Dynamic Uncertainty Quantification in Bayesian Model Combination for Nuclear Extrapolation

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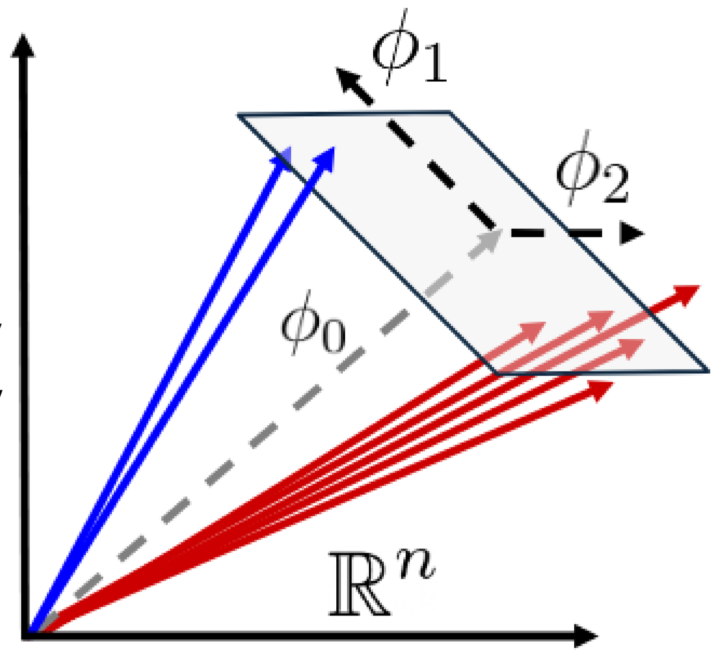
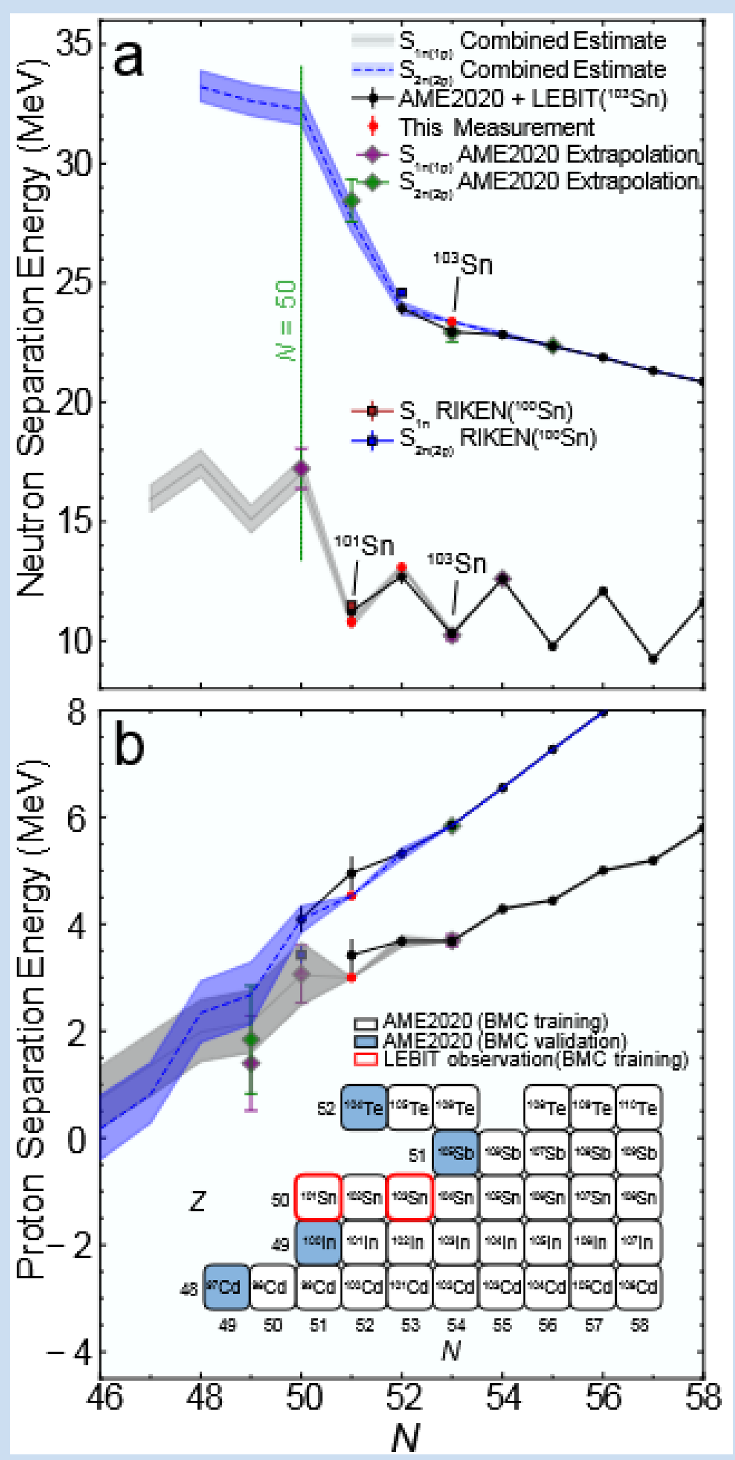
Bayesian Model Combination

- Problem: Single theoretical models have local biases and often don't have well-quantified uncertainties
- Bayesian Model Combination (BMC) is a procedure that takes an input set of theoretical models and constructs a weighted ensemble model that can make predictions on the entire dataset with quantified uncertainties. The resulting model is the best combination of the theory that predicts the training data.
- BMC relies on the assumption that the real truth is within the convex hull of the theory models. For these applications, we use different Energy Density Functionals (EDFs) and Density Functional Theory (DFT) that reflects the microscopic mechanics of nuclei.





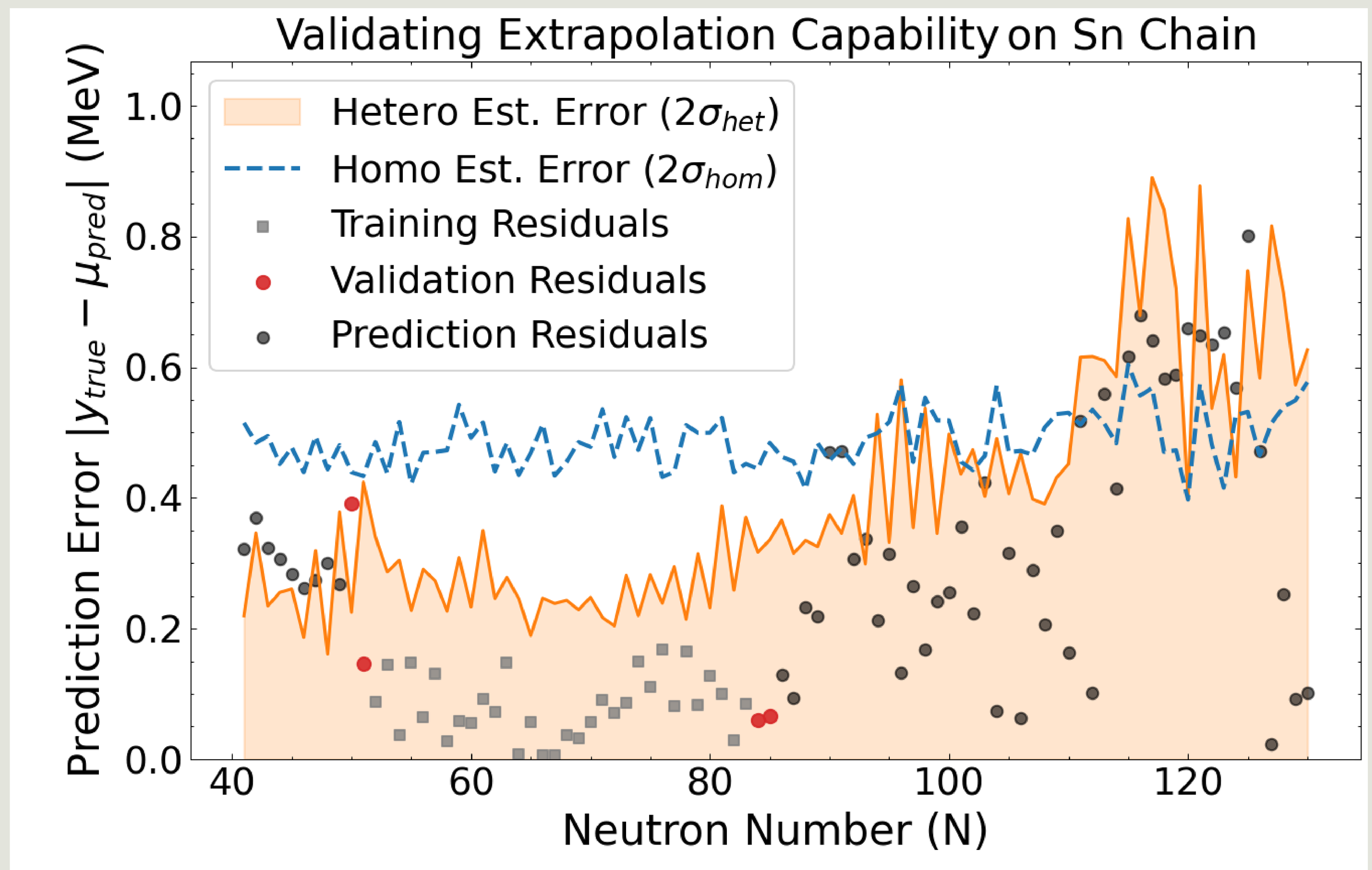
- BMC is an effective tool to perform extrapolations beyond the current limits of experimental data.
- Using Bayesian methods, we can make predictions of unmeasured observables accompanied by rigorous uncertainty bands that reflect how well the models are able to predict experimental data.
- With these predictions, we are able to probe what our experiments and theory tell us probabilistically about the edge of nuclear existence

Error Modeling

To accommodate for a change in the magnitude of uncertainty across the range of the nuclear chart, it is often useful to leverage a heteroscedastic uncertainty scale that changes across the predictive domain.

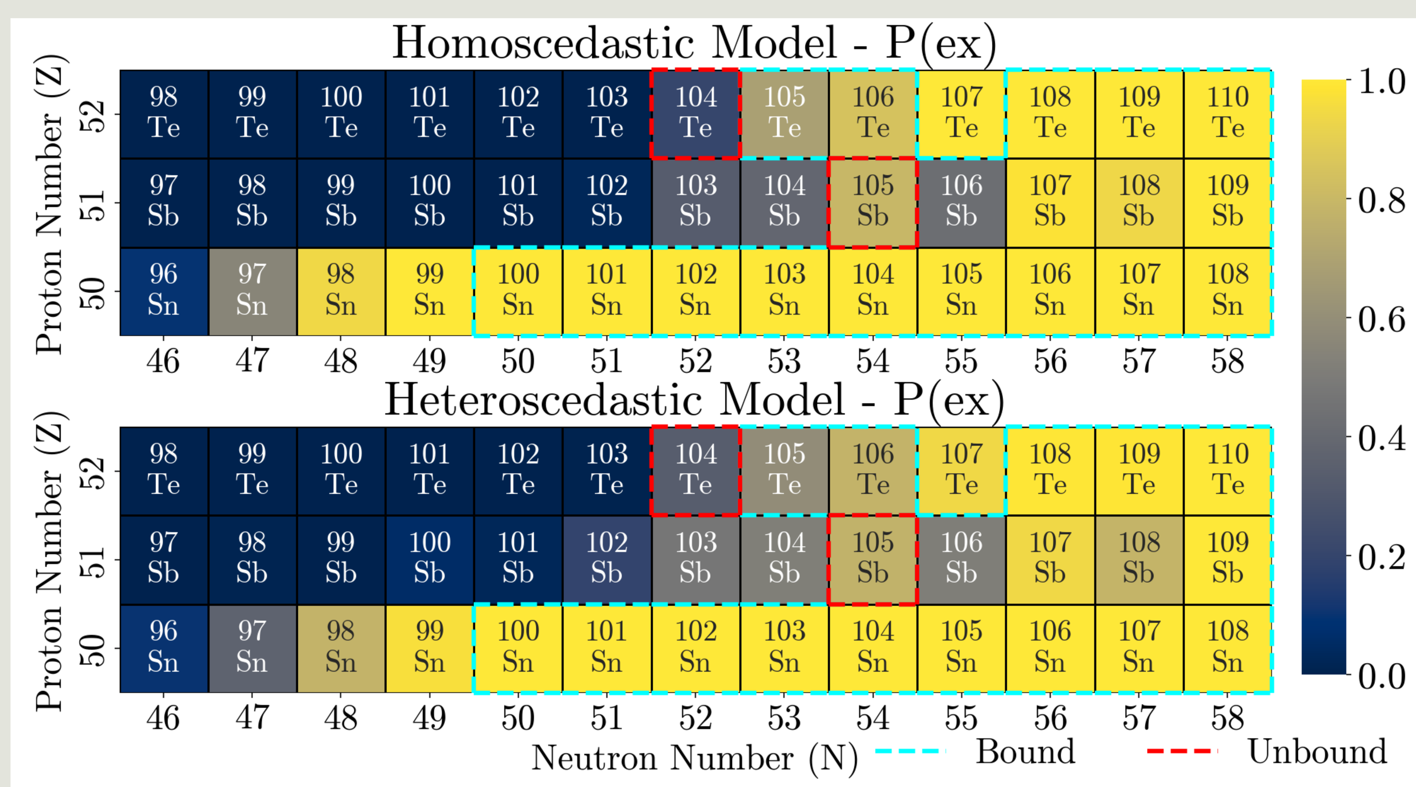
$$\sigma_i^2 = \alpha$$
$$\sigma_i^2 = \alpha + \beta \cdot d_i,$$
$$\sigma_i^2 = \alpha + \beta_1 d_i + \beta_2 d_i^2,$$
$$\sigma_i^2 = \alpha + \beta_d d_i + \beta_v v_i,$$

A sampling of error models. α represents a constant error scale, β is a trained weight, and d/v are metrics of each nucleus.

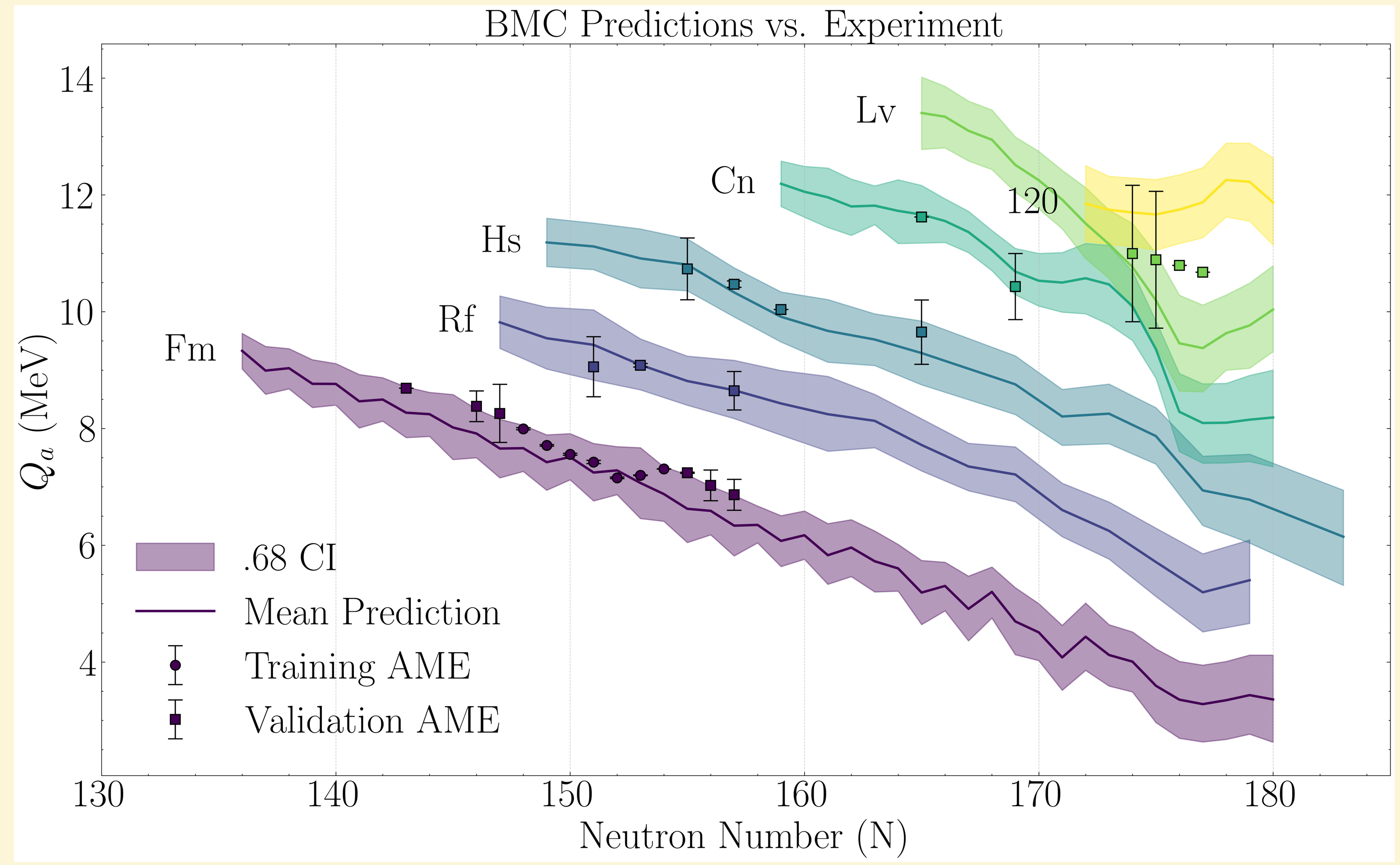


Heteroscedastic Error Quantification:

Allowing the variance to fluctuate across the isotopic regime results in a more accurate estimation of the uncertainty in both the training region and the prediction region in synthetic data experiments.



BMC predictions of the limits of proton-heavy existence in the Sn region



Qα calculations & Generalizability

BMC can be applied to predict any type of nuclear observable. In this demonstration, it predicts the alpha decay Q value for superheavy nuclei with very limited experimental data.

Future Work

Future projects for BMC application:

- Heteroscedastic error applied to the global chart of the nuclides & quality of local vs global fitting regimes
- Comparing ab initio results to BMC DFT results
- Testing non-local calibration quality

Citations

C. M. Ireland, G. Bollen, S. E. Campbell, X. Chen, H. Erington, N. D. Gamage, K. Godbey, A. M. Houff, C. Izzo, B. Knight, S. Lalit, E. Leistenschneider, E. M. Lykiardopoulou, F. M. Maier, W. Nazarewicz, R. Orford, W. S. Porter, C. Quick, A. Ravlic, M. Redshaw, P.-G. Reinhard, R. Ringle, S. Schwarz, C. S. Sumithrarachchi, A. A.Valverde, and A. C. C. Villari, The mass of 101Sn and
Bayesian extrapolations to the proton drip line (2025), arXiv:2510.11815 [nucl-ex]

P. Giuliani, K. Godbey, V. Kejzlar, and W. Nazarewicz, Model orthogonalization and Bayesian forecast mixing via principal component analysis, Phys. Rev. Res. 6, 033266 (2024).

FRIB FACILITY FOR RARE ISOTOPE BEAMS

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