosystem for Physics

Project aims to:

- Provide a **large-compute-scale AI ecosystem for hosting challenges and benchmarks.**
- **Organize a challenge series** initially focused on **measuring and minimizing the effects of systematic uncertainties** in HEP (particle physics and cosmology).

# Large-compute-scale AI ecosystem for hosting challenges and benchmarks

# NERSC: Mission HPC for the Dept. of Energy Office of Science

**Large compute systems**

- E.g. Perlmutter: ~7k A100 GPUs

Also high-capacity/ fast filesystems,
1 Tbit/s WAN and flexible services

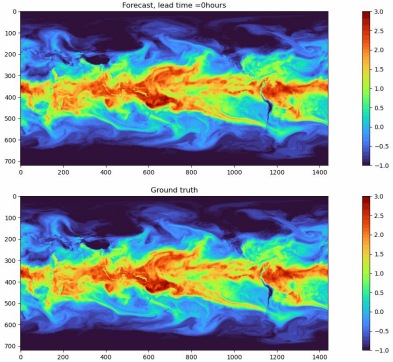
- E.g. SPIN: Rancher/K8s platform for user-defined services

**Broad science user base**

- > 10,000 users,
- > 1000 projects
- Across all DoE Science e.g. HEP; NP; Climate; Fusion Chemistry; Materials; Genomics; etc …

# NERSC-AI Ecosystem:

- ***Deploy*** optimized hardware and software (working with vendors)
  - Improve performance, e.g through benchmarking (MLPerf HPC)
- ***Apply*** cutting edge AI for science: e.g. “NESAP” program with postdocs
- ***Empower*** through e.g. over 20 DL@Scale tutorials, 1000s of total participants: (SC23)
- **Many AI for science highlights** not covered here. e.g.



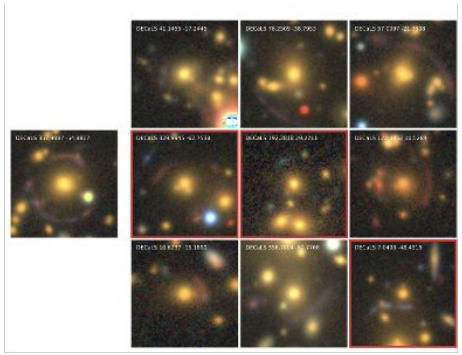

**FourCastNet-** Pathak et al. 2022

Collab with Nvidia, Caltech

First DL model with skill of numerical weather prediction (NWP)

Train up to 1000s of GPUs

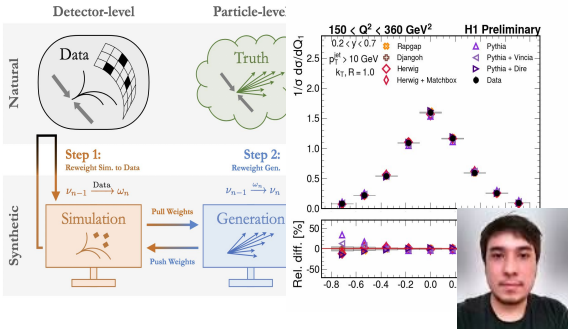
Forecasts 1000s times faster than NWP



**Self-supervised sky surveys** Stein et. al. (2021)

Foundation-like model trained at scale - used for downstream tasks

E.g. uncovered thousands of undiscovered strong-lenses




**Unfolding particle physics**

H1 Collaboration ([...] Mikuni et. al.):

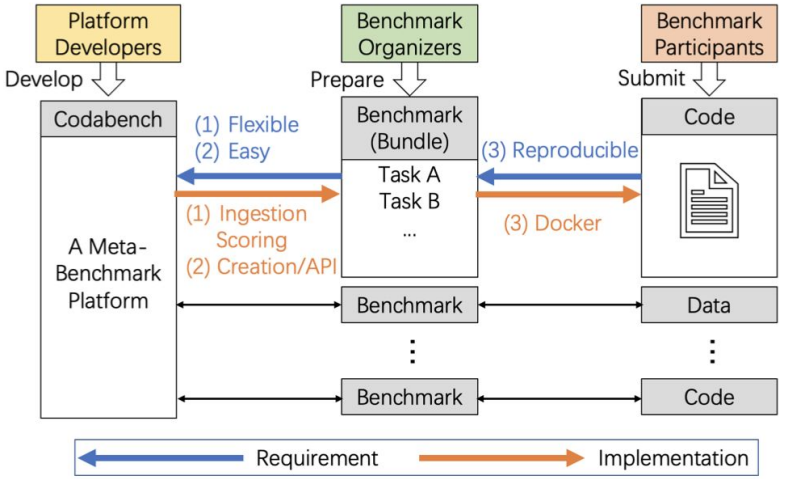
Reanalyzing previous experiment data to unfold many quantities

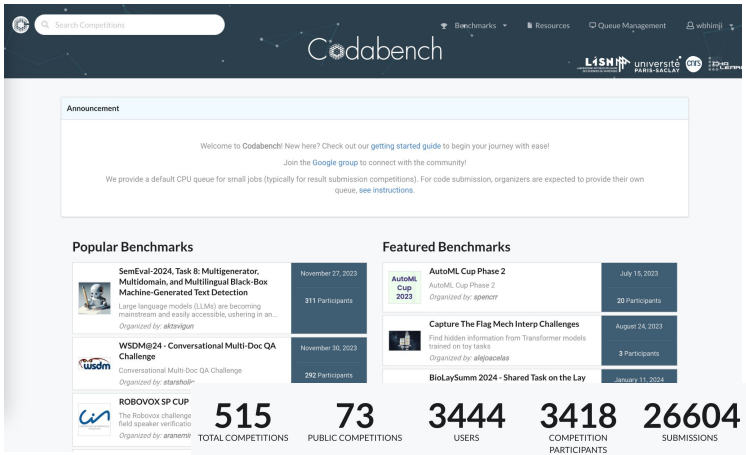
Utilized Perlmutter for 1000s of bootstrapping and UQ runs

# Codabench/“Fair Universe” Platform

Based on https://www.codabench.org/

- Codabench - open source platform for AI benchmarks and challenges
  - Originally (CodaLab) Microsoft/Stanford now a Paris-Saclay/LISN led community
  - > 500 challenges since 2013
  - Allows code submission as well as results e.g. for evaluation timing or reproducibility
  - Also data-centric AI “inverted competitions”
  - Organizers can define scoring functions
  - Queues for evaluation can run on diverse compute resources
  - Platform itself can be deployed on different compute resources




“Fair Universe” brings Codabench to HPC at NERSC!

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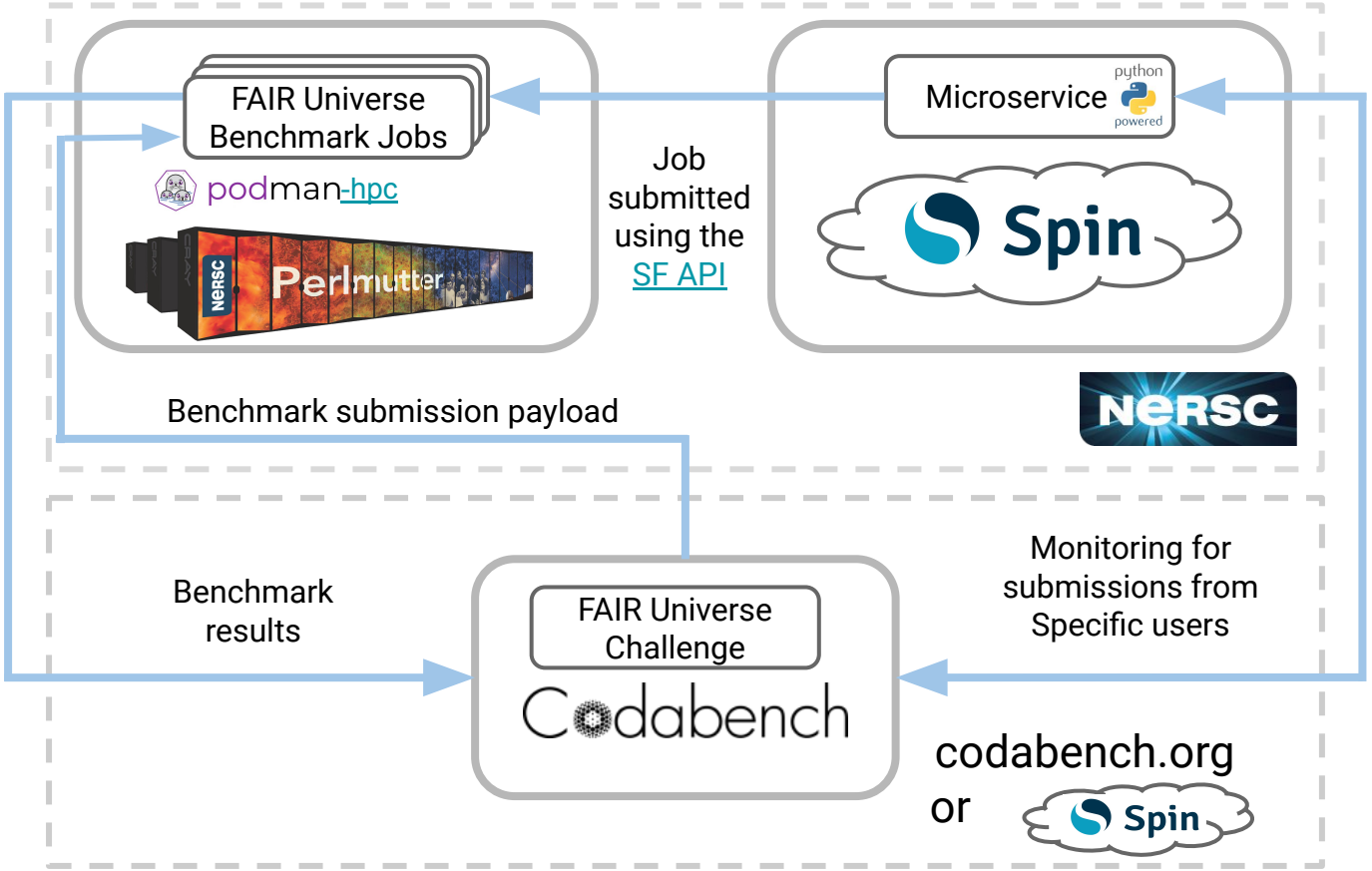
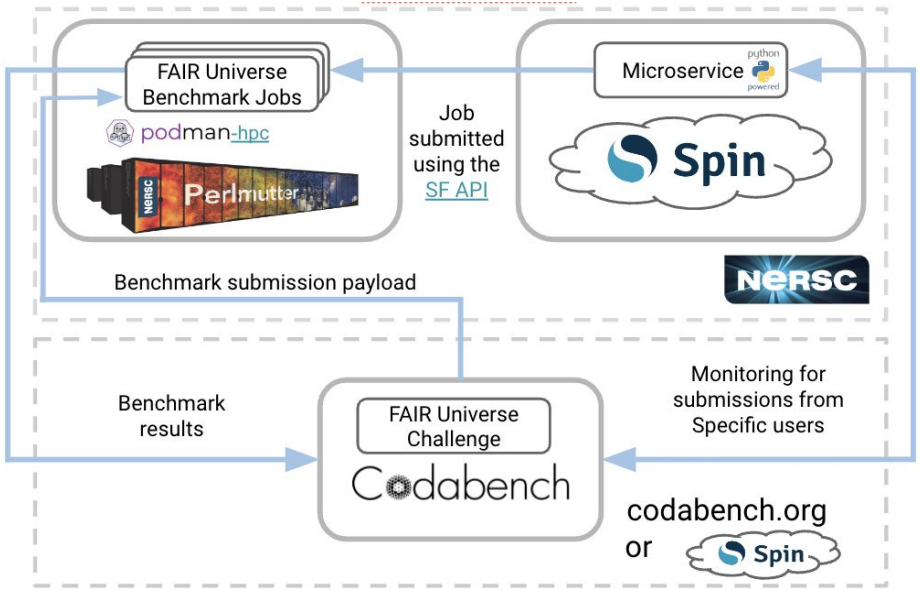
# Fair Universe Platform: Codabench/NERSC integration



# Fair Universe Platform: Codabench/NERSC integration

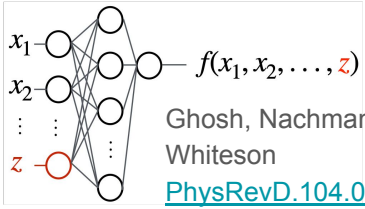
- Benchmark submissions pulled to workers running on Perlmutter:
  - Use podman(-hpc) container runtime: secure and scalable
  - Enable parallelism/scale for
    - **Intensive methods** - use multiple A100 GPUs for training or evaluation
    - **Many participants** - through running many parallel workers
    - **Many evaluations** - e.g for Uncertainty Quantification
- Workers submitted as needed by microservice on SPIN service platform
  - NERSC's "SF API" for job submission
  - Monitor/filter submissions




- Also deploy instances of Codabench platform itself within SPIN
  - Customization and future OIDC integration with NERSC authorization

Organize a challenge series focused on measuring and minimizing the effects of systematic uncertainties in HEP

# Bias and uncertainty in ML in HEP

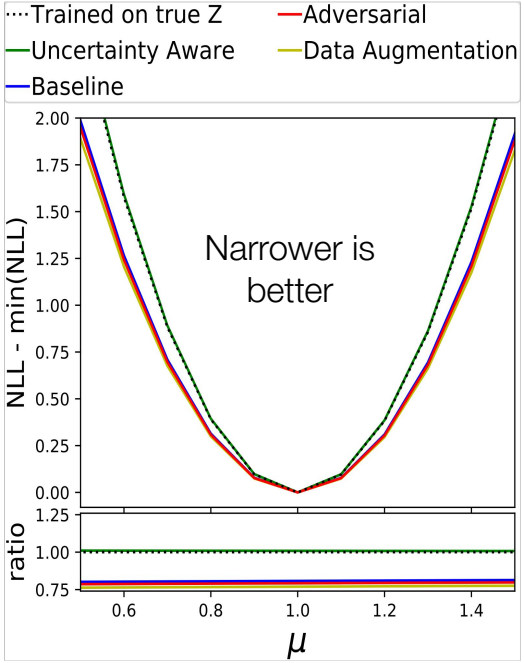



Ghosh, Nachman, Whiteson PhysRevD.104.056026

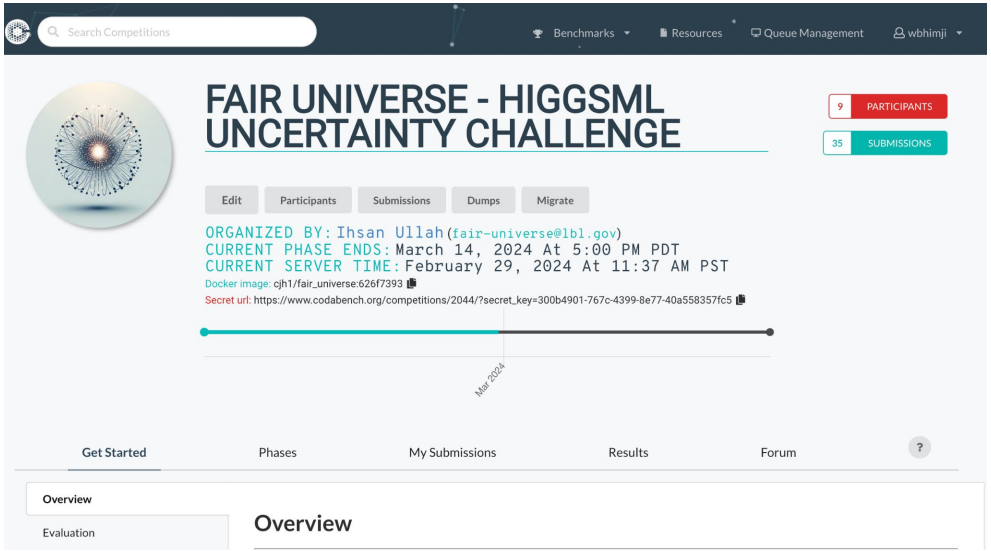
- ML trained on simulation with estimated systematics (“Z”)
  - Then applied in data with different state Z’
  - Commonly dealt with by shifting Z and measuring impact

Non-optimal so many other techniques proposed - e.g.:

- Decorrelation - augmentation; adversarial training
- “Uncertainty-aware” Ghosh, Nachman, Whiteson PhysRevD.104.056026
  - Parameterize classifier using Z
- Other novel approaches e.g. (not comprehensive)
  - Inferno: arxiv:1806.04743;
  - Full profile-likelihood: e.g. arxiv:2203.13079
- Mainly demonstrated on single systematic with limited data
  - Can be hard to scale, e.g. retraining and profiling expensive
- Need for larger datasets and novel metrics to compare uncertainty quantification for ambitious approaches



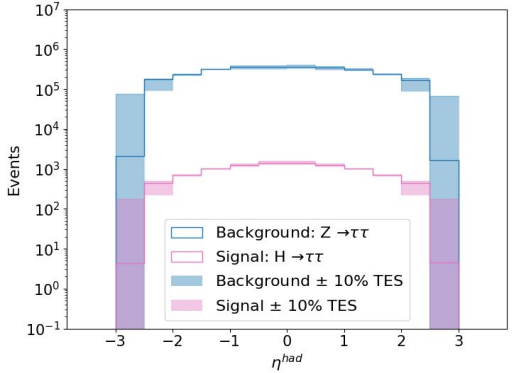
# Fair Universe: HiggsML Uncertainty Challenge

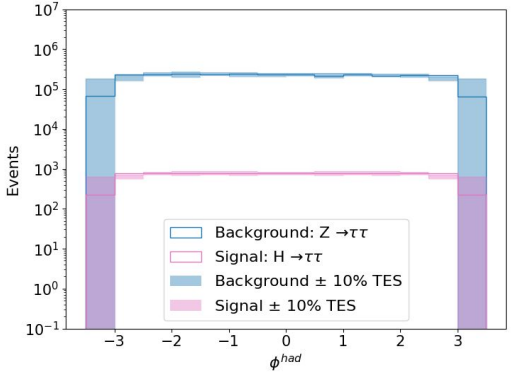


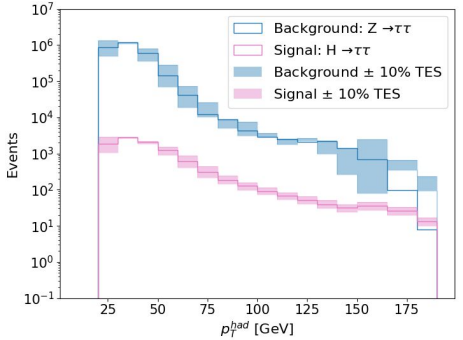

- Extension of HiggsML Kaggle challenge (H→ττ) from 2014
- HiggsML Uncertainty Challenge Pilot - launched today → http://go.lbl.gov/fair-universe-higgsml-spring24
  - Evaluate methods and metrics and gain feedback
- Full HiggsML Uncertainty Challenge ~May-Oct 2024
  - Submitted as NeurIPS competition - results presented at NeurIPS in December

# HiggsML Uncertainty Challenge - Datasets

- Much larger datasets than original HiggsML challenge ($12*10^6$ training events)
- *Delphes* detector simulation (see “Data” tab on competition page for details)
- Apply parameterized systematics (Nuisance Parameters) :
  - In current pilot: Tau Energy Scale - shift hadronic Tau Pt (and correlated MET)
  - Further planned for full competition: Jet Energy Scale (and correlated MET impact); Additional randomised Soft MET; Background normalisation; W-boson background normalisation
  - Also ongoing work to add systematics into Delphes generation for comparison

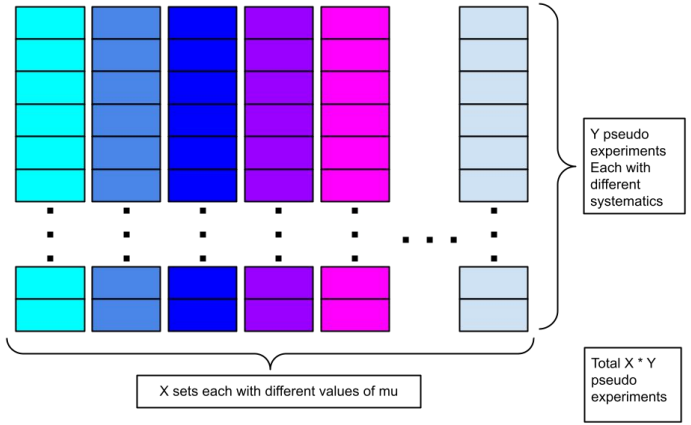


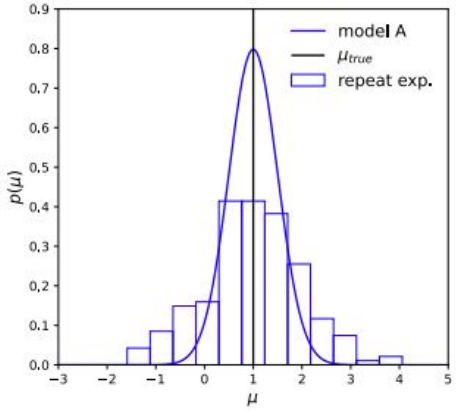



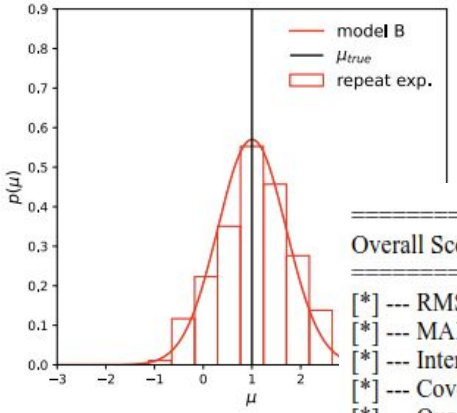



# HiggsML Uncertainty Challenge - Evaluation

- Form multiple pseudo-experiment test sets: different signal strengths ($\mu$) and systematics
  - Current pilot - 4$\mu$ and 50 pseudo-experiments
- Task: predict uncertainty interval [$\mu_{16}$, $\mu_{84}$]
  - E.g. 68% quantile of likelihood or assume 1$\sigma$
- Score: balance accuracy and precision with matching the true uncertainty and accuracy

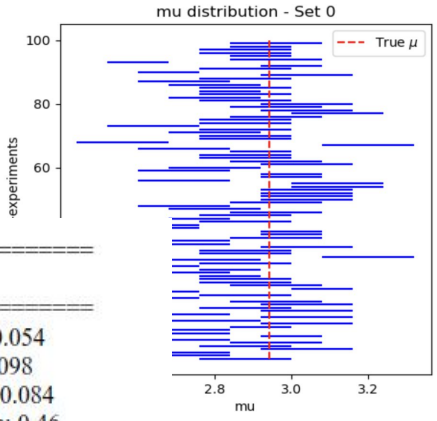


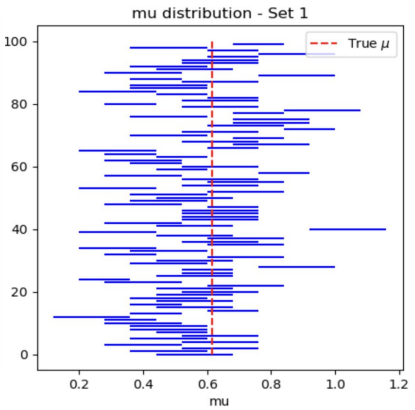




Overall Score

[*] --- RMSE: 0.054
[*] --- MAE: 0.098
[*] --- Interval: 0.084
[*] --- Coverage: 0.46
[*] --- Quantiles score: -1.651



# Uncertainty Quantification Metric

- **Interval width (w)** averaged over N test sets
- **Coverage (c)**: fraction of time $\mu$ is contained
- Combined using a **coverage function f(x):**

$$x \geq 0.68 - 2\sigma_{68} \text{ and } x \leq 0.68 + 2\sigma_{68} : 1.$$

$$x < 0.68 - 2\sigma_{68} : 1 + \left|\frac{x-(0.68-2\sigma_{68})}{\sigma_{68}}\right|^4$$

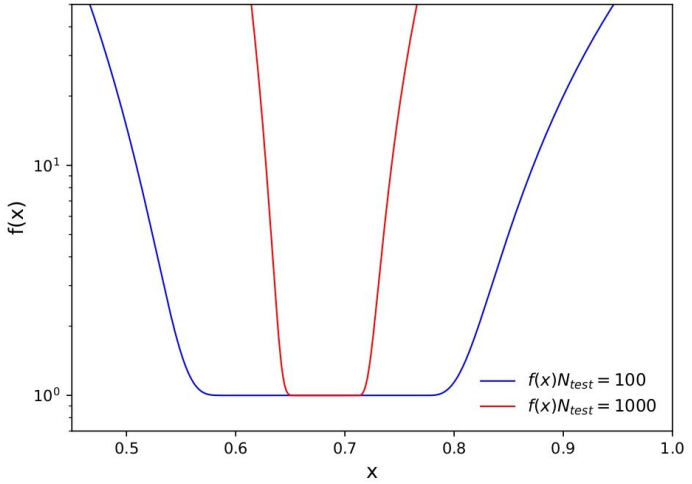
$$x > 0.68 + 2\sigma_{68} : 1 + \left|\frac{x-(0.68+2\sigma_{68})}{\sigma_{68}}\right|^3$$

$$\text{with } \sigma_{68} = \frac{\sqrt{(1-0.68)0.68N)}}{N}$$

- N dependance for equivalent ideal coverage
- Penalizes undercoverage more
- **Final score (s)** designed to avoid large values or gaming

$$w = \frac{1}{N}\sum_{i=0}^{N} \left|\mu_{84,i} - \mu_{16,i}\right|$$

$$c = \frac{1}{N}\sum_{i=0}^{N} 1 \text{ if}(\mu_{true,i} \in [\mu_{84,i} - \mu_{16,i}])$$

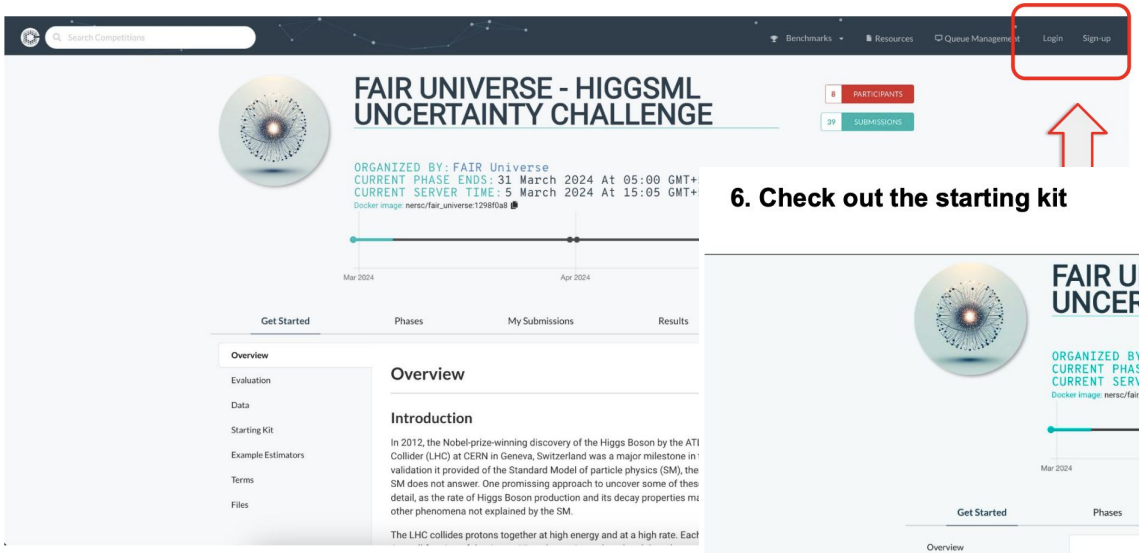



$$s = -\ln\left((w+\epsilon)f(c)\right)$$

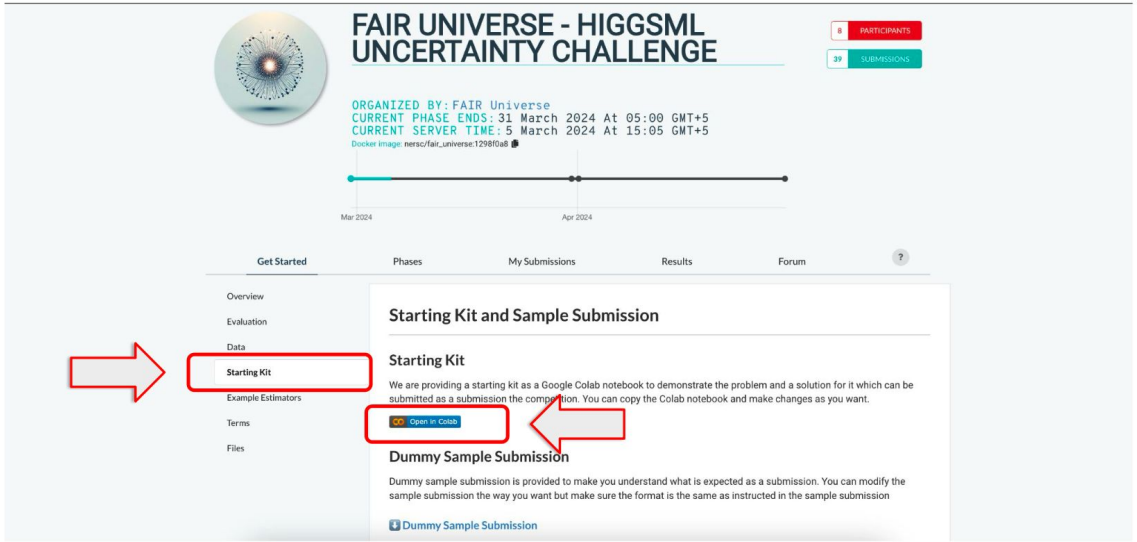
# Enter the HiggsML Uncertainty Challenge Pilot!

http://go.lbl.gov/fair-universe-higgsml-spring24

- See more detailed: walkthrough slides; and “starting kit”

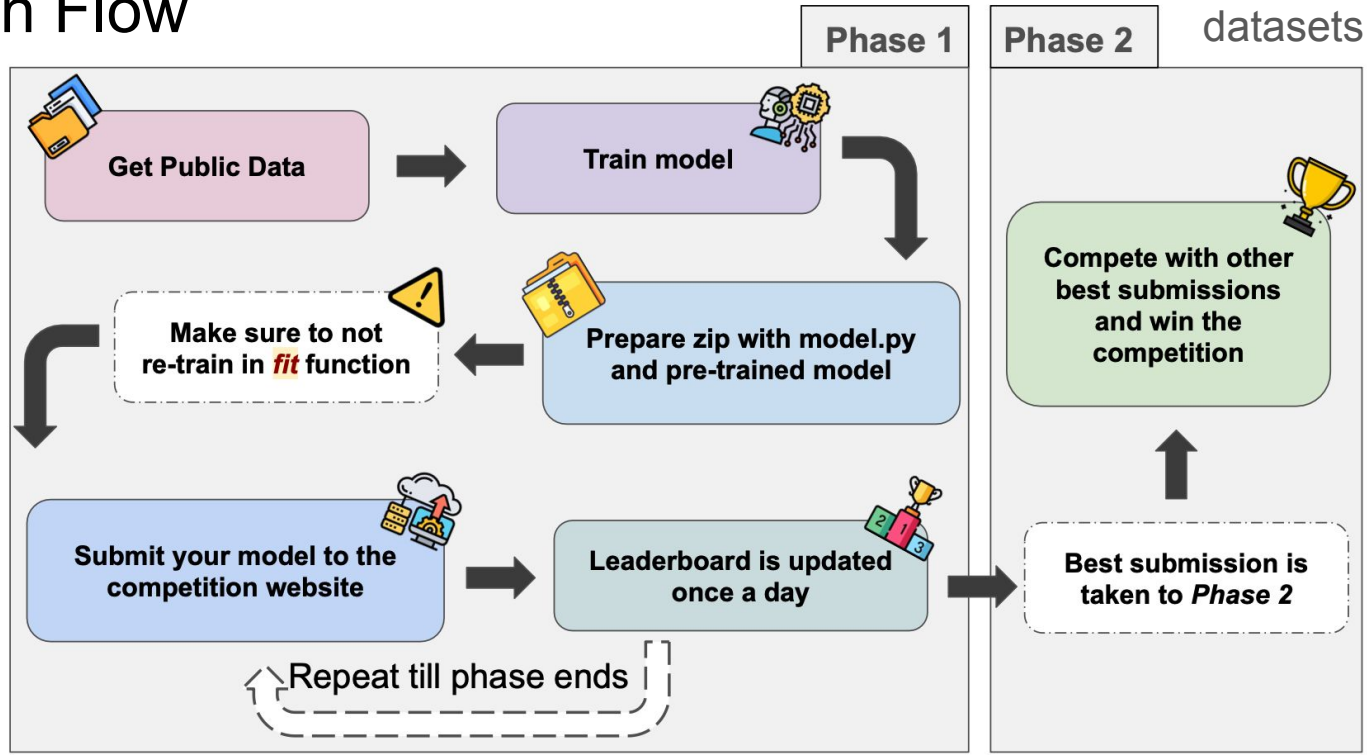



**6. Check out the starting kit**



# Competition Flow

New, hidden $\mu$ datasets




- Submissions are run, and the leaderboard updated, at least once a day
- Participants code is run on the platform, in parallel on many test sets, so there can be differences to when tested locally - contact us on slack with any issues

# Conclusions

- We have built a flexible platform for hosting challenges and benchmarks - extending Codabench, backed by HPC at NERSC
- Launching a series of challenges for uncertainty aware methods for HEP
  - You can enter the HiggsML Uncertainty Challenge Pilot now!
    - http://go.lbl.gov/fair-universe-higgsml-spring24
- Open to feedback on metrics/datasets to encourage advanced approaches and ensure challenge is interesting

Help and feedback: #higgsml-uncertainty-challenge-spring-24 channel on the Fair Universe Slack workspace
Ongoing information Google Group: Fair-Universe-Announcements
Collaborations, questions, comments: fair-universe@lbl.gov
General collaboration on NERSC-AI: wbhimji@lbl.gov