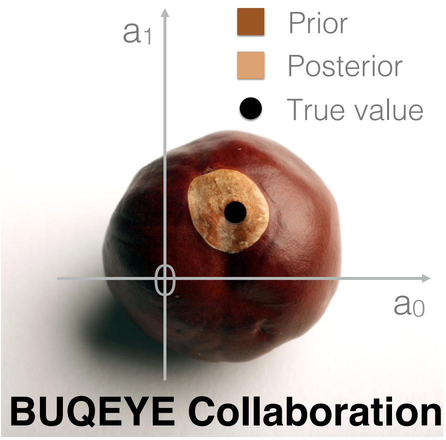
Uncertainty Quantification for Nuclear Models

Dick Furnstahl
MSU Nuclear Seminar, March 2023
THE OHIO STATE UNIVERSITY

Slides:



https://buqeye.github.io/

Jupyter notebooks here!

LENPIC

https://www.lenpic.org/

NUCLEI
Nuclear Computational Low-Energy Initiative

https://nuclei.mps.ohio-state.edu/

BAND
Bayesian Analysis of Nuclear Dynamics

https://bandframework.github.io/

U.S. DEPARTMENT OF ENERGY

NSF

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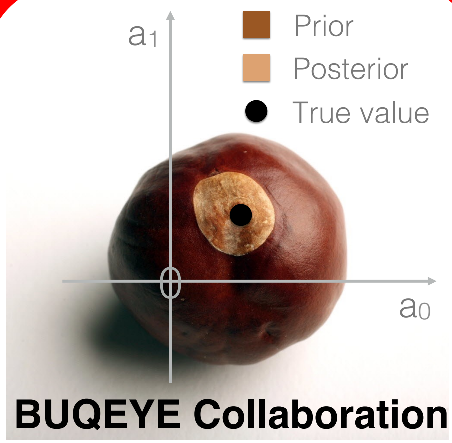

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Outline

- Thinking about uncertainty quantification (UQ) for models
- **BAND:** emulators, calibration, model mixing, expt. design
- Outlook: Frontiers of UQ for nuclear models

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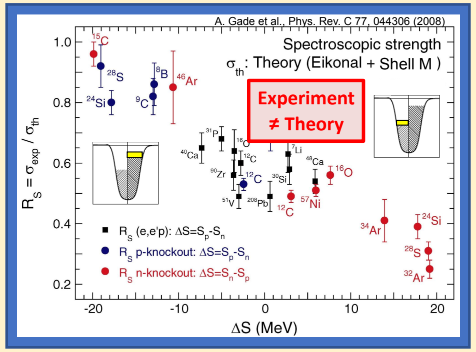
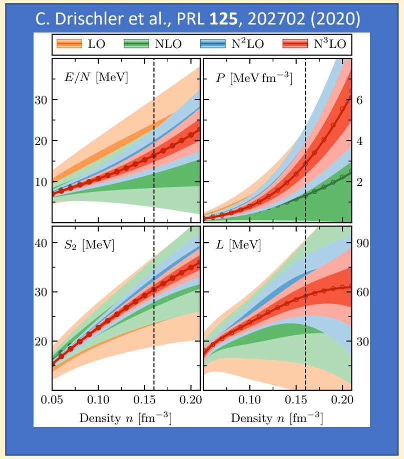
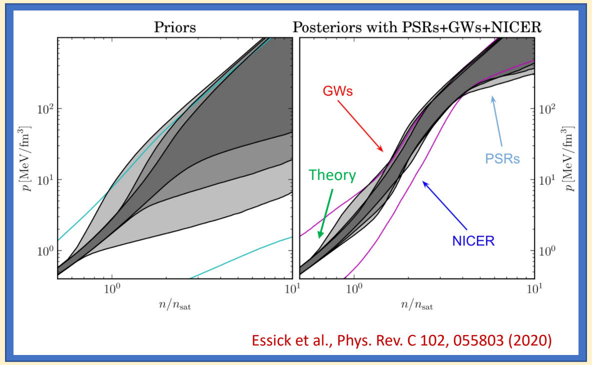
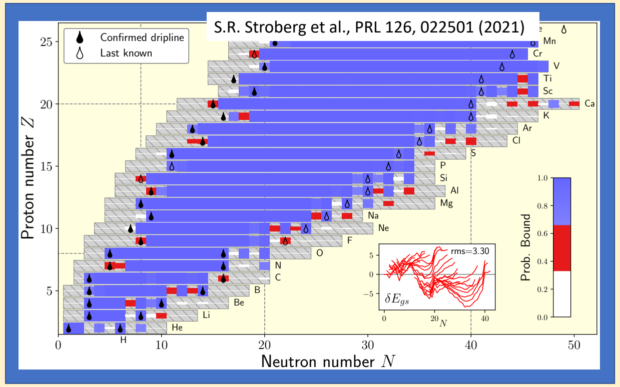
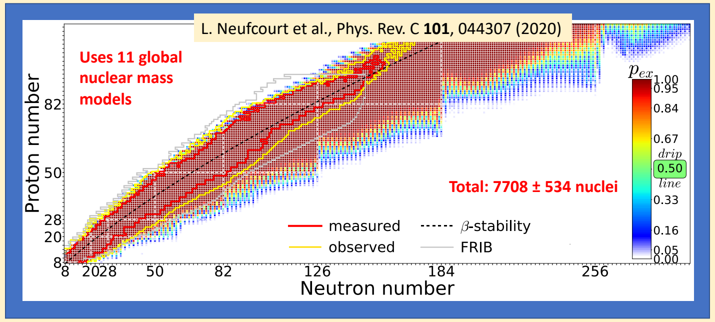
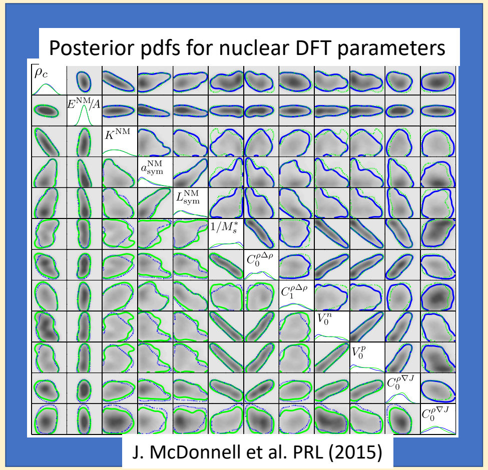

A. Gade et al., Phys. Rev. C 77, 044306 (2008)
Spectroscopic strength
σth: Theory (Eikonal + Shell M)
Experiment ≠ Theory
RS = σexp / σth
RS (e,e'p): ΔS=Sp-Sn
RS p-knockout: ΔS=Sp-Sn
RS n-knockout: ΔS=Sn-Sp
ΔS (MeV)

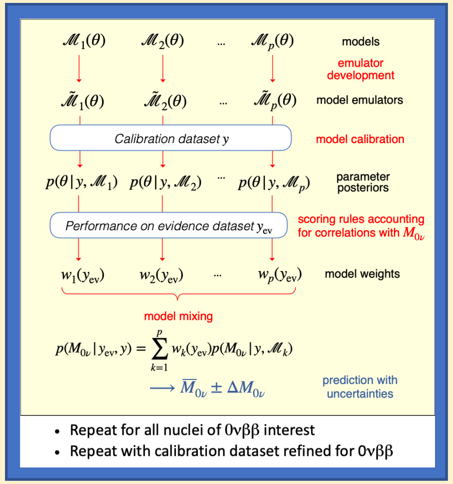

C. Drischler et al., PRL 125, 202702 (2020)
LO
NLO
N2LO
N3LO
E/N [MeV]
P [MeV fm−3]
S2 [MeV]
L [MeV]
Density n [fm−3]

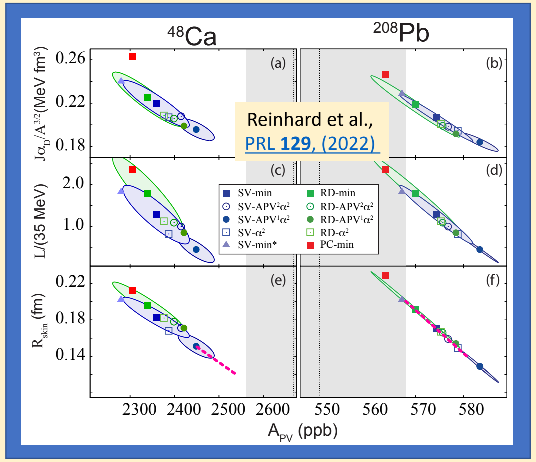

Priors
Posteriors with PSRs+GWs+NICER
GWs
Theory
PSRs
NICER
p [MeV/fm3]
n/nsat
Essick et al., Phys. Rev. C 102, 055803 (2020)

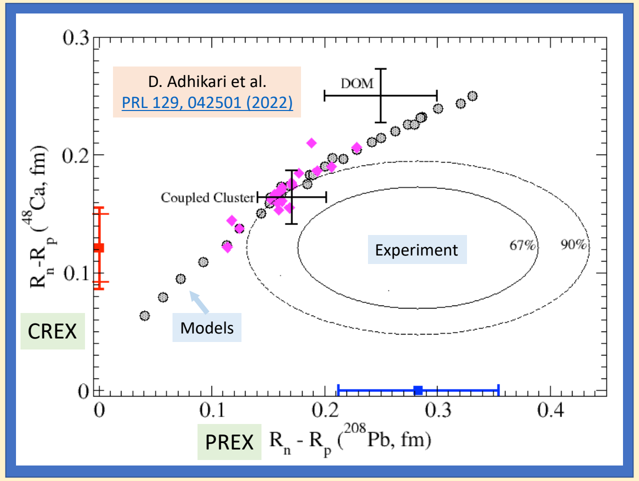

S.R. Stroberg et al., PRL 126, 022501 (2021)
Confirmed dripline
Last known
Proton number Z
Neutron number N
Prob. Bound
rms=3.30
δEgs

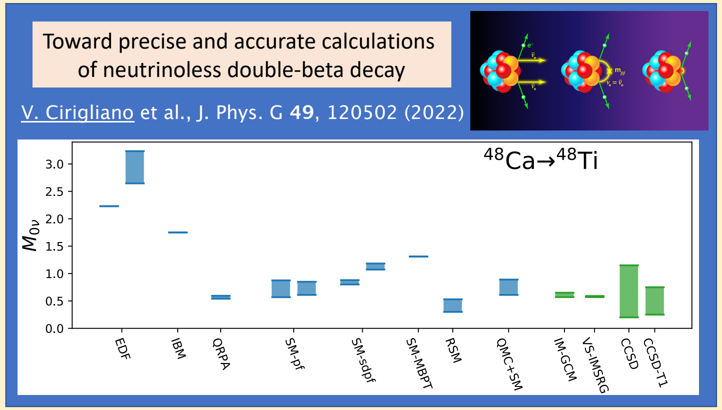

L. Neufcourt et al., Phys. Rev. C 101, 044307 (2020)
Uses 11 global nuclear mass models
Total: 7708 ± 534 nuclei
measured
observed
β-stability
FRIB
pex
drip line
Proton number
Neutron number

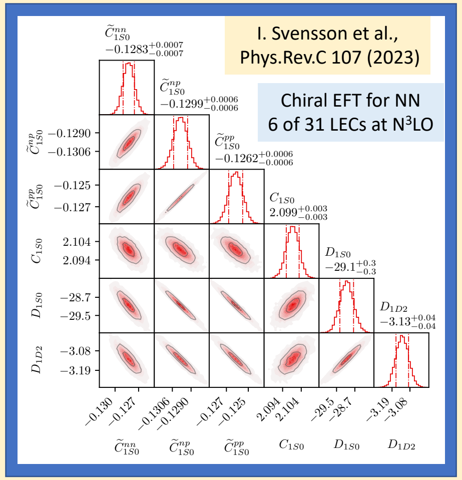

Posterior pdfs for nuclear DFT parameters
J. McDonnell et al. PRL (2015)

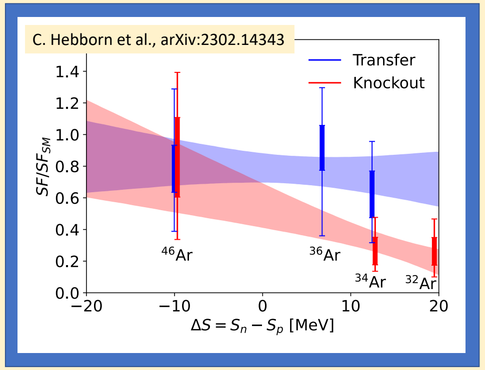

models
emulator development
model emulators
Calibration dataset y
model calibration
parameter posteriors
Performance on evidence dataset yev
scoring rules accounting for correlations with M0ν
model weights
model mixing
prediction with uncertainties
Repeat for all nuclei of 0νββ interest
Repeat with calibration dataset refined for 0νββ


48Ca
208Pb
Reinhard et al.,
PRL 129, (2022)
SV-min
SV-APV2α2
SV-APV1α2
SV-α2
SV-min*
RD-min
RD-APV2α2
RD-APV1α2
RD-α2
PC-min
L(35 MeV)
Rskin (fm)
APV (ppb)


D. Adhikari et al.
PRL 129, 042501 (2022)
DOM
Coupled Cluster
Experiment
Models
CREX
PREX
Rn - Rp (208Pb, fm)
Rn-Rp (48Ca, fm)


Toward precise and accurate calculations of neutrinoless double-beta decay
V. Cirigliano et al., J. Phys. G 49, 120502 (2022)
48Ca→48Ti
M0ν
EDF
IBM
QRPA
SM-pf
SM-sdpf
SM-MBPT
RSM
QMC+SM
IM-GCM
VS-IMSRG
CCSD
CCSD-T1


I. Svensson et al.,
Phys.Rev.C 107 (2023)
Chiral EFT for NN
6 of 31 LECs at N3LO


C. Hebborn et al., arXiv:2302.14343
Transfer
Knockout
SF/SFSM
ΔS = Sn − Sp [MeV]

Checklist for statistically sound Bayesian inference

- ☑ Interact with the experts (i.e., statisticians, applied mathematicians)
- ❑ Incorporate all sources of experimental and *theoretical* errors
- ❑ Formulate *statistical models* for uncertainties
- ❑ Use as informative priors as is reasonable; test sensitivity to priors
- ❑ Account for correlations in inputs (type x) and observables (type y)
- ❑ Propagate uncertainties through the calculation
- ❑ Use *model checking* to validate our models

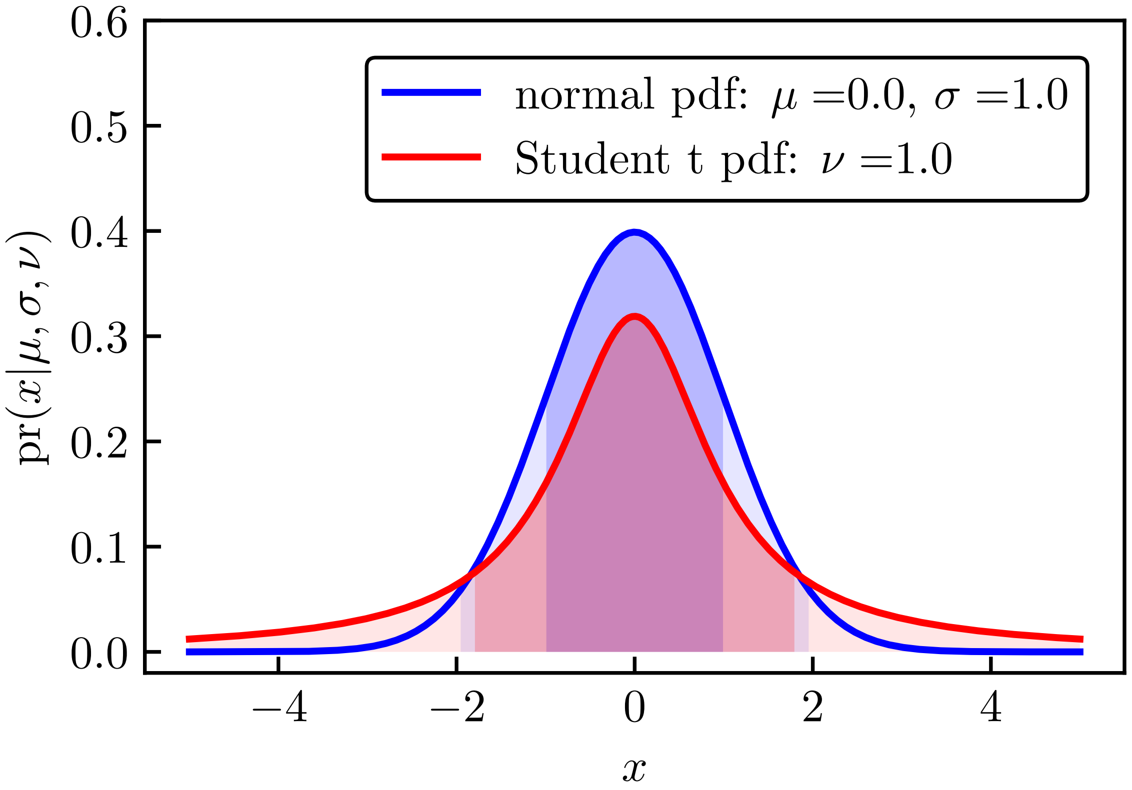
Bayesian updating of knowledge

$$\mathrm{pr}(A|B,I) = \frac{\mathrm{pr}(B|A,I)\,\mathrm{pr}(A|I)}{\mathrm{pr}(B|I)} \Longrightarrow \underbrace{\mathrm{pr}(\boldsymbol{\theta}|\mathbf{y}_{\mathrm{exp}},I)}_{\text{posterior}} \propto \underbrace{\mathrm{pr}(\mathbf{y}_{\mathrm{exp}}|\boldsymbol{\theta},I)}_{\text{likelihood}} \times \underbrace{\mathrm{pr}(\boldsymbol{\theta}|I)}_{\text{prior}}$$

State of knowledge as probability distributions (pdfs)

- pr(A, B | C) "joint probability (density) of A and B given C" (*contingent* on C)
- A, B, C can be observables, parameters, uncertainties, propositions, models, …
- cf. quantum mechanics $|\psi(\mathbf{x}_1, \mathbf{x}_2)|^2$ or $|\psi(\mathbf{x}_1)|^2 = \int |\psi(\mathbf{x}_1, \mathbf{x}_2)|^2 \, d\mathbf{x}_2$ (*marginalization*)
- Bayesian confidence (credible) interval:

$$\mathrm{pr}(a \le x \le b) = \int_a^b |\psi(x)|^2 \, dx$$



State of knowledge as probability distributions (pdfs)

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- A, B, C can be observables, parameters, ur
- cf. quantum mechanics $|\psi(\mathbf{x}_1, \mathbf{x}_2)|^2$ or $|\psi($
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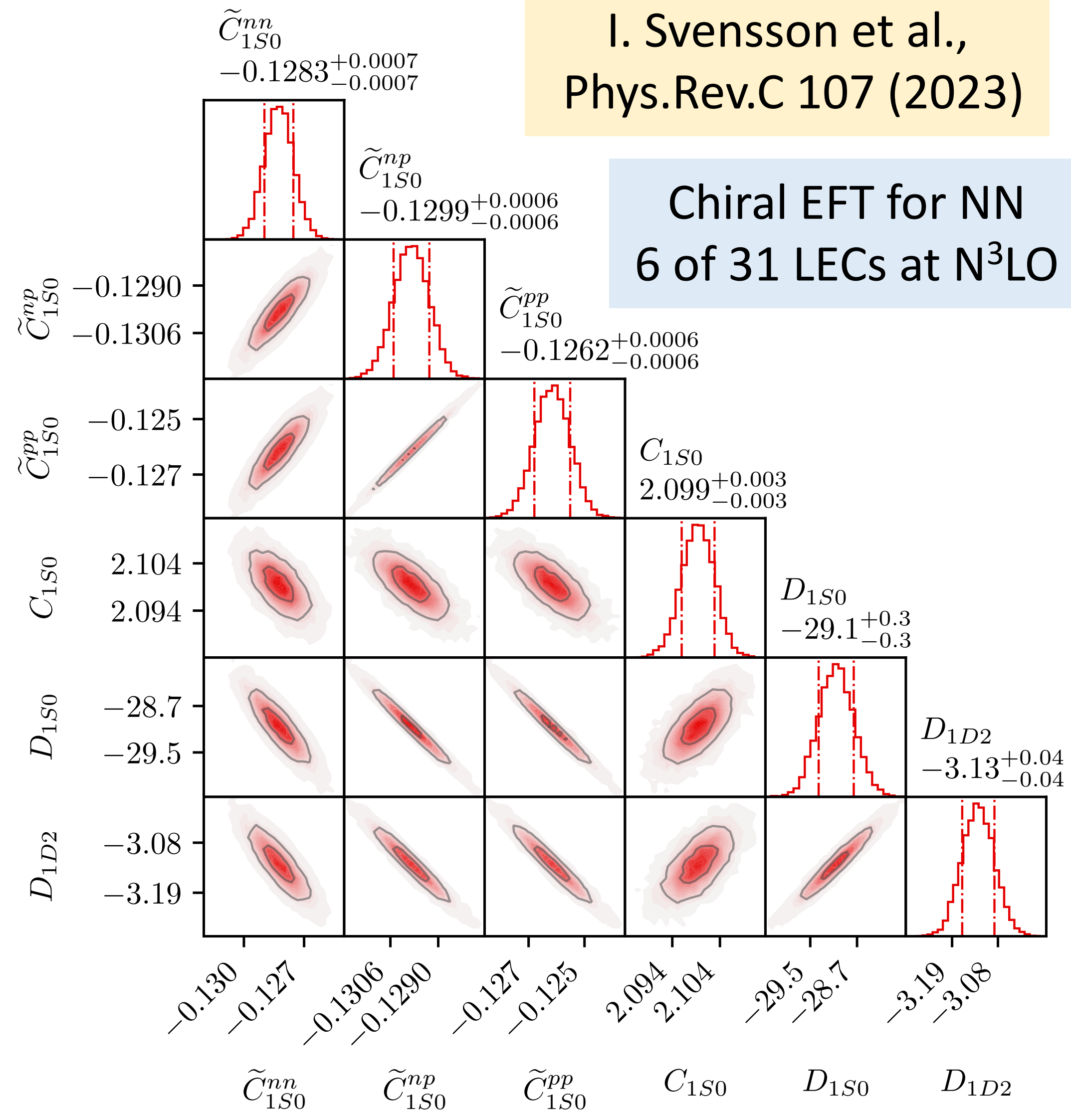
Examples of pdfs for model UQ:

$\mathrm{pr}(\boldsymbol{\theta} \mid \mathbf{y}_{exp}, \Sigma_{exp}, \Sigma_{th}, I) \Rightarrow$

pdf of model parameters **θ** given data y_{exp} and experiment/theory errors Σ, plus other information I



I. Svensson et al., Phys.Rev.C 107 (2023)

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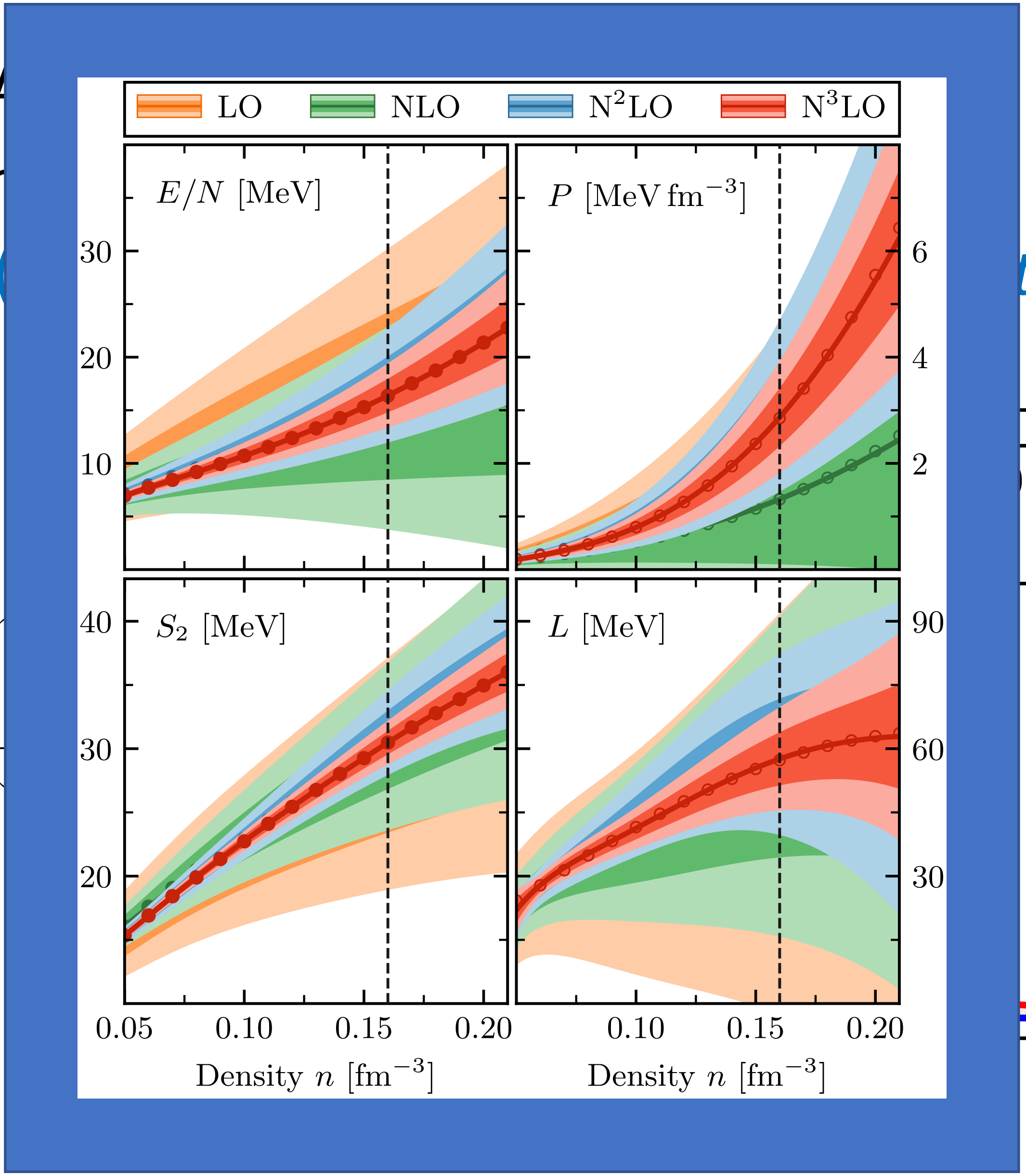

Examples of pdfs for model UQ:

pr($\delta\mathbf{y}_{th}$ | $\mathbf{y}_{th}$, I) ⇒
pdf of *model discrepancy* $\delta\mathbf{y}_{th}$ (model error) given order-by-order theory calculations $\mathbf{y}_{th}$ plus other information I

State of knowledge as probability distributions (pdfs)

- pr(A, B | C) "joint probability (density) of A
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- cf. quantum mechanics $|\psi(\mathbf{x}_1, \mathbf{x}_2)|^2$ or $|\psi($ … $on)$
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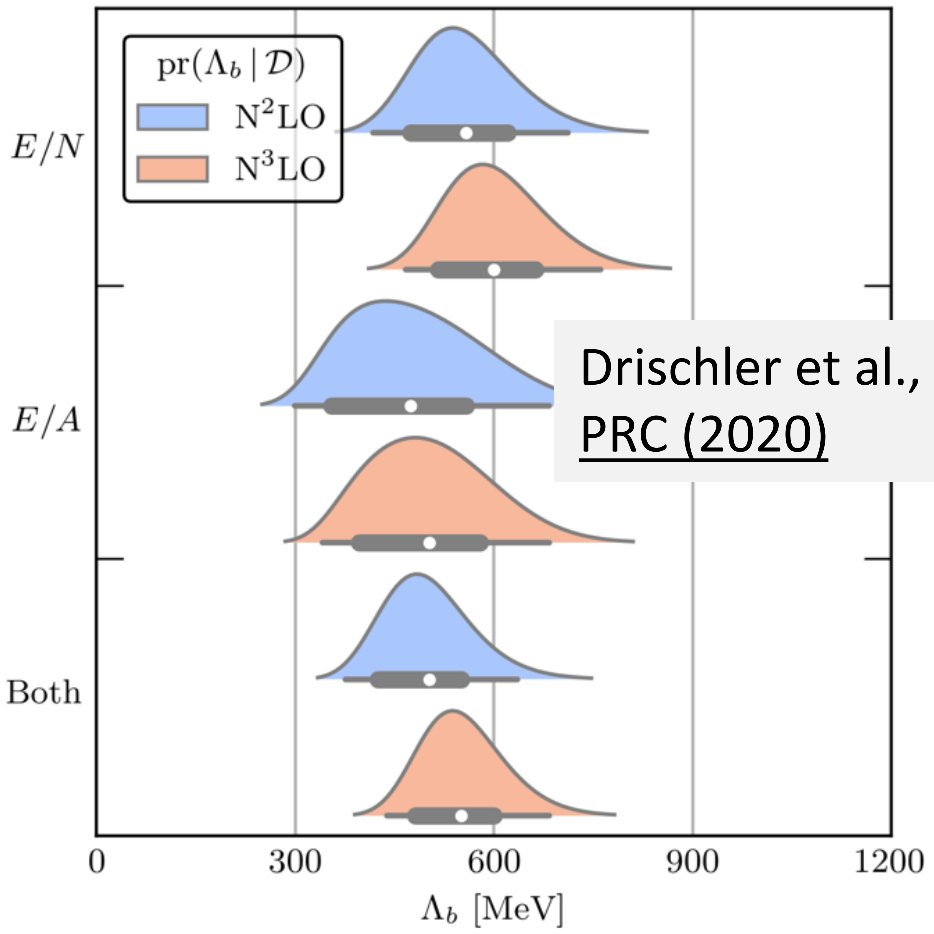
Examples of pdfs for model UQ:

pr(Λ_b | $\mathbf{y}_{th}$, I) ⇒
pdf of breakdown scale of EFT expansion given order-by-order theory calculations $\mathbf{y}_{th}$ plus other information I

Λ_b from infinite matter



Drischler et al., PRC (2020)

Bayes's Theorem: How to update knowledge in PDFs

Bayesian updating of knowledge

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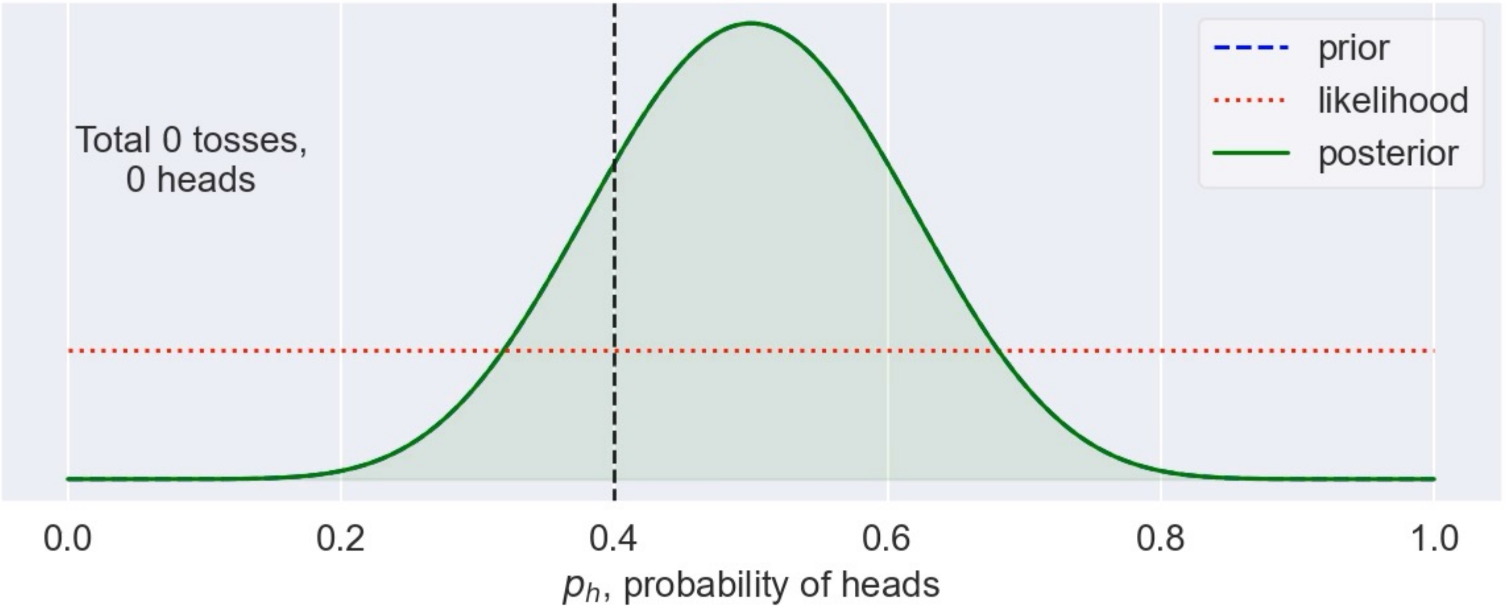
Example: tossing a *biased* coin. True probability of heads is p_h=0.4, but we don't know that. So p_h is a distribution updated with each toss of the coin.



Likelihood is

$$\mathrm{pr}(H \text{ heads in } N \text{ tosses} \mid p_h, I)$$
$$\propto p_h^H (1-p_h)^{N-H}$$

Priors can suppress too wide likelihoods to inhibit overfitting (cf. regularization for ANNs) but data wins in the end.

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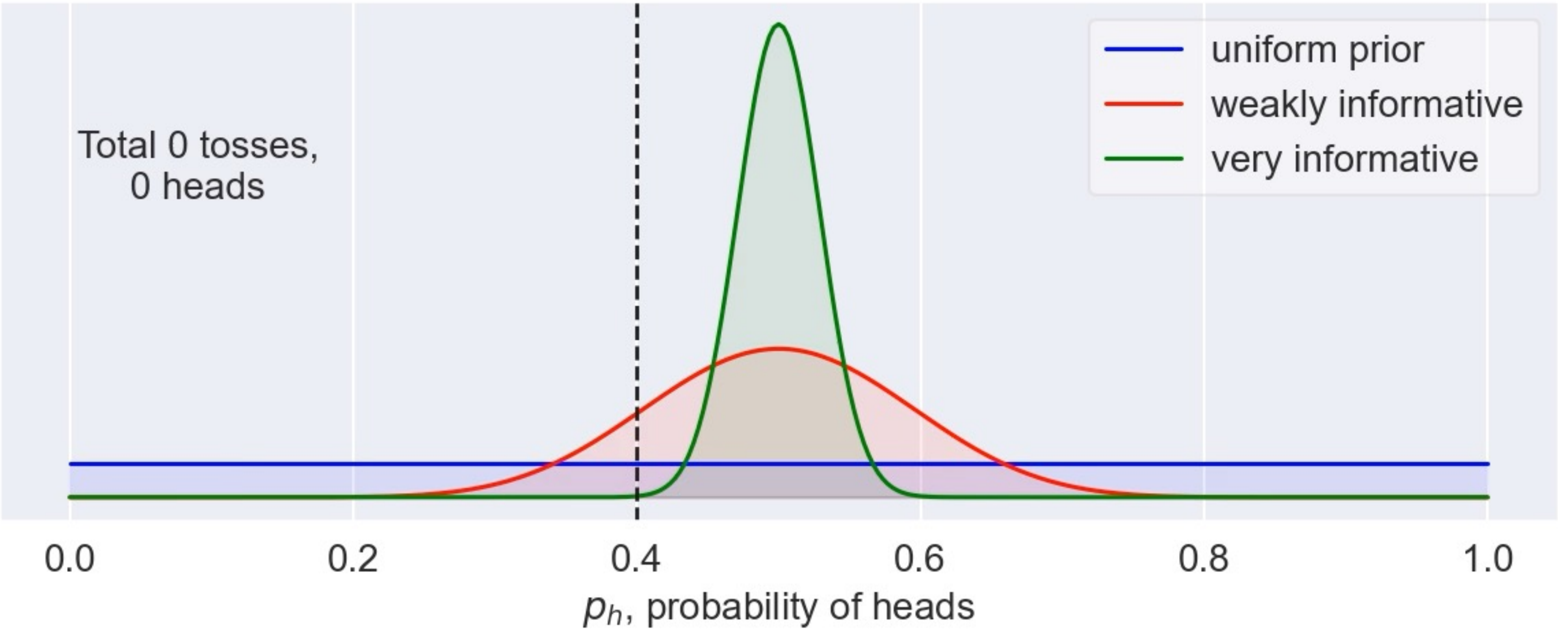

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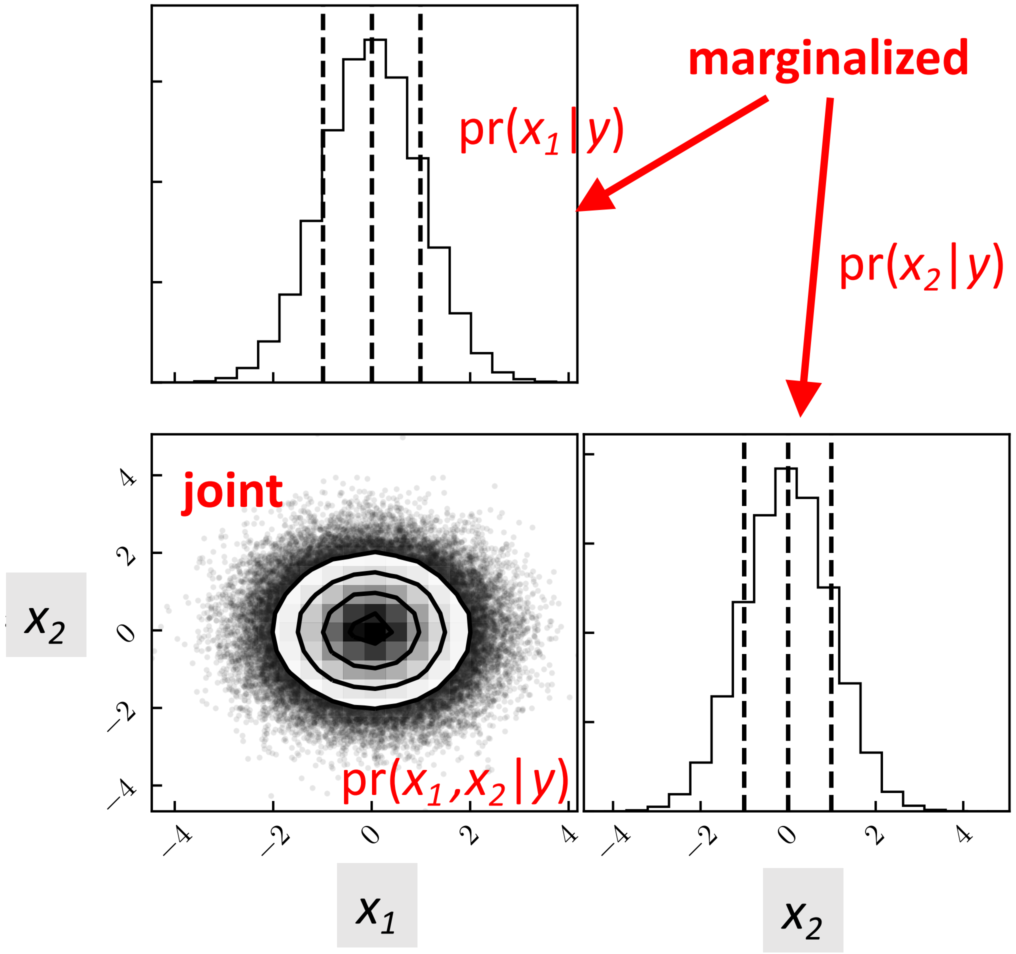
- ❑ Use *model checking* to validate our models

❑ Account for correlations in inputs and observables

- pr(x_1, x_2| y) "joint probability (density) of x_1 and x_2 given y" (*contingent* on y)



$$\mathcal{N}e^{-\frac{1}{2}\mathbf{r}^\intercal \Sigma^{-1}\mathbf{r}} = \mathcal{N}e^{-\frac{(x_1-\mu)^2}{2\sigma_{x1}^2}}\, e^{-\frac{(x_2-\mu)^2}{2\sigma_{x2}^2}}$$

$$\mathbf{r} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad \Sigma = \begin{bmatrix} \sigma_{x_1}^2 & 0 \\ 0 & \sigma_{x_2}^2 \end{bmatrix}$$

❑ Account for correlations in inputs and observables

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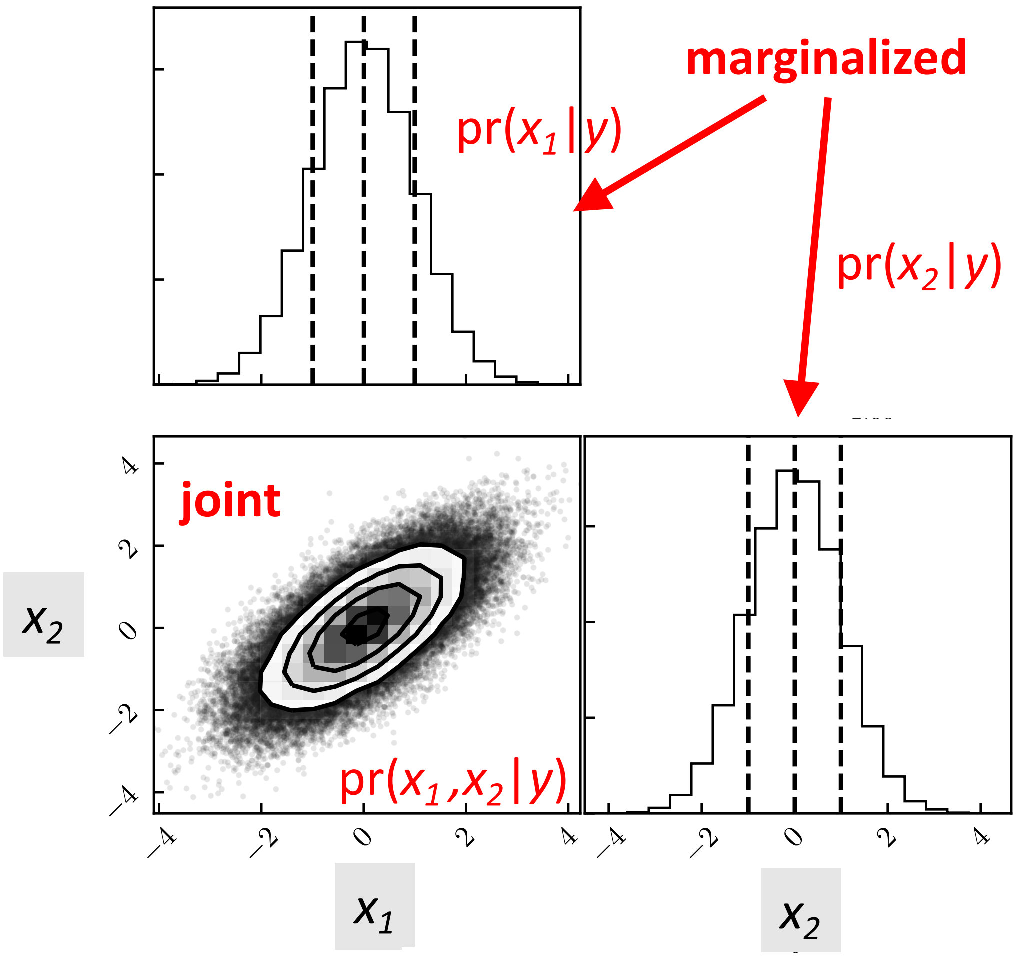

$$\mathcal{N} e^{-\frac{1}{2}\mathbf{r}^\intercal \Sigma^{-1}\mathbf{r}} = \textit{correlated gaussian}$$

$$\mathbf{r} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad \Sigma = \begin{bmatrix} \sigma^2_{x_1} & \rho\sigma_{x_1}\sigma_{x_2} \\ \rho\sigma_{x_1}\sigma_{x_2} & \sigma^2_{x_2} \end{bmatrix}$$

❑ Formulate *statistical models* for uncertainties

❑ Interact with the experts: statisticians say any model better than none!

George Box: “All models are wrong, but some are useful”

In what ways can a theoretical model be wrong?

- **Uncertainty from numerical method**
- **Truncation of Hilbert space** (e.g., lattice volume/spacing or ho model space)
- **Model discrepancy**
  - Incomplete or in parts incorrect physical model
  - Effective field theory expansion truncation error

❑ Incorporate all sources of expt. and *theoretical* errors

Mostly systematic and correlated (doesn’t mean they can’t be treated as random!).

- **Systematic:** error is not reduced when more observations are averaged
- **Correlated:** e.g., model error in binding energy for oxygen chain all in same direction

Bayesian statistics is ideal for modeling, combining, and propagating theory errors!

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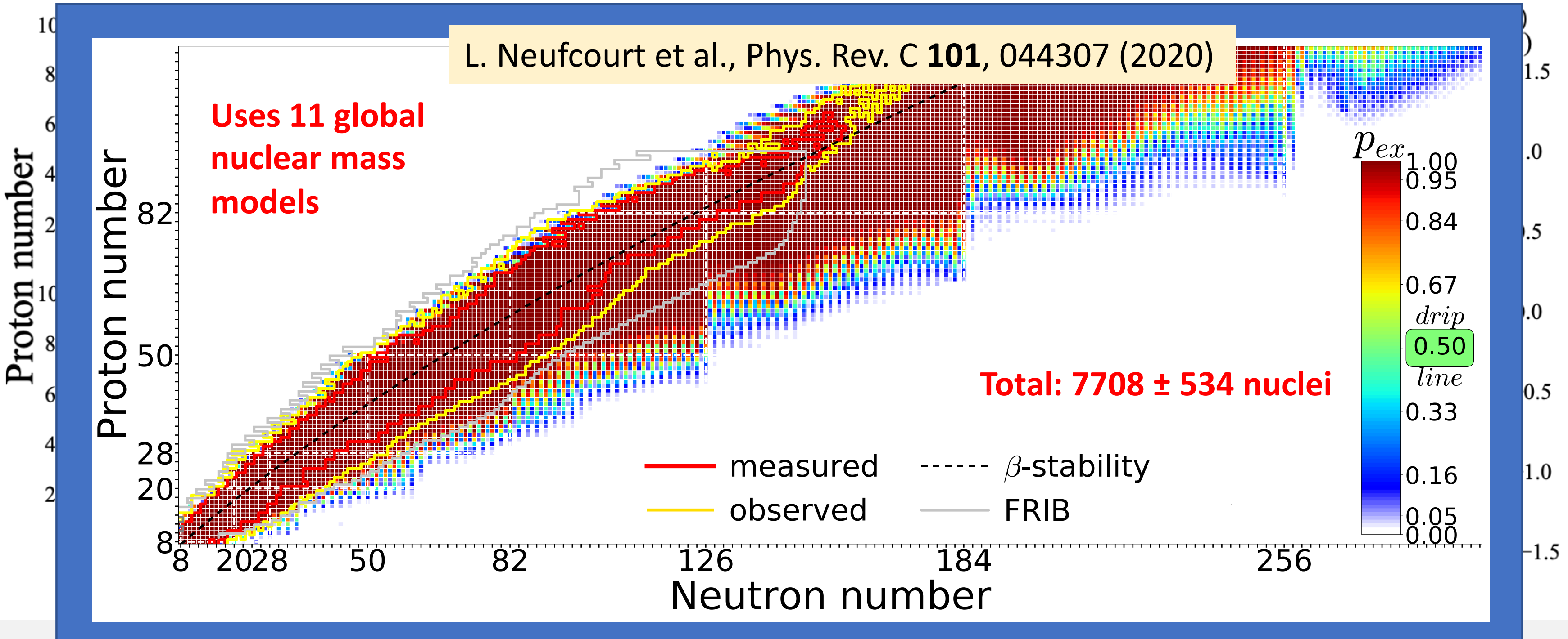
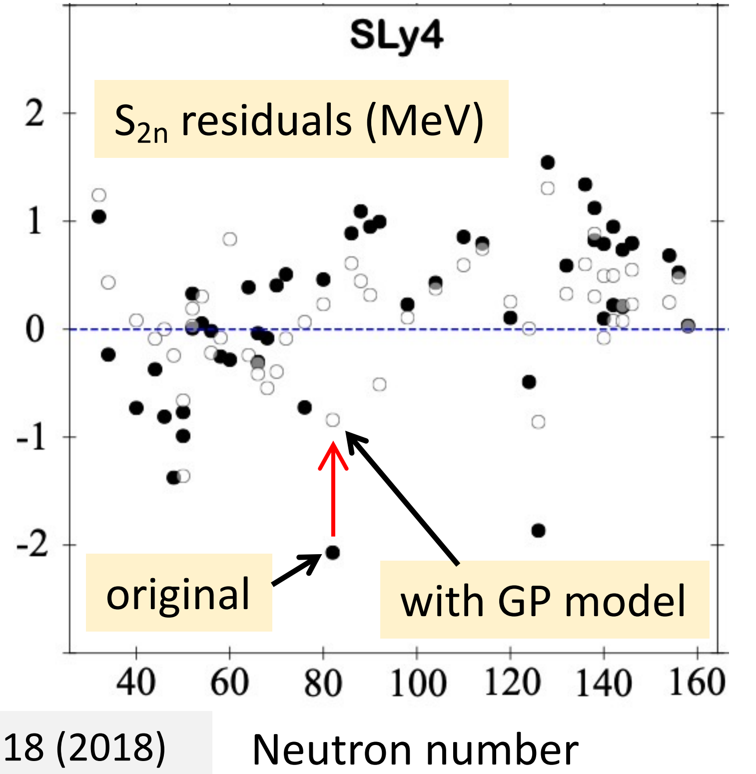
1. Model distribution of *residuals*: $\delta \equiv \mathbf{y}_{\rm exp} - \mathbf{y}_{\rm th} = \delta\mathbf{y}_{\rm exp} + \delta\mathbf{y}_{\rm th}$

Train the residuals on Gaussian Process model or with Bayesian Neural Network on one set; *test* on another set





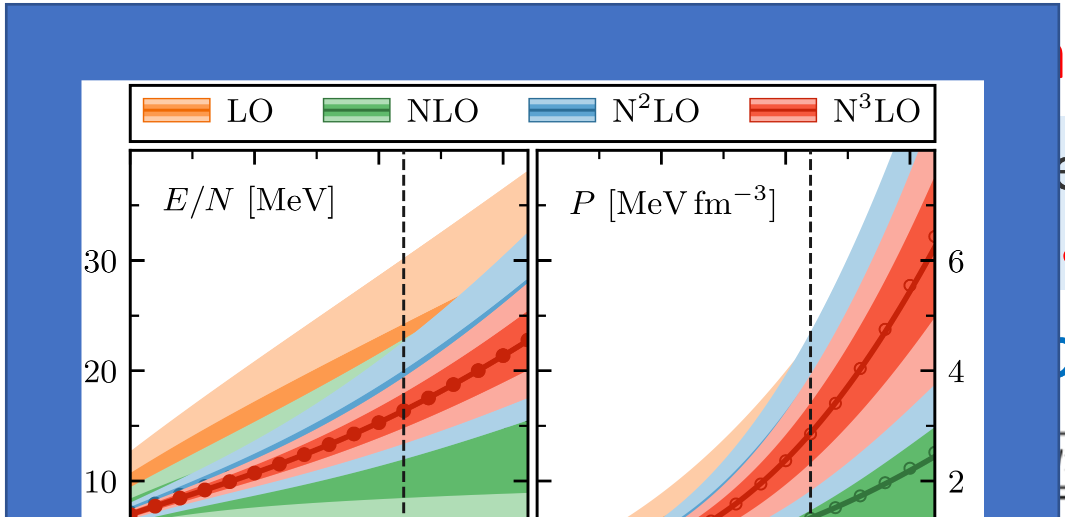
Fig… 034318 (2018)

❑ Formulate *statistical models* for uncertainties

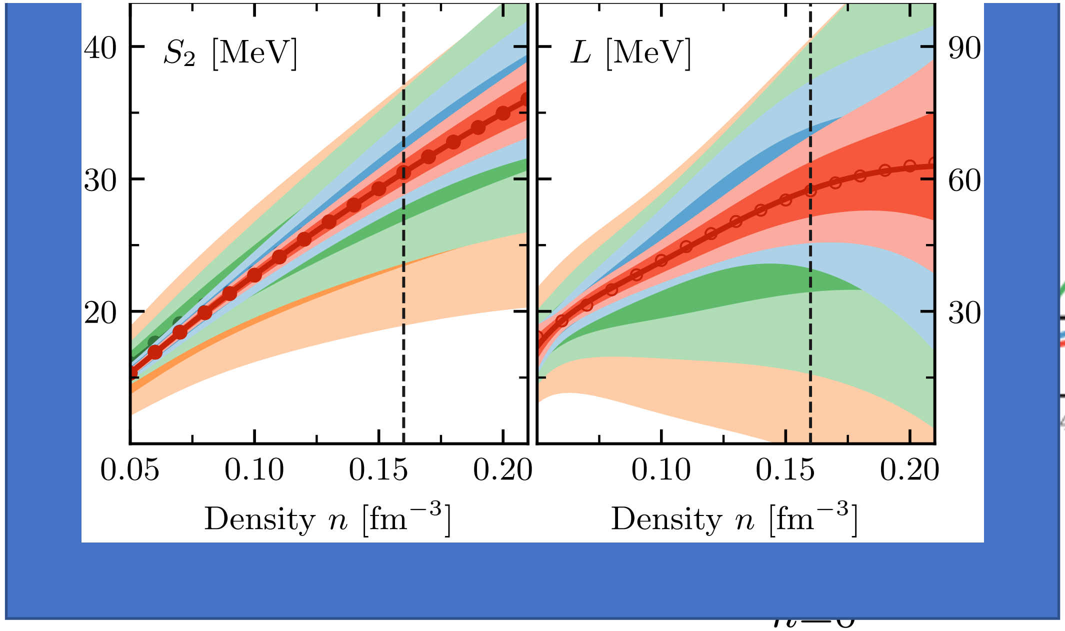
tisticians say any model better than none!

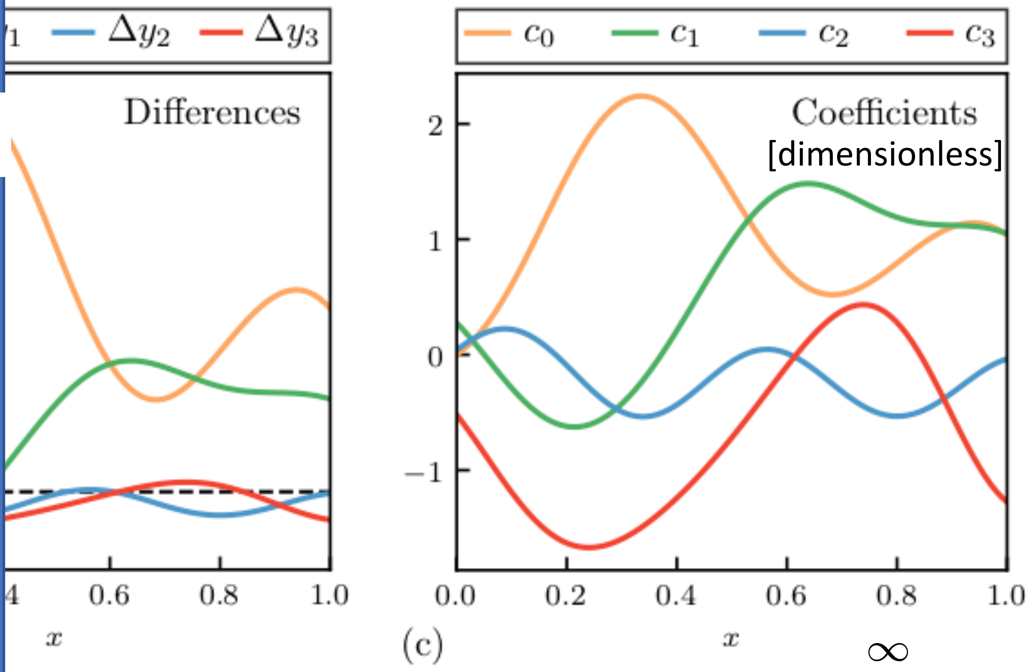
els are wrong, but ~~some~~ models that *know* are wrong, are useful.”

onvergence pattern of observables



❑ Use *model checking* to validate our models





Estimate variance → $\bar{c}$

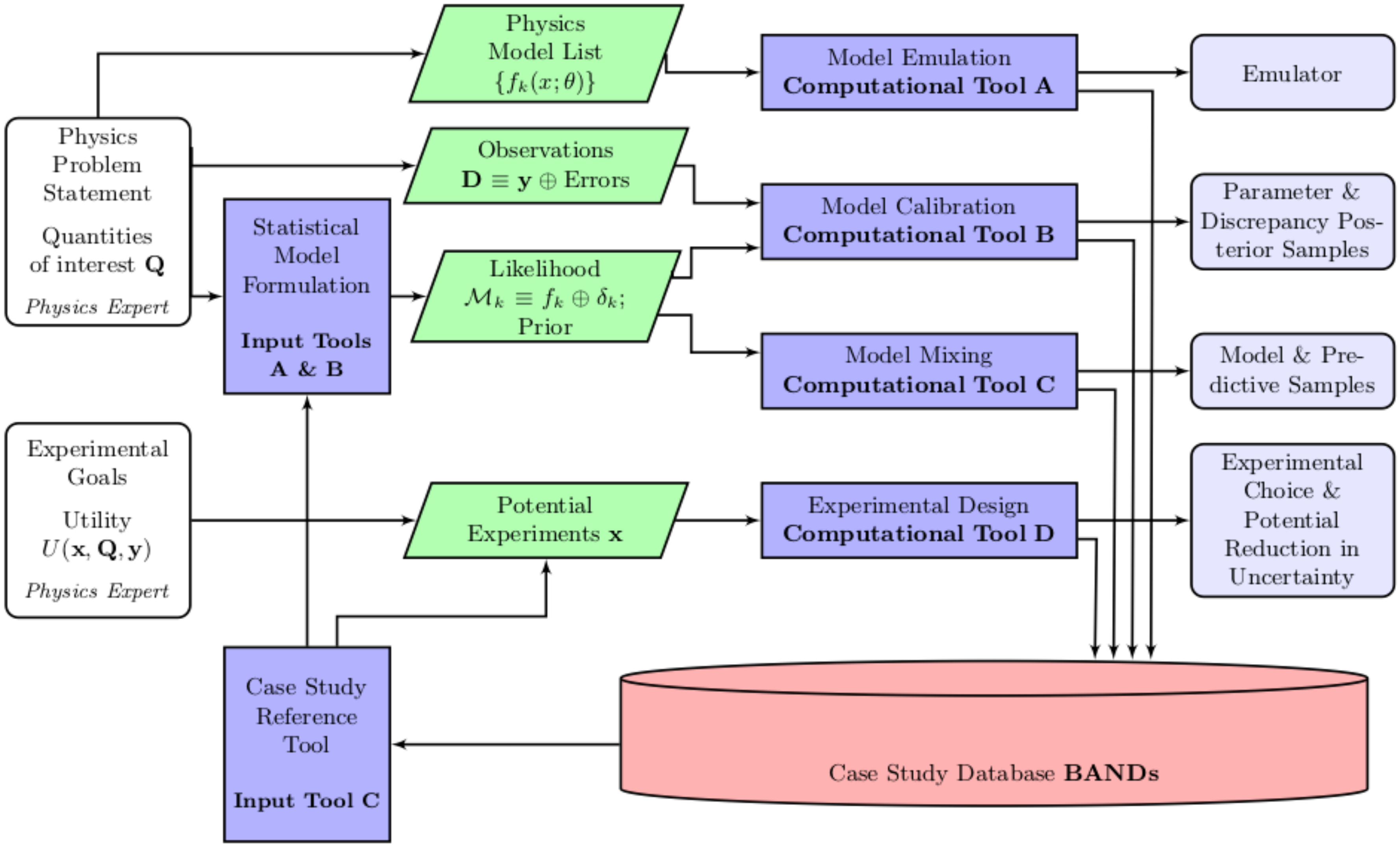
Omitted orders: $\delta \boldsymbol{y}_{\mathrm{th}} = \boldsymbol{y}_{\mathrm{ref}} \sum_{n=k+1}^{\infty} c_n Q^n$

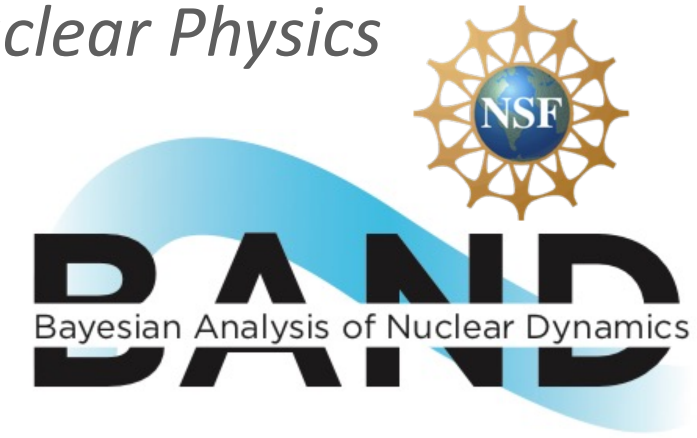
Outline

- Thinking about uncertainty quantification (UQ) for models
- **BAND:** emulators, calibration, model mixing, expt. design
- Outlook: Frontiers of UQ for nuclear models

BAND (Bayesian Analysis of Nuclear Dynamics)

***Goal:** Facilitate principled Uncertainty Quantification in Nuclear Physics*





An NSF CSSI Framework (started 7/2020)

Look to https://bandframework.github.io/ for papers, talks, and software!

BAND (Bayesian Analysis of Nuclear Dynamics)

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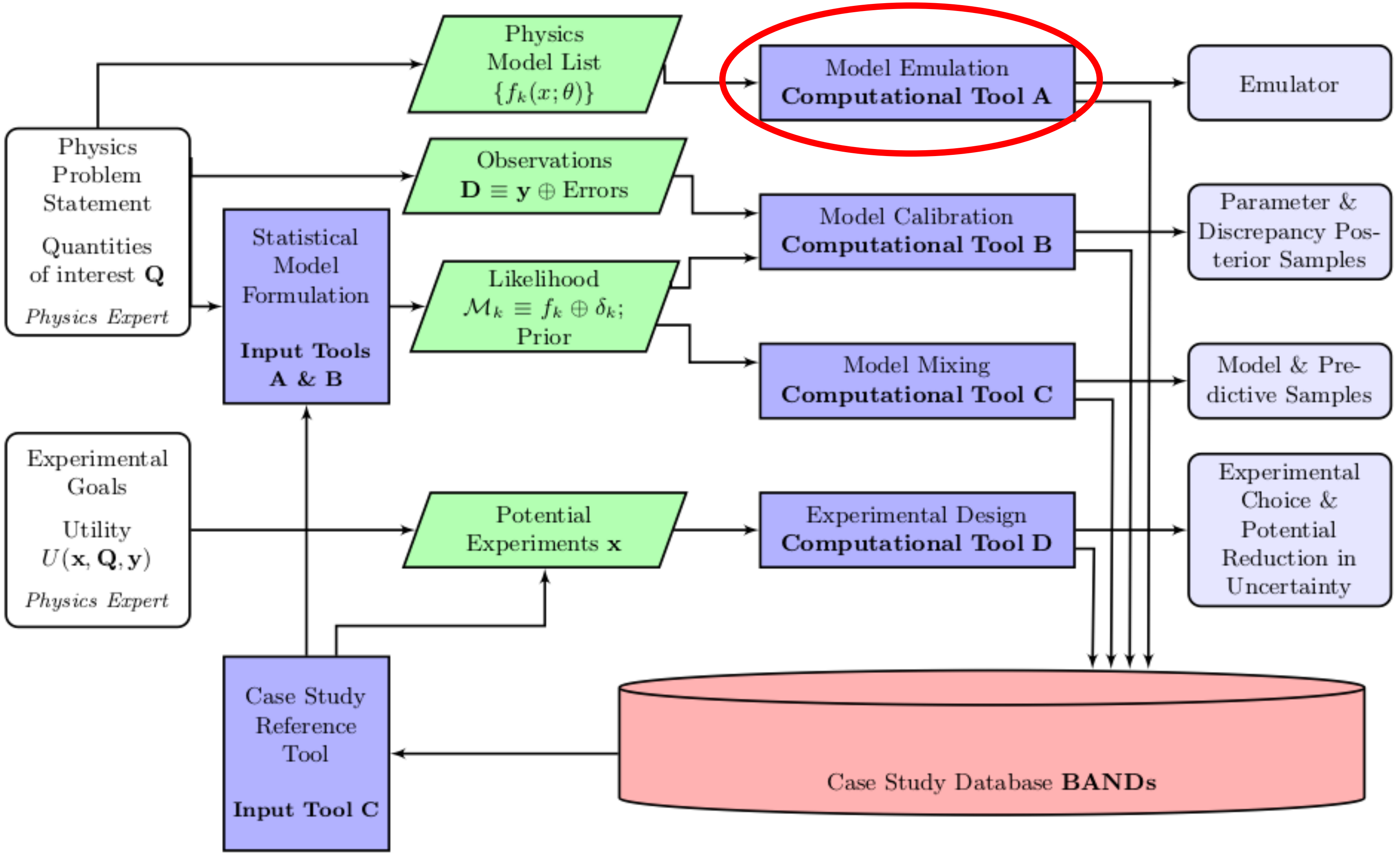
High-fidelity models may be too expensive → use an emulator instead!



Bayesian Analysis of Nuclear Dynamics

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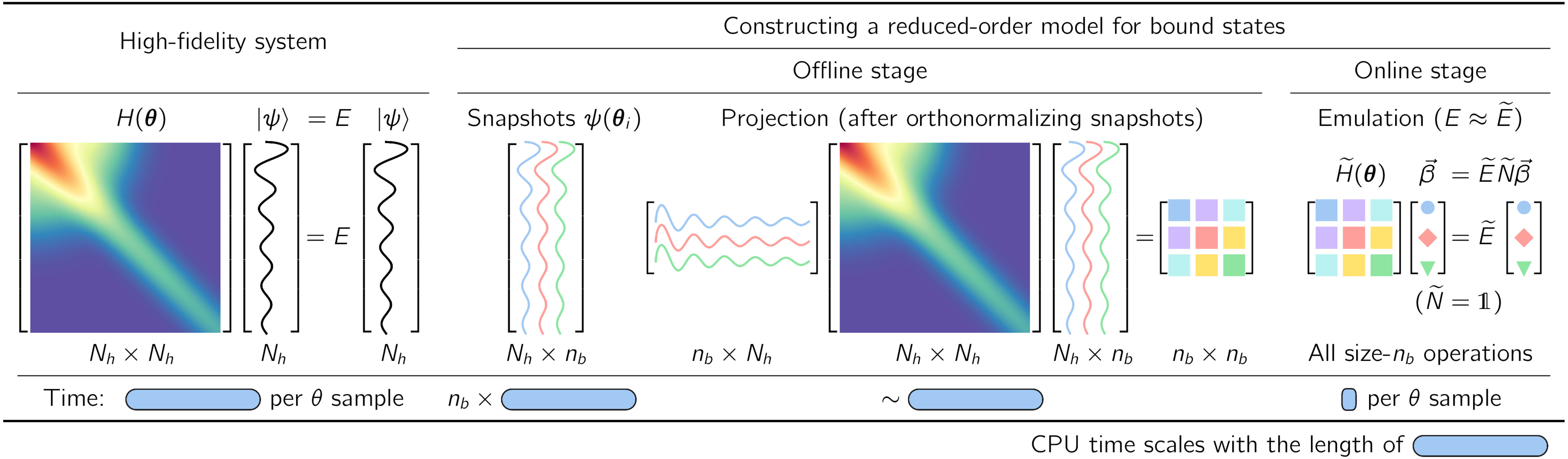
Constructing a reduced-basis model (aka emulator)



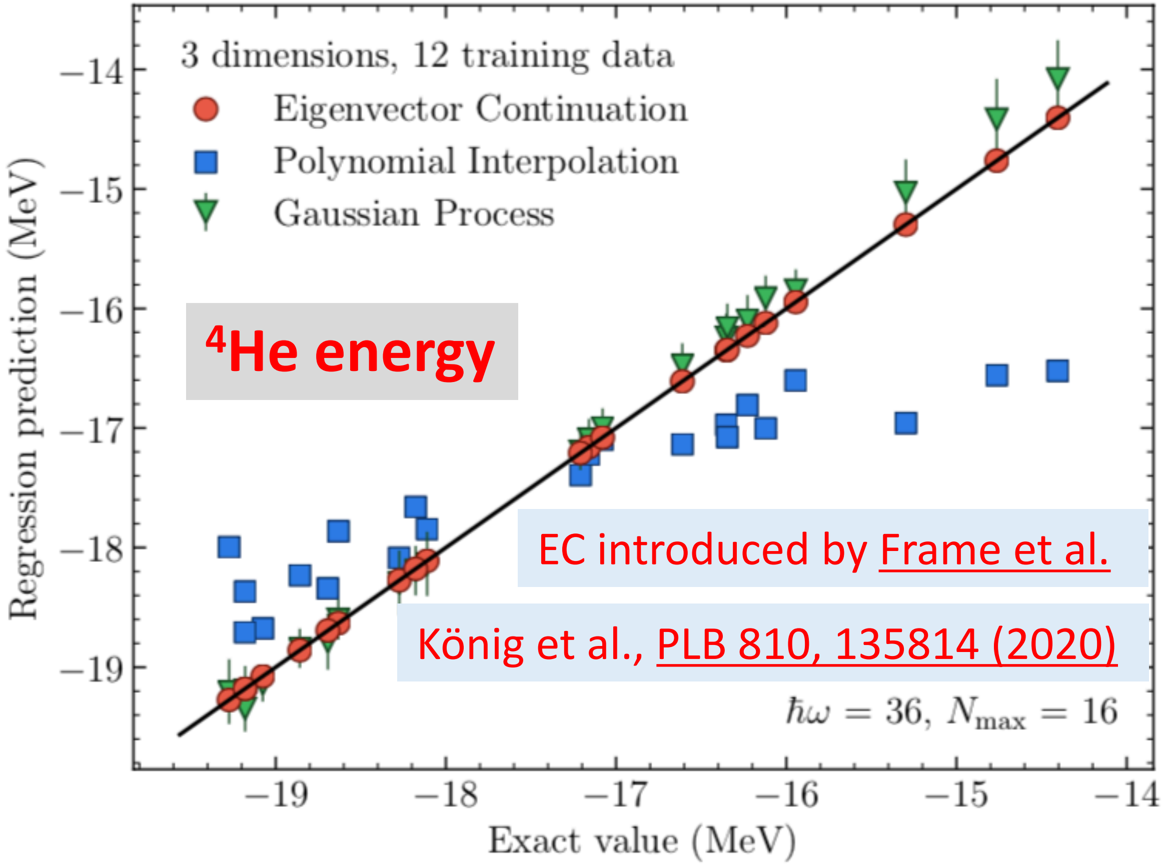
- Offline stage (pre-calculate):
  - Construct basis using snapshots from high-fidelity system (simulator)
  - Project high-fidelity system to small-space using snapshots
- Online stage (emulator):
  - Make many predictions fast & accurately (e.g., for Bayesian analysis)

- *J. A. Melendez et al., J. Phys. G 49, 102001 (2022)*
- *E. Bonilla, P. Giuliani et al., Phys. Rev. C 106, 054322*
- *P. Giuliani, K. Godbey et al., arXiv:2209.13039.*
- *C. Drischler et al., Quarto + arXiv:2212.04912*

Eigenvector continuation emulators for nuclear observables

Basic idea: a small # of ground-state eigenvectors from a selection of parameter sets is an extremely effective variational basis for other parameter sets.

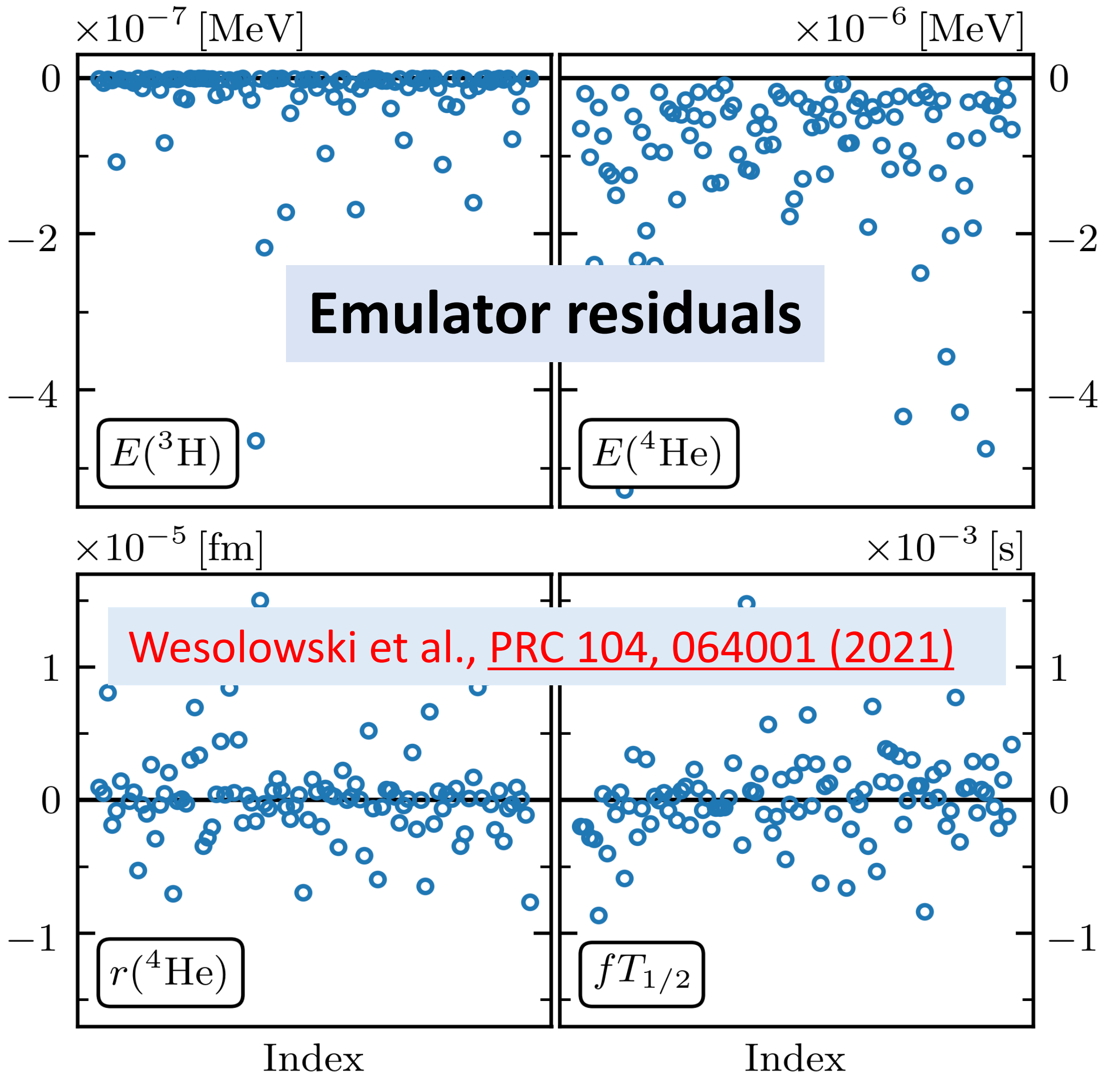
Characteristics: fast and accurate!



^{4}He energy

EC introduced by Frame et al.

König et al., PLB 810, 135814 (2020)



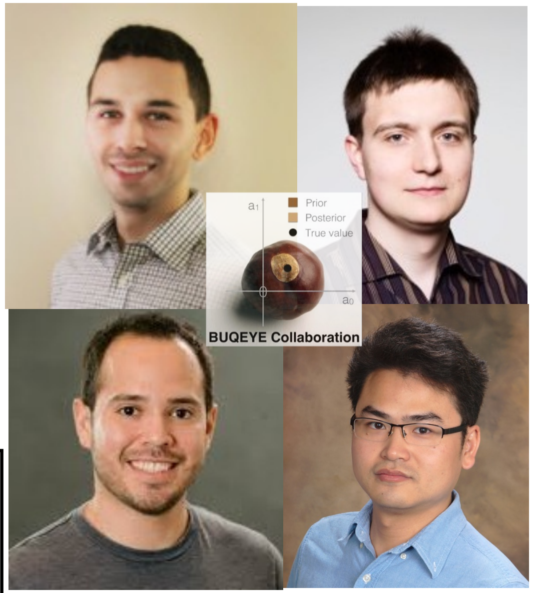
Emulator residuals

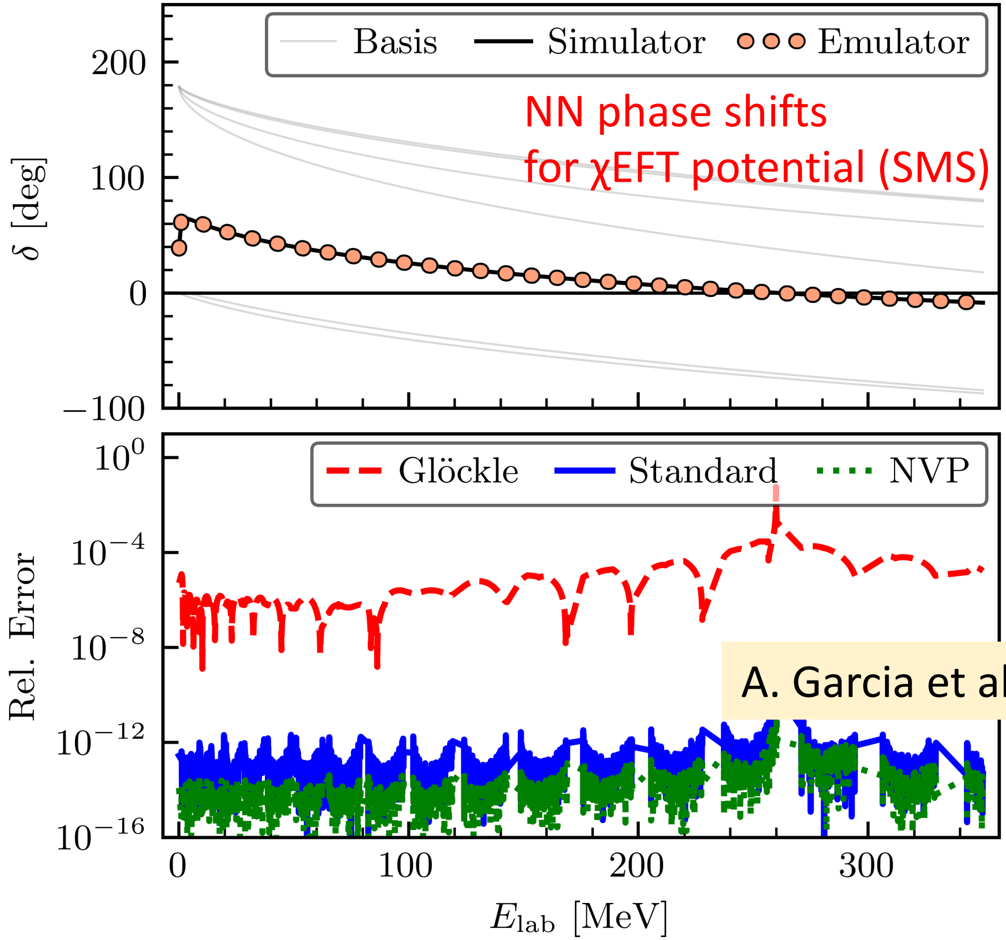
Wesolowski et al., PRC 104, 064001 (2021)

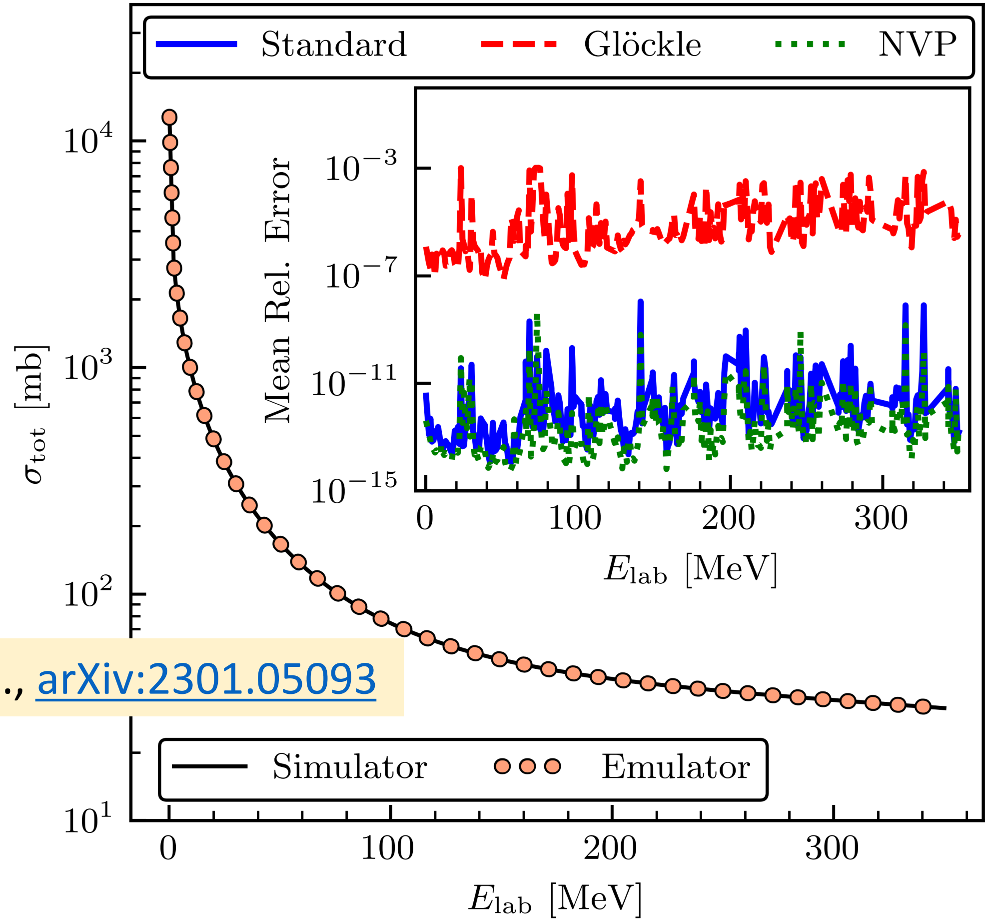
Emulator doesn't require specialized calculations!

RBM emulators for NN and 3N scattering

- NN scattering by rjf et al., PLB (2020) using the Kohn variational principle.
- Improved by Drischler et al., PLB (2021) (e.g., mitigate Kohn anomalies).
- Two-body emulation w/o wfs by Melendez et al., PLB (2021).





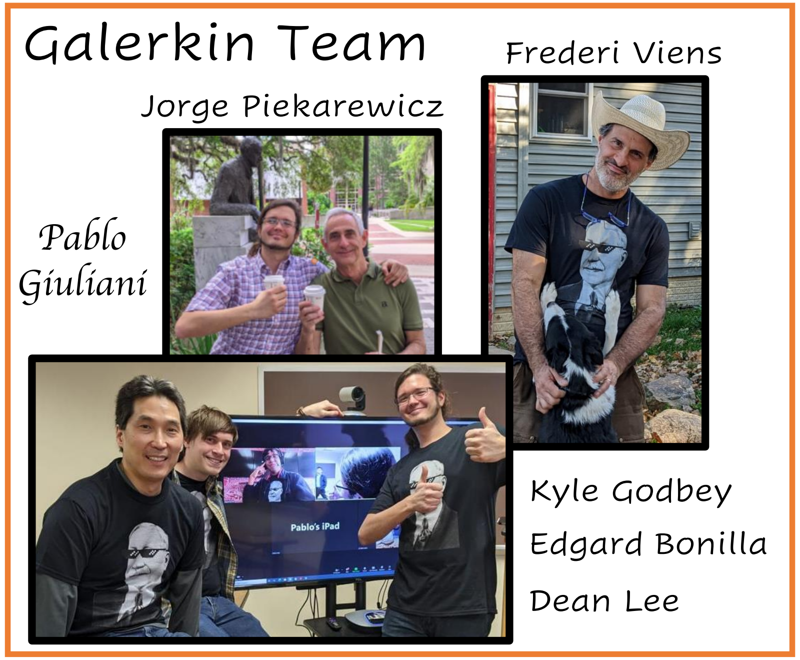


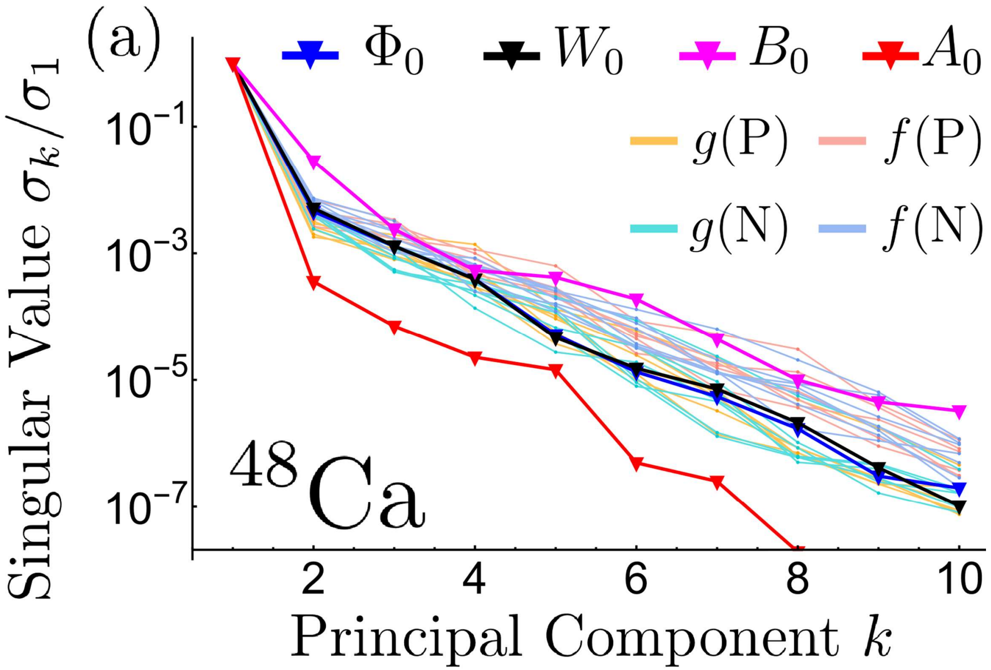
A. Garcia et al., arXiv:2301.05093

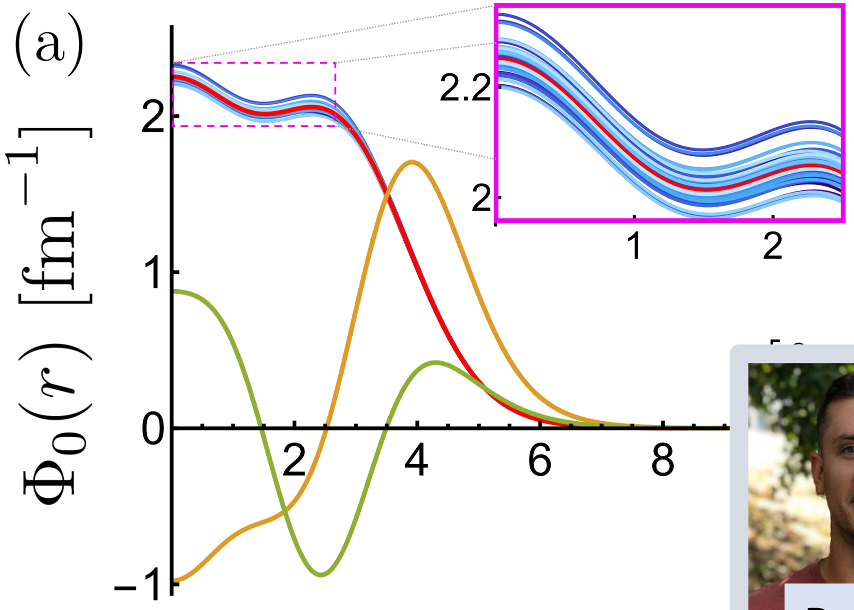
3-body scattering?
E.g, for Bayesian χEFT LEC estimation.
→ X. Zhang, rjf proof of principle (2022).

RBM emulators for EDFs

- Energy density functionals (EDFs) present new challenges.
- P. Giuliani et al., "Bayes goes fast …" (also "Training and Projecting")
  → apply Galerkin RBM to EDFs (covariant mean field, Skyrme)
- Efficient basis to evaluate functional for many parameter sets.
- → Fast and accurate emulation, ideal for Bayesian inference!



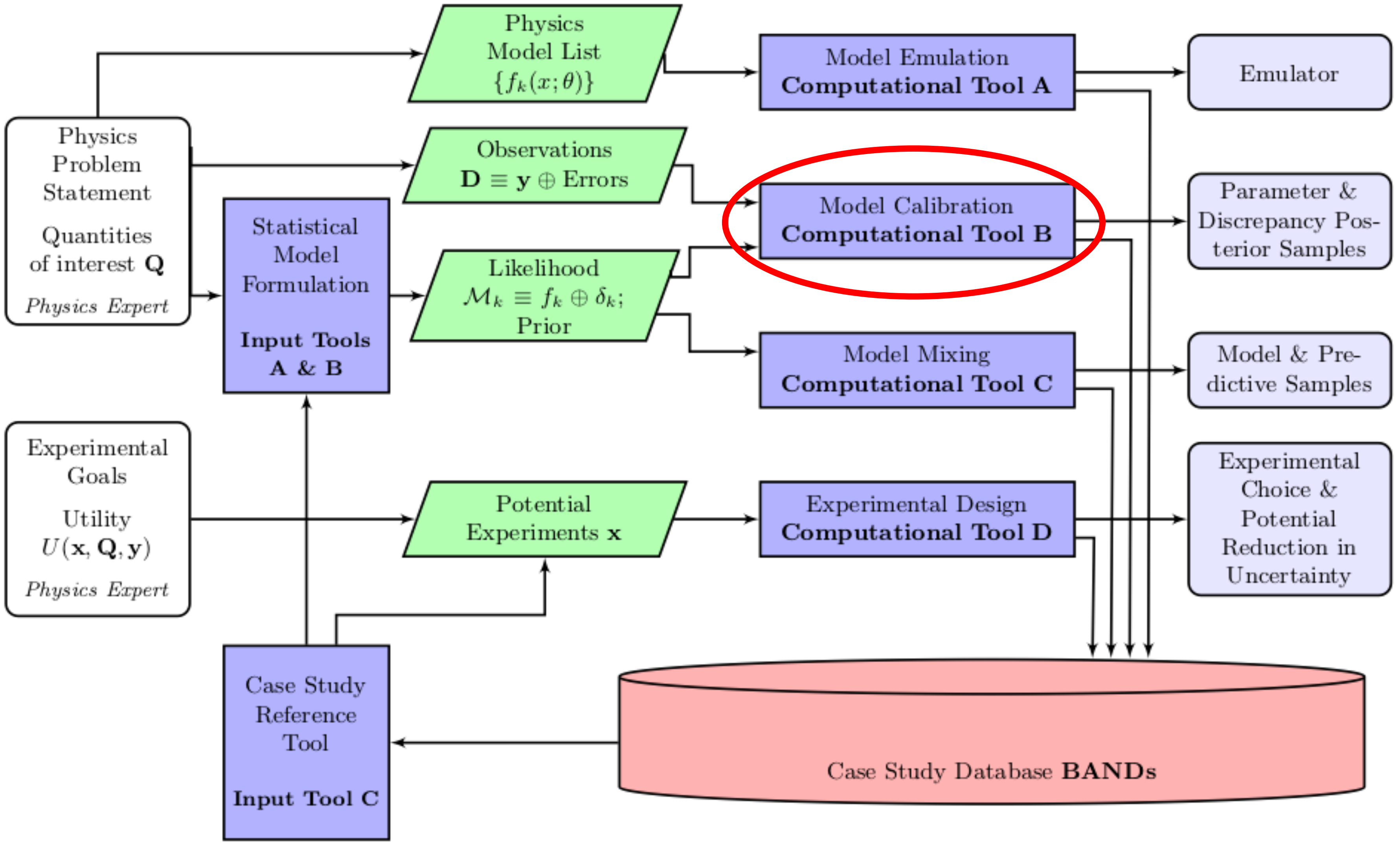




Under development in BAND: ROSE software for non-linear, non-affine problems (e.g., opt. potl.)

BAND (Bayesian Analysis of Nuclear Dynamics)

Calibrating a model means to update distributions of its parameters based on data.

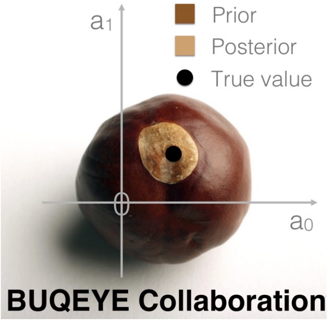


An NSF CSSI Framework (started 7/2020)

Look to https://bandframework.github.io/ for papers, talks, and software!

Rigorous constraints on three-nucleon forces in chiral effective field theory from fast and accurate calculations of few-body observables

Wesolowski, Svensson, Ekström, Forssén, rjf, Melendez, and Phillips, PRC **104**, 064001 (2021)



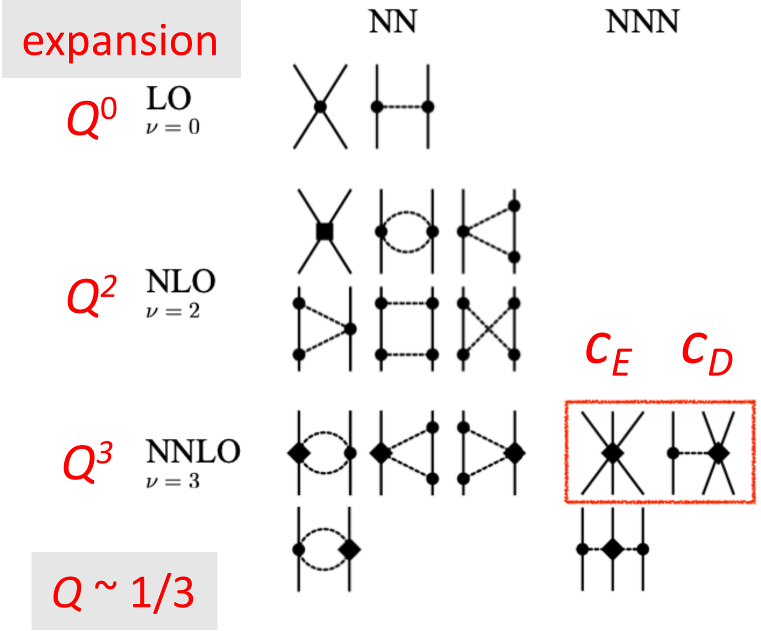
BUQEYE Collaboration

Notebook with all figures at

https://buqeye.github.io

See also: Djärv et al., PRC (2022) on A=6 nuclei; Svensson et al., PRC (2023) on Bayesian LEC estimation; Alnamlah et al., Front. Phys. (2022) on EFT for rotational bands; Acharya et al. Front. Phys. (2022) on E&M observables; Poudel et al., J. Phys. G (2022) on 3He-α scattering; Baker et al., PRC (2022) on N-A, …

Original title: *Fast & rigorous constraints on chiral three-nucleon forces from few-body observables*



Chiral 3N forces: estimate constraints on c_D and c_E

Few-body observables (cf. other possibilities):

^{3}H ground-state energy; ^{3}H β-decay half-life;
^{4}He ground-state energy; ^{4}He charge radius

Rigorous: statistical best practices for parameter estimation

Fast: uses eigenvector continuation emulators for observables

Full Bayesian approach to calibration parameters

Experimental data

Other info (EFT scheme/scale, etc.)

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 \,|\, \mathbf{y}_{\mathrm{exp}}, I) \propto \mathrm{pr}(\mathbf{y}_{\mathrm{exp}} \,|\, \vec{a}, \Sigma, I)\, \underbrace{\mathrm{pr}(\vec{a}\,|\,I)\;\; \mathrm{pr}(\bar{c}^2\,|\,Q, \vec{a}, I)\;\; \mathrm{pr}(Q\,|\,\vec{a}, I)}_{\text{Individual posteriors; everything has priors!}}$$

NN *and* 3N LECs

EFT expansion parameter

Truncation error variance

All experiment and theory errors

Likelihood: $\mathrm{pr}(\mathbf{y}_{\mathrm{exp}} \,|\, \vec{a}, \Sigma, I) \sim \mathcal{N}(\mathbf{y}_{\mathrm{th}}(\vec{a}),\; \Sigma_{\mathrm{exp}} + \Sigma_{\mathrm{method}} + \Sigma_{\mathrm{th}})$

Uses NNLO chiral EFT without Δ’s based on Carlsson et al. PRX **6**, 011019 (2016), but methods are general (other regulators, Δ’s, other observables)

Sample pdf with MCMC over 15 dimensions (11 NN LECs + c_D, c_E + Q, $\bar{c}^2$)
→ marginalize (integrate out) what you are not considering (trivial!)

Full Bayesian approach to calibration parameters

Experimental data

Other info (EFT scheme/scale, etc.)

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 | \mathbf{y}_{\mathrm{exp}}, I) \propto \mathrm{pr}(\mathbf{y}_{\mathrm{exp}} | \vec{a}, \Sigma, I) \underbrace{\mathrm{pr}(\vec{a}|I)\ \mathrm{pr}(\bar{c}^2 | Q, \vec{a}, I)\ \mathrm{pr}(Q|\vec{a}, I)}_{\text{Individual posteriors: everything has priors!}}$$

NN *and* 3N LECs

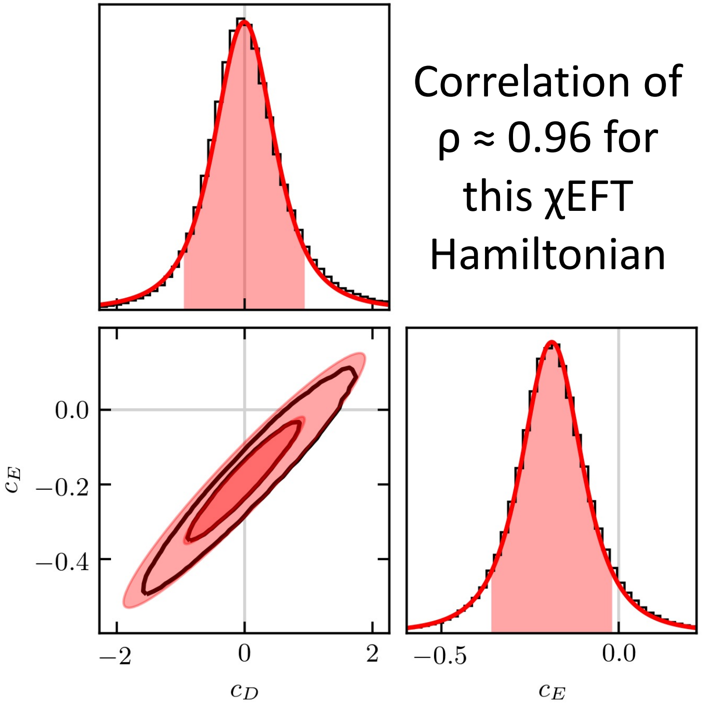
EFT expansion

Truncation

- ☑ Interact with the experts (i.e., statisticians, applied mathematicians)
- ☑ Incorporate all sources of experimental and *theoretical* errors
- ☑ Formulate *statistical models* for uncertainties
- ☑ Use as informative priors as is reasonable; test sensitivity to priors
- ☑ Account for correlations in inputs (type x) and observables (type y)
- ☑ Propagate uncertainties through the calculation
- ☑ Use *model checking* to validate our models

Posteriors from "*Fast & Rigorous*" [PRC 104, 064001 (2021)]

Posterior for c_D and c_E



Correlation of $\rho \approx 0.96$ for this χEFT Hamiltonian

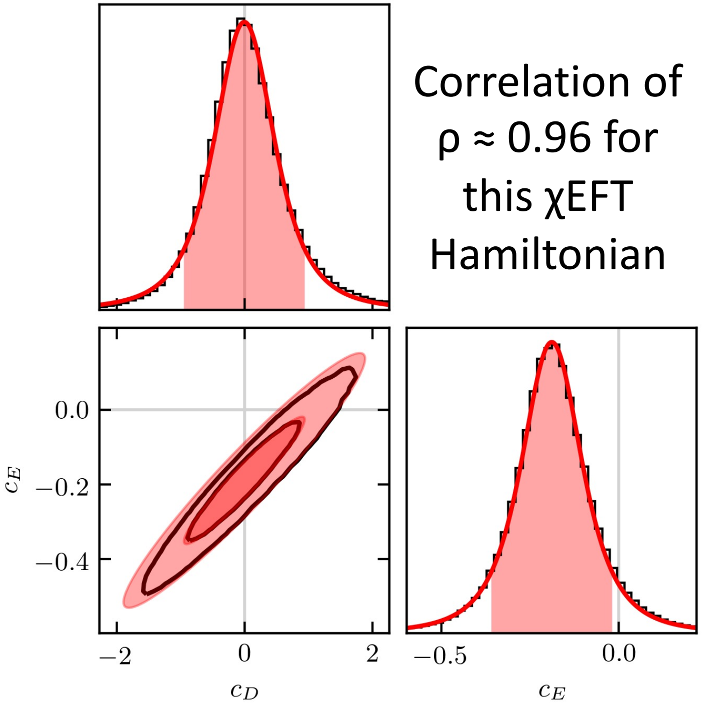
Tails are *not* well approximated by a Gaussian! (But do look like t's!)

Sample pdf with MCMC over 11 NN LECs + c_D, c_E + Q, $\bar{c}^2$ → marginalize (integrate out) what you are not considering

How do student t distributions arise?

Link to blog page
Link to D. Bailey

Posterior for c_D and c_E



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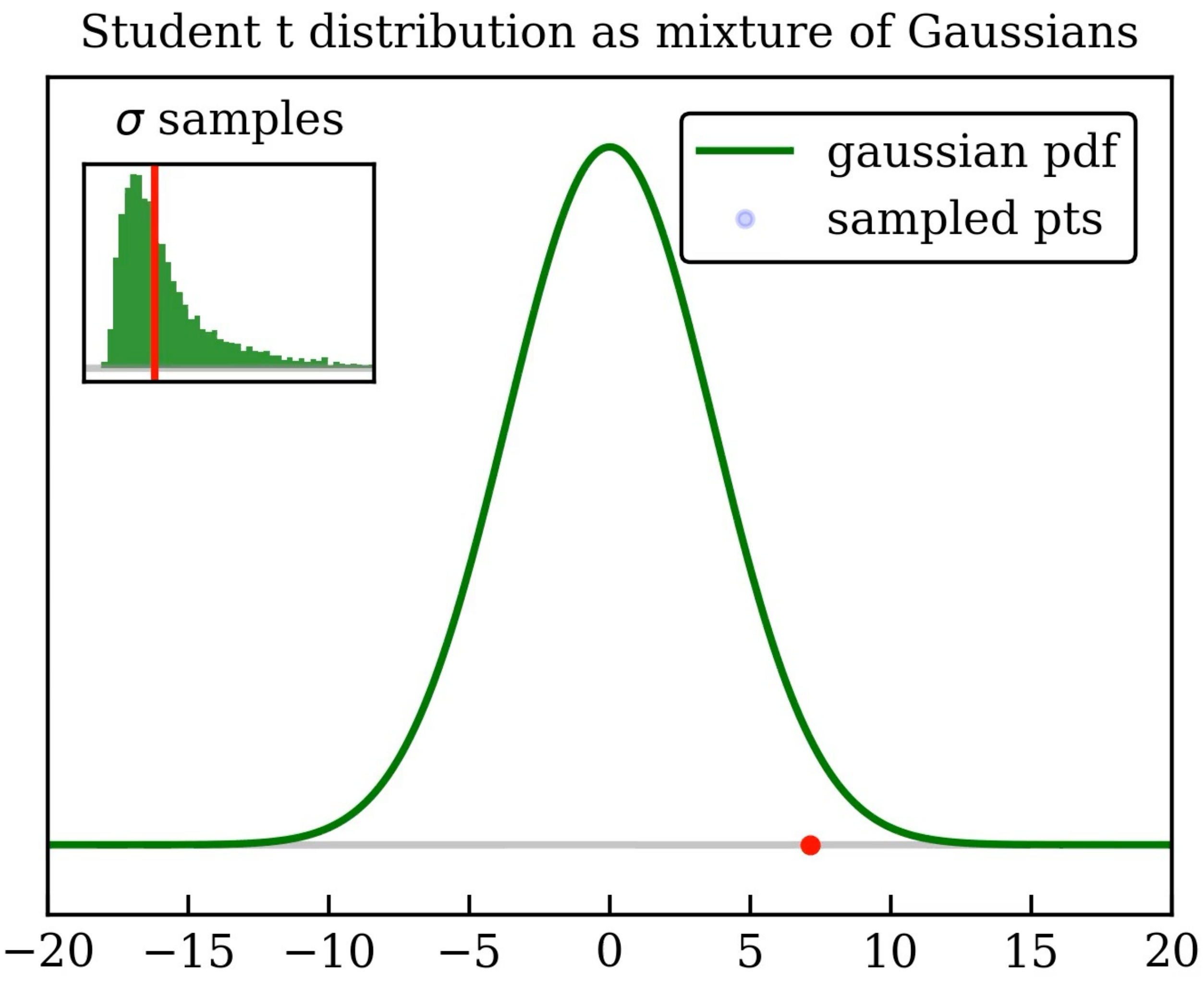
See appendix A of arXiv:2104.04441



Sample pdf with MCMC over 11 NN LECs + c_D, c_E + Q, $\bar{c}^2$ → marginalize (integrate out) what you are not considering

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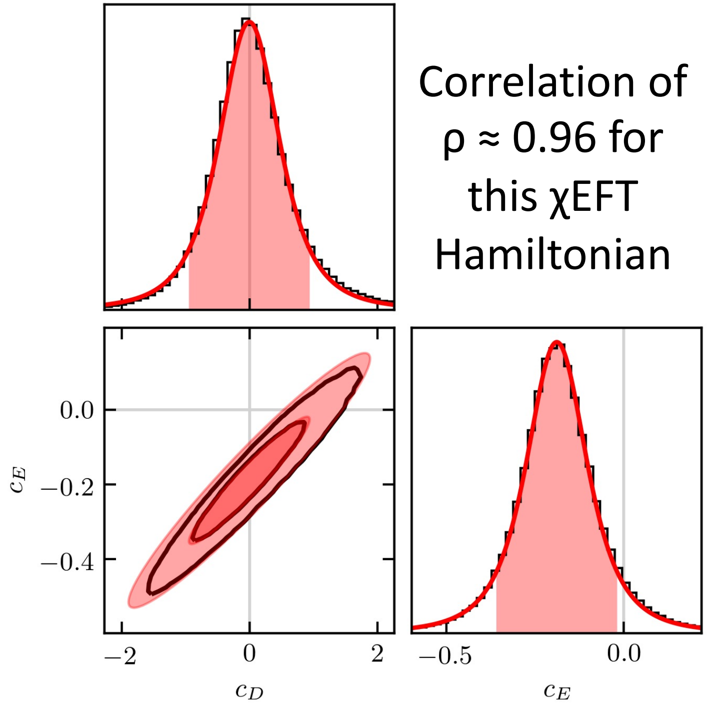
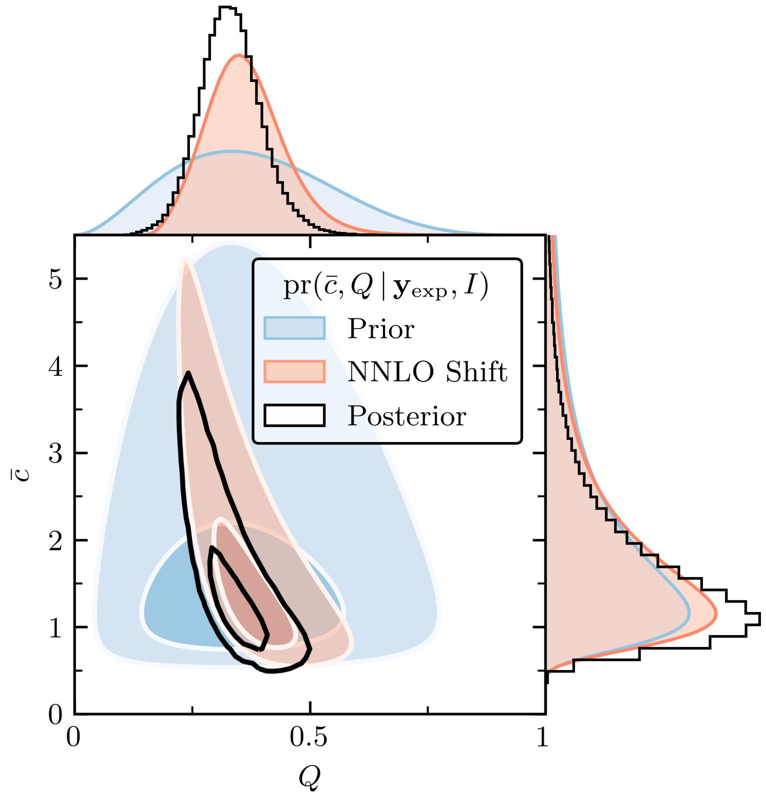
Posterior for c_D and c_E



Correlation of ρ ≈ 0.96 for this χEFT Hamiltonian

Tails are *not* well approximated by a Gaussian! (But do look like t's!)

Posterior for Q and $\bar{c}$



Truncation error for observables:

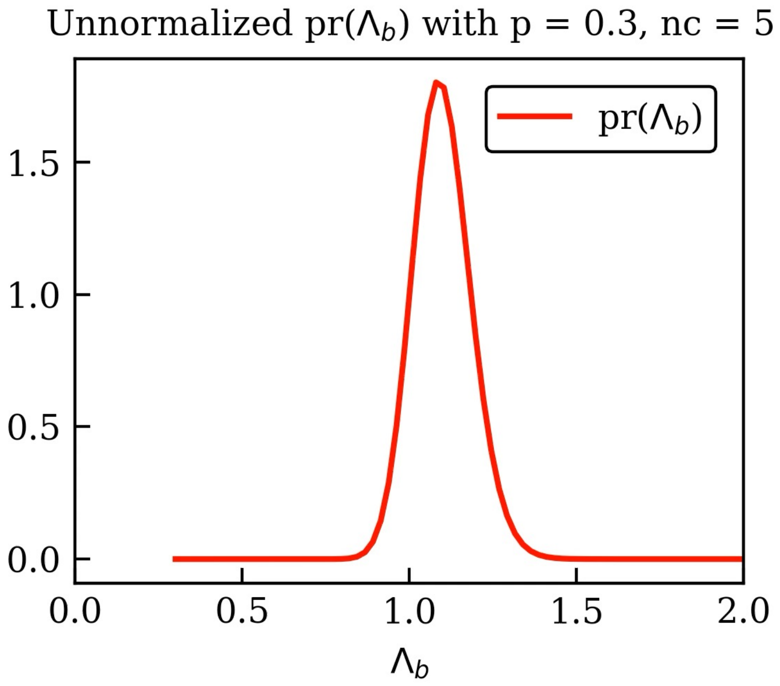
$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 | \mathbf{y}_{\rm exp}, I) \ , \qquad y_{\rm k} = y_{\rm ref} \sum_{n=1}^{k} c_n Q^k \ , \quad \bar{c}^2 \text{ variance for } c_n\text{'s}$$

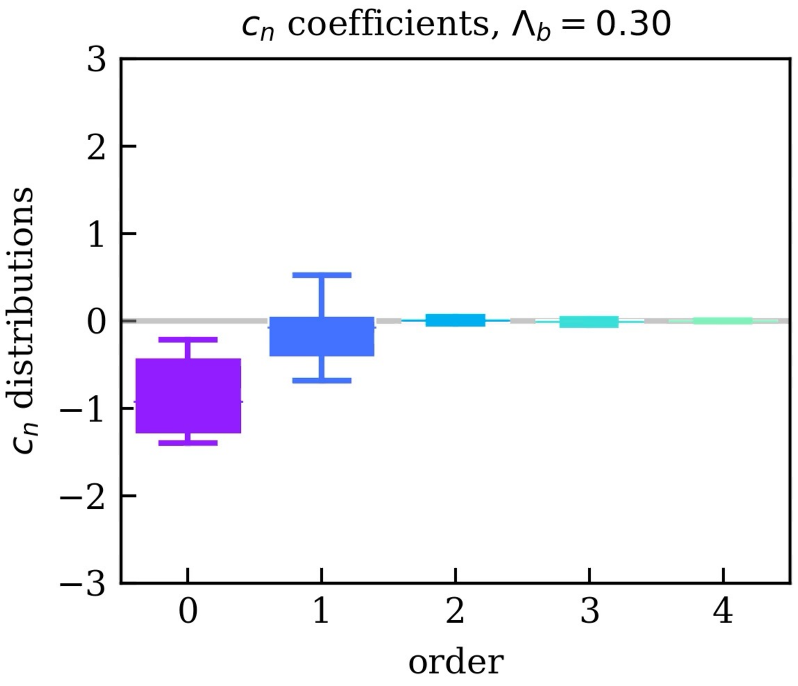
Sample pdf with MCMC over 11 NN LECs + c_D, c_E + Q, $\bar{c}^2$ → marginalize (integrate out) what you are not considering

Limits of EFTs: Learning the expansion parameter

Model: $y_k = y_{\rm ref} \sum_{n=0}^{k} c_n Q^n$

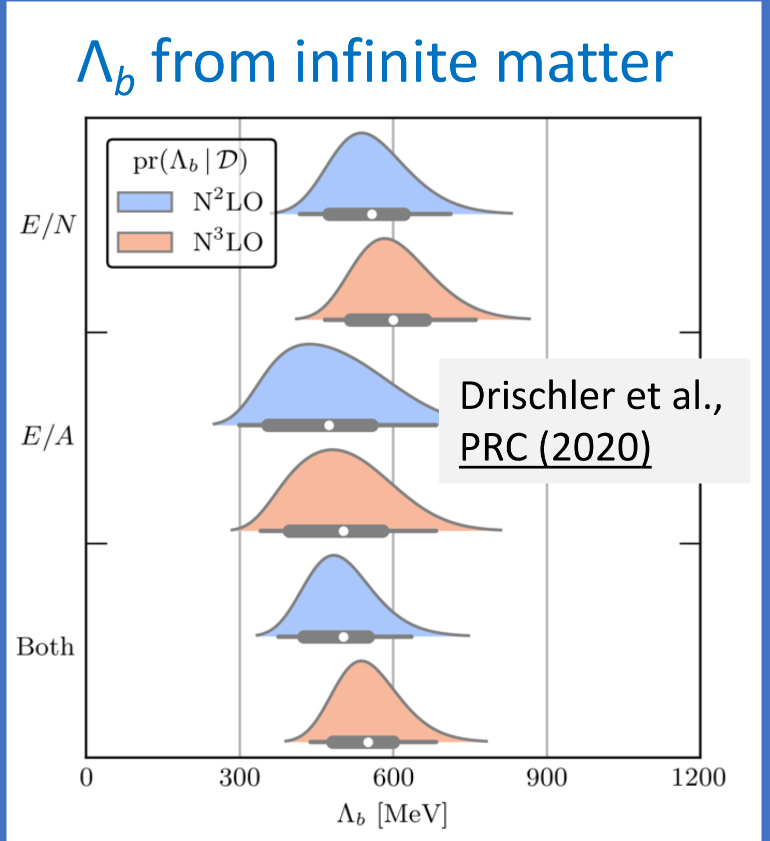
Expectation: $\chi\mathrm{EFT} \Rightarrow Q = \dfrac{\{p, m_\pi\}}{\Lambda_b}, \quad \Lambda_b \approx 600\,\mathrm{MeV}$





Melendez et al. (2019):

$$\mathrm{pr}(\Lambda_b | \{y_n\}, y_{\rm ref}) \propto \frac{\mathrm{pr}(\Lambda_b)}{\tau^\nu \prod_n Q^n}$$

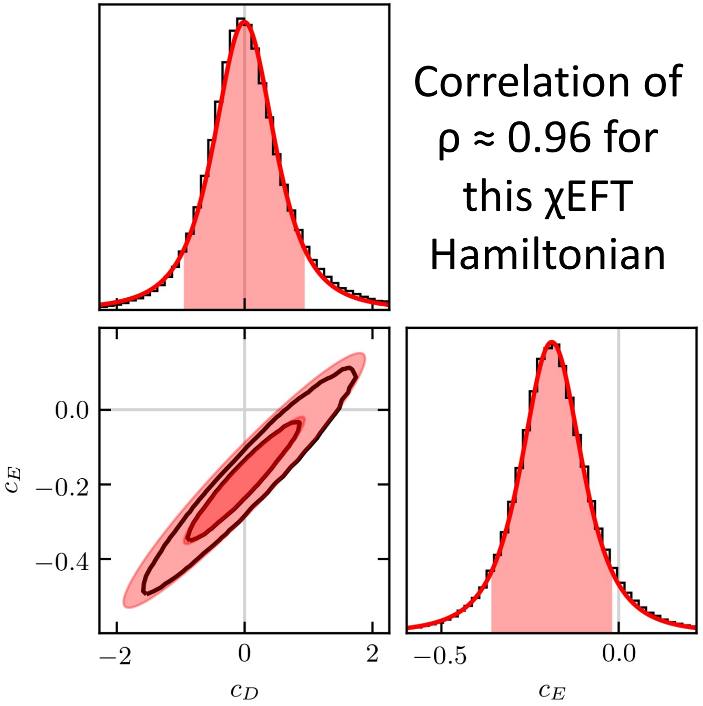


Drischler et al., PRC (2020)

Posteriors from "*Fast & Rigorous*" [PRC 104, 064001 (2021)]

❑ Propagate uncertainties through the calculation

Posterior for c_D and c_E



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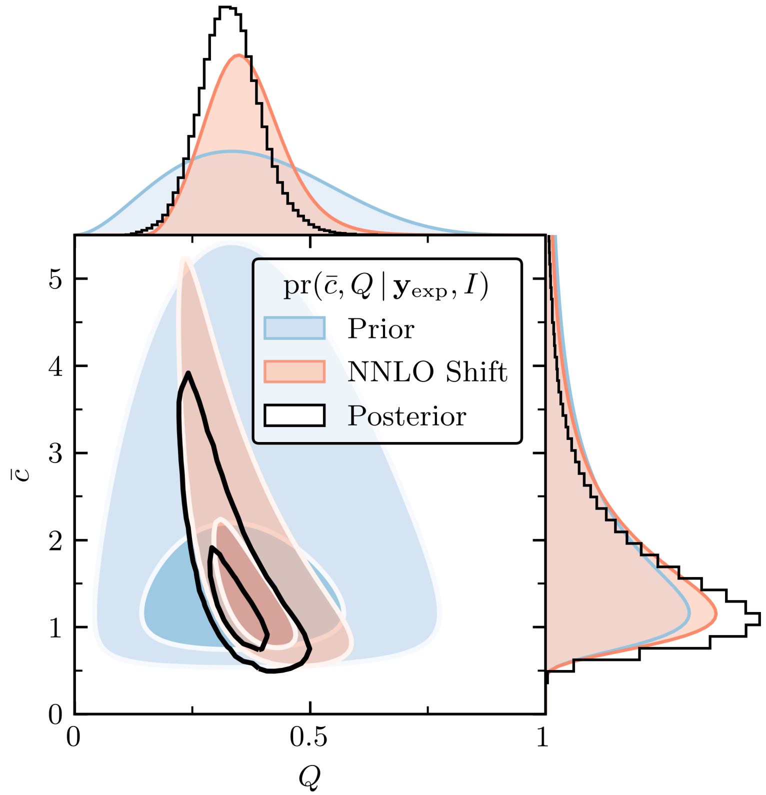
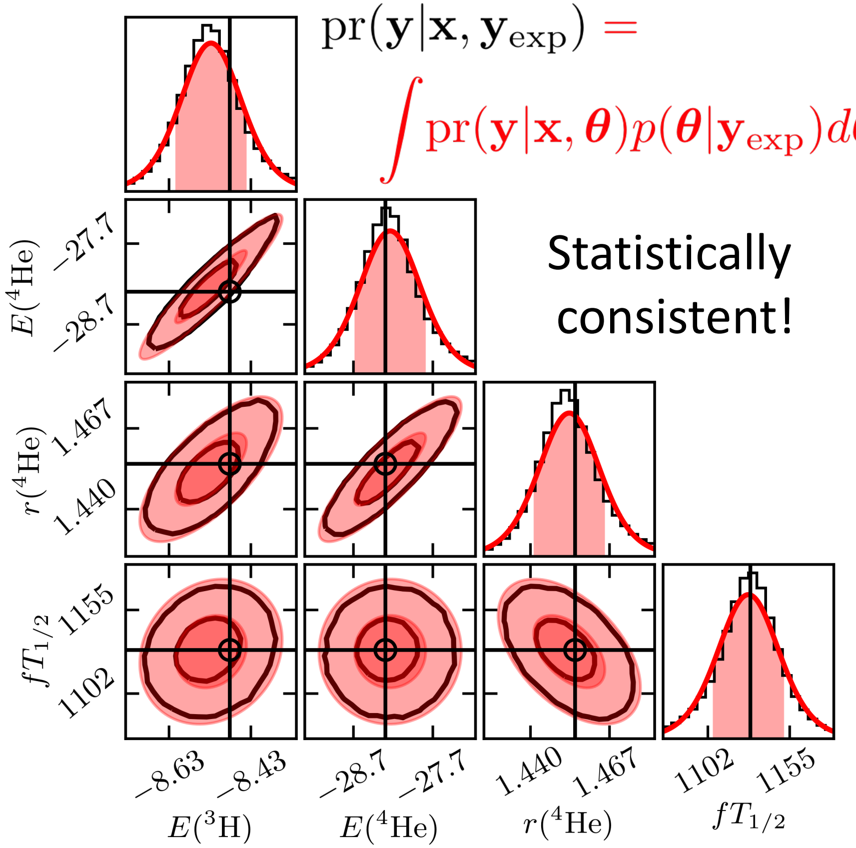
Posterior for Q and $\bar{c}$



Posterior predictive distribution



$$\mathrm{pr}(\mathbf{y}|\mathbf{x}, \mathbf{y}_{\mathrm{exp}}) = \int \mathrm{pr}(\mathbf{y}|\mathbf{x}, \boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathbf{y}_{\mathrm{exp}}) d\boldsymbol{\theta}$$

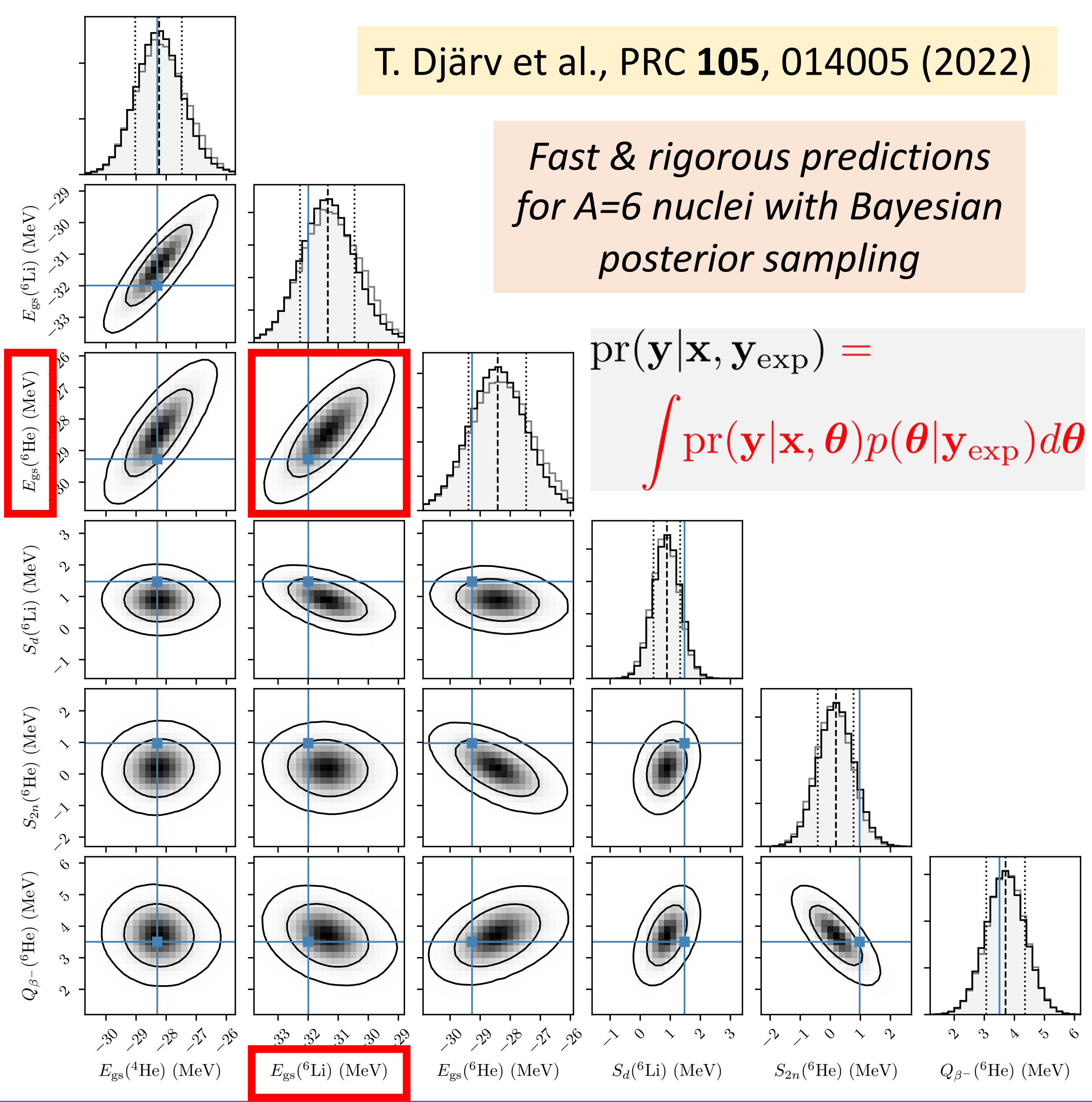
Statistically consistent!

Truncation error for observables:

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 | \mathbf{y}_{\mathrm{exp}}, I) \;, \qquad y_{\mathrm{k}} = y_{\mathrm{ref}} \sum_{n=1}^{k} c_n Q^k \;, \qquad \bar{c}^2 \text{ variance for } c_n\text{'s}$$

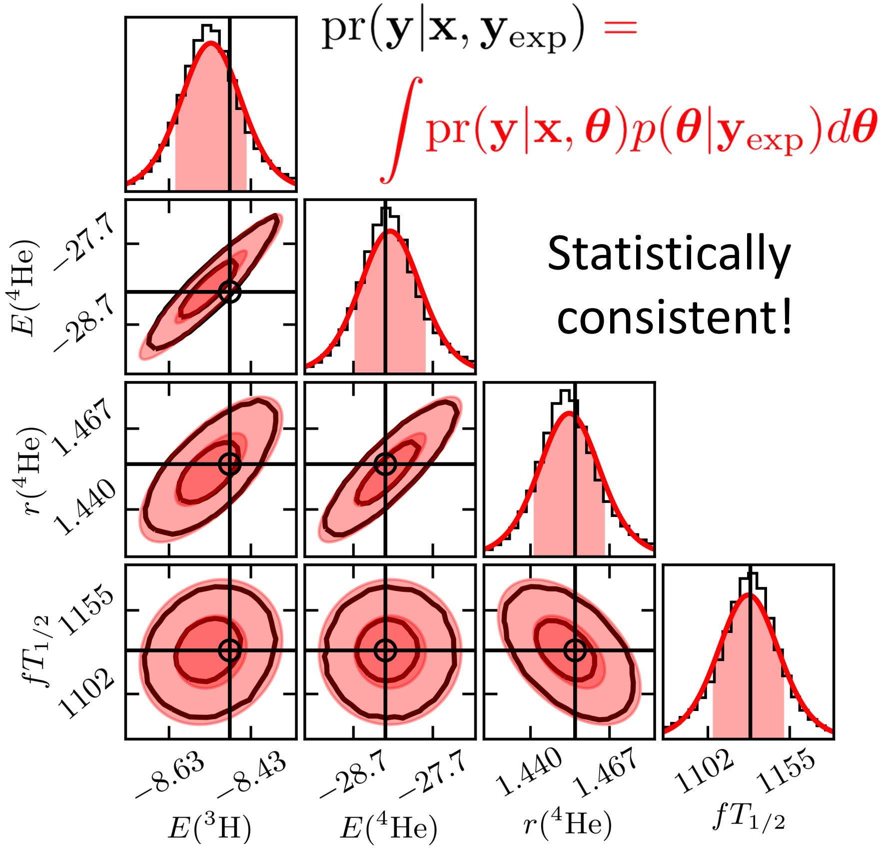
Sample pdf with MCMC over 11 NN LECs + c_D, c_E + Q, $\bar{c}^2$ → marginalize (integrate out) what you are not considering

ous” [PRC 104, 064001 (2021)]



- Propagate uncertainties through the calculation

Posterior predictive distribution



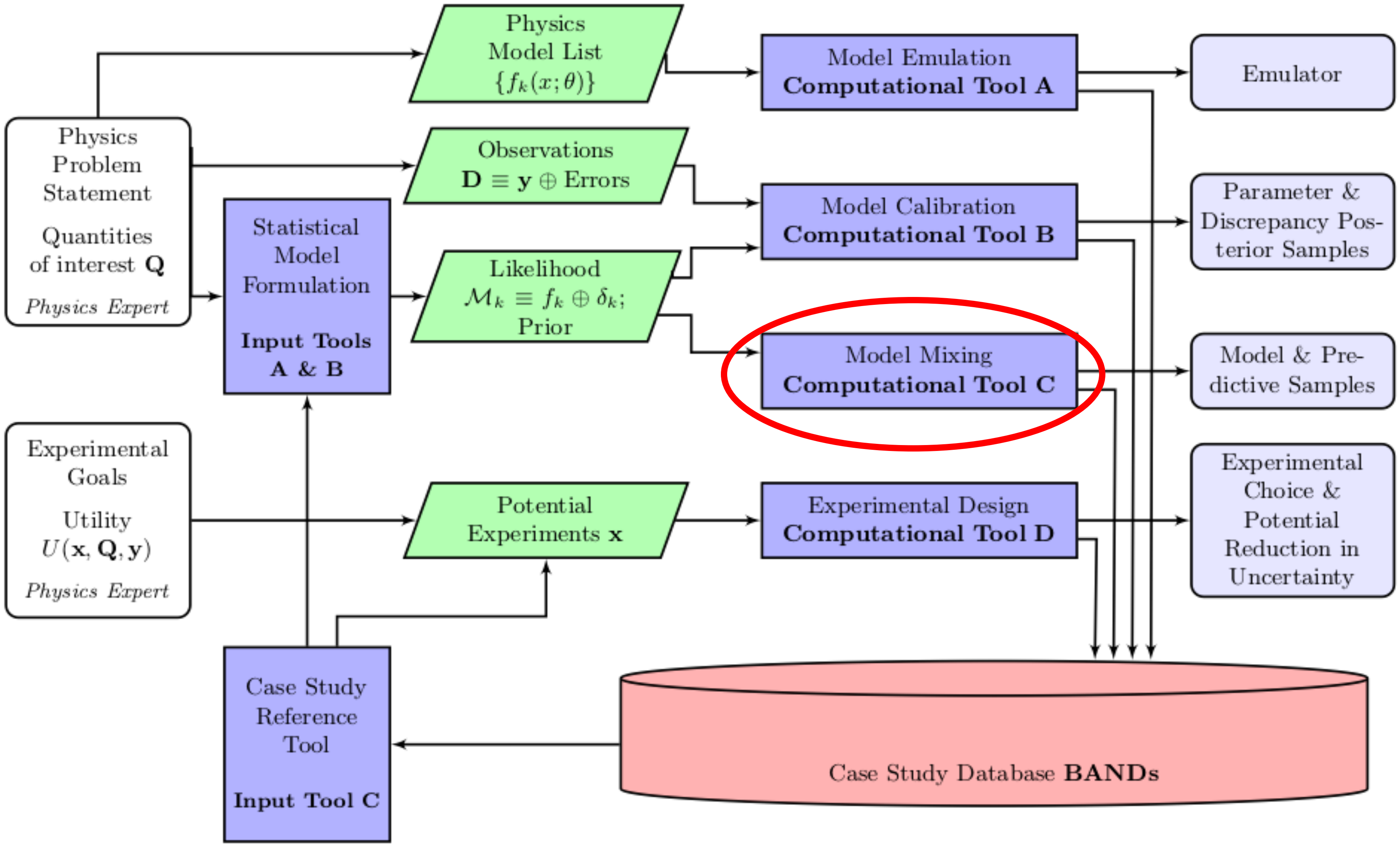
ples:

, $\bar{c}^2$ variance for c_n's

S alize (integrate out) what you are not considering

BAND (Bayesian Analysis of Nuclear Dynamics)

Multiple models predict an observable: how to combine for the *best* prediction?



An NSF CSSI Framework (started 7/2020)

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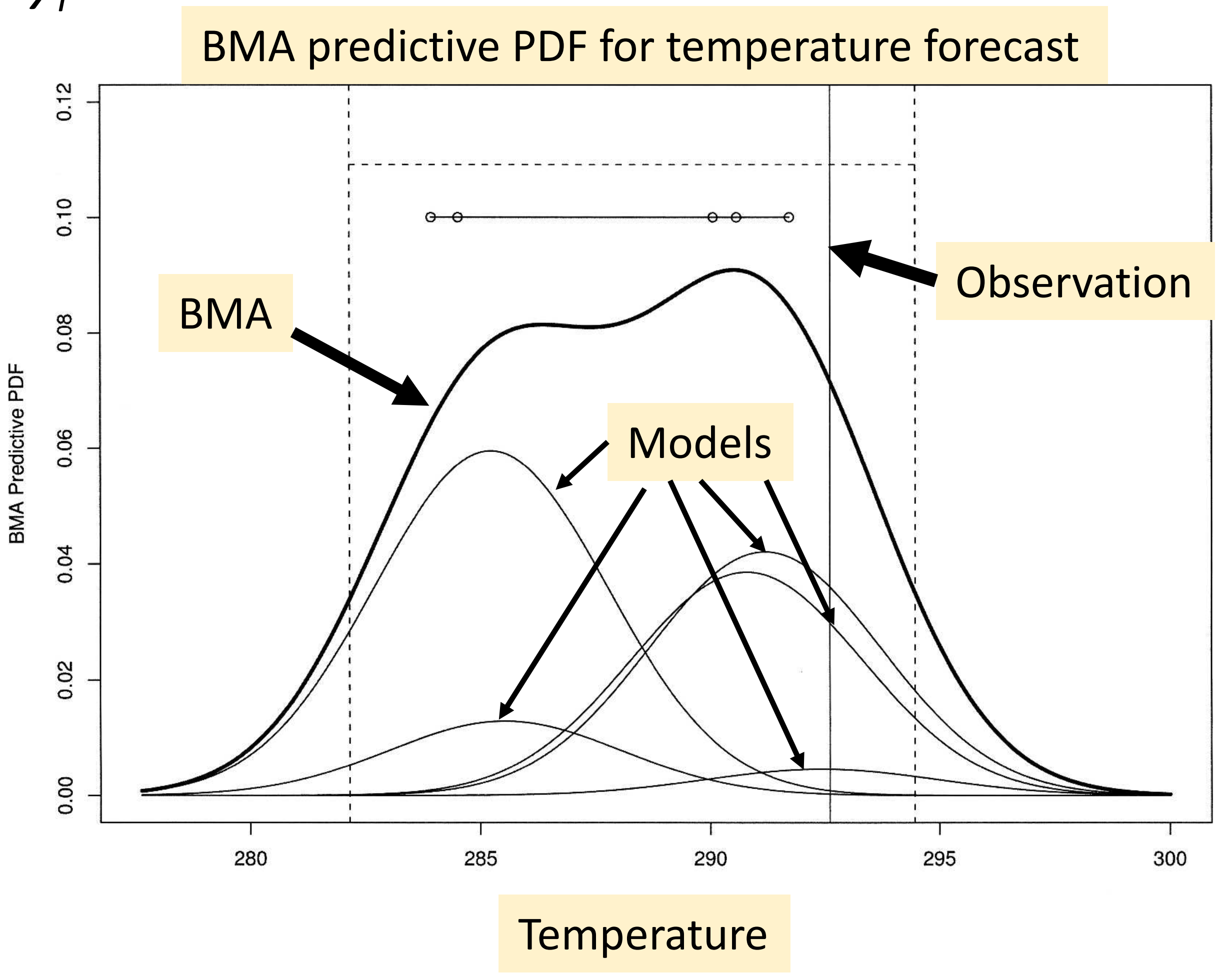
Bayesian model mixing → BMA

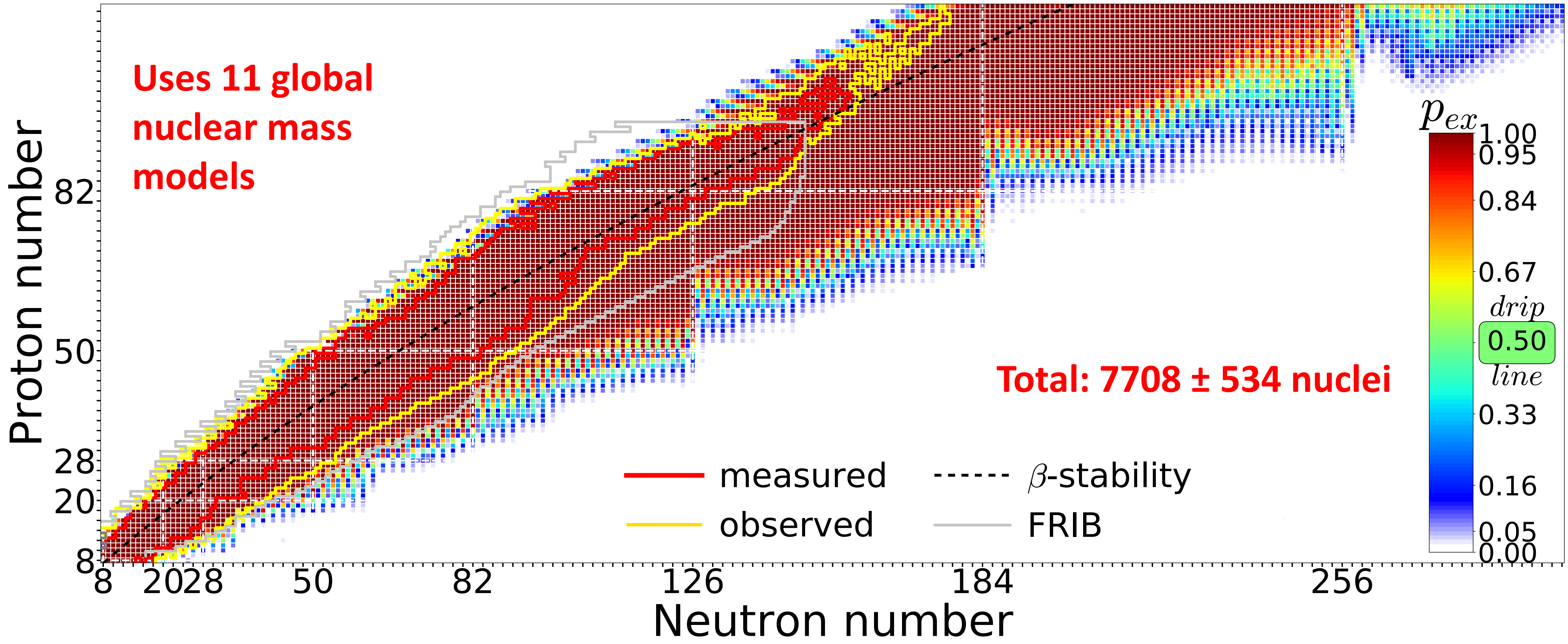
- General: K models $\mathcal{M}_k, (k = 1, \ldots, K)$
- Specify a model by predictions for observations y_i at points x_i → $\mathcal{M}_k : y_i = f_k(x_i) + \varepsilon_{i,k}$
- Predictions at new input points:

$$\mathrm{pr}(\tilde{y}|\tilde{x}) = \sum_{k=1}^{K} \hat{w}_k \mathrm{pr}(\tilde{y}|\tilde{x}, \mathcal{M}_k)$$

- Bayesian Model Averaging (BMA) has constant weights $\hat{w}_k$, determined by predictive power.
- Improves predictive performance in weather forecasting [Raftery et al., (2005)]



Limits of the nuclear landscape: Bayesian model averaging (BMA)



L. Neufcourt et al., Phys. Rev. C **101**, 014319 (2020); arXiv:2001.05924

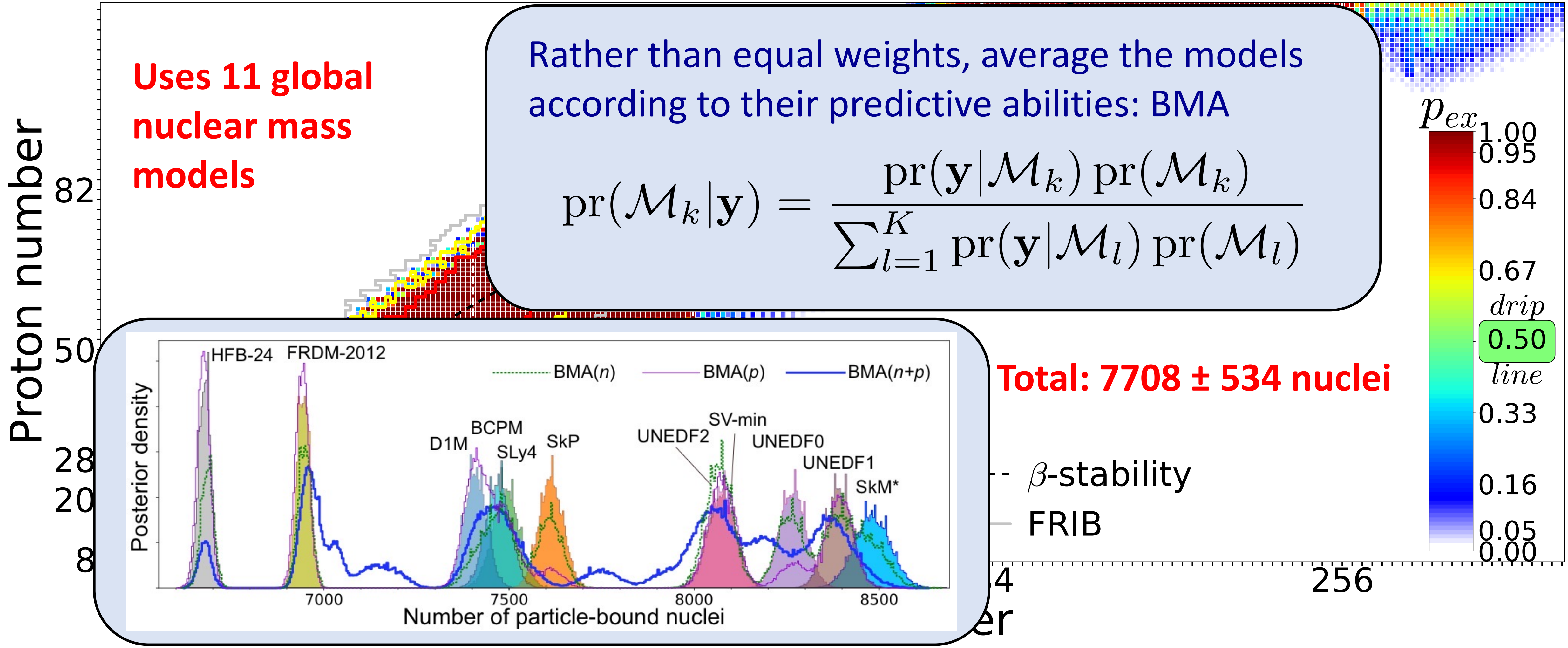
Probability for each nucleus (Z,N) to be bound shown as a color. Dripline at 50%.

Limits of the nuclear landscape: Bayesian model averaging (BMA)

Uses 11 global nuclear mass models

Rather than equal weights, average the models according to their predictive abilities: BMA

$$\mathrm{pr}(\mathcal{M}_k|\mathbf{y}) = \frac{\mathrm{pr}(\mathbf{y}|\mathcal{M}_k)\,\mathrm{pr}(\mathcal{M}_k)}{\sum_{l=1}^{K}\mathrm{pr}(\mathbf{y}|\mathcal{M}_l)\,\mathrm{pr}(\mathcal{M}_l)}$$



Total: 7708 ± 534 nuclei

L. Neufcourt et al., Phys. Rev. C **101**, 014319 (2020); arXiv:2001.05924

Probability for each nucleus (Z,N) to be bound shown as a color. Dripline at 50%.

Toy Bayesian model mixing (BMM) example

- General: K models $\mathcal{M}_k, (k = 1, \ldots, K)$
- Specify a model by predictions for observations y_i at points x_i → $\mathcal{M}_k : y_i = f_k(x_i) + \varepsilon_{i,k}$
- Predictions at new input points:

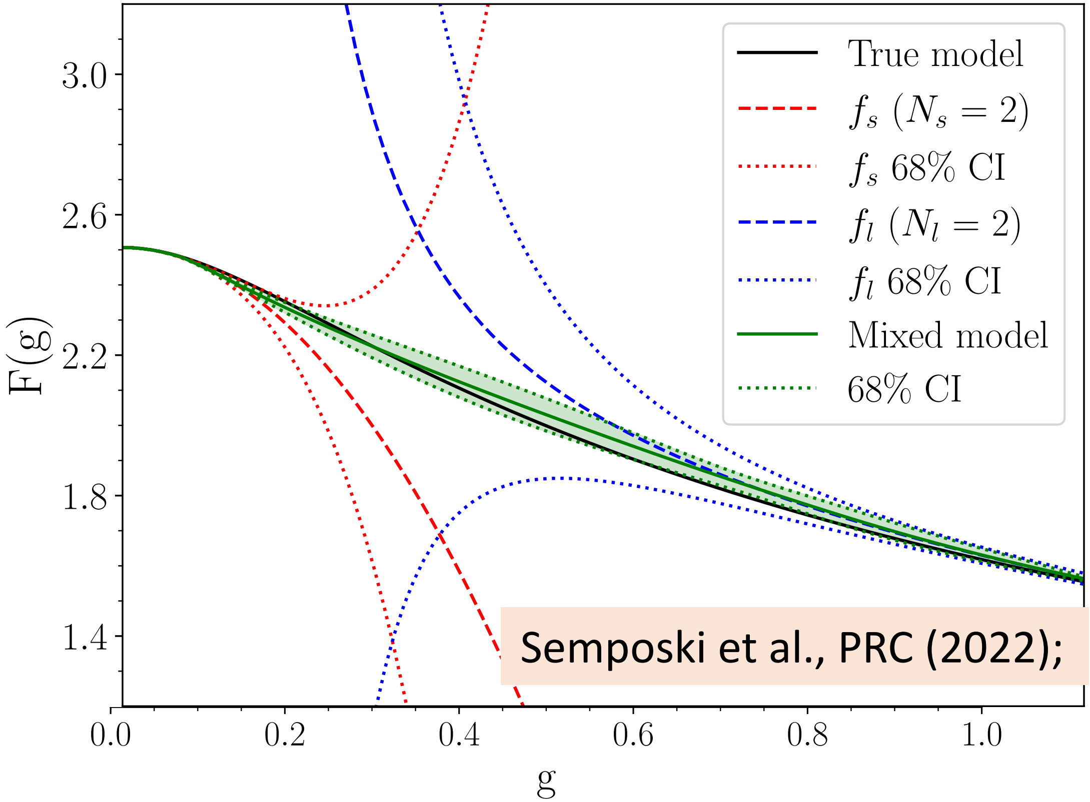
$$\mathrm{pr}(\tilde{y}|\tilde{x}) = \sum_{k=1}^{K} \hat{w}_k \mathrm{pr}(\tilde{y}|\tilde{x}, \mathcal{M}_k)$$

- Bayesian Model Averaging (BMA) has constant weights $\hat{w}_k$; for BMM they depend on x_i.

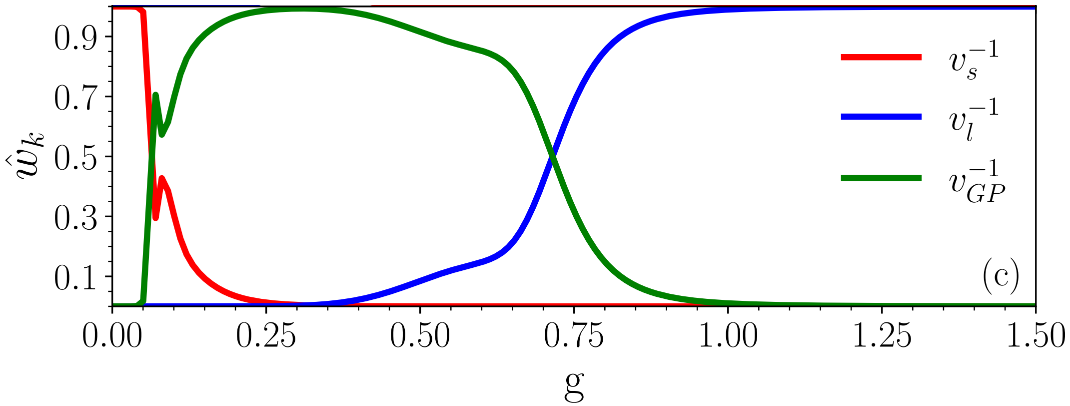
Test strategies with expansions of:

$$F(g) = \int_{-\infty}^{\infty} d\phi \; e^{-\frac{\phi^2}{2} - g^2\phi^4}$$

and truncation error models.



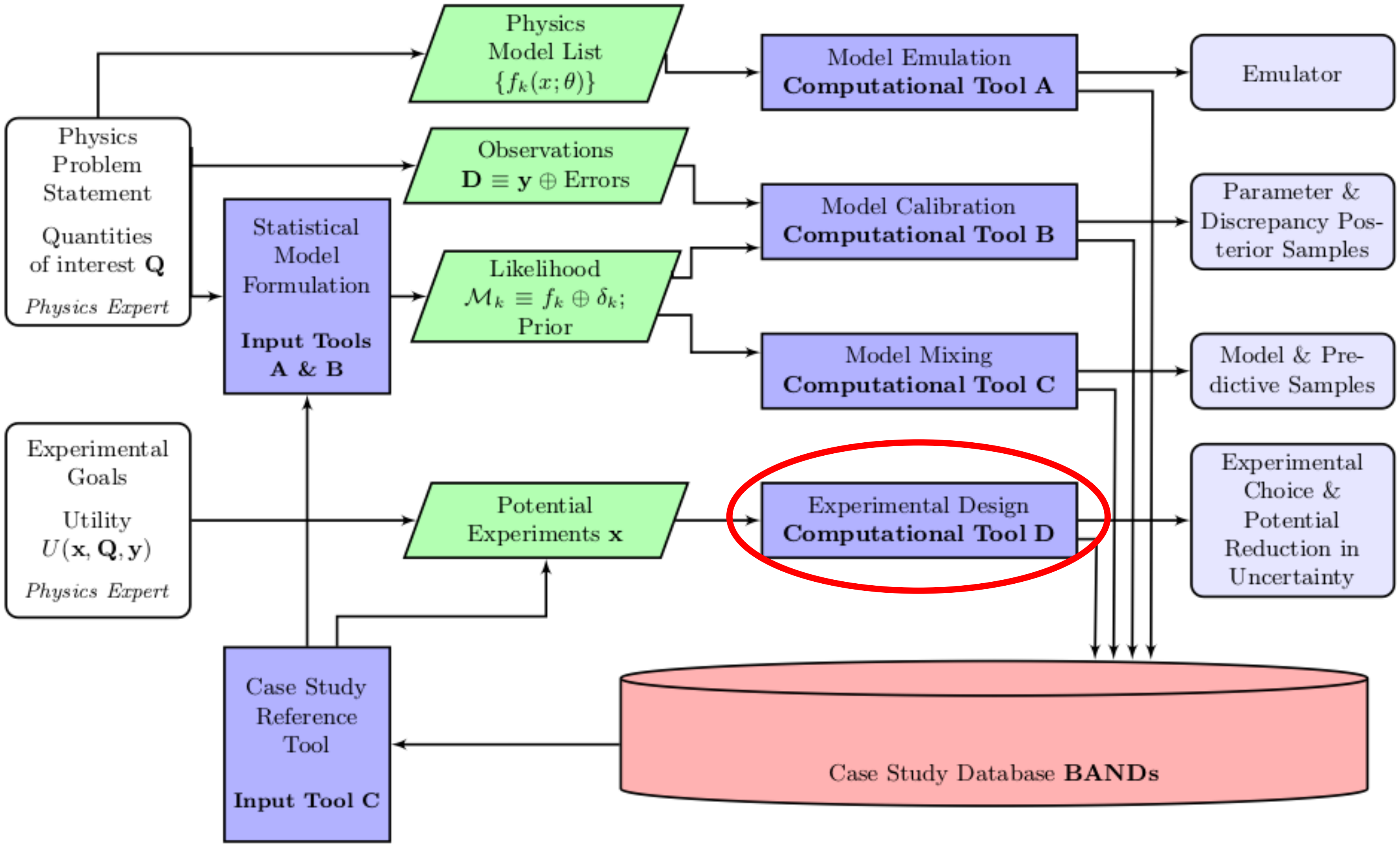
Semposki et al., PRC (2022);



A. Semposki J. Yanotty

BAND (Bayesian Analysis of Nuclear Dynamics)

Experimental design requires uncertainties from both experiment and models



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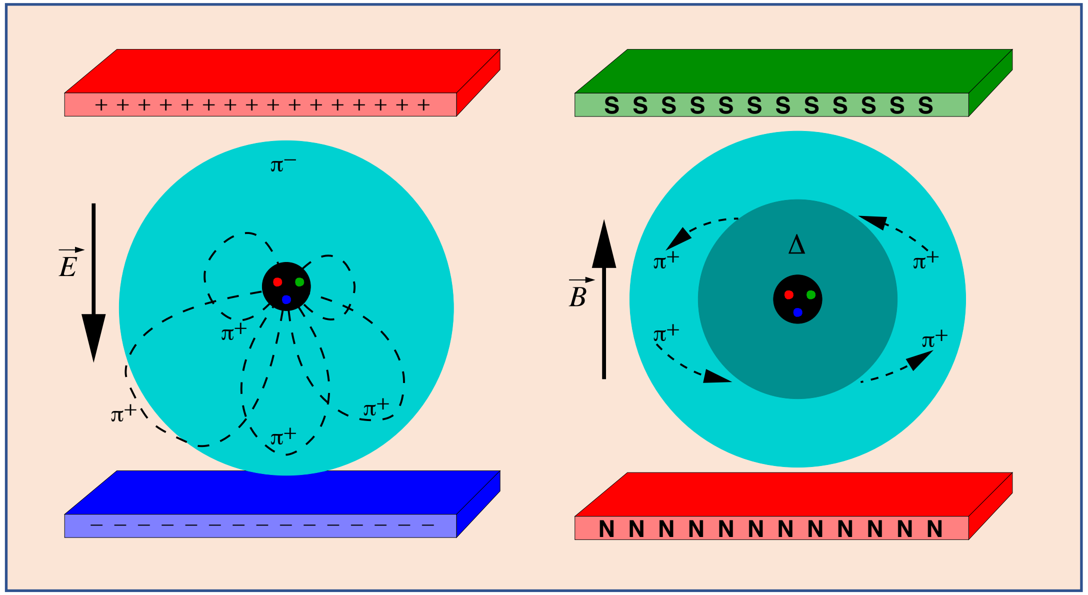
Goal: maximize benefits – minimize cost (time, money, workforce)

Example: Design of future γp Compton scattering experiments

What experimental (ω, θ) are most useful for constraining polarizabilities and testing theory?

Given: (1) Present polarizability error bars; (2) experimental constraints; (3) χEFT accuracy decreases as ω↑.



Nucleon polarizabilities from Compton scattering with χEFT

Griesshammer, McGovern, Phillips, EPJA (2018)

Experiments: HIγS; A2@MAMI
→ tension with χEFT valid range

What does a Bayesian analysis of experimental design look like?

[J. Melendez et al, Eur. Phys. J. A **57,** 3 (2021)]

Example: Design of future γp Compton scattering experiments

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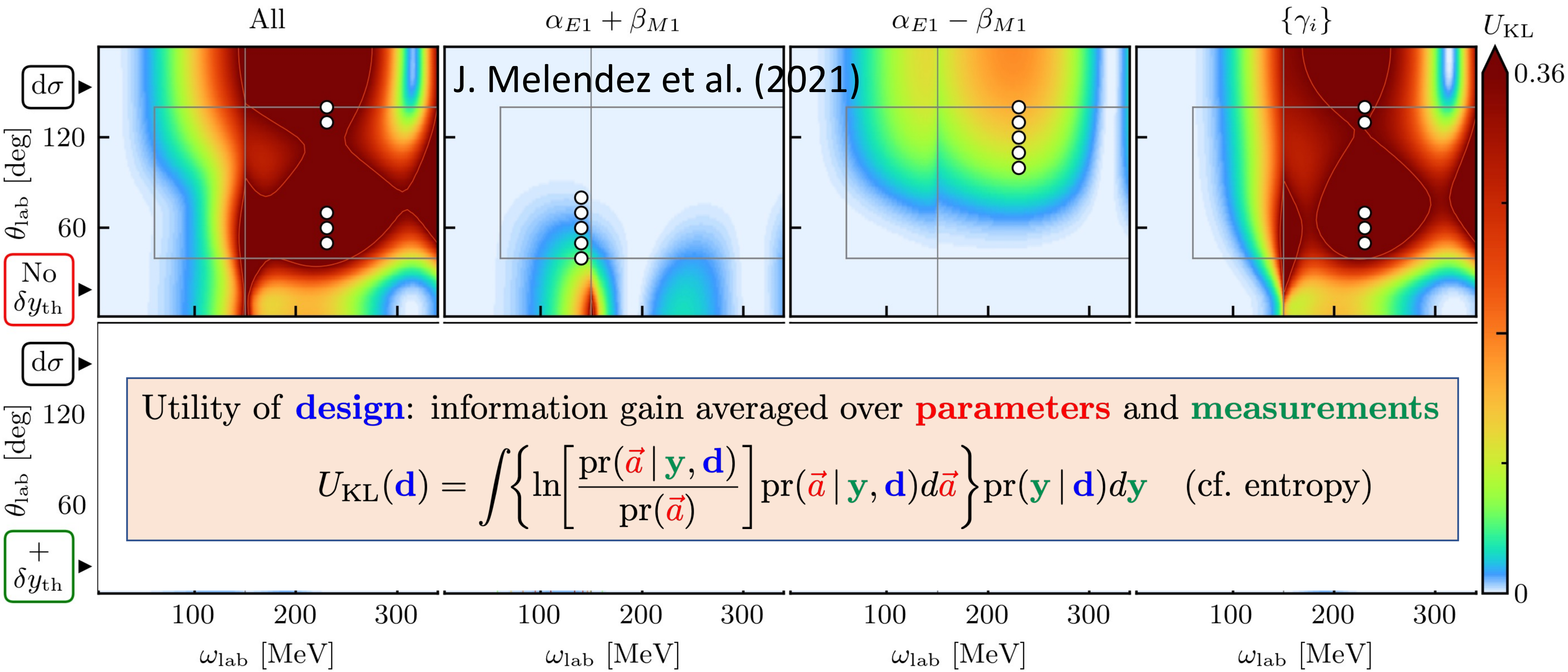


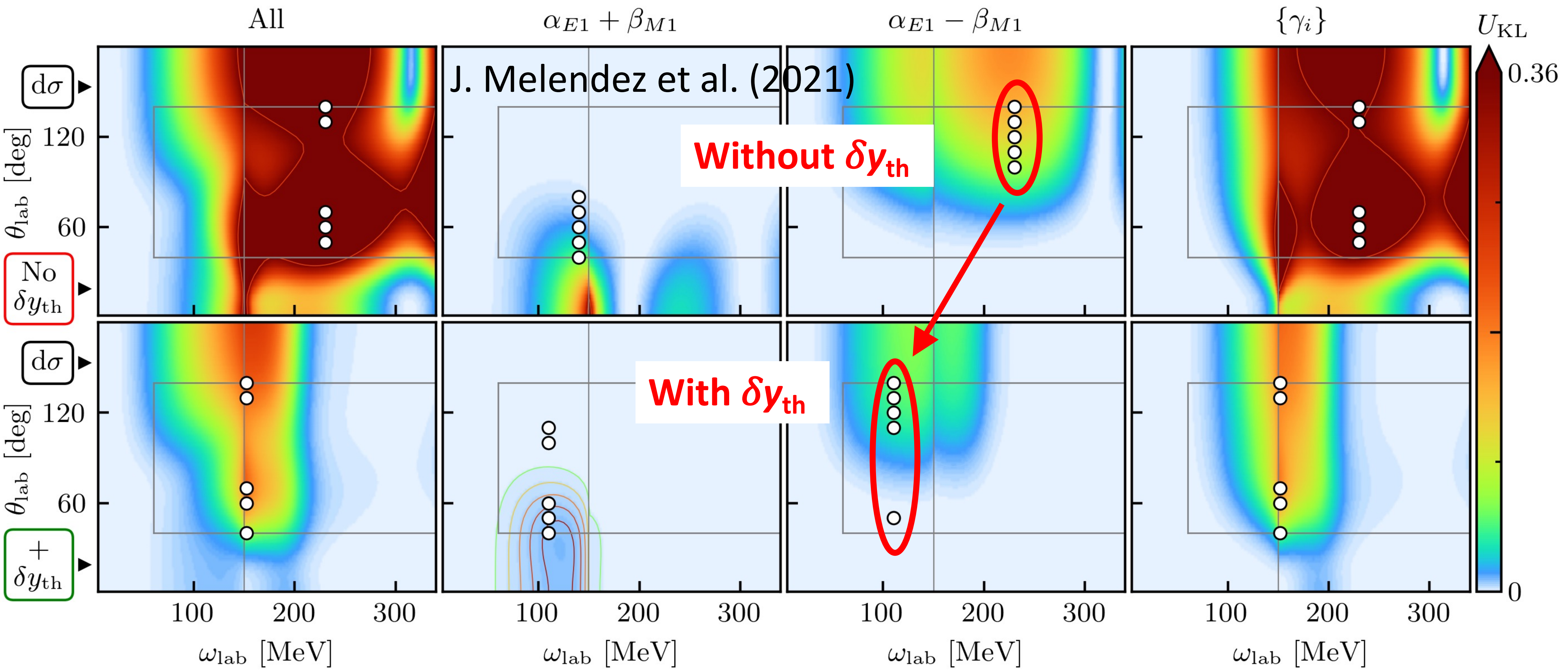
Utility of **design**: information gain averaged over **parameters** and **measurements**

$$U_{\mathrm{KL}}(\mathbf{d}) = \int \left\{ \ln \left[\frac{\mathrm{pr}(\vec{a} \mid \mathbf{y}, \mathbf{d})}{\mathrm{pr}(\vec{a})} \right] \mathrm{pr}(\vec{a} \mid \mathbf{y}, \mathbf{d}) d\vec{a} \right\} \mathrm{pr}(\mathbf{y} \mid \mathbf{d}) d\mathbf{y} \quad \text{(cf. entropy)}$$

Example: Design of future γp Compton scattering experiments

What experimental (ω, θ) are most useful for constraining polarizabilities and testing theory?

Given: (1) Present polarizability error bars; (2) experimental constraints; (3) χEFT accuracy decreases as ω↑.



Compare utility without to with model discrepancy δy_{th} ⇒ very different implications!

Outline

- Thinking about uncertainty quantification (UQ) for models
- **BAND:** emulators, calibration, model mixing, expt. design
- Outlook: Frontiers of UQ for nuclear models

Outlook: Frontiers of UQ for nuclear models

Checklist for statistically sound Bayesian inference

- ☑ Interact with the experts (i.e., statisticians, applied mathematicians)
- ☑ Incorporate all sources of experimental and *theoretical* errors
- ☑ Formulate *statistical models* for uncertainties
- ☑ Use as informative priors as is reasonable; test sensitivity to priors
- ☑ Account for correlations in inputs (type x) and observables (type y)
- ☑ Propagate uncertainties through the calculation
- ☑ Use *model checking* to validate our models

Outlook: Frontiers of UQ for nuclear models

- **Emulators:** new applications to 3N scattering, infinite matter, pairing, …; new technologies explored (e.g., MOR, active learning, AI/machine learning); new workflows enabled (bypass specialized knowledge).
- **Calibration:** full Bayesian parameter estimation and uncertainty propagation.
- **Model mixing:** BAND and other projects on nuclear EOS, EDFs, EFTs, …
- **Experimental design:** exploring alternative approaches; *sampling* is feasible with emulators!
- **Software:** e.g., BAND github repository → surmise, Taweret, ROSE, …
- **Physics *discovery* through statistics:** e.g., exploit statistical correlations using Bayesian tools (spectra, $0\nu\beta\beta$, …); uncover power counting of EFT; …

Thank you!

Coming attractions (sign up now!):

2023: **ISNET-9 + BAND CAMP**, May 22-26 , at Washington U. in St. Louis

2023: **FRIB-TA Summer School on** ***Practical Uncertainty Quantification and Emulator Development in Nuclear Physics***, June 26-28, at FRIB.

Jupyter and Quora books:

Learning from Data (OSU course Physics 8820)

BUQEYE Guide to Projection-Based Emulators in Nuclear Physics

Reduced Basis Methods in Nuclear Physics

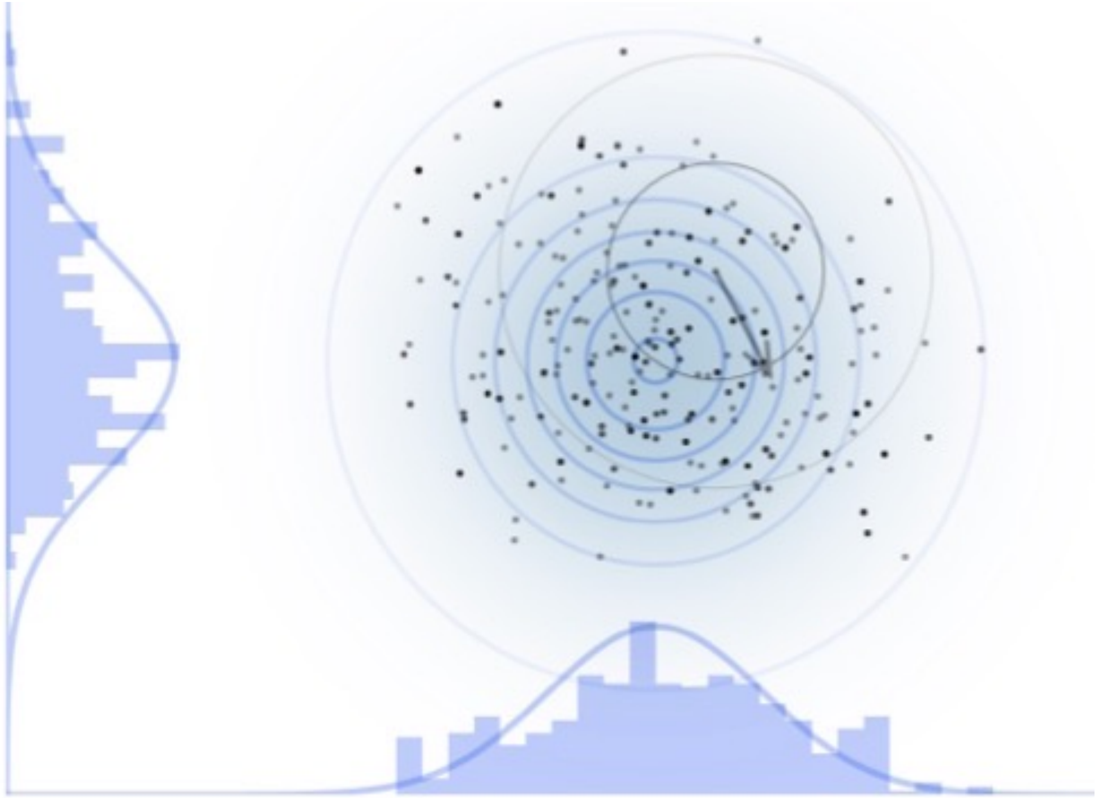
Extra slides

Historical perspective: UQ for nuclear models

- **Pre-2010:** If given, model uncertainties usually from conventional regression
- **2011:** Physical Review A editorial calling for theory uncertainty estimates
- **2013:** ISNET: **I**nformation and **S**tatistics in **N**uclear **E**xperiment and **T**heory
- **2014:** “Error Estimates of Theoretical Models: a Guide” [Dobaczewski et al]
- **2015:** Journal of Physics G Special Focus Issue: *ISNET*
- **2016:** Bayesian Methods in Nuclear Physics (ISNET-4) [INT, Seattle]
- **2020-1:** J. Phys. G Special Focus Issue: *ISNET 2.0*
- **2022:** Frontiers in Physics issue: *Uncertainty Quantification in Nuclear Physics*
- **2023:** **ISNET-9 + BAND CAMP**, May 22-26 , at Washington U. in St. Louis

How do we sample efficiently?

Random walk (Metropolis-Hastings)



Used for most Bayesian sampling to date

For animations, see: [McElreath blog entry on sampling] and Chi Feng's [Markov-chain Monte Carlo Interactive Gallery]

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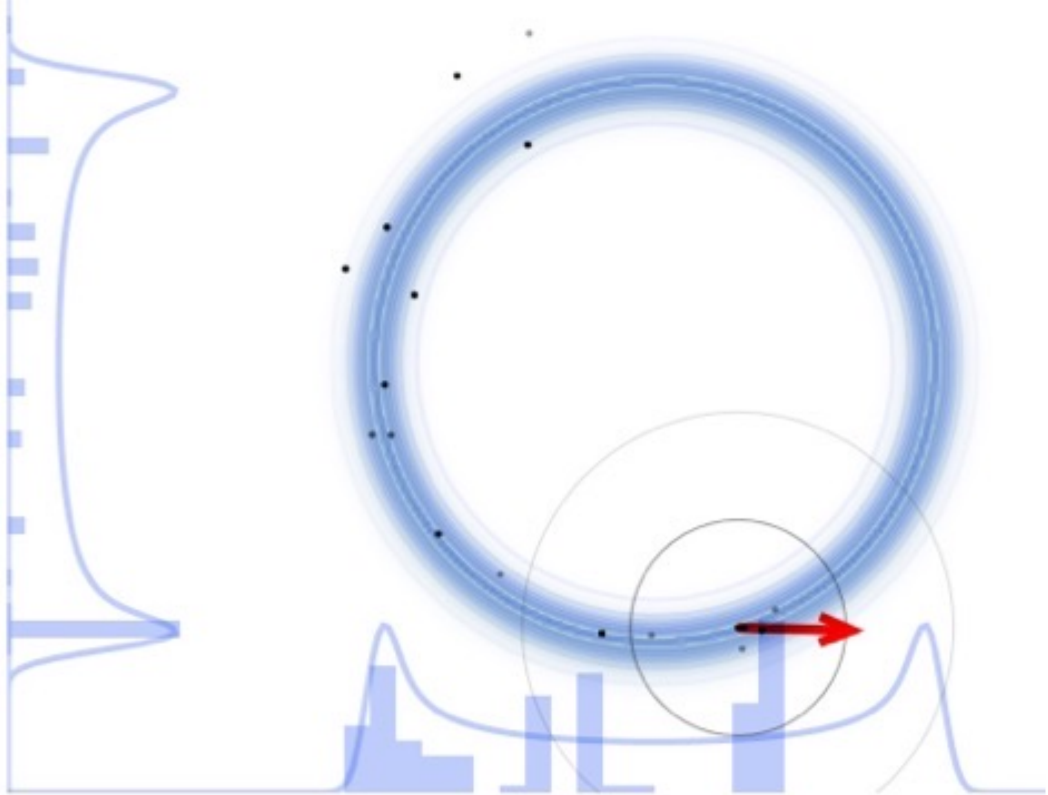
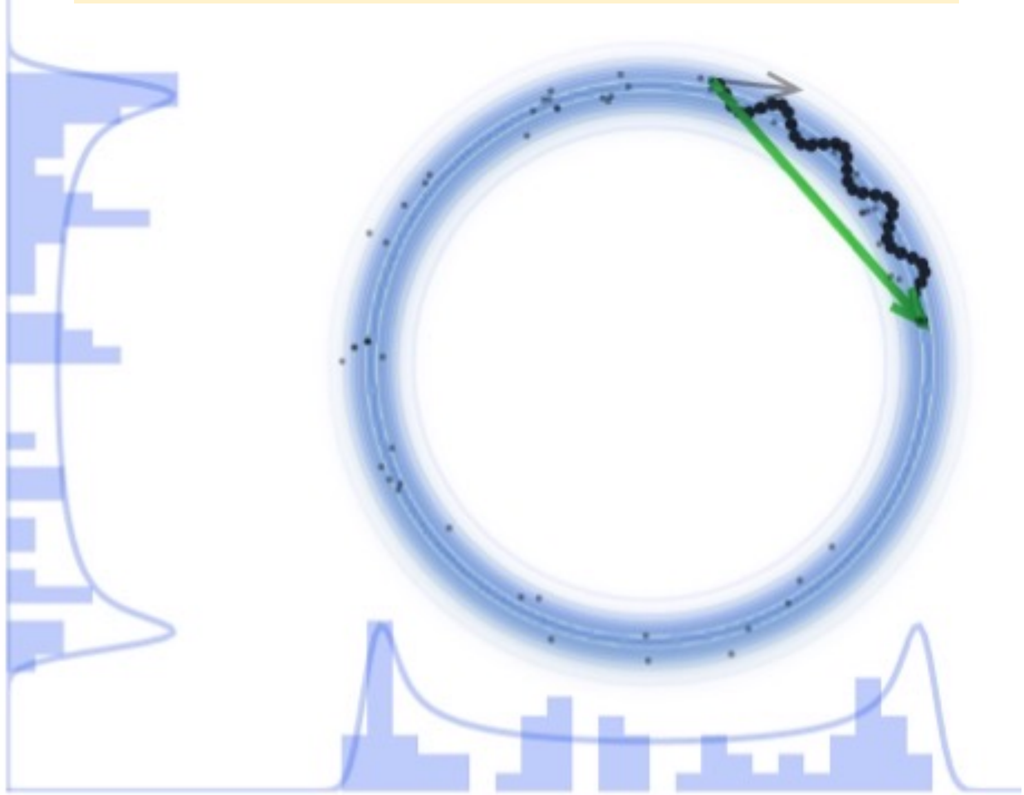


Used for most Bayesian sampling to date

Hamiltonian Monte Carlo (HMC)



Recent work by Chalmers group (arXiv:2206.08250)
→ HMC much more effective for many parameters!

For animations, see: McElreath blog entry on sampling and Chi Feng's Markov-chain Monte Carlo Interactive Gallery

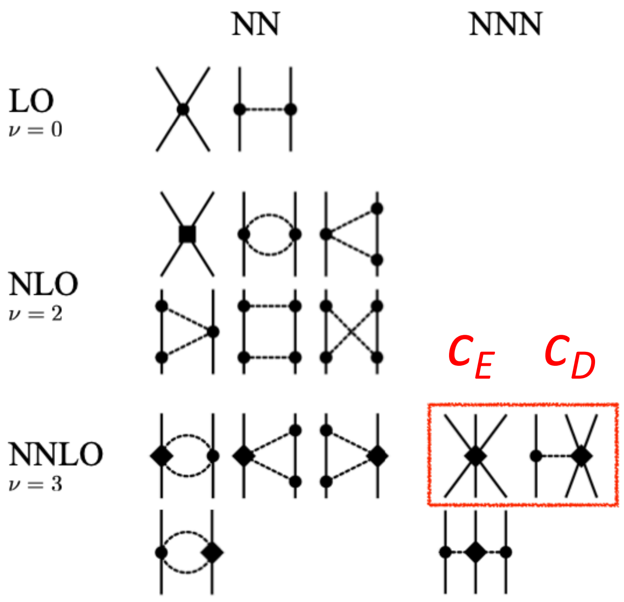
Light nuclei with semilocal momentum-space regularized chiral interactions up to [and beyond] N^2LO

LENPIC Collaboration

https://www.lenpic.org/

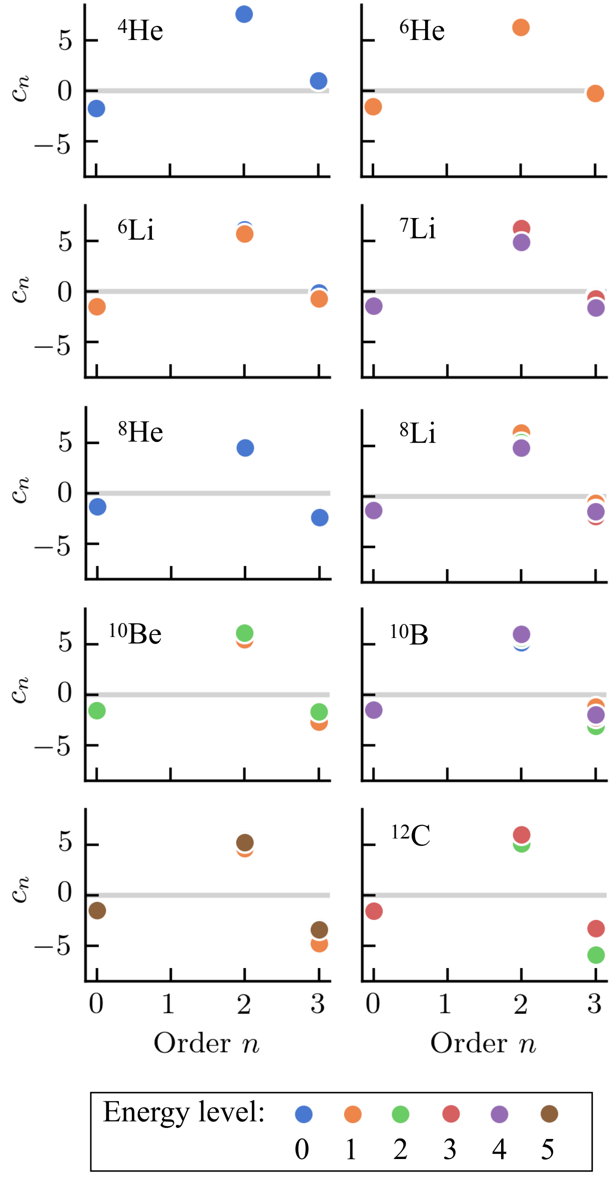
P. Maris et al., PRC **103**, 054001 (2021) arXiv:2104.04441

P. Maris, R. Roth et al., PRC **106**, 064002 (2022) arXiv:2206.13303



- *Consistent* NN and 3N potentials to N^2LO [2022: NN to N^4LO]
- "Semilocal" to reduce regulator artifacts
- c_E and c_D from ^3H binding and *Nd* diff. cross section minimum
- Calculations for few-body and p-shell+ nuclei (NCCI plus SRG)
- Bayesian estimates of EFT truncation errors (also method error)
- Many results (e.g., overbinding at N^2LO and cutoff dependence reduced with higher-order NN; but radii still underpredicted).

Excitation energies are highly correlated



Coefficients for all the levels

- Empirically: calculated excitation energies are better determined than each level.
- Why? If E_1 and E_2 have $\delta \boldsymbol{y}_{\mathrm{th}}$ variance σ^2, then $E_2 - E_1$ has $2\sigma^2$ if uncorrelated but $2(1\text{-}\rho)\sigma^2$ if correlated with ρ!
- Plan: *learn* ρ from $\boldsymbol{y}_{\mathrm{th}}$ coefficients c_n:

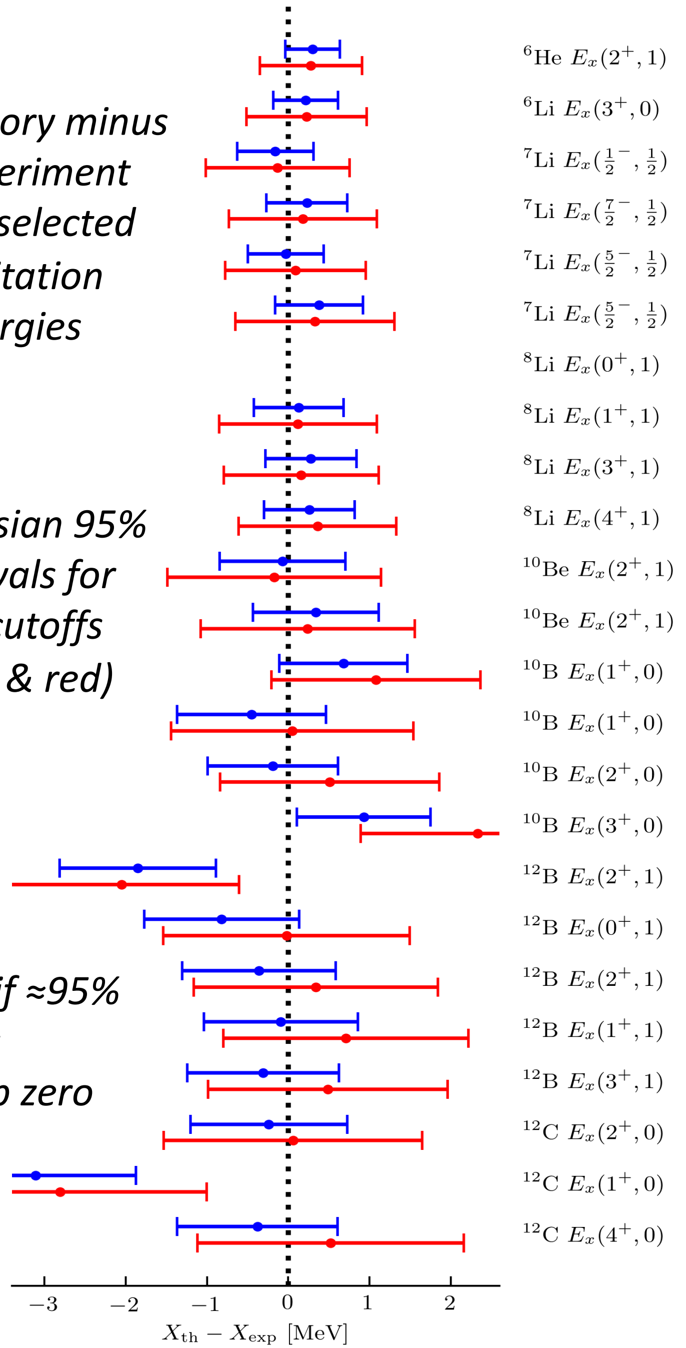
$$\boldsymbol{y}_k = \boldsymbol{y}_{\mathrm{ref}} \sum_{n=0}^{k} c_n Q^n \qquad c_n \equiv \frac{\Delta y_n}{y_{\mathrm{ref}} Q^n}$$

- **Model checking:** empirical coverage in agreement with experiment *if* correlations used for errors.
- **Diagnostic of physics**: exceptions in ^{12}C and ^{12}B point to different theoretical correlations in the nuclear structure.
- **Higher order:** >N^{2}LO enables better estimates of correlations → more insight

Theory minus experiment for selected excitation energies

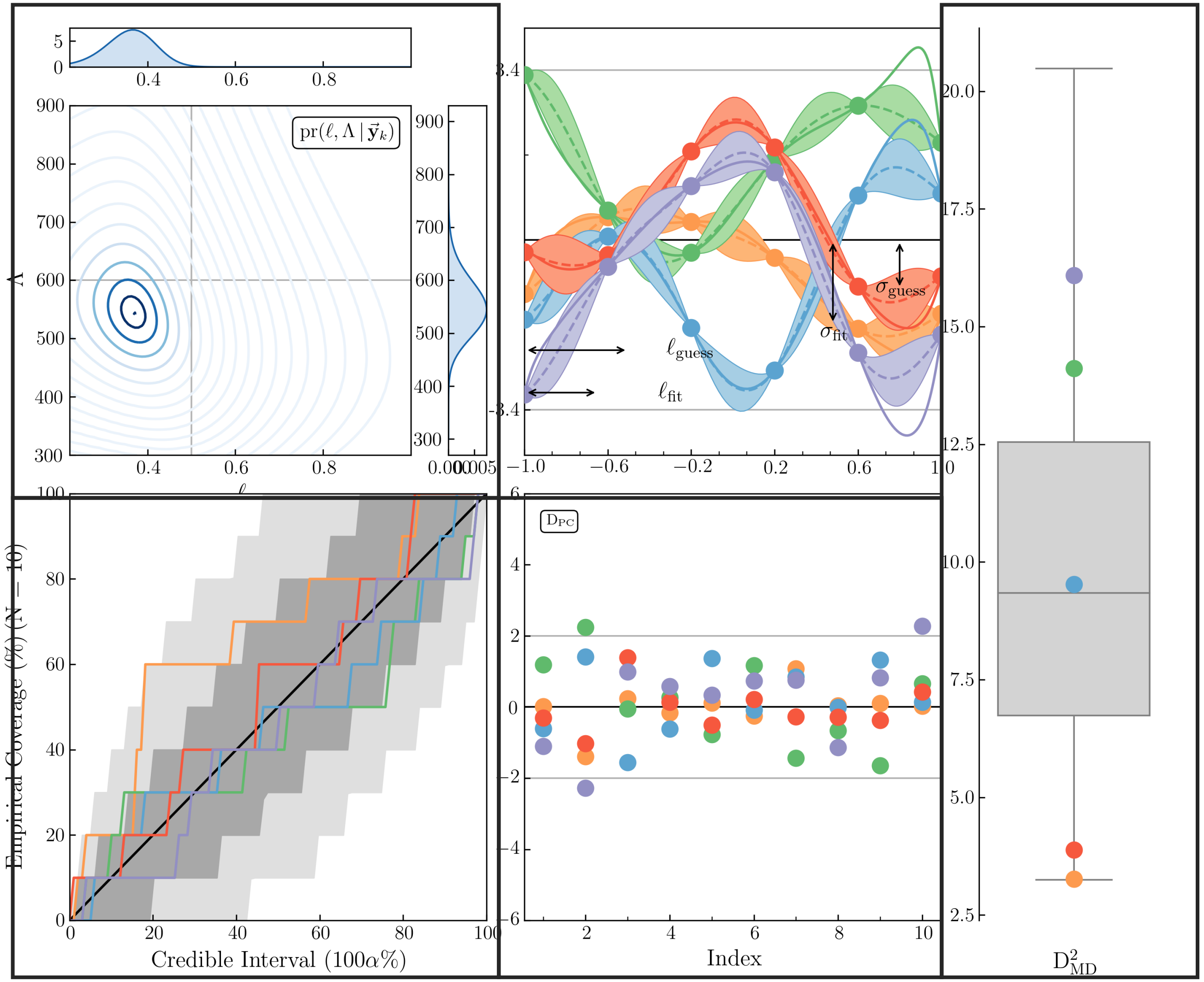
Bayesian 95% intervals for two cutoffs (blue & red)

Check if ≈95% of bars overlap zero



Statistical diagnostics [Melendez et al. (2019) and Millican et al. (2023)]

- Mahalanobis distance (MD) squared
  - Chi-squared with correlations
- Pivoted Cholesky (PC) decomposition
  - Indexed breakdown of MD linear algebra
- Credible interval coverage
  - "Does 68% of the data fall within the 68% confidence intervals of the fitted GP?"
- Λ_b, l_C joint posterior pdf
  - Uses Bayesian statistics to find conditional probabilities



Spin observable D (150 MeV) for SMS 450 MeV potential

Statistical diagnostics [Melendez et al. (2019) and Millican et al. (2023)]

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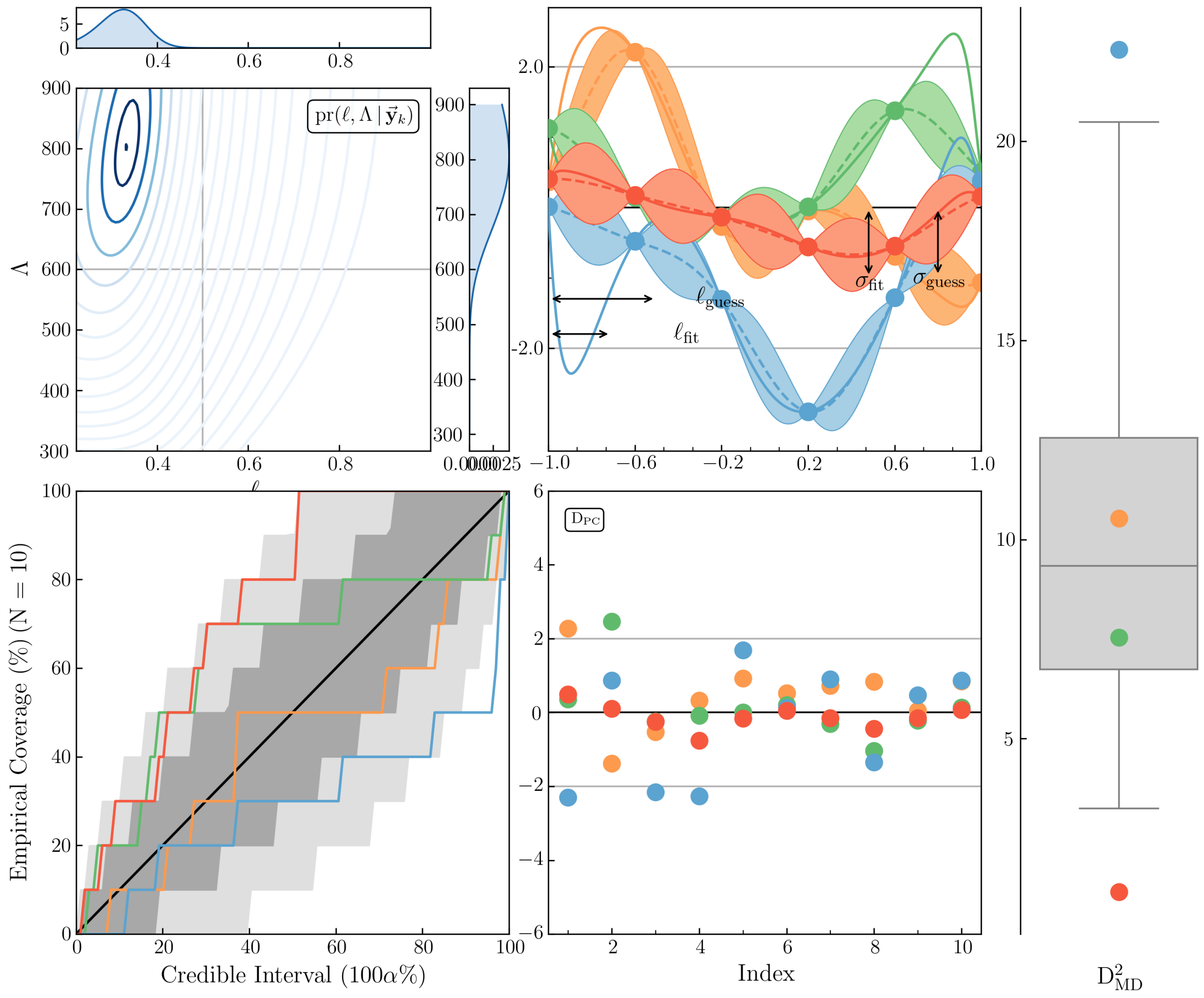
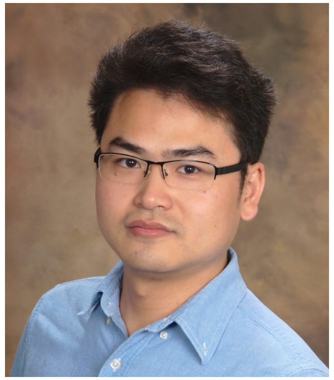
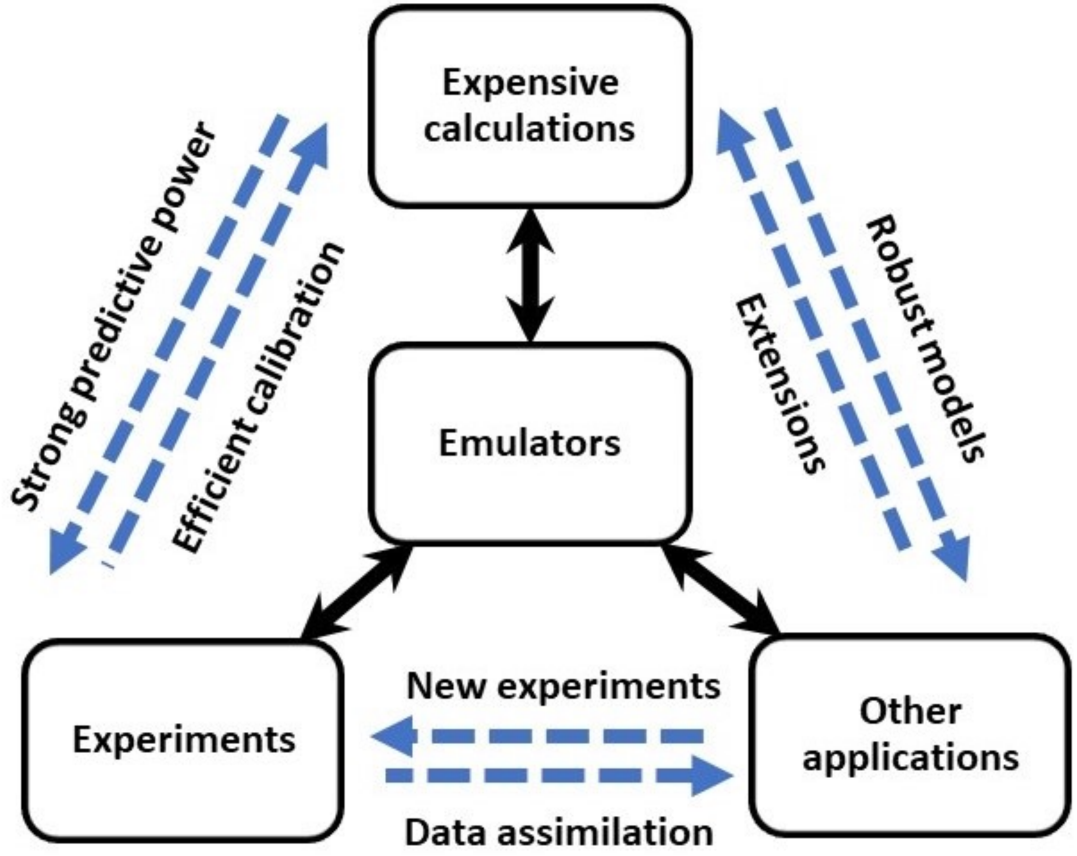


Spin observable D (150 MeV) for SCS 1.2 fm potential

Role of emulators: new workflows for EFT applications

From Xilin Zhang, rjf, *Fast emulation of quantum three-body scattering*, Phys. Rev. C **105**, 064004 (2022).





If you can create fast & accurate™ emulators for observables, you can do calculations without specialized knowledge and expensive resources!

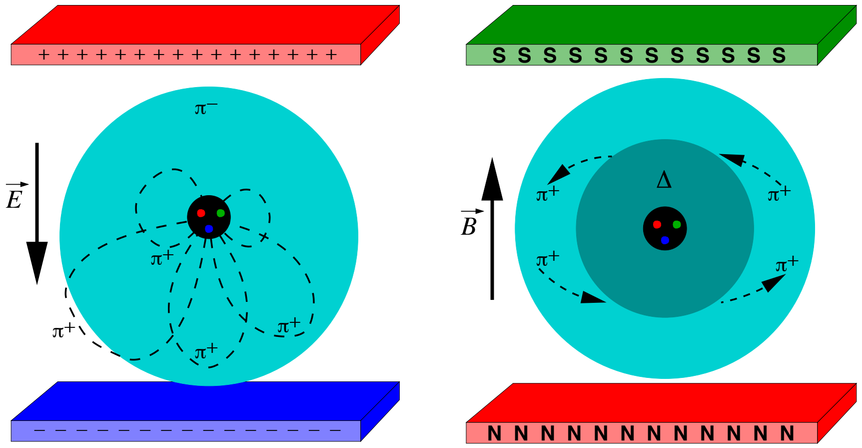
Experimental design: A case study

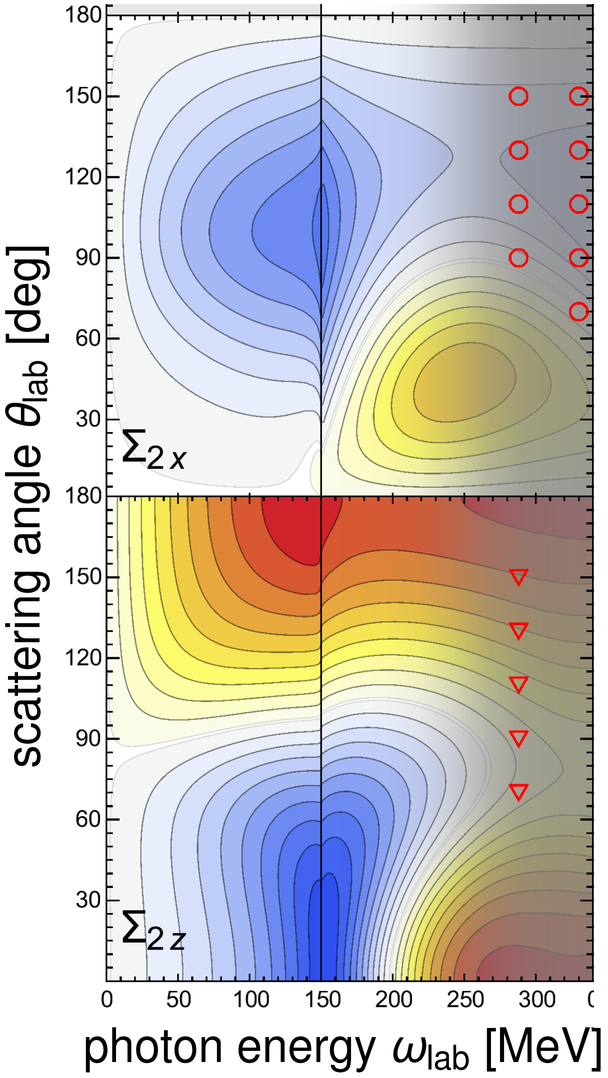
Maximize benefits – minimize cost (time, money, workforce)

Nucleon polarizabilities from Compton scattering with ChiEFT

[Harald Griesshammer, Judith McGovern, Daniel Phillips, EPJA (2018)]

- How do constituents of the nucleon react to external fields?
- How to reliably extract proton, neutron, spin polarizabilities?
- How to plan effective experiments and test theory?





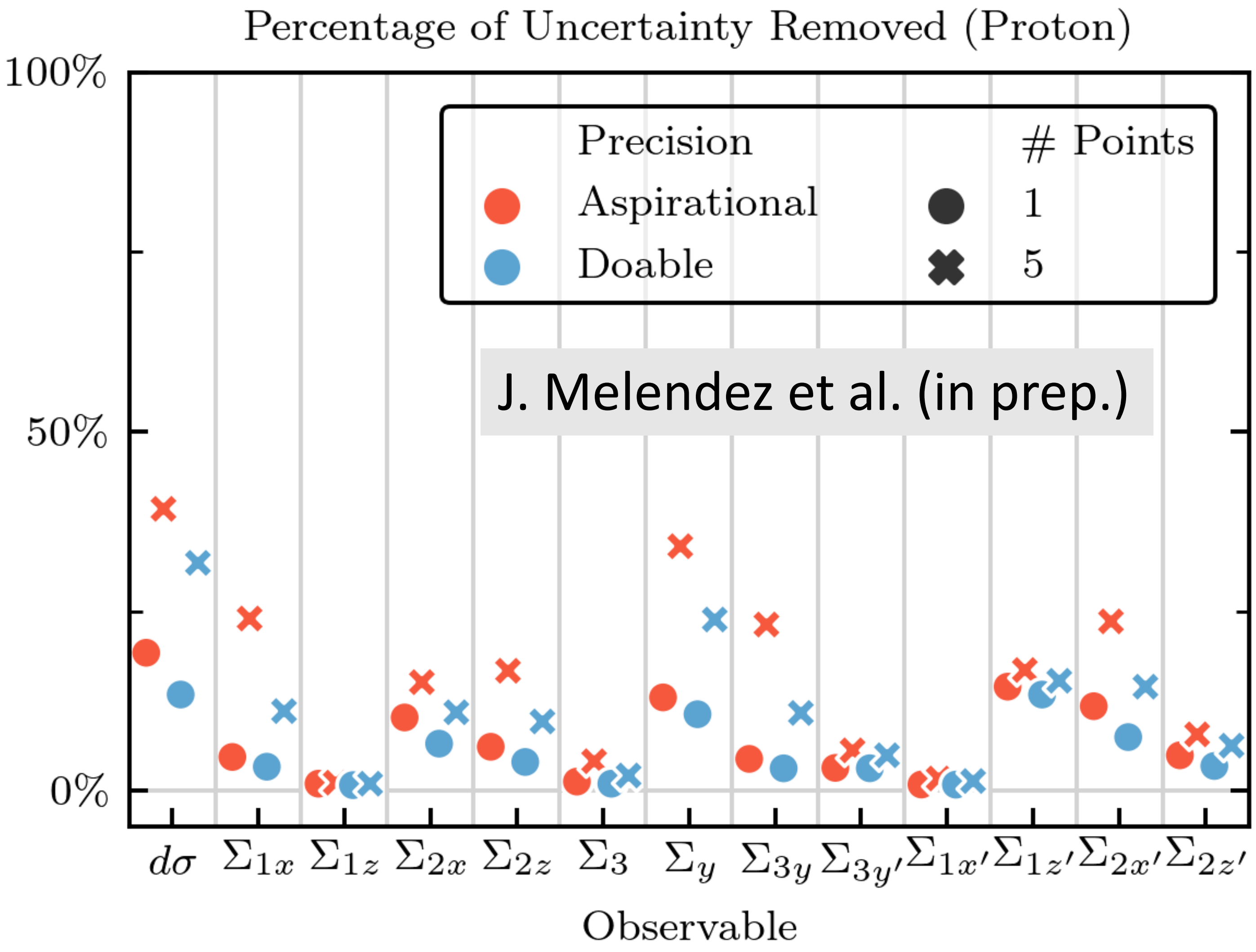
$$2\pi\left[\underbrace{\alpha_{E1}\,\vec{E}^2+\beta_{M1}\,\vec{B}^2}_{\text{electric, magnetic scalar dipole}}+\underbrace{\gamma_{E1E1}\vec{\sigma}\cdot(\vec{E}\times\dot{\vec{E}})+\gamma_{M1M1}\vec{\sigma}\cdot(\vec{B}\times\dot{\vec{B}})+2\gamma_{M1E2}\sigma^i B^j E_{ij}+2\gamma_{E1M2}\sigma^i E^j B_{ij}}_{\text{spin-dependent dipole response of nucleon-spin constituents}}+\dots\right]$$

Experiments: HIγS; A2@MAMI → tension with ChiEFT valid range

Optimizing the design of future Compton scattering experiments

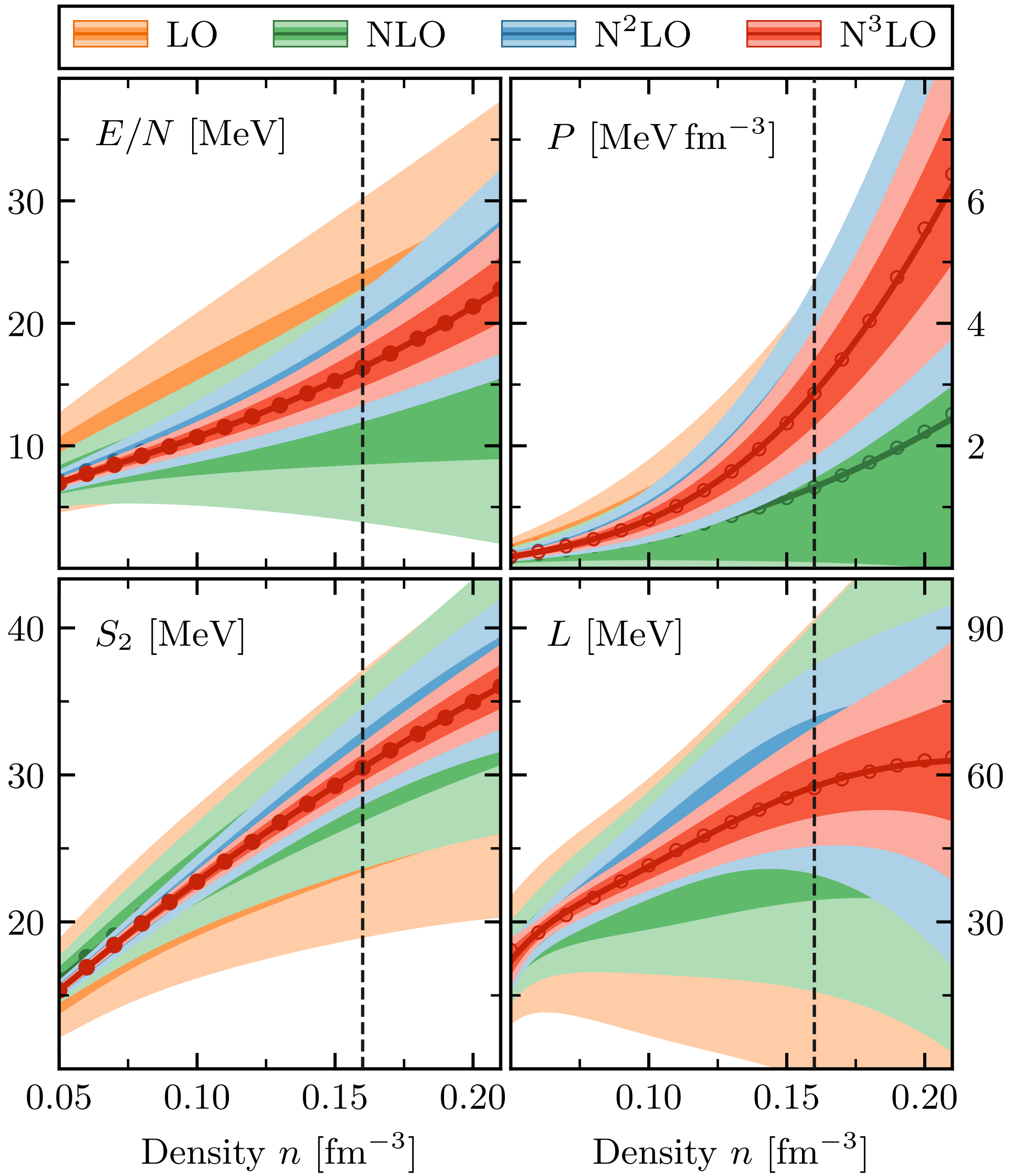
How to plan effective experiments & test theory? What (ω, θ) are most useful for constraining?

Ingredient: Calculate a utility function for sum of variances for each kinematic point on a grid.



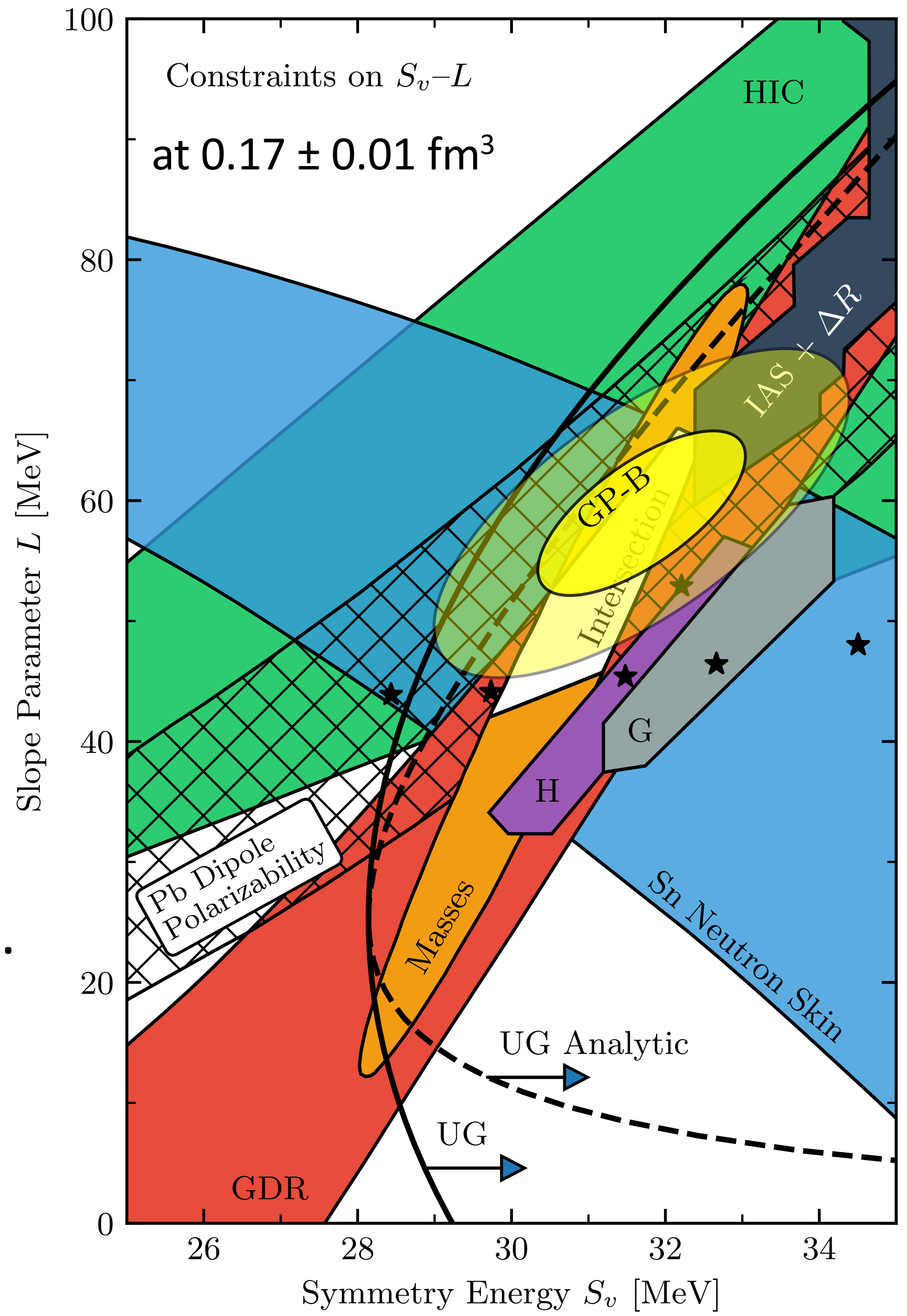
- Apply to decide on trade-off between different allocations of experimental resources (exploration vs. exploitation).
- 1-point vs 5-point?
- Increase precision or more points?

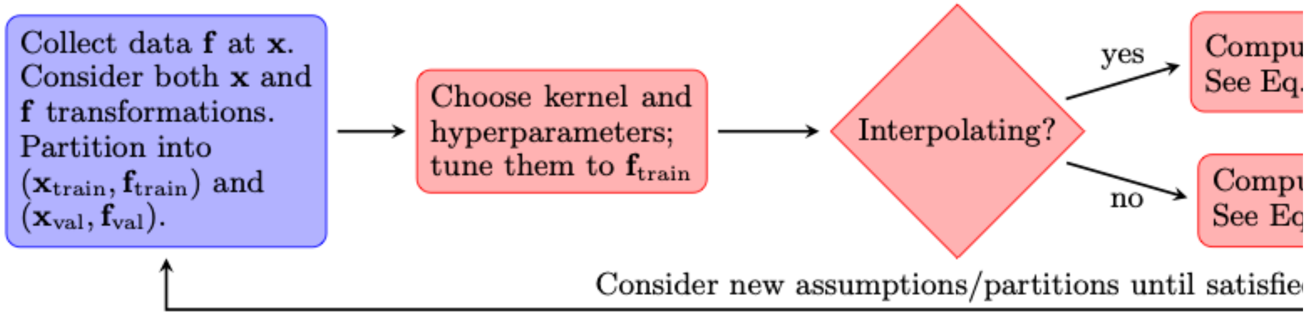
Correlated theory errors for EOS properties



C. Drischler et al.

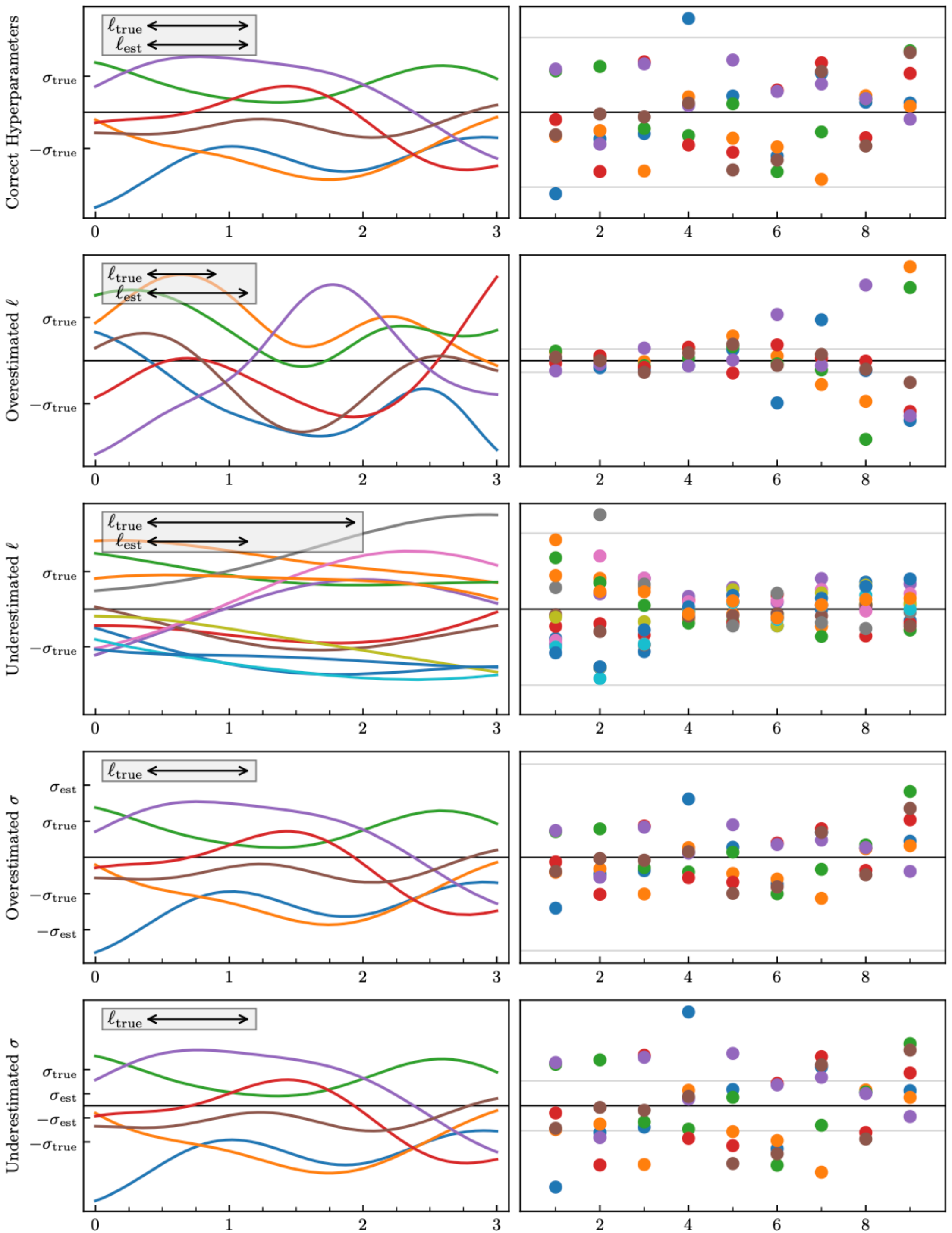
Correlated GP treatment gives better estimates for truncation errors and clean propagation of uncertainties to derived quantities.





Diagnostic	Formula	Motivation
Visualize the function	—	Does $\mathbf{f}_{\text{val}}$ look like a draw from a GP? What kind of GP?
Mahalanobis Distance $\mathrm{D}^2_{\mathrm{MD}}$	$(\mathbf{f}_{\text{val}} - \mathbf{m})^\intercal K^{-1} (\mathbf{f}_{\text{val}} - \mathbf{m})$	Can we *quantify* how much the $\mathbf{f}_{\text{val}}$ looks like a GP?
Pivoted Cholesky $\mathbf{D}_{\mathrm{PC}}$	$G^{-1}(\mathbf{f}_{\text{val}} - \mathbf{m})$	Can we understand why $\mathrm{D}^2_{\mathrm{MD}}$ is failing?
Credible Interval $\mathrm{D}_{\mathrm{CI}}(p)$ for $p \in [0, 1]$	$\dfrac{1}{M}\sum_{i=1}^{M} \mathbf{1}[\mathbf{f}_{\text{val},i} \in \mathrm{CI}_i(p)]$	Do $100p\%$ credible intervals capture data roughly $100p\%$ of the time?

Variance	Length Scale	Observed Pattern
$\sigma_{\text{est}} = \sigma_{\text{true}}$	$\ell_{\text{est}} = \ell_{\text{true}}$	Points are distributed as a standard Gaussian, witl
$\sigma_{\text{est}} = \sigma_{\text{true}}$	$\ell_{\text{est}} > \ell_{\text{true}}$	Points look well distributed at small index but grov
$\sigma_{\text{est}} = \sigma_{\text{true}}$	$\ell_{\text{est}} < \ell_{\text{true}}$	Points look well distributed at small index but shri
$\sigma_{\text{est}} > \sigma_{\text{true}}$	$\ell_{\text{est}} = \ell_{\text{true}}$	Points are distributed in a too-small range at all in
$\sigma_{\text{est}} < \sigma_{\text{true}}$	$\ell_{\text{est}} = \ell_{\text{true}}$	Points are distributed in a too-large range at all in



Limits of EFTs: Learning the expansion parameter

Model: $y_k = y_{\text{ref}} \sum_{n=0}^{k} c_n Q^n$

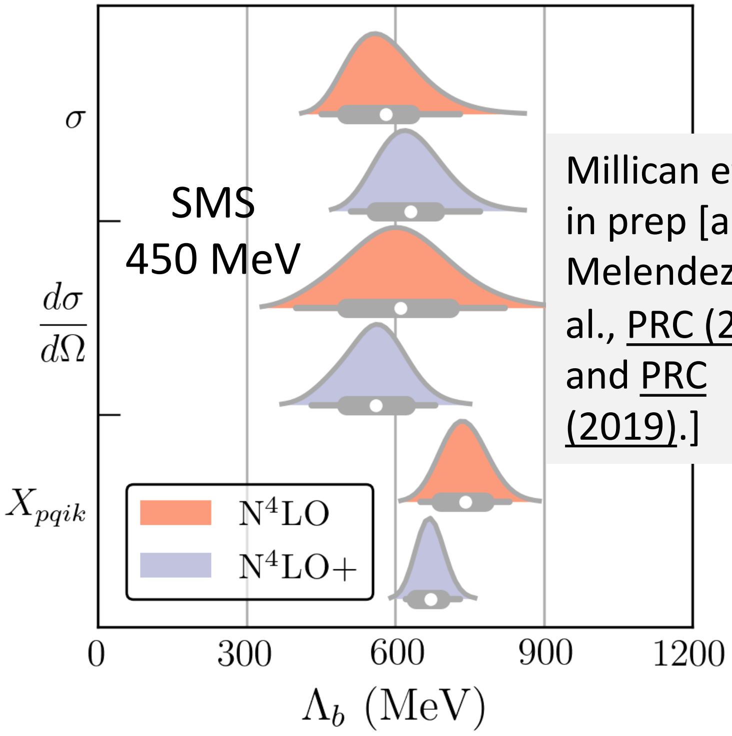
Expectation: $\chi\text{EFT} \Rightarrow Q = \dfrac{\{p, m_\pi\}}{\Lambda_b}, \quad \Lambda_b \approx 600\,\text{MeV}$

Melendez et al. (2019):

$$\text{pr}(\Lambda_b | \{y_n\}, y_{\text{ref}}) \propto \frac{\text{pr}(\Lambda_b)}{\tau^\nu \prod_n Q^n}$$

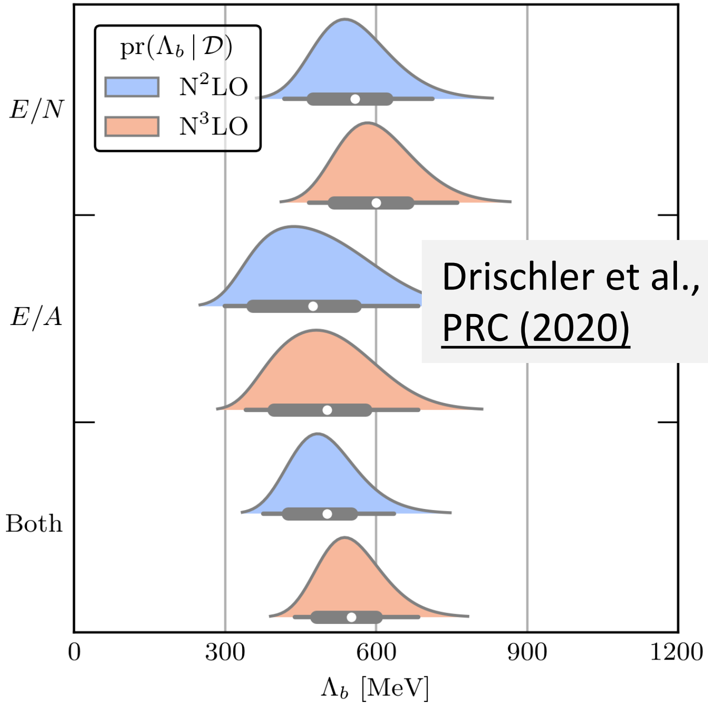
With $Q^n \propto 1/\Lambda_b^n,\ \tau \sim \langle c_n^2 \rangle$, the posterior favors Λ_b with same c_n variance for all n

Λ_b from NN observables



Millican et al., in prep [also Melendez et al., PRC (2017) and PRC (2019).]

Λ_b from infinite matter



Drischler et al., PRC (2020)

- Are different Λ_b posteriors consistent? Other ways?
- How do correlations affect the estimation of the breakdown scale?
- …

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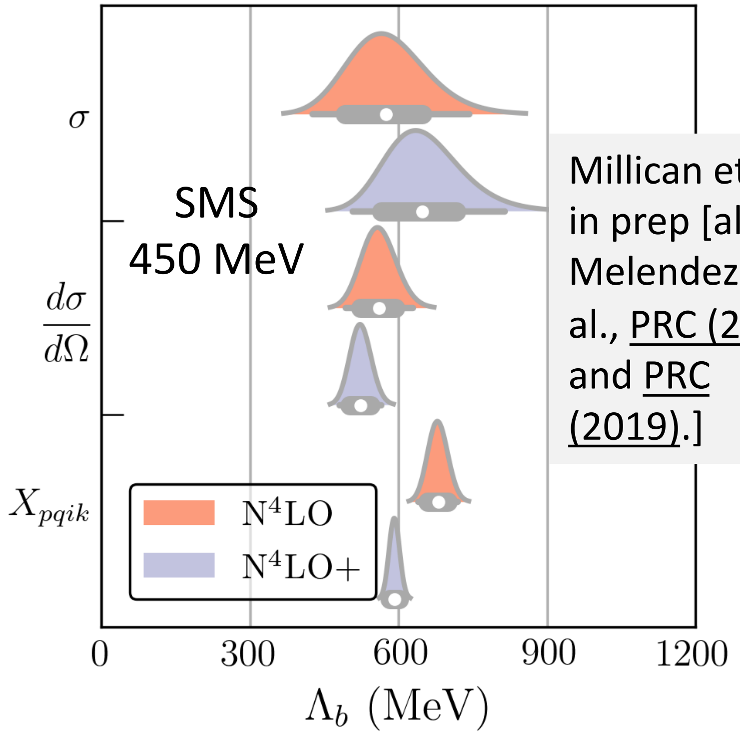

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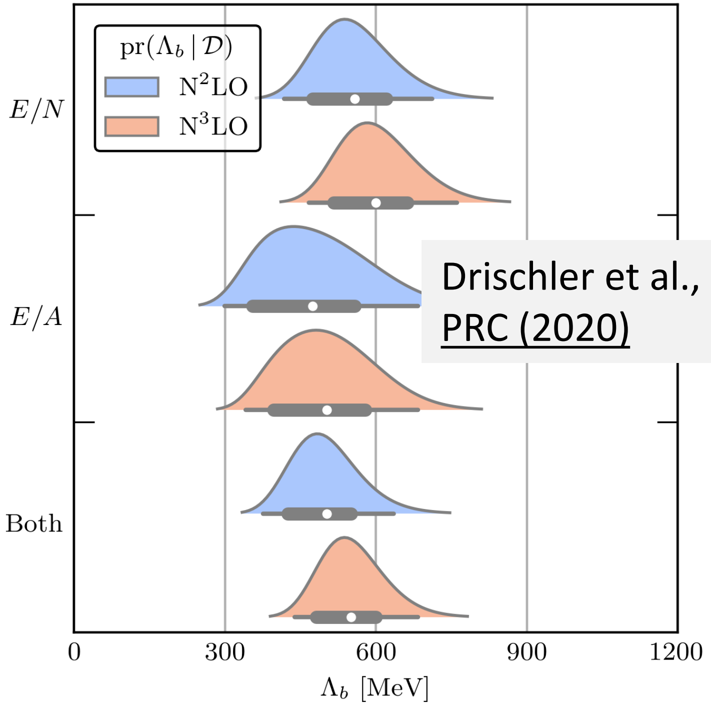

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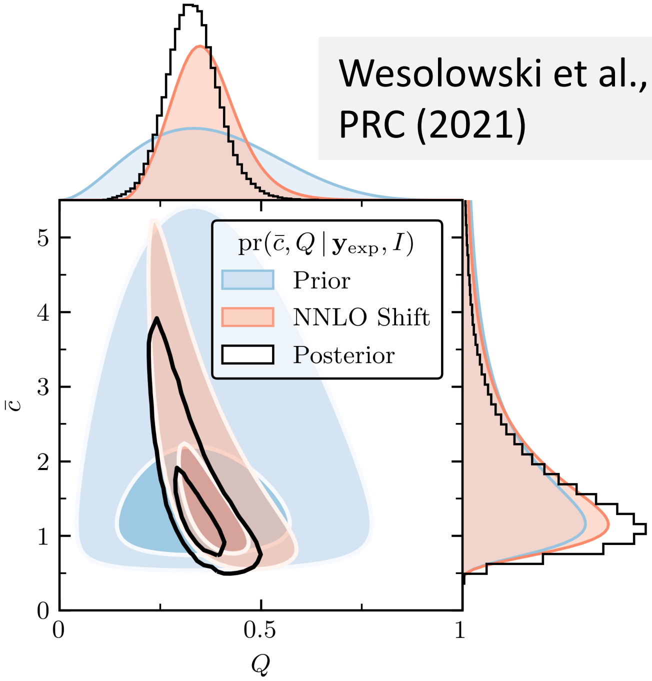
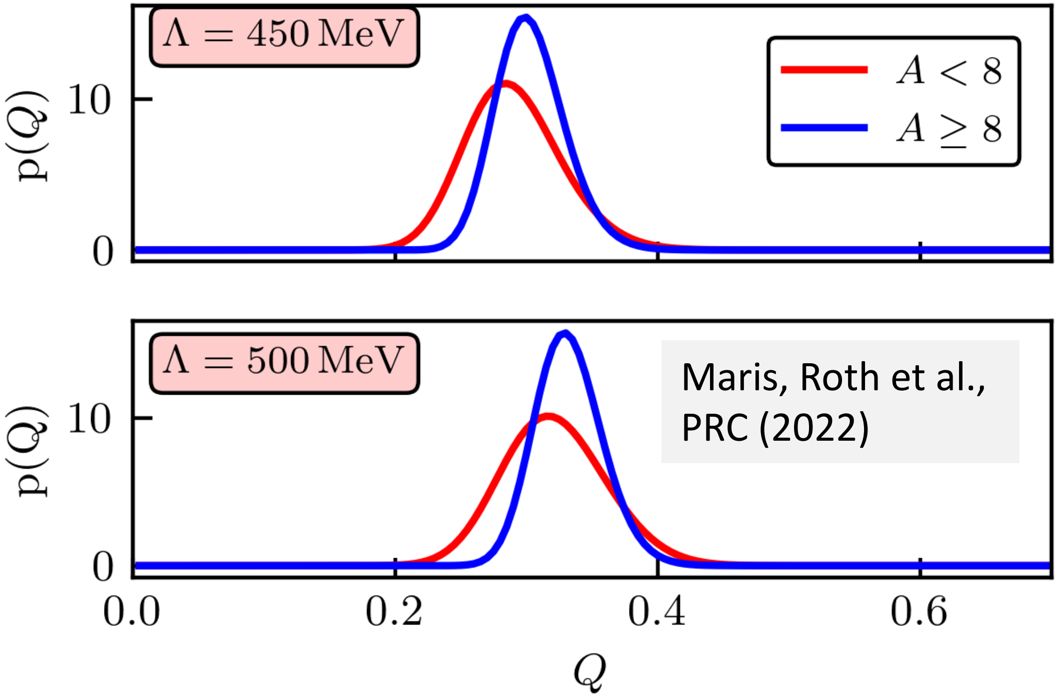
What about spectra of light nuclei?
Convergence pattern obscured at low order by KE vs. PE cancellation.
→ only use higher orders → Q ≈ 0.3
[consistent with $(m_\pi)^{\text{eff.}}/\Lambda_b$ (see Ref.)]

Q from few-body observables



Wesolowski et al., PRC (2021)

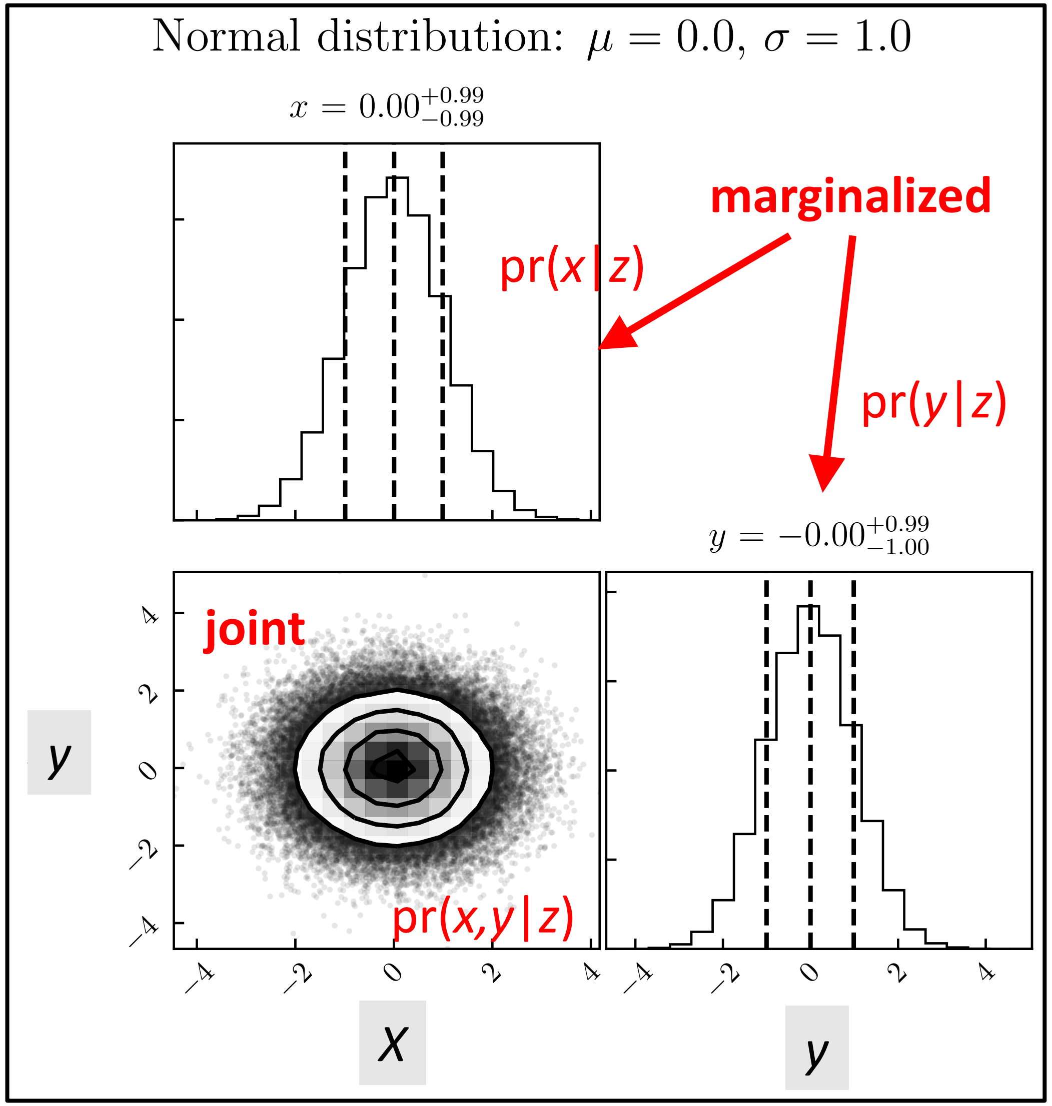
Q from nuclear energies (*A* < 8 vs. *A* ≥ 8)



Maris, Roth et al., PRC (2022)

❑ Account for correlations in inputs and observables

- pr(*x*, *y*| *z*) "joint probability (density) of *x* and *y* given z" (*contingent* on *z*)



$$\mathcal{N} e^{-\frac{1}{2}\mathbf{r}^\intercal \Sigma^{-1}\mathbf{r}} = \mathcal{N} e^{-\frac{(x-\mu)^2}{2\sigma_x^2}} e^{-\frac{(y-\mu)^2}{2\sigma_y^2}}$$

$$\mathbf{r} = \begin{bmatrix} x \\ y \end{bmatrix} \qquad \Sigma = \begin{bmatrix} \sigma_x^2 & 0 \\ 0 & \sigma_y^2 \end{bmatrix}$$

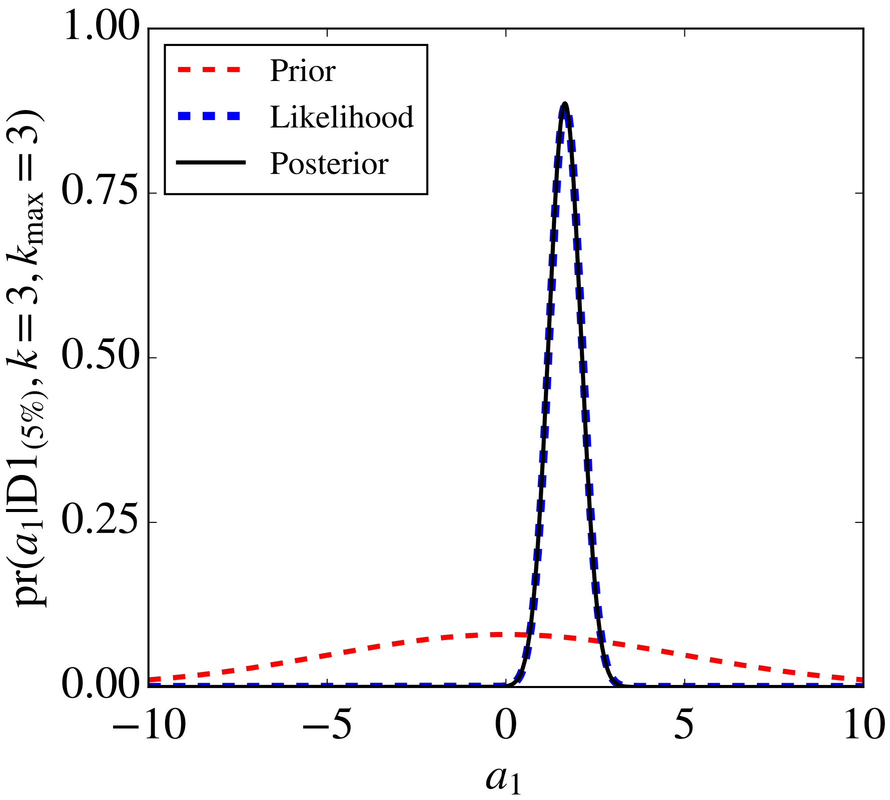
$$\text{e.g., } X - Y \sim \mathcal{N}(\mu_x - \mu_y, \sigma_x^2 + \sigma_y^2)$$

Bayes's Theorem: How to update knowledge in PDFs

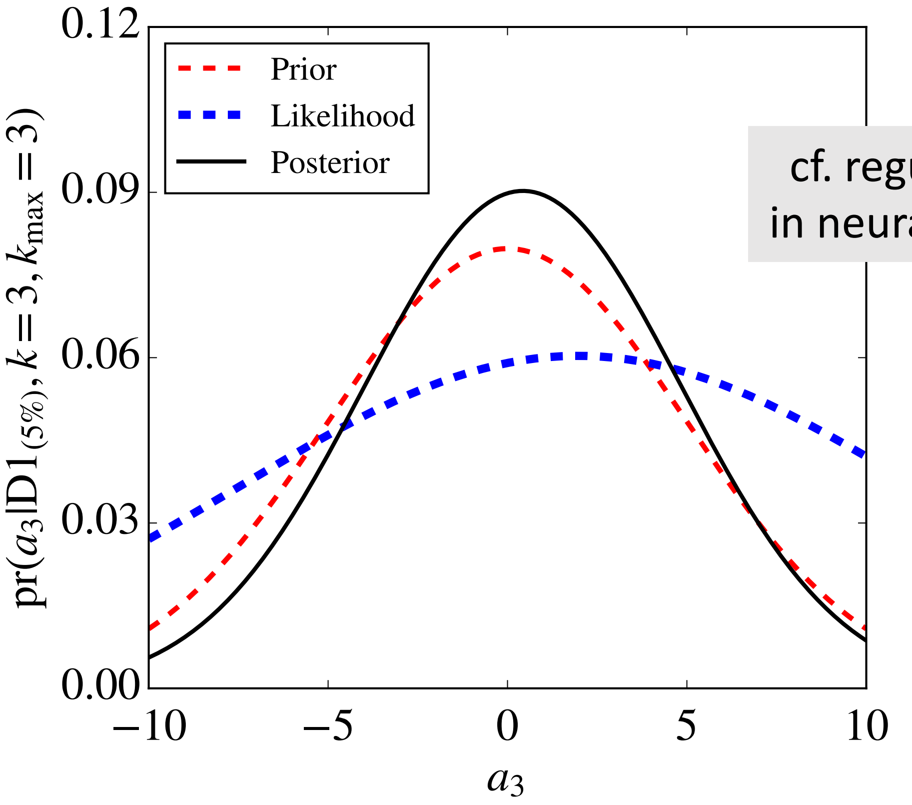
Bayesian updating of knowledge

$$\mathrm{pr}(A|B,I) = \frac{\mathrm{pr}(B|A,I)\mathrm{pr}(A|I)}{\mathrm{pr}(B|I)} \implies \underbrace{\mathrm{pr}(\boldsymbol{\theta}|\mathbf{y}_{\mathrm{exp}},I)}_{\text{posterior}} \propto \underbrace{\mathrm{pr}(\mathbf{y}_{\mathrm{exp}}|\boldsymbol{\theta},I)}_{\text{likelihood}} \times \underbrace{\mathrm{pr}(\boldsymbol{\theta}|I)}_{\text{prior}}$$

Likelihood overwhelms prior



Prior suppresses unconstrained likelihood



cf. regularization in neural networks