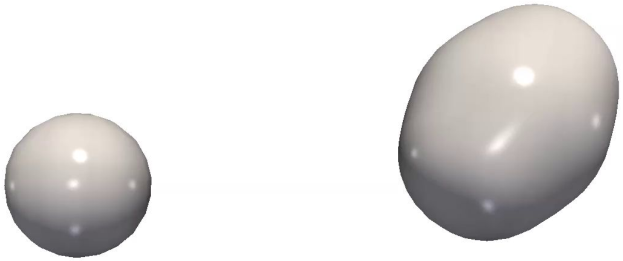
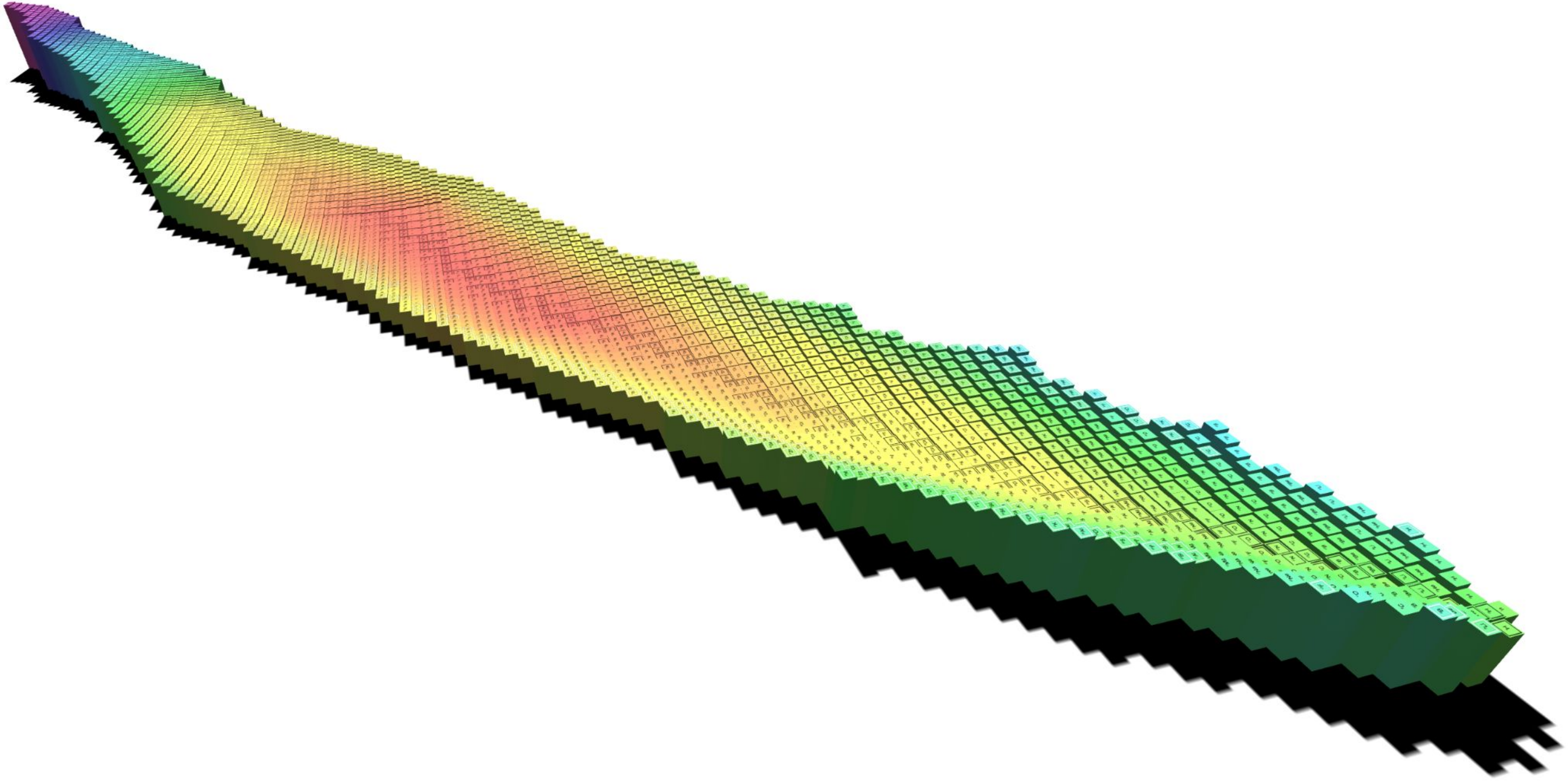
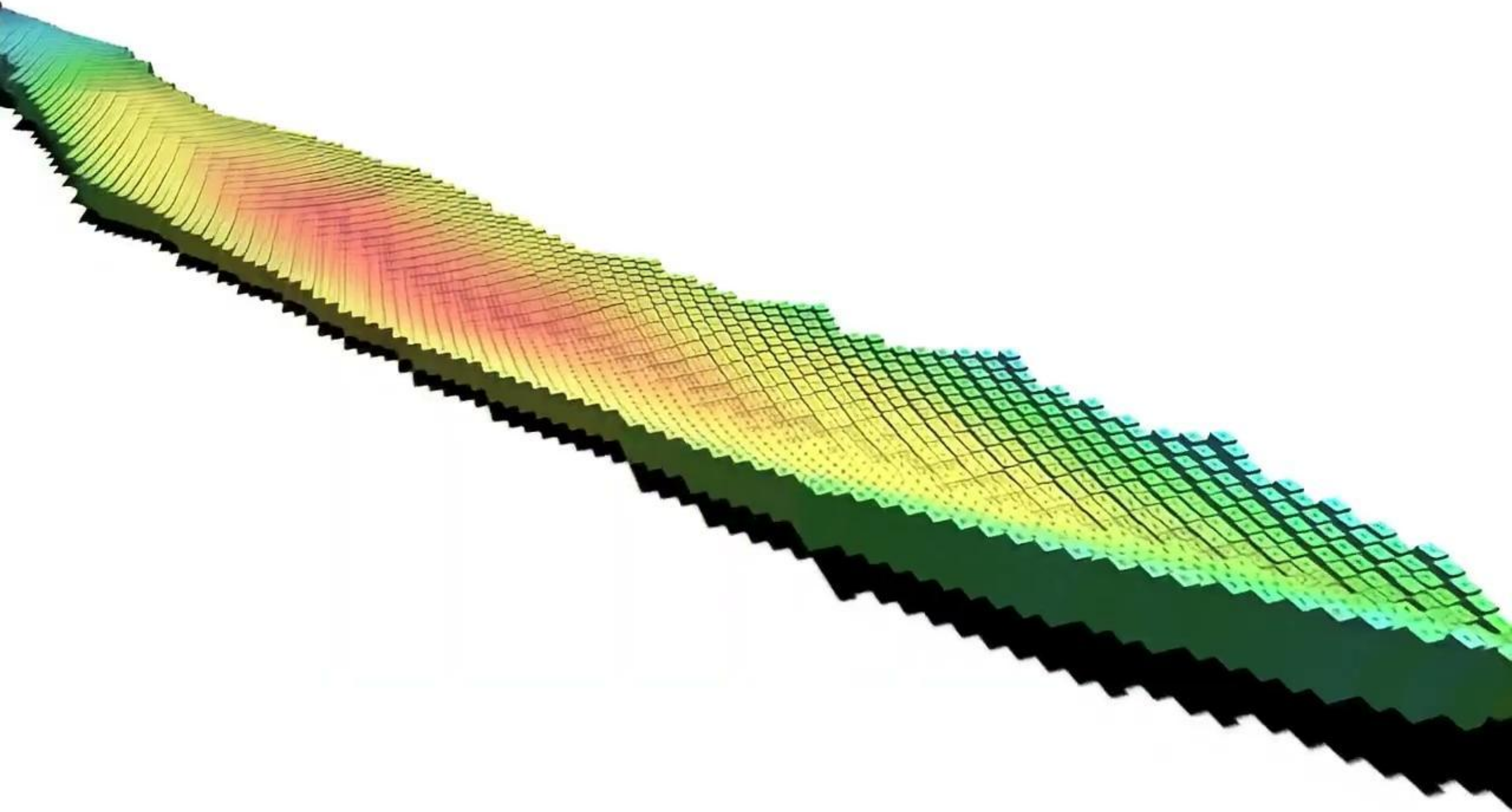
Efficient Bayesian Model Combination With pybmc

Kyle Godbey



Slides with videos: https://docs.google.com/presentation/d/1xRZo72xdc_uwMq-Jl6Gk9myKCNaJ4I2mLoLPHqvQcQo/edit?usp=sharing





What's Model Combination?

Model Combination

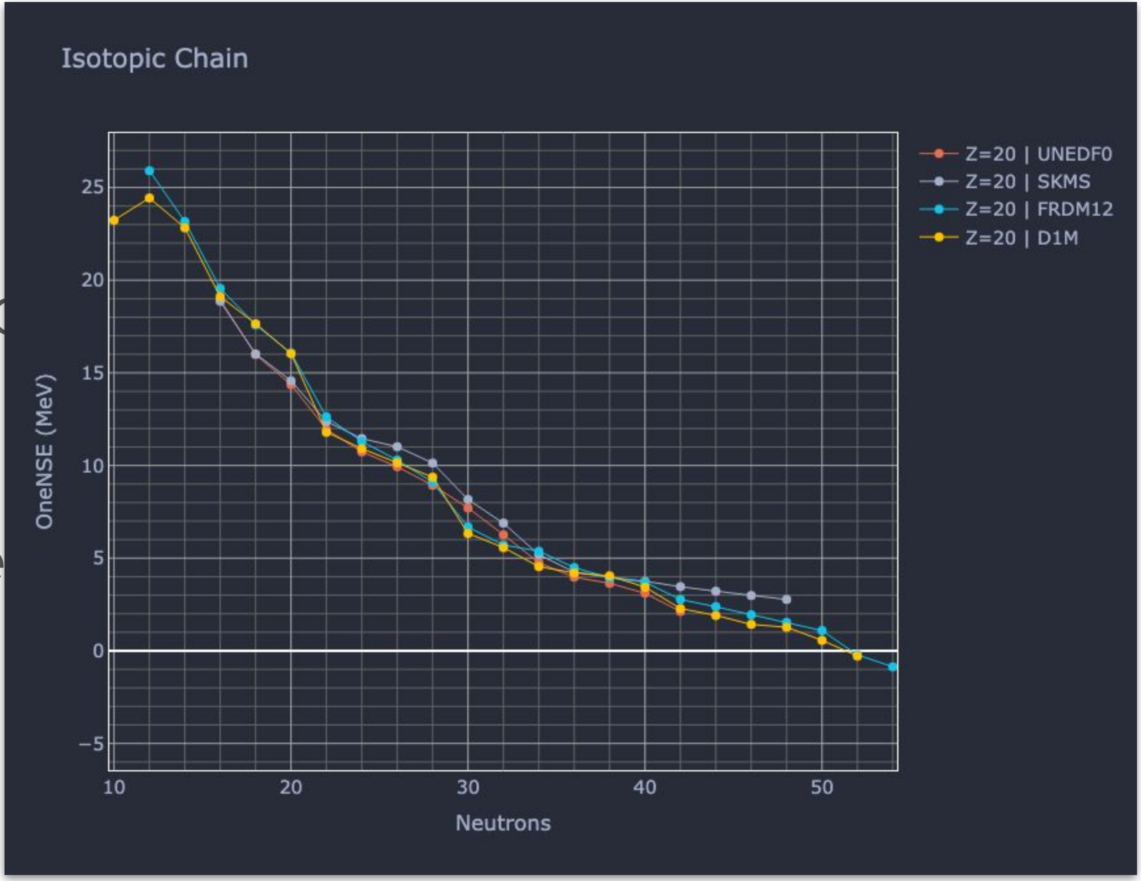
Imagine a scenario where you have many wrong (and potentially useful) models

Will they be wrong in the same ways and places? Are they equally useful?

Model Combination

Imagine a sc
wrong (and

Will they be
places? Are



The Bayesian Mass Explorer
https://bmex.dev

Model Combination

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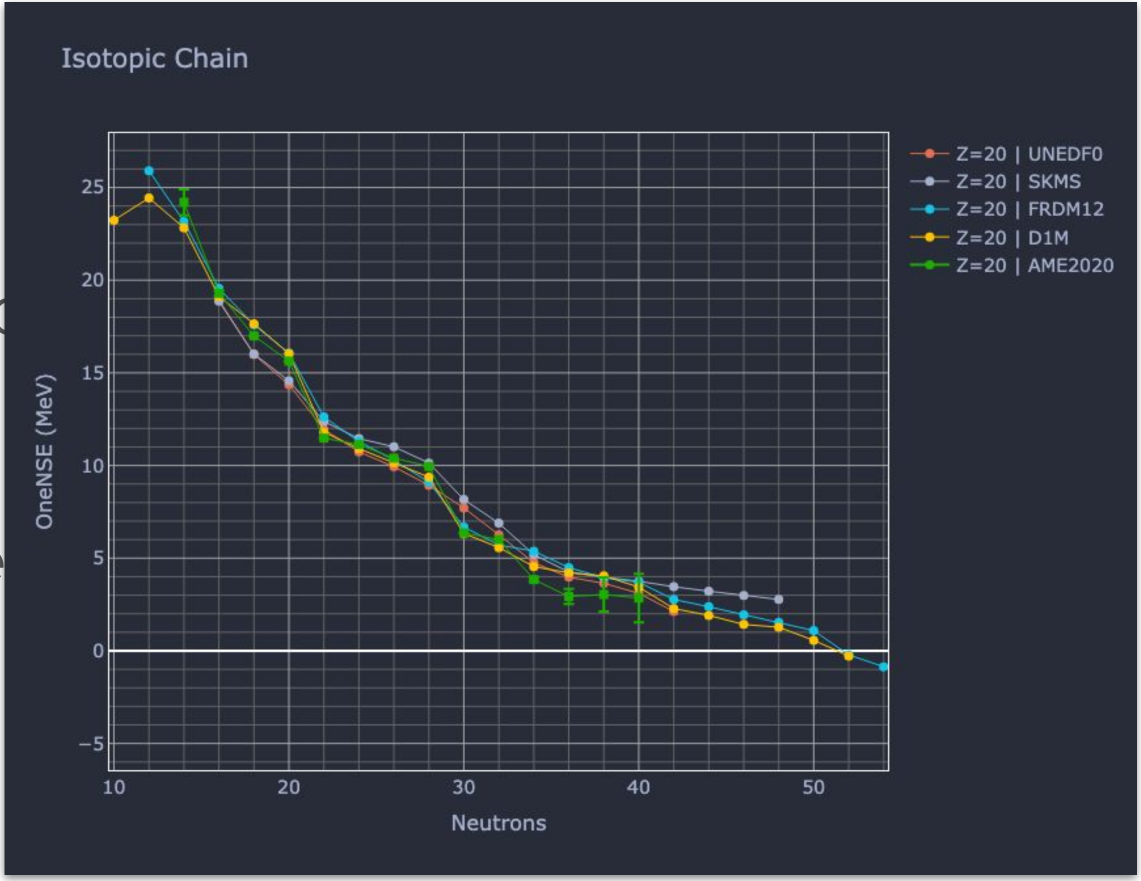

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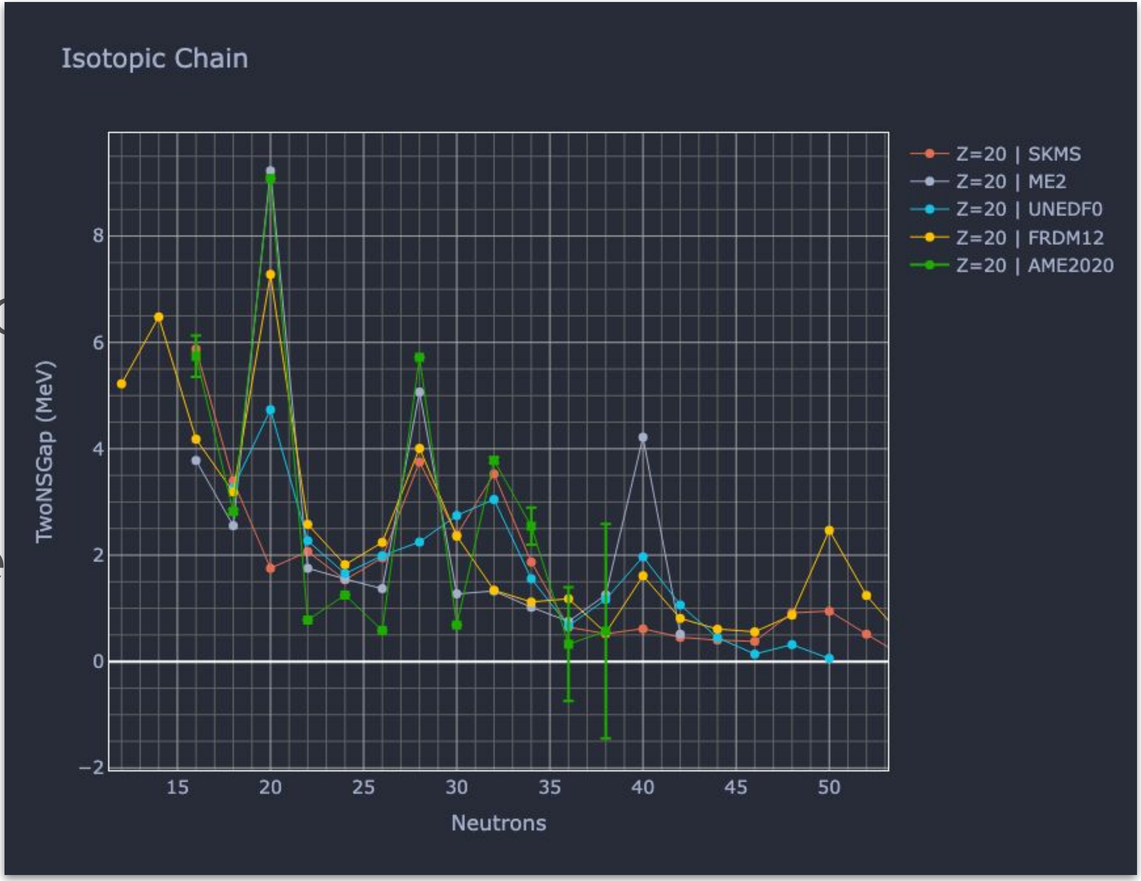
Model Combination



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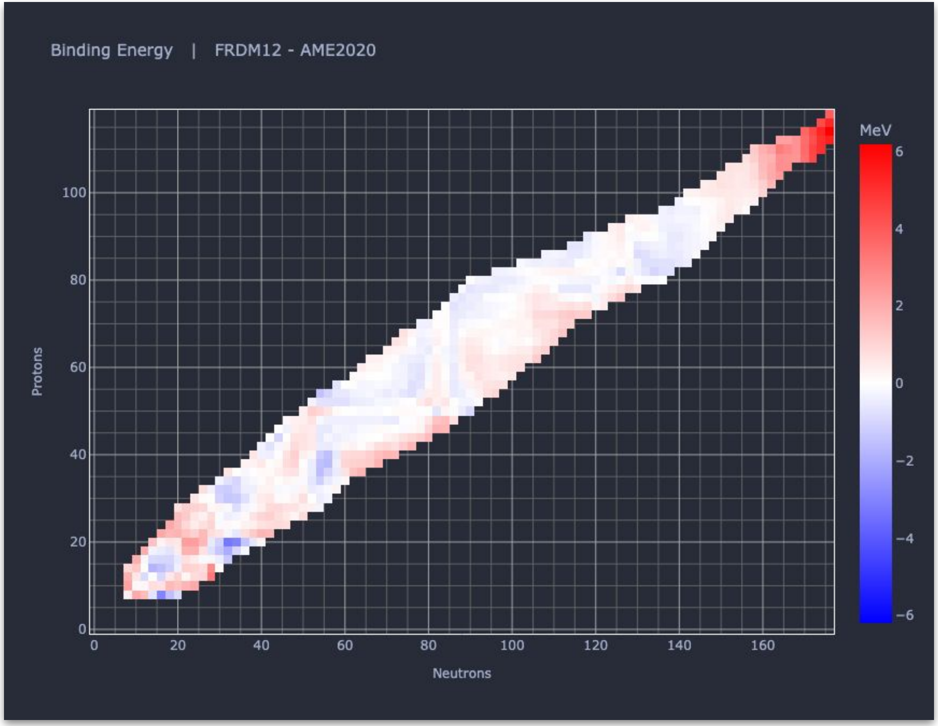
Binding Energy | FRDM12 - AME2020
MeV
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Neutrons
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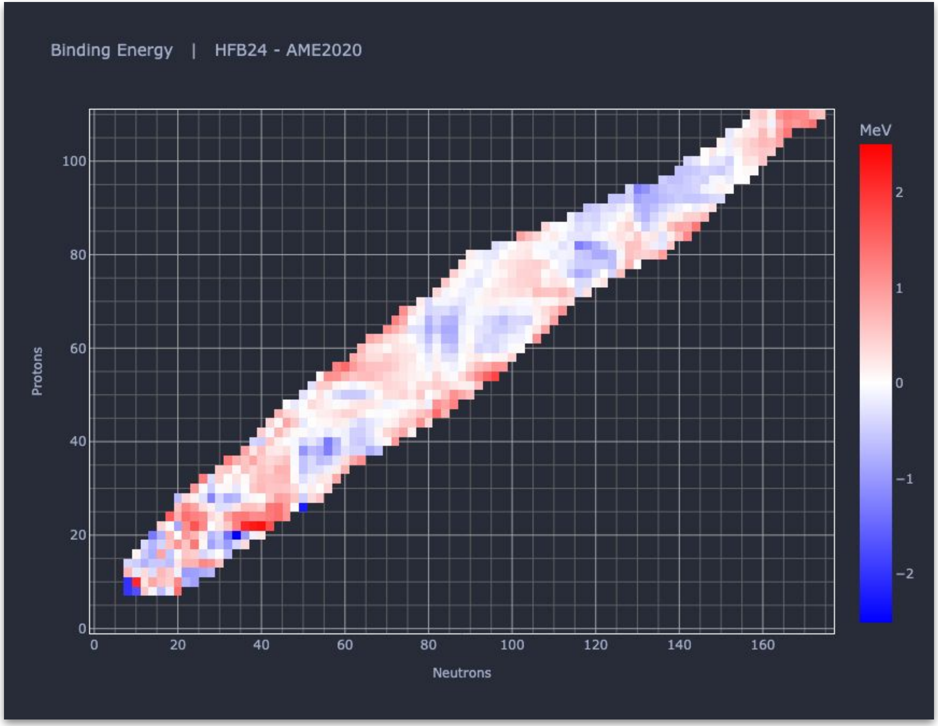
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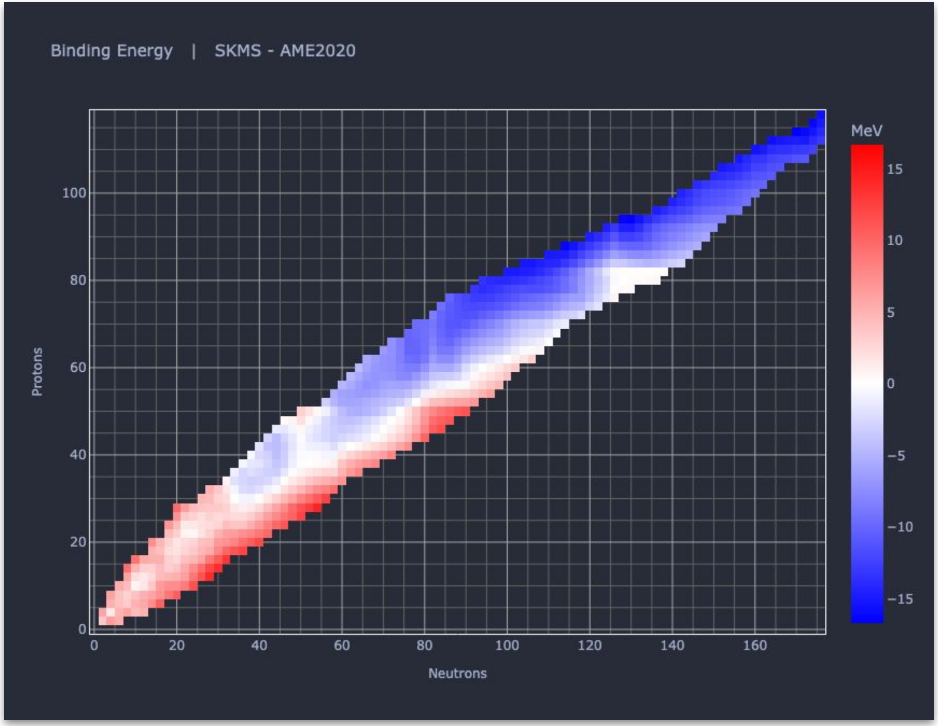

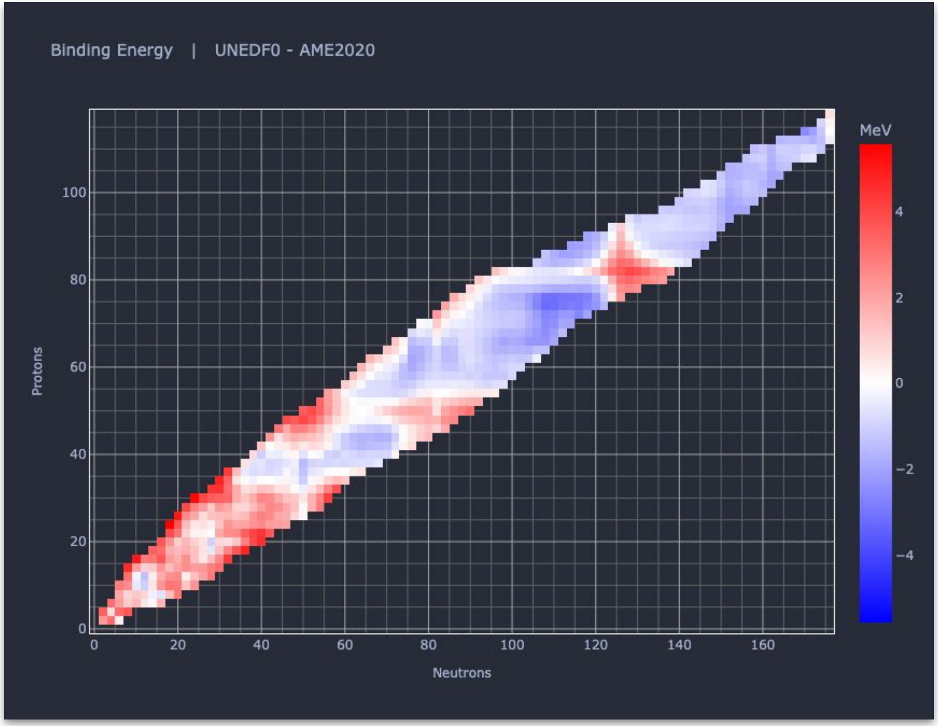

The Bayesian Mass Explorer
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Model Combination

Model combination techniques provide a prescription on how to handle this!

This talk is going to focus on **forecast combination** specifically, i.e. where we already have independent model forecasts prepared

Model Combination (+ orthogonalization)

Additionally, we'll orthogonalize our forecasts to remove model redundancies

Side benefit: we can truncate the principal components to get less overfitting

Model Combination (+ orthogonalization)

First, center your data

$$X_{i,k}^{c} = X_{i,k}^{0} - \phi_0\left(x_i\right)$$

Your models

where

$$\phi_0\left(x_i\right) = \frac{1}{m}\sum_{k=1}^{m} X_{i,k}^{0} = \frac{1}{m}\sum_{k=1}^{m} f_k\left(x_i\right).$$

Model Combination (+ orthogonalization)

Then, reduce the dimensionality:

$$\boldsymbol{X^c}_{n\times m} = \boldsymbol{U}_{n\times n} \quad \boldsymbol{S}_{n\times m} \quad \boldsymbol{V}^T_{m\times m}$$

$$\approx \quad \widehat{\boldsymbol{X^c}}_{n\times p} = \hat{\boldsymbol{U}}_{n\times p} \quad \hat{\boldsymbol{S}}_{p\times p} \quad \hat{\boldsymbol{V}}^T_{p\times m}.$$

n = # of data points, **m** = # of models, **p** = # of kept components

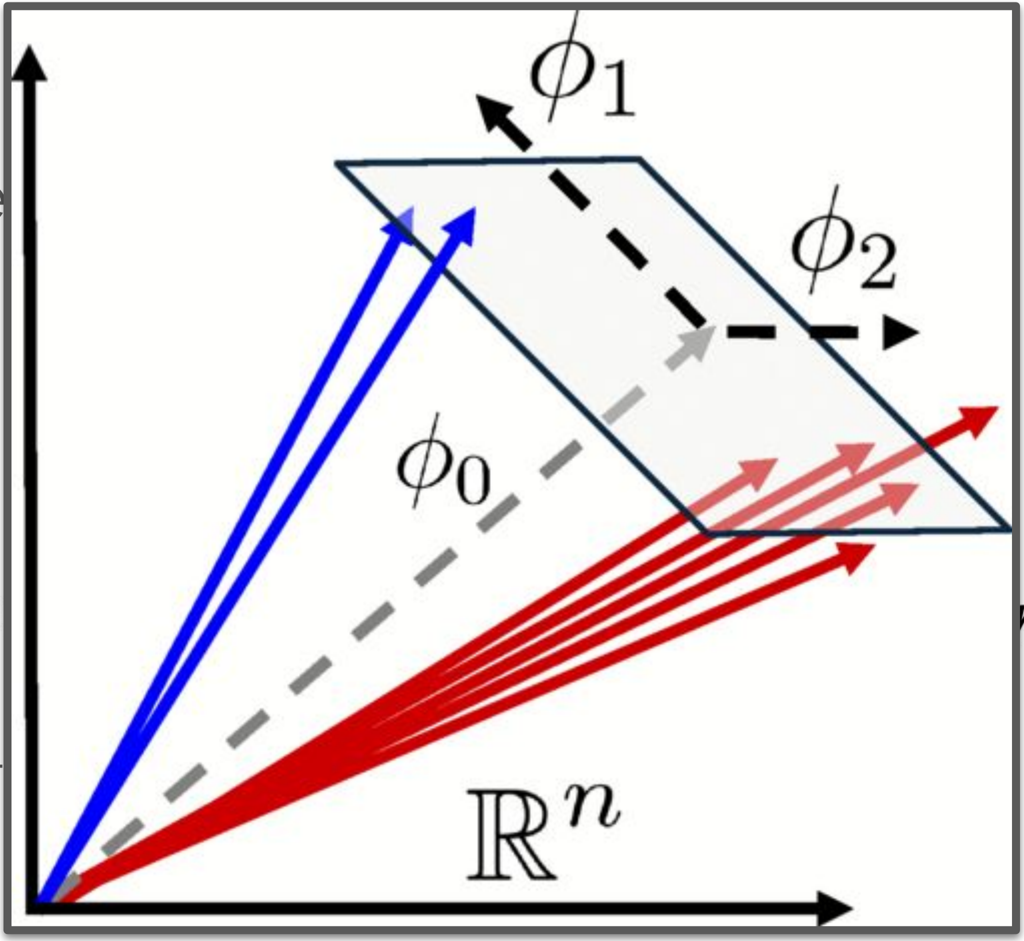
Model Combination (+ orthogonalization)

Then, reduce the dime

$$\boldsymbol{X^c}_{n \times m} = \boldsymbol{U}_{n \times n}$$

$$\approx \widehat{\boldsymbol{X^c}}_{n}$$

m.



n = # of data points, **m** = # ts

Model Combination (+ orthogonalization)

Now construct your combined forecast:

$$f^{\dagger}(\boldsymbol{x};\boldsymbol{b}) = \phi_0(\boldsymbol{x}) + \sum_{j=1}^{p} b_j \phi_j(\boldsymbol{x})$$

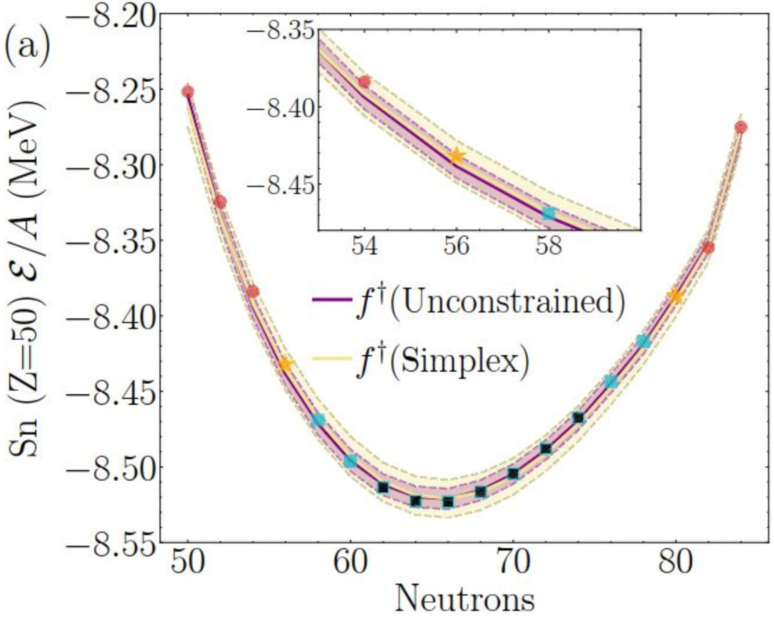
Bringing it Together

Dataset construction is important!

Once you determine the weights, you're ready to go!

P. Giuliani, K. Godbey, V. Kejzlar, and W. Nazarewicz
Phys. Rev. Research 6, 033266

Model	RMSE $\mathcal{X}_0^{\text{tr}}$	RMSE $\mathcal{X}_0^{\text{va}}$	RMSE $\mathcal{X}_0^{\text{te}}$	RMSE $\mathcal{X}_0$
DD-ME2 [39]	2.47	2.48	2.25	2.38
DD-MEδ [40]	2.46	2.19	2.18	2.32
DD-PC1 [41]	1.94	1.77	2.19	2.03
NL3* [42]	2.18	2.15	3.59	2.84
SkM* [43]	4.91	6.34	9.75	7.42
SkP [44]	3.06	3.50	4.41	3.72
SLy4 [45]	4.53	4.84	6.27	5.34
SV-min [46]	2.97	2.99	3.98	3.42
UNEDF0 [47]	1.47	2.02	1.51	1.56
UNEDF1 [48]	1.82	1.83	2.06	1.92
UNEDF2 [49]	1.83	1.66	2.04	1.90
FRDM-12 [38]	0.62	0.62	0.65	0.63
HFB-24 [37]	0.52	0.51	0.52	0.52
BCPM [50]	2.57	2.34	2.44	2.49
D1M [51]	5.02	4.91	5.63	5.27
$f^\dagger(p=7)$	0.38	0.46	0.47	0.43
$f^\dagger(\text{simplex}, p=7)$	0.74	0.69	0.71	0.72



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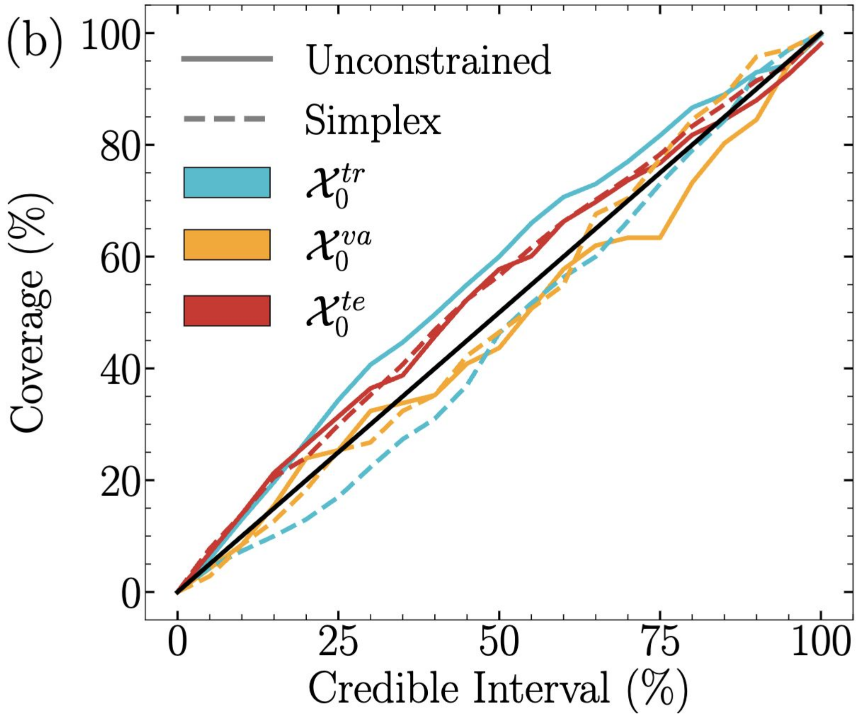

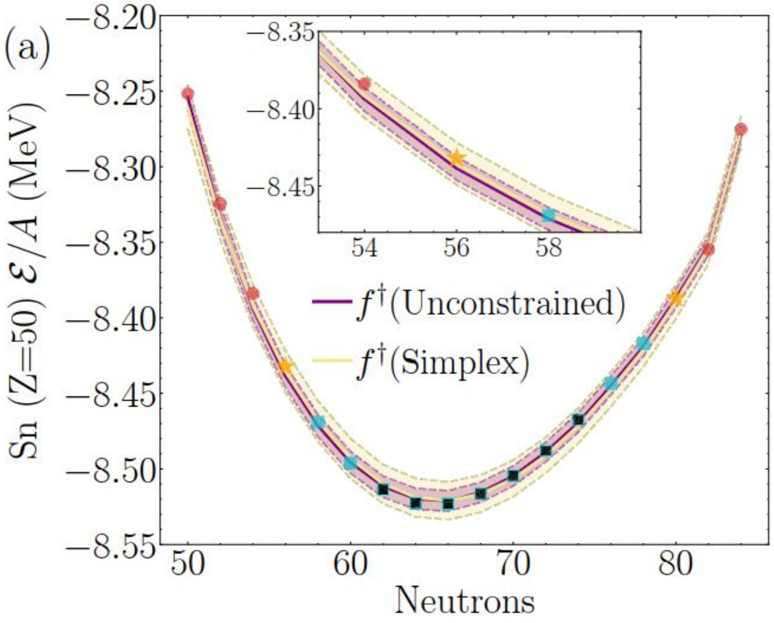

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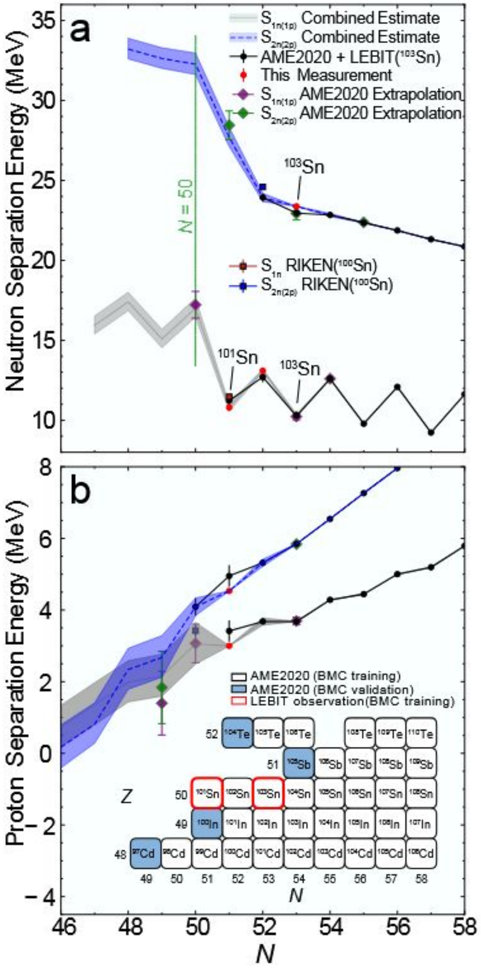
The combination scheme is *very* quick! New (or proposed) experimental data can be easily incorporated



https://arxiv.org/pdf/2510.11815

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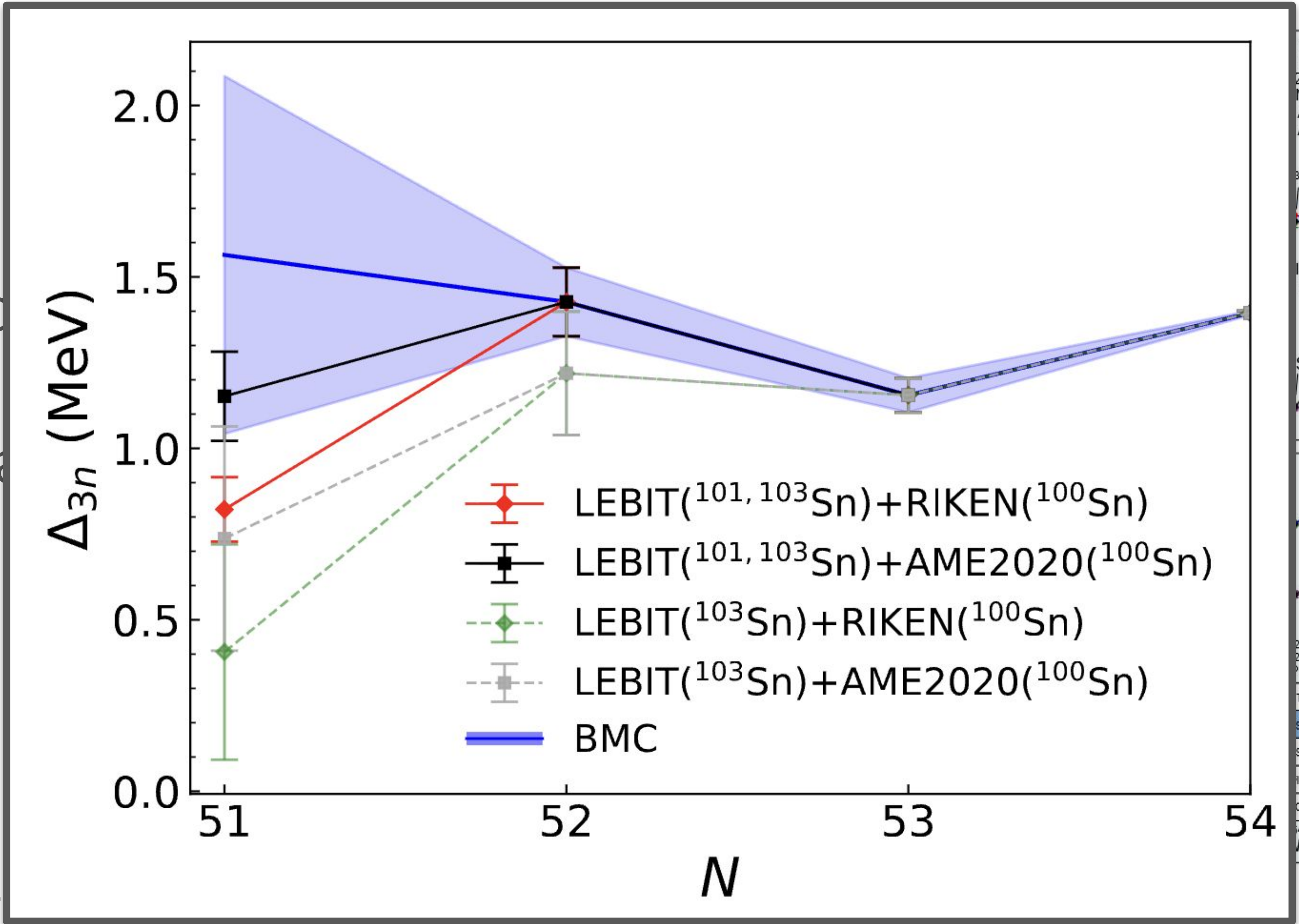

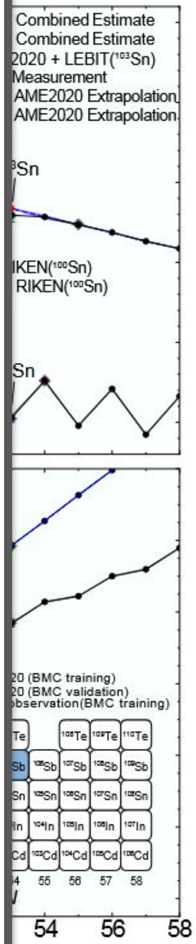

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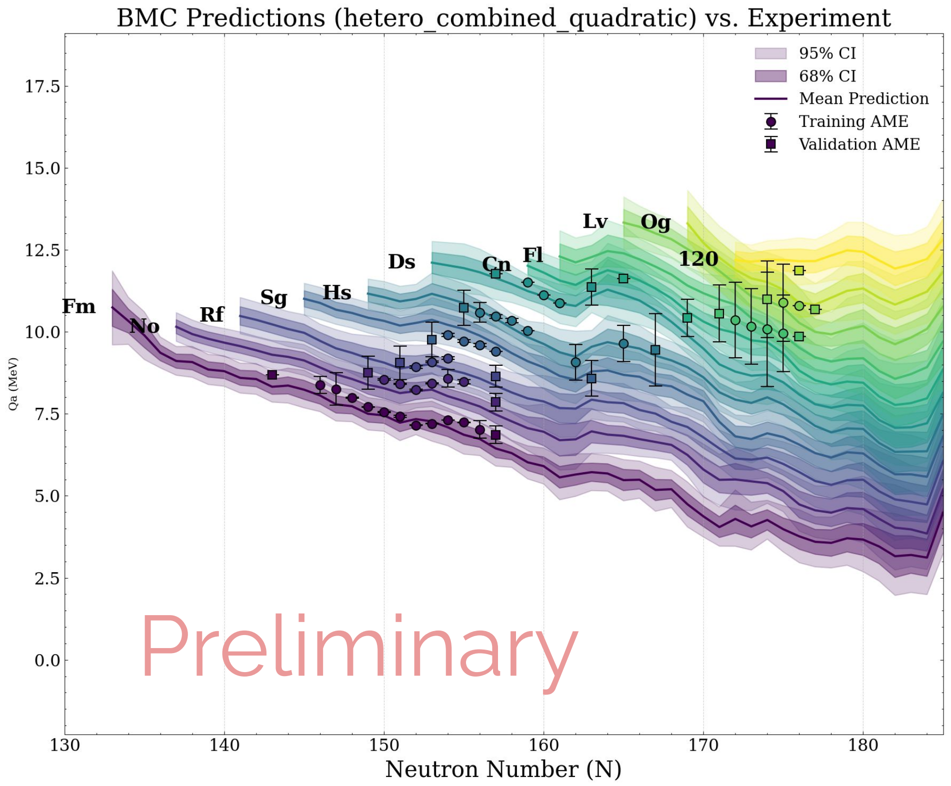
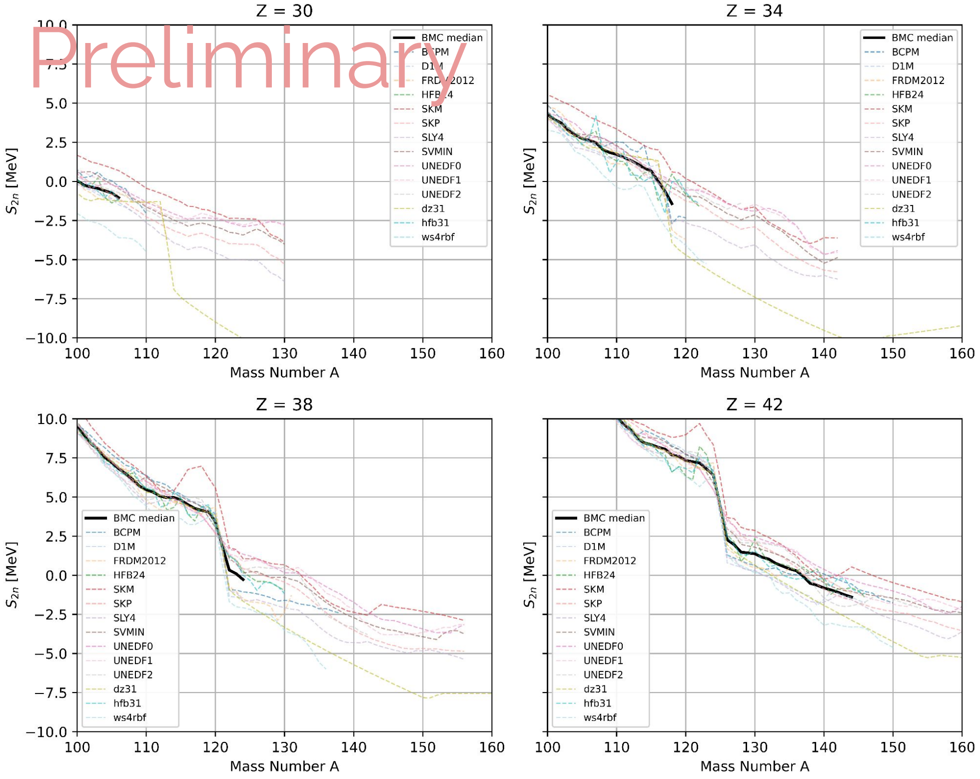
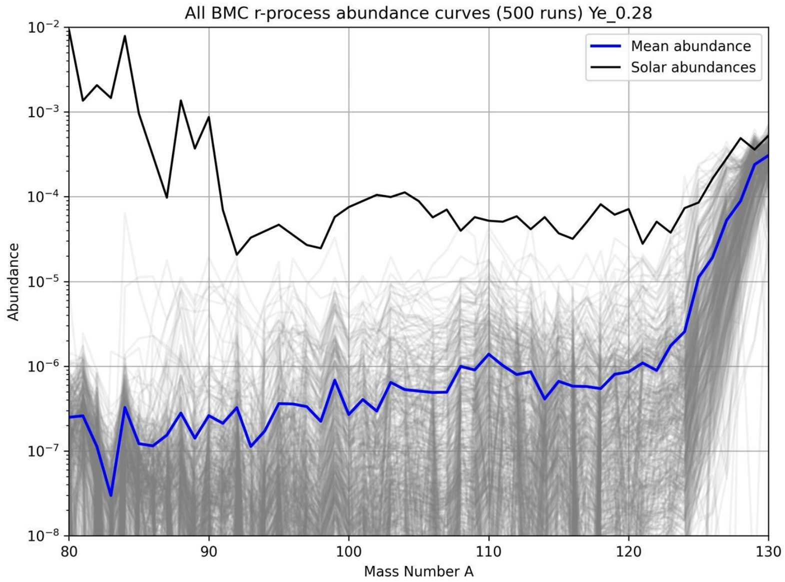


Knight, et al. In Preparation





Agarwal et al. In Preparation

Enter: `pybmc`

Lightweight Python package designed to streamline model orthogonalization and combination tasks

Currently, the core algorithm has been implemented by Undergraduate students Troy Dasher, An Le, and Pranav Agarwal

http://pybmc.ascsn.net/

Sidebar

Putting the effort into making (and releasing) software can pay off immensely!

http://pybmc.ascsn.net/

Wrapping Up: Known Issues

What if your original model space doesn't contain the right behavior (missing physics)?

Model contamination?

Should the error scale be global?

What about the use of global principal components?

Wrapping Up: Known Issues

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Care to help?

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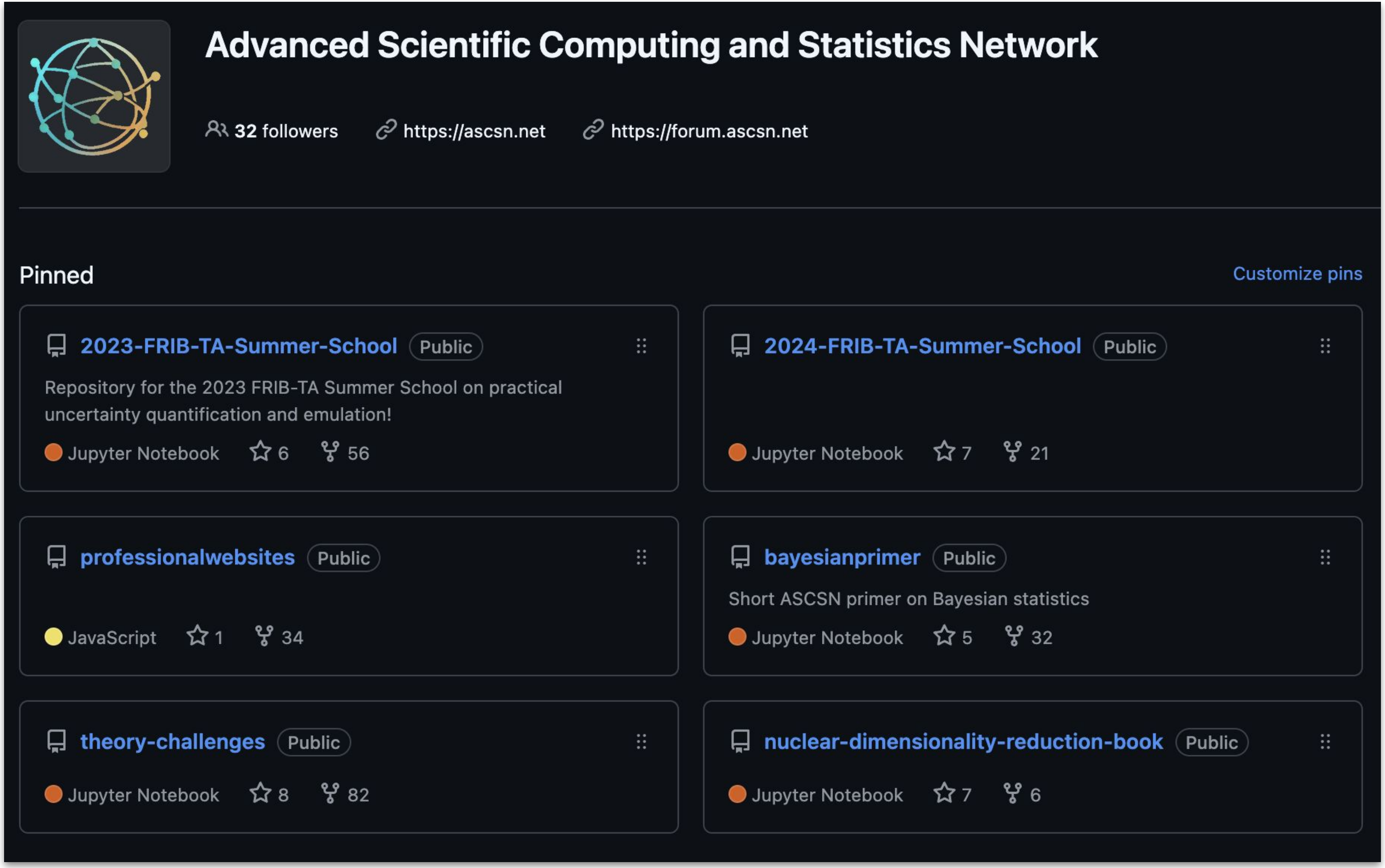
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Dimensionality Reduction in Nuclear Physics
Presented by ASCSN

Aplication 5: Black-Box Methods

- Efficient Emulation of SECAR Beam
- Non-linear and non-affine problem

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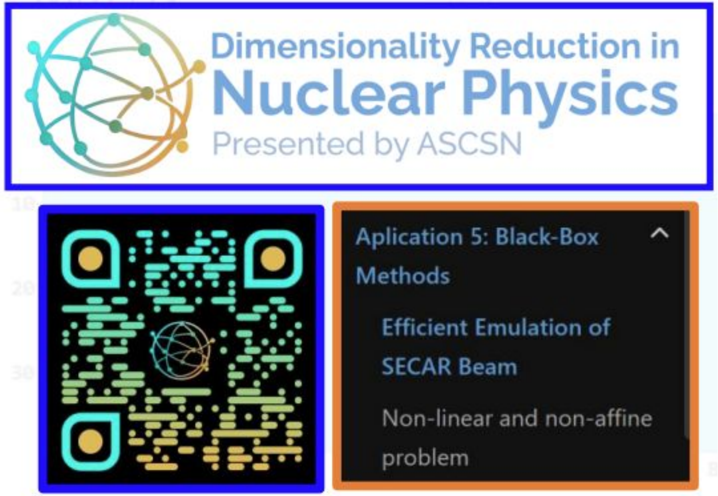
Dimensionality Reduction in Nuclear Physics
Presented by ASCSN

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)
- Aplication 5: Black-Box Methods
- Contributors



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Immense Gratitude to All Collaborators!

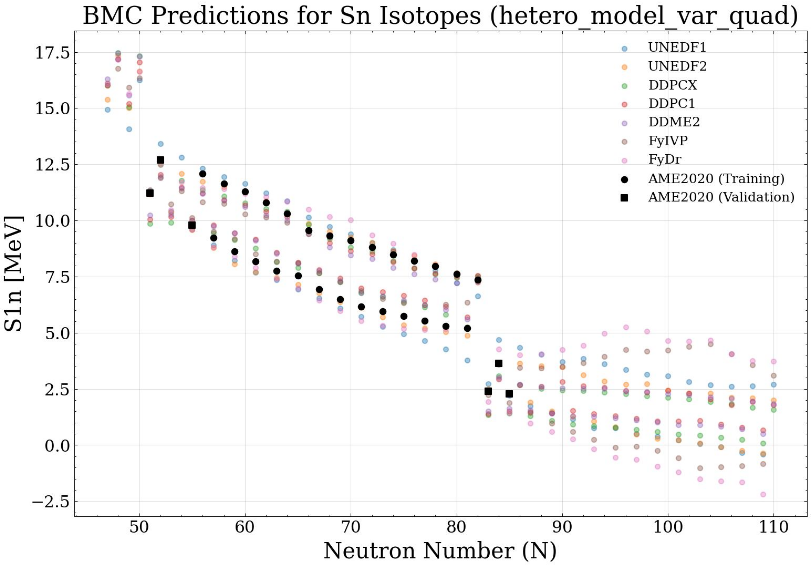
Funding

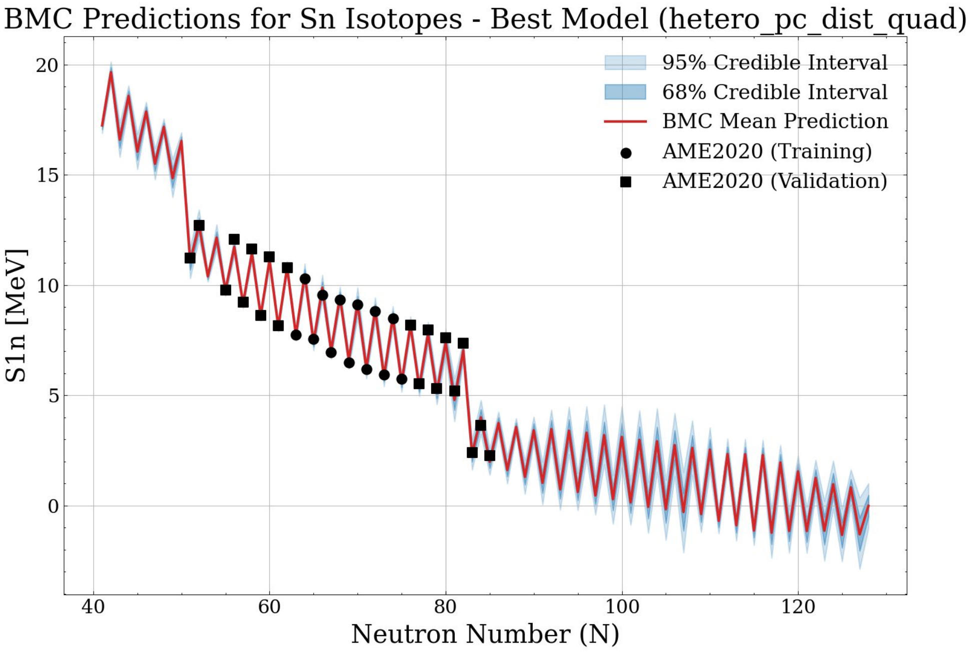
DOE NNSA Grant No. DE-NA0004074
DOE Grant Nos. DE-SC0013365, DE-SC0023175
NSF CSSI Program No. 2004601

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

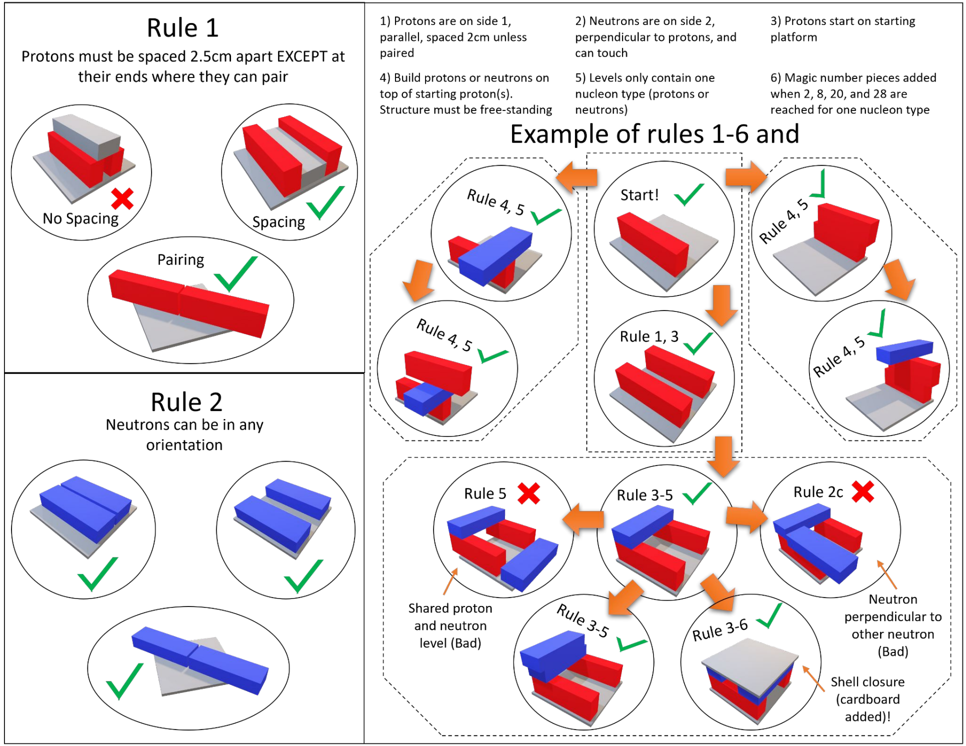
Heteroscedastic Uncertainty





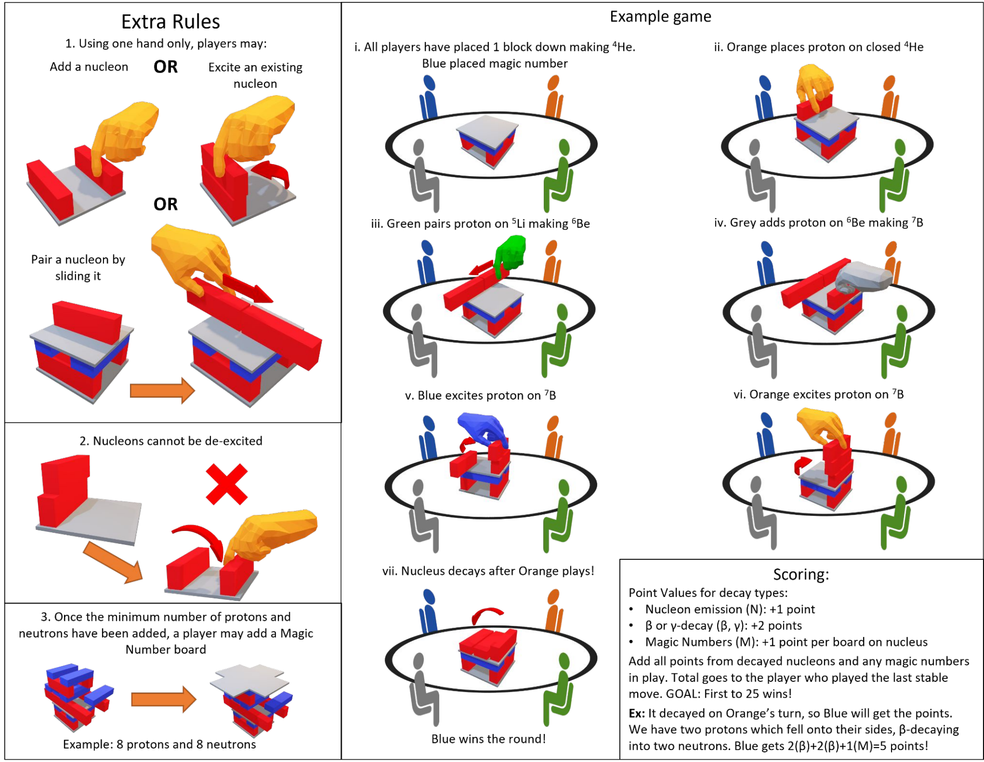
Interface of Technology and Education

- We focus on highlighting structure with dynamic decays
- Rule sets for varying student level (younger students to adults)
    - Coulomb repulsion
    - Pairing
    - Nucleon Excitations
    - Magic numbers



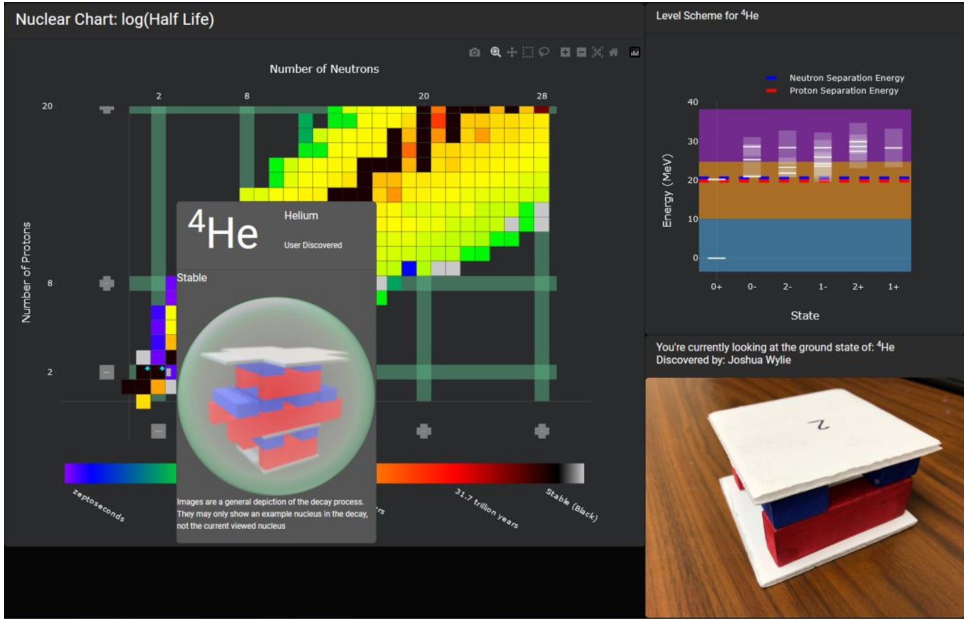
Interface of Technology and Education

- We focus on highlighting structure with dynamic decays
- Alternate multiplayer rule set:
  - Highlights competing forces and effects that may make nuclei more unstable
  - Promotes focus on excitation or more proton or neutron-rich systems



Interface of Technology and Education

- Website will be available:
  - User may click on a nucleus to see the relation between in-game view and real nuclear properties (a translation tool)
  - User-input for “discoveries” (blue diamonds) of ground state, excited state, and second excited state configurations
  - “Discovered” nuclear states are shown with user-submitted photos



Interface of Technology and Education

- Website will be available:
  - User may click on a nucleus to see the relation between in-game view and real nuclear properties (a translation tool)
  - Supplement so users can see game representation of actual physical phenomena (decay modes)