

# 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>



# 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.)

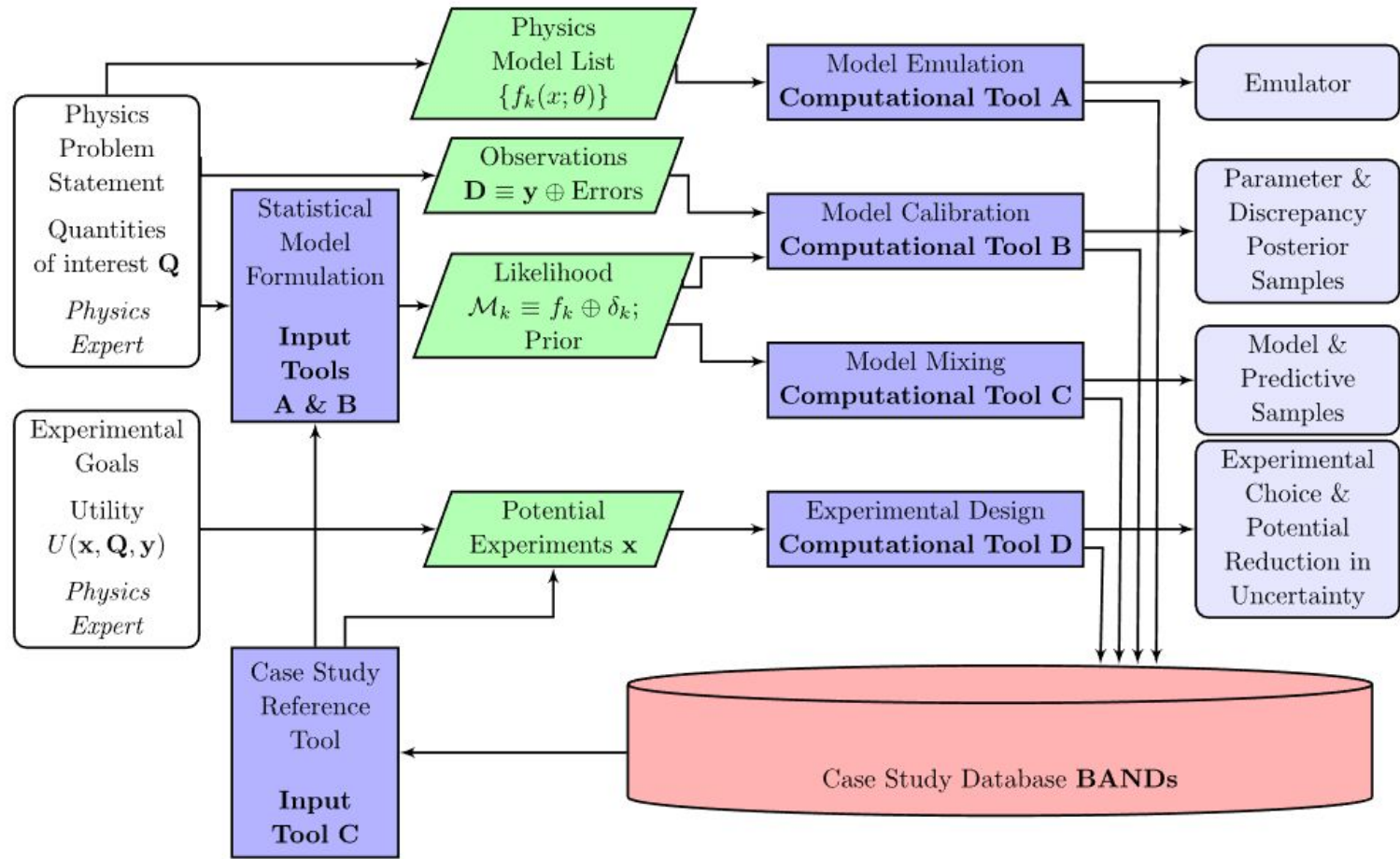
> Com  
model

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

> Aid in  
(again, in a principled way)

To cite this article: 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



Application 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

Introduction to Dimensionality  
Reduction in Nuclear Physics

Introduction

Application 1: The Quantum Harmonic  
Oscillator

Application 2: Two body single channel  
nuclear scattering

Application 3: The Empirical  
Interpolation Method

Application 4: Time Dependent Systems  
(evolution in the reduced space)

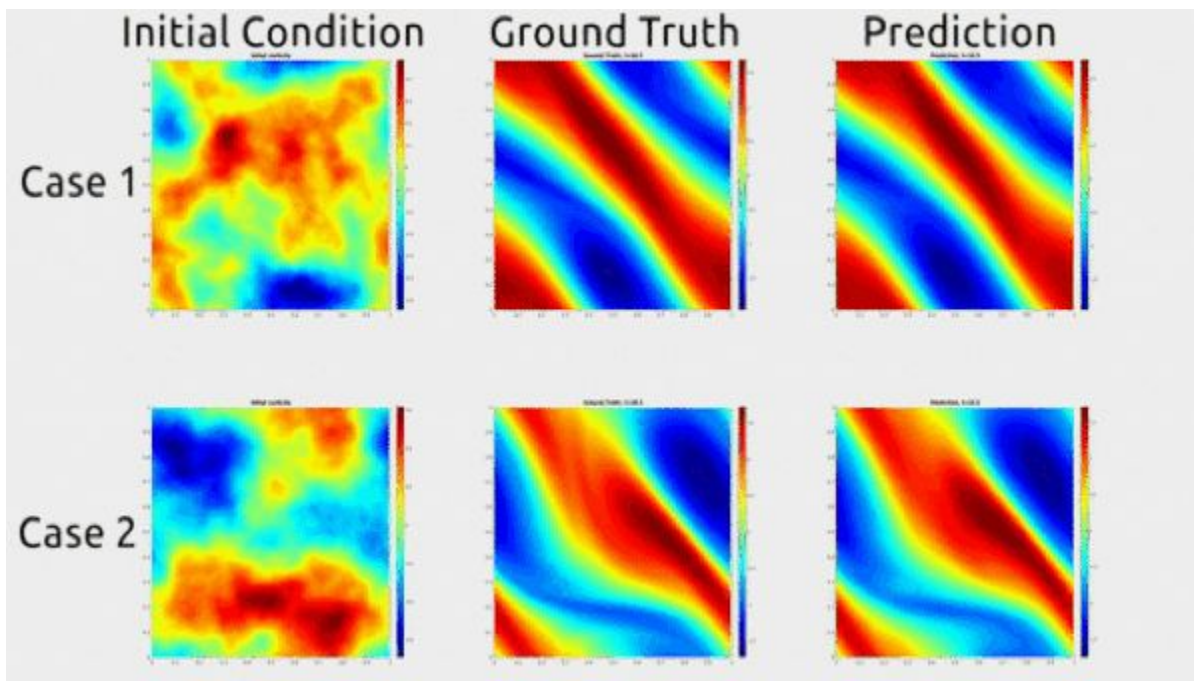
Application 5: Black-Box Methods

Contributors



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





Topics

My Posts

Review

Admin

More

Categories

Educational Programs

2023 FRIB-TA Summer Sc...

CM and QM Thriving S...

General

Highlights and Discussion

Questions and Answers

Site Feedback

Staff

All categories

all categories

all tags

Latest

Unread (1)

Top

Categories

Topic

Fall 2023 Statistical Mechanics

MSU Help Desk



Fall 2023 Help Desk Announcements

MSU Help Desk



Building a database backed website

Questions and Answers website-development



Cool RBM application - "Reduced basis surrogates for quantum spin systems based on tensor networks"

Highlights and Discussion rbms, tensor-networks, spin-systems



Nobel Prize in Physics

ASCSN Scholars physics, news, nobel-prize



# 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

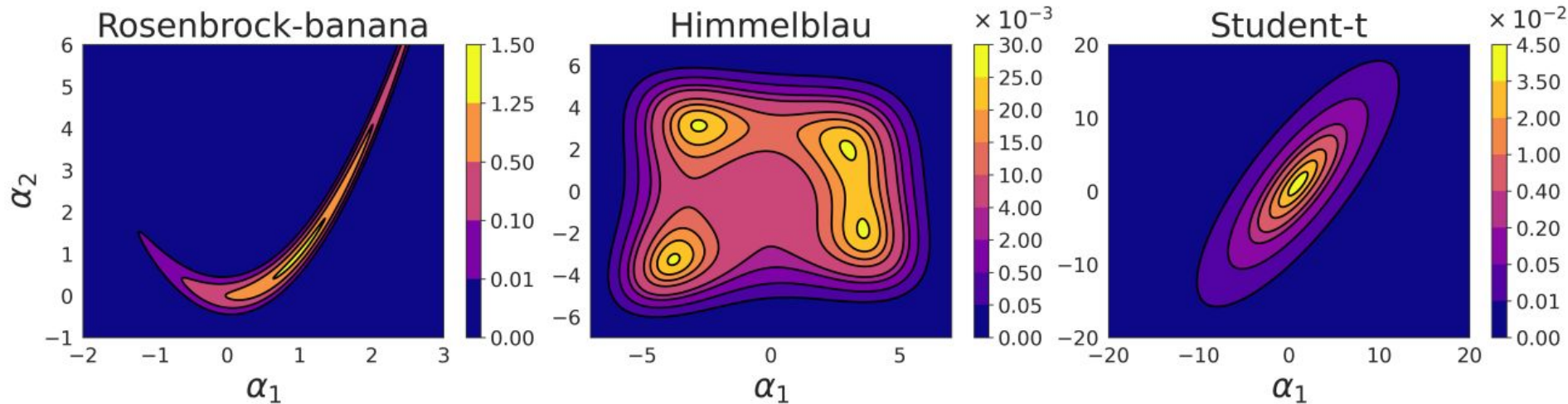
A few challenges include:

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



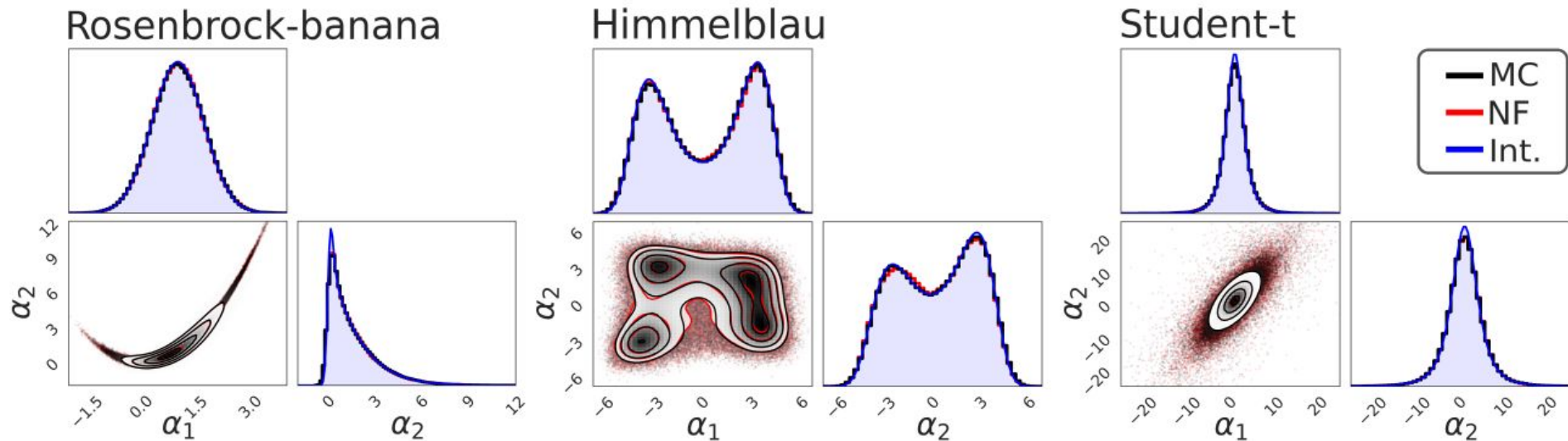
# Reproducibility and Accessibility

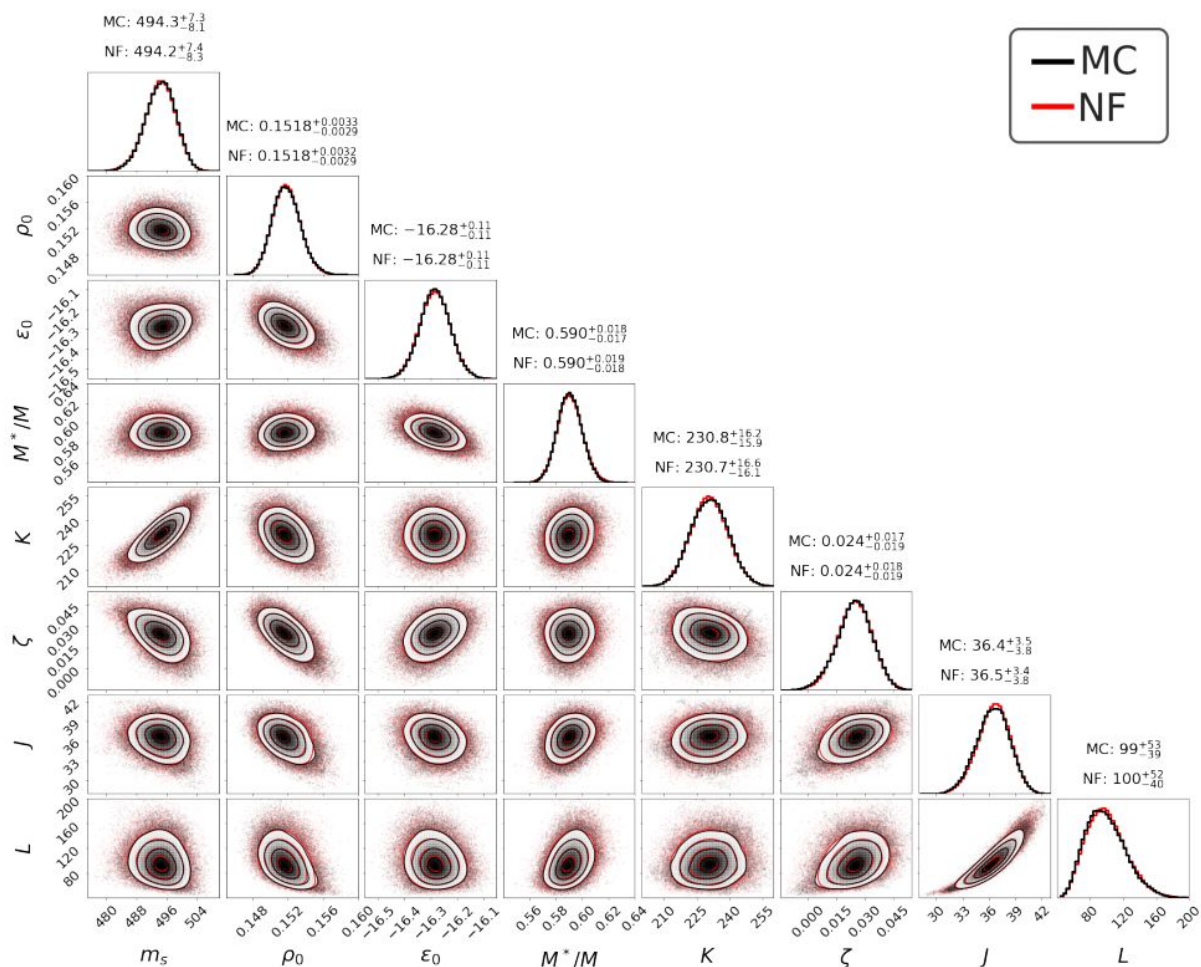
Our approach: use an ML approach to learn normalizing flows for the high-dimensional posterior distributions



# Reproducibility and Accessibility

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









# Advanced Scientific Computing and Statistics Network

29 followers <https://ascsn.net> <https://forum.ascsn.net>

## Pinned

[Customize pins](#)

 [2023-FRIB-TA-Summer-School](#) Public 

Repository for the 2023 FRIB-TA Summer School on practical uncertainty quantification and emulation!

 Jupyter Notebook  6  52

 [2024-FRIB-TA-Summer-School](#) Public 

 Jupyter Notebook  7  21

 [professionalwebsites](#) Public 

 JavaScript  1  38

 [bayesianprimer](#) Public 

Short ASCSN primer on Bayesian statistics

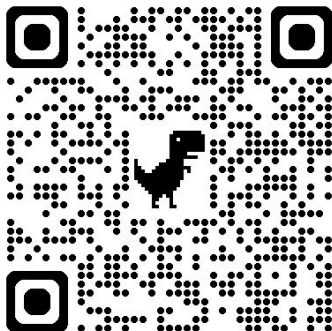
 Jupyter Notebook  5  31

 [theory-challenges](#) Public 

 Jupyter Notebook  8  61

 [nuclear-dimensionality-reduction-book](#) Public 

 Jupyter Notebook  6  6



IRL-NPA |

Dense Matter EOS Workshop  
October 31st, 2024

<https://github.com/ascsn>

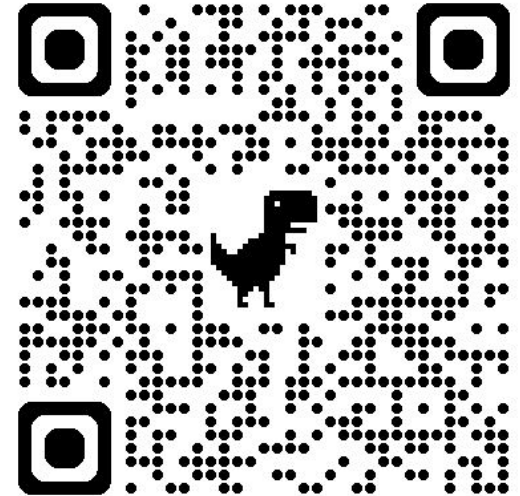


# Model Mixing



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>

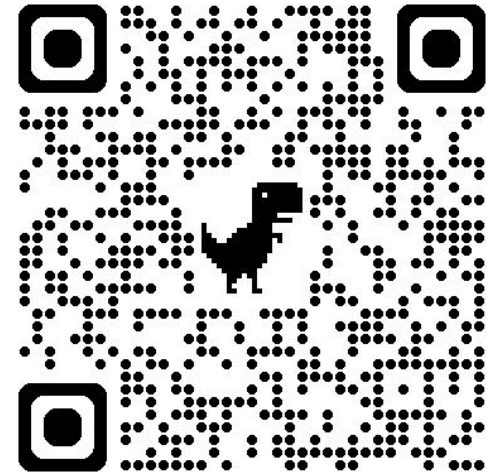


# Practical Bayes

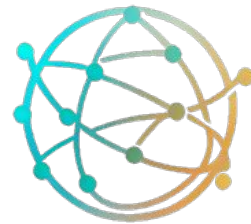


For the challenges on practical Bayes, visit:

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



# Practical Bayes

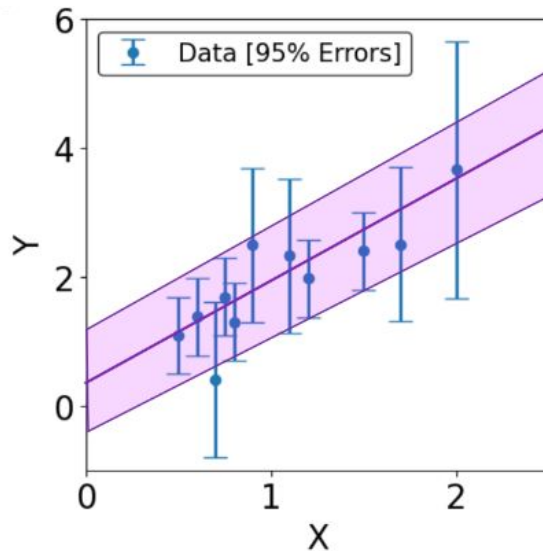


Prior and likelihood building

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



Theory Alliance  
FACILITY FOR RARE ISOTOPE BEAMS

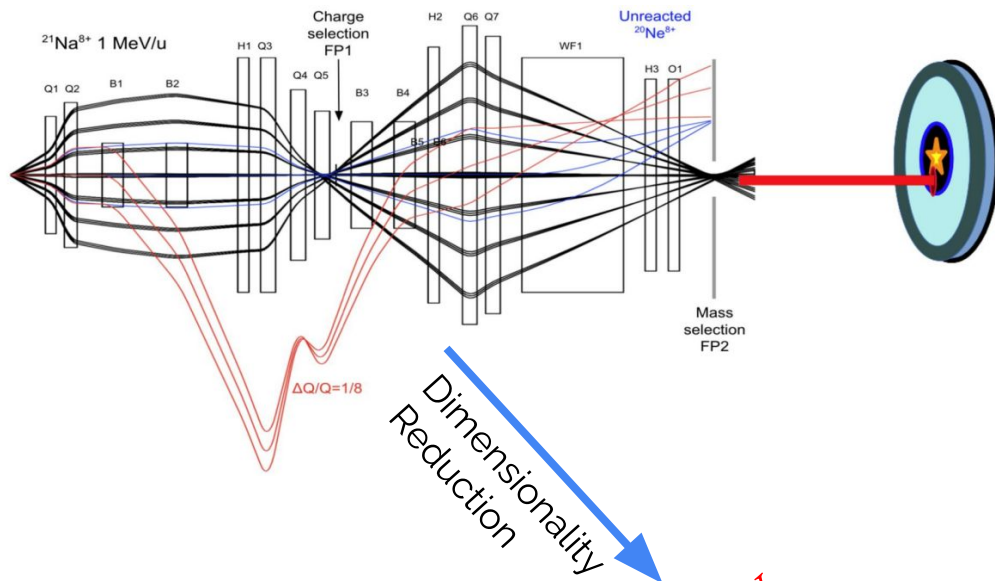
# FRIB-TA Summer School: Practical Uncertainty Quantification and Emulator Development in Nuclear Physics



Social, too!



equations  
data



**PRELIMINARY**

# of Bases	Emulation Time (to FP1)	Max Position Error (x)	Max angular Error ( $\alpha_x$ )
3	$(9.7 \pm 0.3)$ ms*	1 $\mu\text{m}$	1 nrad
10	$(10.9 \pm 0.6)$ ms*	0.01 $\mu\text{m}$	7.5 prad
15	$(12.1 \pm 0.2)$ ms*	0.7 nm	0.3 frad

↑  
Fast

↙ ↘  
Accurate

