FAIR Universe 2024: Higgs ML Uncertainty Challenge

Yulei Zhang

University of Washington, Seattle

Team: Wahid Bhimji, **Paolo** Calafiura, **Ragansu** Chakkappai, **Yuan-Tang** Chou, **Sascha** Diefenbacher, **Jordan** Dudley, **Steven** Farrell, **Aishik** Ghosh, **Isabelle** Guyon, **Chris** Harris, **Shih-Chieh** Hsu, **Elham** Khoda, **Rémy** Lyscar, **Alexandre** Michon, **Benjamin** Nachman, **Benjamin** Thorne, **Peter** Nugent, **Po-Wen** Chang, **Mathis** Reymond, **Benjamin** Sluijter, **David** Rousseau, **Ihsan** Ullah, **Daniel** Whiteson, **Yulei** Zhang

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FAIR Universe

FAIR Universe

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

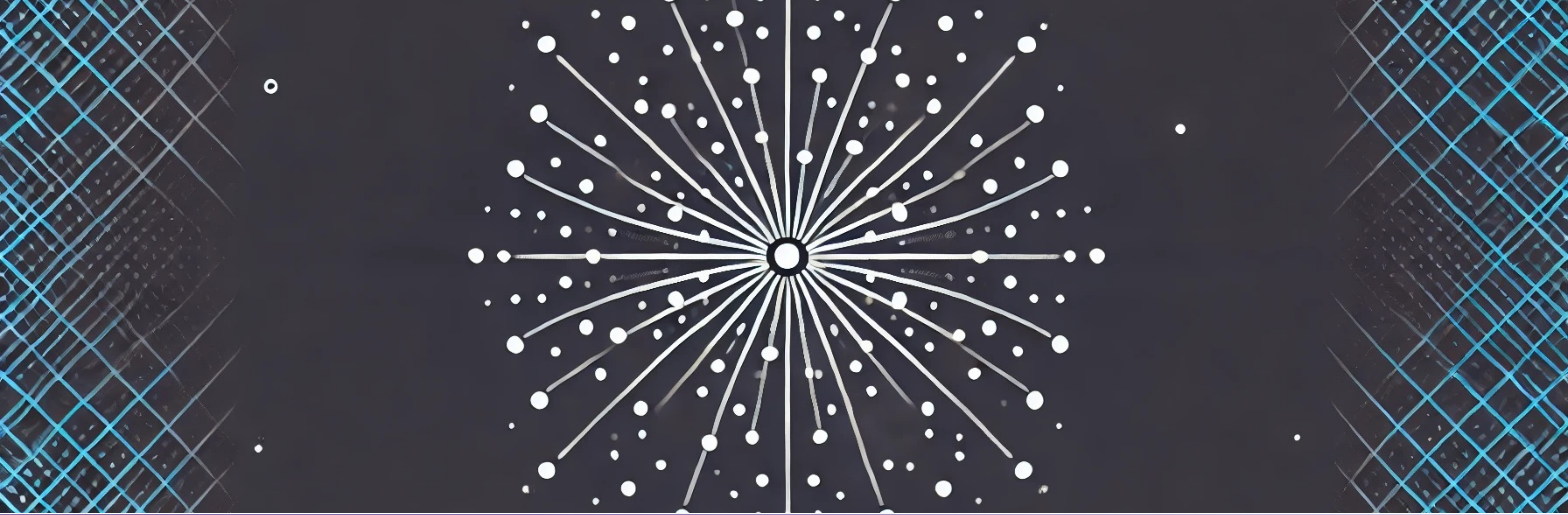
Collaborators: U. Berkeley, U. Washington, Chalearn, IJCLab-Orsay, UC Irvine, UCSD, Universiteit Leiden

Project Aims:

- An Open, **Large-Compute-Scale AI Ecosystem** for sharing datasets, training large models, and **hosting challenges and benchmarks**
- Progressive **challenge series** on **measuring and minimizing the effects of systematic uncertainties** in HEP (particle physics and cosmology)

Broad team Involvement in major AI and HEP challenges like HiggsML, TrackML, LHC Olympics, Fast Calorimeter Simulation Challenge, and wider (e.g NeurIPS competition, MLPerf HPC)

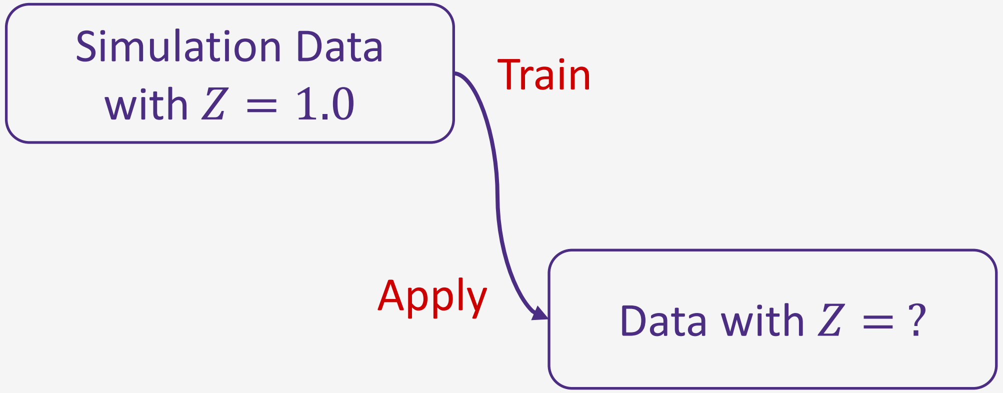
➢ ***Fair Universe HiggsML Uncertainty Challenge : NeurIPS competition*** 🥳

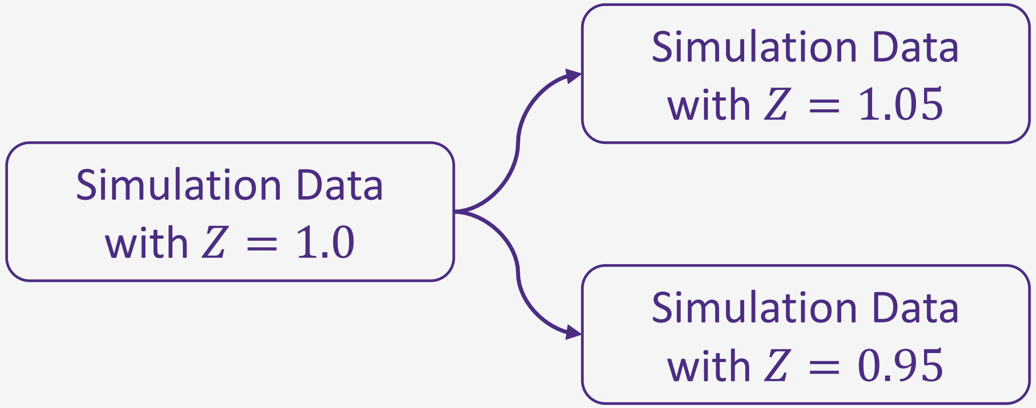


Measuring and minimizing the effects of systematic uncertainties in HEP

Bias and Uncertainty in Fundamental Sciences

- Machine learning models in HEP are typically **trained using simulations**, which include **certain assumptions** and **systematic uncertainties** (called "epistemic" uncertainties, **labeled as "Z"**).
- However, when these models **are applied to real-world data**, the conditions (detector states) may differ, leading to an unknown Z value.
- **Common Approach:** First, train the model on standard simulation data (Z = 1). Then, estimate uncertainties by comparing results from simulations with different Z values. Shift Z slightly and examine how it affects the results or use **a full profile likelihood** to evaluate the impact.





Simple estimation of uncertainty

FAIR Universe: HiggsML Uncertainty Challenge

- **Focus on novel approaches** to address model uncertainty, including decorrelation, adversarial training, and uncertainty-aware techniques.
  - Example techniques: "Pivot" by Louppe et al. (arXiv:1611.01046), Ghosh et al. (PhysRevD.104.056026), Inferno (arXiv:1806.04743), and others.
  - **Challenge:** Scaling methods to handle multiple values of systematic uncertainties (Z), which increases training complexity and cost.
- **Key gaps**: Current benchmarks rely on **single systematic uncertainties** and **limited datasets** (based on HiggsML 2014), which restrict scaling and broader adoption.
- **New dataset for the challenge**: Extension of the original HiggsML dataset.
  - **Improvements**: Larger dataset (from 800k to ~**300M events**), faster simulation, **parameterized systematics** (nuisance parameters).
  - **Task:** Provide a confidence interval on signal strength in a pseudo-experiment with a given signal.

Dataset Overview

- **Simulated Dataset** (**280 million events**): Representative of high-energy proton collision data from the **ATLAS experiment** at the Large Hadron Collider (LHC).
- **Pythia 8.2** and **Delphes 3.5.0** for simulation, and data organized in a tabular format with **28 features** per event.
- Includes a **biasing script** introducing systematic uncertainties (Nuisance Parameters) for realistic challenges.

Process	Number Generated	LHC Events	Label
Higgs	52101127	1015	**signal**
Z Boson	221724480	1002395	**background**
Di-Boson	2105415	3783	**background**
$t\bar{t}$	12073068	44190	**background**

Public

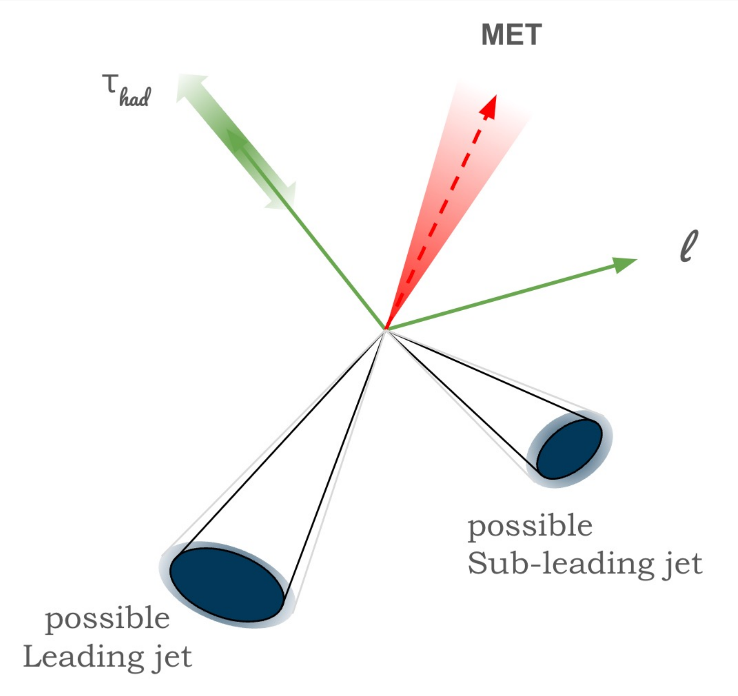
- **Train/Val**: **100** $\times$ LHC @ 10 fb^{-1}
- **Pseudo**: **60** $\times$ LHC @ 10 fb^{-1}

Private

- **Pseudo**: **60** $\times$ LHC @ 10 fb^{-1}

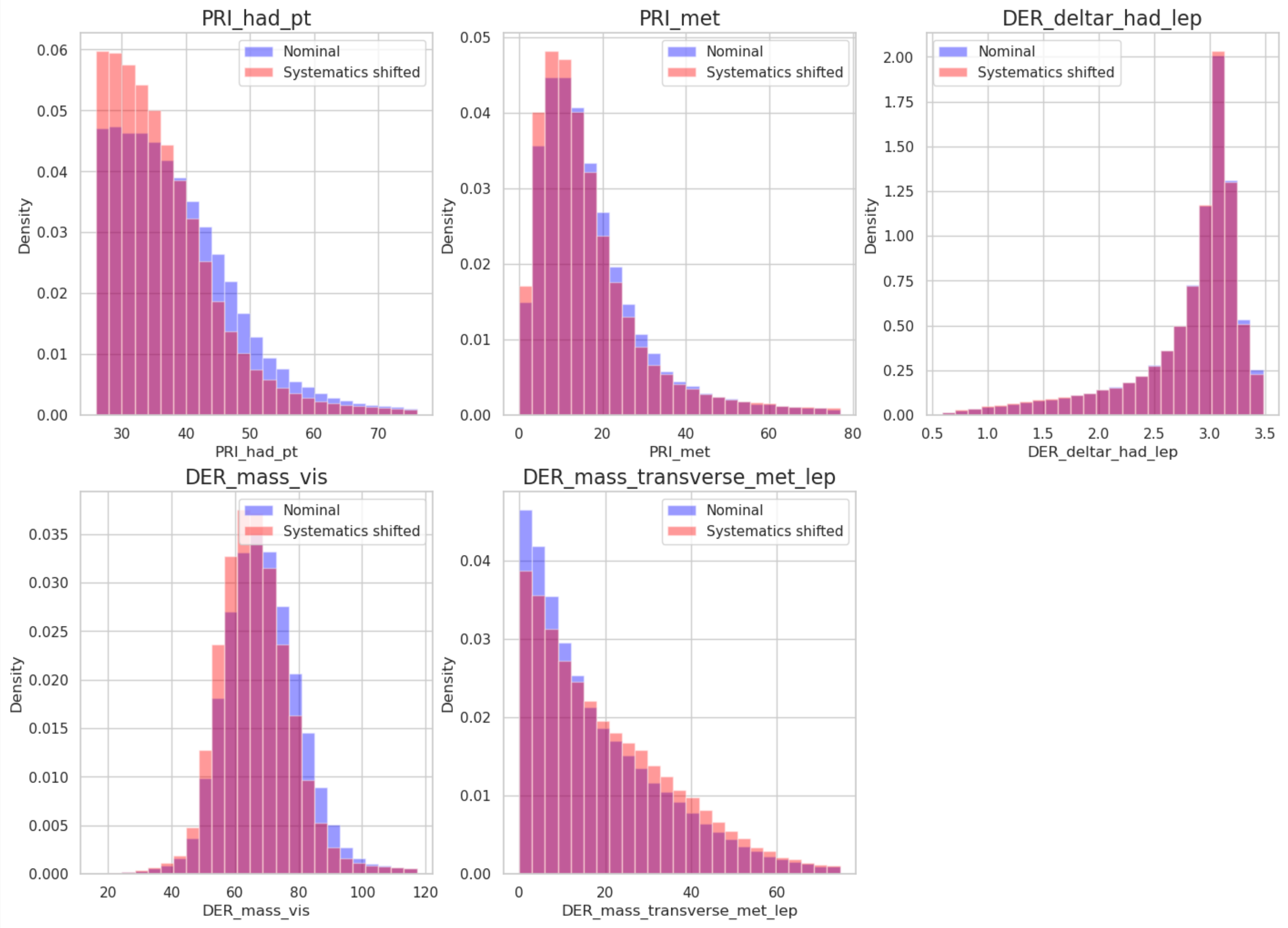
Systematics Parameterization: Nuisance Parameters

- New systematic parameterization method [white paper, github]
- 6 systematic uncertainties!
- **Object-level uncertainties:**
  - Tau Energy Scale (and correlated MET) $[0.9, 1.1, \sigma = 0.01]$
  - Jet Energy Scale (and correlated MET impact) $[0.9, 1.1, \sigma = 0.01]$
  - Additional randomized Soft MET $[0, 5, \sigma = 1.0]$
- **Event category normalization:**
  - Overall Background norm $[0.99, 1.01, \sigma = 0.001]$
  - VV background norm $[0, 2, \sigma = 0.25]$
  - $t\bar{t}$ background norm $[0.8, 1.2, \sigma = 0.02]$



We operate within the framework of '**known unknowns**,' while addressing '**unknown unknowns**' remains a more complex challenge beyond this scope.

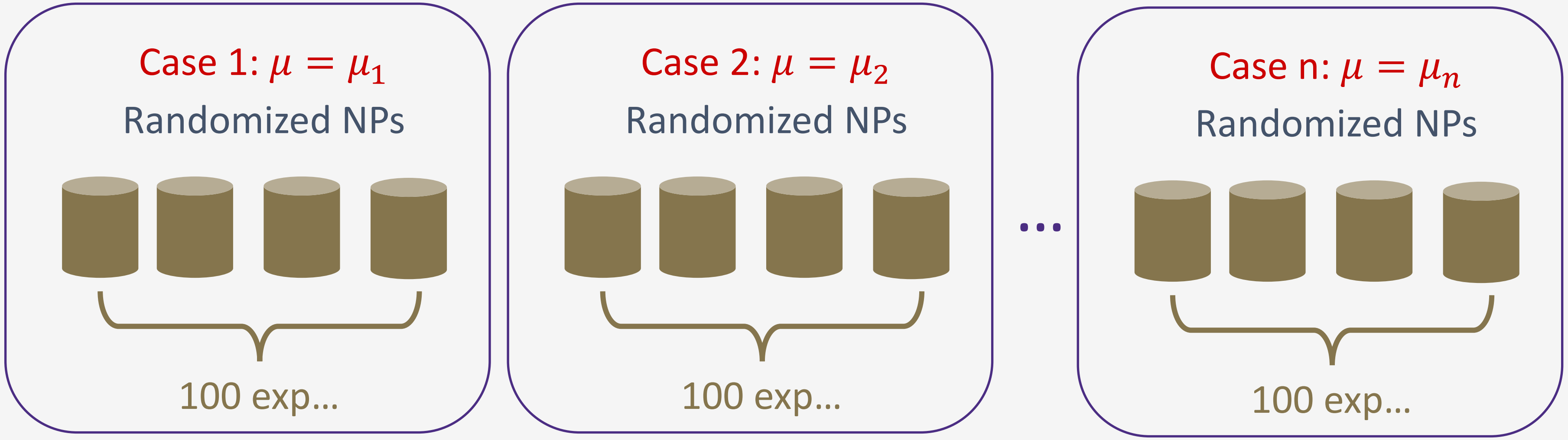
Example of one NP: Tau Energy Scale Impact

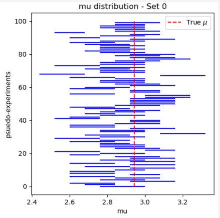


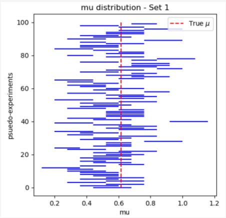
- Histogram between nominal (TES = 1) and shifted (TES = 0.9)
- TES = 0.9 is an exaggeration, in practice it is sampled with $\mathcal{g}(\mathbf{1}, \mathbf{0.01})$ and with boundary $[\mathbf{0.9}, \mathbf{1.1}]$

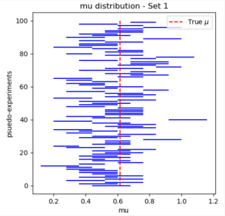
Evaluation Metrics

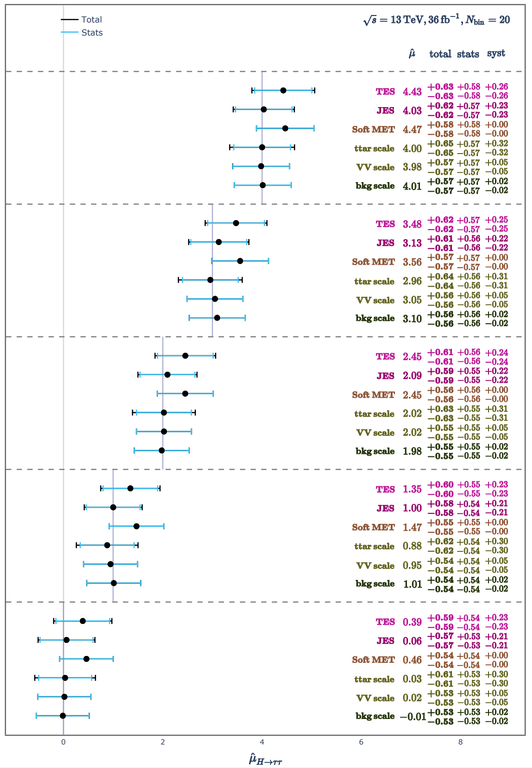
- Pseudo-experiments
  - dataset representative of what would be measured from 10fb^{-1}~800 billion LHC pp collisions for a given value of μ and of the Nuisance Parameters











Evaluation Metrics

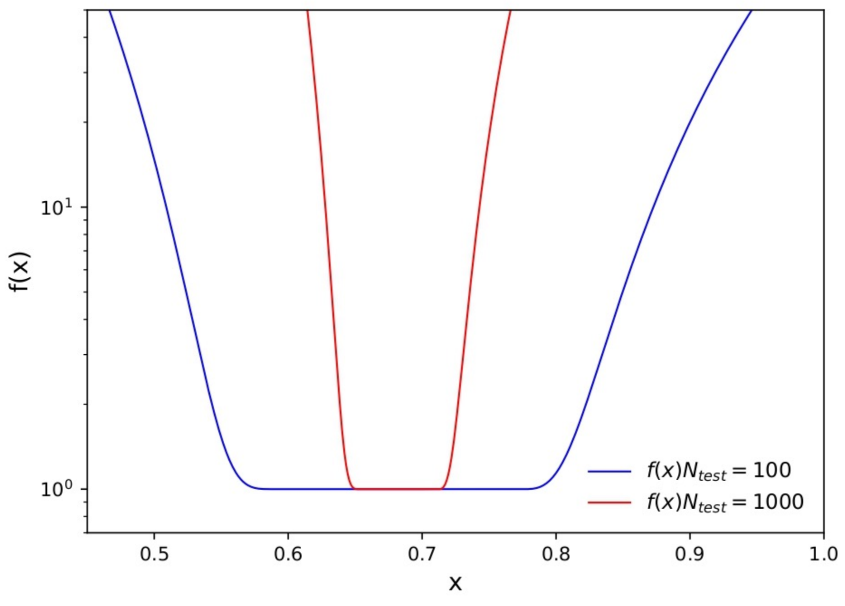
- **Interval width (ω)** averaged over N test sets $w = \frac{1}{N}\sum_{i=0}^{N} |\mu_{84,i} - \mu_{16,i}|$
- **Coverage (c)**: fraction of time $\boldsymbol{\mu}$ is contained $$c = \frac{1}{N_{test}}\sum_{i=1}^{N} 1 \text{ if } \mu_{\text{true},i} \in [\mu_{16,i} - \mu_{84,i}]$$
- Combined using a **coverage function $f(c)$:**

$$c \in [0.6827 - 2\sigma_{68}, 0.6827 + 2\sigma_{68}] : f(c) = 1$$

$$c < 0.6827 - 2\sigma_{68} : f(c) = 1 + \left|\frac{c - (0.6827 - 2\sigma_{68})}{\sigma_{68}}\right|^4$$

$$c > 0.6827 + 2\sigma_{68} : f(c) = 1 + \left|\frac{c - (0.6827 + 2\sigma_{68})}{\sigma_{68}}\right|^3$$

$$\sigma_{68} = \sqrt{\frac{(1 - 0.6827)0.6827}{N_{\text{test}}}}$$



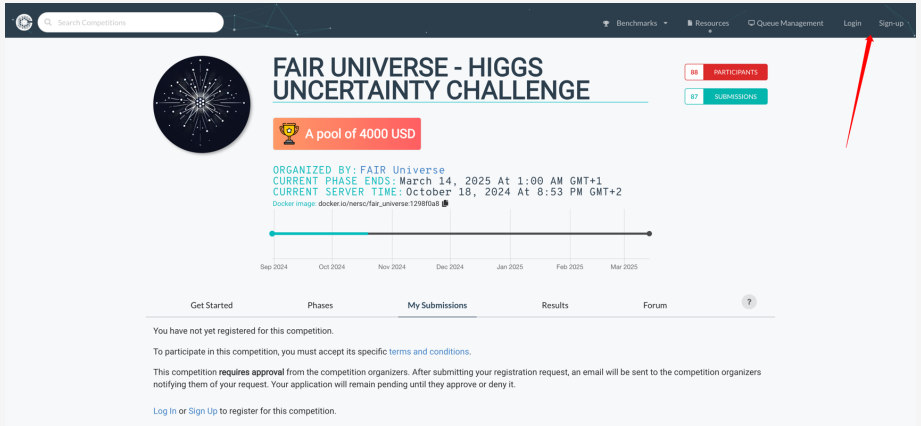
- N dependance for equivalent ideal coverage
- Penalizes undercoverage more
- **Final score (s)** designed to avoid large values or gaming: $-\ln((\omega + \epsilon)f(c))$ ($\epsilon = 10^{-2}$)
- More details in White paper

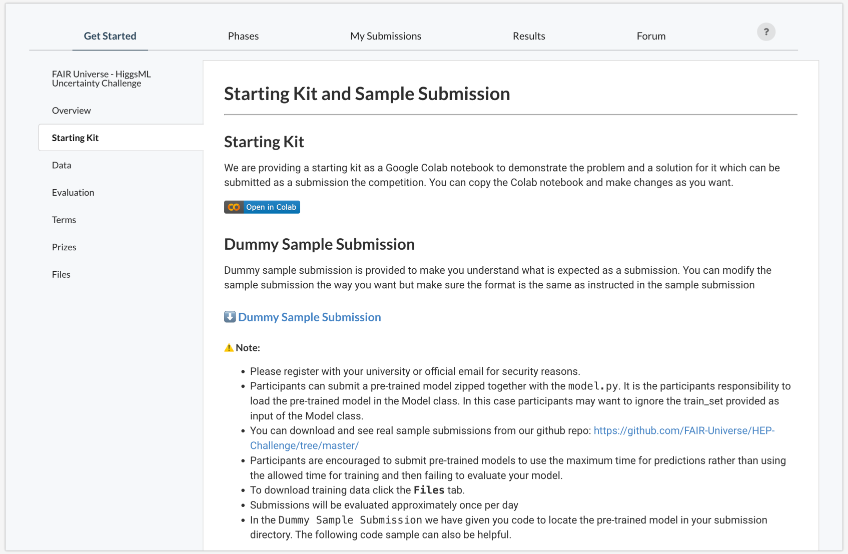
Enter the HiggsML Uncertainty Challenge!

Total pool of 4000 USD

- **First Place: $2000**
- **Second Place: $1500**
- **Third Place: $500**

- **Competition page**: https://www.codabench.org/competitions/2977/
- **Current Phase ends**: March 14, 2025 @ 0:00 GMT+0
- **Documentations**: https://fair-universe.lbl.gov/docs/
- **White paper**: this serves as a full breakdown of the competition in detail [Arxiv:2410.02867]
- Please apply to the competition with your institute's email address.

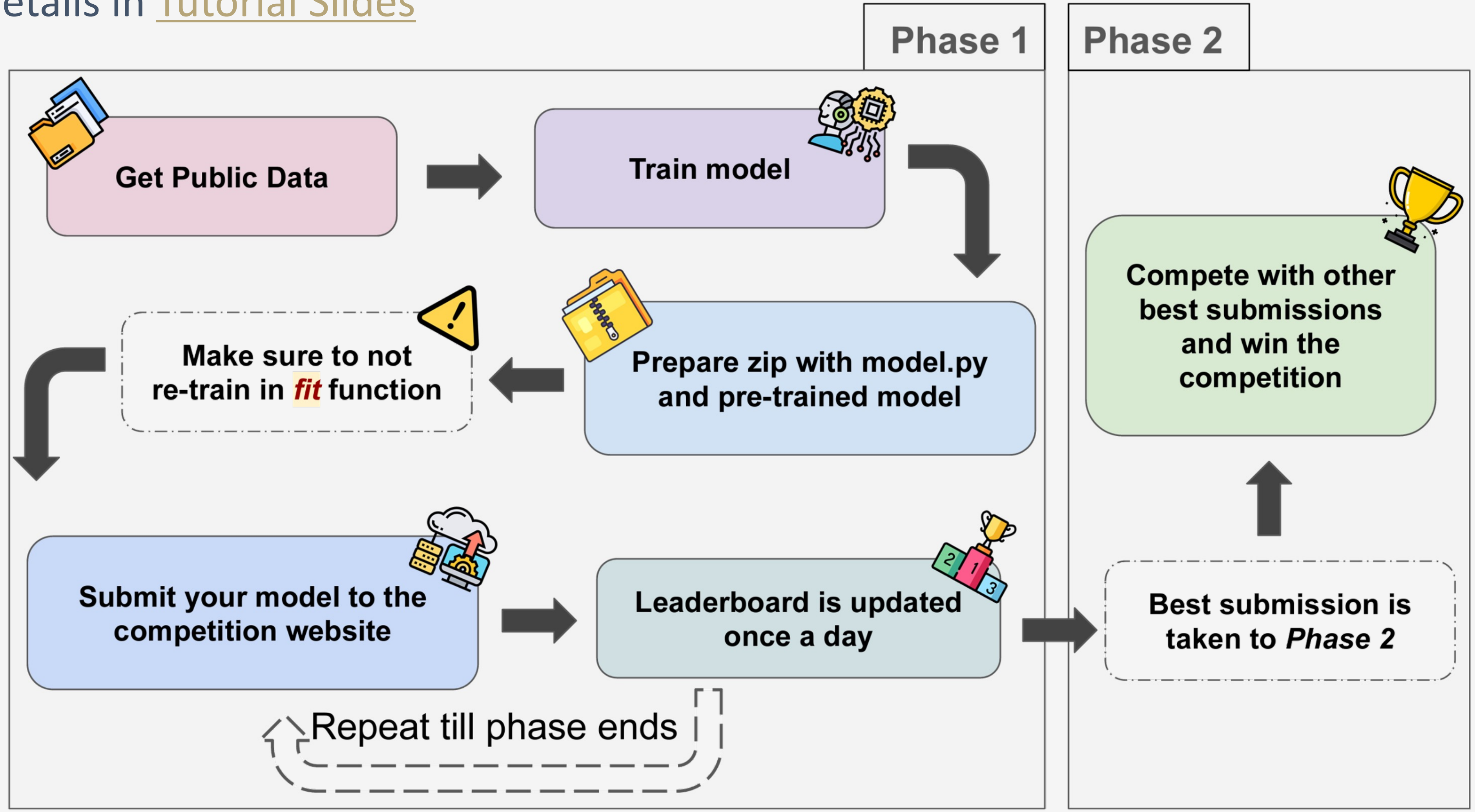




FAIR Universe

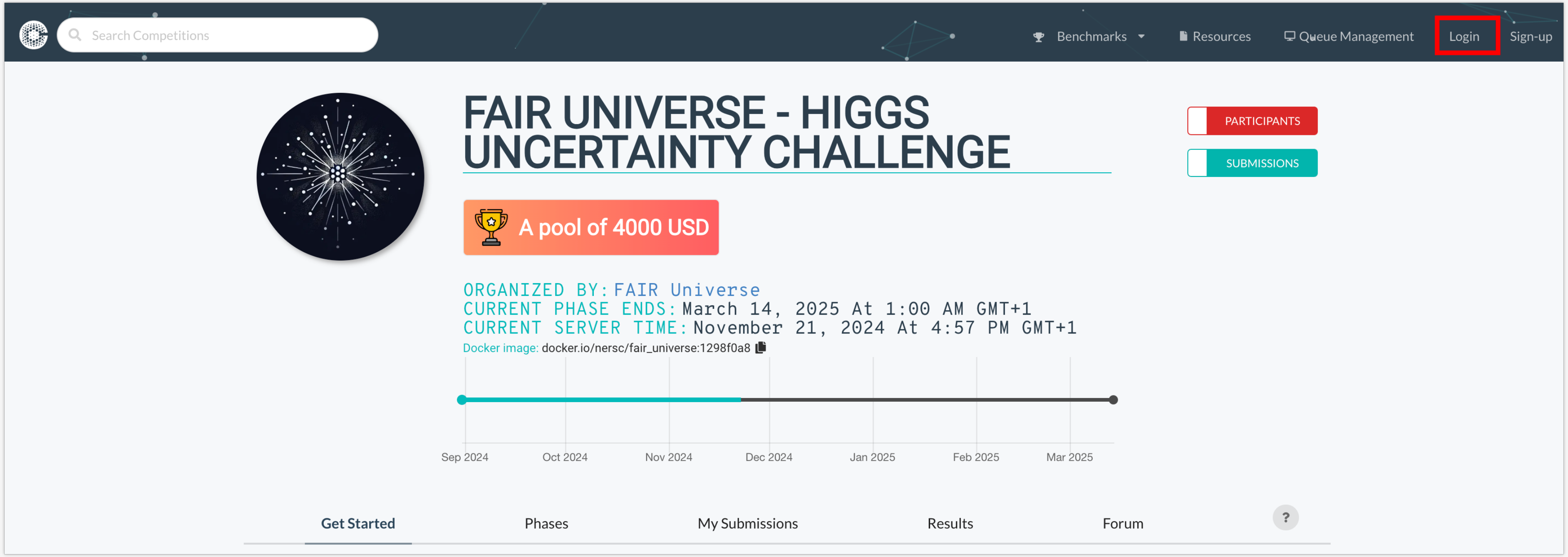
Competition Flow

- More details in Tutorial Slides



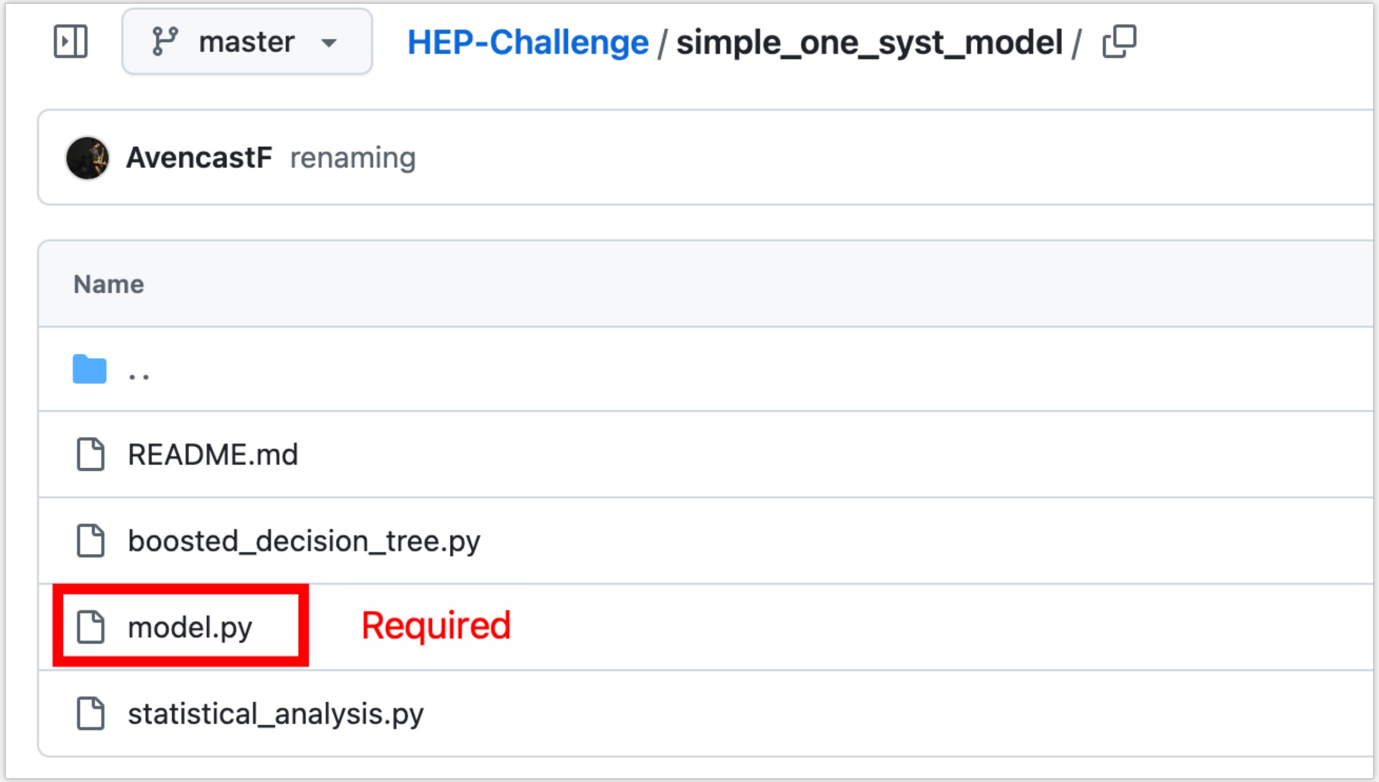
Hands-On

- Login https://www.codabench.org/competitions/2977/#/participate-tab



Hands-On

- Example model: https://github.com/FAIR-Universe/HEP-Challenge/tree/master/simple_one_syst_model
- Required script: `model.py`



Hands-On

- Required script: `model.py`
  - __init__(self): -> None
  - fit(self): -> None (To train model)
  - predict(self, test_set): -> dict (predict $\hat{\mu}$ with uncertainties)

```python
def predict(self, test_set):
    """
    Predicts the values for the test set.

    Args:
        * test_set (dict): A dictionary containing the data and weights

    Returns:
        dict: A dictionary with the following keys:
        - 'mu_hat': The predicted value of mu.
        - 'delta_mu_hat': The uncertainty in the predicted value of mu.
        - 'p16': The lower bound of the 16th percentile of mu.
        - 'p84': The upper bound of the 84th percentile of mu.
    """

    test_data = test_set["data"]
    test_weights = test_set["weights"]

    print("[*] -> test weights sum = ", test_weights.sum())

    predictions = self.model.predict(test_data)


    result = self.stat_analysis.compute_mu(
        predictions,
        test_weights,
    )

    print("Test Results: ", result)

    return result
```

Hands-On

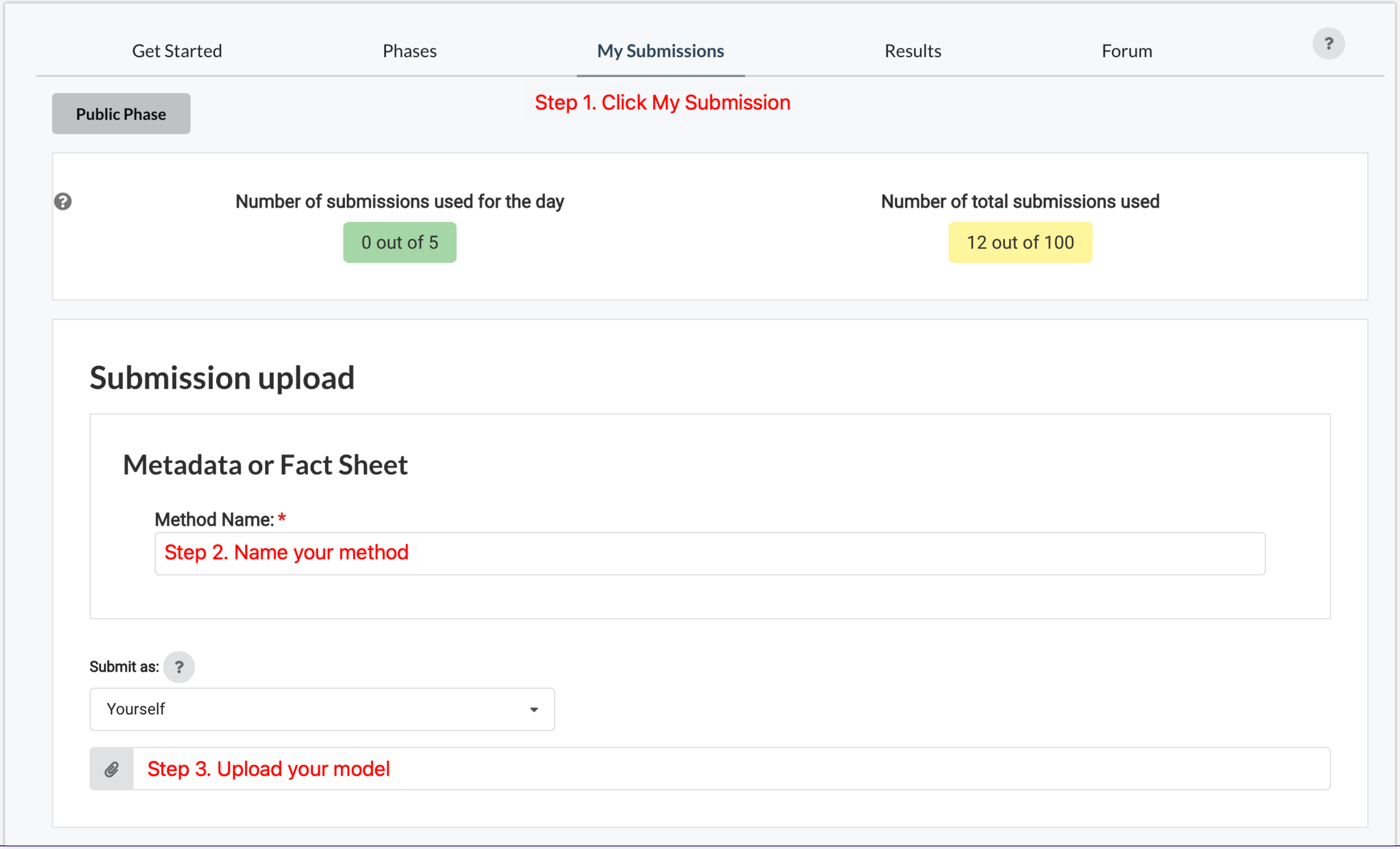
- Prepare for submission: zip the model

My_awesome_model/
- model.py
- necessary_scripts.py

→ My_awesome_model.zip

Hands-On

- Submit your model



Hands-On

Summary

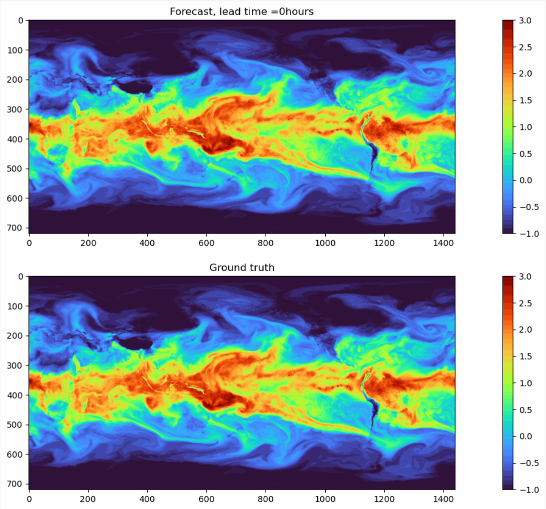
FAIR Universe

- We've built a **flexible platform** for hosting challenges and benchmarks, extending Codabench, and powered by **HPC at NERSC**.
- Launching a series of challenges focused on **uncertainty-aware methods for High-Energy Physics (HEP)**.
- A NeurIPS competition running from September 2024 to March 2025
- **Enter the HiggsML Uncertainty Challenge** now: https://www.codabench.org/competitions/2977/
- **We welcome feedback** on the challenge to keep it engaging and beneficial for advanced methods.
- **Get involved and stay updated:**
  - Help and feedback: Join the **#higgsml-uncertainty-challenge** channel on the Fair Universe Slack workspace.
  - Ongoing updates: Subscribe to the **Fair-Universe-Announcements Google Group**.
  - Questions or collaborations: Contact **fair-universe@lbl.gov**.

Backup

NERSC-AI Ecosystem

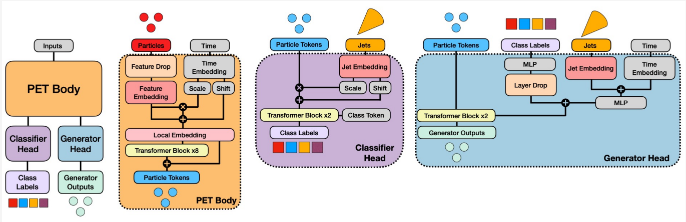
- ***Deploy*** optimized hardware and software (working with vendors)
  - Improve performance, e.g through benchmarking (MLPerf HPC)
- ***Apply*** cutting edge AI for science: e.g., “NESAP” program with postdocs
- ***Empower*** through e.g., over 20 DL@Scale tutorials, 1000s of total participants: (SC23)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



FourCastNet- Pathak et al. 2022

Collab with Nvidia, Caltech

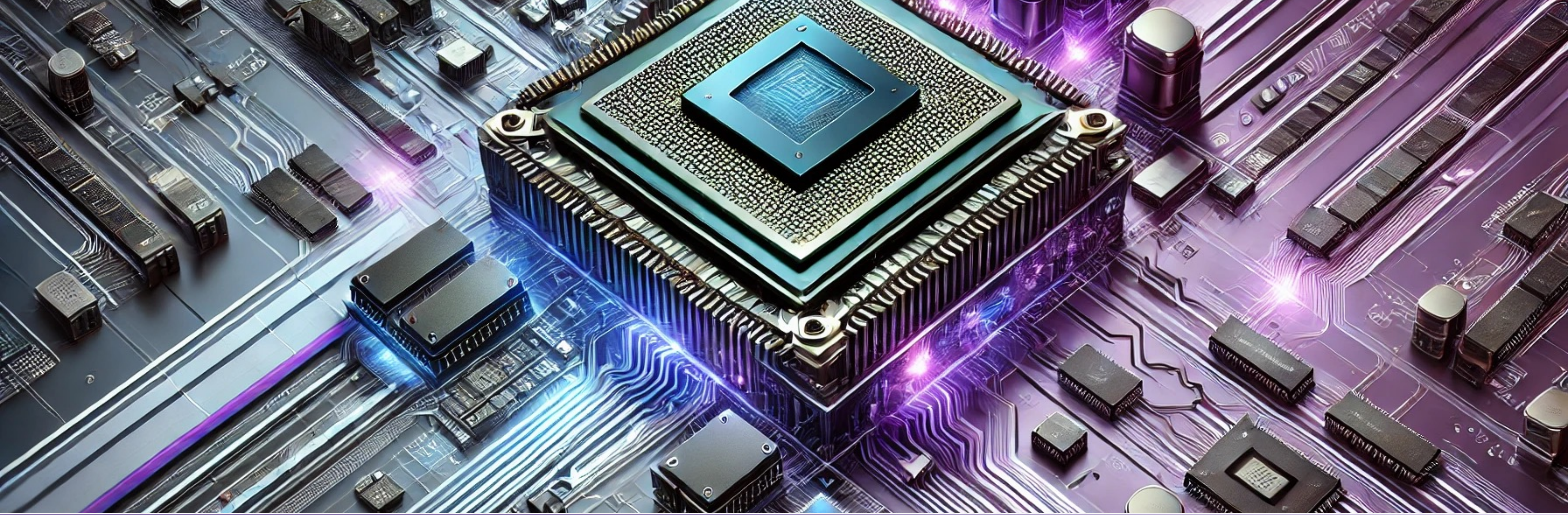
- First DL model with skill of numerical weather prediction (NWP)
- Train up to 1000s of GPUs
- Forecasts 1000s times faster than NWP



OmniLearn

H1 Collaboration (Mikuni et. al.):

jet physics analyses by enhancing accuracy, precision, and speed across multiple tasks using **a unified machine learning model**.

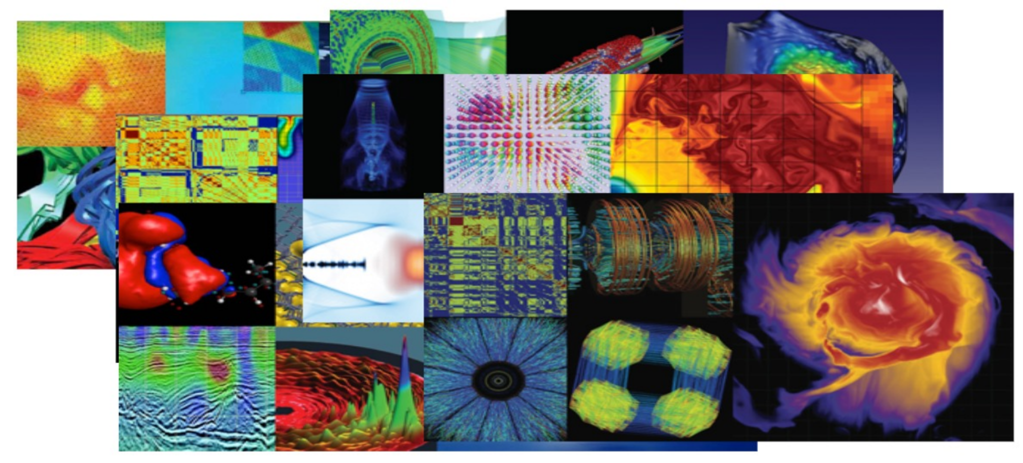


Large-compute-scale AI Ecosystem for hosting challenges and benchmarks

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

- Large compute systems
  - Perlmutter: ~7k A100 GPUs, Also high-capacity / fast filesystems, 1 Tbit/s WAN and flexible services
  - SPIN: Rancher/K8s platform for user-defined services

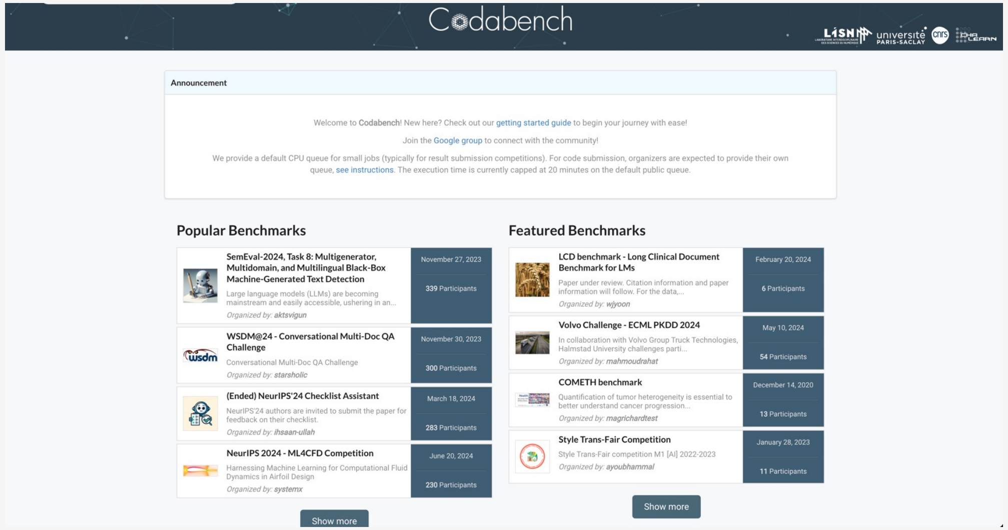
- Broad science user base
  - $>$ 10,000 users
  - $>$ 1,000 projects
  - Across all DoE Science e.g. HEP; NP; Climate; Fusion Chemistry; Materials; Genomics; etc …



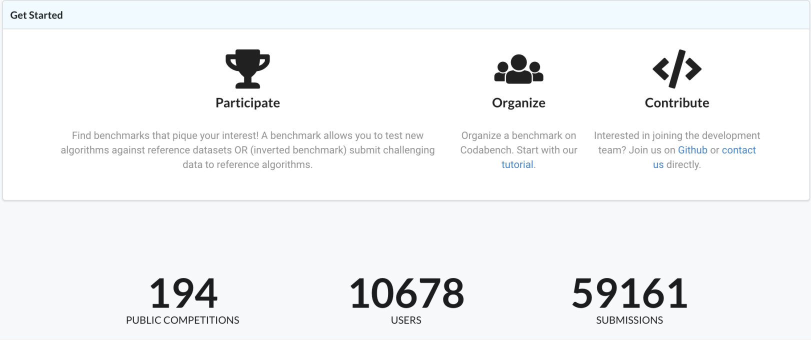
Condabench/FAIR Universe Platform

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

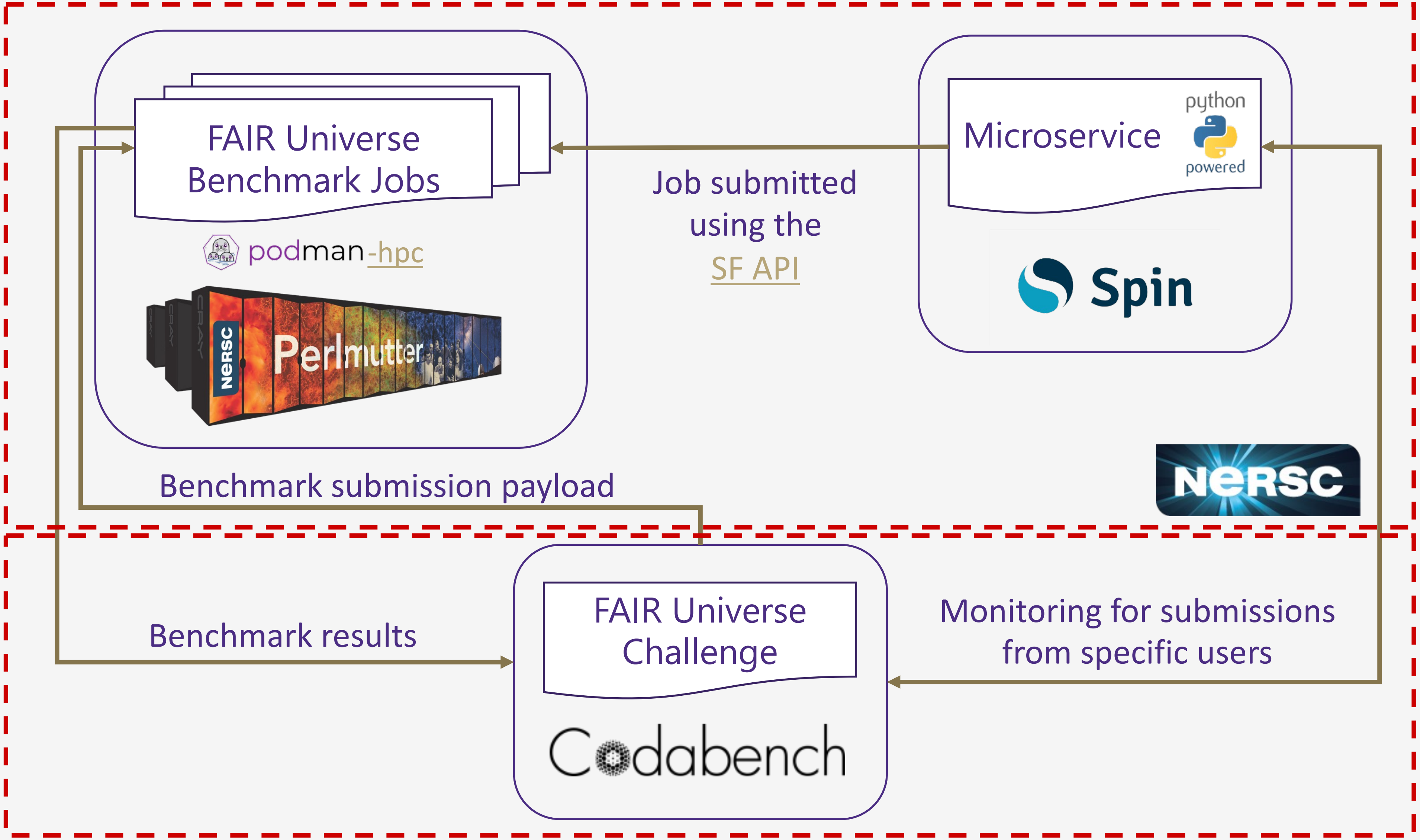
- Codabench - open-source platform for AI benchmarks and challenges
  - Originally (CodaLab) Microsoft/Stanford now a Paris-Saclay/LISN led community
  - **> 500 challenges** since 2013
  - Allows code submission as well as results e.g., for evaluation timing or reproducibility
  - Also, data-centric 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!



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