Quantified Density Functional Theory

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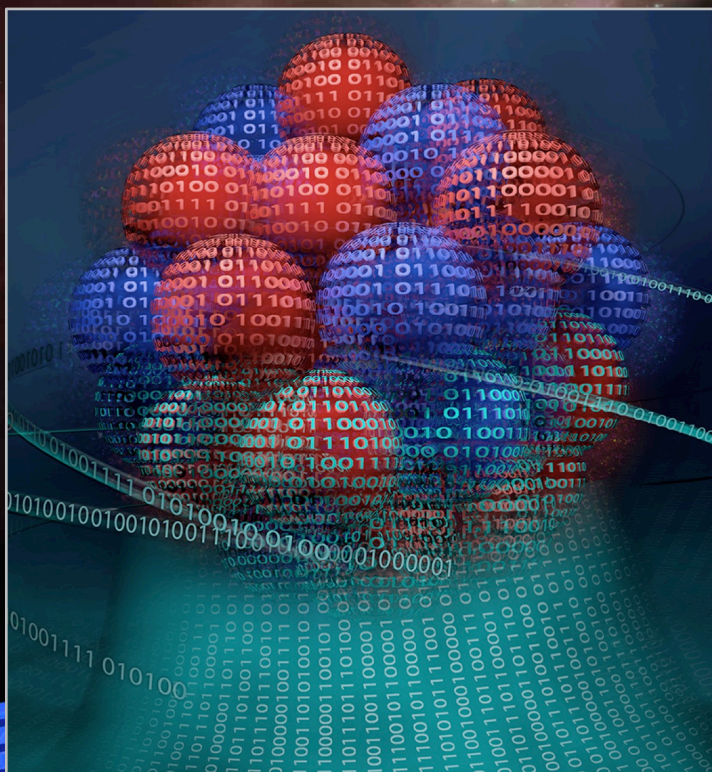
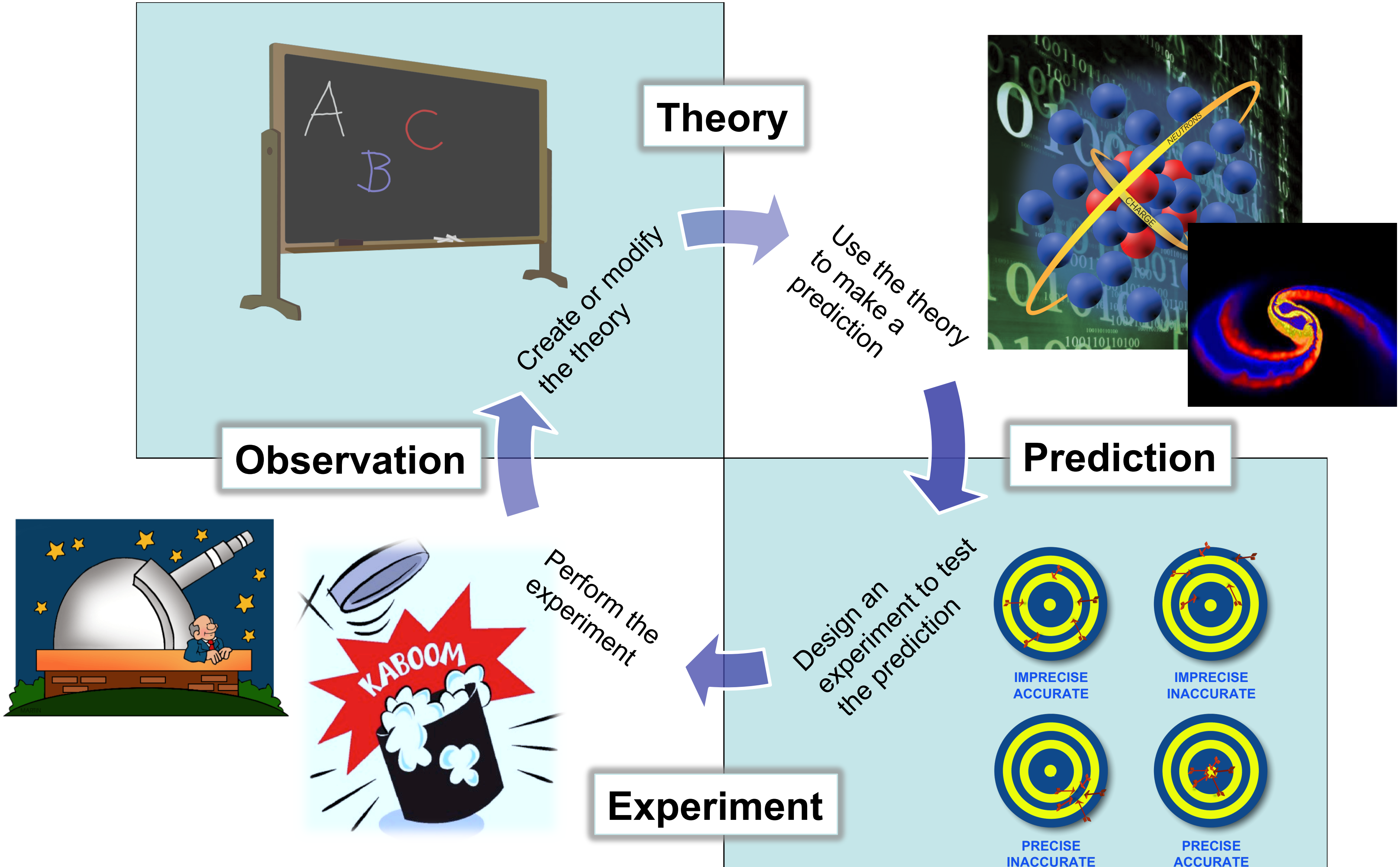


Menu

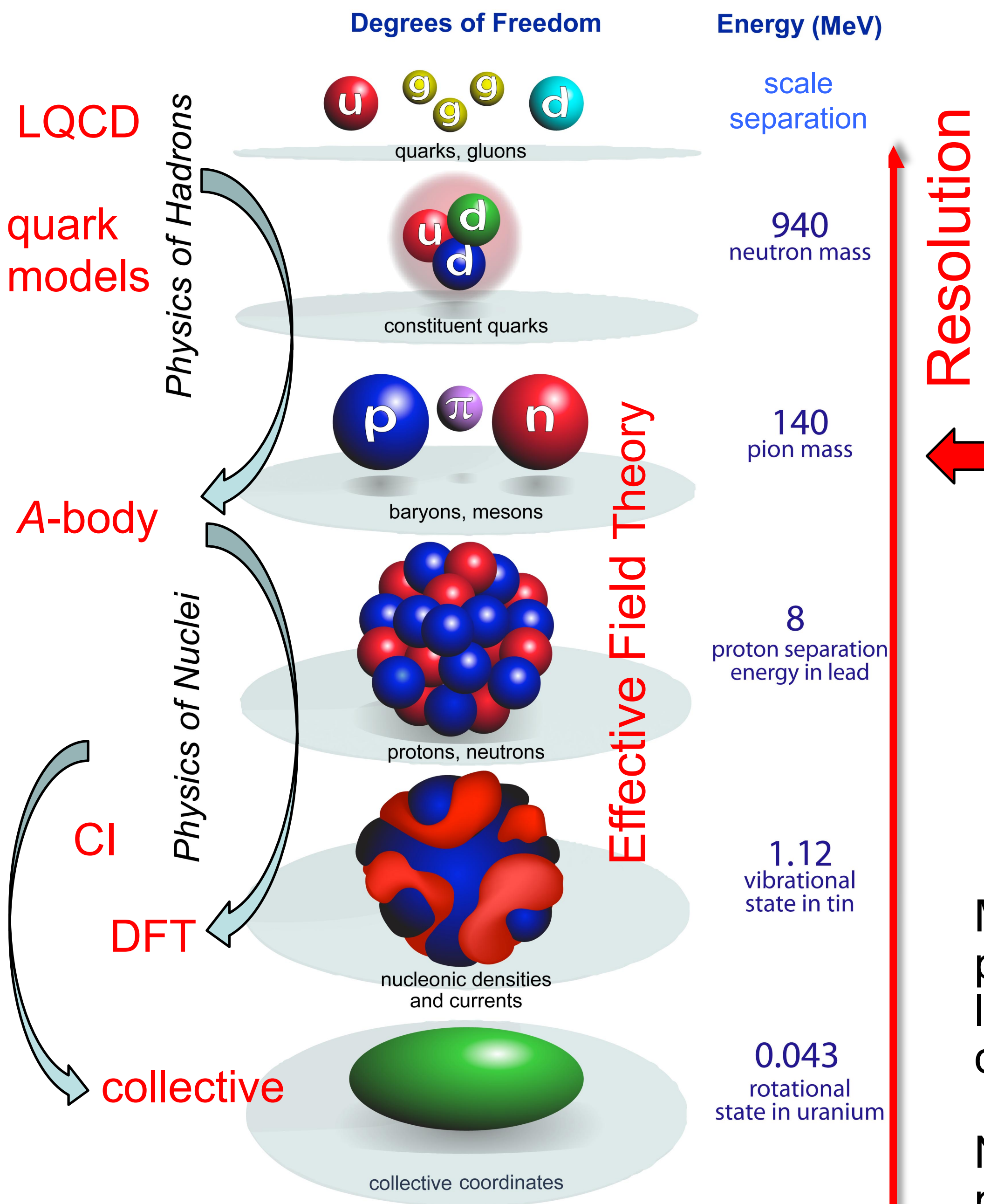
- Introduction to nuclear DFT
- Global applications: charge radii
- Model extrapolations and machine learning
- Conclusions

Guiding principle: the scientific method…



J. Phys. G 43, 044002 (2016)

No precision science without UQ!



J. Phys. G 43, 044002 (2016)

Hot and dense quark-gluon matter
Hadron structure

Nuclear-Particle Physics

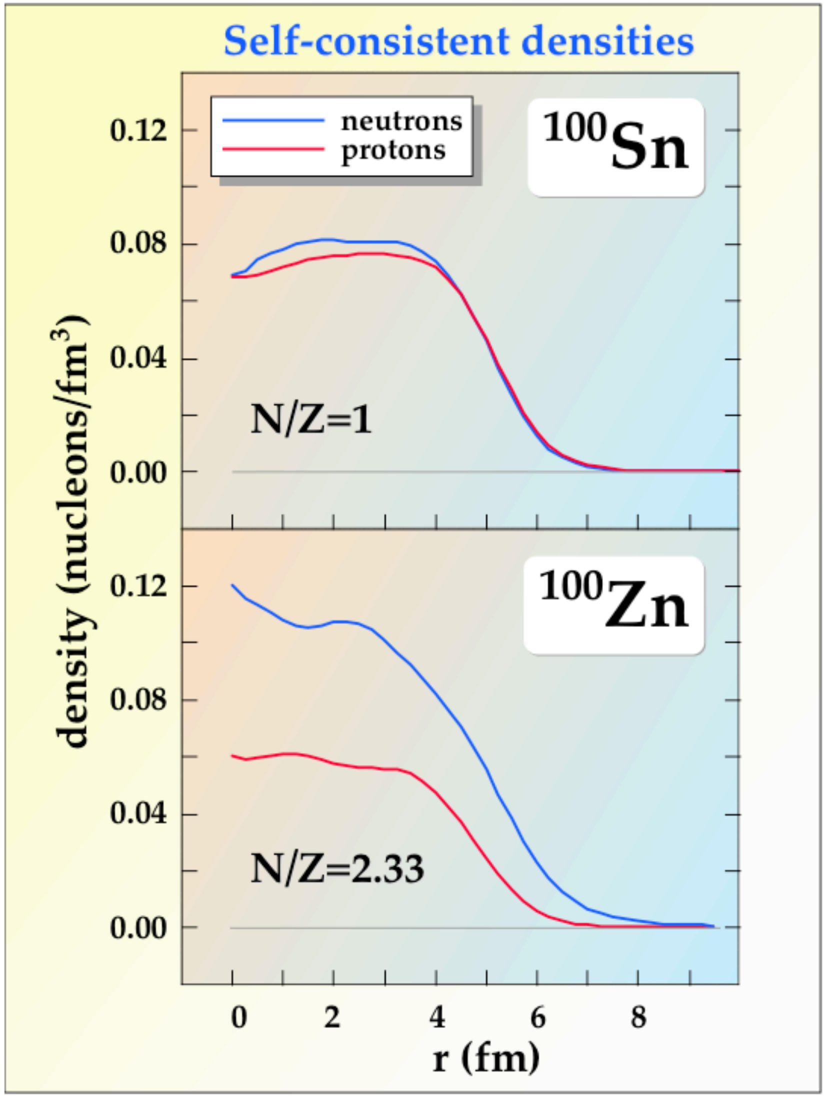
Nuclear structure
Nuclear reactions
New standard model

Most *efficient* approach: resolving power of a theoretical model taken as low as reasonably possible for the question at hand

Nuclear models must reproduce physical reality: phenomenology

Mean-Field Theory ⇒ Density Functional Theory

Degrees of freedom: nucleonic densities



Nuclear DFT

- two fermi liquids
- self-bound
- superfluid

- mean-field ⇒ one-body densities
- zero-range ⇒ local densities
- finite-range ⇒ gradient terms
- particle-hole and pairing channels
- Does not have to be related to a force
- Has been extremely successful. A broken-symmetry generalized product state does surprisingly good job for nuclei.

Nuclear Energy Density Functional

isoscalar (T=0) density $\left(\rho_0 = \rho_n + \rho_p\right)$

isovector (T=1) density $\left(\rho_1 = \rho_n - \rho_p\right)$

+isoscalar and isovector densities:
spin, current, spin-current tensor,
kinetic, and kinetic-spin
+ pairing densities

$$E = \int \mathcal{H}(r) d^3 r$$

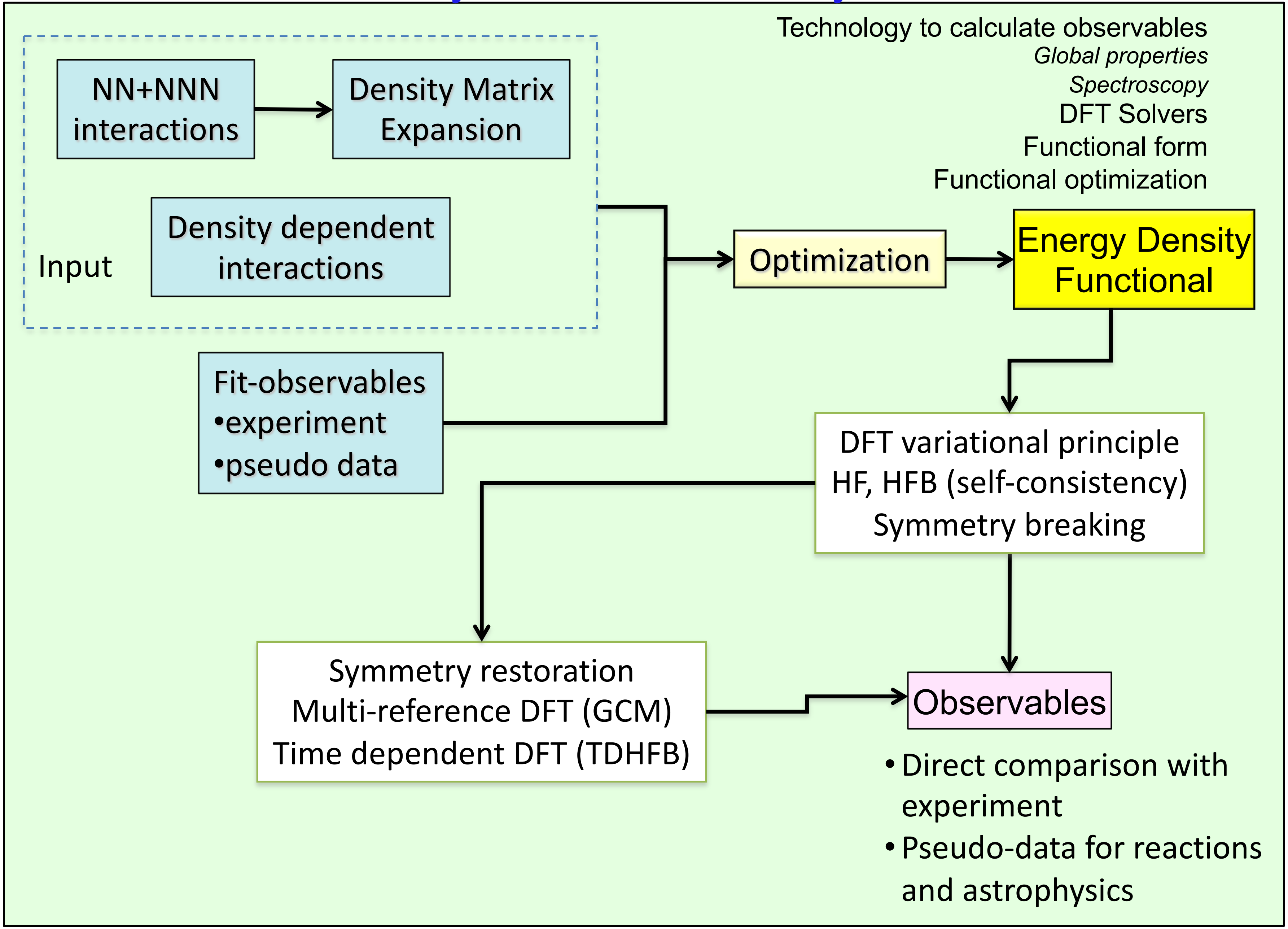
p-h density   p-p density (pairing functional)

$$\mathcal{H}(r) = \frac{\hbar^2}{2m}\tau_0(r) + \sum_{t=0,1} \left(\chi_t(r) + \breve{\chi}_t(r)\right)$$

Expansion in densities and their derivatives

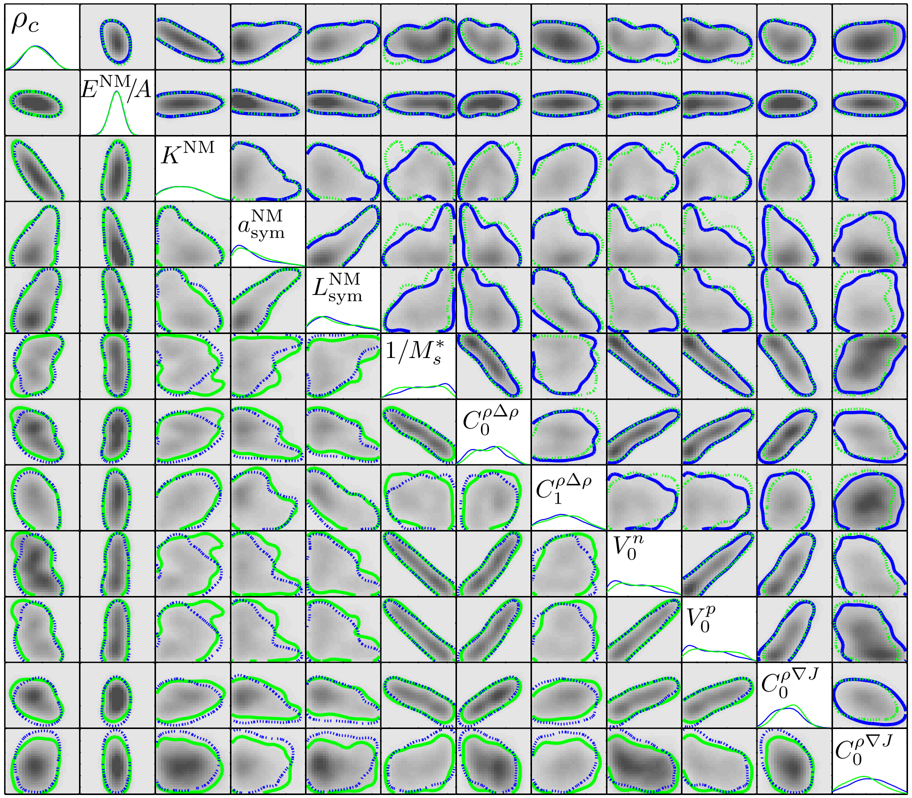
- Constrained by microscopic theory: ab-initio functionals provide quasi-data!
- Not all terms are equally important. Usually ~12 terms considered
- Some terms probe specific experimental data
- Pairing functional poorly determined. Usually 1-2 terms active
- Most popular: Skyrme, Gogny, Covariant
- Becomes very simple in limiting cases (e.g., unitary limit)
- Can be extended into multi-reference DFT (GCM) and projected DFT

Nuclear Density Functional Theory and Extensions



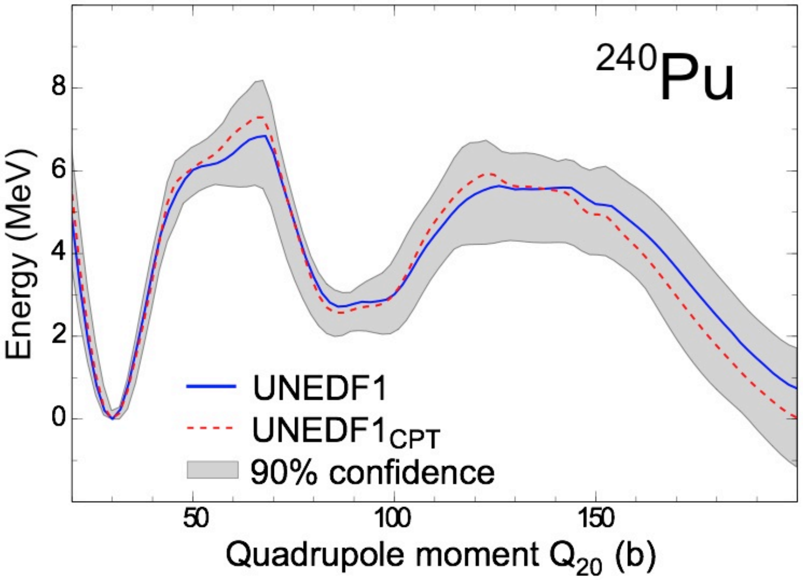
Quantified EDF

J. McDonnell et al. Phys. Rev. Lett. 114, 122501 (2015)



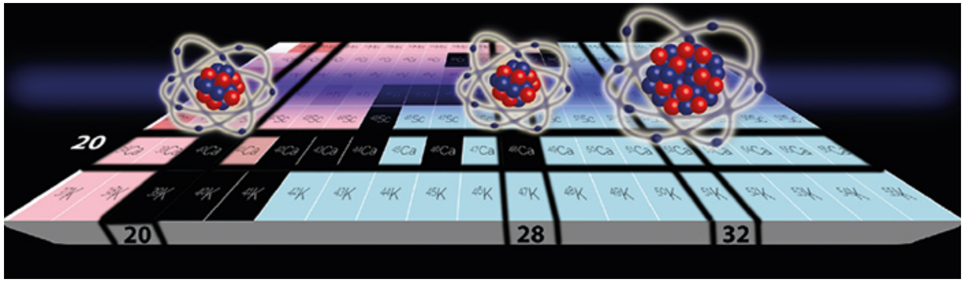
Bivariate marginal estimates of the posterior distribution for the 12-dimensional DFT UNEDF1 parameterization.

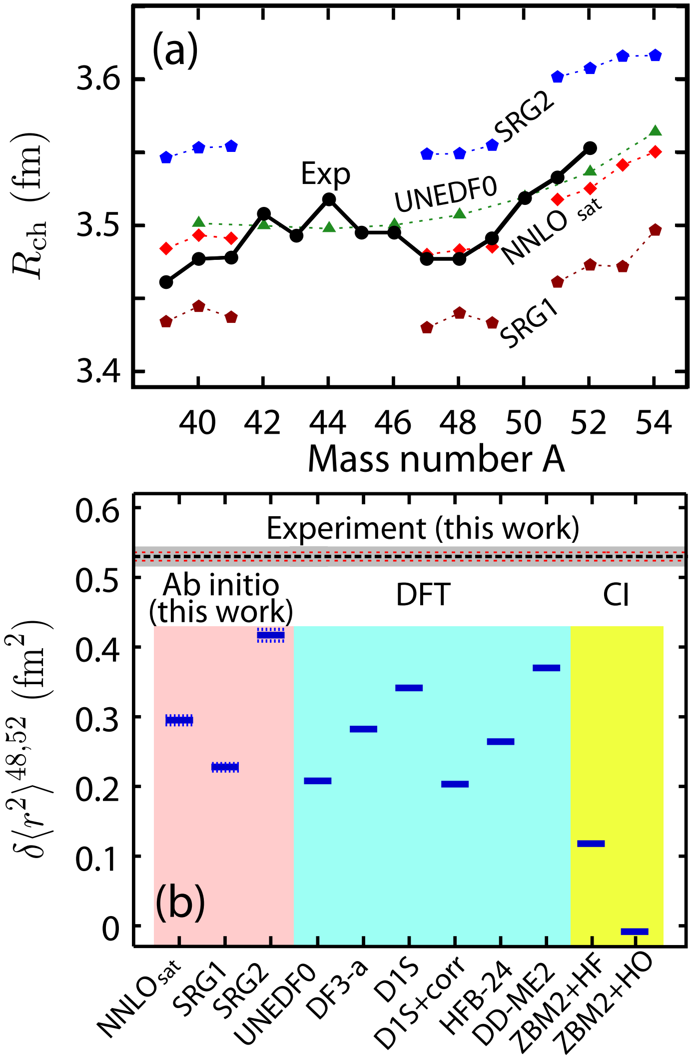
- Developed a Bayesian framework to quantify and propagate statistical uncertainties of EDFs.
- Showed that new precise mass measurements do not impose sufficient constraints to lead to significant changes in the current DFT models (models are not precise enough)



Example: Charge radii of calcium isotopes
Where *A*-body and DFT meet…

Garcia-Ruiz et al, Nature Physics **12**, 594 (2016)



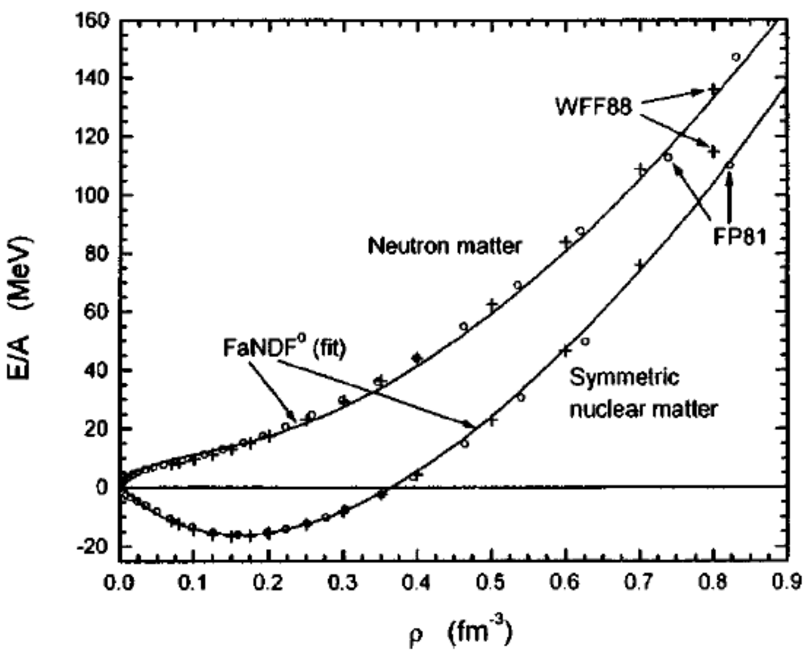


The local Fayans functional offers superb description of binding energies and charge radii: S. A. Fayans, JETP Lett. 68, 169 (1998)

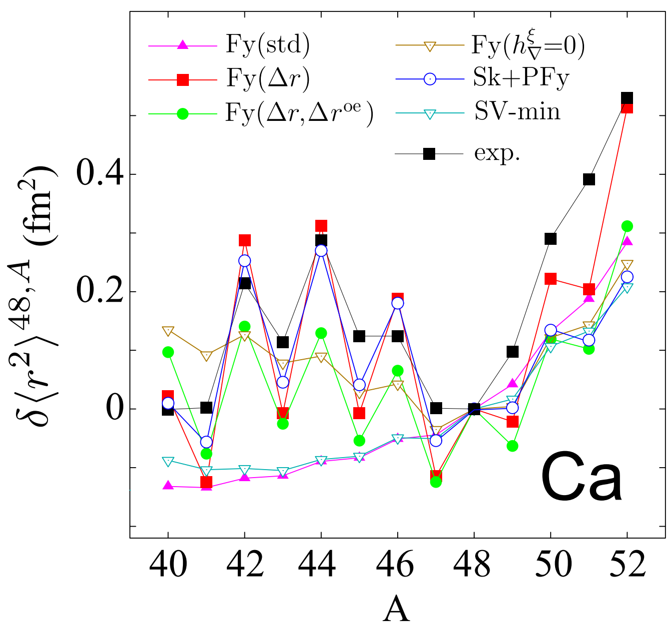
$$x_t = \frac{\rho_t}{\rho_{\rm sat}}, \quad x_{\rm pair} = \frac{\rho_0}{\rho_{\rm pair}}$$

$$\mathcal{E}^{\rm s}_{\rm Fy} = \tfrac{1}{3}\varepsilon_F \rho_{\rm sat} \frac{a^{\rm s}_{+} r_s^2 (\boldsymbol{\nabla} x_0)^2}{1 + h^{\rm s}_{+} x_0^{\sigma} + h^{\rm s}_{\nabla} r_s^2 (\boldsymbol{\nabla} x_0)^2}$$

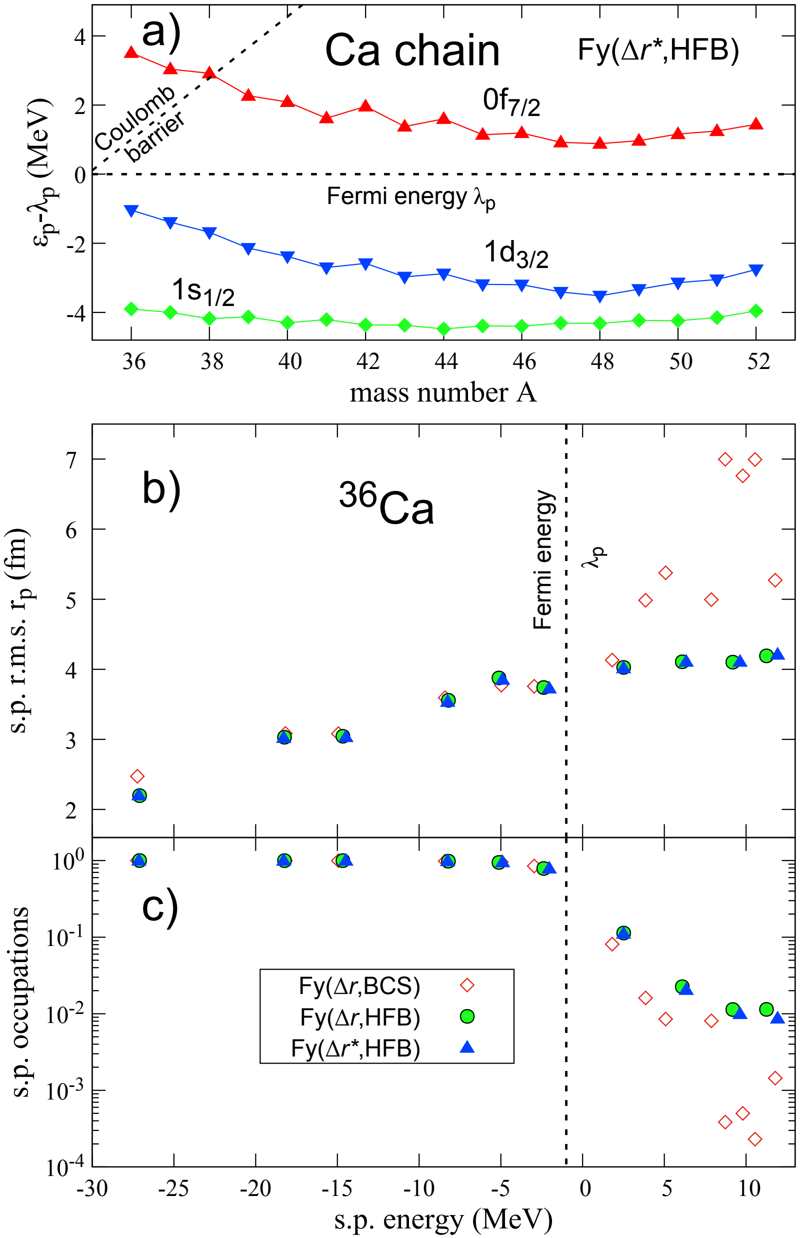
$$\mathcal{E}^{\rm pair}_{{\rm Fy},q} = \frac{2\varepsilon_F}{3\rho_{\rm sat}} \breve{\rho}_q^2 \left[f^{\xi}_{\rm ex} + h^{\xi}_{+} x^{\gamma}_{\rm pair} + h^{\xi}_{\nabla} r_s^2 (\boldsymbol{\nabla} x_{\rm pair})^2 \right]$$

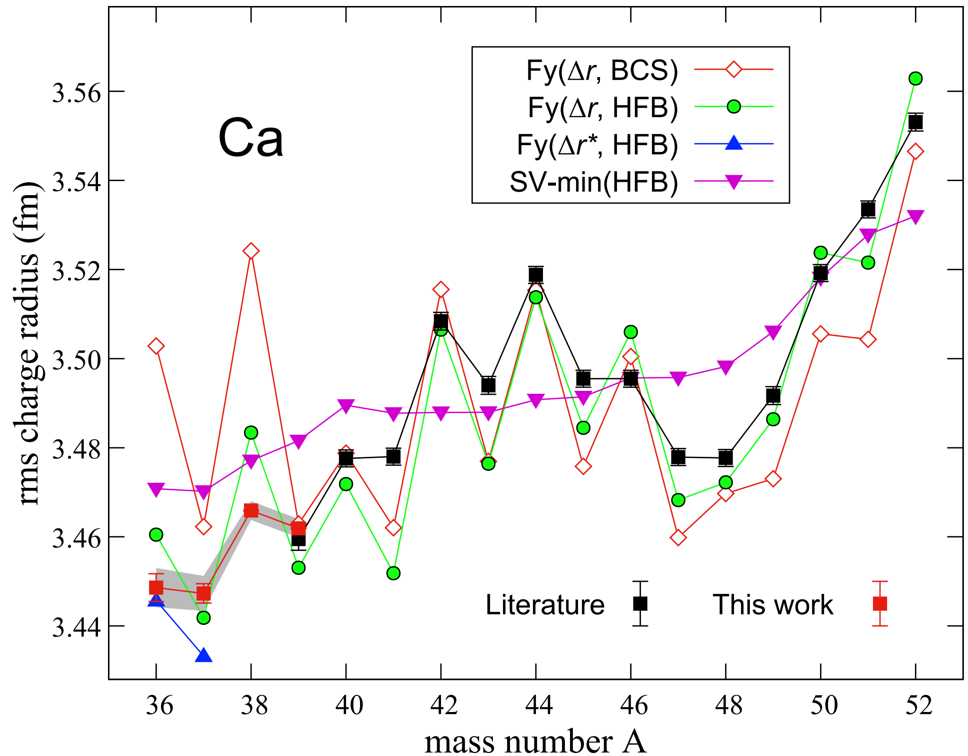


Recent optimization Fy(Δr): P.G. Reinhard and WN, Phys. Rev. C 95, 064328 (2017)



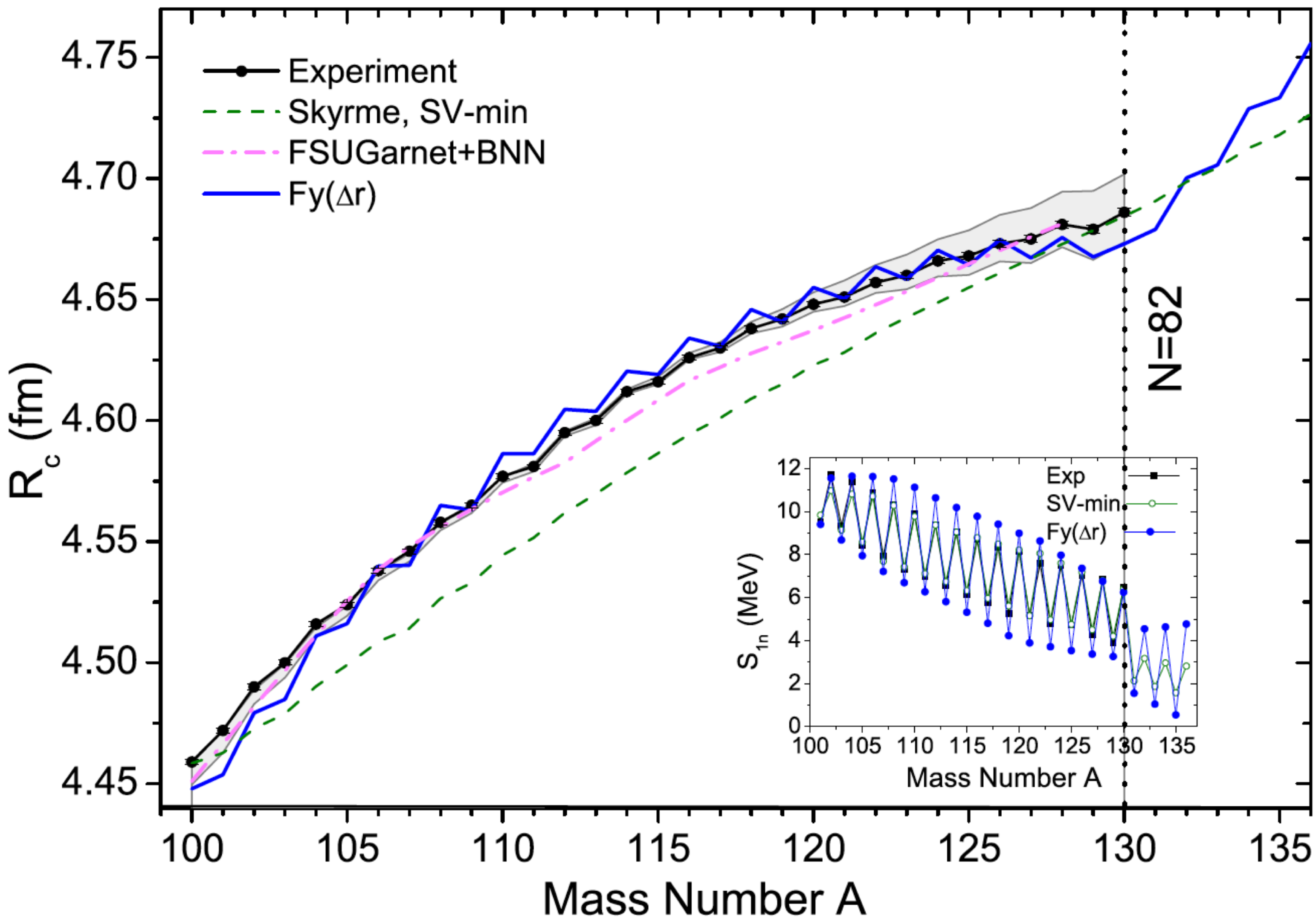
A.J. Miller et al: Proton superfluidity and charge radii in proton-rich calcium isotopes, submitted





From Calcium to Cadmium

M. Hammen et al. Phys. Rev. Lett. 121, 102501 (2018)



Summary (novel functionals, charge radii)

By using the tools of numerical optimization and linear regression, we developed new local Fayans energy density functional Fy(Δr, HFB). This functional provide excellent description of selected nuclear properties, such as charge radii and separation energies.

Microscopically based energy density functionals for nuclei using the density matrix expansion. II. Full optimization and validation

R. Navarro Pérez, N. Schunck, A. Dyhdalo, R. J. Furnstahl, and S. K. Bogner
Phys. Rev. C **97**, 054304 – Published 2 May 2018

TABLE II. Root mean square (rms) deviations between experimental and theoretical binding energies. Experimental values are taken from the 2016 Atomic Mass Evaluation [60,61]; see text for additional details.

EDF	rms	Number of nuclei
UNEDF2	1.98	620
LO	1.99	617
NLO	2.02	617
N2LO	1.57	616
N2LO+3N	1.58	613
NLOΔ	1.41	618
NLOΔ+3N	1.46	617
N2LOΔ	1.26	615
N2LOΔ+3N	1.72	617

Bayesian approach to model-based extrapolation of nuclear observables

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

Editors' Suggestion

Bayesian approach to model-based extrapolation of nuclear observables

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In order 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 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).

Separation energy residual:

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

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

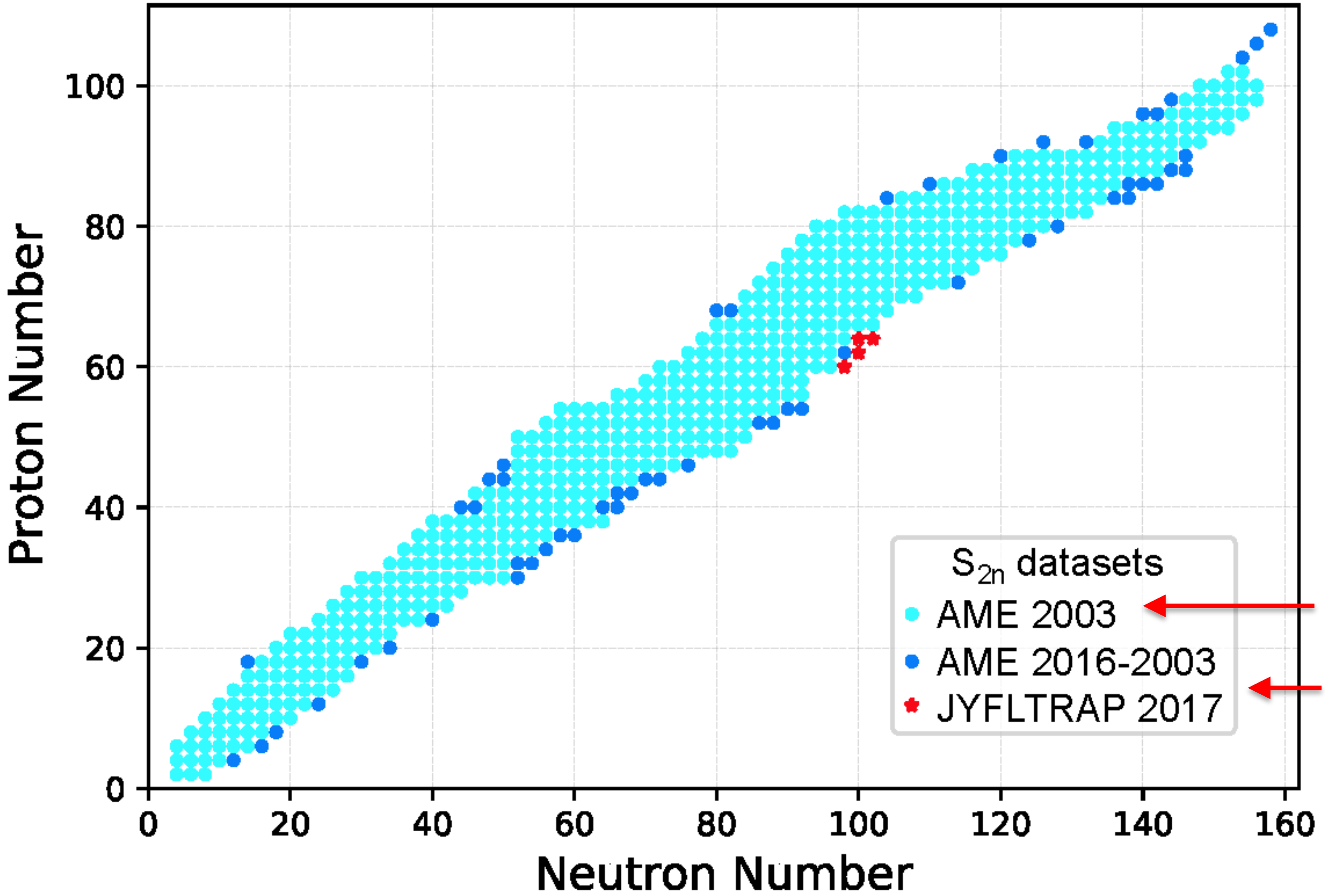
emulator of residual

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

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

We are not interested in mass formulae: “With four parameters I can fit an elephant, and with five I can make him wiggle his trunk” (John von Neumann)

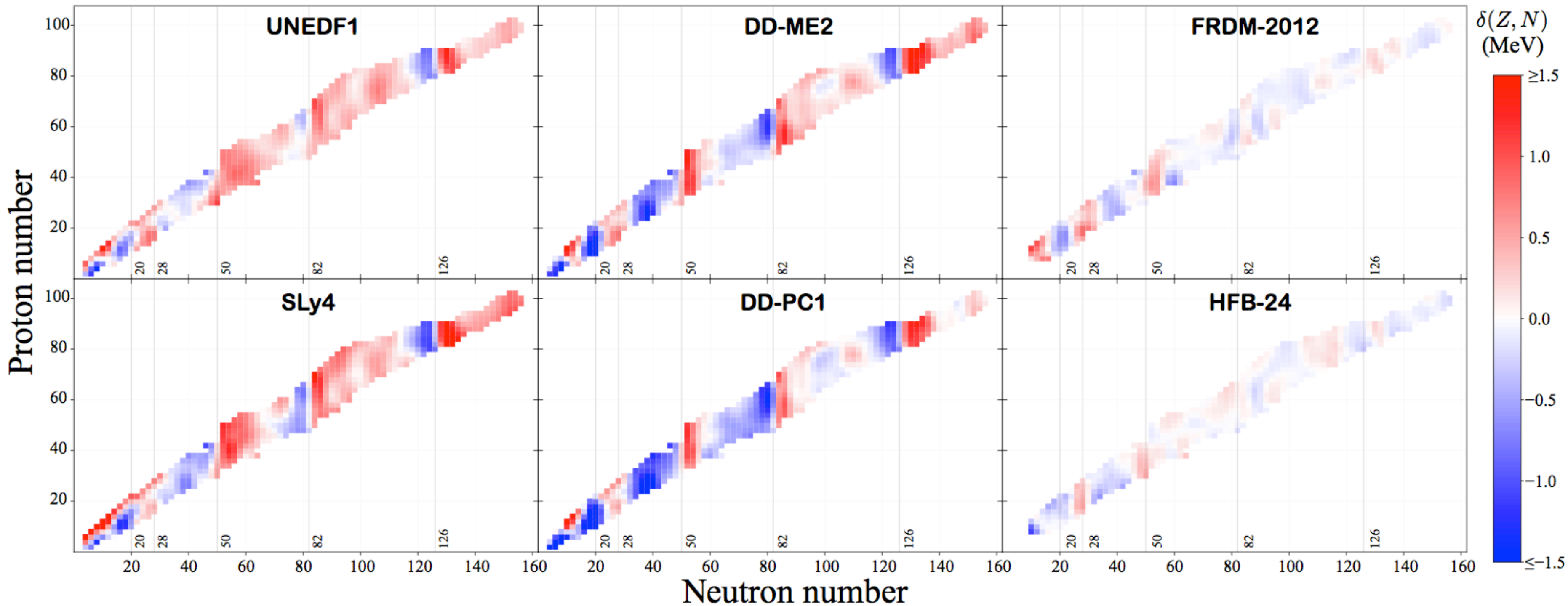
Our objective: extrapolations



Training set:
537 points

Testing sets:
55+4 points

Residuals exhibit local trends



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

Bayesian approach

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

$(Z,N)_i$

$$p(\theta, \sigma|y) \propto p(y|\theta, \sigma)\pi(\theta, \sigma)$$ Bayes' theorem

$$p(y^*|y) = \int p(y^*|y, \theta, \sigma)p(\theta, \sigma|y)\, d\theta d\sigma$$

Prediction of unknown observable *y** given known data *y*

Two statistical models used:

- Gaussian process (**3** parameters)
- Bayesian neural network with sigmoid function (30 neurons, 1 layer; **181** parameters)

100,000 iterations of an ergodic Markov chain produced by the Metropolis-Hastings algorithm

Some refinements added based on our knowledge of trends

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

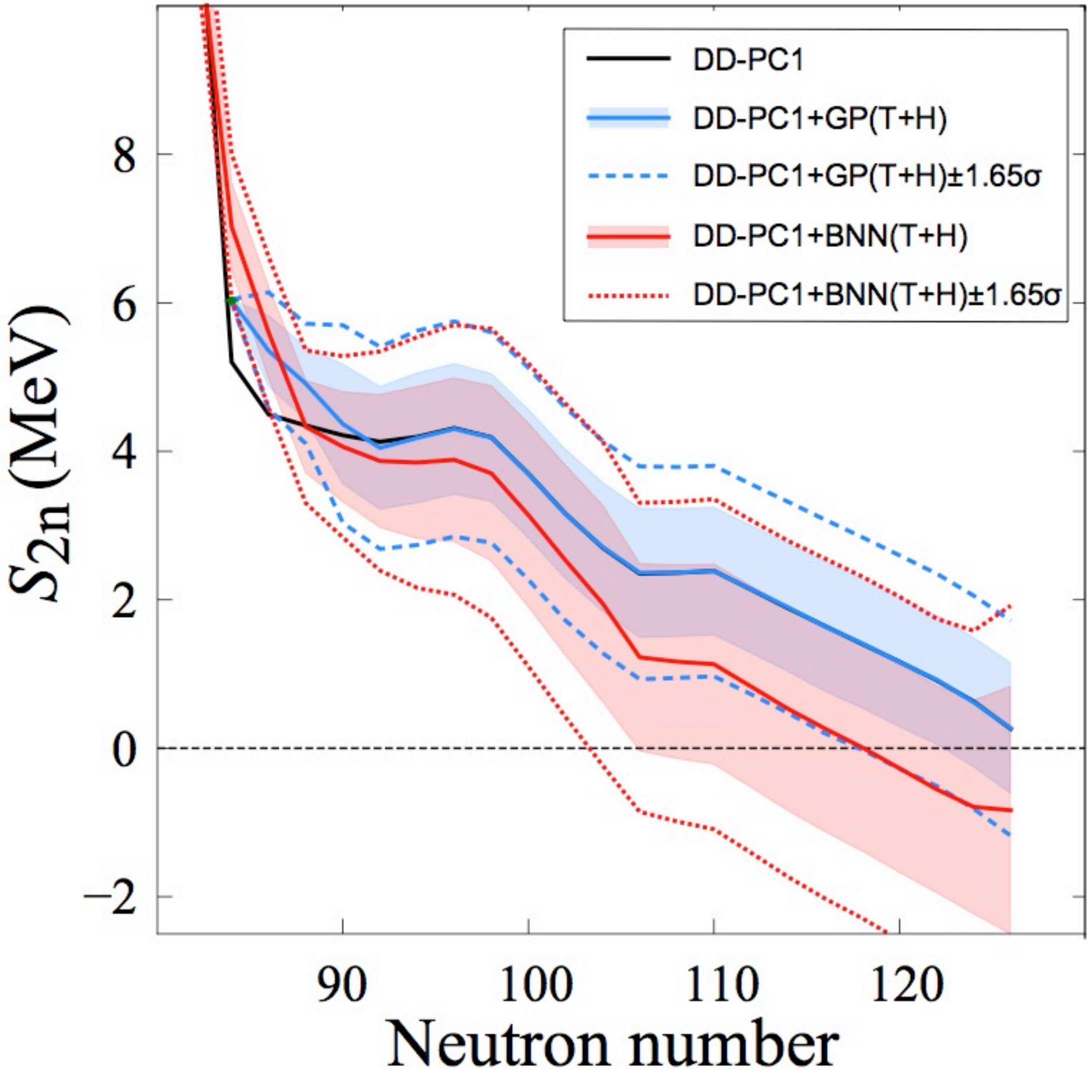
BNN

training dataset: AME2003

testing dataset: AME2016-AME2003

Overall, for the testing dataset AME2016-2003, the rms deviation from experimental S_{2n} values is 400-500 keV in the GP variant for *all* theoretical models employed in our study, which suggests that our statistical methods capture most of the residual structure.

BUT the predicted mean value is certainly not the whole story!

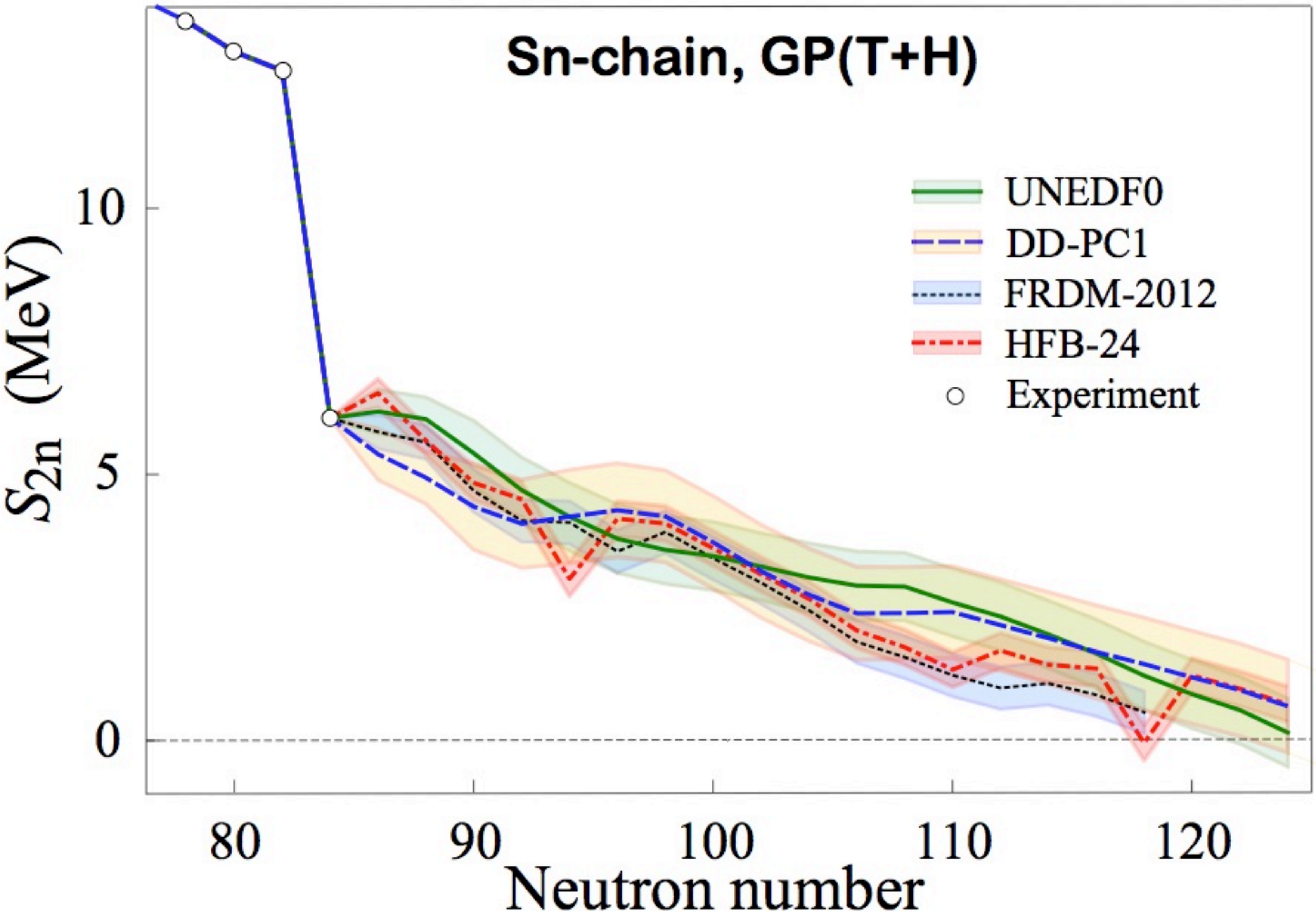


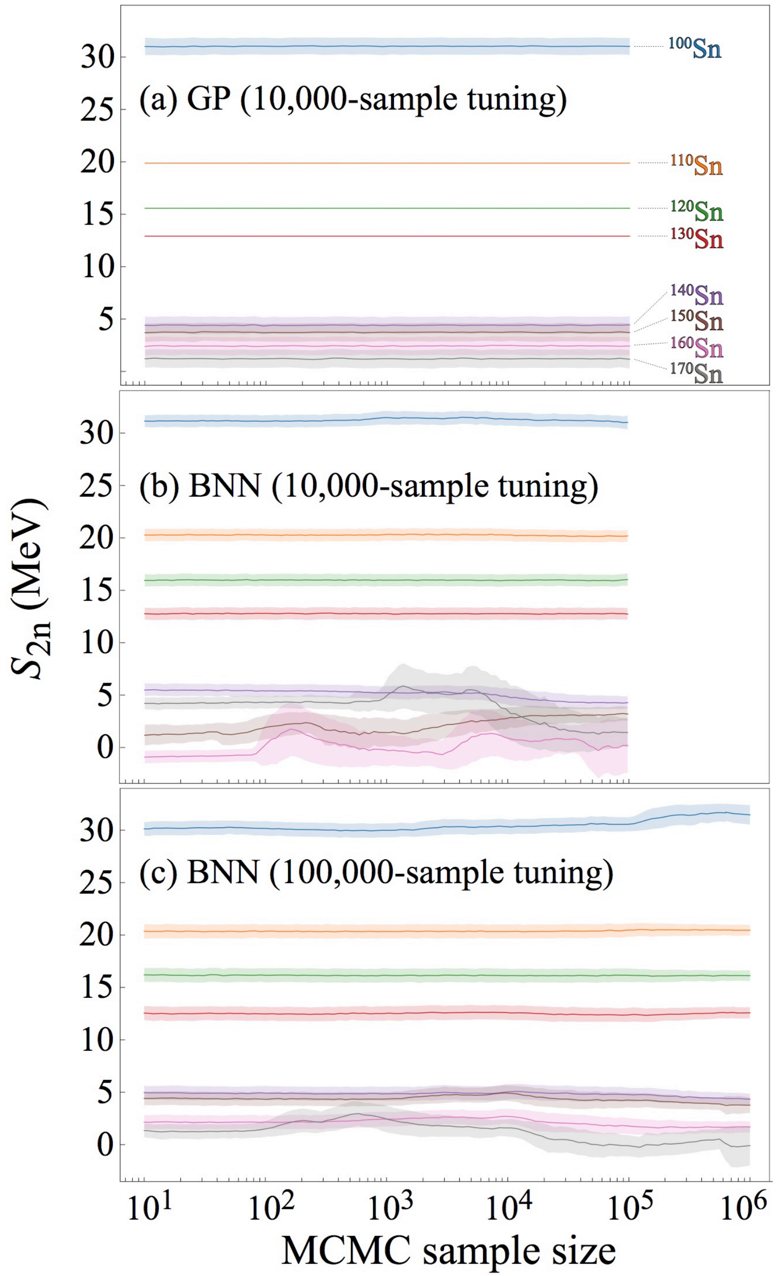
model: N*=126

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

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

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


Sn-chain, GP(T+H)
UNEDF0
DD-PC1
FRDM-2012
HFB-24
Experiment
S_{2n} (MeV)
10
5
0
80
90
100
110
120
Neutron number



Massive MCMC runs: BNN shows convergence issues!

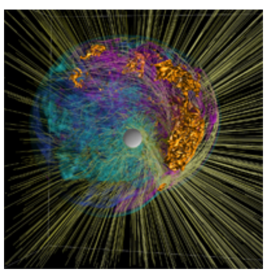
Summary (Bayesian treatment)

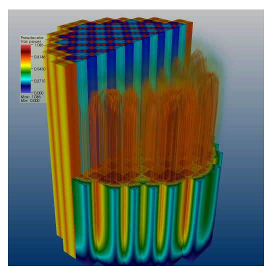
Beam time and compute cycles are difficult to get and expensive

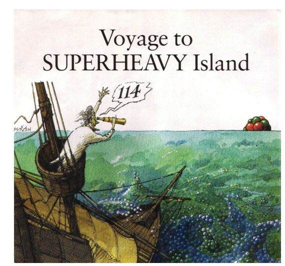
- What is the information content of measured observables?
- Are estimated errors of measured observables meaningful?
- What experimental data are crucial for better constraining current nuclear models?

New technologies are essential for providing predictive capability, to estimate uncertainties, and to assess extrapolations

- Theoretical models are often applied to entirely new nuclear systems and conditions that are not accessible to experiment







Statistical tools can help us revealing the structure of our models

- Parameter reduction
- Uncertainty quantification

Thank You