Bayesian Model Combination for Nuclear Extrapolation

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May 11, 2026

Nuclear Masses in Astrophysics for the Next 25 Years, East Lansing

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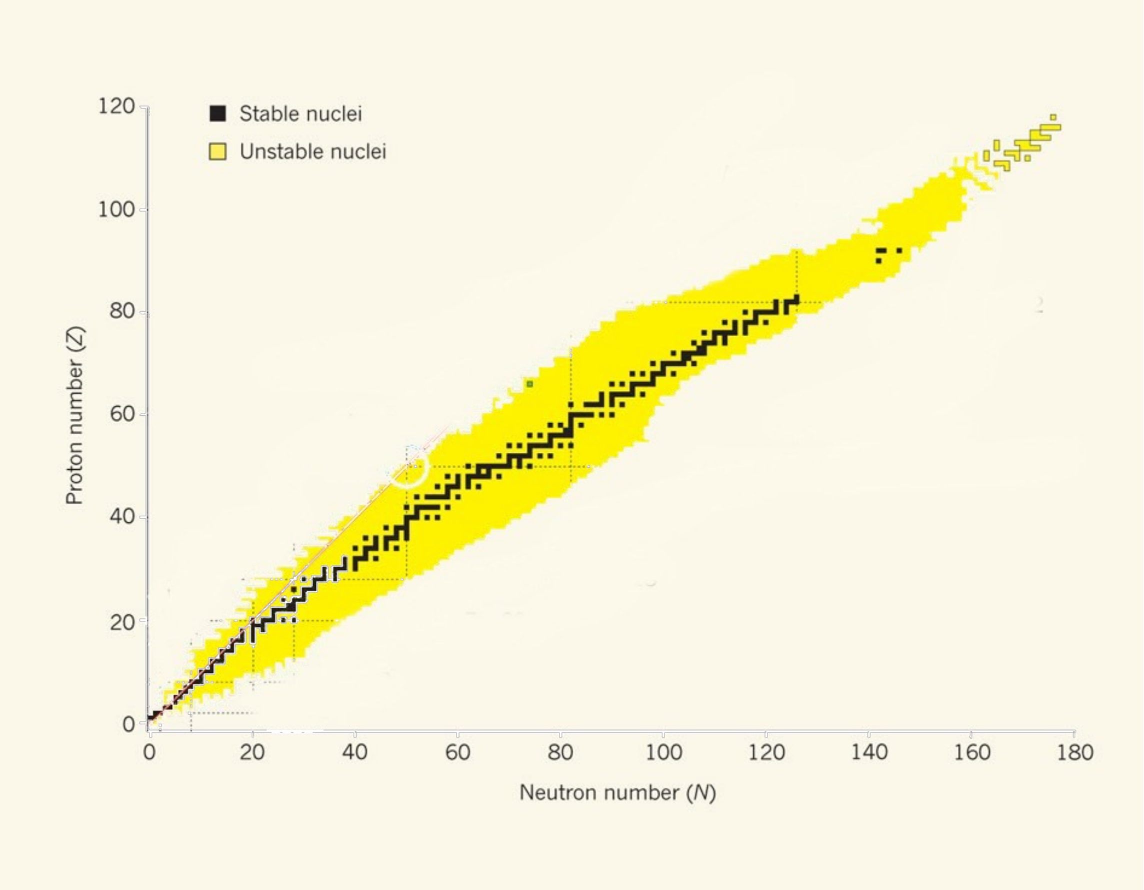
Nuclear Masses: Key to Nuclear Physics



Why this talk?
Nuclear Masses are not known everywhere

Nuclear Structure

- Binding energy, shell structure, deformation and magic numbers

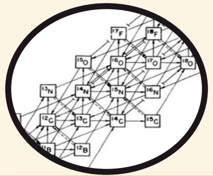
Weak Interactions

β

- Governs β-decay, electron capture, and stability

Nuclear Astrophysics

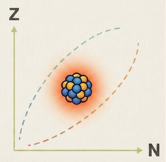
- r- and rp-process paths and waiting points
- Abundance patterns of the elements



Nuclear Statistical Equilibrium

- Composition in hot, dense matter
- Masses control equilibrium abundances

Limits of Nuclear Existence



- Driplines from separation energies:
  - $S_n \rightarrow 0$ and $S_p \rightarrow 0$

Fig. Credit: Bailey Knight

Nuclear Density Functional Theory

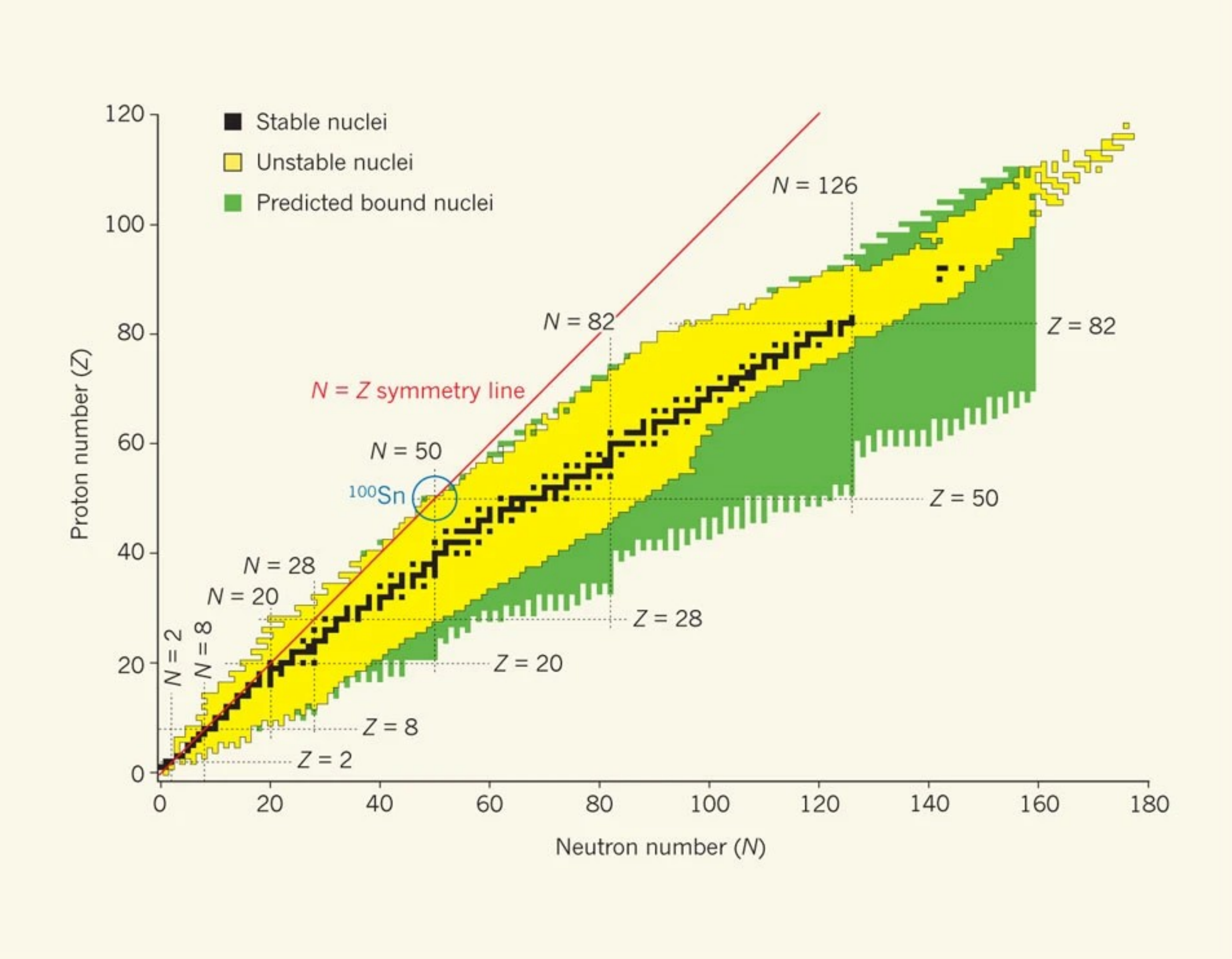


Fig. Credit: Bailey Knight

Why DFT?

Microscopic many-body problem is computationally impossible globally

Density Functional Theory

Global Coverage

Self-consistent treatment

Deformation and pairing

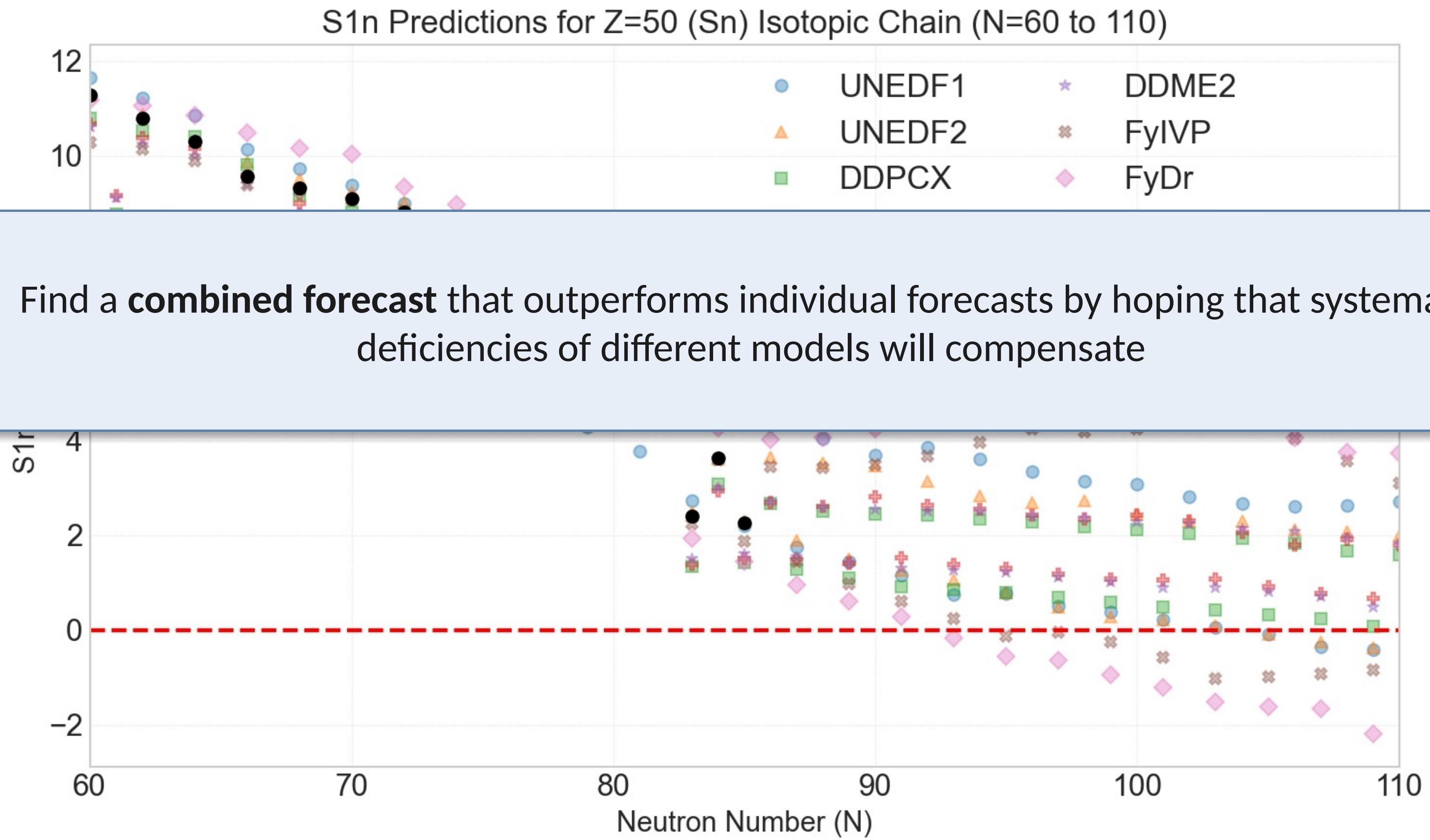
Scalability across the nuclear chart

E[ρ, κ] → solve HFB Equations → M(Z, N)

Energy
Density
Functional

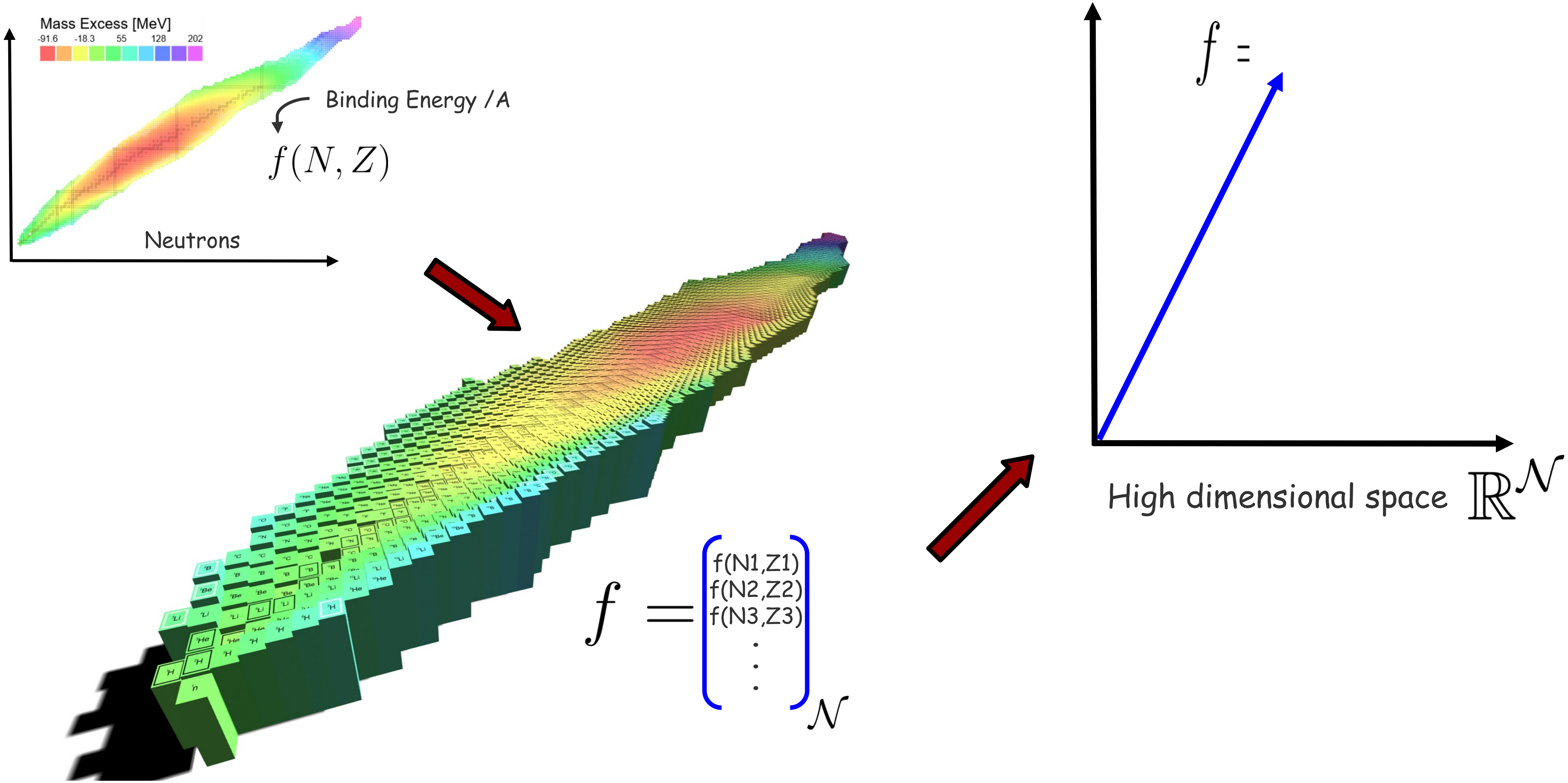
Divergence away from Stability

Goal



Find a **combined forecast** that outperforms individual forecasts by hoping that systematic deficiencies of different models will compensate

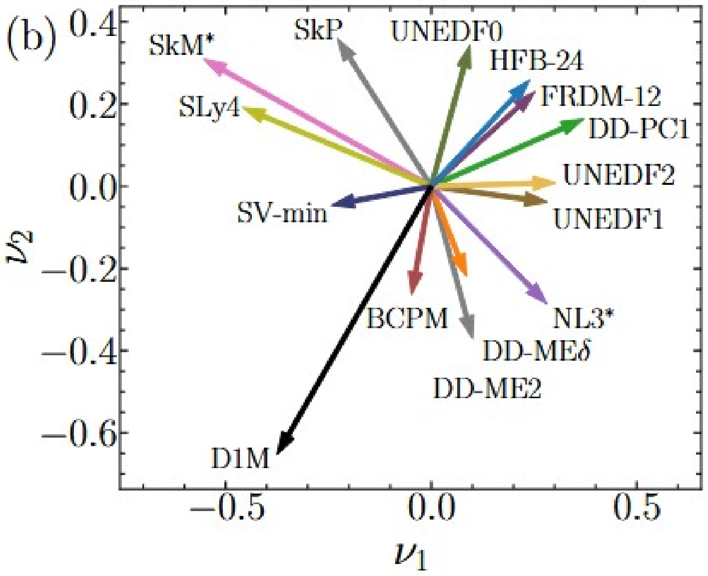
Bayesian Model Combination

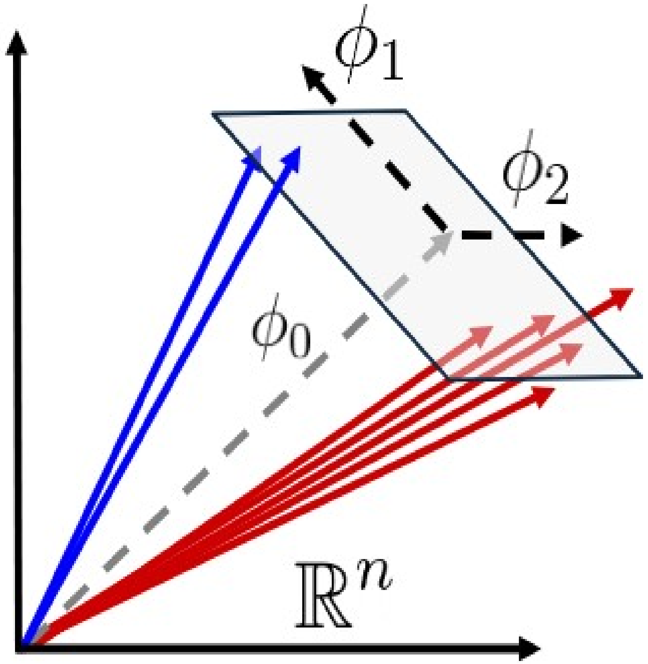


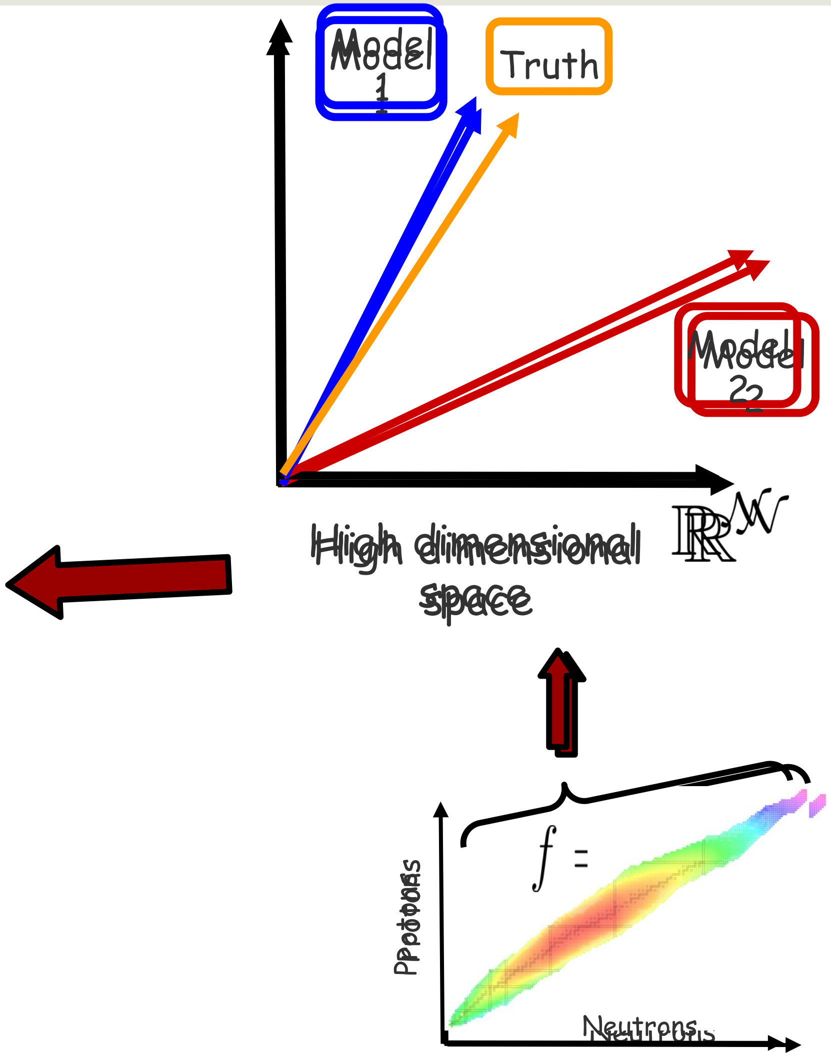
$$f = \begin{pmatrix} f(N1,Z1) \\ f(N2,Z2) \\ f(N3,Z3) \\ \vdots \end{pmatrix}_{\mathcal{N}}$$

Courtesy: P. Giuliani

Model Redundancy



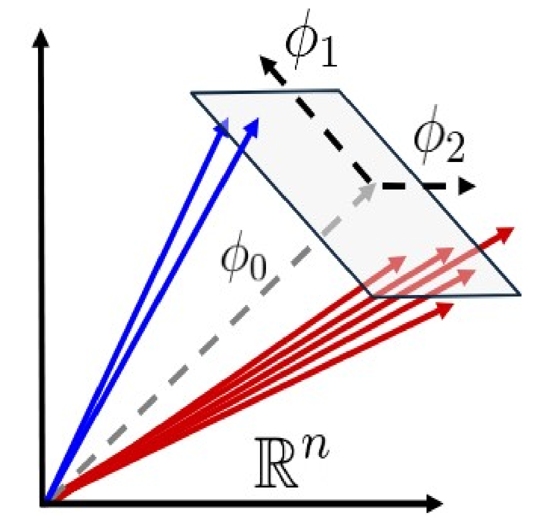


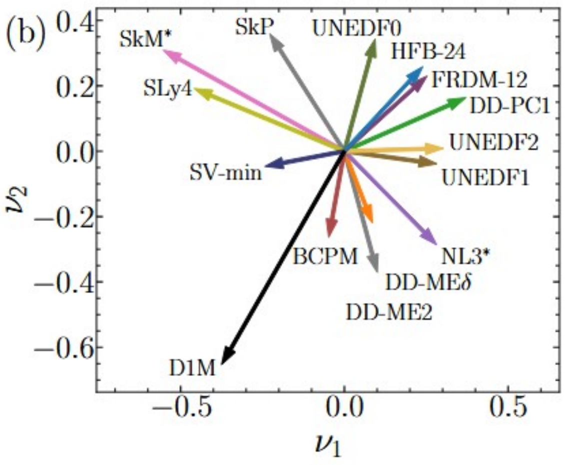


Principal Components

Giuliani P., et al., PRR 6, 2024

Bayesian Model Combination



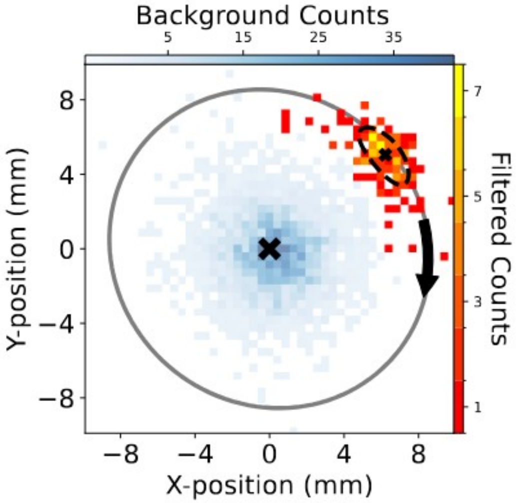


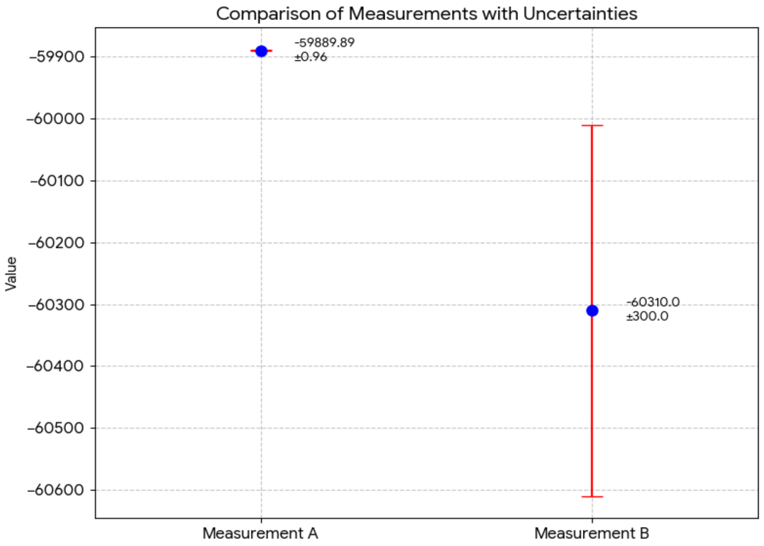
$$\underbrace{f^{\dagger}(\boldsymbol{x};\boldsymbol{b})}_{\text{Combined model}} = \underbrace{\phi_0(\boldsymbol{x})}_{\text{Average forecasts of all the models}} + \underbrace{\sum_{j=1}^{p} b_j \phi_j(\boldsymbol{x})}_{\text{Principal components}}$$

Giuliani P., et al., PRR 6, 2024

Applications

Experimental Measurements





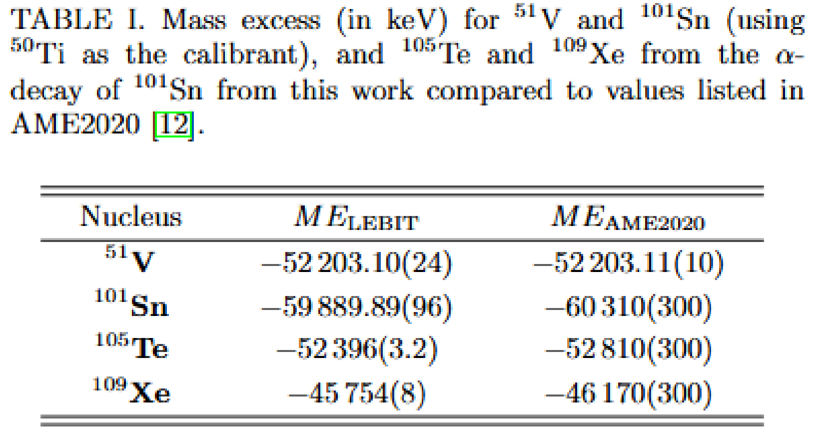


TABLE I. Mass excess (in keV) for ^{51}V and ^{101}Sn (using ^{50}Ti as the calibrant), and ^{105}Te and ^{109}Xe from the α-decay of ^{101}Sn from this work compared to values listed in AME2020 [12].

Nucleus	ME_{LEBIT}	ME_{AME2020}
^{51}**V**	−52 203.10(24)	−52 203.11(10)
^{101}**Sn**	−59 889.89(96)	−60 310(300)
^{105}**Te**	−52 396(3.2)	−52 810(300)
^{109}**Xe**	−45 754(8)	−46 170(300)

Precision Mass Measurements (LEBIT)

^{101}Sn: a precision anchor at the doubly-magic boundary

LEBIT improves mass precision by a factor of 300 over prior estimates

Result: ^{101}Sn is less bound than AME2020 predicted

Provides a critical experimental constraint for theoretical models near ^{100}Sn

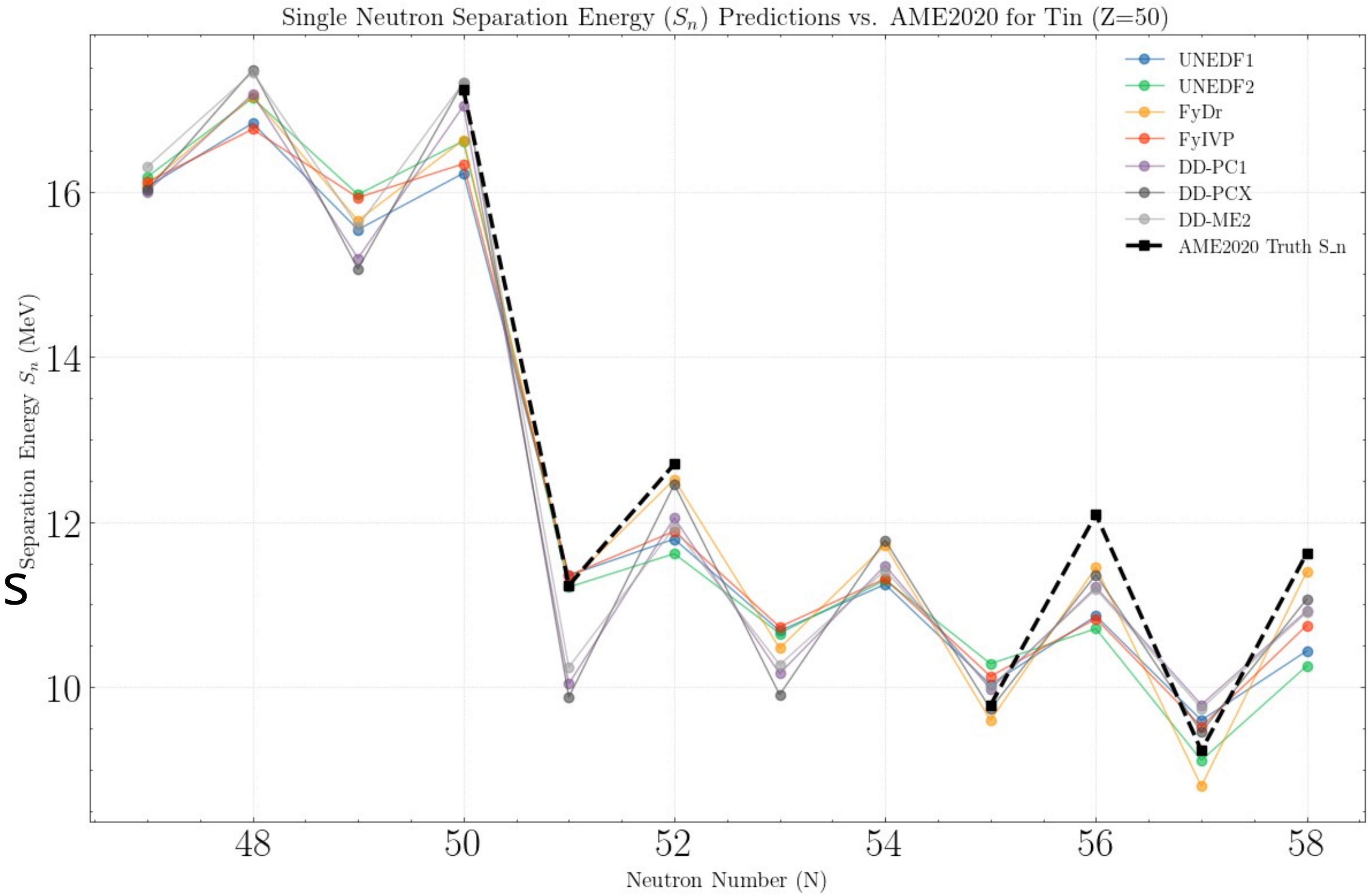
See **Hannah**’s talk for more details!

Ireland, C. M., et al., PRC 113 L021302, 2026

DFT Predictions

Seven DFT models were used:

- Two Skyrme EDFS
    - UNEDF1, UNEDF2
- Two Fayans EDFS
    - Fy(Dr), Fy(IVP)
- Three covariant relativistic models
    - DD-PC1, DD-PCX, DD-ME2



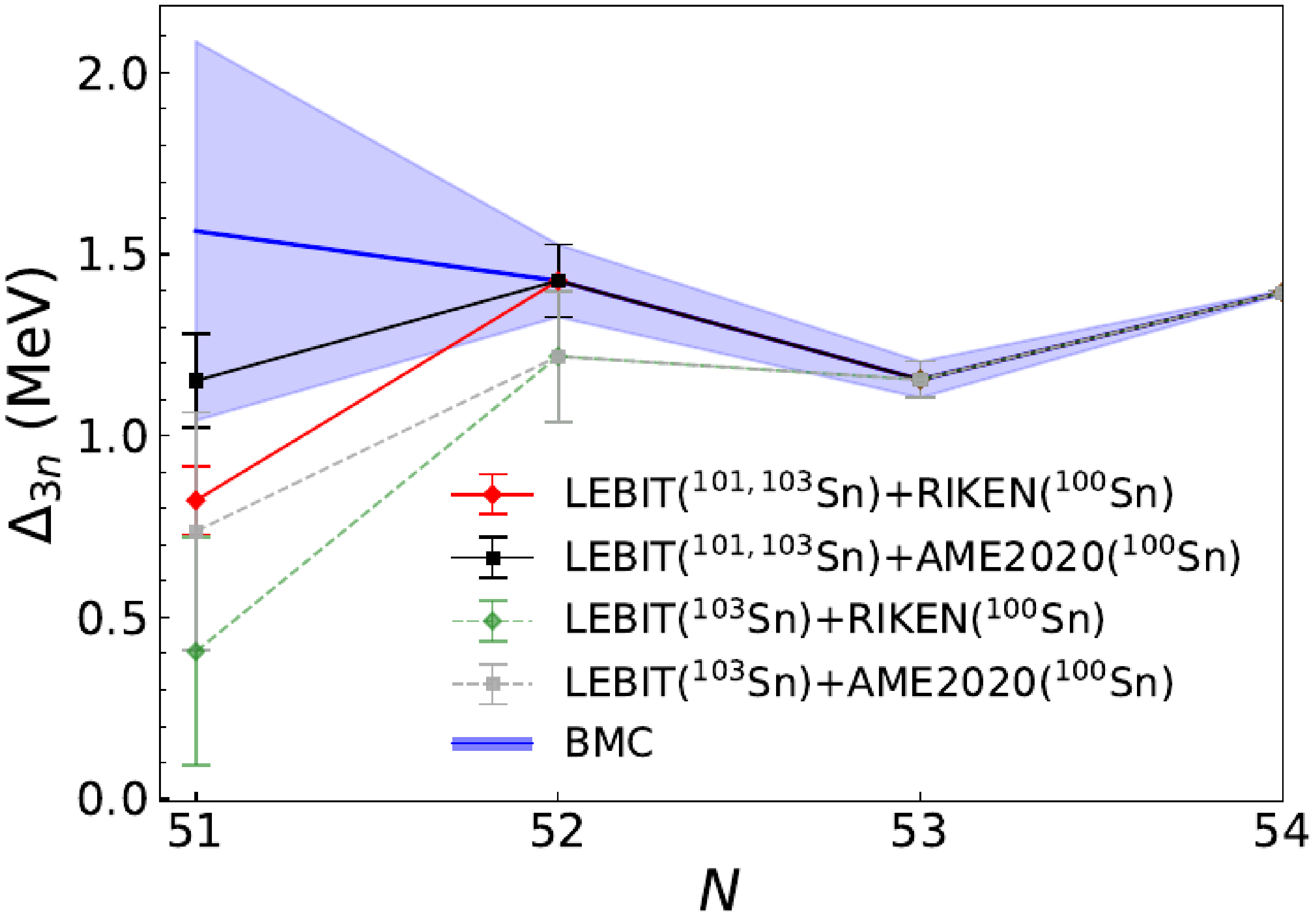
Ireland, C. M., et al., PRC 113 L021302, 2026

Experimental discrepancy: ^{100}Sn

The disagreement between GSI and RIKEN values is exacerbated by the precision of this measurement

The three-point estimator for neutron odd-even staggering, Δ_{3n}, helps probe shell properties.

^{100}Sn: Minor preference for the GSI measurement over RIKEN



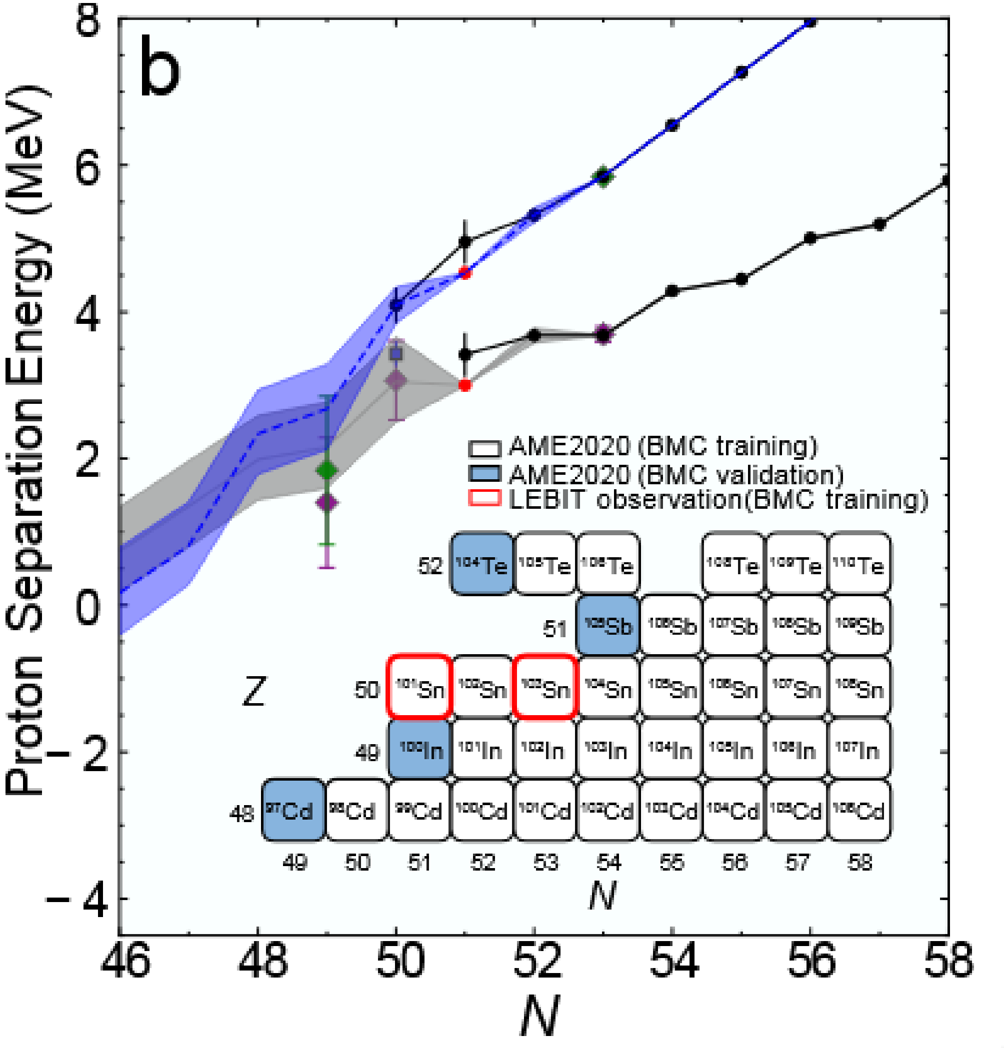
Ireland, C. M., et al., PRC 113 L021302, 2026

Extrapolation: Proton dripline

Proton drip line defined by $S_p < 0$

^{96}Sn – ^{99}Sn: bound to one-proton emission

^{96}Sn: two-proton stability uncertain — sits at the drip-line boundary



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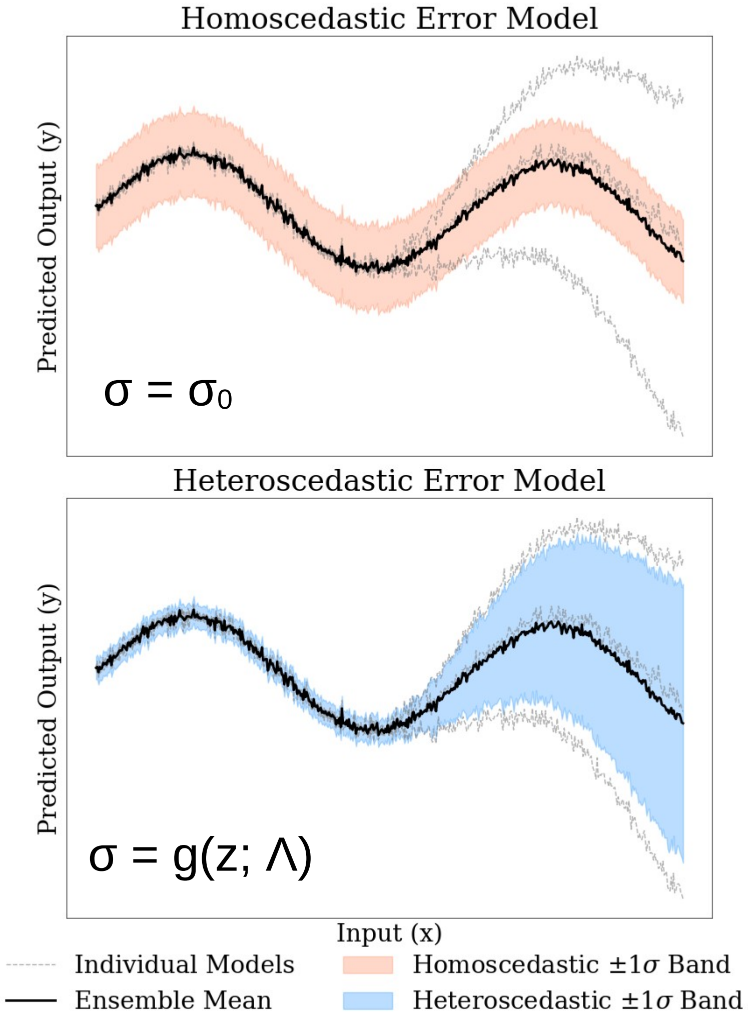
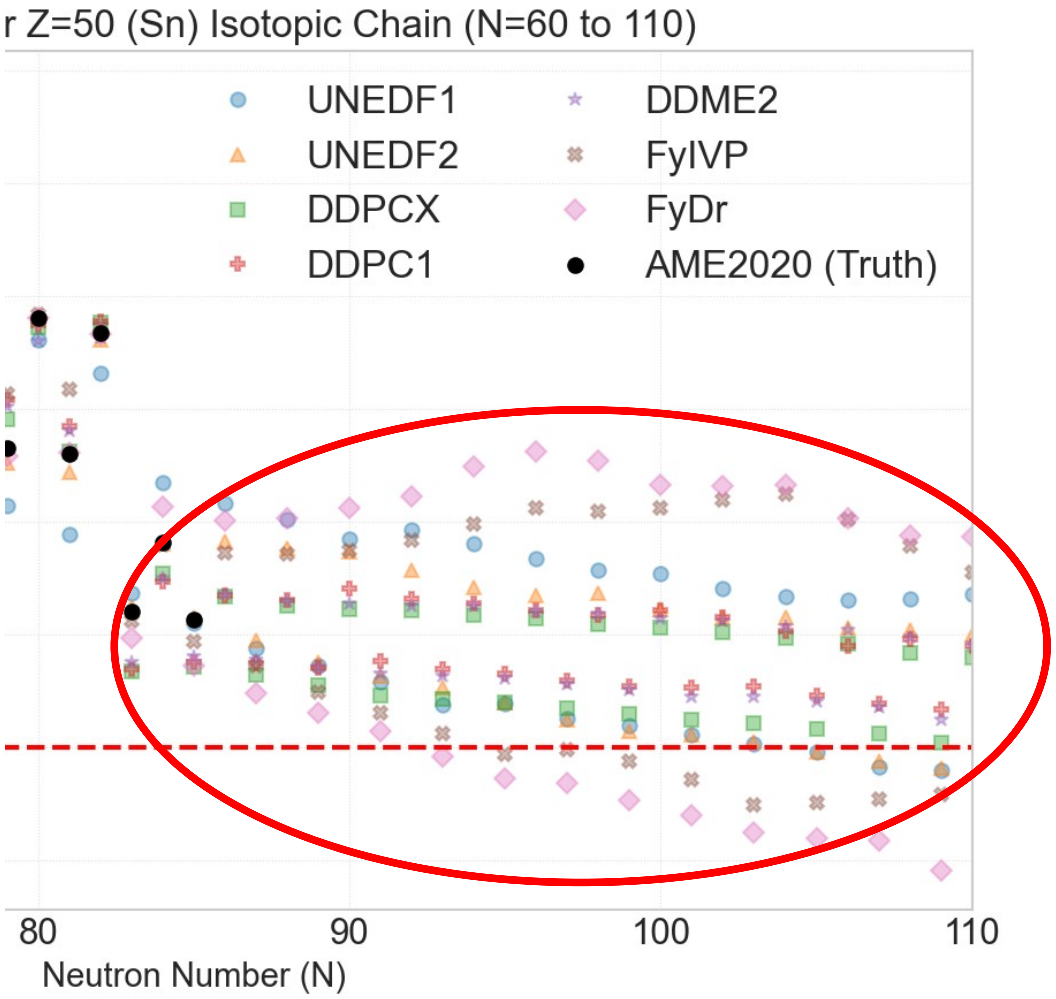
Ireland, C. M., et al., PRC 113 L021302, 2026

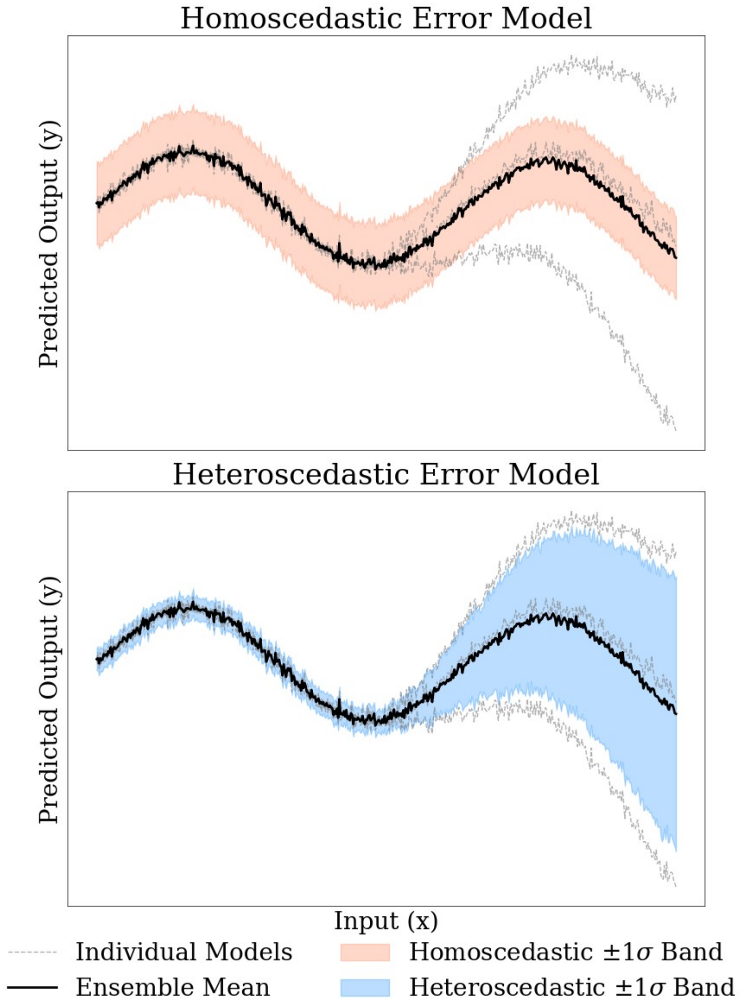
Extrapolations: Neutron Dripline



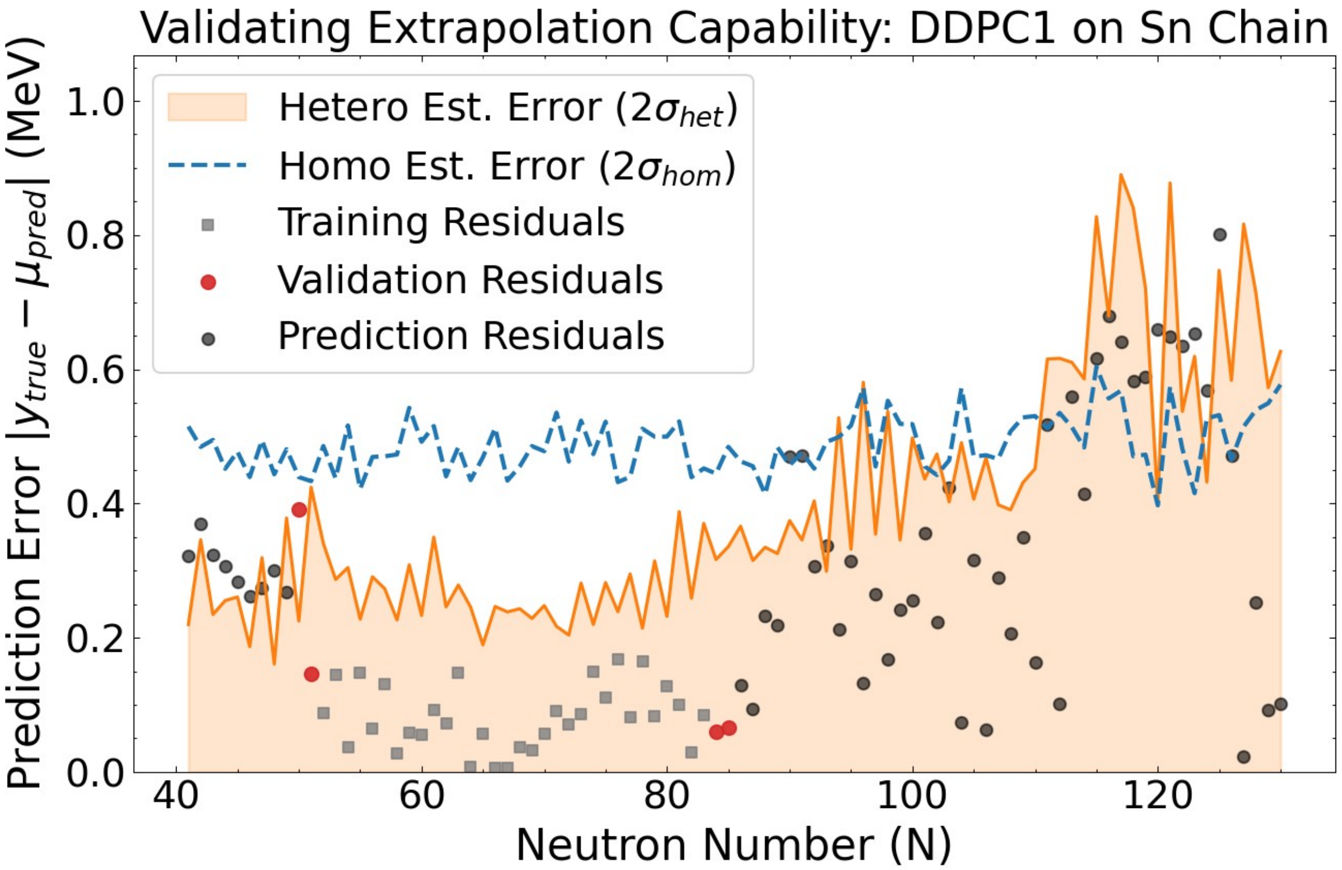


Knight, B., **Lalit, S.**, et al., in prep.

Extrapolations: Neutron Dripline


Homoscedastic Error Model

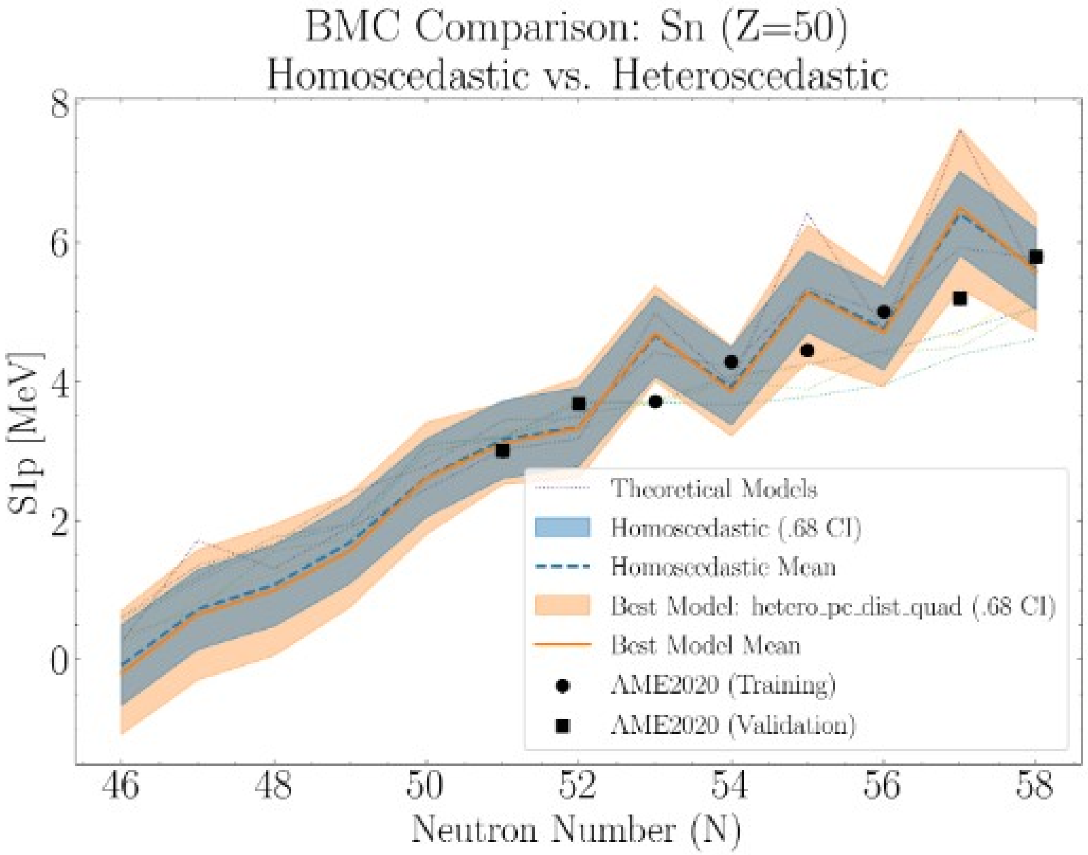
Heteroscedastic Error Model

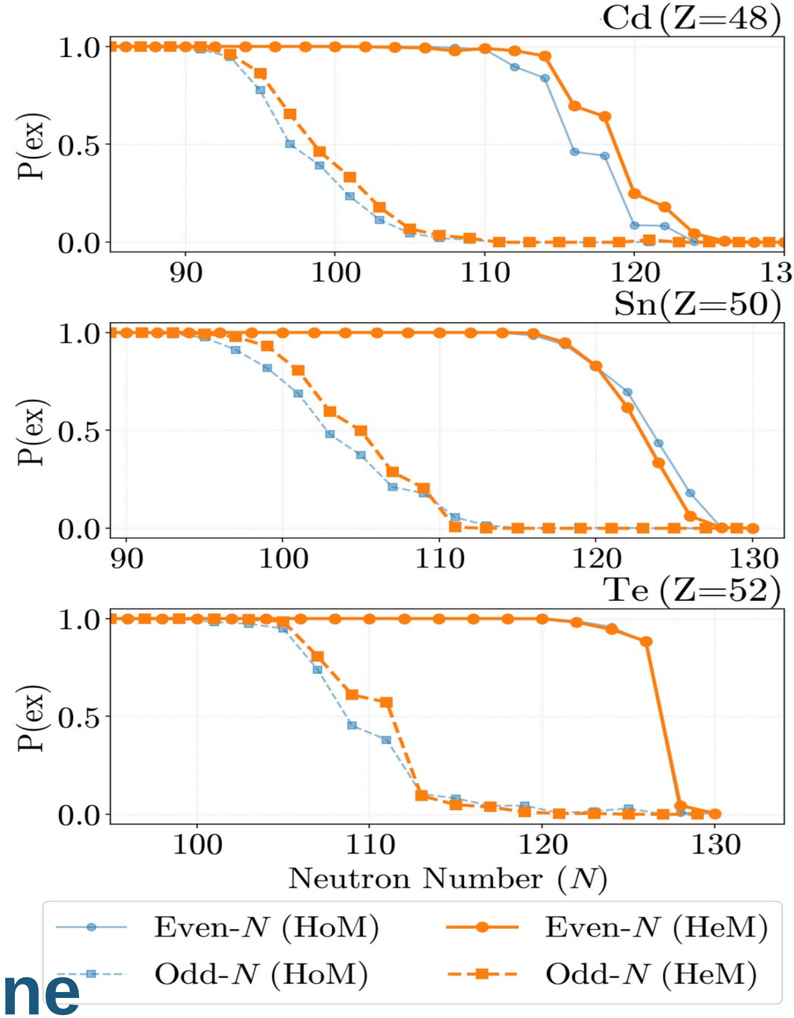

Validating Extrapolation Capability: DDPC1 on Sn Chain

Knight, B., **Lalit, S.**, et al., in prep.

Homoscedastic/Heteroscedastic Predictions

Proton dripline



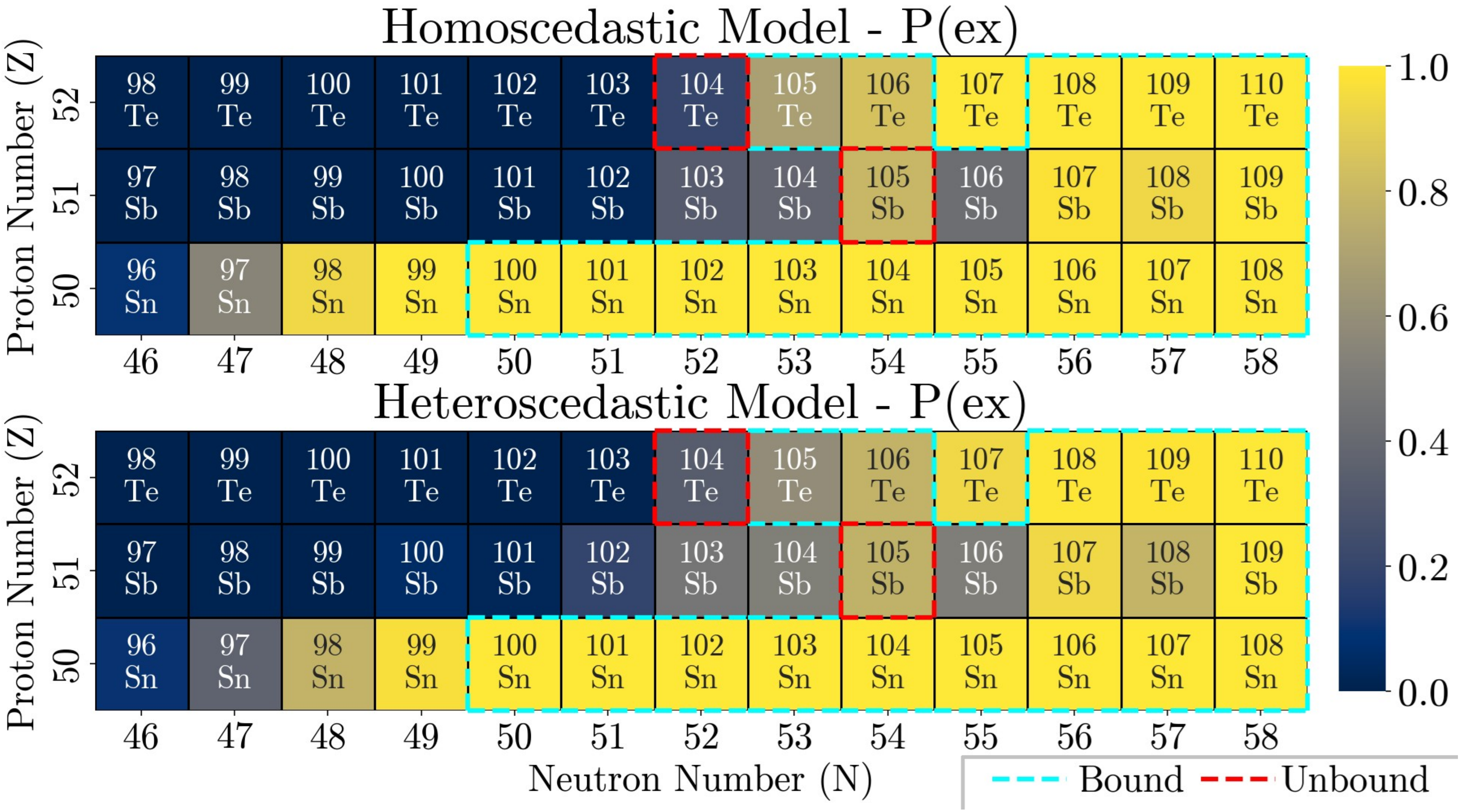


Neutron dripline

Knight, B., **Lalit, S.**, et al., in prep.

Probabilistic Landscape

Local, physics-informed uncertainties are essential for providing realistic maps to guide future experiments

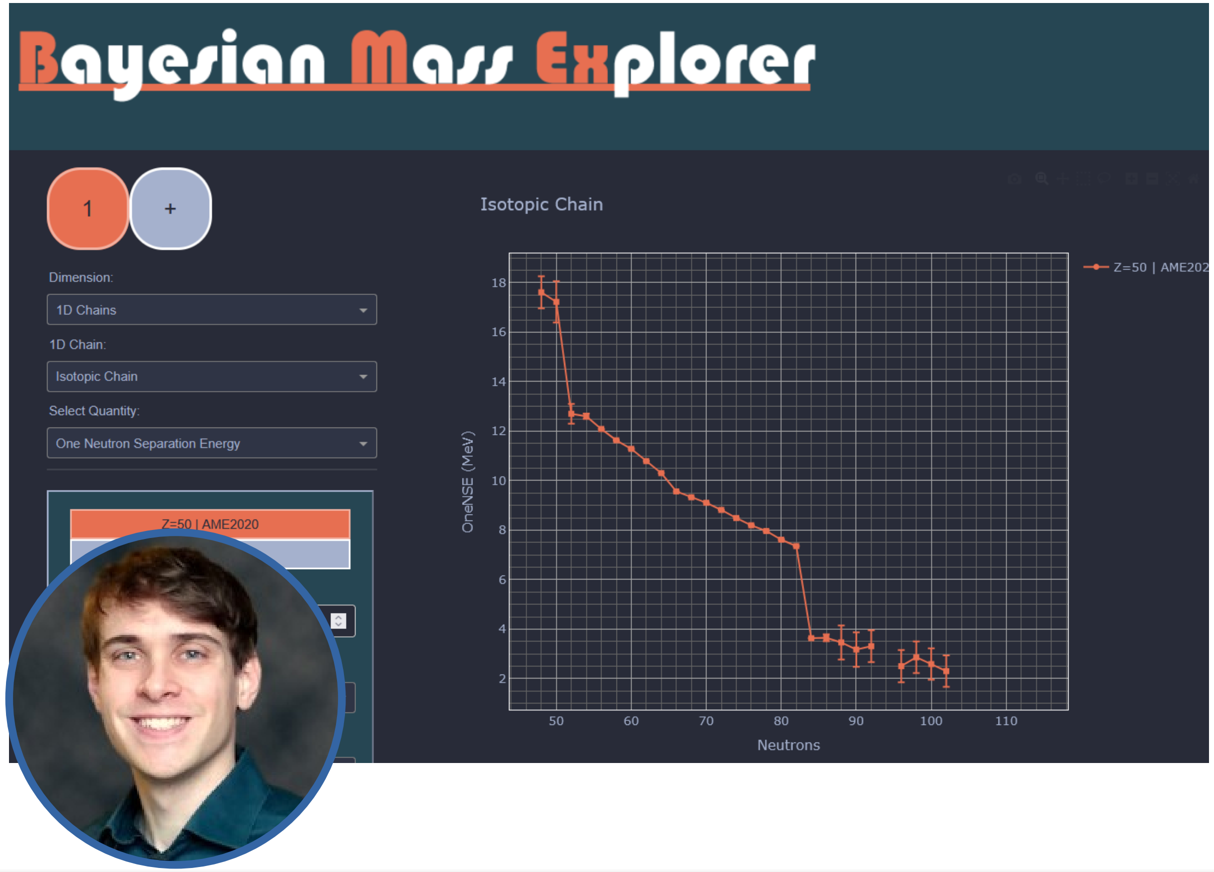


Courtesy: B. Knight

Knight, B., **Lalit, S.**, et al., in prep.

Community Tools

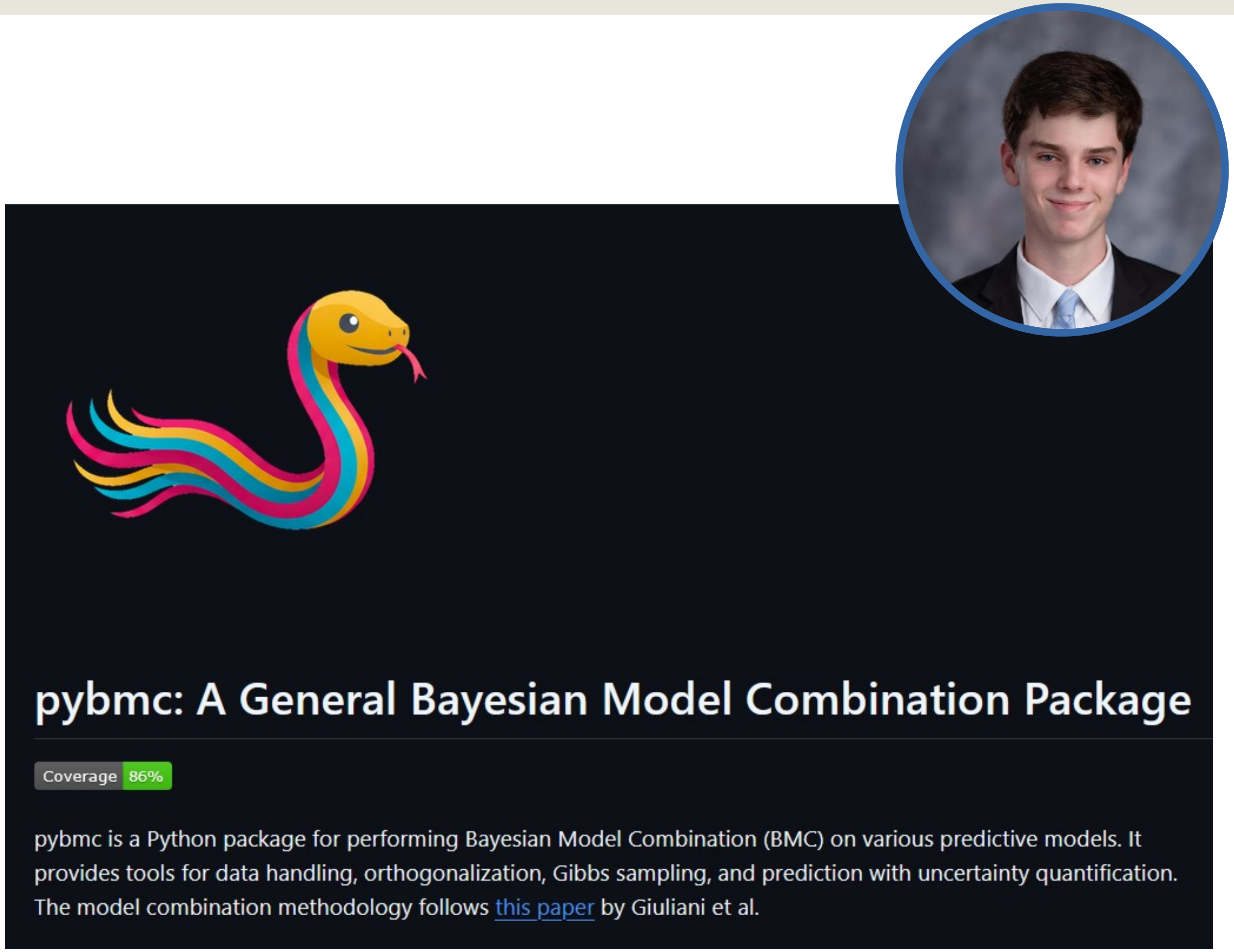
https://bmex.dev/masses



Dimension: 1D Chains

1D Chain: Isotopic Chain

Select Quantity: One Neutron Separation Energy



pybmc: A General Bayesian Model Combination Package

pybmc is a Python package for performing Bayesian Model Combination (BMC) on various predictive models. It provides tools for data handling, orthogonalization, Gibbs sampling, and prediction with uncertainty quantification. The model combination methodology follows this paper by Giuliani et al.

https://github.com/ascsn/pybmc

Courtesy: B. Knight

Summary and Conclusion

- Bayesian Model Combination has been successful in making useful predictions for experimental measurements.
- Addition of a new measurement does not affect the predictions of the BMC models drastically.
- Homoscedastic error models (constant error) are useful for predictions near the line of stability, while Heterscedastic error models (error as a function) cover the expected error for predictions far from stability.

Thank you!

Collaborators


Bailey Knight


Christian Ireland


Kyle Godbey


Troy Dasher


Pablo Giuliani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P. -G. Reinhard


Witek Nazarewicz

U.S. DEPARTMENT OF ENERGY

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