Beyond the proton drip line with Bayesian analysis

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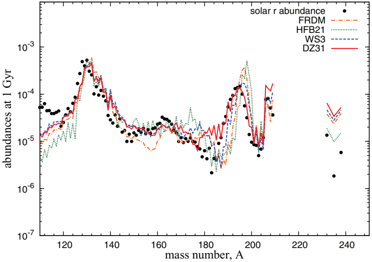
Motivation

- Knowledge of nuclear binding energy crucial for basic science and applications.
- Global mass models show significant discrepancies far from stability.

Mendoza-Temis *et al.*, PRC 92, 0055805 (2015)



- Goal: combine Bayesian analysis and global mass models
  - Uncertainty quantification through credibility intervals.
  - Increase predictive power by reducing systematic deviations.
  - Model mixing based on most current experimental data.
- This talk: Study of proton drip line and 2-proton emitters.

Separation energies and GP

L. Neufcourt *et al.*, PRC98, 034318 (2018)

- Model 1- and 2- proton separation energies (residuals):

$$\delta(Z,N) = S_p^{\text{exp}}(Z,N) - S_p^{\text{theo}}(Z,N)\,.$$

- Use emulators to improve models' predictions:

$$S_p^{\text{em}}(Z,N) = S_p^{\text{theo}}(Z,N) + \delta^{\text{em}}(Z,N)\,.$$

- Emulators posteriors constructed from Gaussian Processes (GP):

$$\delta^i(Z,N) \equiv \delta^i(x) \sim \mathcal{GP}(\mu, k_{\eta,\rho}(x,x')) \quad \text{with} \quad k_{\eta,\rho}(x,x') = \eta^2 e^{-\frac{(Z-Z')^2}{2\rho_Z^2} - \frac{(N-N')^2}{2\rho_N^2}}\,.$$

- Residuals corrections and uncertainties constructed from posteriors distributions:

$$\delta^{\text{em}}(Z,N) = \frac{1}{n_{MC}} \sum_{i=1}^{n_{MC}} \delta^i(Z,N)\,,$$

$$\sigma(Z,N) = \sqrt{\frac{1}{n_{MC}} \sum_{i=1}^{n_{MC}} (\delta^i - \delta^{\text{em}})^2}\,.$$

Results: model performance

L. Neufcourt *et al.*, PRC101, 0141319 (2020)

- 11 global mass models (7 Skyrme, 1 Gogny, 3 astrophysics).
- Training Data: AME03. Testing data: AME16-03

		SkM*	UNEDF1	FRDM
raw	S_{1p}:	0.86	0.54	0.44
	S_{2p}:	1.87	0.62	0.71
$\mu = 0$	S_{1p}:	0.65	0.47	0.40
	S_{2p}:	1.14	0.50	0.55
$\mu \neq 0$	S_{1p}:	0.54	0.38	0.40
	S_{2p}:	0.76	0.39	0.55

Table 1: S_{1p} and S_{2p} rms deviations (in MeV) for individual models.

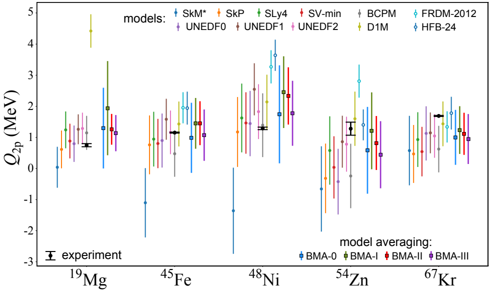
- GP reduce rms by $\sim 25\%$ (additional $\sim 15\%$ with $\mu \neq 0$).
- Smaller impact on more phenomenological models fitted to larger datasets.
- Similar corrected rms: most of systematic has been captured.

Bayesian model averaging (BMA)

- Model mixing performed by averaging individual mass models' posteriors.
- Prior weights w_k: capability of a model $\mathcal{M}_k$ to predict known $2p$ emitters.

$$w_k(\mathrm{I}) \propto p\left(\mathcal{M}_k | Q_{2p} > 0, S_{1p} > 0 \text{ for } x_{2p,\text{known}}\right) ,$$
$$w_k(\mathrm{II}) \propto p\left(\mathcal{M}_k | Q_{2p} \text{ of } x_{2p,\text{known}}\right) .$$

L. Neufcourt *et al.*, PRC101, 0141319 (2020)



	BMA-I	BMA-II
SkM*	0.00	0.00
UNEDF1	0.14	0.71
FRDM	0.17	0.00

Table 2: Model posterior weights.

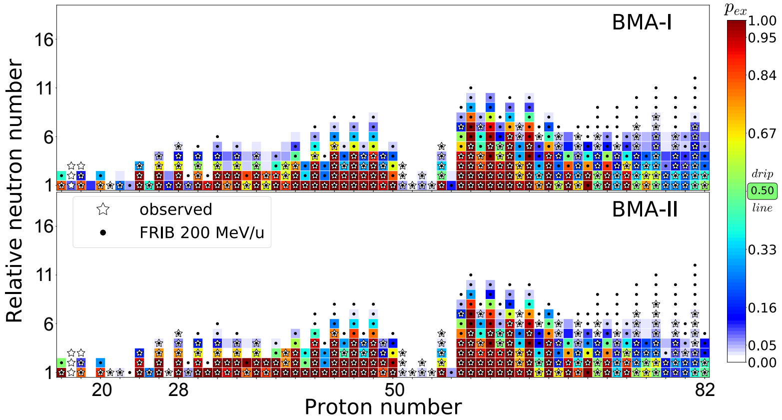
	BMA-I	BMA-II
S_{1p}	0.38	0.38
S_{2p}	0.35	0.37

Table 3: S_{1p} and S_{2p} rms (in MeV).

BMA: Proton drip line

$$p_{\mathrm{ex}} = p(S^*_{1p/2p} > 0 | S_{1p/2p}).$$

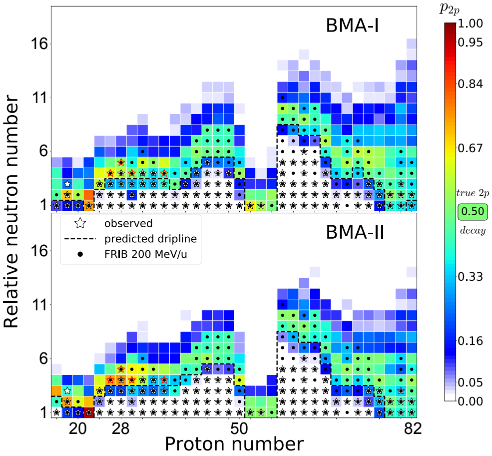
L. Neufcourt *et al.*, PRC101, 0141319 (2020)



BMA: 2p emitters

$$p_{2p} = p(S^*_{2p} < 0 \cap S^*_{1p} > 0 | S_{1p/2p}),$$

L. Neufcourt *et al.*, PRC101, 0141319 (2020)



Conclusions

- Statistical correction greatly improves models' accuracy:
  - $\sigma(S_{2p}) = 400 - 600$ keV.
  - GP with $\mu \neq 0$ better reproduces extrapolative data.
- BMA obtained using different weights:
  - On testing data, BMA outperforms single models.
  - BMA $\sigma(S_{1p})/\sigma(S_{2p}) = 380/360$ keV: precision limit of current models?
- No $2p$ emitters with $\tau > 10^{-7}$ s are predicted above $Z = 54$.
- **Future work:**
  - Propagate posteriors on network calculations for astrophysical studies.
  - Employ statistical analysis to fission.

Backup

GP parameters: distributions of posteriors samples

L. Neufcourt *et al.*, PRC101, 0141319 (2020)