Reproducible Bayesian Workflows for Model Mixing and Calibration

Kyle Godbey

Slides with videos:
https://docs.google.com/presentation/d/1DkuXaGHSvYAYYSaTS-uZHLDs3-rkDhgp2Ck9OLrswvg/edit?usp=sharing

IRL-NPA | Dense Matter EOS Workshop
October 31st, 2024

What to expect?

> Tiny introduction and motivation

> `Brief` and `Biased` rundown of cool Bayesian things happening in nuclear physics

> Hands-on session for beginners and experts

What's our goal?

> Predictions and analyses using `Quantified Nuclear Models`

> We can quantify our `Uncertainty` as well as the `Information Content` of new (and old) measurements

What's our goal? (cont.)

> Combine the `wisdom of multiple models` in a principled way

> Aid in the `design of new experiments` (again, in a principled way)

What's our goal? (cont.)

> Com

model

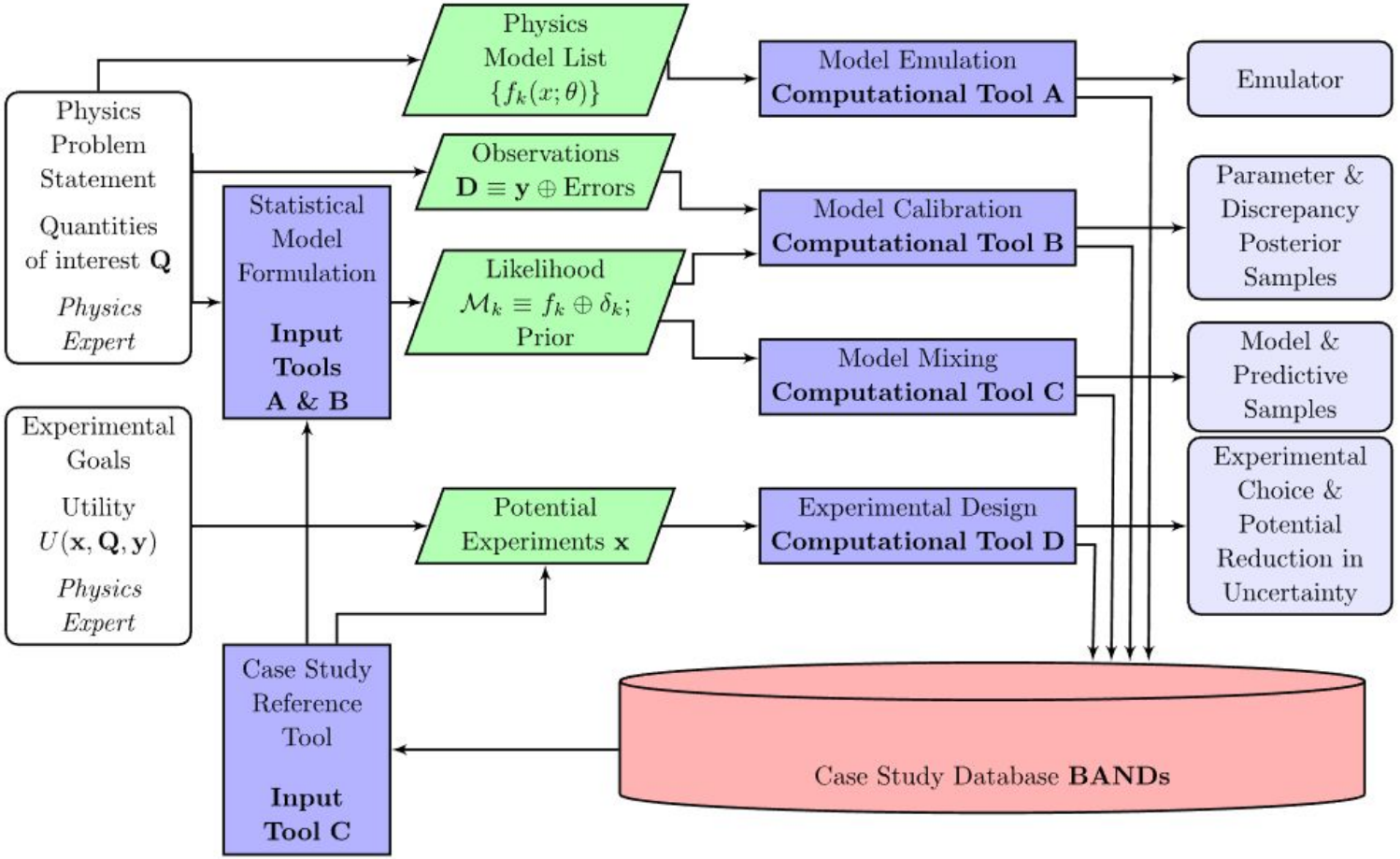
> Aid i

(again, in a principled way)

Get on the BAND Wagon: a Bayesian framework for quantifying model uncertainties in nuclear dynamics

To cite this article: D R Phillips *et al* 2021 *J. Phys. G: Nucl. Part. Phys.* **48** 072001

D R Phillips *et al* 2021 *J. Phys. G: Nucl. Part. Phys.* 48 072001



D R Phillips *et al* 2021 *J. Phys. G: Nucl. Part. Phys.* 48 072001

A note on Emulation

Does your model take a “long time” to evaluate? Maybe a surrogate model is for you!

There has been incredible progress on `Model-driven` and `Data-driven` emulation techniques in nuclear physics contexts

Dimensionality Reduction in Nuclear Physics
Presented by ASCSN

Aplication 5: Black-Box Methods

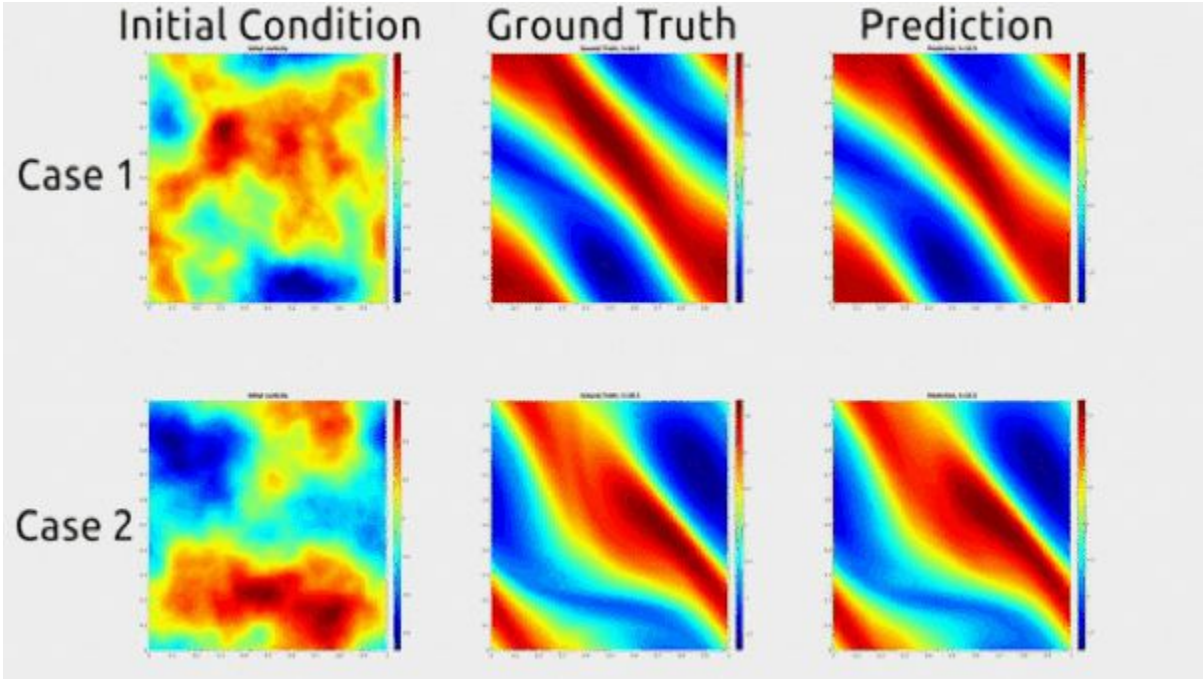
Efficient Emulation of SECAR Beam

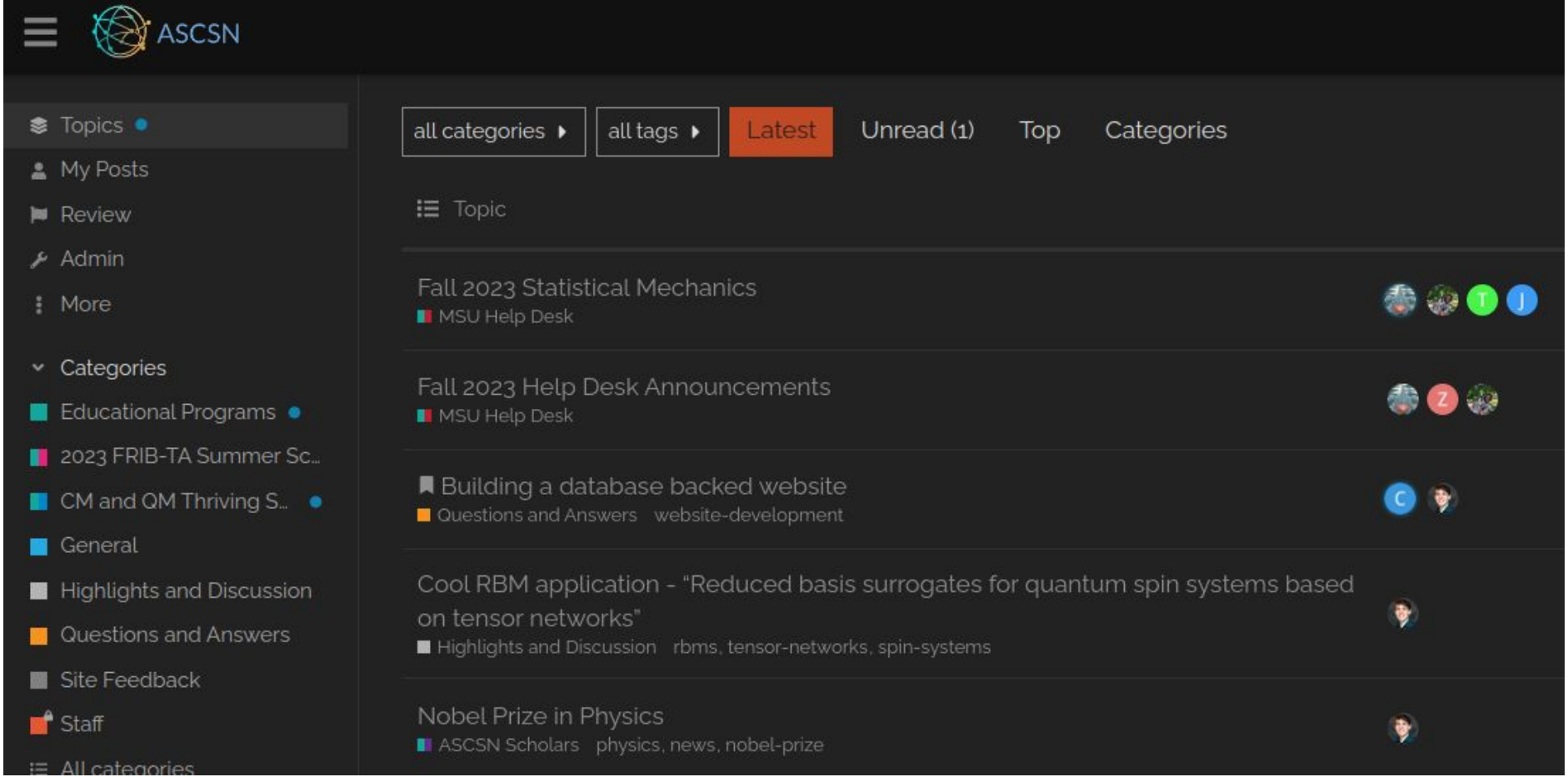
Non-linear and non-affine problem

Always accepting new examples!

https://dr.ascsn.net

Dimensionality Reduction in Nuclear Physics
Presented by ASCSN


Initial Condition
Ground Truth
Prediction
Case 1
Case 2



https://forum.ascsn.net

Onto the Challenges!

Who here has done a few Bayesian analyses in the past?

For the experienced, I recommend either exploring:

1) Posterior storage and distribution
2) Model Mixing
3) Or whatever else seems fun :)

Reproducibility and Accessibility

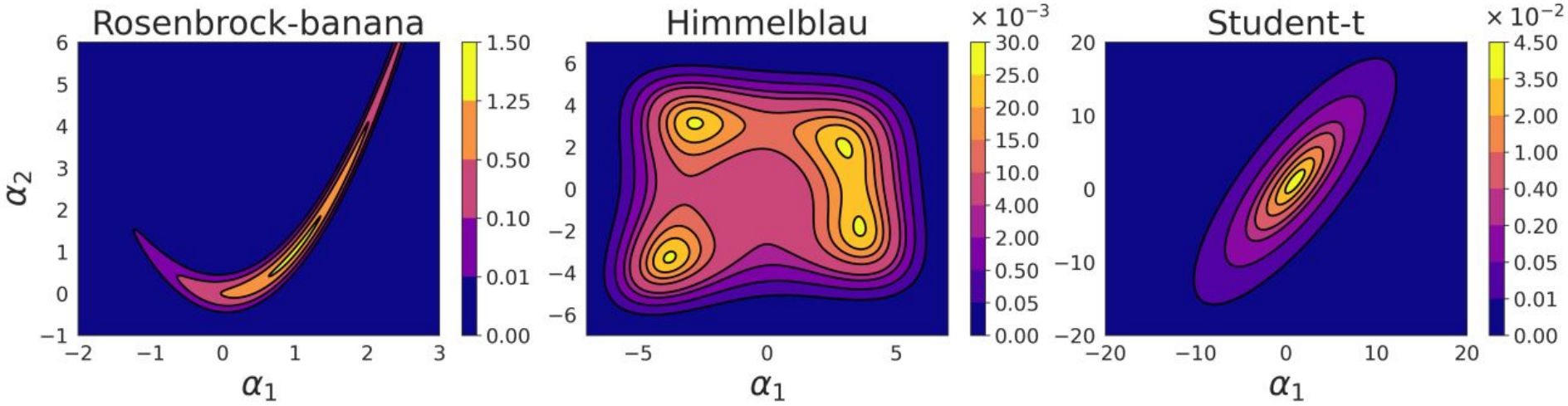
A few challenges include:

- Agility in the face of new data
- Efficiency of calibration
- Distribution of Bayesian posteriors (not just samples!)
- Traceability and reproducibility of results

Y. Yamauchi, L. Buskirk, P. Giuliani, K. Godbey, Normalizing Flows for Bayesian Posteriors: Reproducibility and Deployment, (submitted) (2023).

Reproducibility and Accessibility

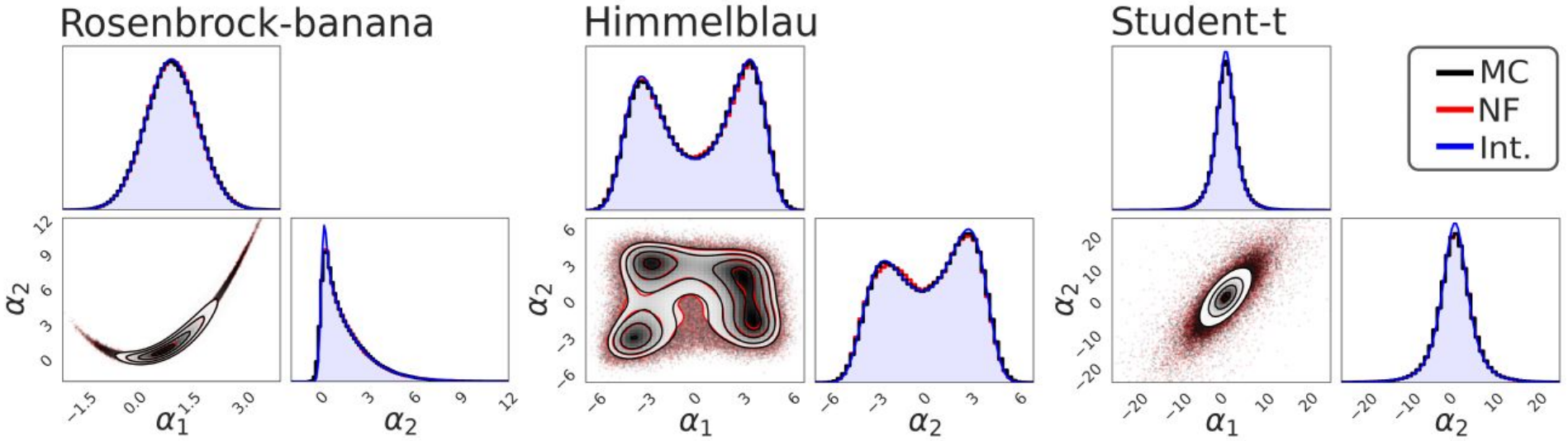
Our approach: use an ML approach to learn normalizing flows for the high-dimensional posterior distributions



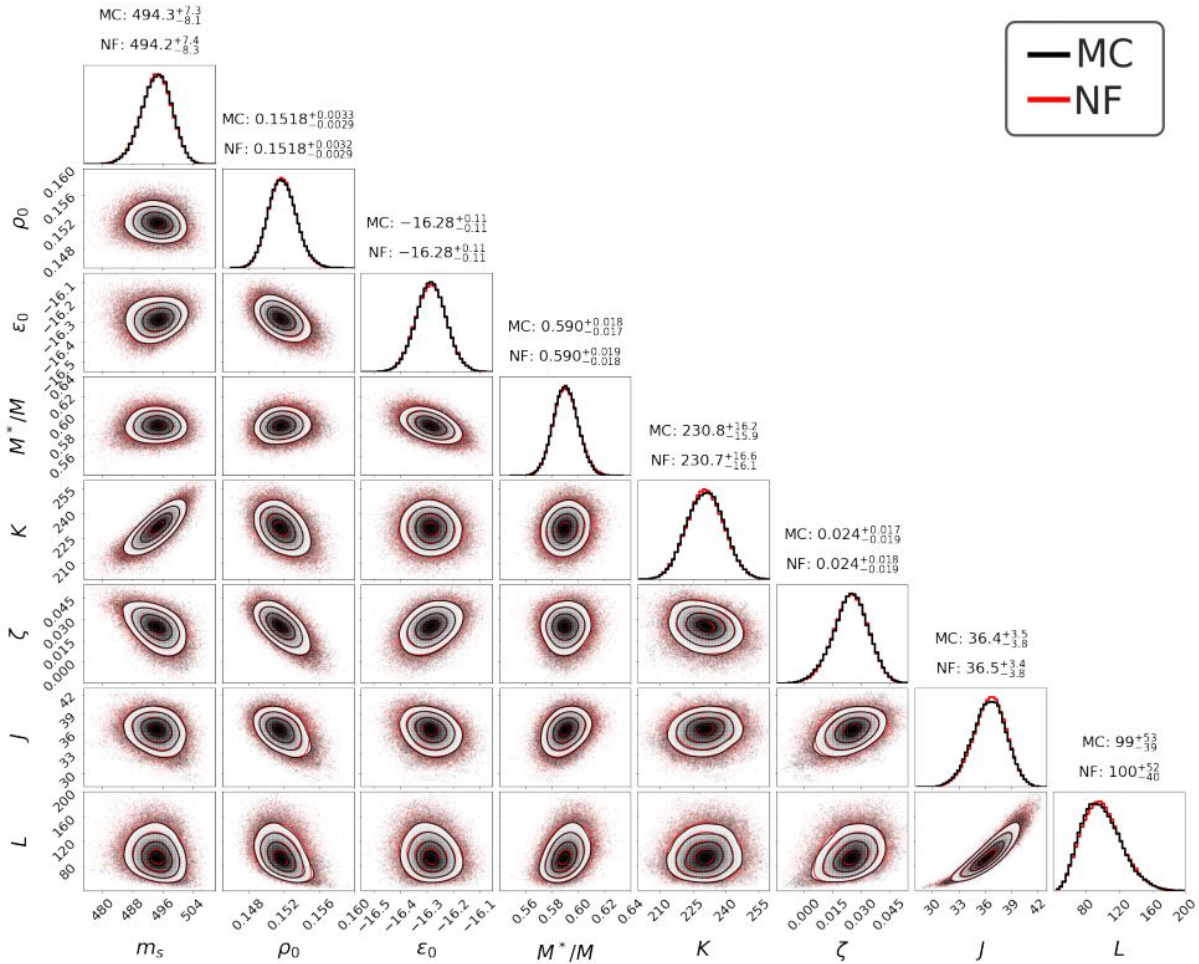
Y. Yamauchi, L. Buskirk, P. Giuliani, K. Godbey, Normalizing Flows for Bayesian Posteriors: Reproducibility and Deployment, (submitted) (2023).

Reproducibility and Accessibility

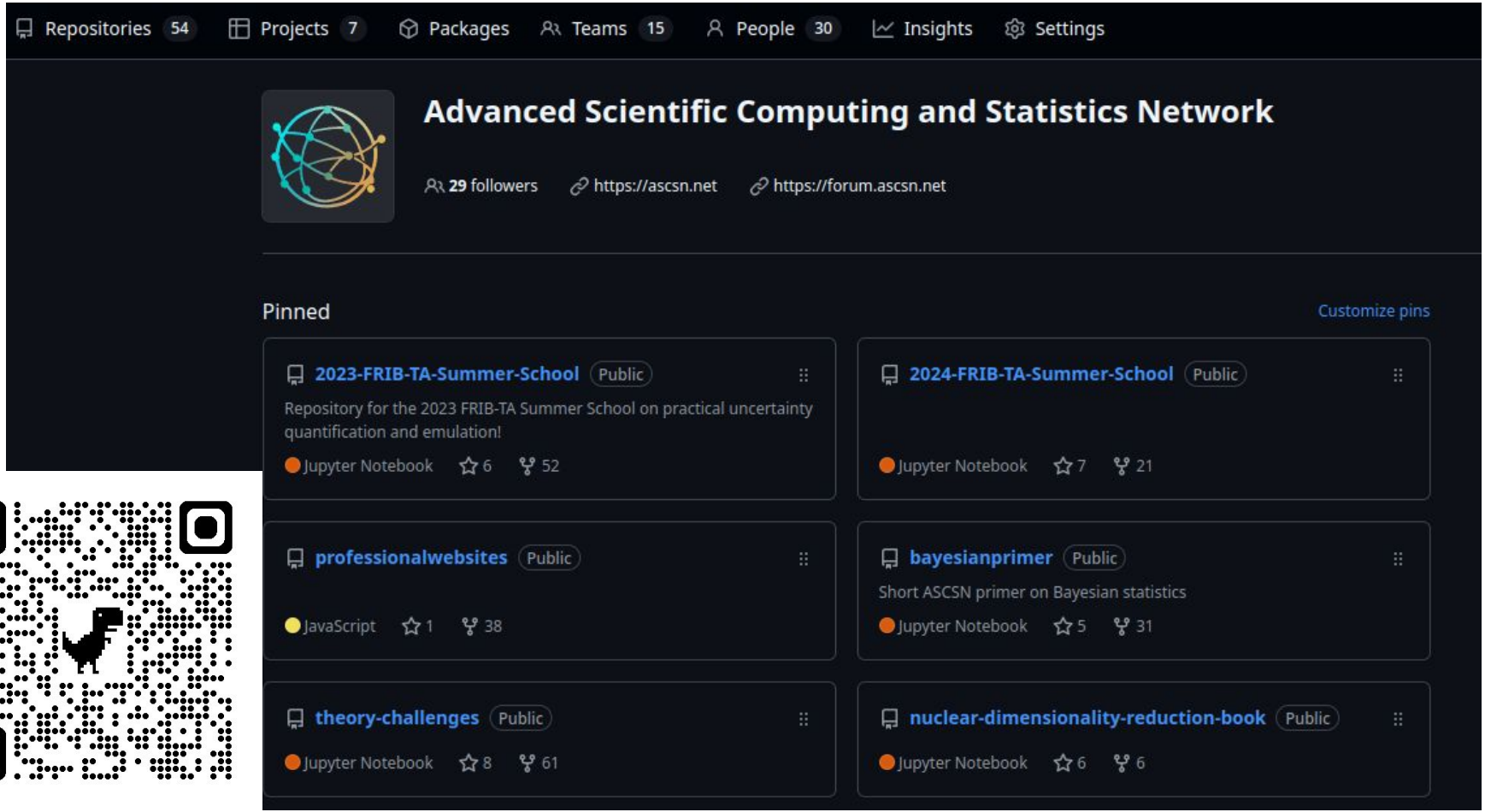
Our approach: use an ML approach to learn normalizing flows for the high-dimensional posterior distributions



S. Yamauchi, L. Buskirk, P. Giuliani, K. Godbey, Normalizing Flows for Bayesian Posteriors: Reproducibility and Deployment, (submitted) (2023).



Y. Yamauchi, L. Buskirk, P. Giuliani, K. Godbey, Normalizing Flows for Bayesian Posteriors: Reproducibility and Deployment, (submitted) (2023).



https://github.com/ascsn

Model Mixing

For a directed challenge, check out:

https://github.com/ascsn/2023-FRIB-TA-Summer-School/tree/main/model-mixing

Model Mixing

For nice model mixing details, visit the following:

https://bandframework.github.io/Taweret/landing.html

Practical Bayes

For the challenges on practical Bayes, visit:

https://github.com/ascsn/2023-FRIB-TA-Summer-School/tree/main/practical-bayes

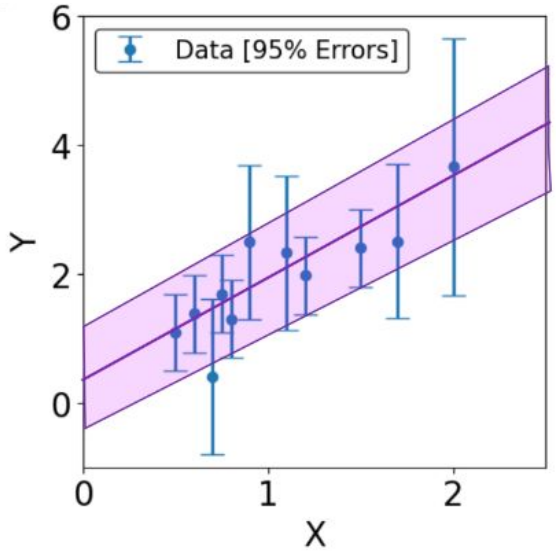
Practical Bayes

Prior and likelihood building

Sampling from posterior and plotting it

Calculating new things

$$f(x, \alpha) = \alpha_0 + \alpha_1 x$$



Immense Gratitude to All Collaborators!

Funding

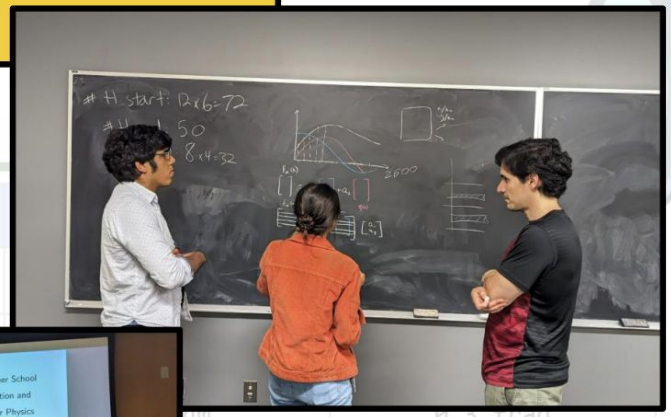
DOE NNSA Grant No. DE-NA0004074
DOE Grant Nos. DE-SC0013365, DE-SC0023175
NSF CSSI Program No. 2004601

Computing Resources

Australian National Computational Infrastructure Raijin and Gadi
Oak Ridge Leadership Computing Facility Summit and Frontier
Argonne Leadership Computing Facility Polaris
Texas A&M High Performance Research Computing Terra and Ada
Michigan State University HPCC

Theory Alliance
FACILITY FOR RARE ISOTOPE BEAMS

FRIB-TA Summer School: Practical Uncertainty Quantification and Emulator Development in Nuclear Physics

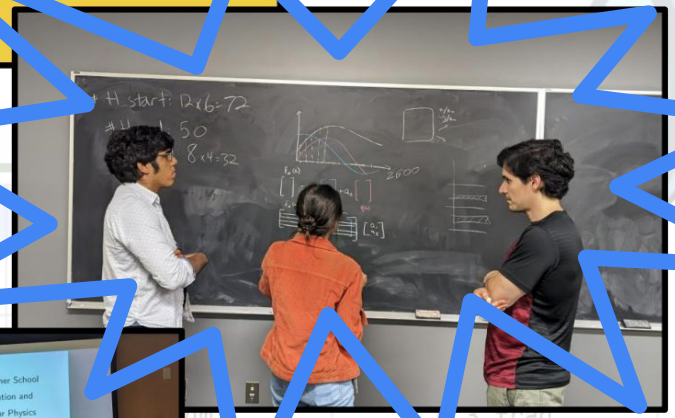


~60 participants spanning a wide audience

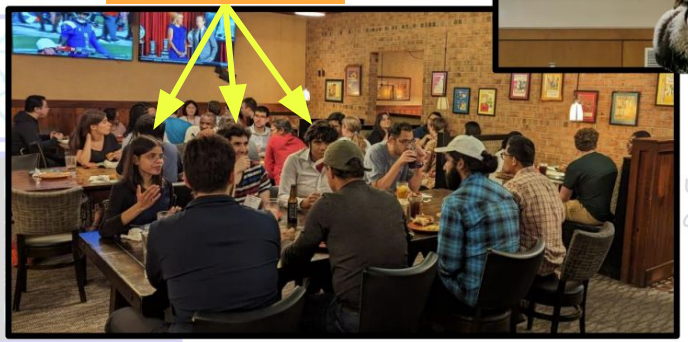
Slide from Pablo Giuliani

Theory Alliance
FACILITY FOR RARE ISOTOPE BEAMS

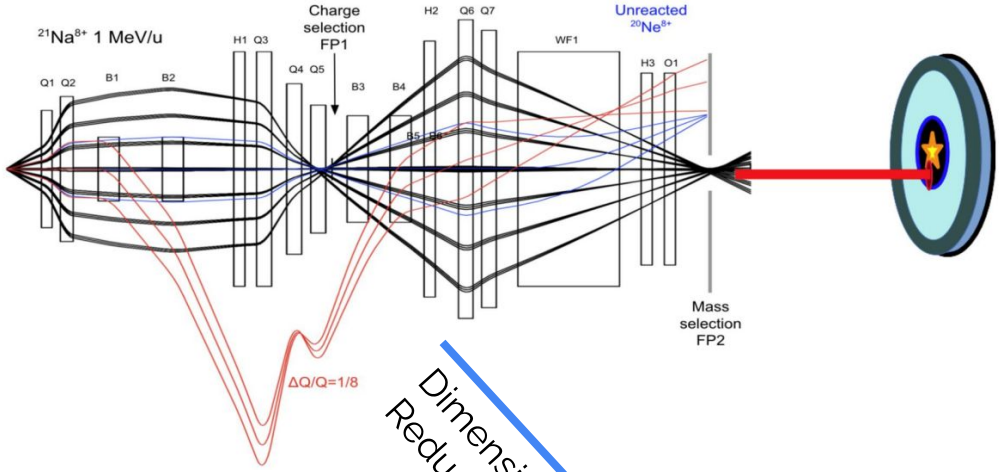
FRIB-TA Summer School: Practical Uncertainty Quantification and Emulator Development in Nuclear Physics



Social, too!



Slide from Pablo Giuliani



Dimensionality Reduction

PRELIMINARY

# of Bases	Emulation Time (to FP1)	Max Position Error (x)	Max angular Error (ax)
3	(9.7 ± 0.3) ms*	1 µm	1 nrad
10	(10.9 ± 0.6) ms*	0.01 µm	7.5 prad
15	(12.1 ± 0.2) ms*	0.7 nm	0.3 frad

Fast

Accurate