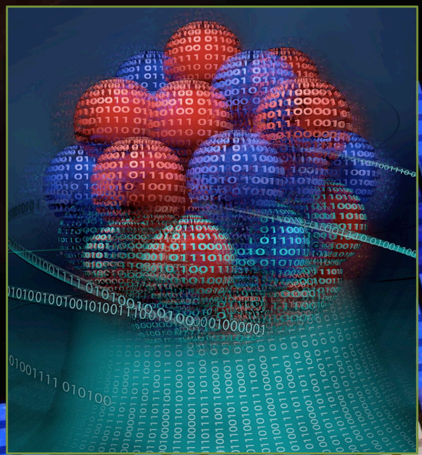
Assessing the progress through quantified nuclear structure theory

Witold Nazarewicz, FRIB@MSU

INTRANS 2024 Workshop, Orsay, Jan. 22-25, 2024



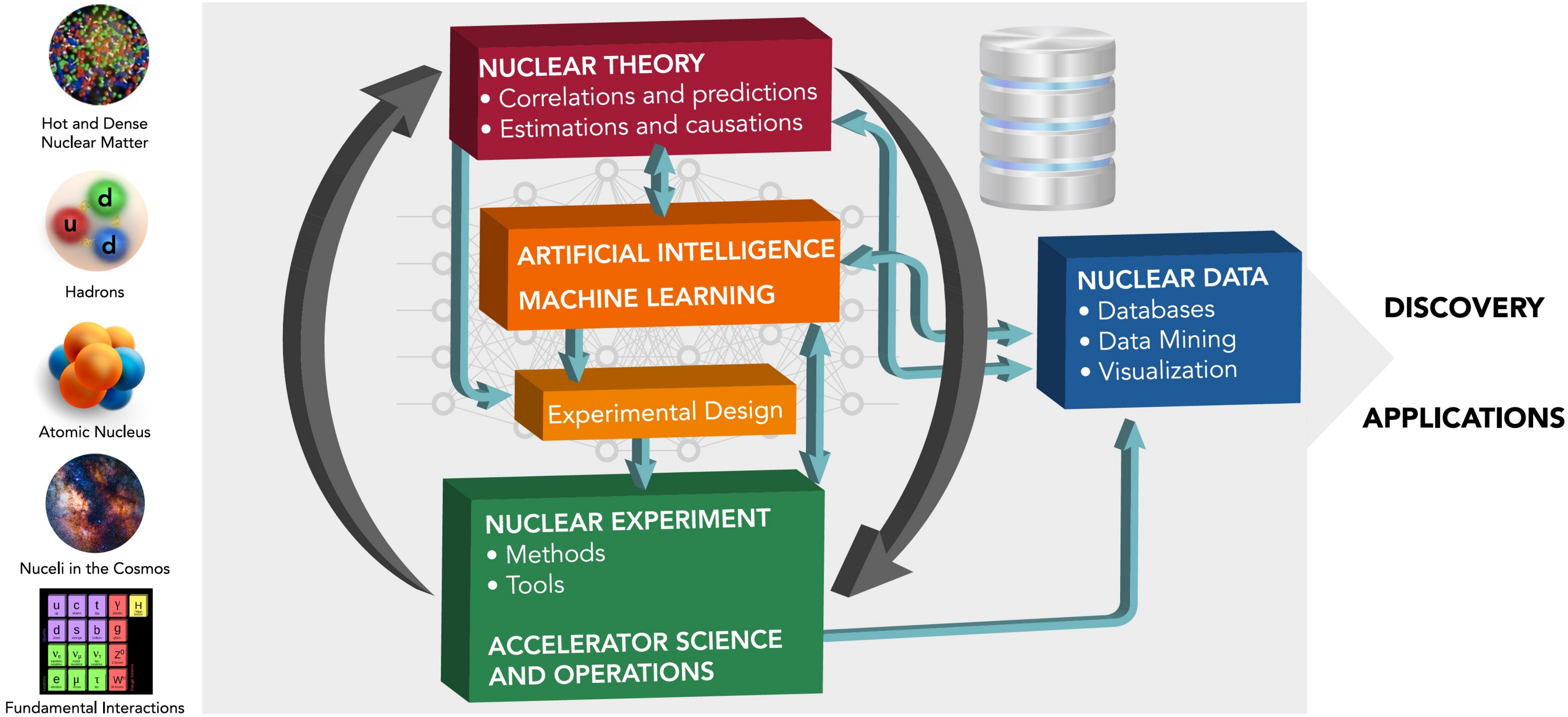
Menu

- Uncertainty quantification in nuclear theory
- Importance of controlled extrapolations
- Help is on the way!

Machine learning and nuclear theory: big picture

Artificial Intelligence and Machine Learning in Nuclear Physics
A. Boehnlein et al., Rev. Mod. Phys. Rev. Mod. Phys. 94, 031003 (2022)

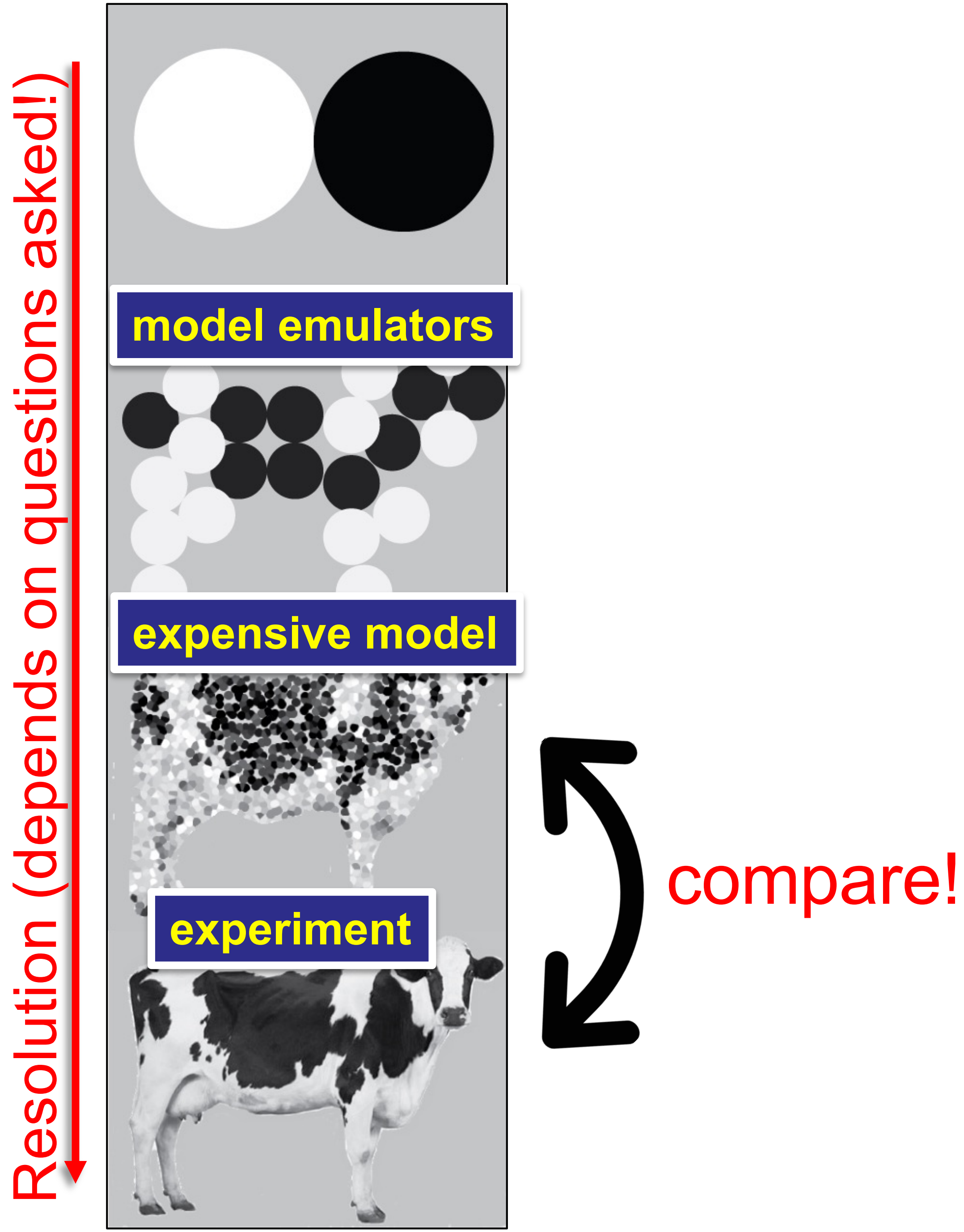
Many examples can be found there!



Speeding-up *the cycle of the scientific method*

The nucleus is a complex many-body system. Exact* realistic nuclear models do not exist.

*parameter-free; fully-microscopic



Machine learning & quantified low-energy nuclear theory: Why?

ML tools can help us to speed up the scientific method cycle and hence facilitate discoveries

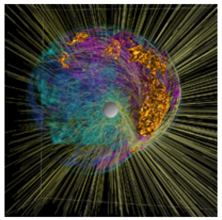
- Enabling big simulations by fast emulation of expensive models
- Providing meaningful input to applications and planned measurements by means of experimental design

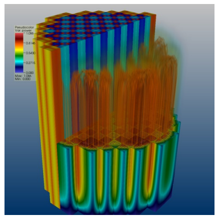
ML tools can help us to reveal the structure of our models

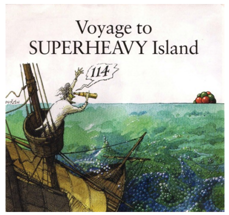
- Model reduction by eliminating redundant parameters
- Identifying crucial experimental data for better constraining theory and revealing the information content of measured observables

ML tools can help us to provide predictive capability

- ML enables uncertainty quantification (UQ)
- Theoretical models are often applied to entirely new nuclear systems and conditions that *are not accessible to experiment*







Parameter estimation

$\mathcal{M}(\boldsymbol{x})$ Model described by parameters $\boldsymbol{x}$

$\mathcal{D}$ Dataset

Calibration

$p(\boldsymbol{x}|\mathcal{D})$ Posterior distribution of parameters given data

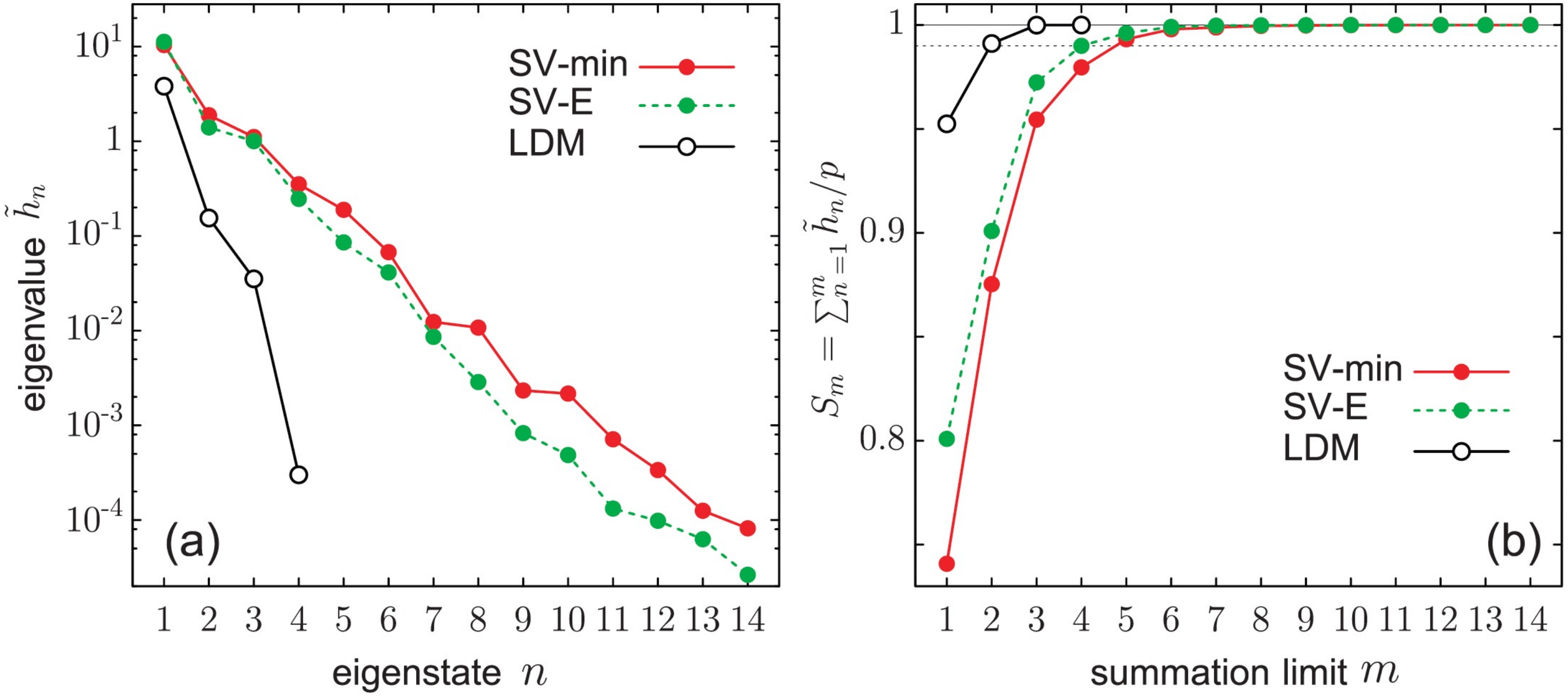
Models are defined by posterior distribution functions of parameters, not just by mean values of parameters!

- Bayesian calibration
- Linear regression (χ^2)

Model reduction

Estimation of effective model parameter space through the principal component analysis

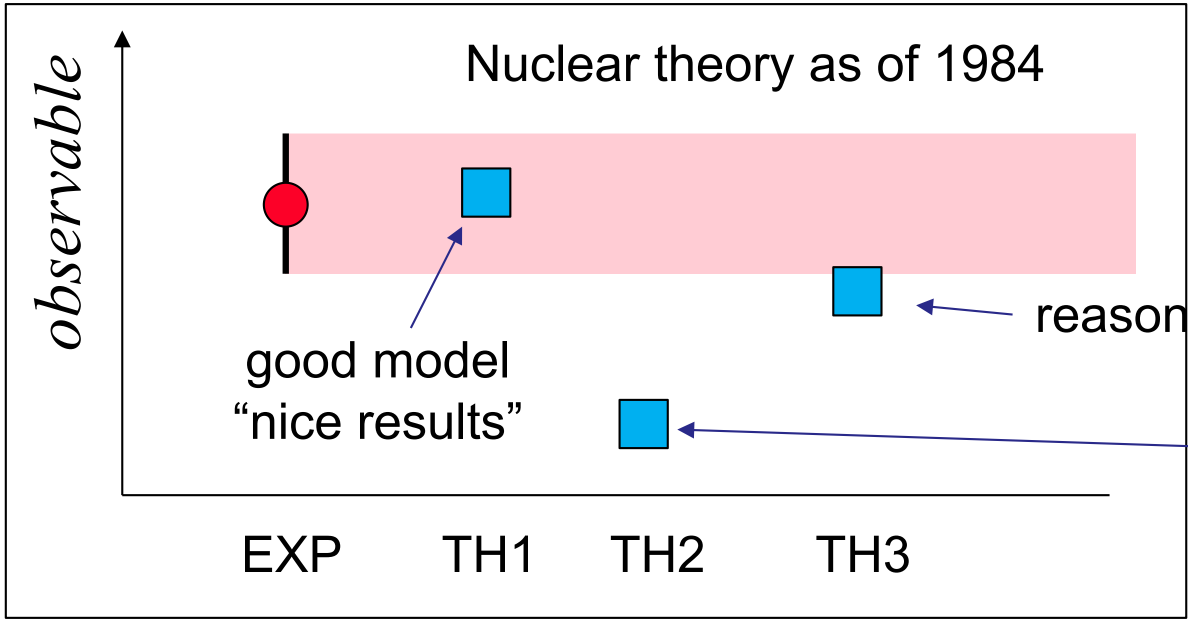
J. Phys. G 47, 094001 (2020)



Eigenvalues of the conditioned Hessian matrix and cumulative percentages

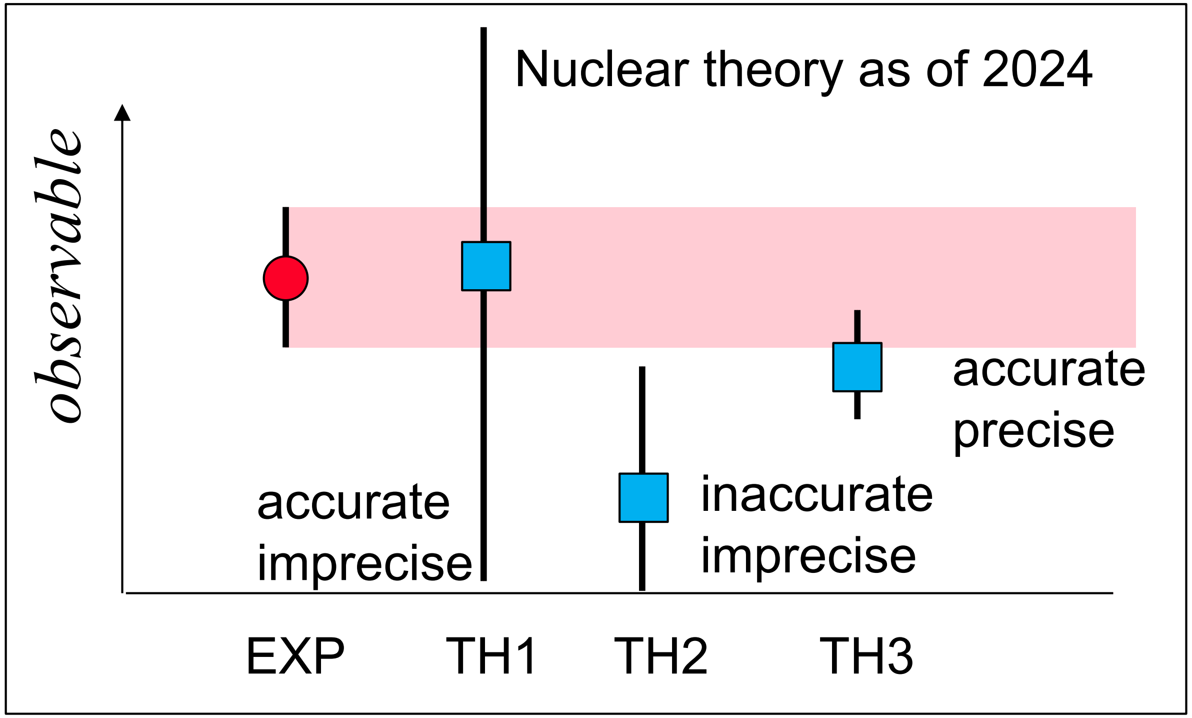
The eigenvalues quantify the relevance of an effective parameter associated with the principal component. Large eigenvalue means that this principal component has a large impact on the objective function while very small eigenvalues indicate irrelevant parameters having little consequences for the parameter estimation.

Assessment through quantification



tenor.com

How can one meaningfully assess the progress based on the average values only?



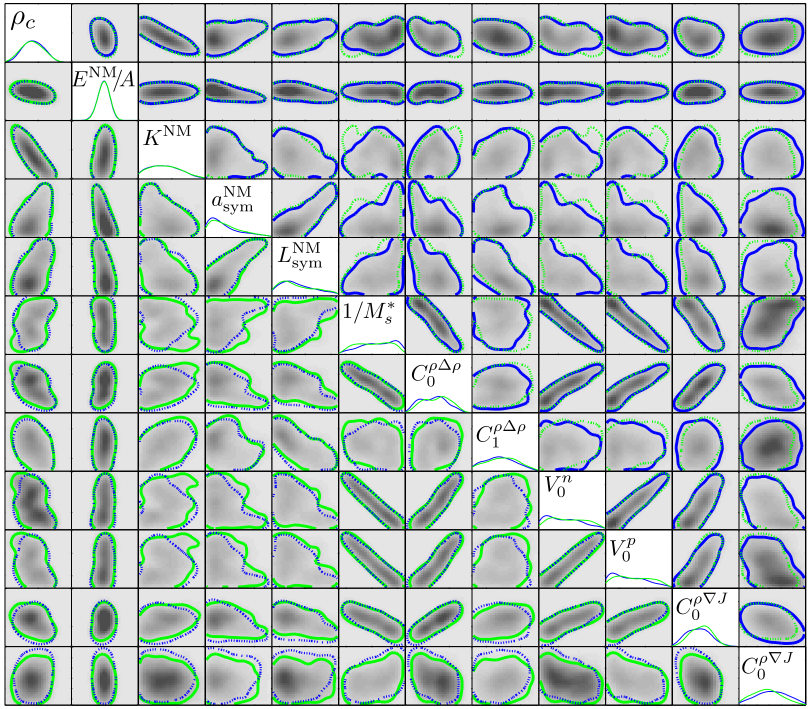
Is new more precise measurement warranted? Are more data needed?

Some examples

Example: Quantified DFT

- Mean values
- Covariances
- PDFs: Posterior probability density functions

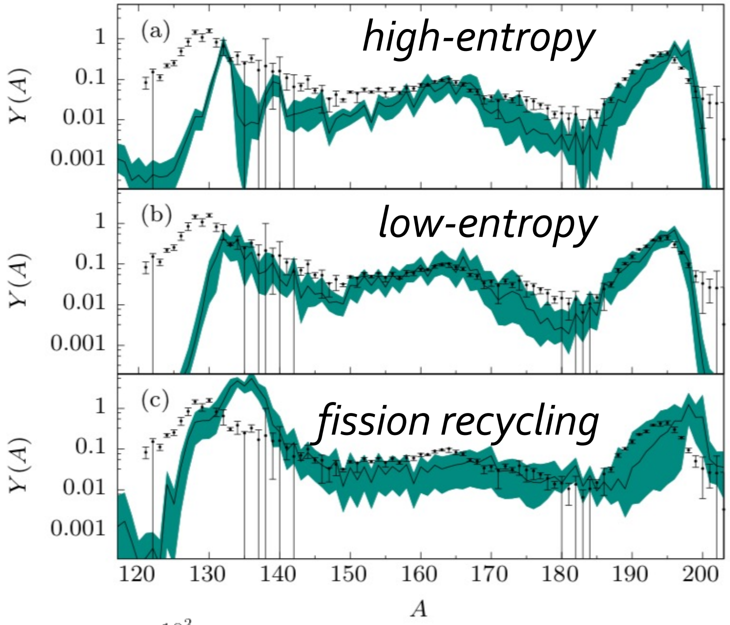
Phys. Rev. Lett. 114, 122501 (2015)



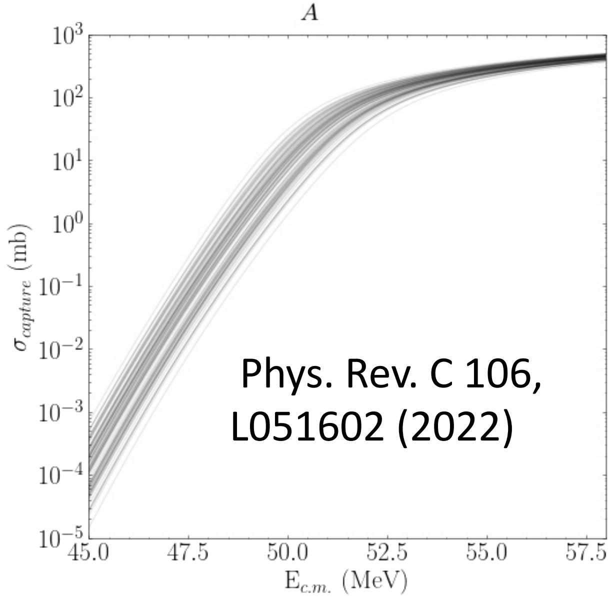
Bivariate marginal estimates of the posterior distributions for the 12-dimensional DFT UNEDF$_1$ parameterization.

r-process modeling

Phys. Rev. C 101, 055803 (2020)



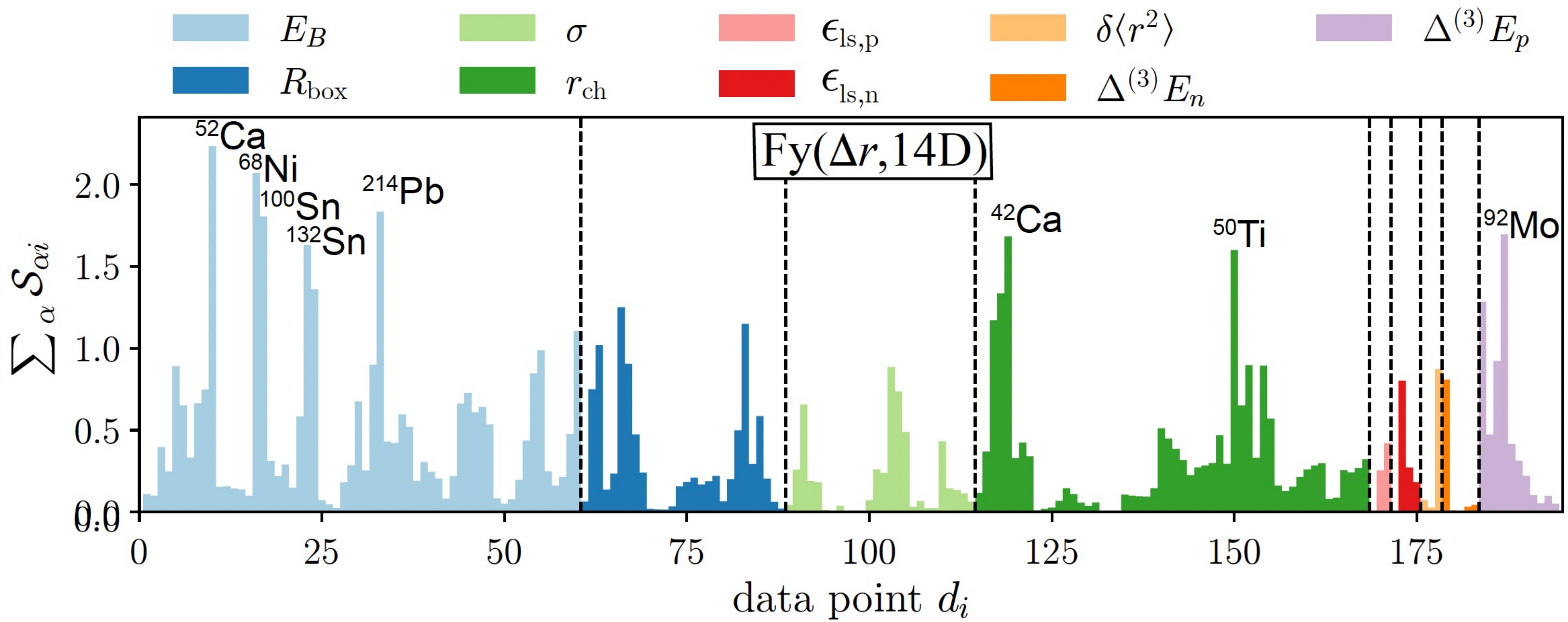
heavy-ion fusion



Phys. Rev. C 106, L051602 (2022)

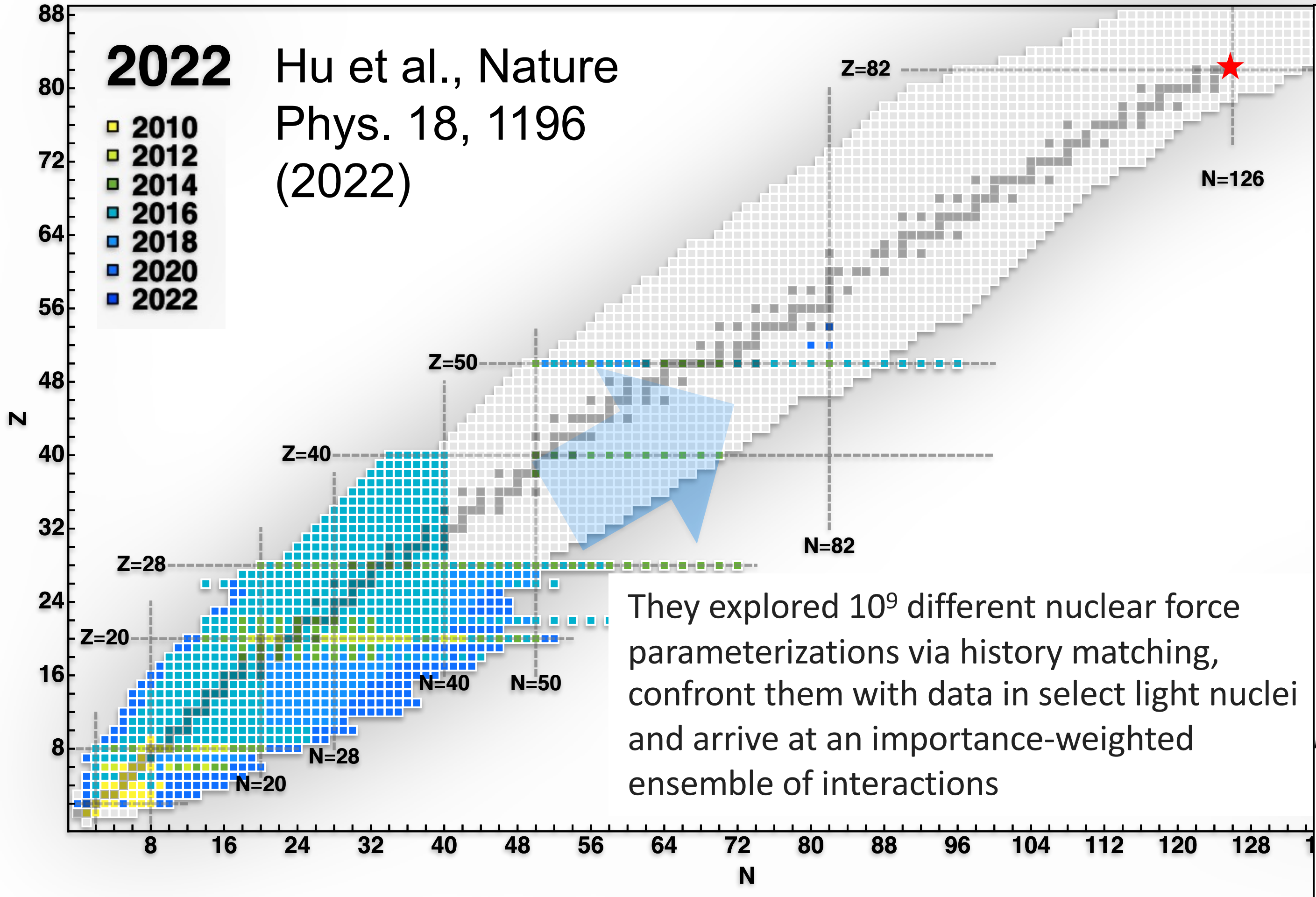
Identifying crucial experimental data

Example: Fayans functional calibration
O'Neal et al., in preparation (2024)



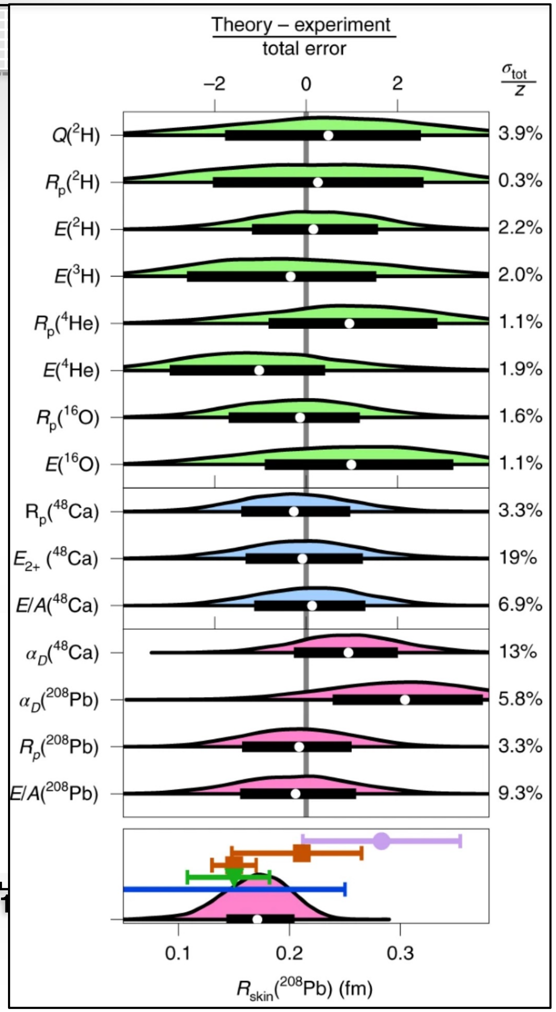
The total impact of a data point on the parameters of the functional

Fast emulation of expensive models



Hu et al., Nature Phys. 18, 1196 (2022)

They explored 10^9 different nuclear force parameterizations via history matching, confront them with data in select light nuclei and arrive at an importance-weighted ensemble of interactions



$$\varepsilon = \varepsilon_{\mathrm{exp}} + \varepsilon_{\mathrm{em}} + \varepsilon_{\mathrm{method}} + \varepsilon_{\mathrm{model}}$$

Nuclei from NN+NNN interactions: CC, IM-SRG, MBPT

Covariances and posterior distribution functions

Correlations are important!

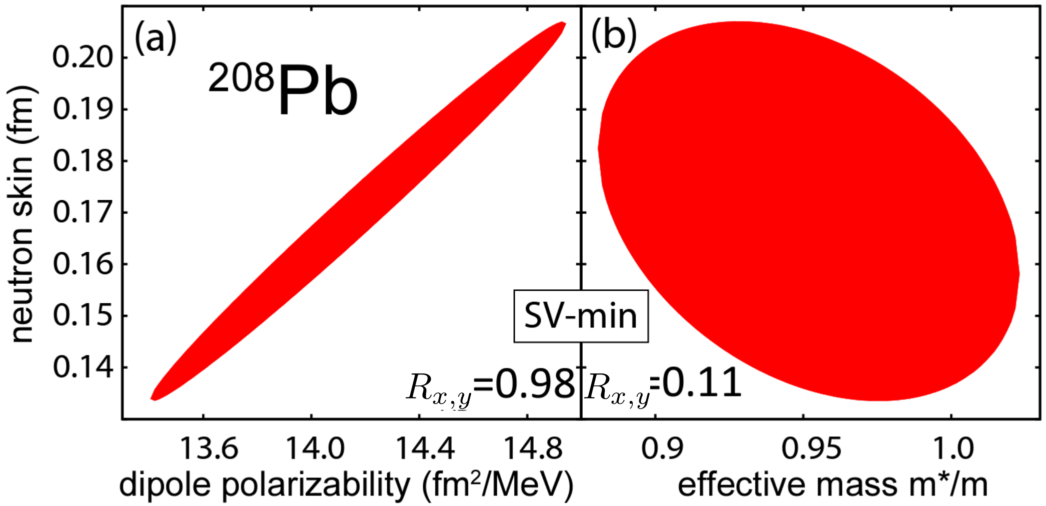
$$R_{x,y} = \frac{\mathrm{cov}(x,y)}{\sigma_x \sigma_y}$$

bivariate correlation coefficient

$$\mathrm{CoD}(x,y) = R^2_{x,y}$$

coefficient of determination

Phys.Rev.C81, 051303 (2010)



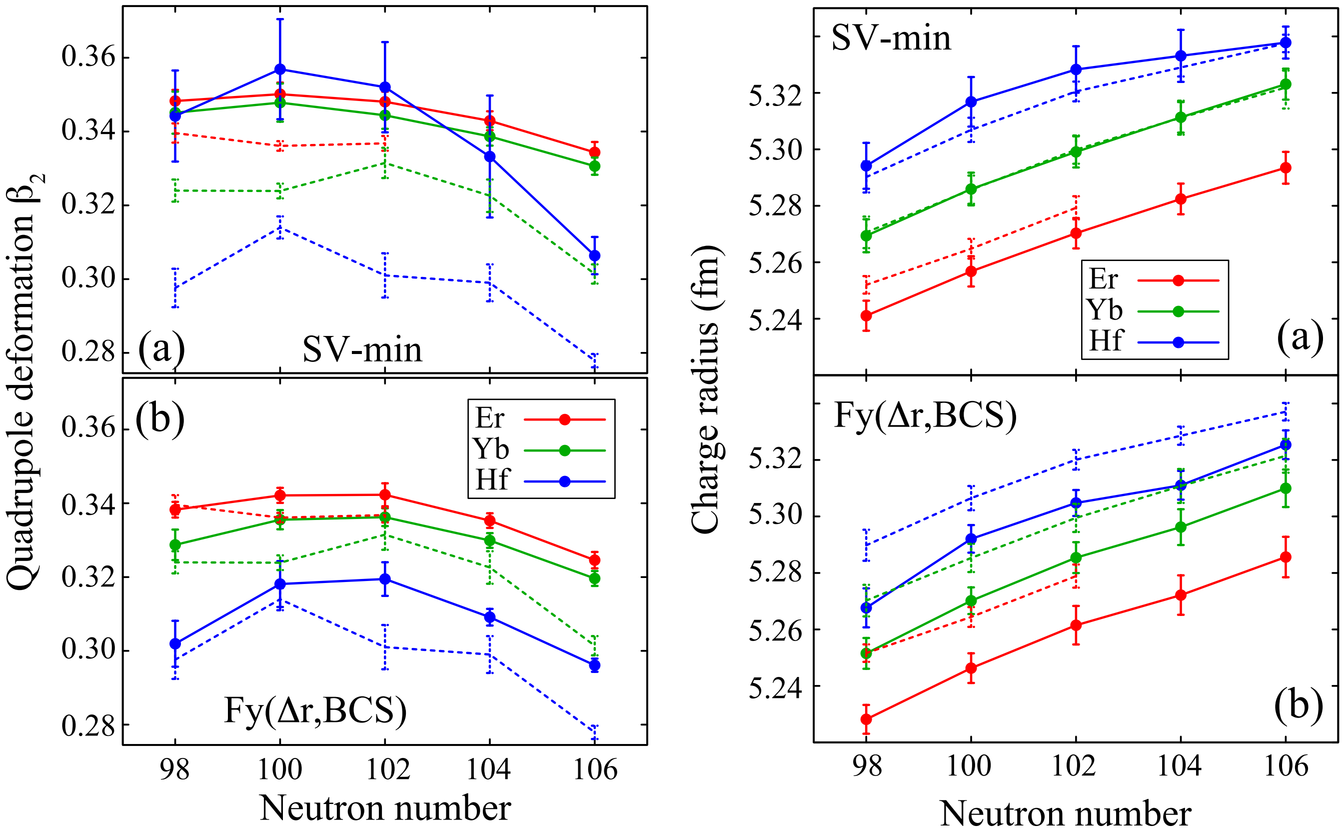
Consider observable $z = x - y$

Variance of difference: $\sigma_z^2 = \sigma_x^2 + \sigma_y^2 - 2R_{x,y}\sigma_x\sigma_y$

$R_{x,y} \approx 1 \longrightarrow \sigma_z \approx |\sigma_x - \sigma_y|$(reduced) $\quad R_{x,y} \approx 0 \longrightarrow \sigma_z \approx \sqrt{\sigma_x^2 + \sigma_y^2}$

Statistical correlations of nuclear quadrupole deformations and charge radii

P.-G. Reinhard & WN, Phys. Rev. C 106, 014303 (2022)

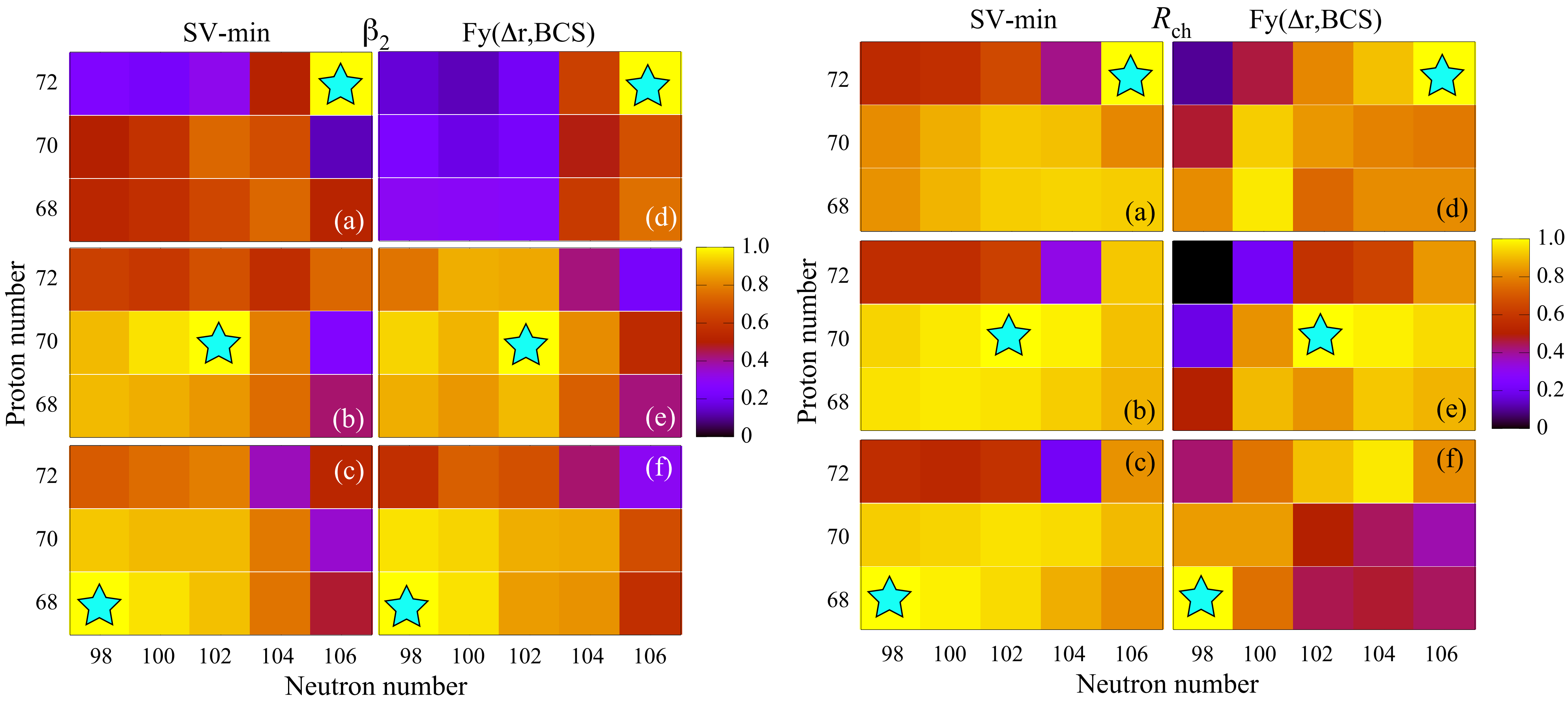


Quadrupole deformations and charge radii vary smoothly! But what about correlations?

- The smoo[...] *[...]hat difference*[...]
- Because the points did not jump around, the *errors must be correlated*.

Until you calculate you do not know!

?



- The calculated CoD diagrams show patterns that are fairly localized as compared to the smooth trends of observables.
- The local variations of CoDs reflect the underlying deformed shell structure and changes of single-particle configurations.
- The errors on radii differences are actually important to know!

Systematic errors

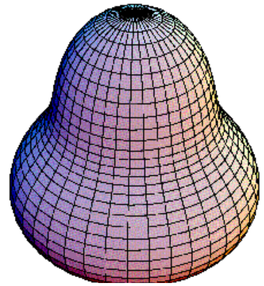
Model mixing

Extrapolations

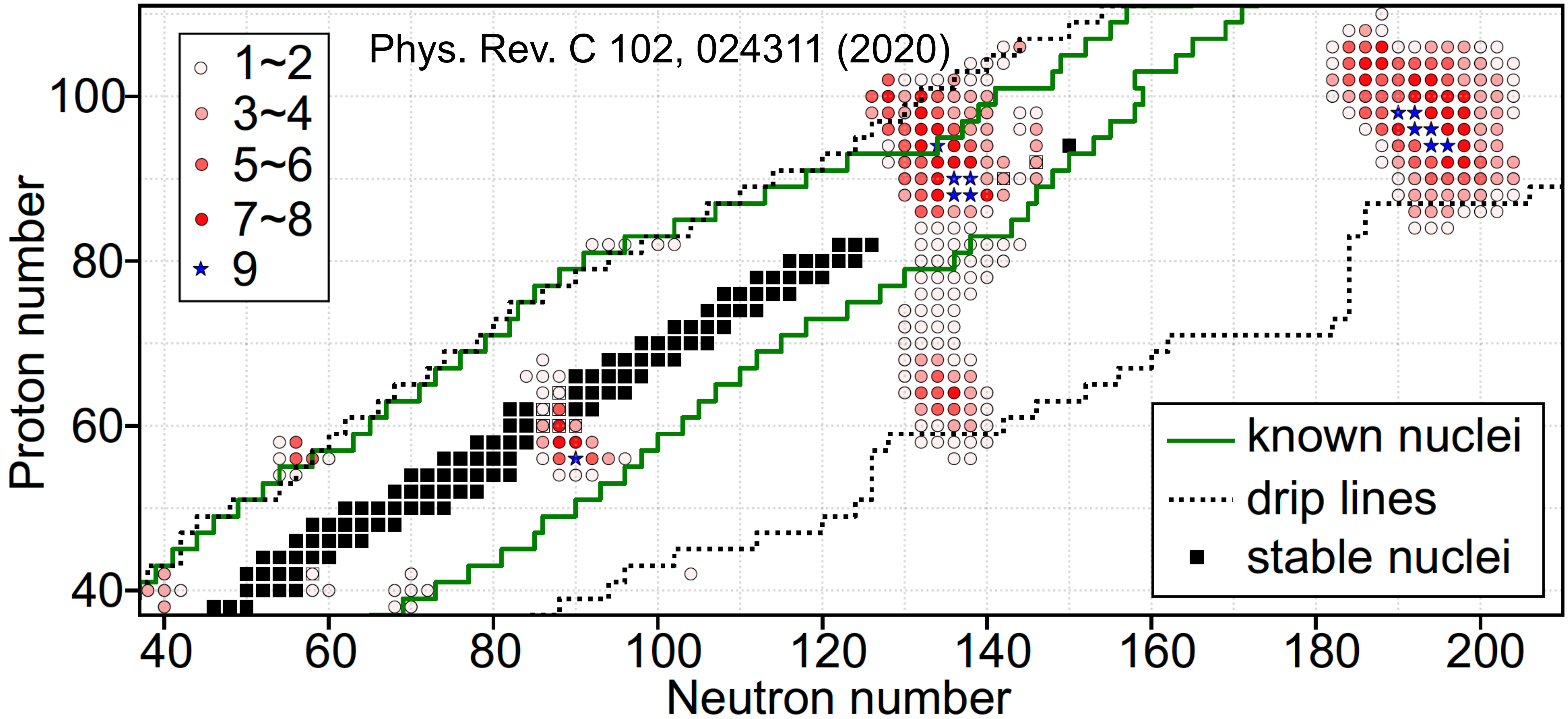
Naïve nuclear theorist's approach to a systematic (model) error estimate (trends analysis):

- Take a set of *reasonable* global models *Mi*, hopefully based on different assumptions/formalism, that satisfy basic theoretical requirements (here comes the expert belief thing).
- Make predictions.
- Compute average and variation within this set
- Compute rms deviation from existing experimental data.

Example: Assessing systematic uncertainty by comparing *different* models



Landscape of pear-shaped even-even nuclei



We can do better by mixing models!

In this way, collective wisdom of several models is maximized by providing the best prediction rooted in the most current experimental information.

Bayesian Model Averaging (BMA) or Bayesian Model Mixing (BMM) incorporate insights from different models into a unified prediction in a statistically rigorous way.

BMA: the total pdf is an average over pdf's of individual models.

$$p(y^*|y, y_{ev}) = \sum_k w_k(y_{ev}) p(y^*|y, \mathcal{M}_k)$$

observable of interest

evidence (target) dataset

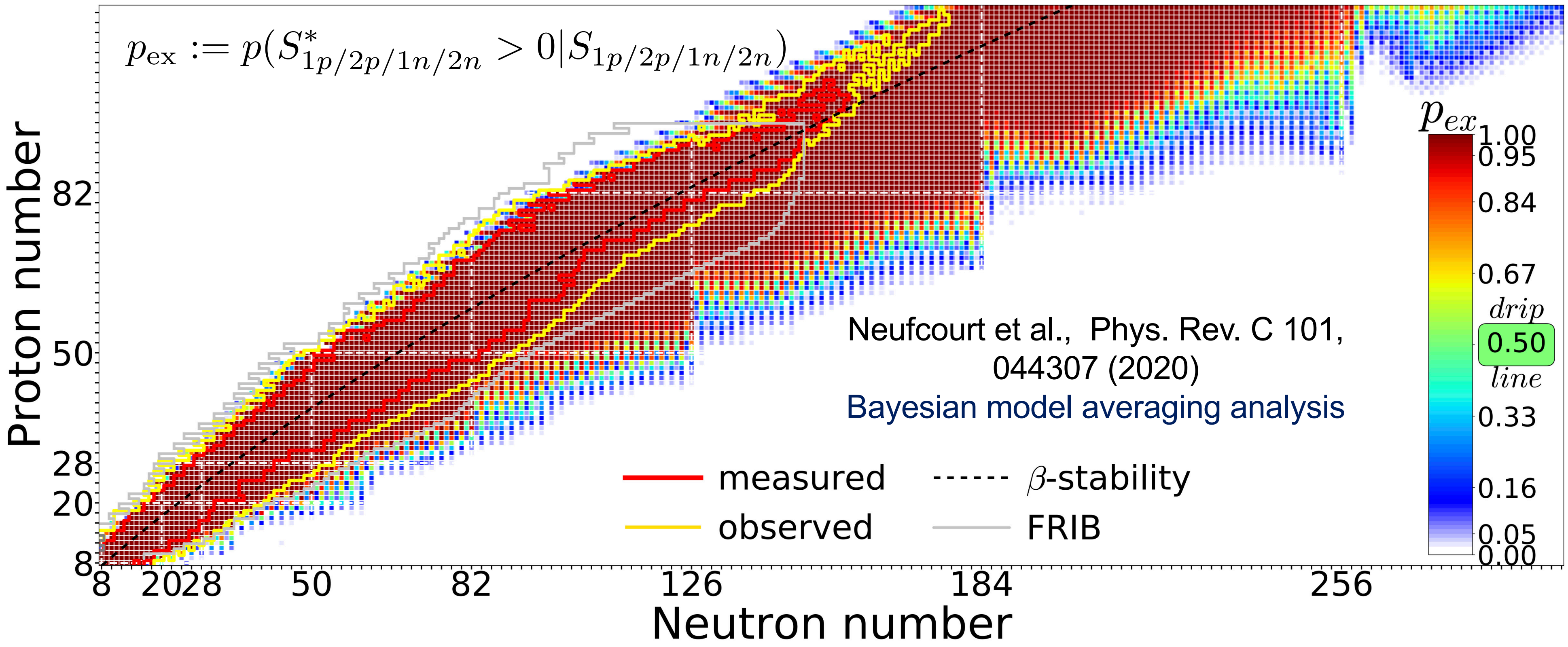
model weight

model

In the more advanced BMM, it is assumed that the total prediction is an average over predictions of individual models.

$$y^*(x) = \sum_k w_k\, y_{\rm th}(x, \theta)$$

Nuclear landscape and particle drip lines



Neufcourt et al., Phys. Rev. C 101, 044307 (2020)
Bayesian model averaging analysis

NEW:

Local Bayesian Dirichlet mixing of imperfect models

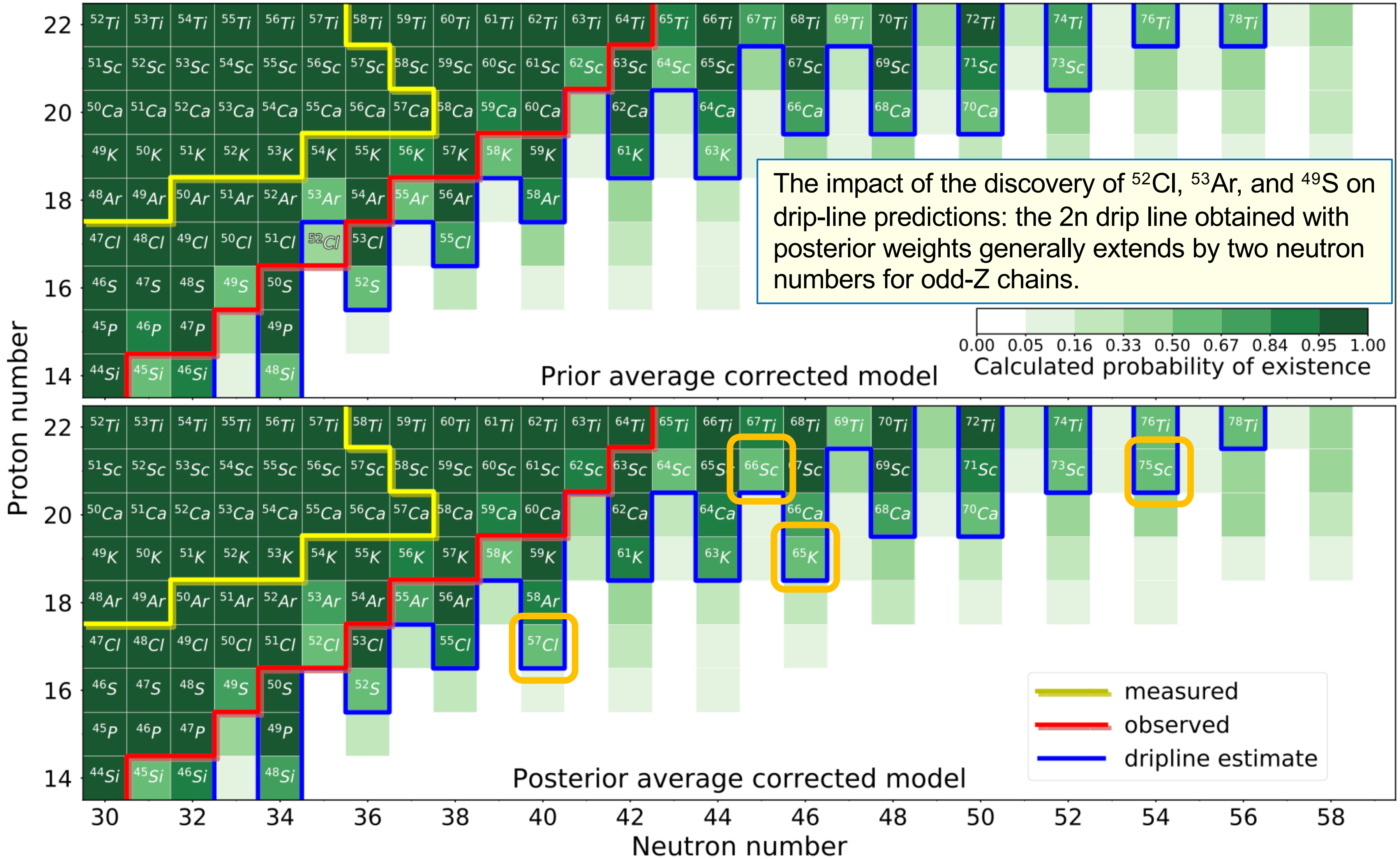
Vojtech Kejzlar, Léo Neufcourt & Witold Nazarewicz

Scientific Reports **13**, Article number: 19600 (2023) | Cite this article

Existence experiments provide strong constraints on theory and help assessing the progress

Discovery of ^{60}Ca: Phys. Rev. Lett. 121, 022501 (2018)

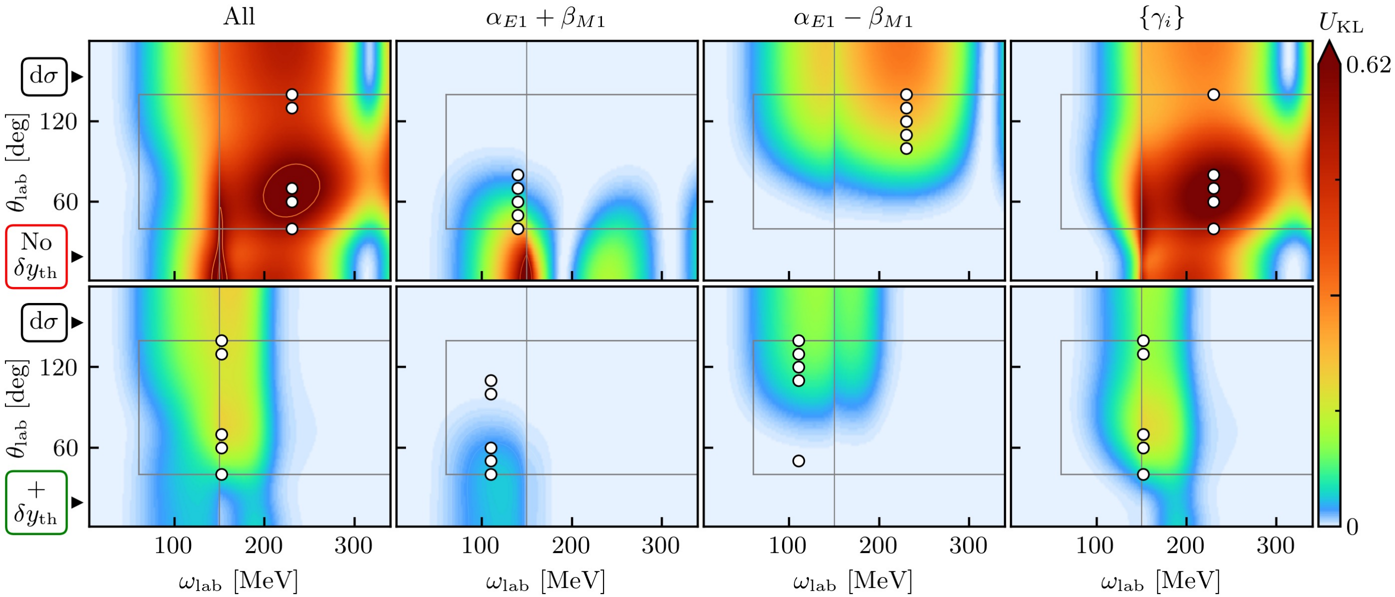
Bayesian model averaging: Phys. Rev. Lett. 122, 062502 (2019)



The future: Experimental design

Beam time and compute cycles are expensive!

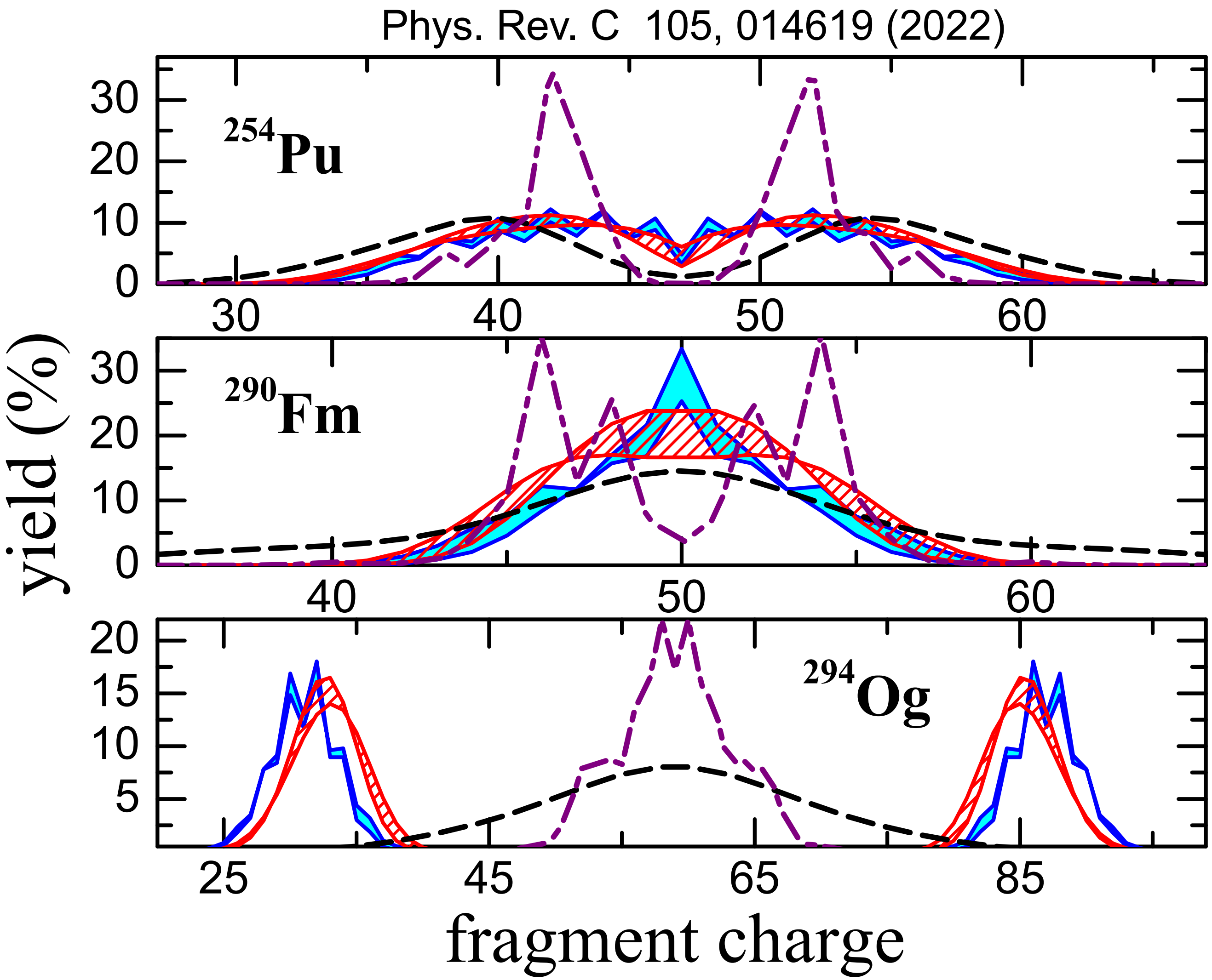
- Bayesian experimental design provides a framework in which experiments can be designed using *the best experimental and theoretical information available*
- *The utility function* is designed to encode the goals of the experiment and the constraints inherent in carrying it out.
- Once the utility function and the possible designs have been specified, the optimal design is simply the scenario that maximizes the expected utility function over the domain of possible designs.



The expected utility of proton differential cross section measurements. The circles show the optimal design kinematics for five measurement points at the same energy but different angles.

Designing optimal experiments: An application to proton Compton scattering EPJA 57, 81(2021)

Fission in the r-process and superheavy nuclei



Fragment charge distributions of ^{254}Pu, ^{290}Fm, and ^{294}Og obtained in DFT+stat work (blue bands) and predicted in previous work by neglecting odd-even staggering (red dashed bands). Predictions of BSM and SPM models are shown by dashed and dash-dotted lines, respectively.

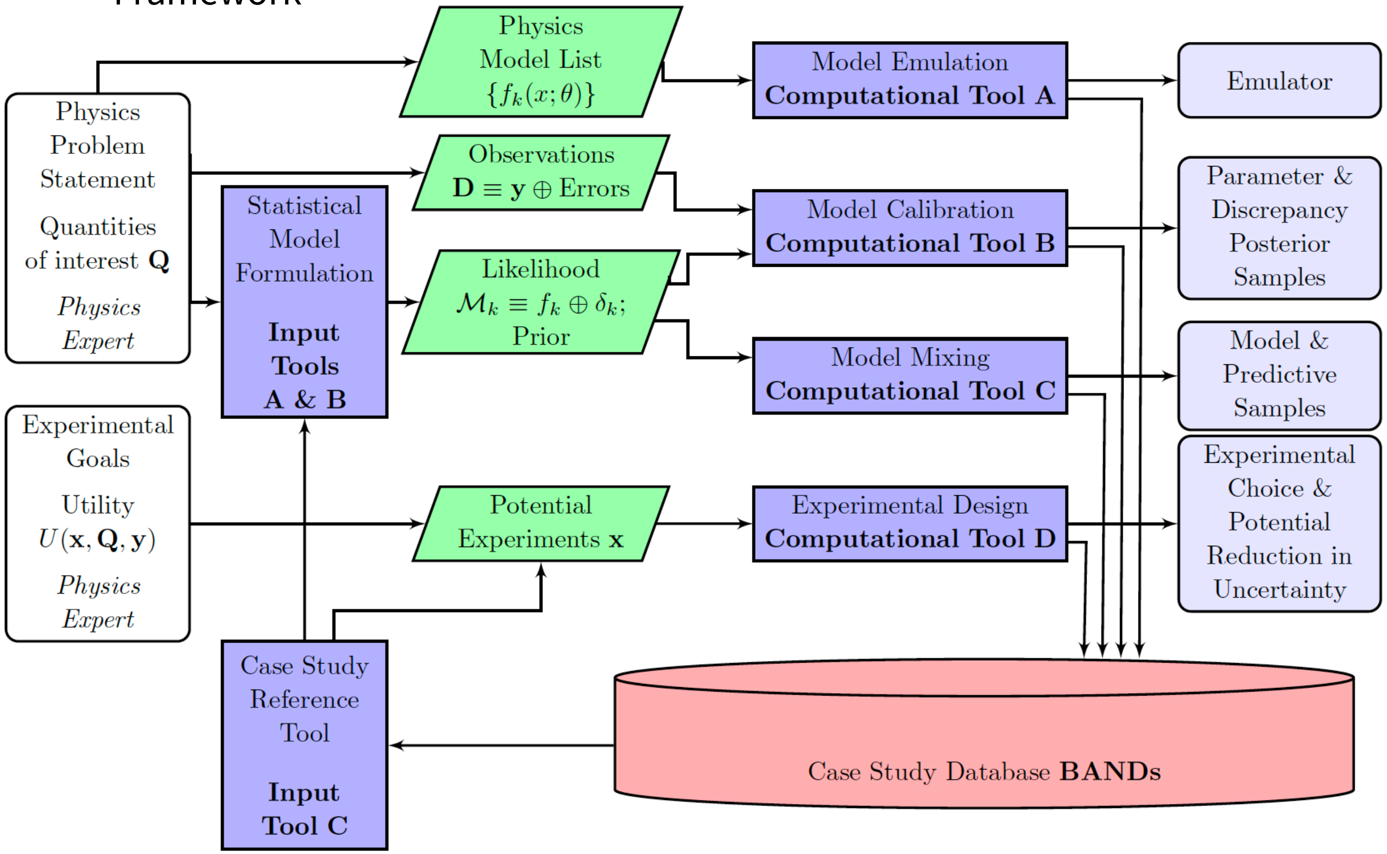
Challenge: uncertainty quantification of current theories of fission. Little has been done!

Cyberinfrastructure for Sustained Scientific Innovation Framework

Bayesian Analysis of Nuclear Dynamics

https://bandframework.github.io

Ohio U.
Michigan State U.
Ohio State U.
Northwestern U.



BAND Manifesto: D R Phillips *et al. J. Phys. G* **48,** 072001 (2021)

BAND provides tools (Python codes) and examples (notebooks) that facilitate principled UQ in nuclear physics

Summary

- The nucleus is a complex many-body system. Exact quantitative nuclear models do not exist.
- Imperfect models are used for making far extrapolations.
- While all models are wrong, models that know how and when they are wrong are useful. (after G. Box)
- One can assess the progress in in nuclear physics theory by means of uncertainty quantification and machine learning.
- To solve many complex problems in the field and facilitate discoveries, multidisciplinary efforts efforts are required involving scientists in nuclear physics, statistics, computational science, and applied math.

Thank you!