Bayesian extrapolation of nuclear observables towards the neutron drip line

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Nuclear and astrophysics aspects for the rapid neutron capture process
in the era of multimessenger observations
ECT*, July 3, 2019

This is not about better nuclear models. This is about better predictions.

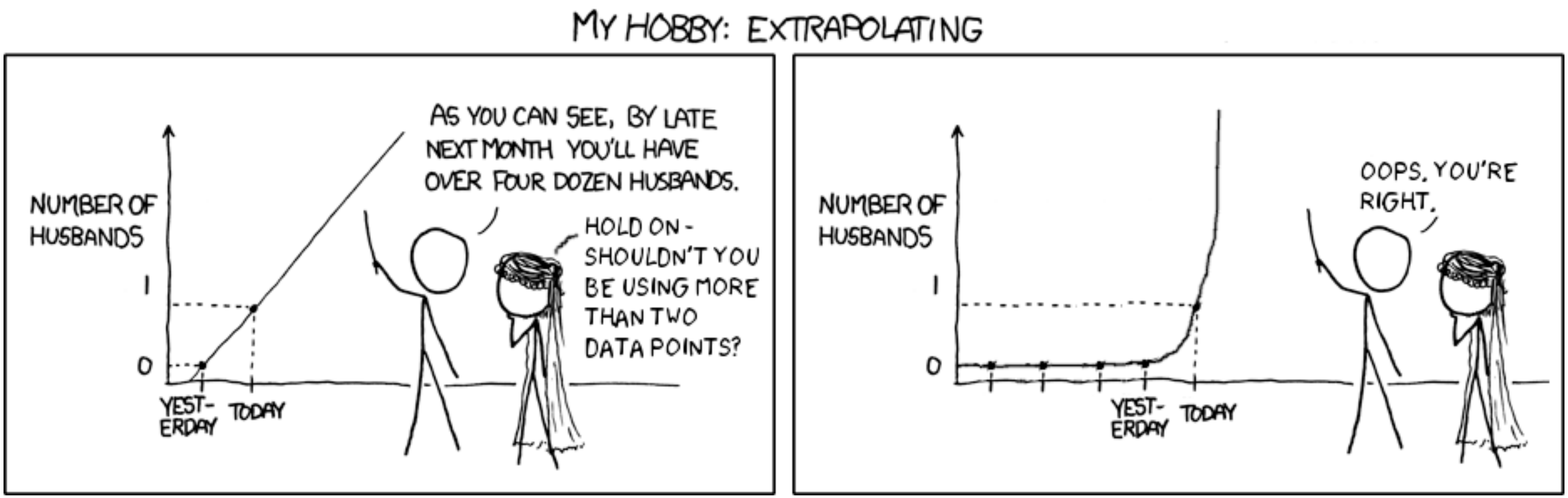
W. Nazarewicz
Y. Cao, S. Giuliani, E. Olsen
O. Tarasov
V. Kejzlar, F. Viens

Menu

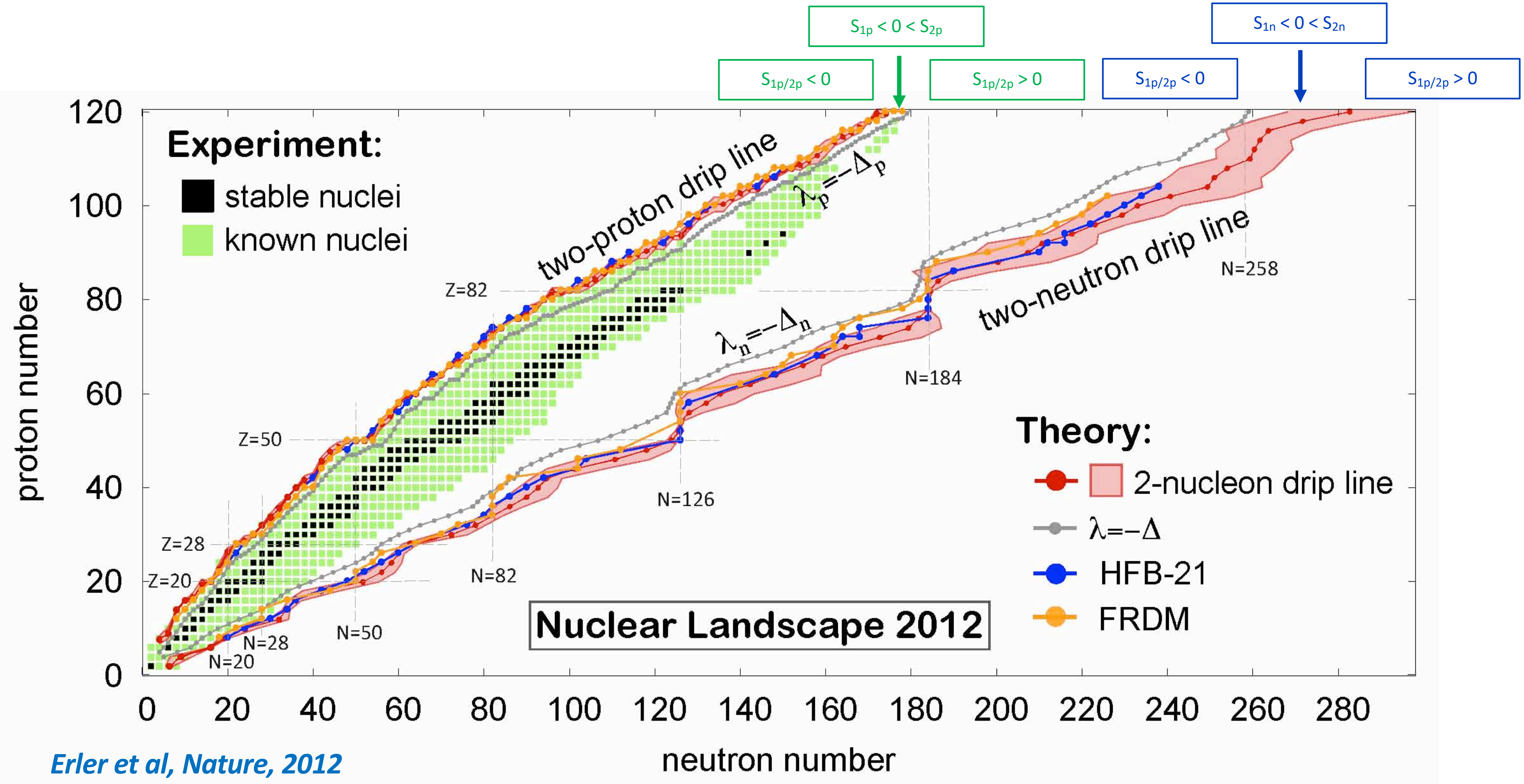
- Model-based extrapolations and Bayesian machine learning
- Separation-energy applications
- Stability of ^{60}Ca and drip line in the Ca region
- Conclusions

“Remember that all models are wrong; the practical question is *how wrong do they have to be to not be useful”* (E.P. Box)

In many cases, nuclear input MUST involve massive extrapolations based on predicted quantities. And extrapolations are ~~impossible~~ tough.



Uncertainty on the nuclear landscape



Erler et al, Nature, 2012

PHYSICAL REVIEW C **98**, 034318 (2018)

Editors' Suggestion

Bayesian approach to model-based extrapolation of nuclear observables

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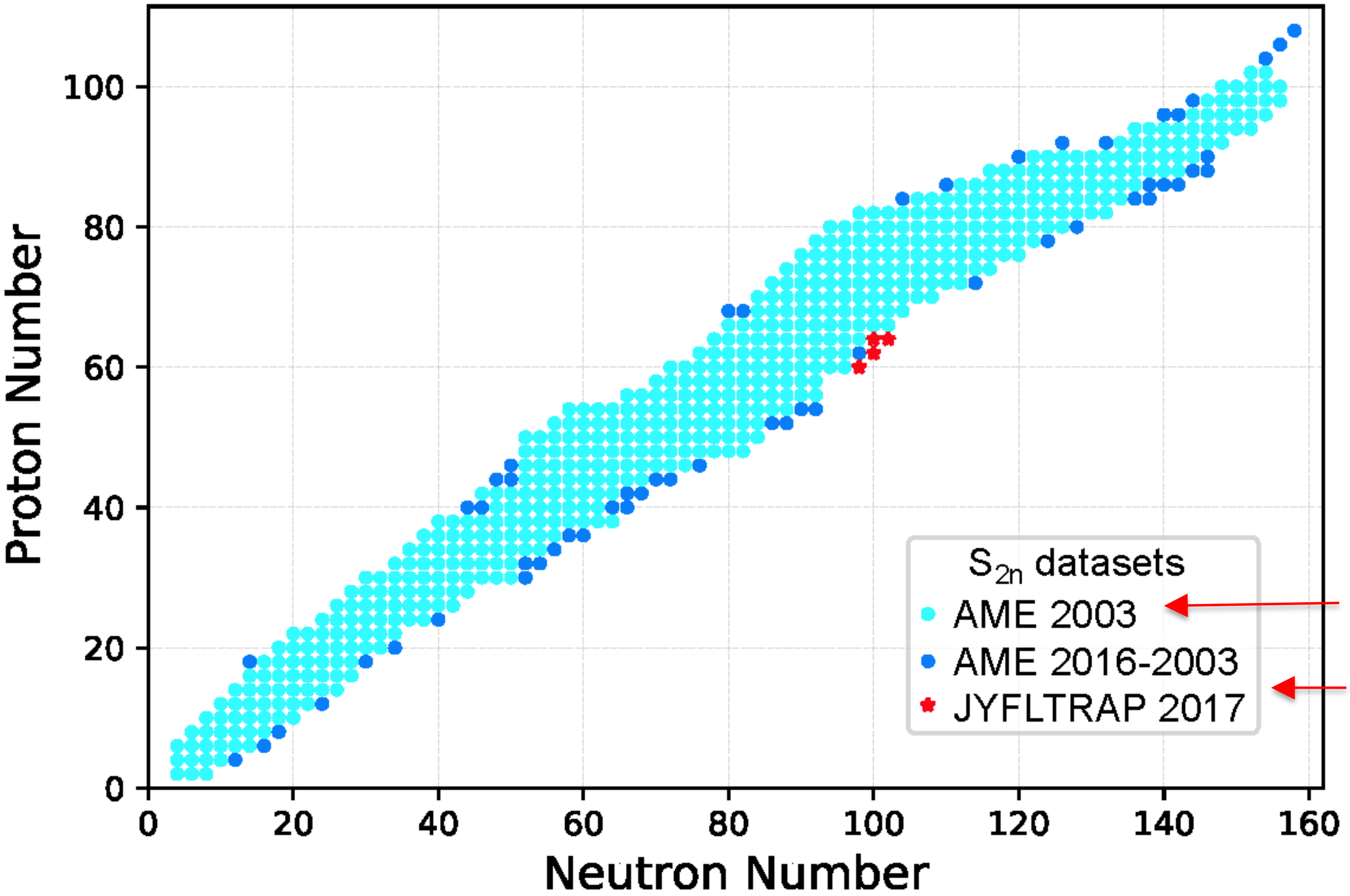
To improve the quality of model-based predictions of nuclear properties of rare isotopes far from stability, **we consider the information contained in the residuals in the regions where the experimental information exist**.
As a case in point, we discuss two-neutron separation energies $\boldsymbol{S_{2n}}$ **of even-even nuclei**. Through this observable, we **assess the predictive power of global mass models towards more unstable neutron-rich nuclei and provide uncertainty quantification of predictions**.

Some recent relevant references…

- S. Athanassopoulos, E. Mavrommatis, K. Gernoth, and J. Clark, Nucl. Phys. A 743, 222 (2004).
- R. Utama, J. Piekarewicz, and H. B. Prosper, Phys. Rev. C 93, 014311 (2016).
- G. F. Bertsch and D. Bingham, Phys. Rev. Lett. 119, 252501 (2017).
- H. F. Zhang et al.,J. Phys. G 44, 045110 (2017).
- Z. Niu and H. Liang, Phys. Lett. B 778, 48 (2018).
- R. Utama and J. Piekarewicz, Phys. Rev. C 97, 014306 (2018).

Data



Training set:
537 points

Testing sets:
55+4 points

Separation energy residual:

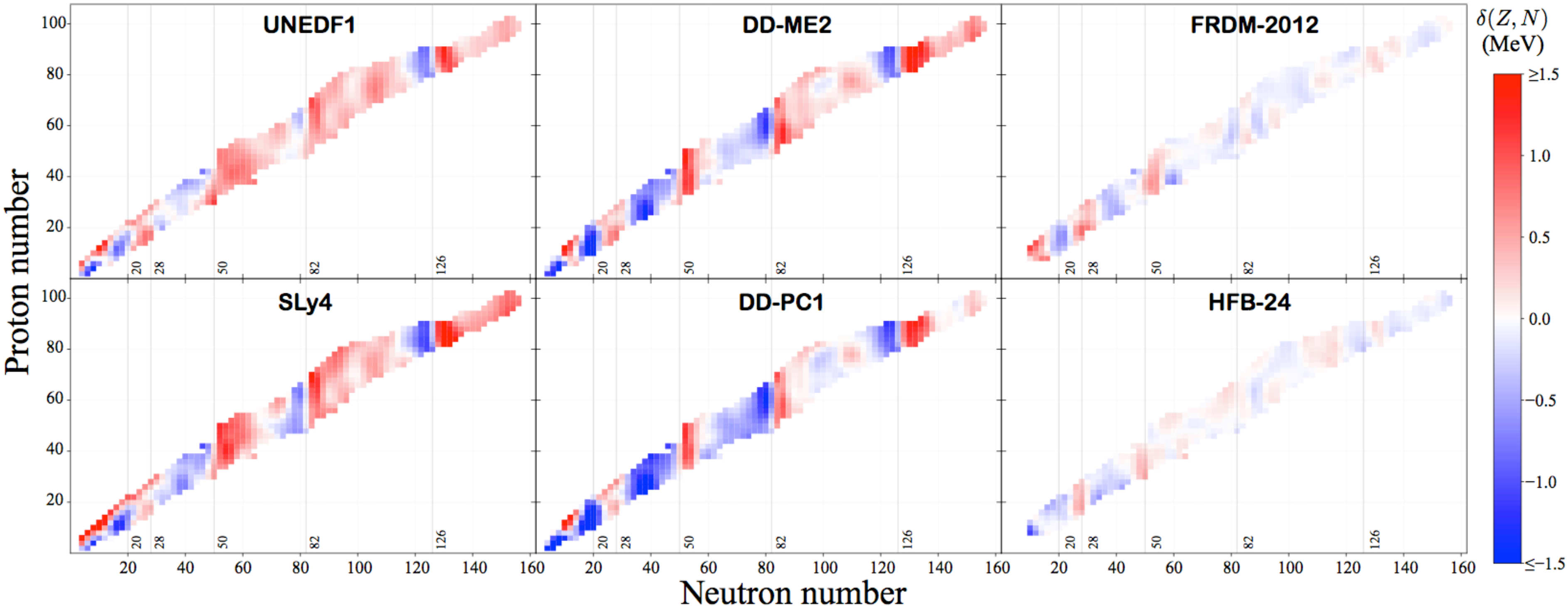
$$\delta(Z,N) = S_{2n}^{\mathrm{exp}}(Z,N) - S_{2n}^{\mathrm{th}}(Z,N,\vartheta)$$

The residuals contain mostly theoretical errors,
which correspond mostly to systematic errors

$$S_{2n}^{\mathrm{est}}(Z,N) = S_{2n}^{\mathrm{th}}(Z,N,\vartheta) + \delta^{\mathrm{em}}(Z,N)$$

emulator of residual

Residuals exhibit local trends



This information can be used to our advantage to improve model-based predictions!

We consider 10 global models based on nuclear Density Functional Theory with realistic energy density functionals as well as two more phenomenological mass models.

FRDM-2012, HFB-24: rms mass deviation ~0.6 MeV
SkM*, SkP, SLy4, SV-min, UNEDF0, UNEDF1: 1.5-6 MeV
NL3*, DD-ME2, DD-PC1, DDMEδ: 2-3 MeV

The emulators of S_{2n} residuals and confidence intervals defining theoretical error bars are constructed using Bayesian Gaussian processes (GP) and Bayesian neural networks (BNN).

We consider a large training dataset pertaining to nuclei whose masses were measured before 2003. For the testing datasets, we considered those exotic nuclei whose masses have been determined after 2003. By establishing statistical methodology and parameters, we carried out extrapolations towards the *2n* dripline.

Bayesian approach I

- Statistical model :

$$y_i = f(x_i, \theta) + \sigma\epsilon_i$$

- $x_i = (Z, N)_i$
- y_i : mass residual
- $f(x_i, \theta)$: statistical model for systematic error
- $\sigma\, \epsilon_i$: statistical uncertainty
- parameters : $\Theta \coloneqq (\theta, \sigma)$

- Bayes theorem gives the posterior distribution of the parameters :

$$p(\Theta|y) \propto p(y|\Theta)\boldsymbol{\pi}(\Theta) \qquad \text{[i.e. } p(\Theta|y) = \frac{p(y|\Theta)\boldsymbol{\pi}(\Theta)}{\int p(y|\Theta)\boldsymbol{\pi}(\Theta)d\Theta}\text{]}$$

- Posterior prediction of unknown observable y* given known data y :

$$p(y^*|y) = \int p(y^*|y, \Theta)\pi(\Theta)d\Theta$$

Bayesian approach II

- Two statistical models used:
  - Gaussian process (**3** parameters)
  - (Bayesian) Neural Network with sigmoid function (30 neurons, 1 layer; **181** parameters)

- BNN refinement: non-linear transformation of x based on our knowledge of trends added to input, namely
  - $d_N(x)$ (distance to closest neutron magic number)
  - $p(x) := \frac{d_Z(x) d_N(x)}{d_Z(x) + d_N(x)}$ (promiscuity factor)

- Samples $\widehat{\Theta}_1, \widehat{\Theta}_2, \dots, \widehat{\Theta}_m \sim p(\Theta|y)$ are produced from 100,000-1,000,000 iterations of an ergodic Markov chain

- Metropolis(-Hastings):
  - start from any point : $\widehat{\Theta}_1 := x$
  - and, iteratively,
    - sample from proposal distribution $g(\Theta)$: $\widetilde{\Theta} \sim g(\widetilde{\Theta})$
    - with probability $\alpha \wedge 1$, with $\alpha := \frac{p(\widetilde{\Theta}|y)}{g(\widetilde{\Theta})}$, accept : $\widehat{\Theta}_{m+1} := \widetilde{\Theta}$
    - with probability $1 - \alpha$, reject : $\widehat{\Theta}_{m+1} := \widehat{\Theta}_{m+1}$
  - "burn in" the first m_0 samples

- More advanced methods for high-dimensional spaces : Hamiltonian Monte Carlo

Gaussian Processes

$$f(x,\theta) \sim \mathcal{GP}(0, k_{\eta,\rho})$$

$$k_{\eta,\rho}(x,x') := \eta^2 e^{-\frac{(Z-Z')^2}{2\rho_Z^2} - \frac{(N-N')^2}{2\rho_N^2}}$$

quadratic exponential covariance kernel

likelihood :

$$p(y|\eta,\rho,\sigma) := \frac{1}{\sqrt{\det(2\pi\Sigma)}} e^{-\frac{1}{2}y^T\Sigma^{-1}y}$$

$$\Sigma_{i,j} = k_{\eta,\rho}(x_i,x_j) + \sigma^2\delta_{i,j}$$

model prediction :

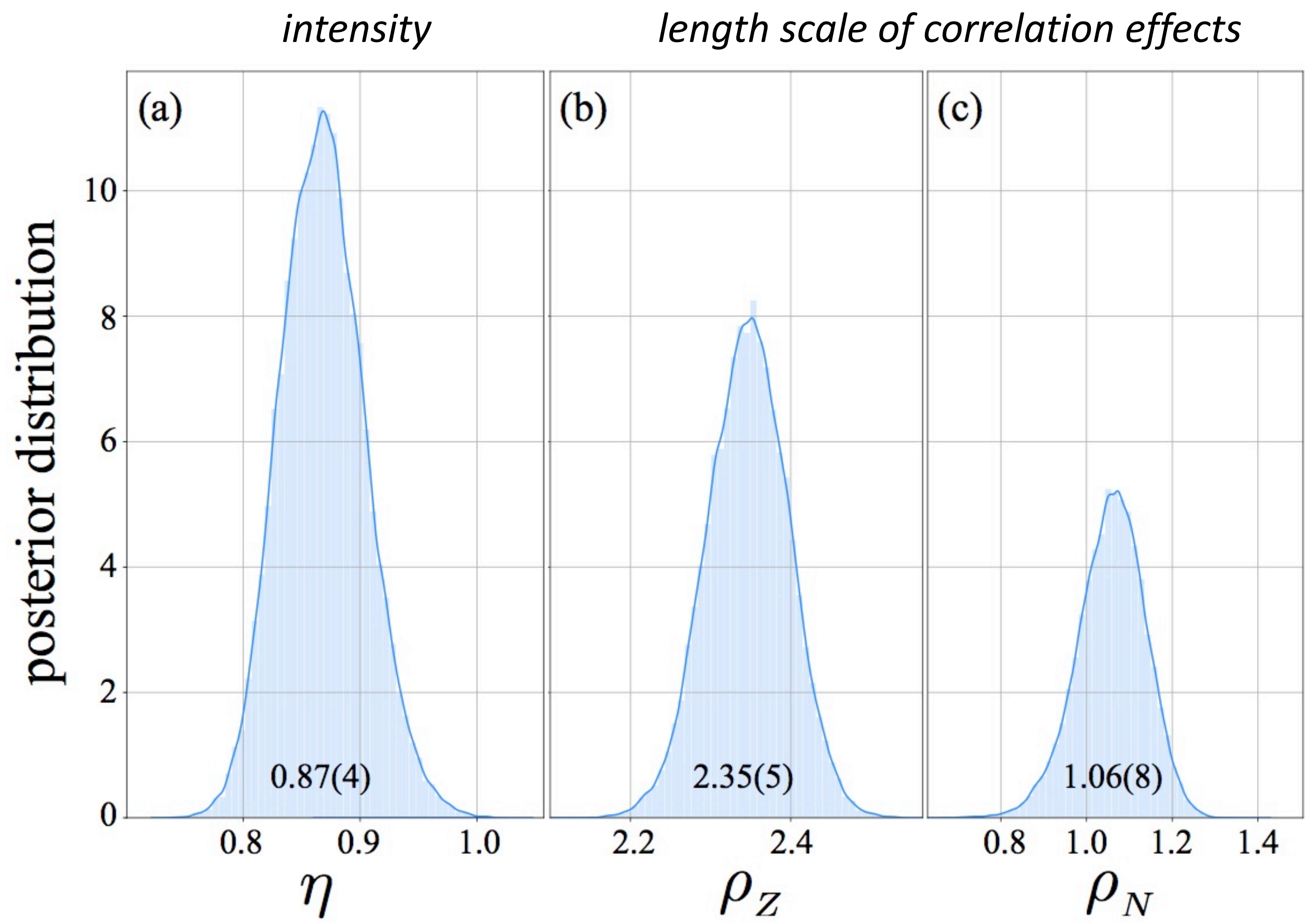
$$y^*|\boldsymbol{y},\eta,\rho,\sigma \sim \mathcal{N}(\Sigma^*\Sigma^{-1}\boldsymbol{y}, \Sigma^{**} - \Sigma^*\Sigma^{-1}\Sigma^*)$$

$$\Sigma^*_{i,j} = k_{\eta,\rho}(x_i^*, x_j)$$

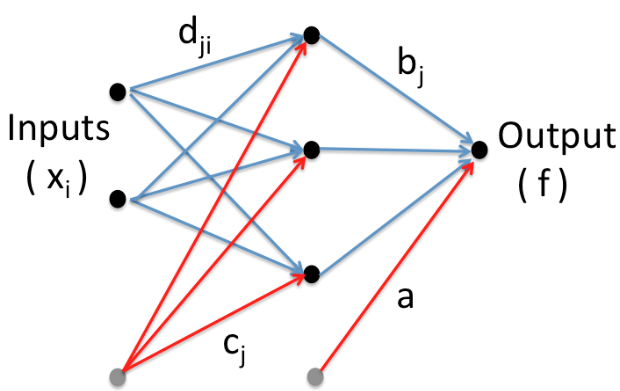
$$\Sigma^{**}_{i,j} = k_{\eta,\rho}(x_i^*, x_j^*) + \sigma^2\delta_{i,j}$$

the training data contains more predictive information than the model parameters

GP parameters



Neural Networks



Utama & Piekarewicz, PRC, 2017

# of hidden neurons

$$f(x,\theta) := a + \sum_{j=1}^{H} b_j \phi \left(c_j + \sum_i d_{ji} x_i \right)$$

NN with 1 layer

activation function (tanh)

$$p(y|\theta,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\sum_i \frac{(y_i - f(x_i,\theta))^2}{2\sigma^2}}$$

likelihood

$$y^*|\theta,\sigma \sim \mathcal{N}(f(x^*,\theta),\sigma^2)$$

model prediction

RMS deviations

training dataset: AME2003
testing dataset: AME2016-AME2003

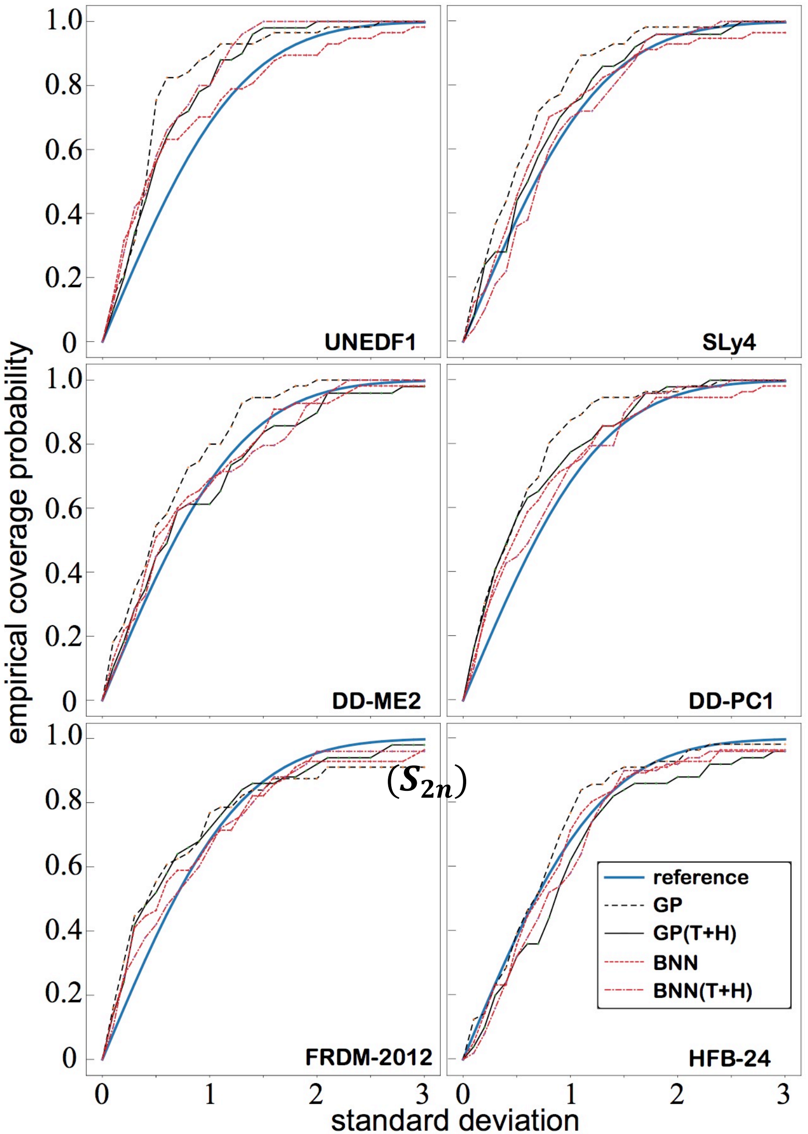
model	Std	T	H	T+H
SkM*	0.96(23)	0.96(23)	0.49(52)	0.49(52)
1.25/1.01	0.99(20)	0.81(35)	0.73(28)	0.53(47)
SLy4	0.82(13)	0.82(13)	0.52(35)	0.52(35)
0.95/0.80	0.91(3)	0.82(14)	0.71(11)	0.56(30)
SkP	0.75(11)	0.75(11)	0.38(39)	0.38(39)
0.84/0.62	0.76(9)	0.74(12)	0.59(5)	0.45(27)
SV-min	0.70(10)	0.70(10)	0.32(34)	0.33(34)
0.78/0.49	0.72(8)	1.35(-73)	0.50(-1)	0.43(12)
UNEDF0	0.73(6)	0.73(6)	0.34(37)	0.34(37)
0.78/0.54	0.87(-12)	0.73(7)	0.55(0)	0.46(16)
UNEDF1	0.61(8)	0.61(8)	0.34(30)	0.34(30)
0.66/0.49	0.79(-20)	0.74(-12)	0.53(-10)	0.32(33)
NL3*	0.84(29)	0.84(29)	0.46(47)	0.45(47)
1.19/0.86	1.10(7)	0.90(24)	0.83(4)	0.69(20)
DD-MEδ	0.73(35)	0.74(35)	0.55(42)	0.55(42)
1.13/0.96	1.08(4)	0.91(19)	0.89(7)	0.75(22)
DD-ME2	0.71(32)	0.71(31)	0.63(34)	0.62(34)
1.04/0.95	1.00(4)	1.32(-27)	0.90(5)	0.61(36)
DD-PC1	0.79(28)	0.79(28)	0.46(50)	0.46(50)
1.10/0.91	1.00(9)	1.33(-22)	0.85(7)	0.54(41)
FRDM-2012	0.57(9)	0.57(9)	0.36(25)	0.36(26)
0.63/0.49	0.61(4)	0.72(-15)	0.48(2)	0.45(7)
HFB-24	0.40(-1)	0.40(-1)	0.40(-8)	0.40(-8)
0.40/0.37	0.59(-48)	0.44(-10)	0.37(1)	0.35(6)

GP
BNN

- rms deviation is 400-500 keV in the GP(T+H) variant for <u>all</u> theoretical models employed in our study
- this suggests that most of the residual structure is captured
- <u>but</u> : the predicted mean value is certainly not the whole story!

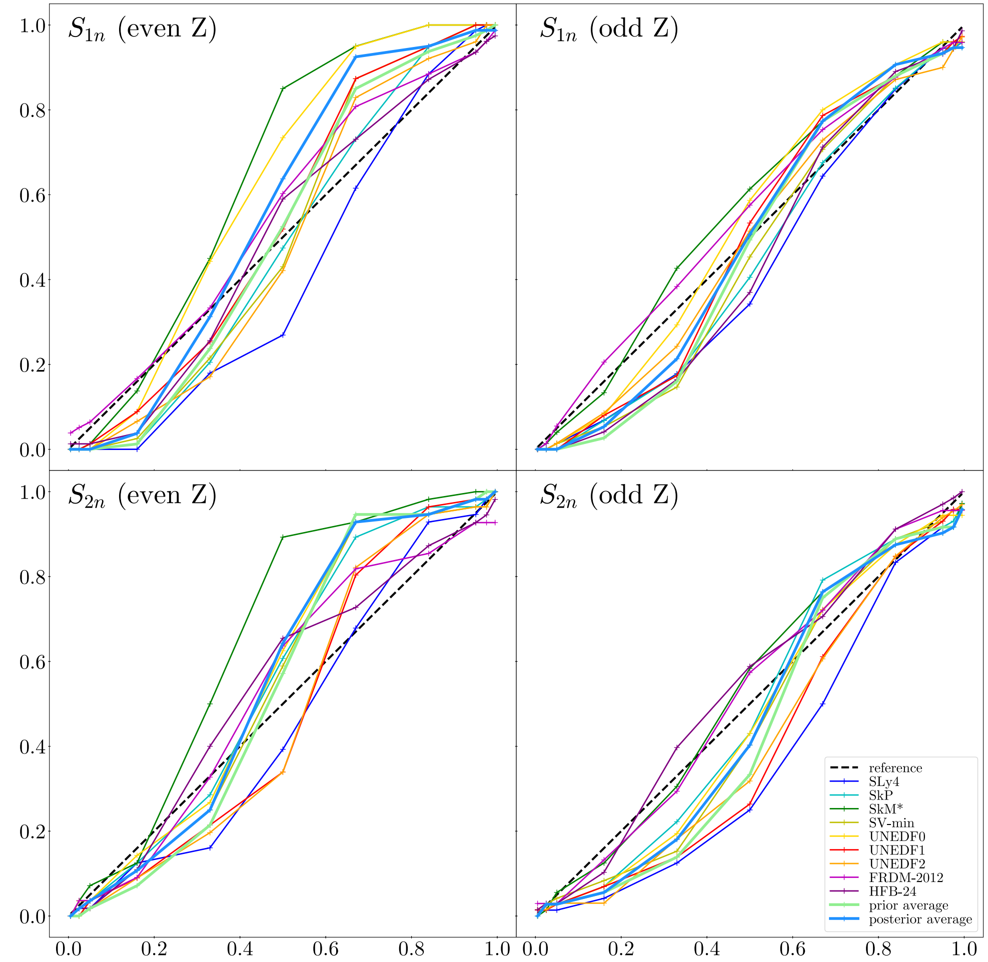
Empirical Coverage Probability I

- ECP is a simple and intuitive metric for assessing the quality of a statistical model's UQ (Gneiting et al., 2007)
- The reference curve shows the **fraction of predictions which should theoretically fall in a CI** centered around the posterior mean prediction according to the model, as a function of the interval width
- The other curves give the **proportion of data which actually falls in the corresponding CI**.
- Values for the ECP **matching** the reference curve are **desirable**.
- A point **above** the reference curve represents a prediction which is too **conservative** (or **pessimistic**).
- A point **below** the reference curve represent a CI which is too narrow (**optimistic**). This should be considered **dishonest**, since it is claiming a level of assurance which is higher than it should be.

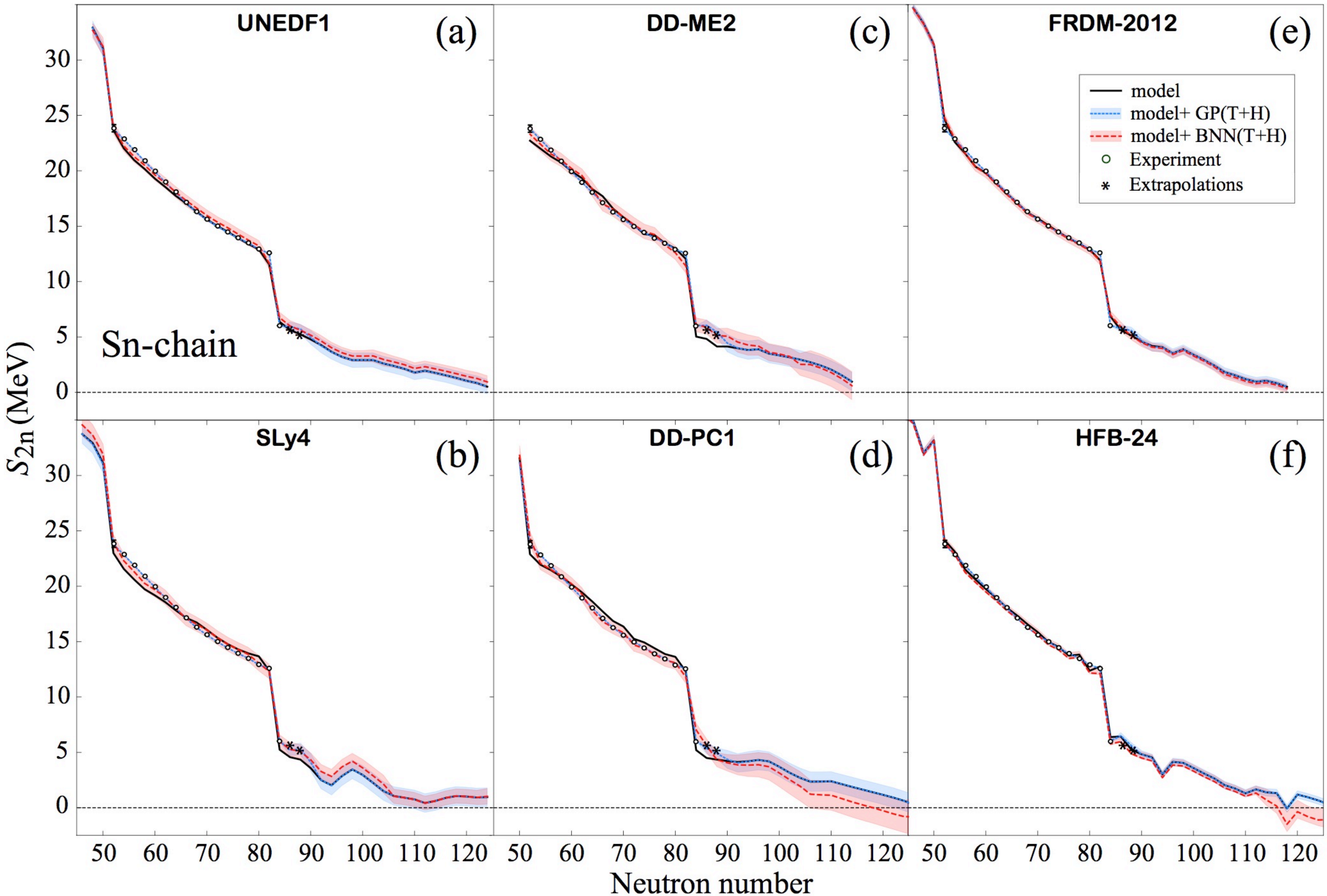


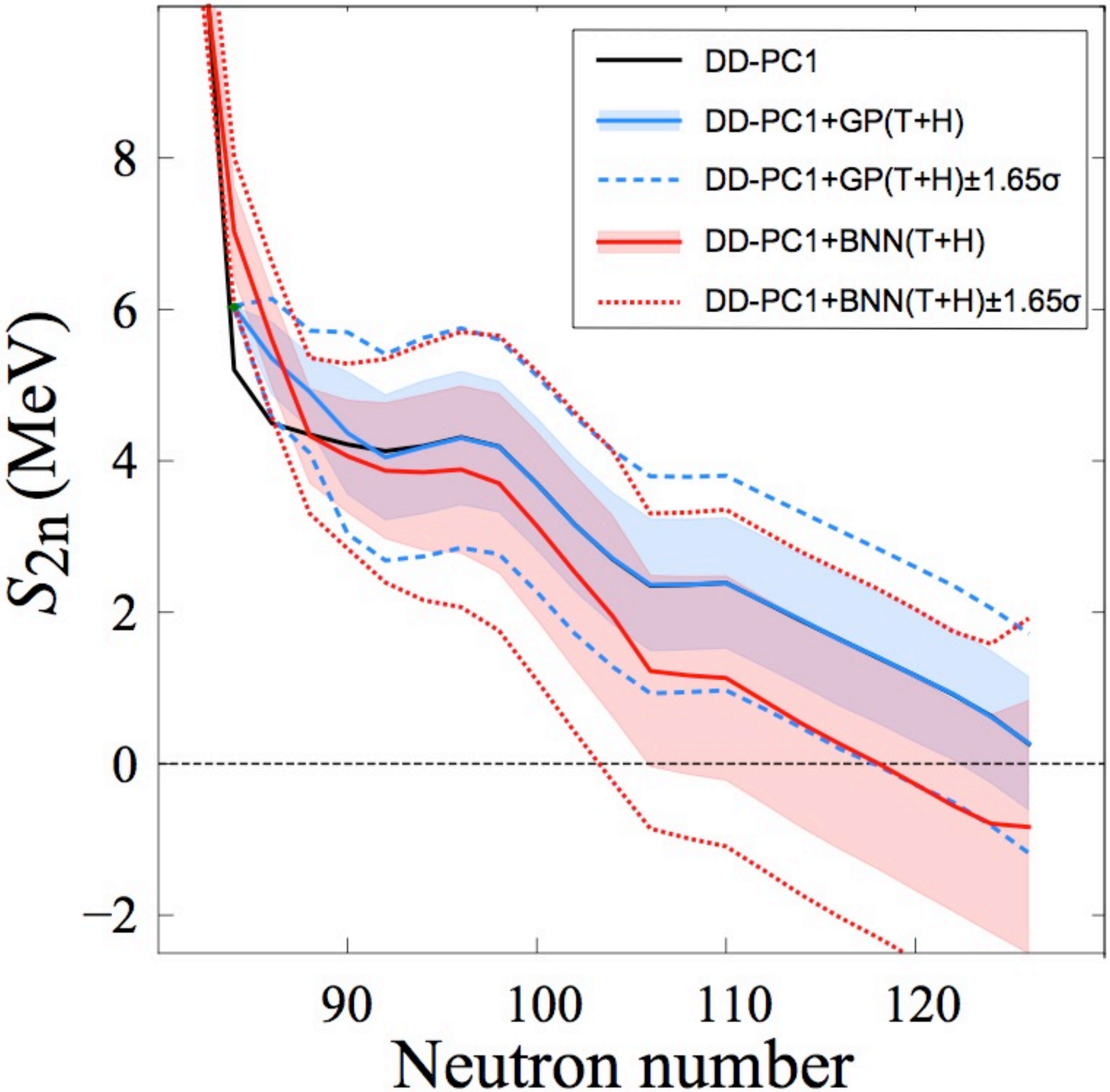
ECP II

- ECP for $S_{1n/2n}$ in the Ca region
- ECP for GP model on separation energy residuals
- $\boldsymbol{x}$ is the nominal value of the credibility interval
- $\boldsymbol{y}$ is the actual fraction of testing data falling into it



Extrapolations



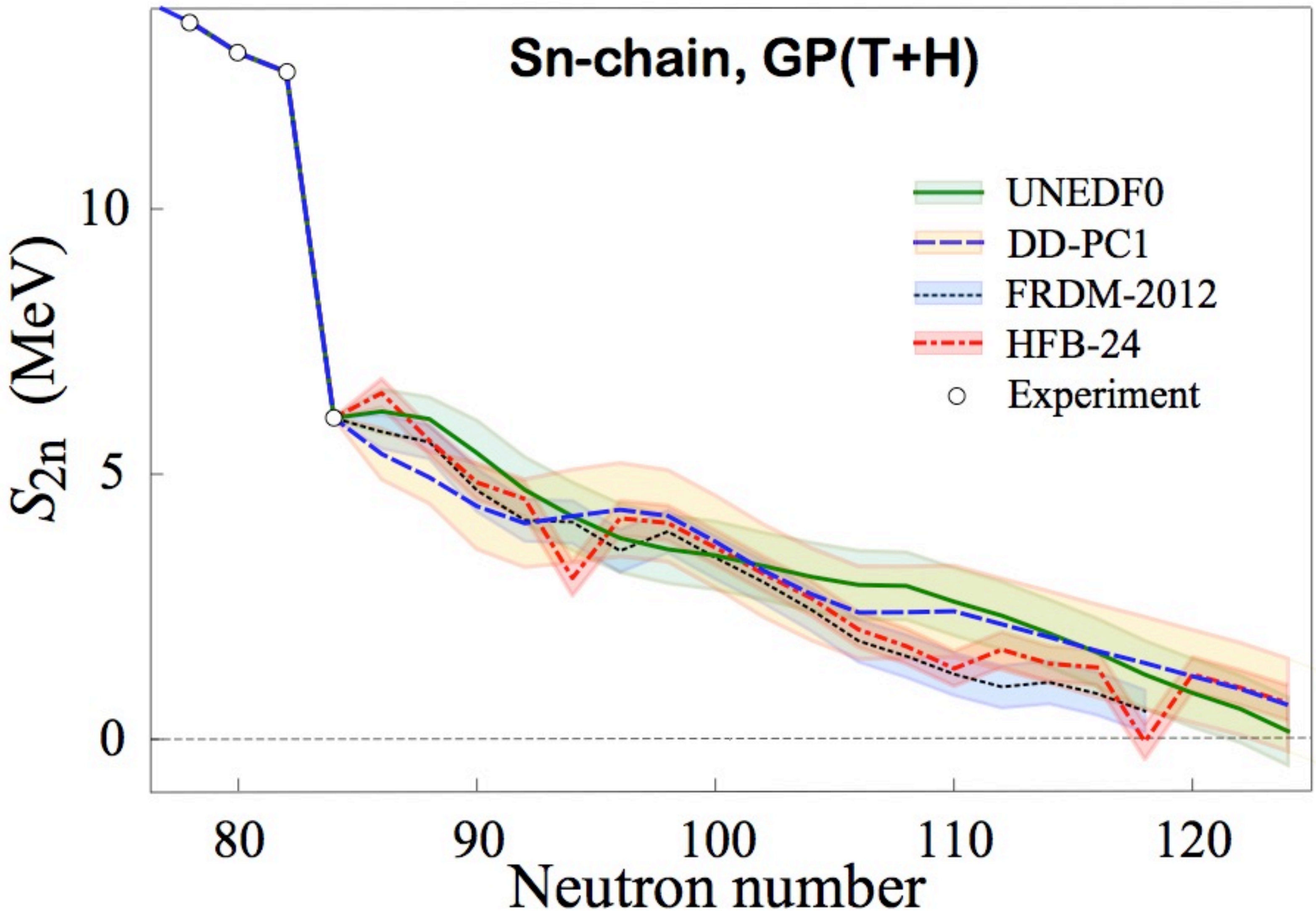


model: N*=126

model+GP: N*=126 (N*=122 at 1s and N*=118 at 1.65s one-sided/credibility 95%)

model+BNN: N*=118 (N*=104 at 1s and N*=102 at 1.65s)

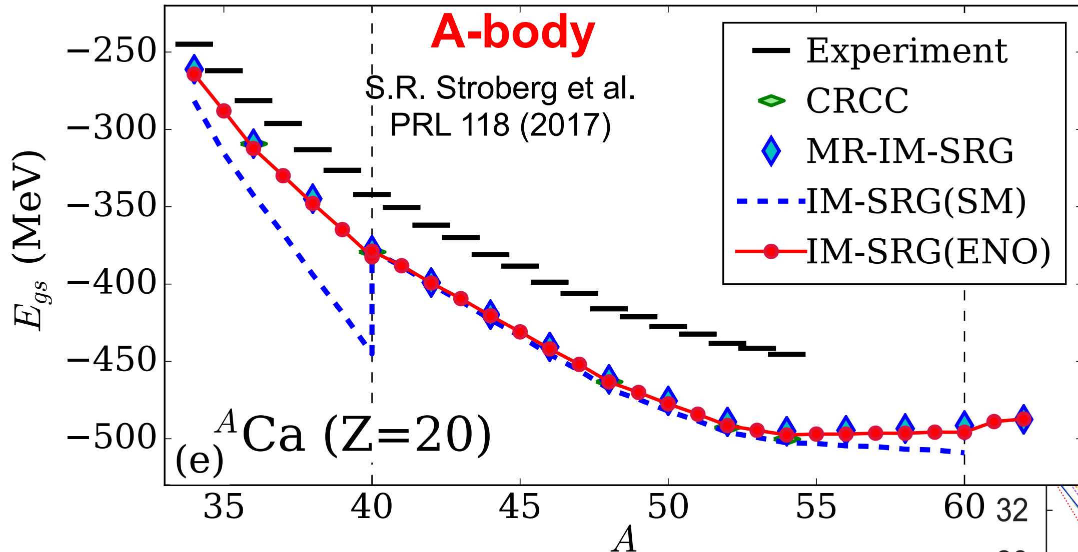
Can one say: “DD-PC1 predicts the 2n dripline at N=126” ?



The increase in the predictive power of microscopic models aided by the statistical treatment is quite astonishing: The resulting rms deviations from experiment on the testing dataset are similar to those of more phenomenological models.

How many Ca nuclei exist?

L.N., Y. Cao, W. Nazarewicz, E. Olsen & F. Viens, Phys. Rev. Lett. (2019)

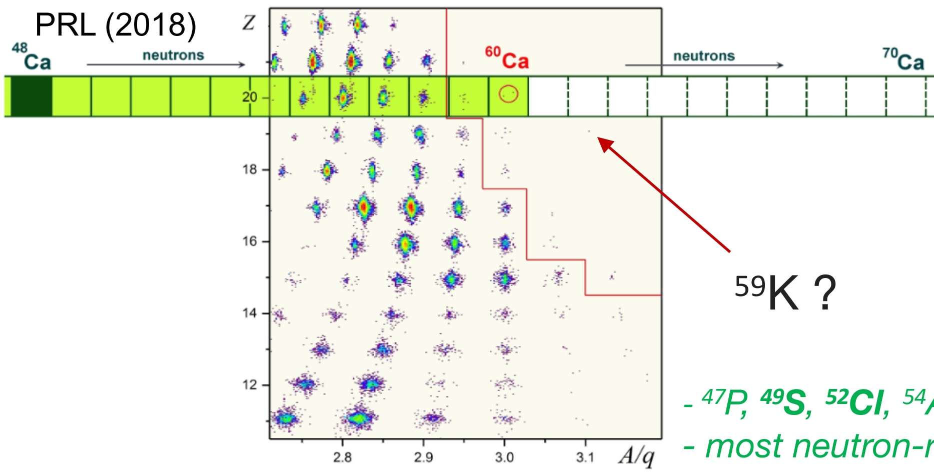


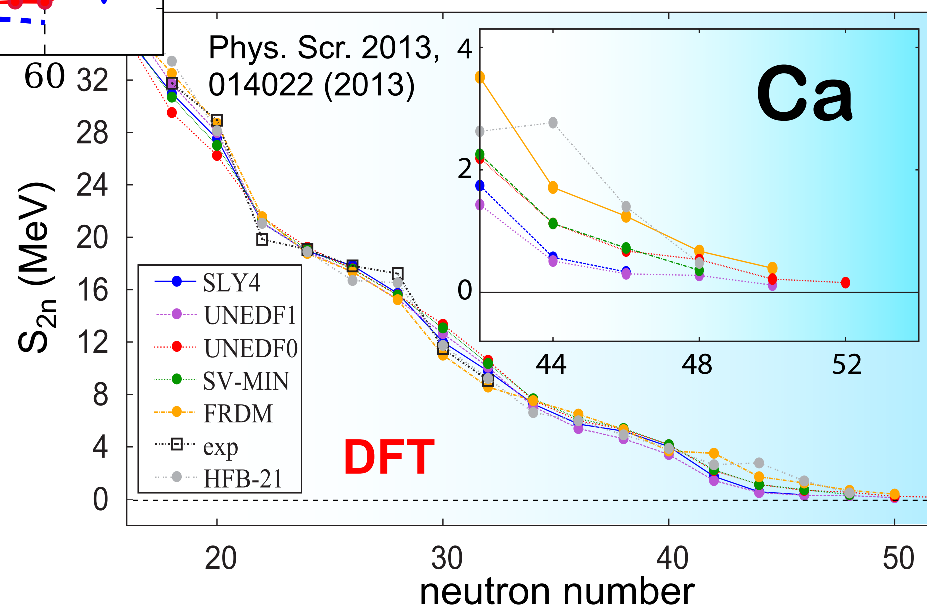
^{60}Ca weakly bound/unbound, $^{61-62}$Ca are located right at the neutron thresholds

Calcium isotopes bound out to about ^{70}Ca

Discovery of ^{60}Ca

O. Tarasov et al.
PRL (2018)

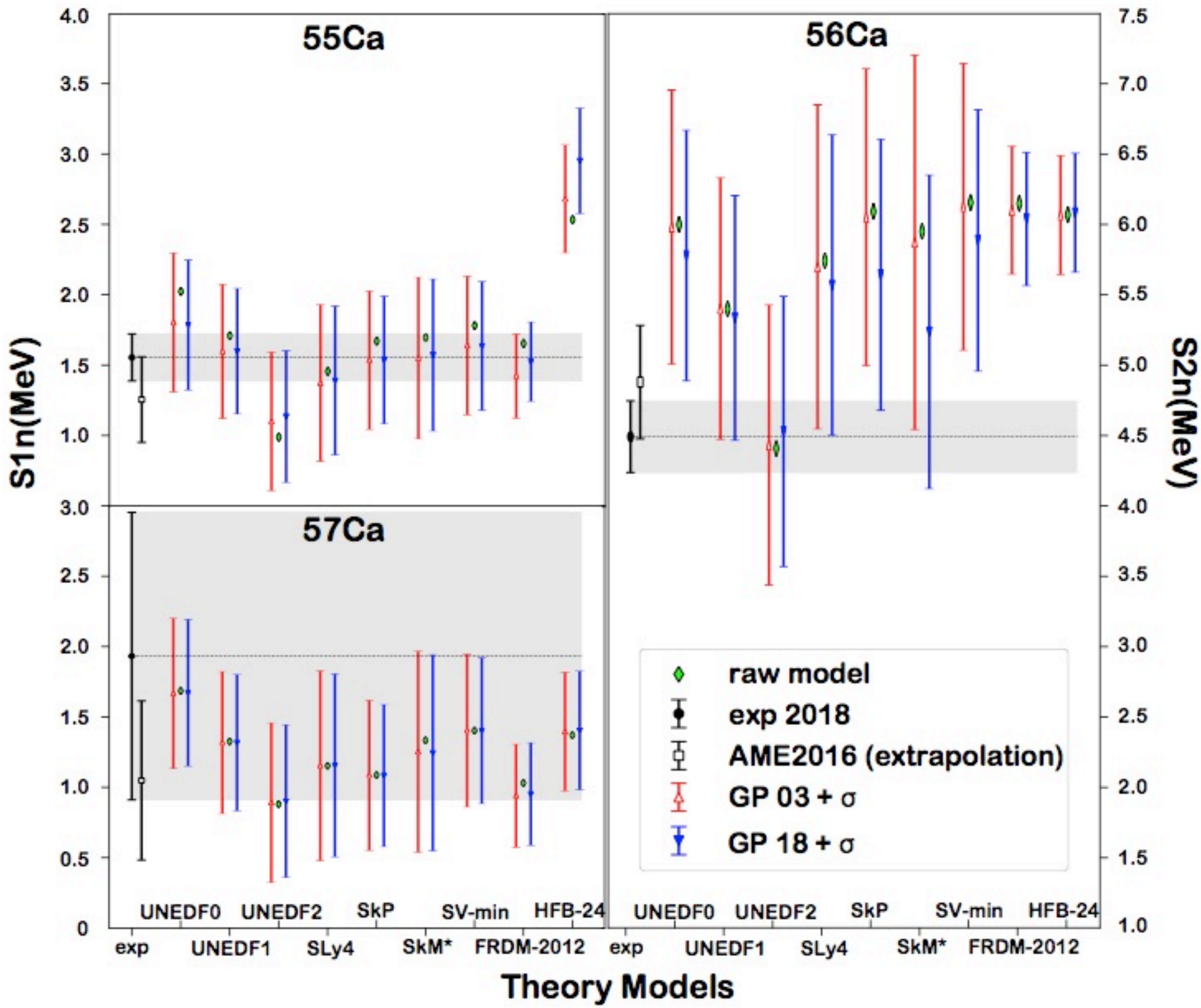




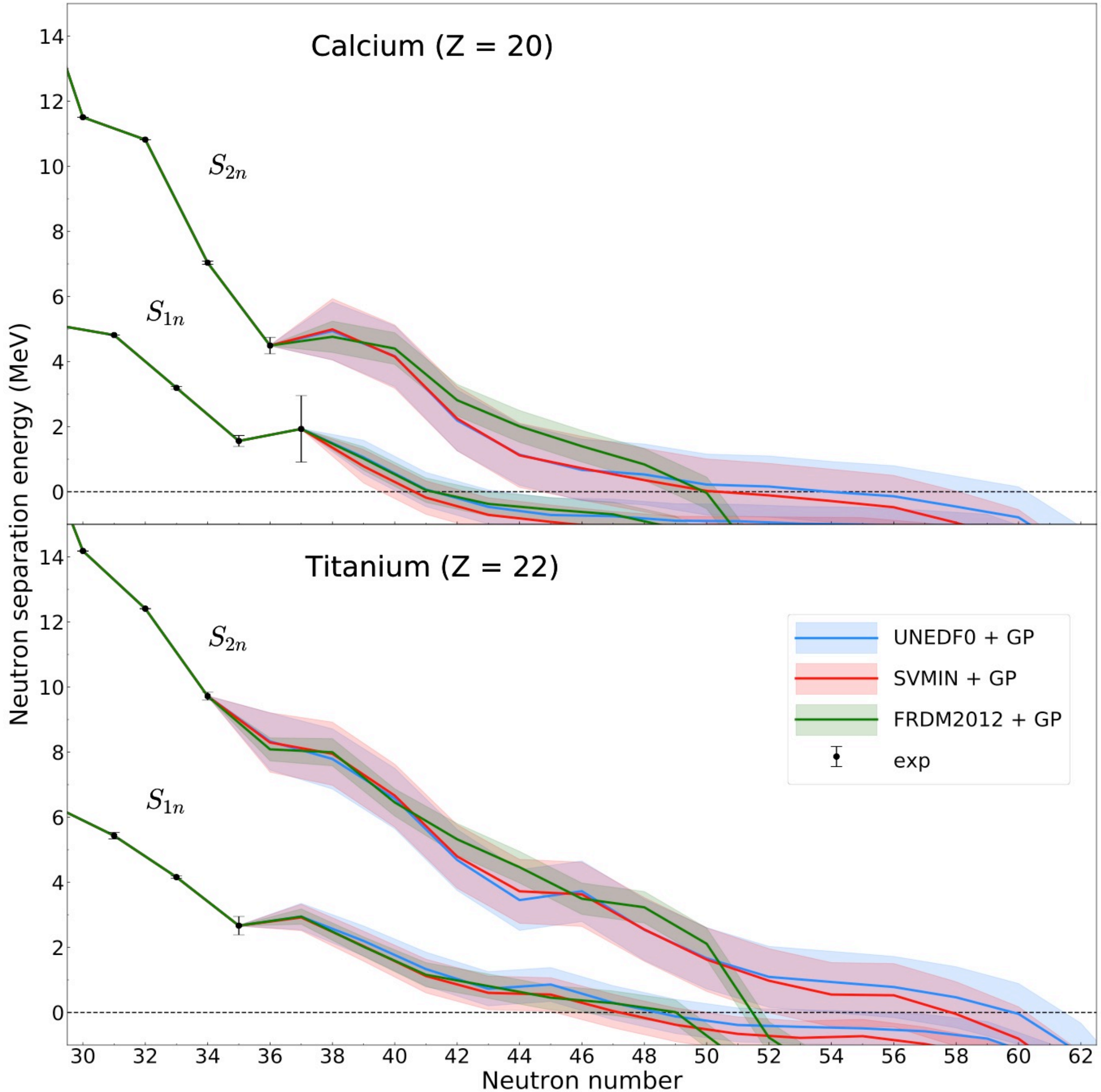
- *^{47}P, **^{49}S**, **^{52}Cl**, ^{54}Ar, ^{57}K, ^{59,60}Ca, and ^{62}Sc, discovered*
- *most neutron-rich isotopes of elements)*
- *one event consistent with ^{59}K*

Validation: new masses of $^{55-57}Ca$

S. Michimasa, et al., Phys. Rev. Lett. 121, 022506 (2018)



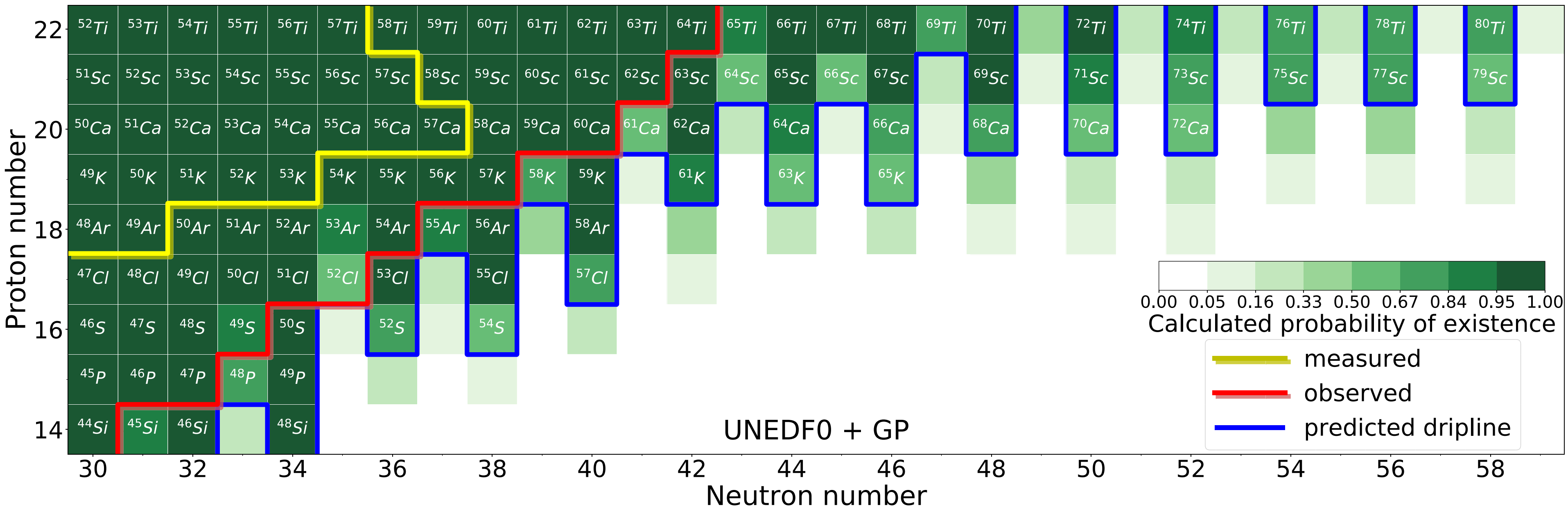
$S_{1n/2n}$ extrapolations for Ca and Ti

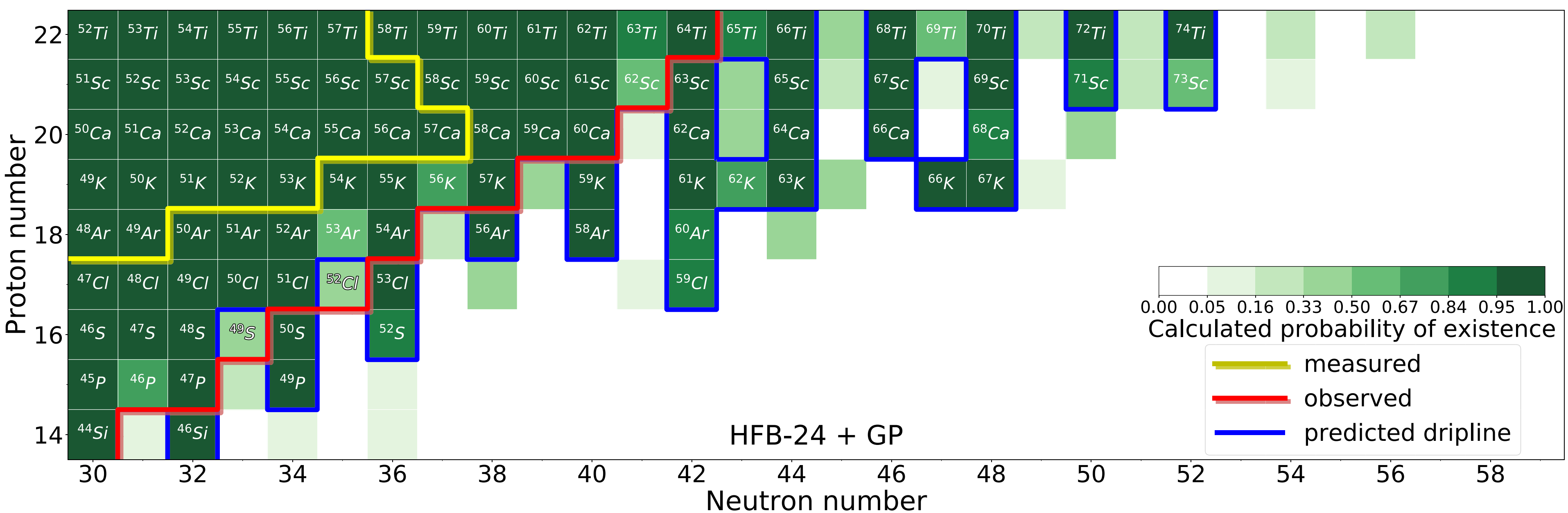


Posterior probability of existence

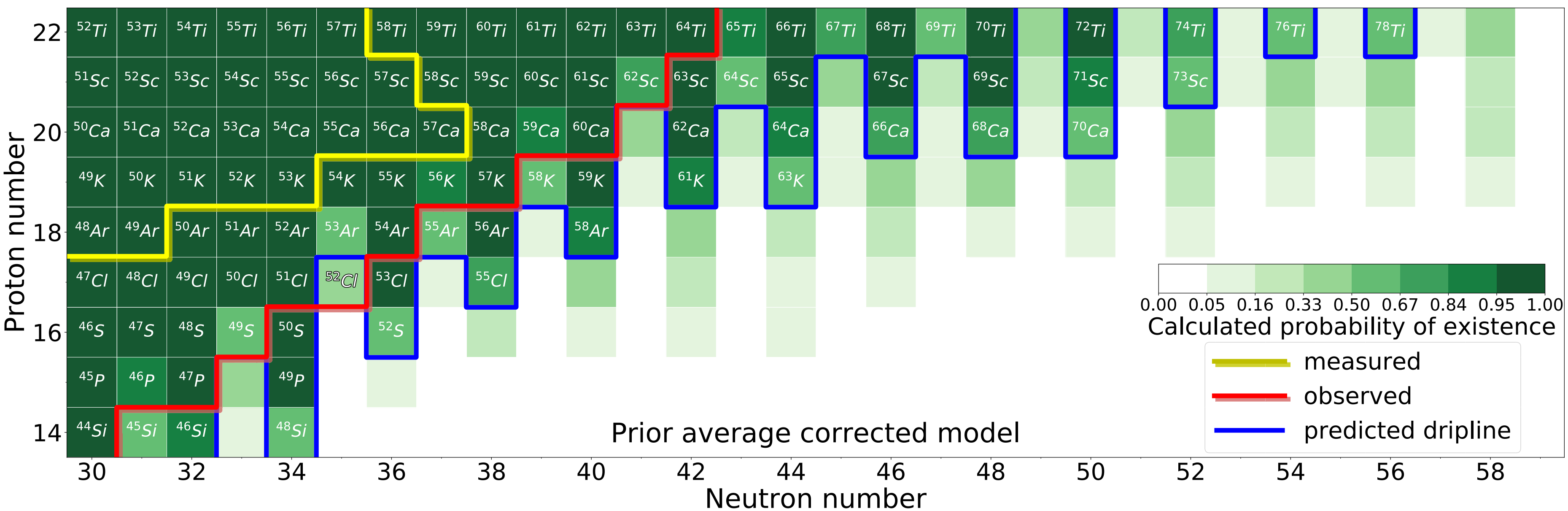
We introduce the posterior proba*bility $p_{ex}(Z,N)$ of the predicted separation energy $S_{1n/2n}(Z,N)$ being positive:

$$p_{ex}(Z,N) := p(S^*_{1n/2n}(Z,N) > 0 | S_{1n/2n})$$


UNEDF0 + GP
Proton number
Neutron number
0.00 0.05 0.16 0.33 0.50 0.67 0.84 0.95 1.00
Calculated probability of existence
measured
observed
predicted dripline


HFB-24 + GP
Proton number
Neutron number
0.00 0.05 0.16 0.33 0.50 0.67 0.84 0.95 1.00
Calculated probability of existence
measured
observed
predicted dripline

Probability of existence : naïve average model



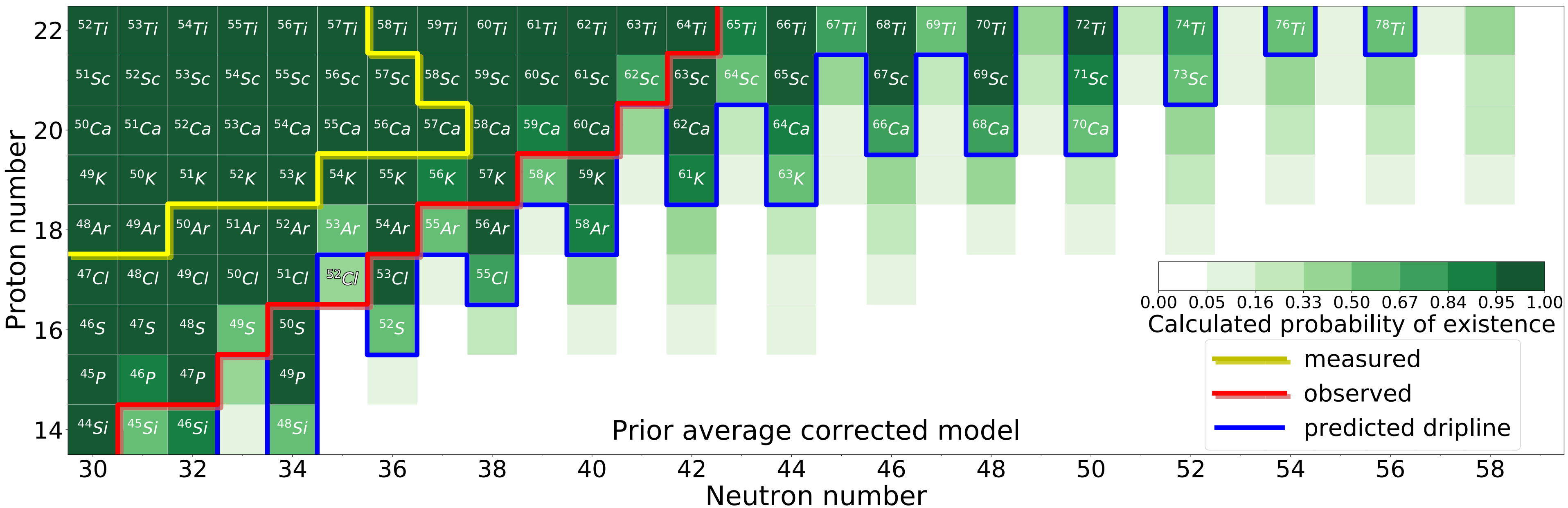
Bayesian model mixing

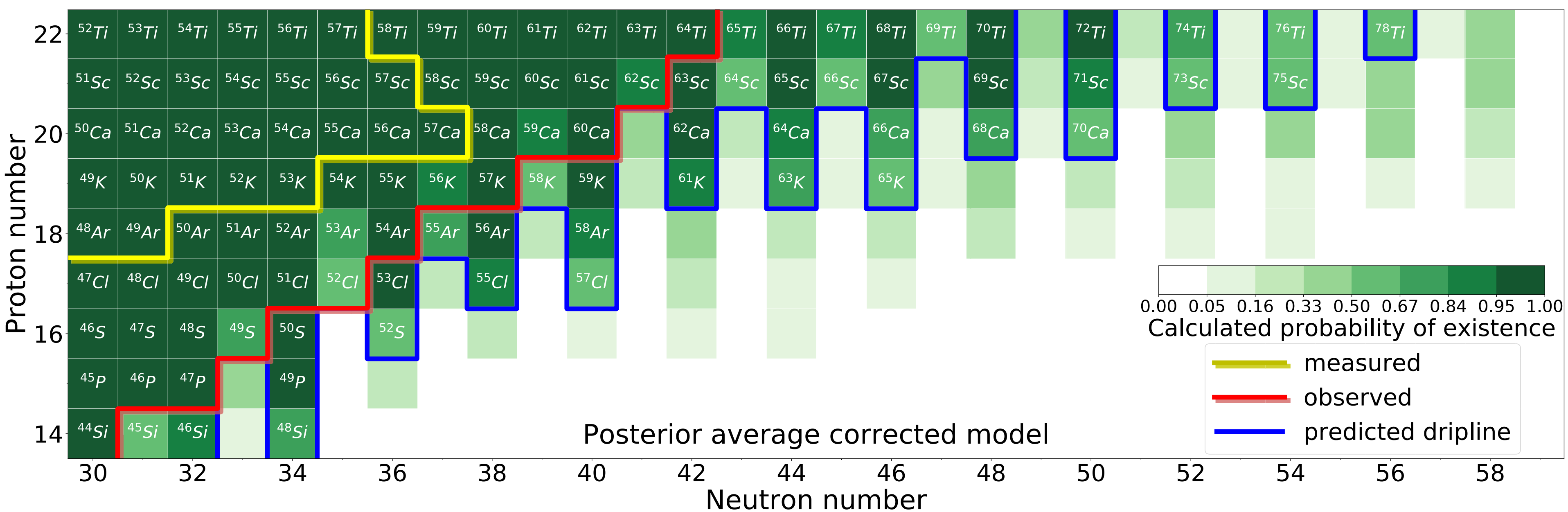
Our model mixing calculations were done by averaging posteriors obtained with individual models.

In the first averaging variant, we assumed model-independent *prior* weights.

In the second *posterior* averaging variant, the weights were obtained as the Bayesian posterior probabilities that a model M_k predicts the existence of the key nuclei ^{52}Cl, ^{53}Ar, and ^{49}S, namely:

$$w_k := p\left(\mathcal{M}_k | {}^{52}\mathrm{Cl}, {}^{53}\mathrm{Ar}, {}^{49}\mathrm{S\ exist}\right)$$
$$\propto p\left(S_{1n}\ \mathrm{of}\ {}^{49}\mathrm{S}, {}^{52}\mathrm{Cl},\ \mathrm{and}\ {}^{53}\mathrm{Ar} > 0 | \mathcal{M}_k\right) \pi(\mathcal{M}_k),$$


52Ti 53Ti 54Ti 55Ti 56Ti 57Ti 58Ti 59Ti 60Ti 61Ti 62Ti 63Ti 64Ti 65Ti 66Ti 67Ti 68Ti 69Ti 70Ti 72Ti 74Ti 76Ti 78Ti
51Sc 52Sc 53Sc 54Sc 55Sc 56Sc 57Sc 58Sc 59Sc 60Sc 61Sc 62Sc 63Sc 64Sc 65Sc 67Sc 69Sc 71Sc 73Sc
50Ca 51Ca 52Ca 53Ca 54Ca 55Ca 56Ca 57Ca 58Ca 59Ca 60Ca 62Ca 64Ca 66Ca 68Ca 70Ca
49K 50K 51K 52K 53K 54K 55K 56K 57K 58K 59K 61K 63K
48Ar 49Ar 50Ar 51Ar 52Ar 53Ar 54Ar 55Ar 56Ar 58Ar
47Cl 48Cl 49Cl 50Cl 51Cl 52Cl 53Cl 55Cl
46S 47S 48S 49S 50S 52S
45P 46P 47P 49P
44Si 45Si 46Si 48Si
Proton number
22
20
18
16
14
Neutron number
30 32 34 36 38 40 42 44 46 48 50 52 54 56 58
0.00 0.05 0.16 0.33 0.50 0.67 0.84 0.95 1.00
Calculated probability of existence
measured
observed
predicted dripline
Prior average corrected model


52Ti 53Ti 54Ti 55Ti 56Ti 57Ti 58Ti 59Ti 60Ti 61Ti 62Ti 63Ti 64Ti 65Ti 66Ti 67Ti 68Ti 69Ti 70Ti 72Ti 74Ti 76Ti 78Ti
51Sc 52Sc 53Sc 54Sc 55Sc 56Sc 57Sc 58Sc 59Sc 60Sc 61Sc 62Sc 63Sc 64Sc 65Sc 66Sc 67Sc 69Sc 71Sc 73Sc 75Sc
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0.00 0.05 0.16 0.33 0.50 0.67 0.84 0.95 1.00
Calculated probability of existence
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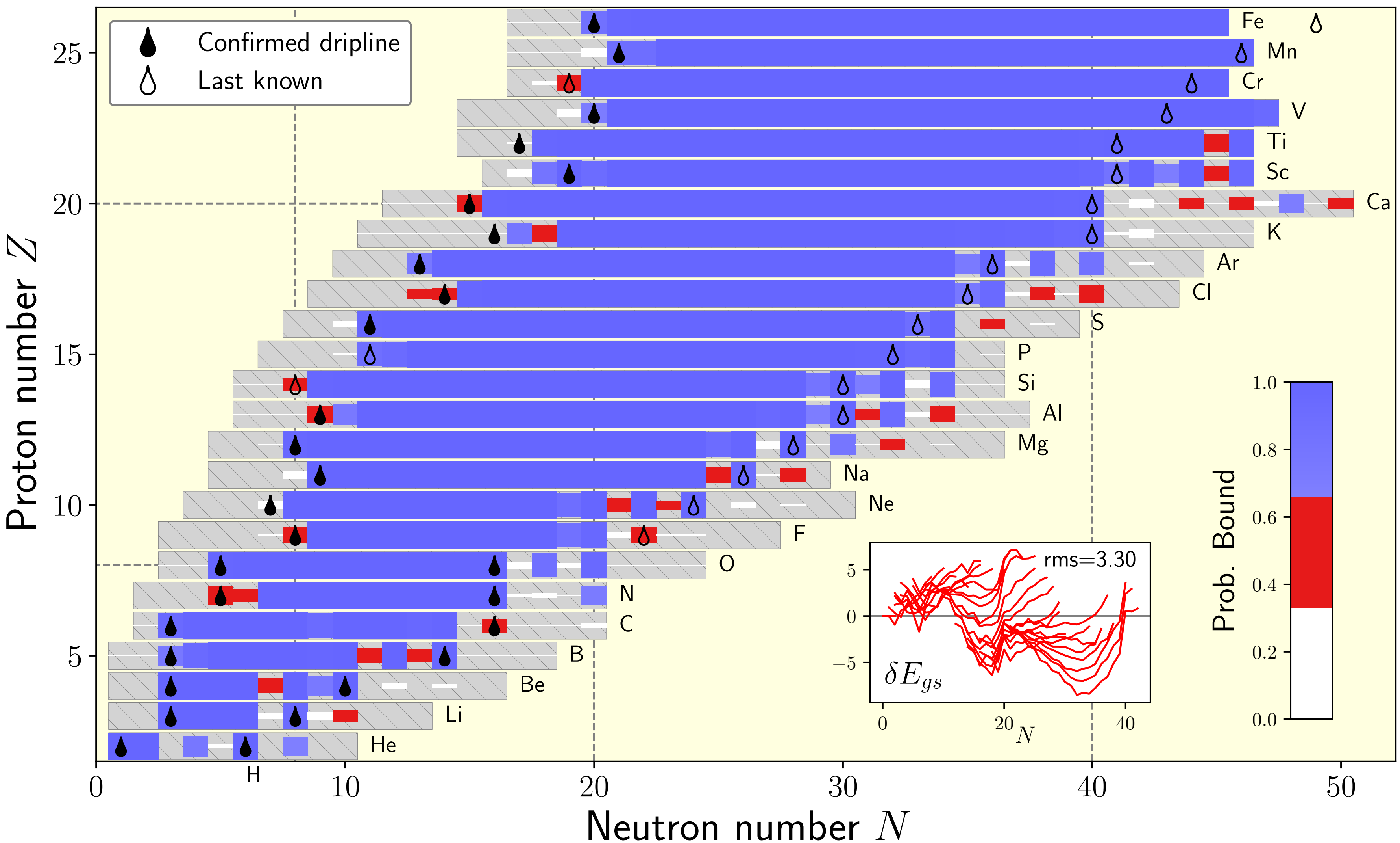
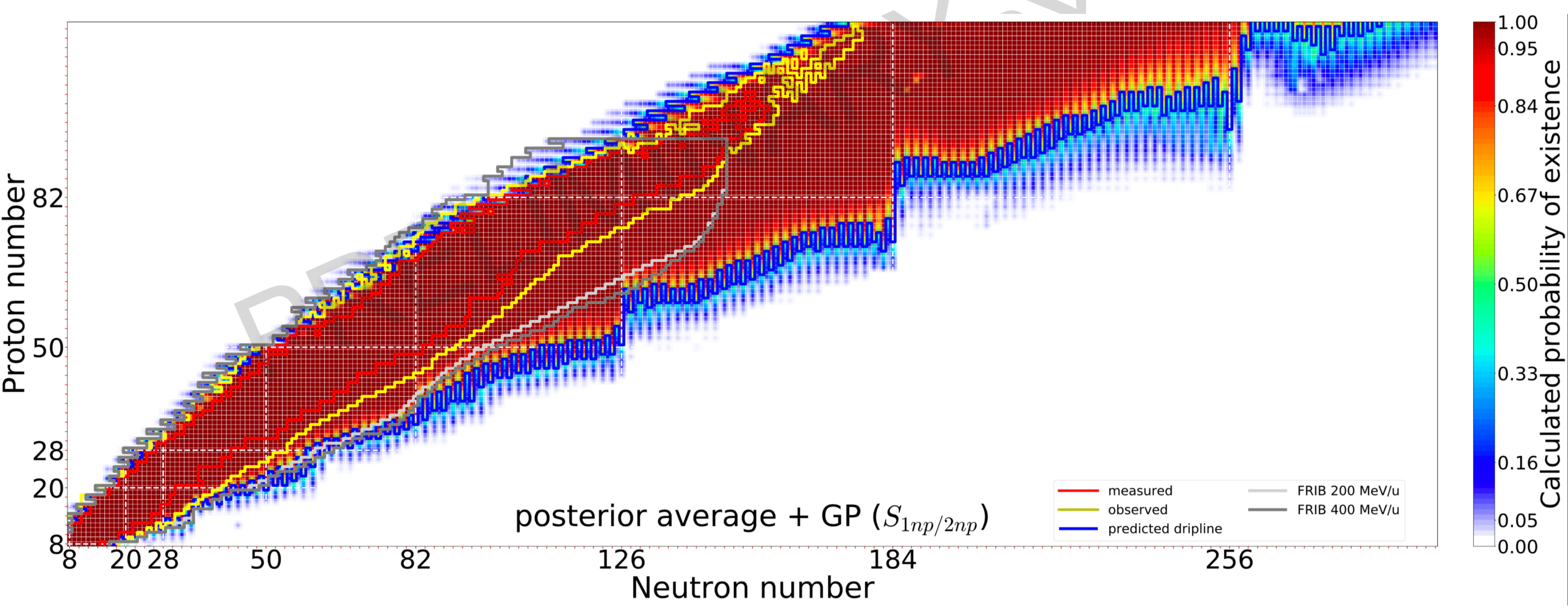
Posterior average corrected model

Ab initio limits of atomic nuclei, J.D. Holt et al. arXiv:1905.10475



VS-IMSRG with 1.8/2.0(EM) potential, NN+NNN

Quantified existence predictions for the full nuclear landscape

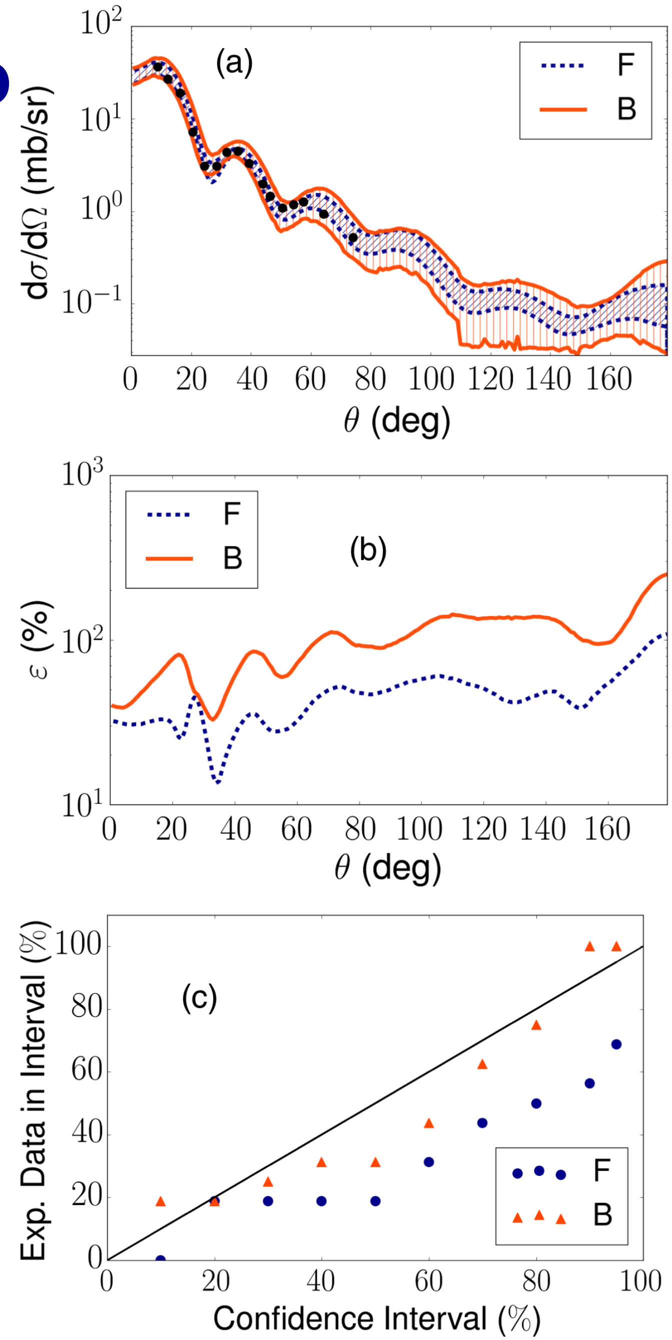


Why Bayesian ?

Direct comparison between Bayesian and frequentist uncertainty quantification for nuclear reactions; King, Lovell, Neufcourt, Nunes, PRL (2019)

- Deuteron induced reactions on heavy ions
- Optical potential model
- Trained on elastic p/n scattering
- Test on independent transfer data
- Model: adiabatic wave approximation (ADWA)

- Figure: Transfer cross sections for ^{48}Ca(d,p)
  - (a) predicted 95% confidence intervals from the Bayesian (orange vertical hash) and the frequentist approach (blue slashed hash)
  - (b) percent uncertainty of the confidence intervals
  - **(c) comparison of the percentage of data falling within the given confidence interval**



Nuclear physics perspective

- The extrapolation outcomes discussed can guide future experiments at rare-isotope facilities against which they will be tested**.**
- New mass measurements on neutron-rich nuclei will help to develop increasingly more quantitative models of the atomic nucleus and also allow for a higher-fidelity statistical analysis. As illuminated by our Bayesian analysis of ^{49}S, ^{52}Cl, and ^{53}Ar, experimental discoveries of new nuclides will also be crucial for delineating the detailed behavior of the nuclear mass surface, including the placement of particle drip lines.
- Potential improvements for statistical model: expert elicitation (models), stylized facts, sophistication
- Extensions: identify proton emitters and calculate half-lives, in superheavy nuclei

Astrophysical perspective

- Goal: uncertainty quantification of nuclear abundances
- Feed quantified mass tables / Bayesian posterior samples to nucleosynthesis codes for abundance calculations
- First step: evaluation of sensitivity to nuclear masses
- <u>Next step: combined analysis of sources of uncertainty</u>

Summary

- Model-based Bayesian methodology which can be easily generalized
- Quantified nuclear mass landscape with accuracy improvement and robust UQ
- Resulting rms deviations from experiment on the testing dataset are similar for DFT and more phenomenological models
- GP offers a better and more stable performance than NN
- The estimated confidence intervals on predictions make it possible to evaluate predictive power of individual models
- We quantified the neutron-stability of the nucleus in terms of its existence probability p_{ex}. Our results are fairly consistent with recent experimental findings: ^{60}Ca is expected to be well bound (S_{2n}~ 5 MeV) while ^{49}S, ^{52}Cl, and ^{53}Ar are predicted by UNEDF0, SV-min, and FRDM-2012 to be marginally-bound threshold systems. One event consistent with ^{59}K was registered. According to our calculations, this nucleus is expected to be firmly neutron-bound.

Thank you!

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