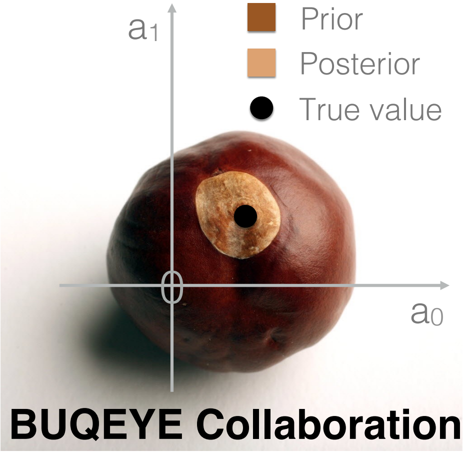
Statistically rigorous analyses of light nuclei with chiral interactions

Dick Furnstahl
Chiral Dynamics 2021, November 2021

The Ohio State University



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

Outline

- Bayesian methods for uncertainty quantification
- Challenges for analyses of light nuclei
- “Sampling” of applications to light nuclei
- Recap and future prospects

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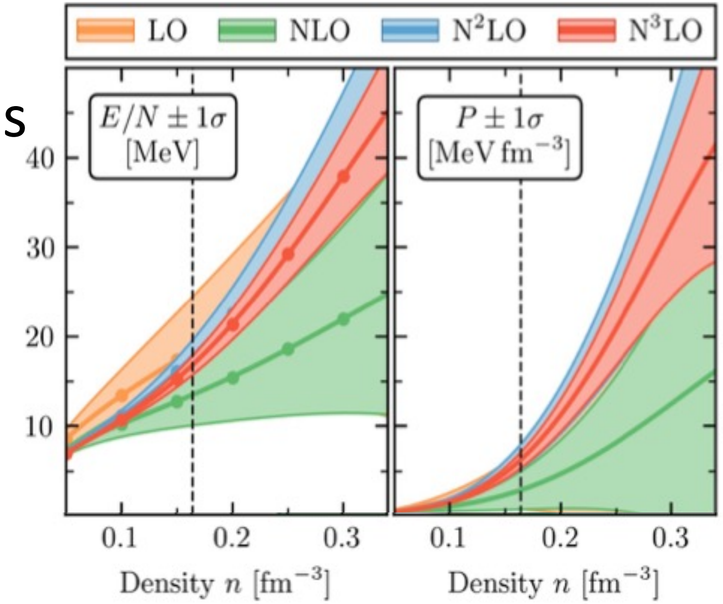
Goals of uncertainty quantification (UQ) for chiral EFT

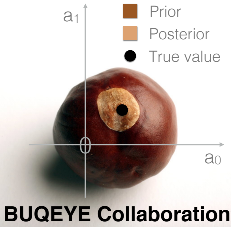
- Full accounting of experiment and theory uncertainties
- Propagation of errors from LEC fits to observables
- Order-by-order error bars or bands for observables
- Statistical assumptions are explicit and testable
- Provide advice on what experiment to do next
- Comparison or *combination* of EFT implementations

Bayesian statistics enables *all* of these goals!

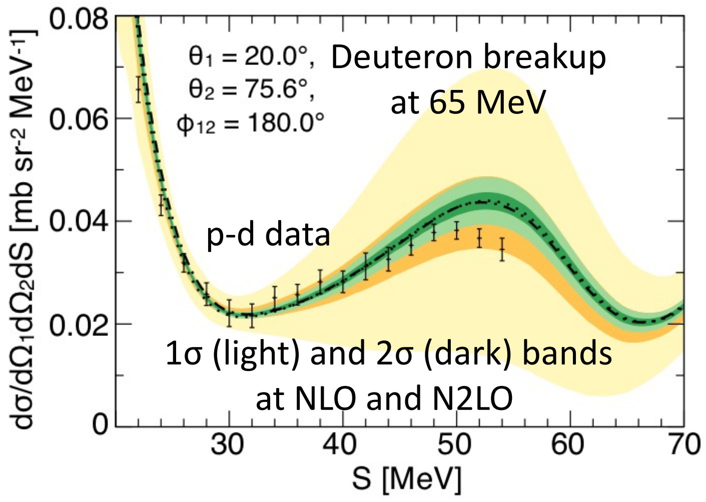
$$\mathrm{pr}(A|B,I) = \frac{\mathrm{pr}(B|A,I)\,\mathrm{pr}(A|I)}{\mathrm{pr}(B|A)}$$



From Drischler et al., PRL 125 (2020)



See talk by C. Drischler, Friday 21:20



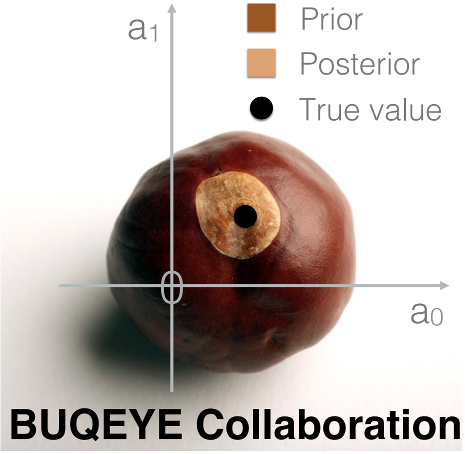
From Maris et al., PRC 103 (2021)

LENPIC

See talk by H. Krebs, Thursday 20:20

What makes Bayesian UQ statistically rigorous?

- Incorporate all sources of experimental and *theoretical* errors
- Formulate *statistical models* for uncertainties
- Use informative priors (at least weakly informative)
- Account for correlations in inputs (type x) and observables (type y)
- Propagate errors through the calculation (e.g., LECs → observables)
- Use *model checking* to validate the model
- Include oversight by experts (statisticians)



For publications and talks, see https://buqeye.github.io/

Jupyter notebooks also!

Bayesian updating of knowledge

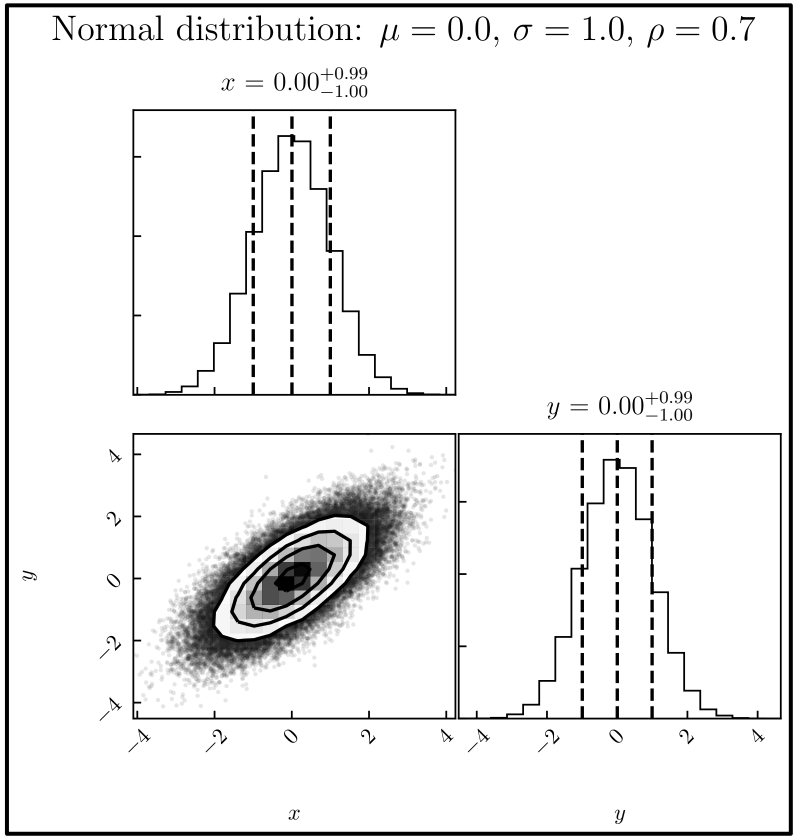
$$\mathrm{pr}(A|B,I) = \frac{\mathrm{pr}(B|A,I)\,\mathrm{pr}(A|I)}{\mathrm{pr}(B|I)} \Longrightarrow \underbrace{\mathrm{pr}(\boldsymbol{\theta}|\mathbf{y}_{\mathrm{exp}},I)}_{\text{posterior}} \propto \underbrace{\mathrm{pr}(\mathbf{y}_{\mathrm{exp}}|\boldsymbol{\theta},I)}_{\text{likelihood}} \times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

Characteristics of Bayesian statistics

- Update knowledge as new information comes in (prior → posterior)
- Almost everything has a probability distribution function (PDF)
- Takes advantage of hierarchical models (sub-models with parameters)
- Marginalize rather than optimize (integrate vs. point estimate)
- With many parameters most often *sample* the posterior with MCMC
- Can model, combine, and propagate systematic, correlated theory errors!

Bayesian updating of knowledge

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



$$\mathrm{pr}(\boldsymbol{\theta}|\mathrm{y}_{\rm exp}, \Sigma_{\rm exp}, \Sigma_{\rm th}, I) \propto e^{-\frac{1}{2}\mathbf{r}^\intercal(\Sigma_{\rm exp}+\Sigma_{\rm th})^{-1}\mathbf{r}} \times e^{-\boldsymbol{\theta}^2/2\bar{\theta}^2}$$

Two ways to treat the theory model discrepancy

Statistical model for observable ***y***: $\boldsymbol{y}_{\rm exp} = \boldsymbol{y}_{\rm th} + \delta\boldsymbol{y}_{\rm th} + \delta\boldsymbol{y}_{\rm exp}$

Advice from statisticians: *any* model for theory discrepancy is better than no model!

1. Model the distribution of residuals: $\boldsymbol{r} \equiv \boldsymbol{y}_{\rm exp} - \boldsymbol{y}_{\rm th}$

- $(\delta\boldsymbol{y}_{\rm exp})_n$ is often a Gaussian with mean $\mu = 0$ and variance σ_n^2 → error bars of size σ_n
- For $\delta\boldsymbol{y}_{\rm th}$, look at pattern of residuals and *model* it (train and test; correlated → GP).

2. For effective field theories (EFT), learn from *convergence pattern*

- Expect that each order will *roughly* improve by expansion parameter $Q < 1$:

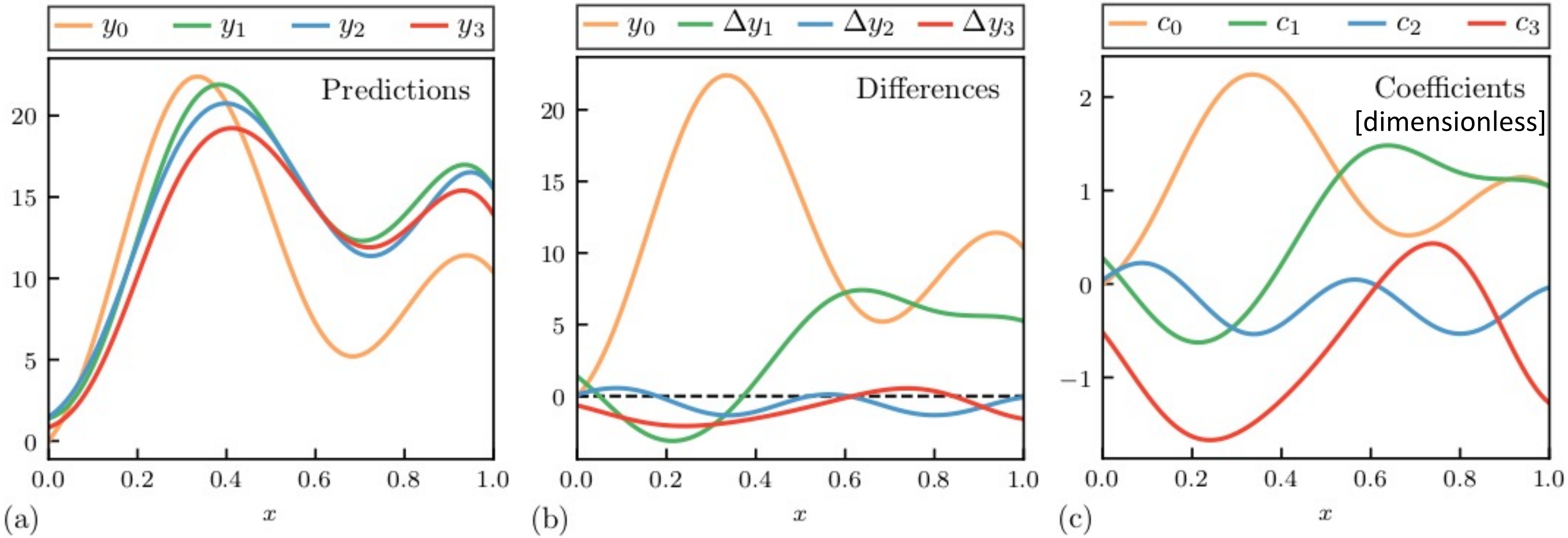
Theory at order k: $\boldsymbol{y}_k = \boldsymbol{y}_{\rm ref} \sum_{n=0}^{k} c_n Q^n$ Omitted orders: $\delta\boldsymbol{y}_{\rm th} = \boldsymbol{y}_{\rm ref} \sum_{n=k+1}^{\infty} c_n Q^n$

- **Treat the c_ns as random variables and learn their distribution from calculated orders**

Coefficients for a Bayesian EFT truncation model (not LECs!)

x can be continuous (e.g., energy, angle, density,) or discrete (e.g., nuclear level).

Either case can be correlated!



- Order-by-order predictions of *y*: $y_{\rm th}(x) = y_0 \to y_1 \to \cdots \to y_k$
- Focus on differences: $\Delta y_n = y_n - y_{n-1}$ → rescale by reference and Q^n: $c_n \equiv \dfrac{\Delta y_n}{y_{\rm ref} Q^n}$
- Treat c_ns (*not* LECs!!) as random variables and learn from calculated orders

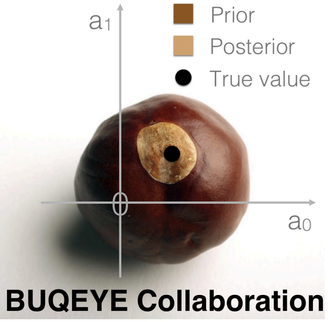
$$\boldsymbol{y}_k = \boldsymbol{y}_{\rm ref} \sum_{n=0}^{k} c_n Q^n \;\rightarrow\; \delta \boldsymbol{y}_{\rm th} = \boldsymbol{y}_{\rm ref} \sum_{n=k+1}^{\infty} c_n Q^n$$

$$\chi{\rm EFT} \Rightarrow Q = \frac{\{p, m_\pi\}}{\Lambda_b}, \quad \Lambda_b \approx 600\,{\rm MeV}$$

Assumption: behavior of c_ns persists across orders with characteristic size $\bar{c}$ (natural)

Fast & rigorous constraints on chiral three-nucleon forces from few-body observables

S. Wesolowski, I. Svensson, A. Ekström, C. Forssén, rjf, J. A. Melendez, and D. R. Phillips

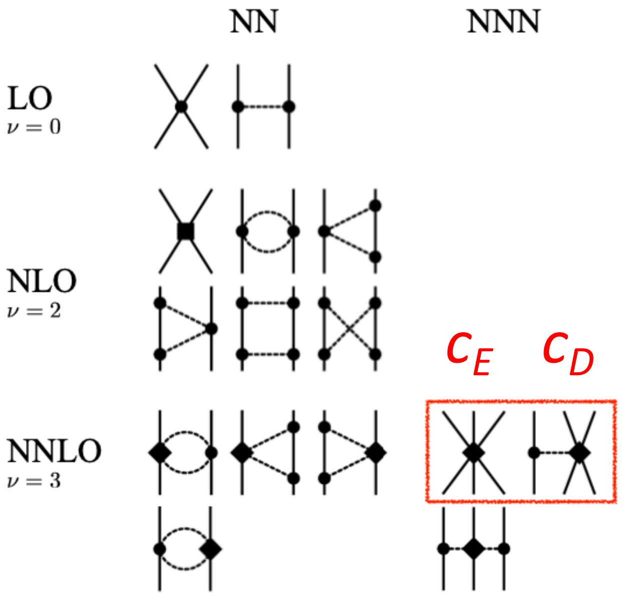


BUQEYE Collaboration

Notebook with all figures at
https://buqeye.github.io

arXiv:2104.04441
PRC (in press)

See talk by Daniel Phillips, Tuesday 20:30 [Few-Body] for physics and stats details



Fast: uses eigenvector continuation emulators for observables

Rigorous: statistical best practices for parameter estimation

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

(almost) Full Bayesian approach to constraining parameters

Experimental data

Other info (EFT scheme/scale, etc.)

$$\mathrm{pr}(\vec{a}, Q, \bar{c}^2 | \mathbf{y}_{\mathrm{exp}}, I) \propto \mathrm{pr}(\mathbf{y}_{\mathrm{exp}} | \vec{a}, \Sigma, I)\, \mathrm{pr}(\vec{a}|I)\;\; \mathrm{pr}(\bar{c}^2 | Q, \vec{a}, I)\;\; \mathrm{pr}(Q|\vec{a}, I)$$

NN *and* 3N LECs

EFT expansion parameter

Truncation error variance

Everything has priors!

All experiment and theory errors

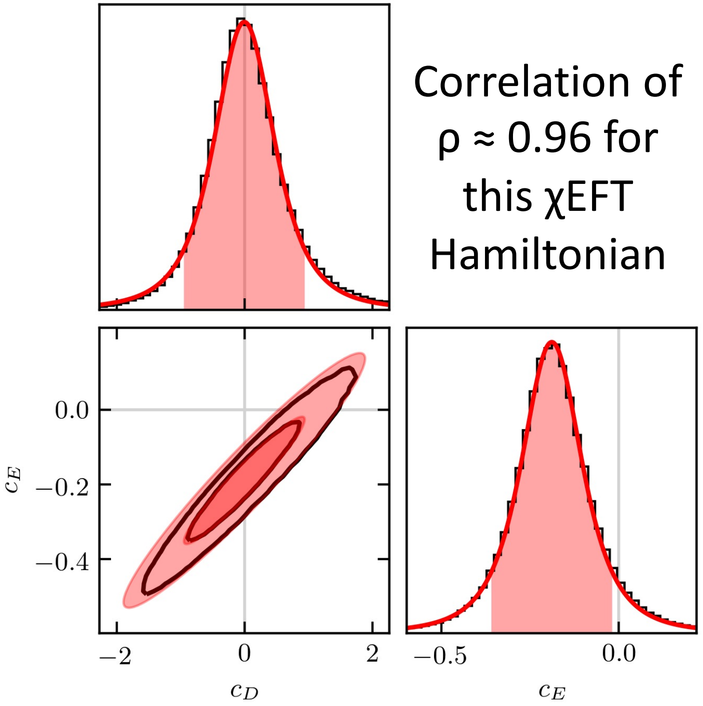
Likelihood: $\mathrm{pr}(\mathbf{y}_{\mathrm{exp}} | \vec{a}, \Sigma, I) \sim \mathcal{N}(\mathbf{y}_{\mathrm{th}}(\vec{a}),\; \Sigma_{\mathrm{exp}} + \Sigma_{\mathrm{method}} + \Sigma_{\mathrm{th}})$

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

Posteriors from "*Fast & Rigorous*" (arXiv:2104.04441)

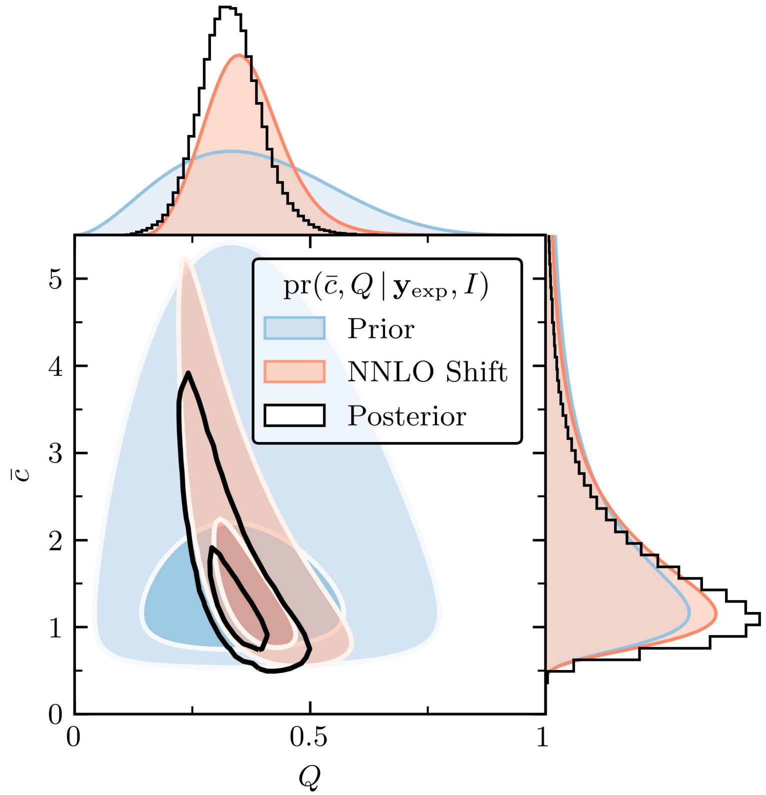
Posterior for c_D and c_E



Correlation of ρ ≈ 0.96 for this χEFT Hamiltonian

Tails are *not* well approximated by a Gaussian! (See Daniel P.'s talk!)

Posterior for Q and $\bar{c}$

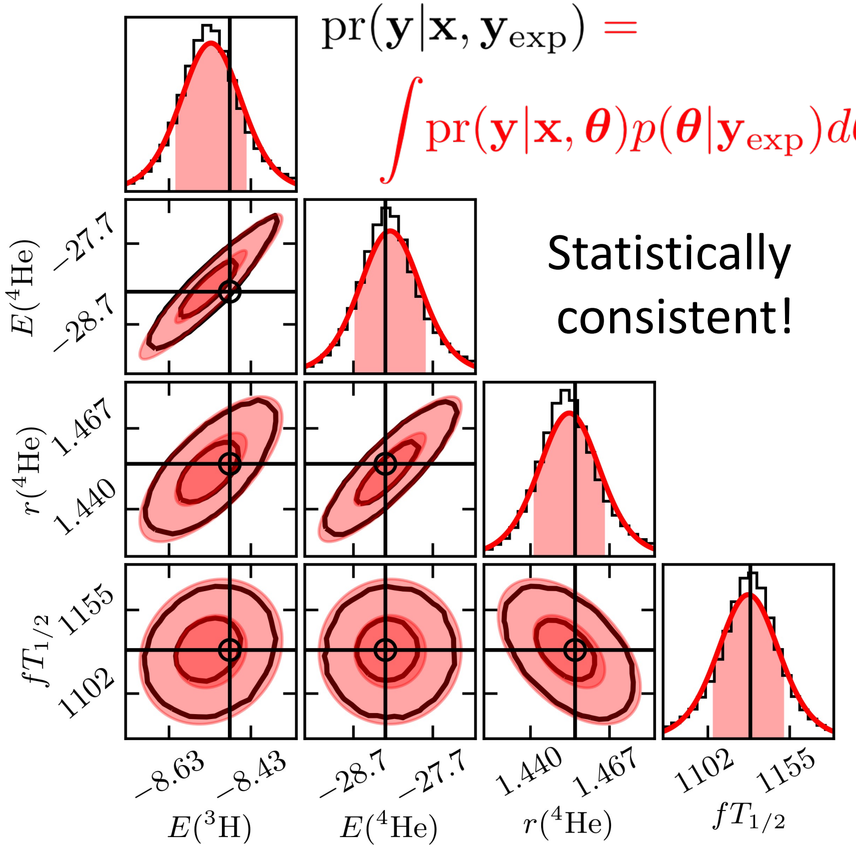


Truncation error for observables:

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

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!

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

Outline

- Bayesian methods for uncertainty quantification
- Challenges for analyses of light nuclei
- "Sampling" of applications to light nuclei
- Recap and future prospects

Challenge 1: Computational cost

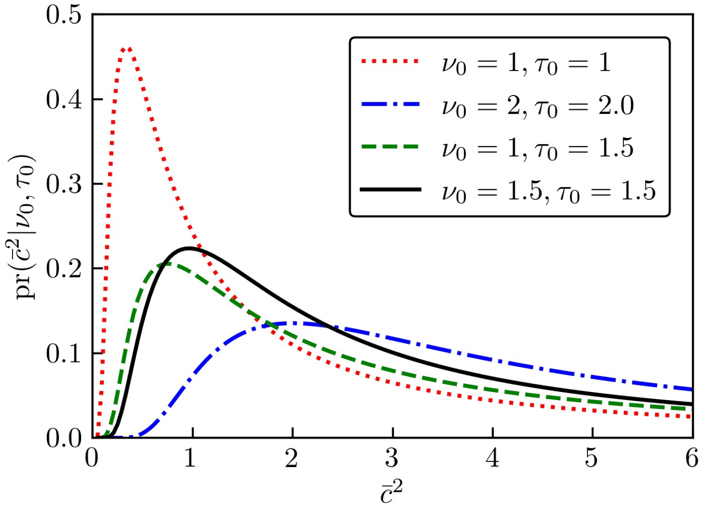
Calculating Bayesian pdfs and expectation values can be prohibitively costly for expensive likelihood. What can we do to mitigate the cost?

→ 1. **Use conjugate priors:** for some likelihoods, posterior pdf is in same family as prior pdf → analytical updating of posterior. An example is the EFT truncation variance:

$$\underbrace{\mathrm{pr}(\bar{c}^2|\{c_n\})}_{\sim\chi^{-2}(\nu,\tau^2)} \propto \underbrace{\mathrm{pr}(\{c_n\}|\bar{c}^2)}_{\sim\mathcal{N}(0,\bar{c}^2)}\ \underbrace{\mathrm{pr}(\bar{c}^2)}_{\chi^{-2}(\nu_0,\tau_0^2)} \leftarrow$$

$$\nu = \nu_0 + n_c$$

$$\nu\tau^2 = \nu_0\tau_0^2 + \sum_n c_n^2$$



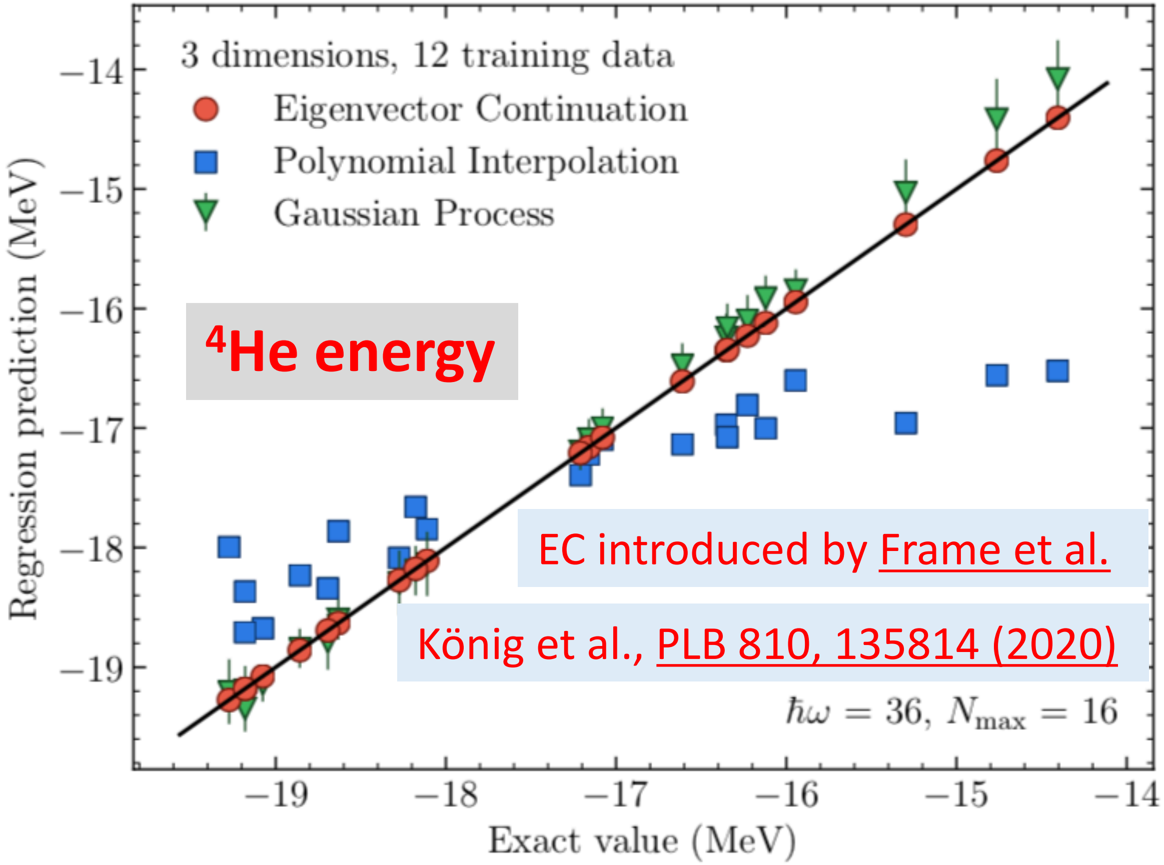
2. **Gaussian approximation** (data >> model complexity)

3. **Variational approximation** (approximate the posterior)

→ 4. Sample with Markov chain Monte Carlo (MCMC) using an ***emulator***
   → Make a computer model of your calculation
   - Gaussian process model emulators [e.g., https://arxiv.org/abs/2004.08474]
   - Eigenvector continuation (EC) and extensions [König et al., PLB 810, 135814 (2020)]

Eigenvector continuation emulators for few-nucleon observables

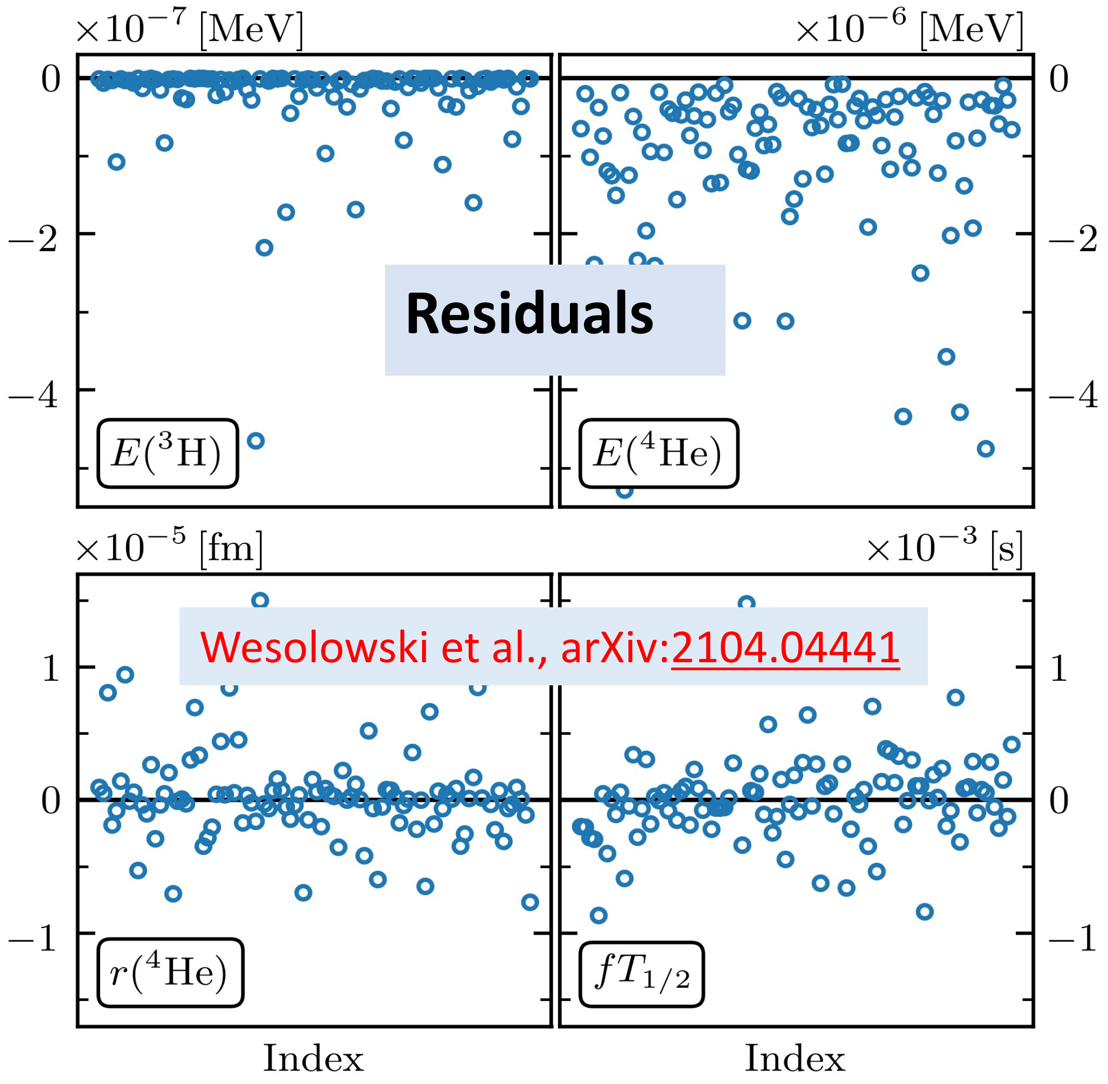
Basic idea: a small # of ground-state eigenvectors from a selection of parameter sets is an extremely effective variational basis for other parameter sets.
Characteristics: fast and accurate!



^{4}He energy

EC introduced by Frame et al.

König et al., PLB 810, 135814 (2020)



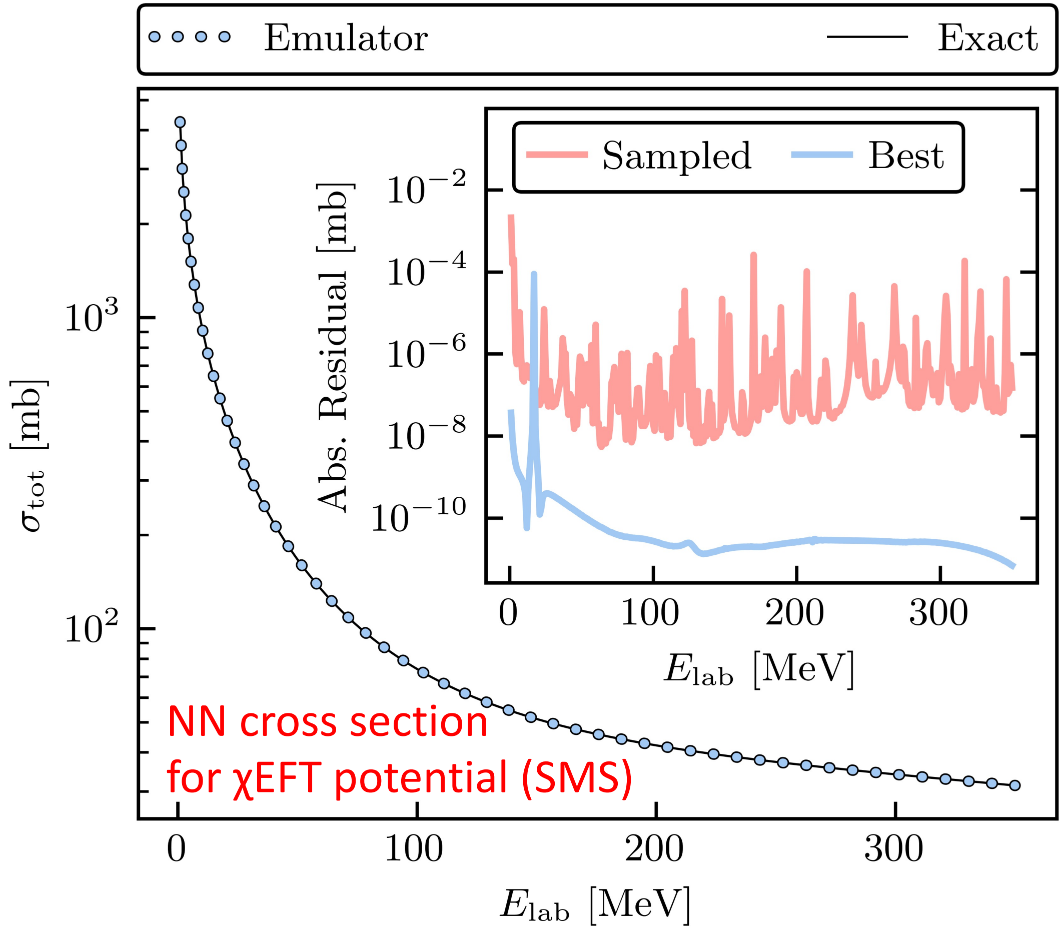
Residuals

Wesolowski et al., arXiv:2104.04441

Works well for transitions, too!

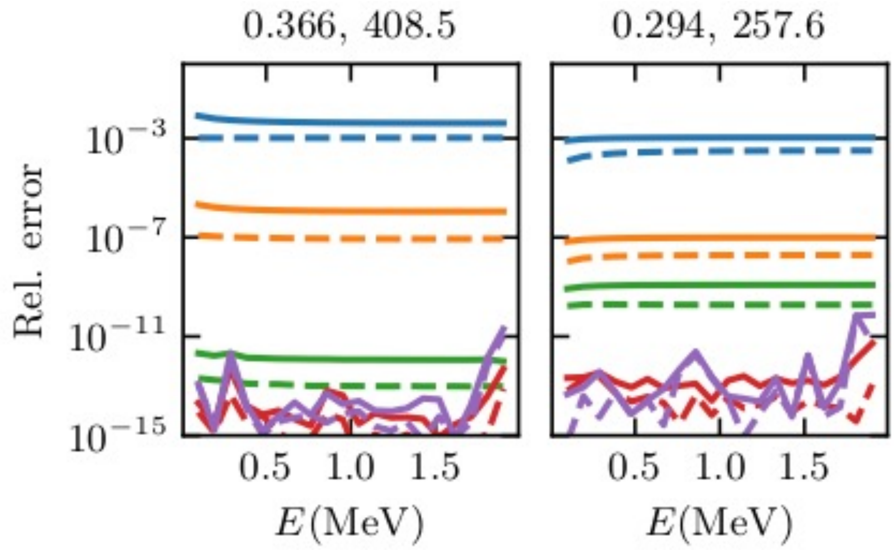
EC emulators for NN and 3N scattering

- EC extended to 2-body scattering by rjf et al., PLB (2020) using the Kohn variational principle.
- Method improved by Drischler et al., arXiv:2108.08269 (e.g., mitigate Kohn anomalies).
- Two-body emulation w/o wfs by Melendez et al., PLB 821, (2021) (Newton variational method).



NN cross section for χEFT potential (SMS)

What about 3-body scattering emulators?
Most useful for Bayesian χEFT LEC estimation.
→ Xilin Zhang recent proof of principle w/ KVP.



3-body S-matrix errors for basis size 3, 6, 9, 12, 14 with schematic potential for two test LEC points.

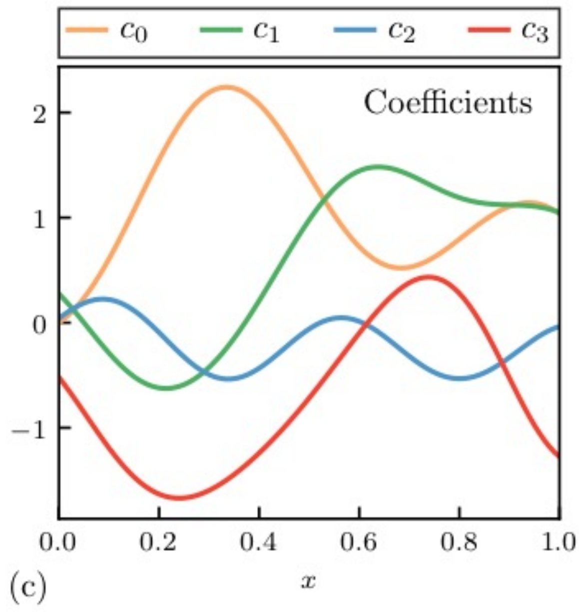
See also Sarkar and Lee, PRL 126 (2021) and arXiv:2017.13449 and Krackow group for Faddeev emulator, EPJA 57 (2021).

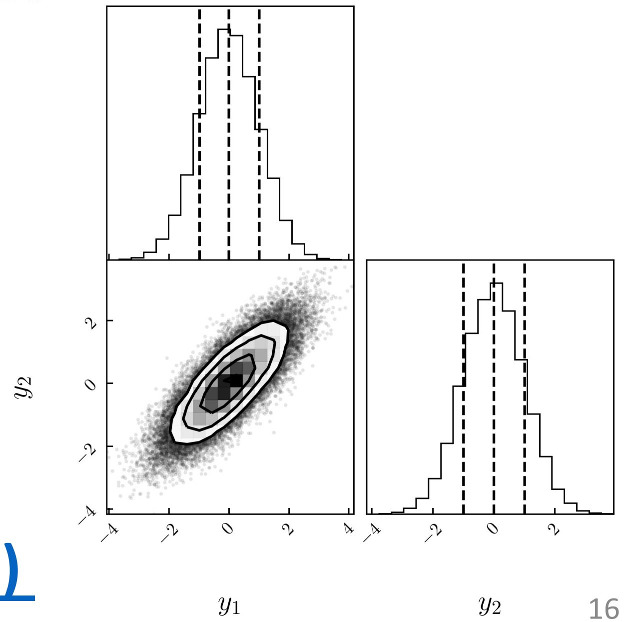
Challenge 2: Accounting for correlations

- **Type *x*:** Between observables *y(x)* and *y(x')* [also discrete]
  - Cross section at nearby energies; EOS at nearby densities
- **Type *y*:** Between observables $y_1(x)$ and $y_2(x)$ [or $y_2(x')$]
  - Symmetric and neutron matter; two energy levels

- **Possible consequences of correlations**
  - Overestimating information provided by correlated inputs
  - Overestimating errors in differences of observables

- **Rigorous statistical treatment of correlations**
  - Learn correlations (e.g., by training a Gaussian process)
  - Incorporate correlated errors (e.g., covariance *matrix* Σ_{th})
  - Model checking (e.g., Mahalanobis distance)





Refs.: Melendez et al., PRC 100 (2019); Drischler et al., PRC 102 (2020)

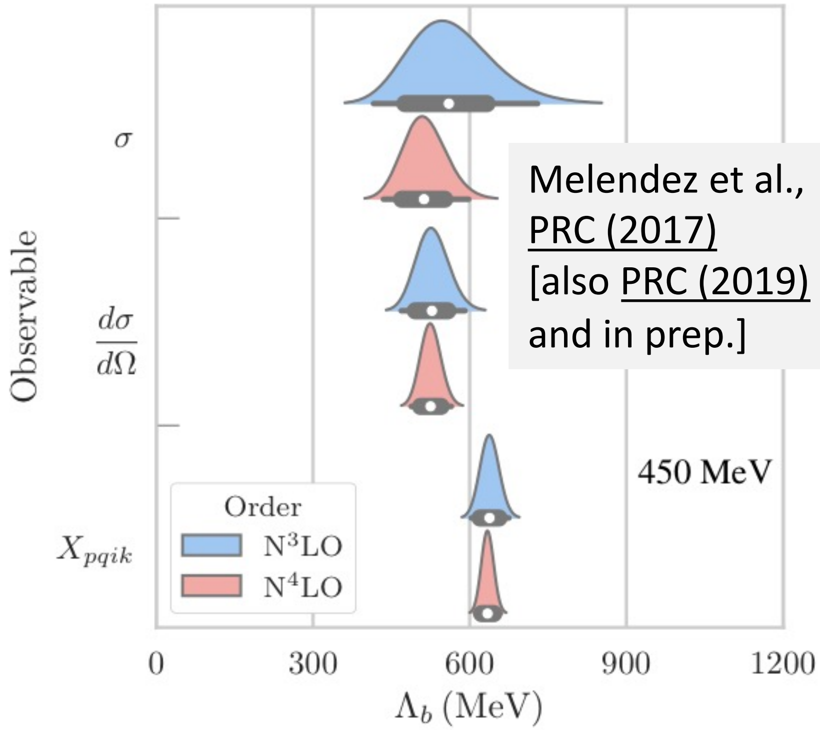
Challenge 3: Estimating the expansion parameter

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

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

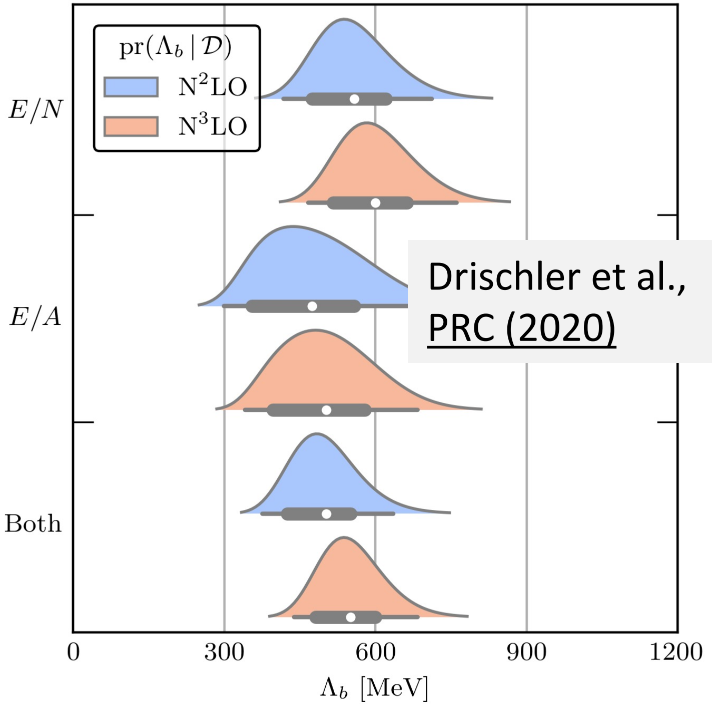
What about spectra of light nuclei?
Convergence pattern obscured at low order by KE vs. PE cancellation.
→ only use higher orders → Q ≈ 0.3
[consistent with $(m_\pi)^{\mathrm{eff.}}/\Lambda_b$ (see Ref.)]

Λ_b from NN observables



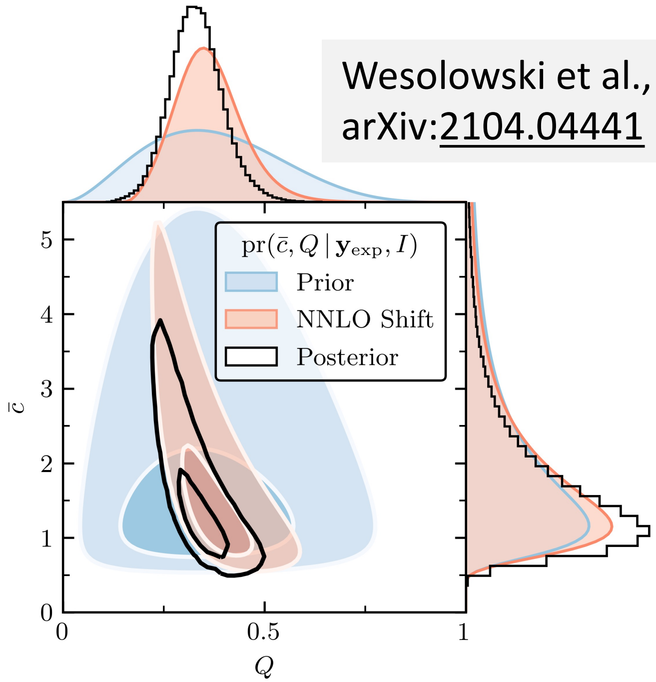
Melendez et al., PRC (2017) [also PRC (2019) and in prep.]

Λ_b from infinite matter



Drischler et al., PRC (2020)

Q from few-body observables



Wesolowski et al., arXiv:2104.04441

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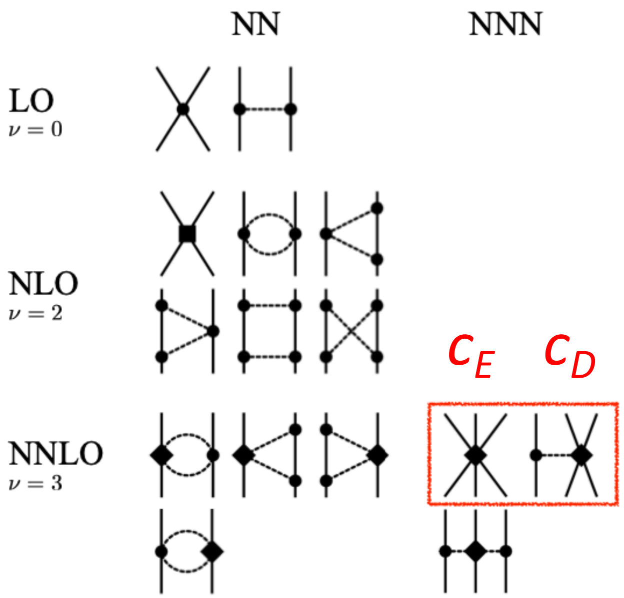
Light nuclei with semilocal momentum-space regularized chiral interactions up to third order

LENPIC Collaboration

https://www.lenpic.org/

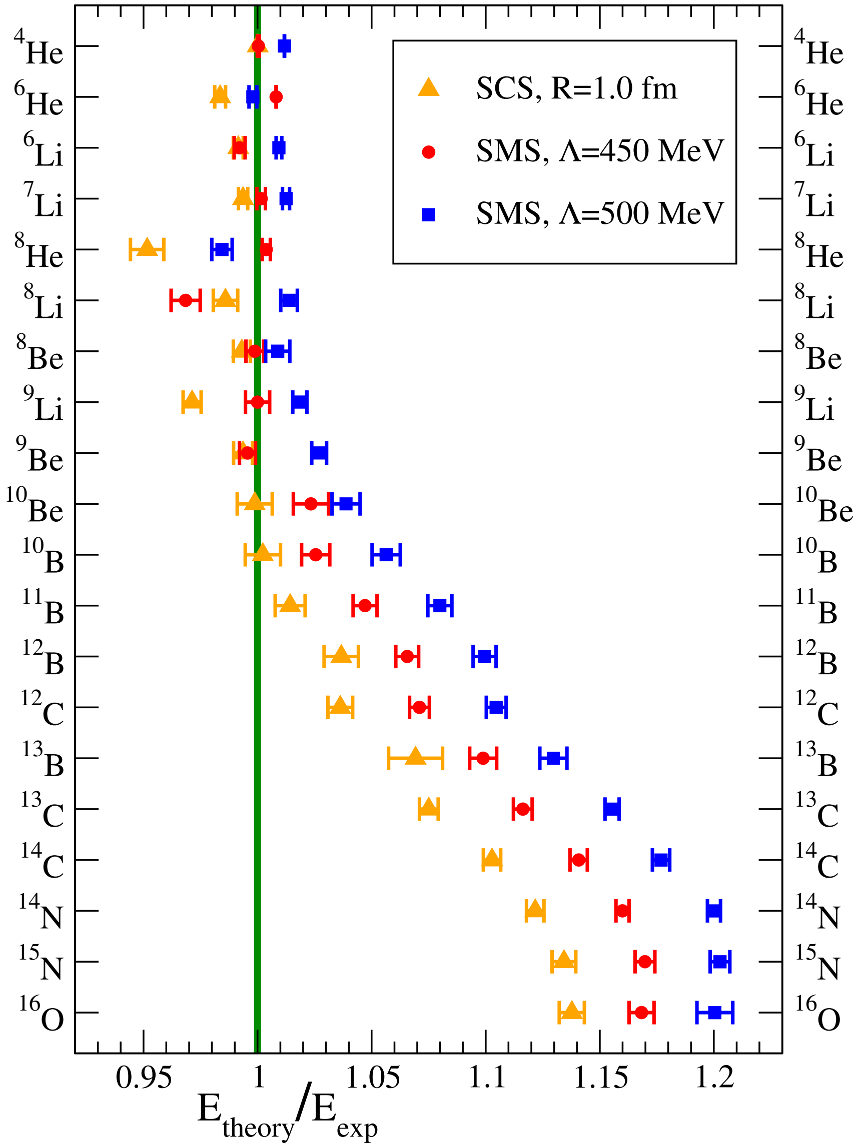
P. Maris et al.,
PRC **103**,
054001 (2021)
arXiv:2104.04441

See talk by Hermann Krebs, Thursday 20:20 for more on LENPIC physics and results



- *Consistent* NN and 3N potentials to N^2LO
- "Semilocal" to reduce regulator artifacts
- c_E and c_D from ^3H binding and *Nd* diff. cross section minimum
- Results for few-body and p-shell nuclei (NCCI plus SRG)
- Bayesian estimates of EFT truncation errors (also method error)
- Here: accounting for correlations in excitation energies

Ground-state energies with Bayesian truncation errors



[Error bars here from extrapolations only]

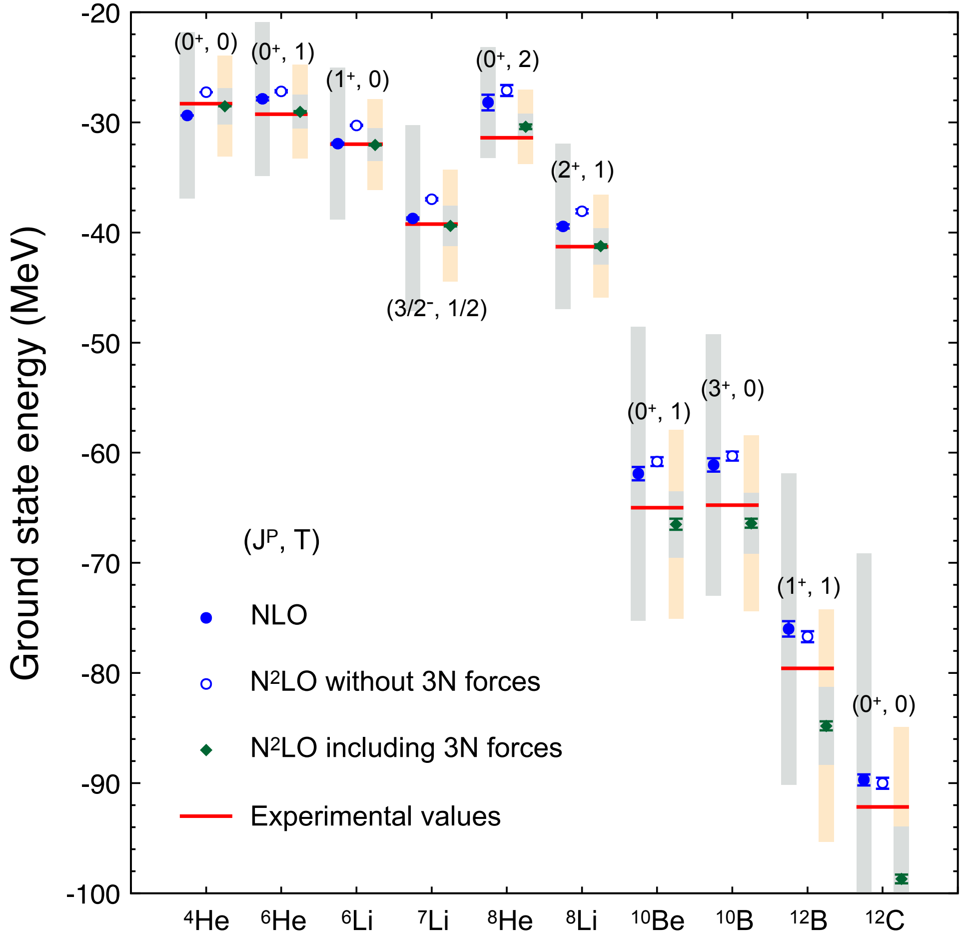
- Apply pointwise Bayesian:

$$\boldsymbol{y}_k = \boldsymbol{y}_{\mathrm{ref}} \sum_{n=0}^{k} c_n Q^n$$

→ learn c_n's from calculated orders and applied to omitted

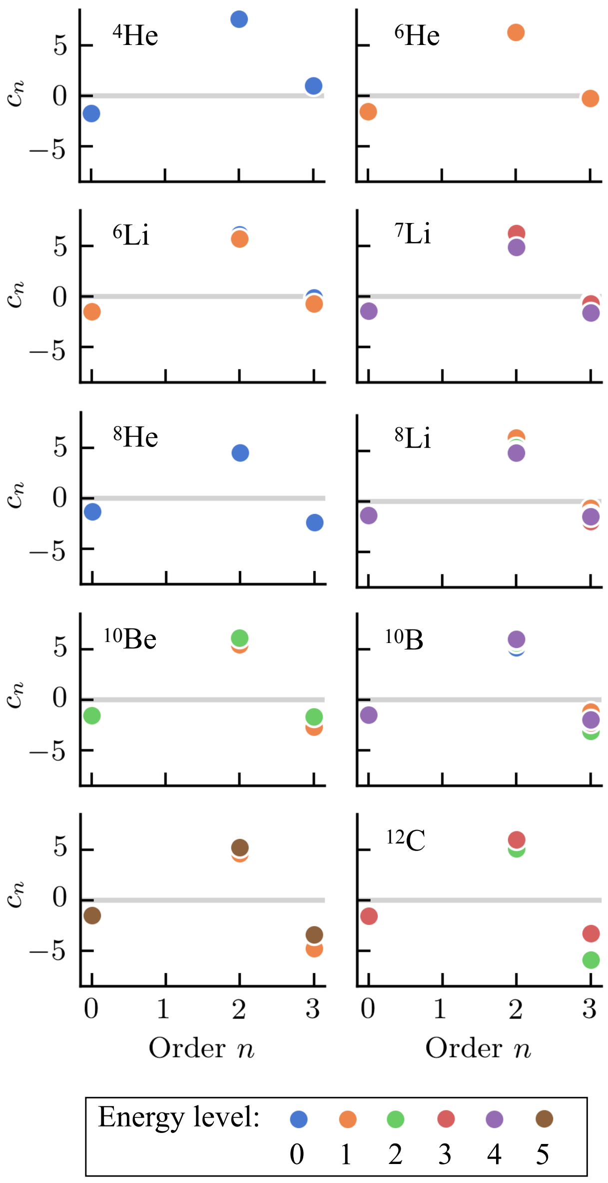
$$\delta \boldsymbol{y}_{\mathrm{th}} = \boldsymbol{y}_{\mathrm{ref}} \sum_{n=k+1}^{\infty} c_n Q^n$$

- Use experiment for $\boldsymbol{y}_{\mathrm{ref}}$
- Expansion param. Q ≈ 0.31
- E_{gs} up to A=10 agrees with experiment within 95% bands; overbound above



What about excitation energies and their errors?

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 $\delta \boldsymbol{y}_{\text{th}}$ 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 $\boldsymbol{y}_{\text{th}}$ coefficients c_n:

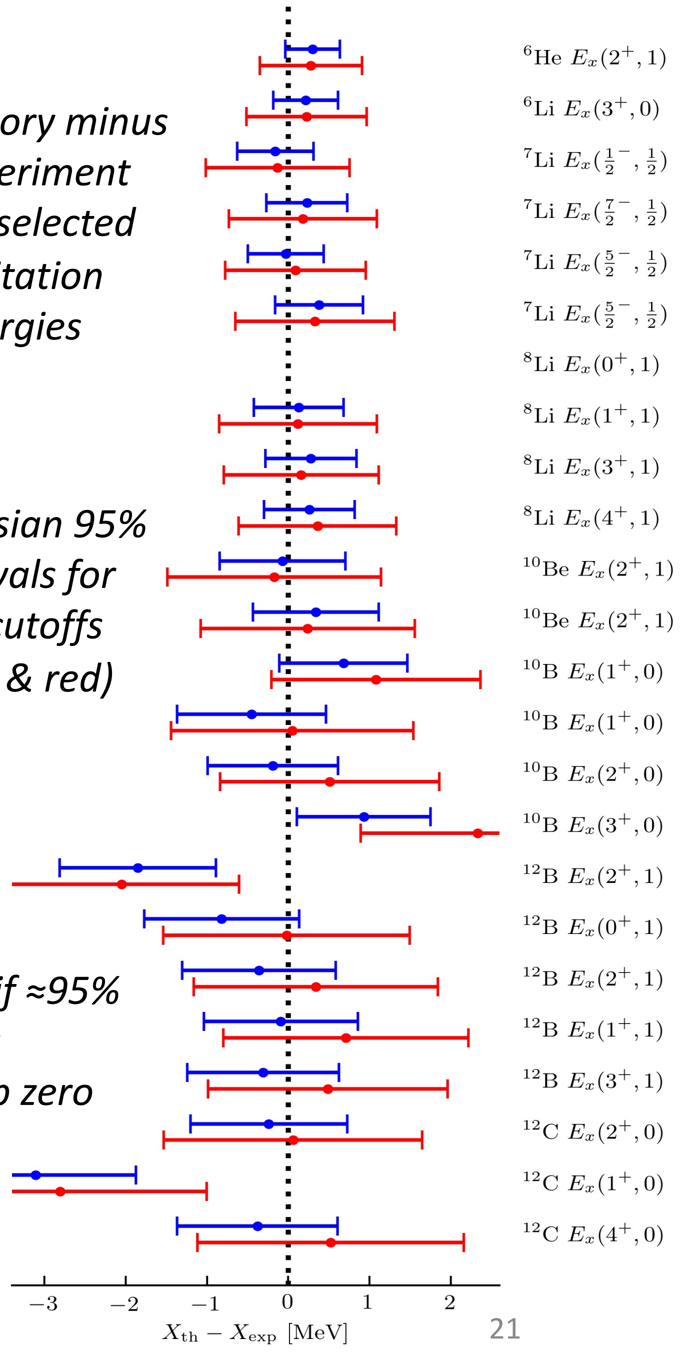
$$\boldsymbol{y}_k = \boldsymbol{y}_{\text{ref}} \sum_{n=0}^{k} c_n Q^n \qquad c_n \equiv \frac{\Delta y_n}{y_{\text{ref}} Q^n}$$

- **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.
- **Future:** N^{3}LO results will enable 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



Other Bayesian-based calculations in light nuclei

Note: this is only a subset of work adopting Bayesian statistical methods

- Mainz group (Acharya and Bacca), ***Gaussian process error modeling for chiral effective-field-theory calculations of np↔dγ at low energies,*** arXiv:2109.13972. χEFT with 1B+2B currents. Extends Bayesian methods for truncation error to an electromagnetic reaction cross section. "…an important step towards calculations with statistically interpretable uncertainties for astrophysical reactions involving light nuclei."

- LLNL/TRIUMF group (Kravvaris et al.), ***Quantifying uncertainties in neutron-alpha scattering with chiral nucleon-nucleon and three-nucleon forces,*** PRC **102** (2021). χEFT with EMN N4LO NN + N2LO 3N. Uses Gaussian Process Model (GPM) emulator. Bayesian UQ with combined uncertainties (incl. uncorrelated NCSM(-C) method and truncation errors). Many results on convergence, cD-cE correlations, phase shifts!

- Chalmers group (Djärv et al.), ***Fast & rigorous predictions for A=6 nuclei with Bayesian posterior sampling,*** arXiv:2108.13313. Non-local-MS-regulated χEFT with NN+3N. Introduces JupyterNCSM → construction and validation of EC emulators. Bayesian UQ with correlated truncation error → more precise predictions for separation energies and beta-decay Q-value. Many results!

Other Bayesian-based calculations in light nuclei

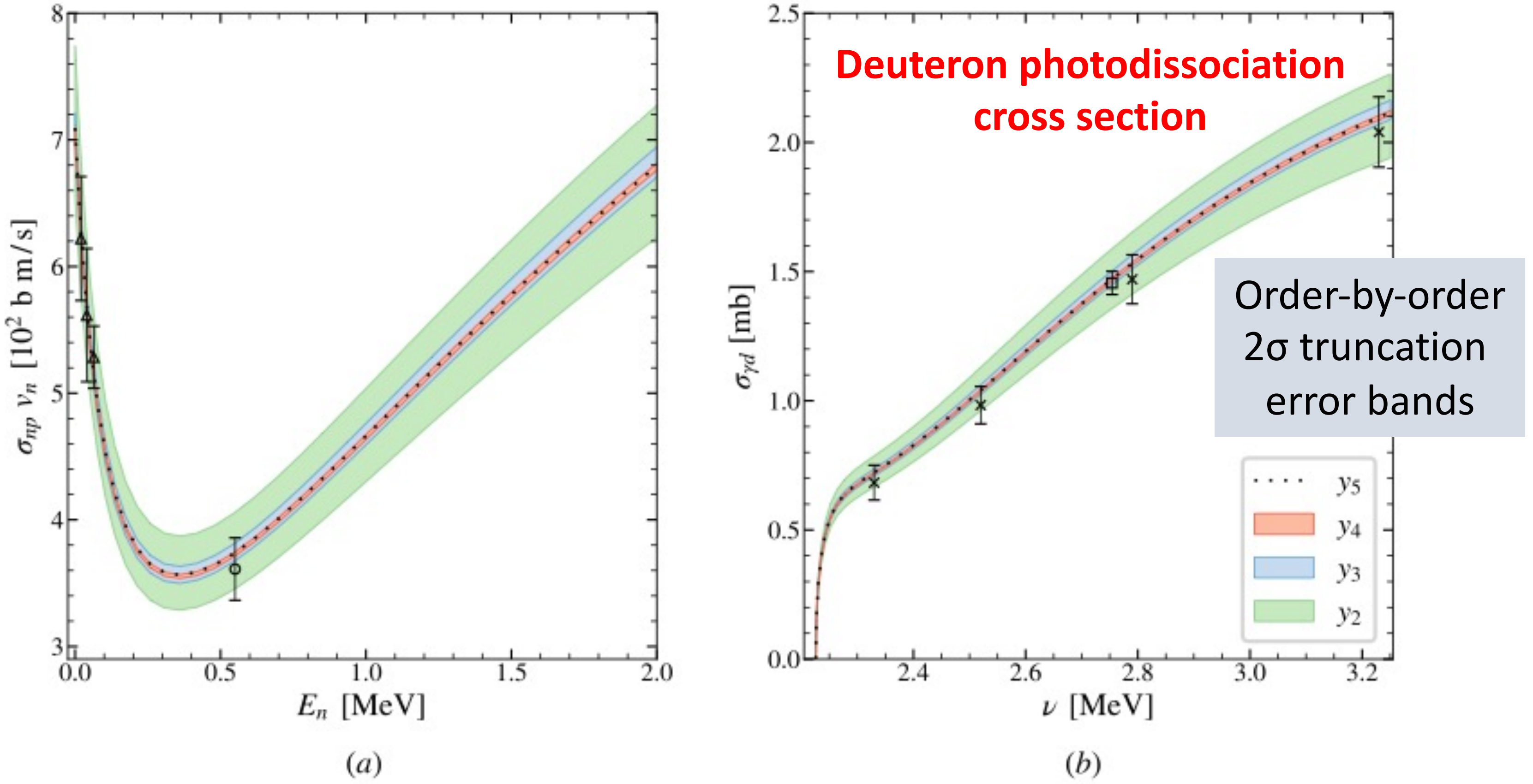


FIG. 3. The 2σ truncation error bands on the χEFT predictions y_k at $k = 2, 3, 4$ along with the prediction y_5 and data from Fig. 1. (a) The product of $p(n,\gamma)d$ cross section and the neutron speed versus the energy of the neutron. (b) The deuteron photodissociation cross section as a function of the photon energy in the rest frame of the deuteron.

Other Bayesian-based calculations in light nuclei

Model checking as in [Melendez et al., PRC (2019)]

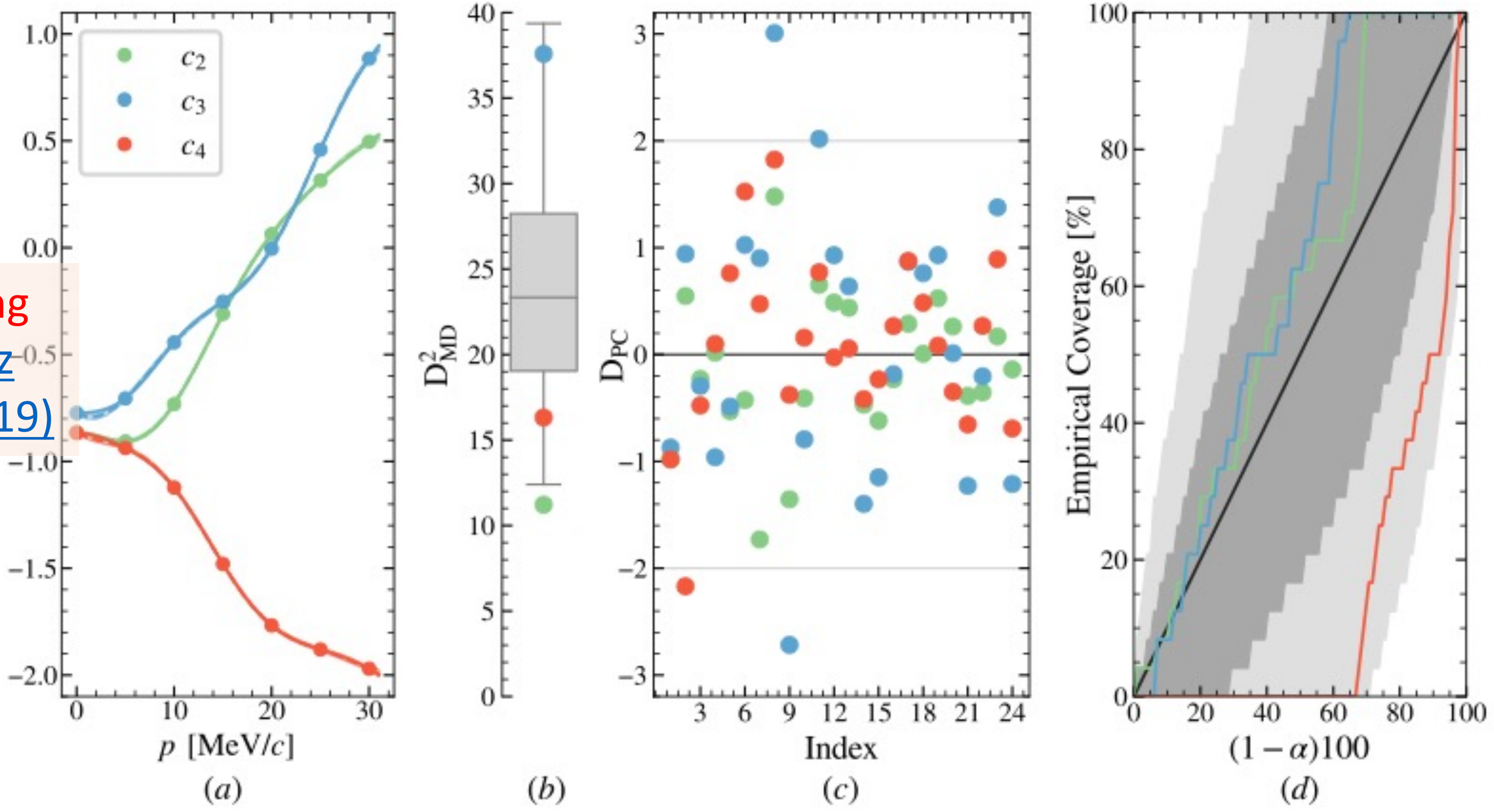


FIG. 2. GP modeling of the χEFT expansion coefficients and its diagnostics. (a) The simulators (solid lines) along with the corresponding GP emulators (dashed lines) and their 2σ intervals (bands). The training data are denoted by filled circles; 4 validation points are located uniformly between each adjacent pair of training points. (b) The Mahalanobis distances compared to the mean (interior line), 50% (box) and 95% (whiskers) credible intervals of the reference distribution. (c) The pivoted Cholesky diagnostics versus the index along with 95% credible intervals (gray lines). (d) The credible interval diagnostics with 1σ (dark gray) and 2σ (light gray) bands estimated by sampling 1000 GP emulators.

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Other Bayesian-based calculations in light nuclei

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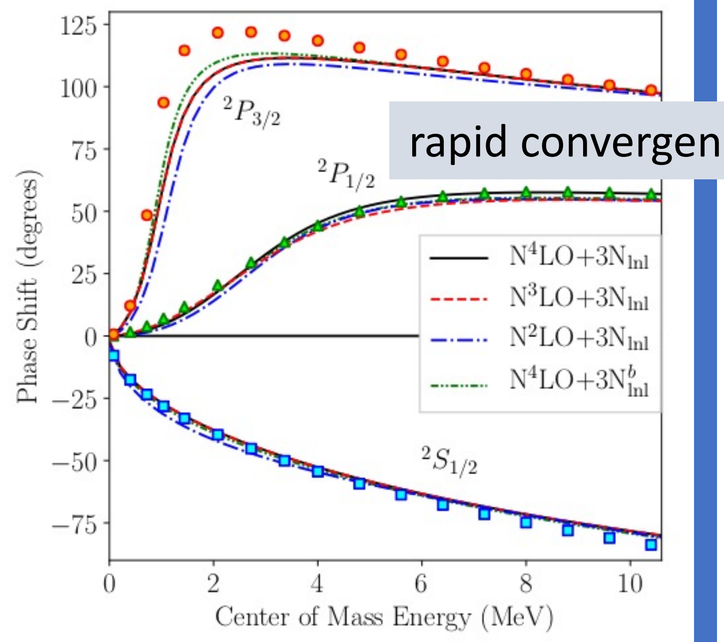

FIG. 3. Evolution of the n-α phase shifts (lines) from third to fifth order of the chiral expansion compared to the empirical phase shifts obtained from an accurate R-matrix analysis of $A = 5$ reaction data [39] (symbols).

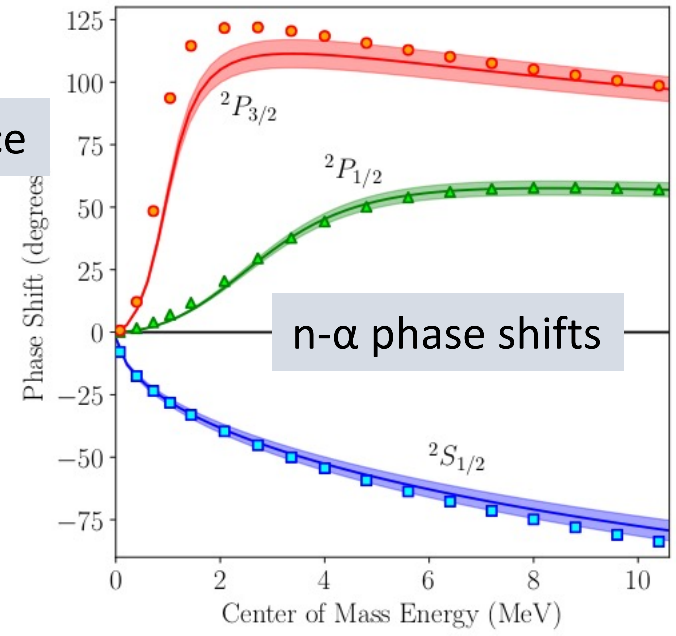

FIG. 4. Bayesian estimation of the uncertainty induced by the truncation of the chiral expasnsion. The bands correpsond to a 90% degree of belief interval estastimate at the fifth order in the chiral expansion.

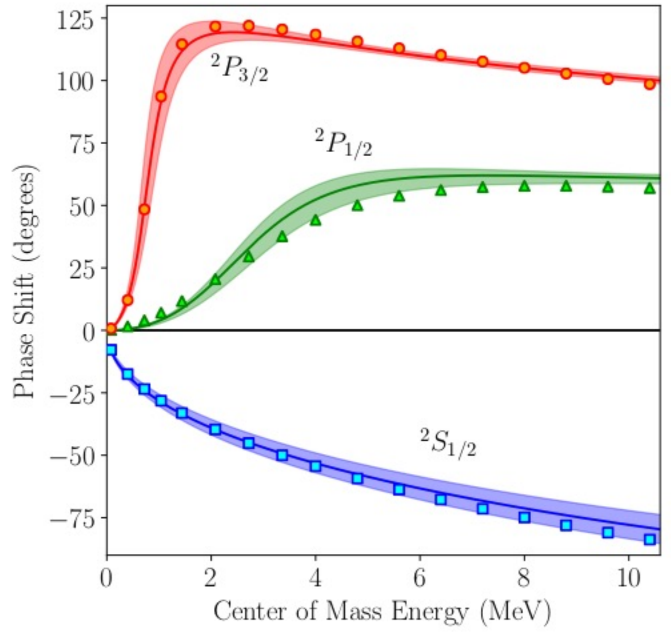

FIG. 9. Same as Fig. 7, but for the N^{3}LO*+3N$_{\rm loc}$ interaction.

Physics pointers from discrepancies

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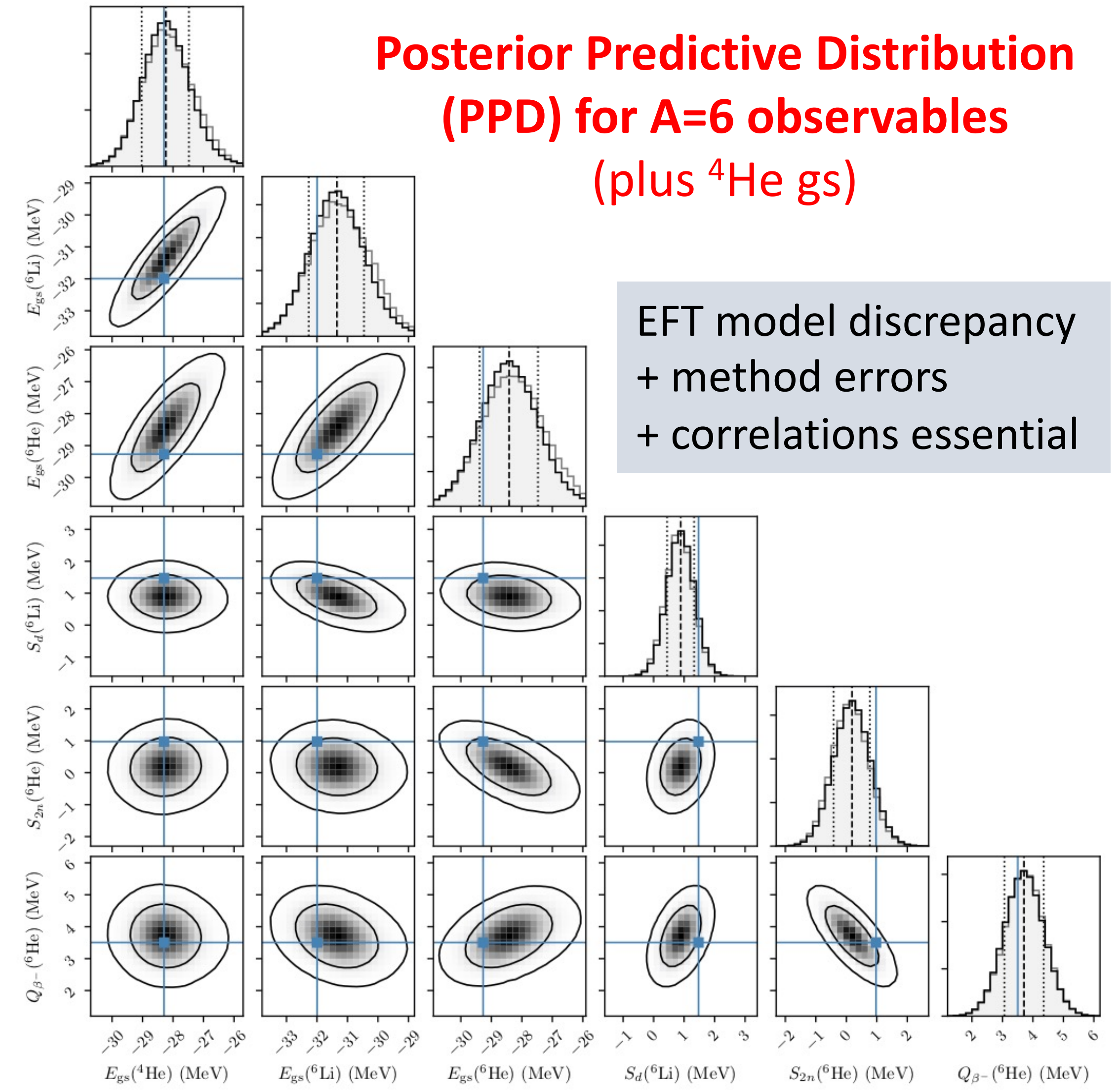
N

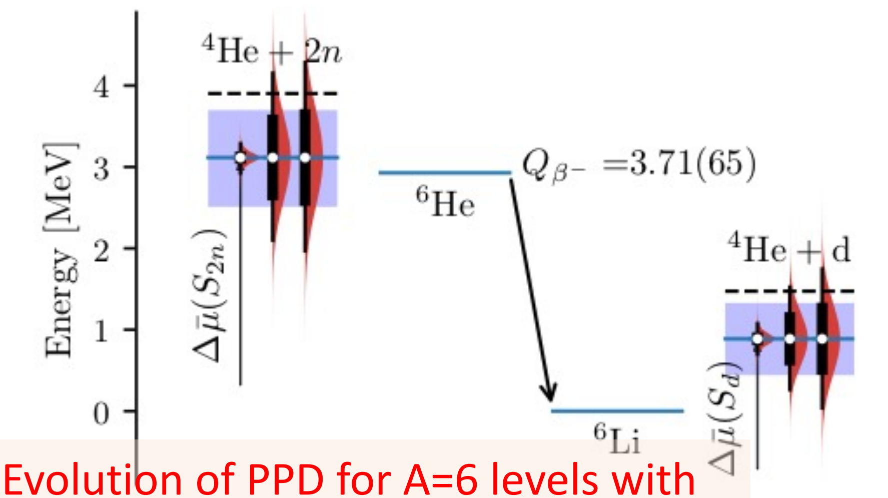
Posterior Predictive Distribution (PPD) for A=6 observables

(plus ^{4}He gs)



EFT model discrepancy
+ method errors
+ correlations essential

FIG. 8. Full PPD for binding energies and thresholds including both method and model (EFT truncation) uncertainties. The dashed (dotted), vertical lines on the diagonal show the median (68% credible interval), while the blue, solid lines indicate the experimental values. See also Table II. The open, grey histograms on the diagonal represent low-statistics results based on only 25 LEC samples (see text for details). The level curves in the off-diagonal panels show the 68% and 95% probability mass regions of the bivariate distributions.



Evolution of PPD for A=6 levels with **method** and EFT truncation errors

FIG. 9. $A = 6$ level scheme. Dashed lines show experimental thresholds for $^4He + 2n$ ($^4He + d$) relative ^6He (^6Li) while the blue line and band show the median and 68% credible interval from the full PPD. The red distributions, from left to right, show the evolution of the PPD as we go from the NCSM prediction, PPD_{NCSM}, to the inclusion of method errors, and finally including the EFT truncation error—with thick (thin) vertical lines indicating the 68%(95%) credible interval. Note that the NCSM prediction for each threshold has been shifted by the mean values of the relevant method errors. The uncertainty in the β^--decay Q-value is dominated by the method (N_{max}-extrapolation) uncertainty.

se

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Outline

- Bayesian methods for uncertainty quantification
- Challenges for analyses of light nuclei
- “Sampling” of applications to light nuclei
- Recap and future prospects

Recap and takeaways

- **Bayesian methods enable statistically rigorous analyses of light nuclei**
  - Chiral power counting → statistical model for truncation error
  - Assumptions are explicit and testable → Bayesian model checking
  - Statistics for *diagnostics* and *discovery* (not just theory error bands)
- **Addressing challenges for analyses of light nuclei**
  - Fast & accurate emulators enable use of full Bayesian machinery
  - Correlations are important (both x,y) → account for them and exploit them
  - Learn chiral EFT expansion parameter from data and test consistency
- **Applications to light nuclei are growing**
  - More nuclei and hypernuclei; more interactions and higher order (e.g., N3LO)
  - More observables; consistent external currents

Future prospects for Bayesian analyses

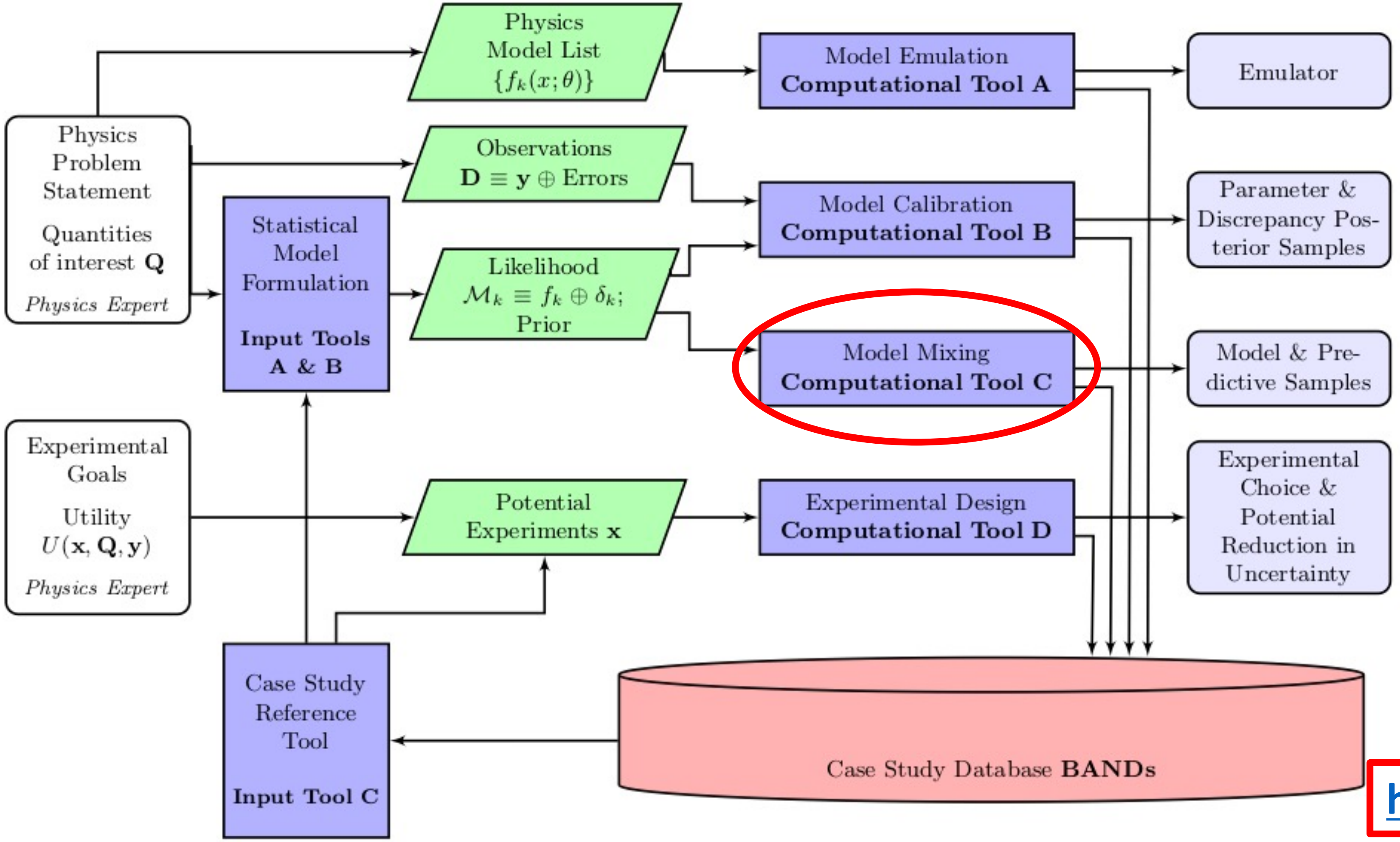
Relevant for light nuclei with chiral forces, but also more generally applicable

- Emulators: 3-body scattering with chiral forces; new emulator technology
- Exploiting statistical correlations in nuclear spectra using Bayesian tools
- Power counting at finite density (see talk by Christian Drischler on matter)
- External currents (see LENPIC talk by Hermann Krebs; talk by Saori Pastore)
- Experimental design (see Compton scattering talk by Harald Griesshammer)
- Bayesian frontier: model mixing (BAND collaboration)
- And much more . . .

BAND (Bayesian Analysis of Nuclear Dynamics)

An NSF Cyberinfrastructure for Sustained Scientific Innovation (CSSI) Framework (from 7/2020)

Look to https://bandframework.github.io/ over the coming years!



Bayesian Analysis of Nuclear Dynamics

ISNET 8 and the Second Annual BAND Camp is Dec. 13-17, 2021.
Hybrid meeting: remote participation by zoom.
See website for details on events and registration.

https://indico.frib.msu.edu/event/47/

Propaganda: Jupyter notebooks for Bayesian UQ

- Jupyter notebooks and Python are great tools for nuclear physics UQ
- E.g., Bayesian methods for EFT and other theory errors (combined with experiment)
  - Many examples from the BUQEYE collaboration [see https://buqeye.github.io/]
- Aspiration: *every* paper should provide a notebook for reproducing figures

- Github repositories with notebooks for learning Bayesian statistics for physics
  - ➢ BAYES 2019 (TALENT course): https://nucleartalent.github.io/Bayes2019/
    [developed by Christian Forssén, rjf, Daniel Phillips]
  - ➢ Christian Forssén's course at Chalmers in Jupyter Book format with notebooks: https://physics-chalmers.github.io/tif285/doc/LectureNotes/_build/html/
  - ➢ rjf course at Ohio State with notebooks: https://furnstahl.github.io/Physics-8820/
    [Jupyter Book based on BAYES 2019 and updates by rjf and C. Forssén]

Thank you!

Extra slides

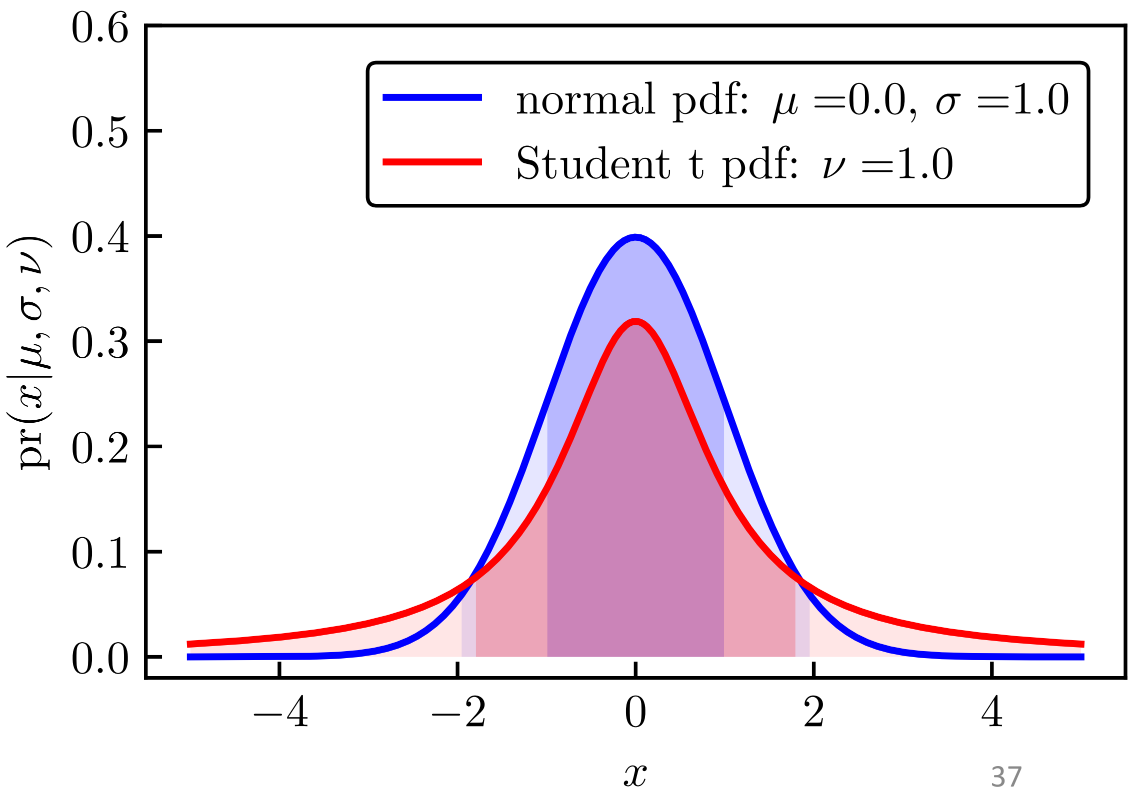
State of knowledge as probability distributions (pdfs)

- 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 $|\psi(x, y)|^2$ or $|\psi(x)|^2 = \int |\psi(x, y)|^2 \, dy$ (*marginalization*)
- Bayesian confidence (credible) interval:

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

Examples of pdfs for theory UQ:

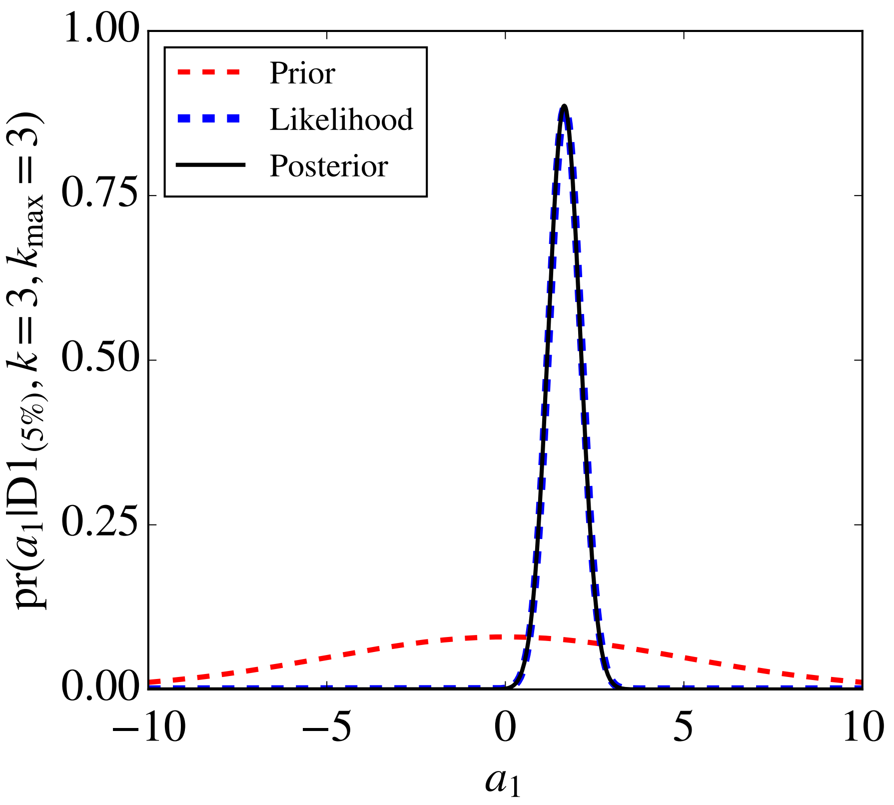
$\mathrm{Pr}(\boldsymbol{\theta} \mid \mathbf{y}_{\mathrm{exp}}, \Sigma_{\mathrm{exp}}, \Sigma_{\mathrm{th}}, I) \Rightarrow$
pdf of model parameters $\boldsymbol{\theta}$ given data y_{exp} and experiment/theory errors Σ, plus other information I



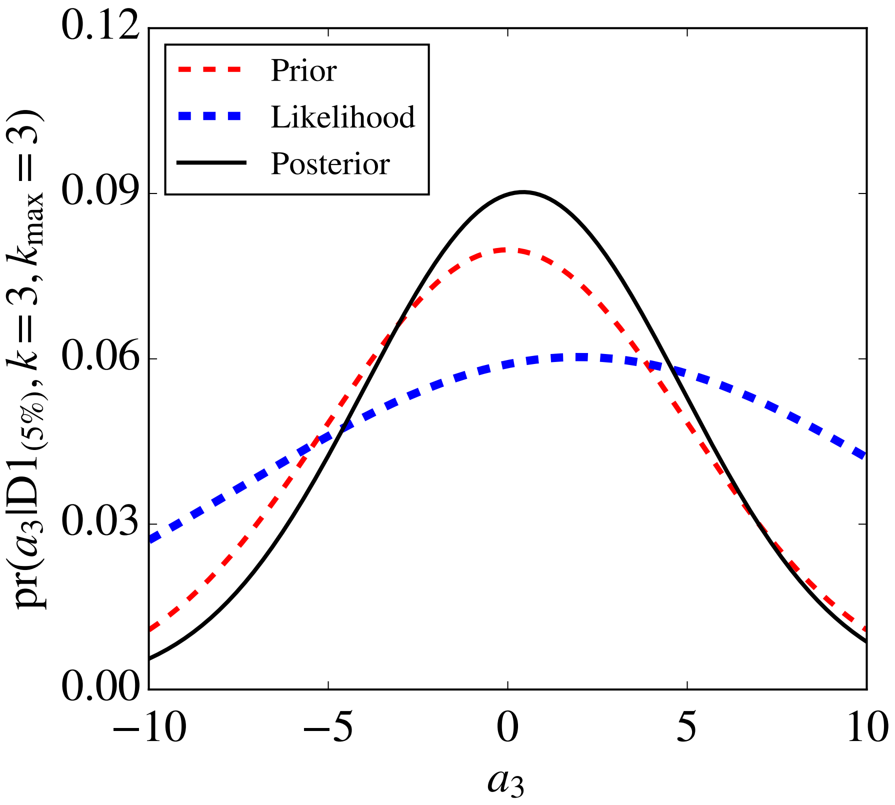
Bayes's Theorem: How to update knowledge in PDFs

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

Likelihood overwhelms prior



Prior suppresses unconstrained likelihood



The BUQEYE Cheatsheet for Pointwise Truncation Errors (arXiv:1904.10581)

From observable y, extract coefficients

$$\vec{y}_k \equiv \{y_0, y_1, \cdots, y_k\} \qquad \text{(A1)}$$
$$\Rightarrow \vec{c}_k \equiv \{c_0, c_1, \cdots, c_k\}$$

Choose ν_0 and τ_0. Update hyperparameters

$$\nu = \nu_0 + n_c \qquad \text{(A7)}$$
$$\nu\tau^2 = \nu_0\tau_0^2 + \vec{c}_k^{\,2} \qquad \text{(A8)}$$

Compute posterior

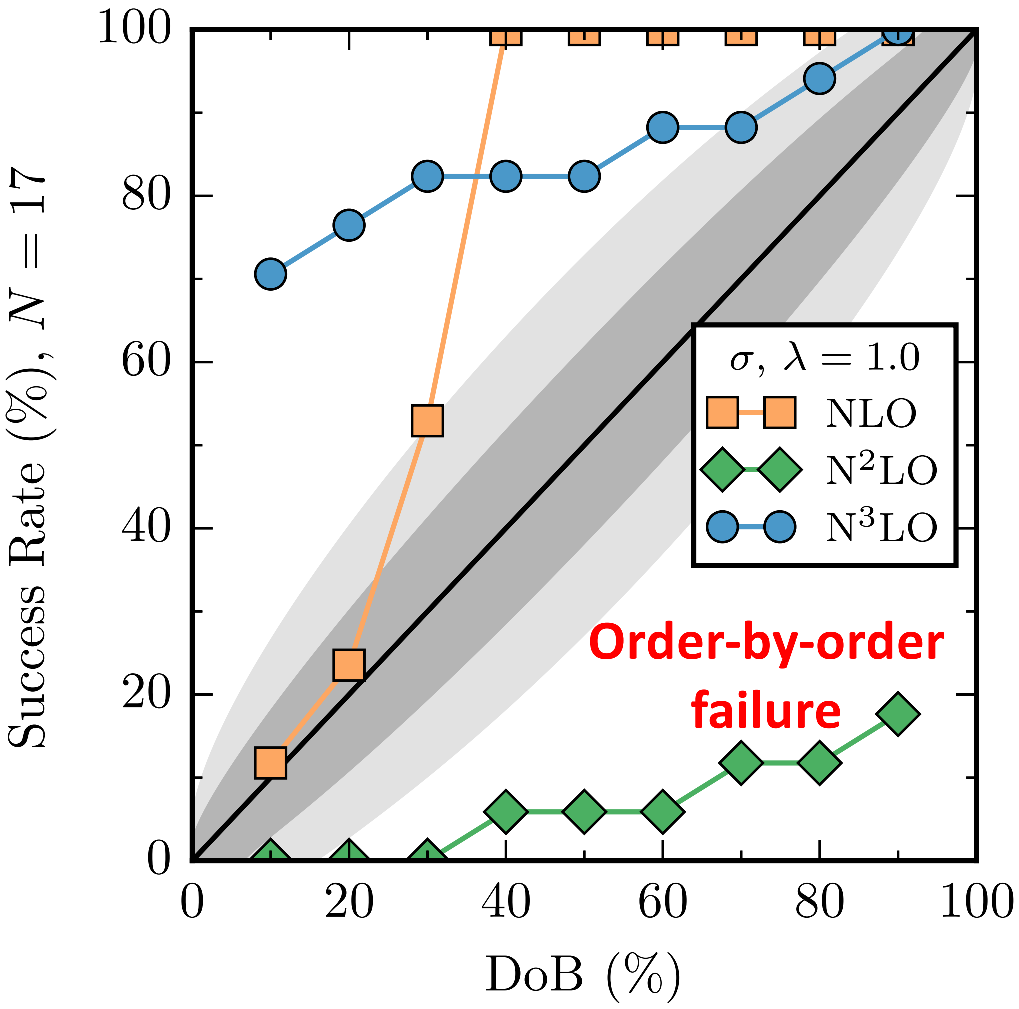
$$\mathrm{pr}(y \mid \vec{y}_k, Q) \sim t_\nu\left[y_k, y_{\mathrm{ref}}^2 \frac{Q^{2(k+1)}}{1-Q^2}\tau^2\right] \qquad \text{(A13)}$$

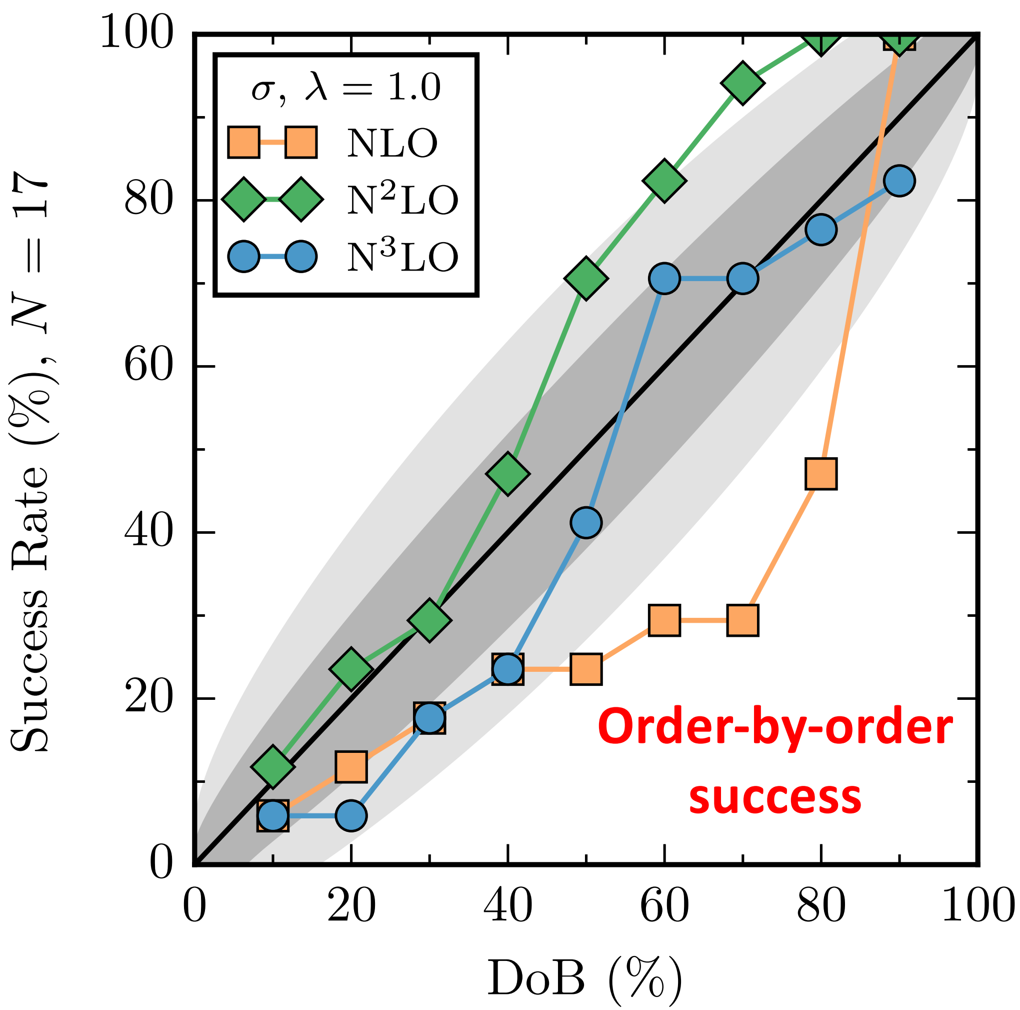
```python
import numpy as np
y_ref = 20.0; Q = 0.3; k = 3
y_k = [21.7, 27.3, 25.4, 26.2]
c_k = np.array([y_k[0] / y_ref] + [
  (y_k[n] - y_k[n-1]) / (y_ref * Q**n)
  for n in range(1, k+1)])

nu_0 = 1; tau_0 = 1 # ~Uninformative
nu = nu_0 + len(c_k)
tau_sq = \
  (nu_0 * tau_0**2 + c_k @ c_k) / nu

from scipy.stats import t
scale = y_ref * Q**(k+1) * \
  ( tau_sq / (1 - Q**2) )**0.5
y = t(nu, y_k[-1], scale)
dob = y.interval(0.95) # (25.7, 26.7)
```

Note: If $n_c \gg 1$, the posterior for y becomes a normal distribution.

From https://buqeye.github.io/

Model Checking I: Weather plots (empirical coverage)





Test of EKM NN chiral EFT potentials from Melendez et al., PRC **96**, 024003 (2017)

In progress (2021): similar analysis of other NN interactions

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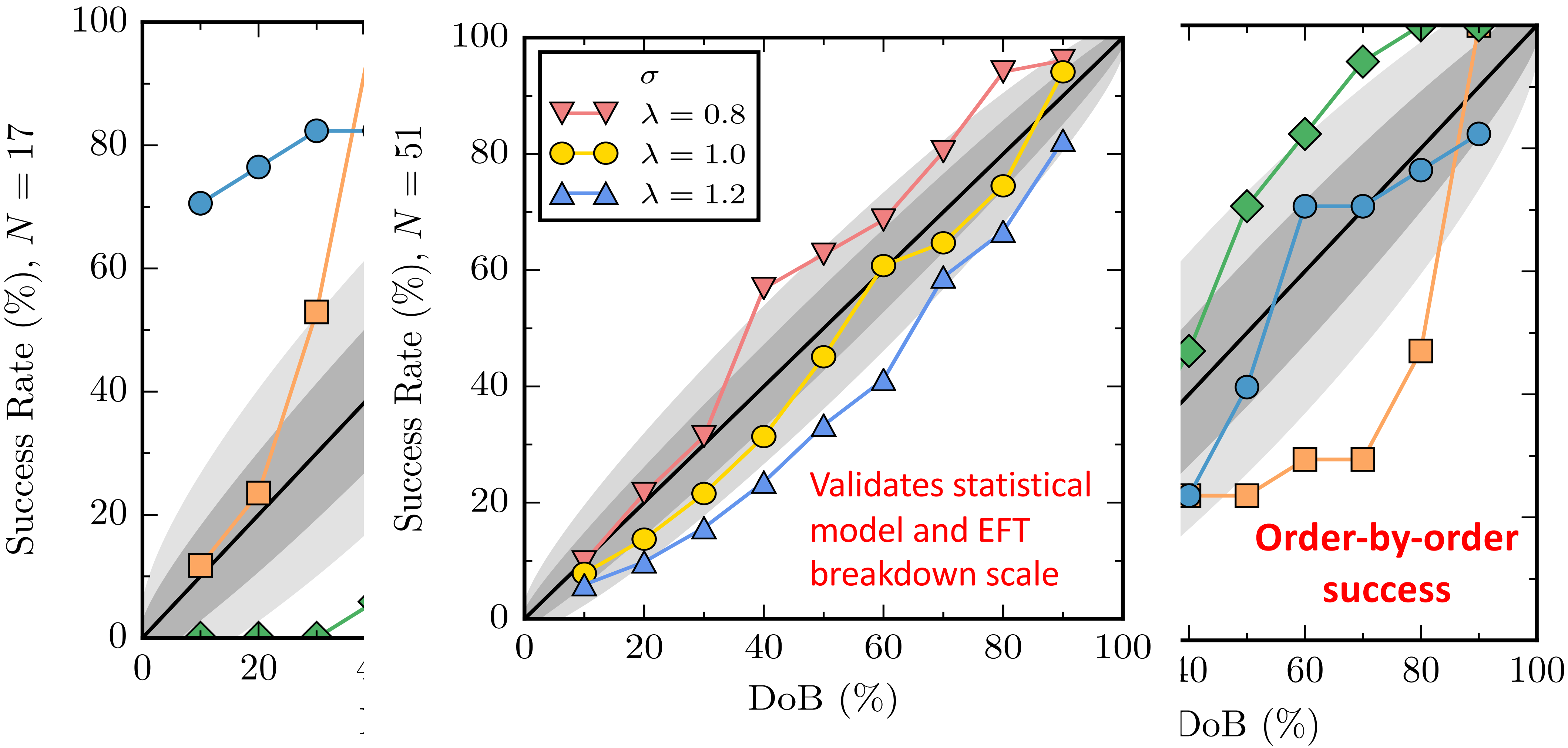

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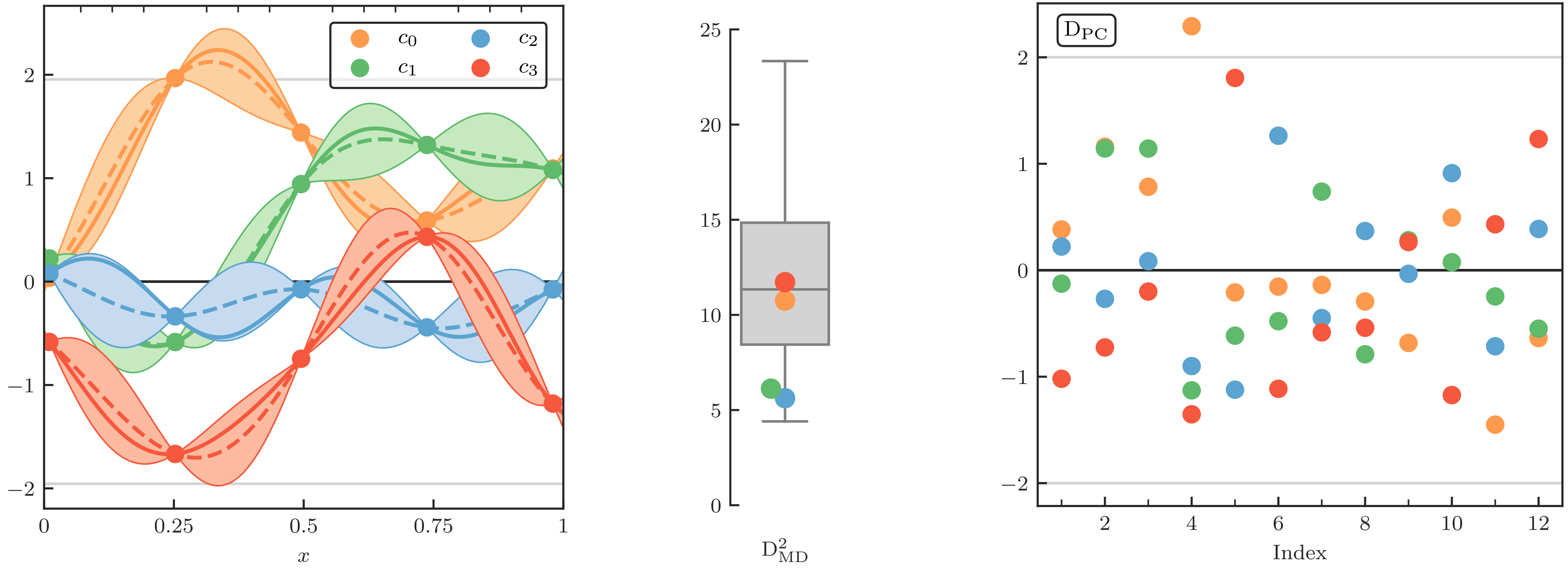
Model checking: Does our model refer to reality?

Use metric to measure GP-ness to test model: Mahalanobis distance

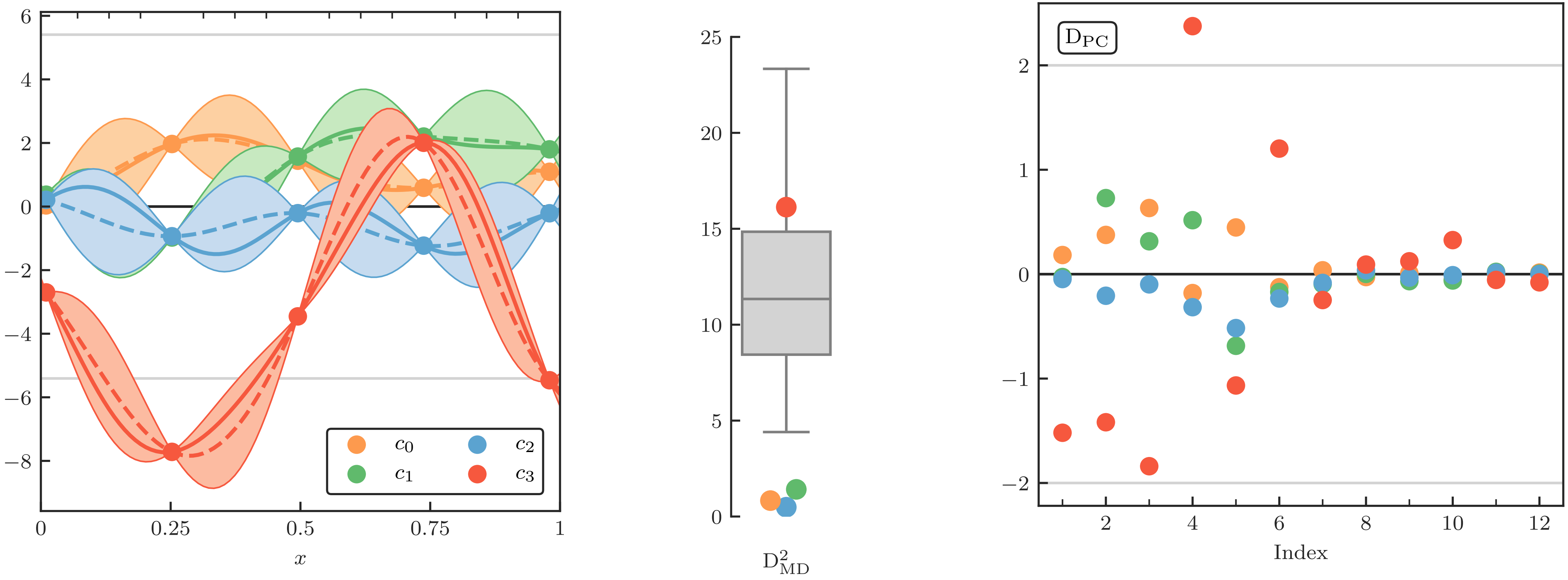


This is what success looks like!

Melendez et al., PRC (2019)

Model checking: Does our model refer to reality?

Use metric to measure GP-ness to test assumption: Mahalanobis distance

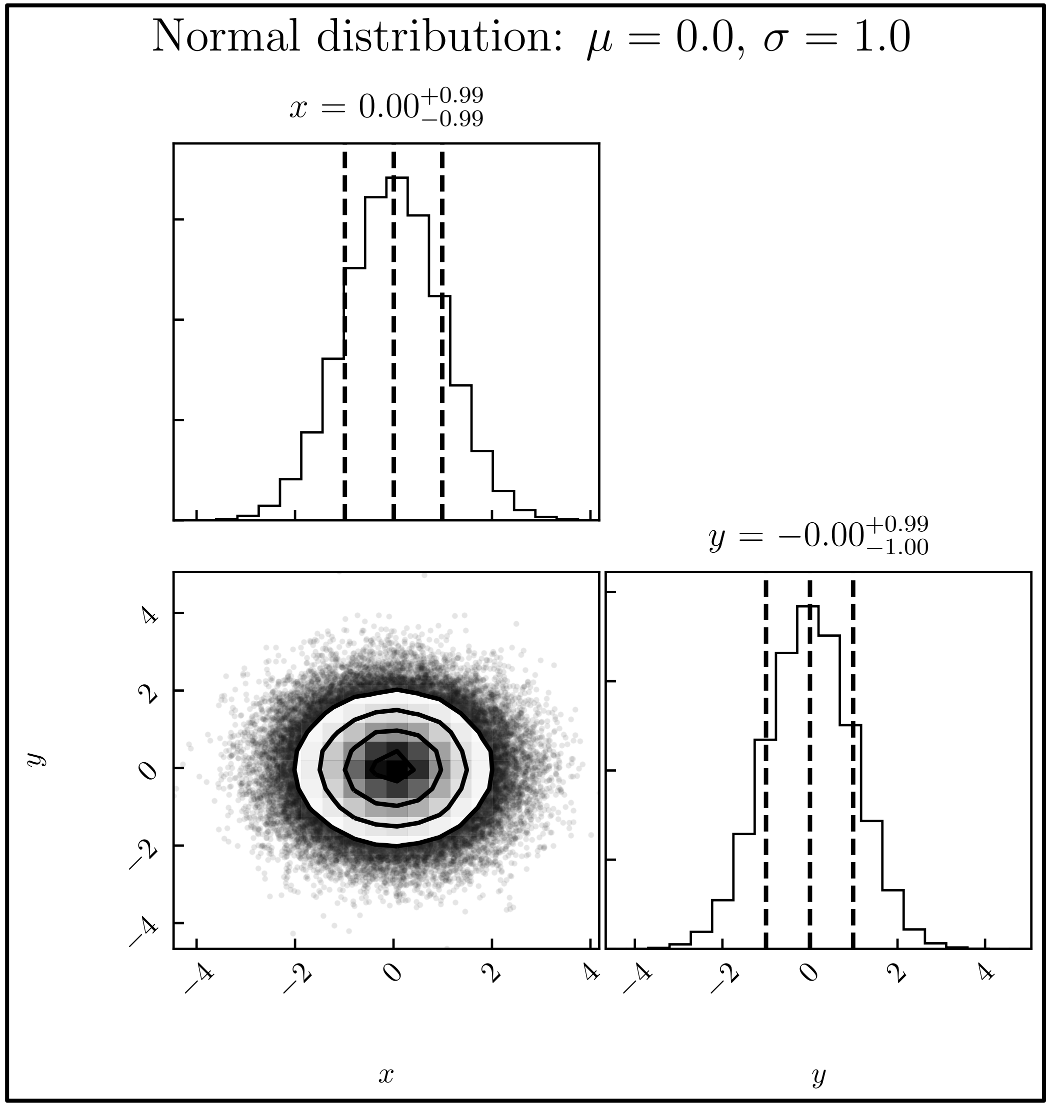


This is what failure looks like!

Melendez et al., PRC (2019)

Reminder about statistical correlations

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



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

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

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

Reminder about statistical correlations

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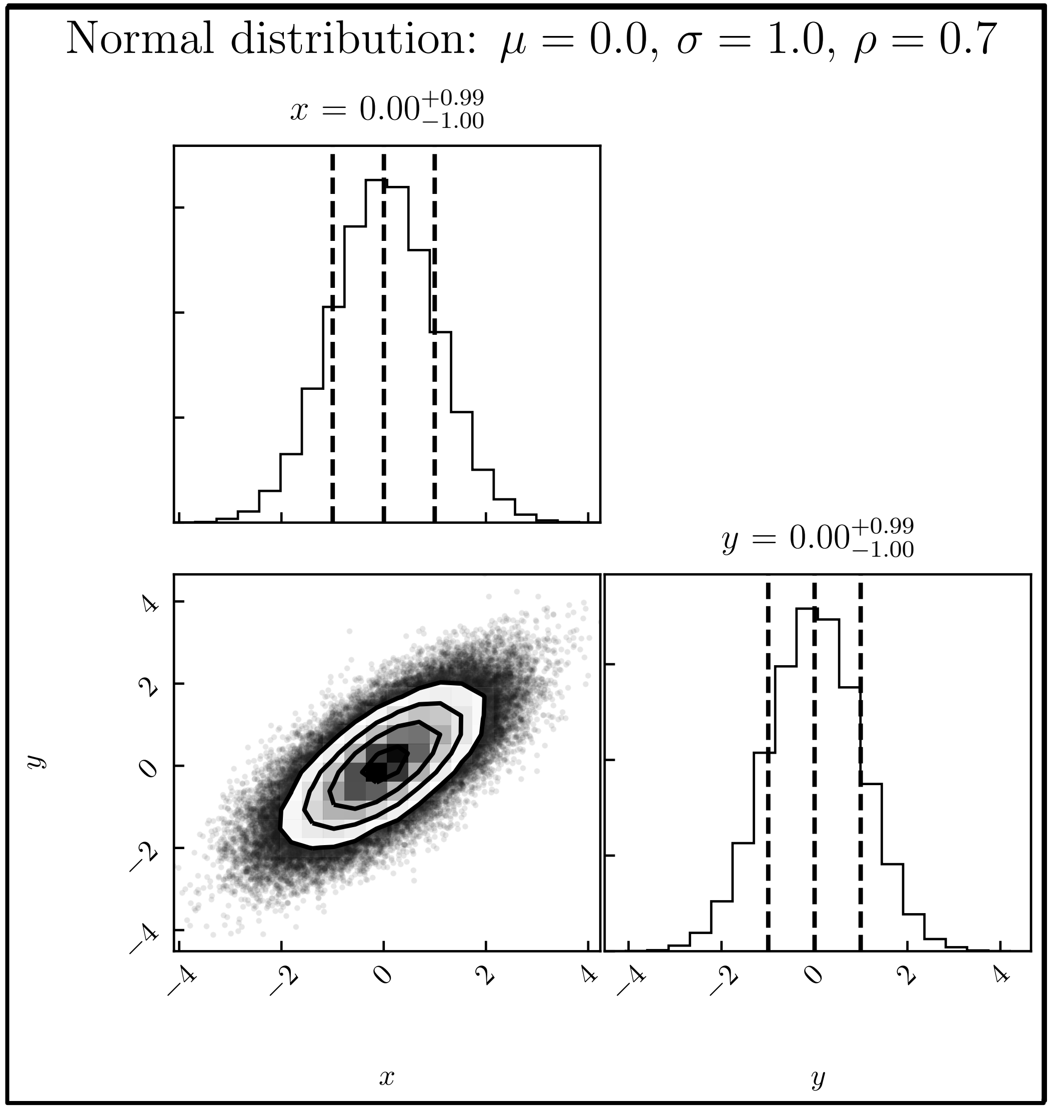


$$\mathcal{N} e^{-\frac{1}{2}\mathbf{r}^\intercal \Sigma^{-1} \mathbf{r}} = \text{correlated gaussian}$$

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

With two points *x* and *y*, -1 ≤ ρ ≤ 1 → correlation. With many points x_1, x_2, … x_N, all pairs have a ρ_{ij} correlation to be learned.

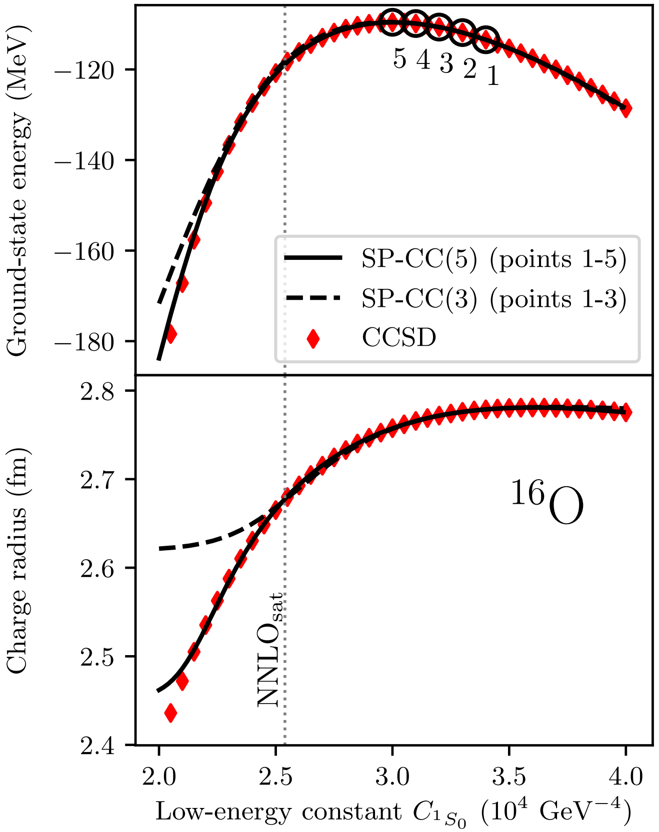
$$X - Y \sim \mathcal{N}(\mu_x - \mu_y, \sigma_x^2 + \sigma_y^2 - 2\sigma_x\sigma_y\rho)$$

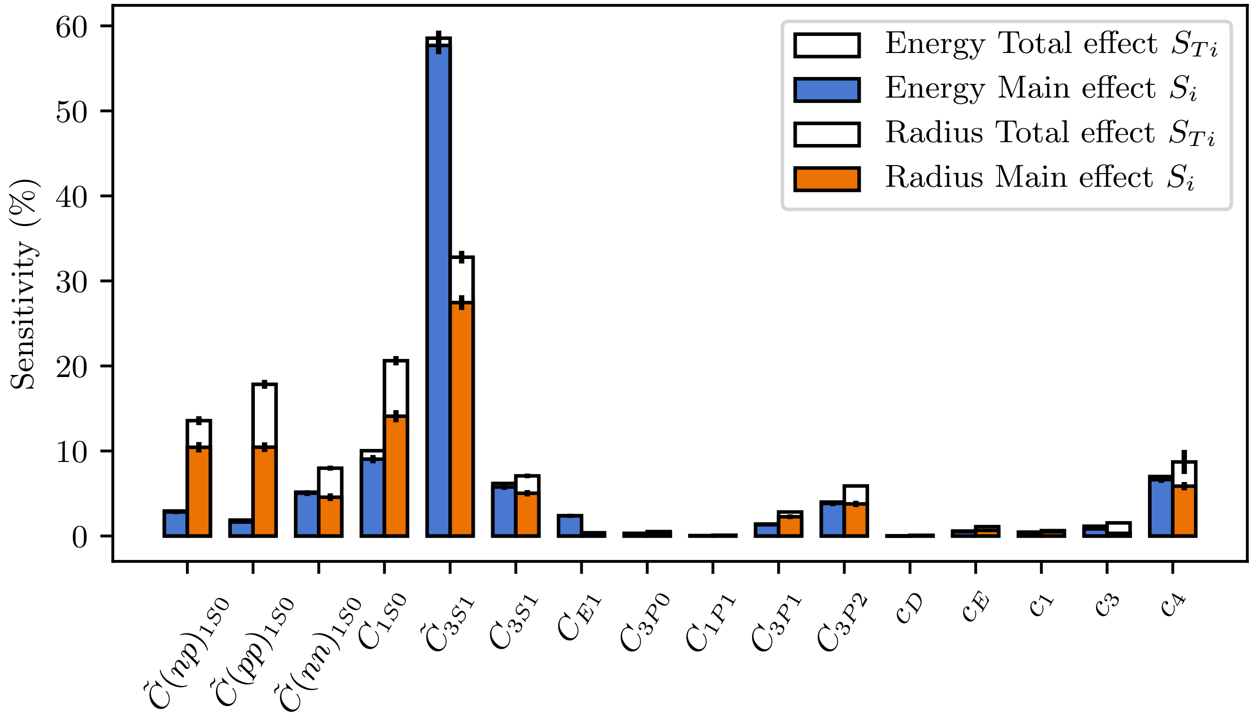
Bayes is great, but won't the sampling be too expensive?

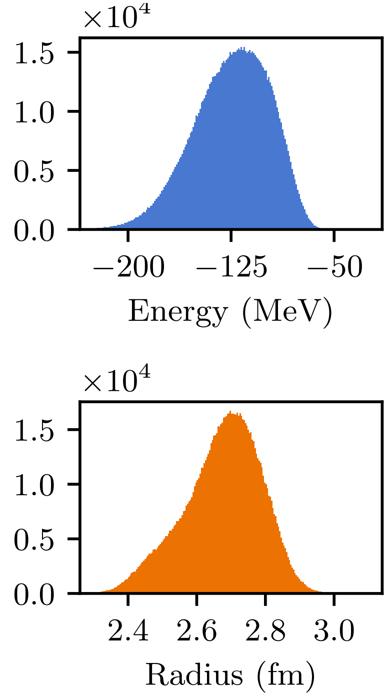
Global sensitivity analysis of bulk properties of an atomic nucleus

A. Ekström and G. Hagen

arXiv: 1910.02922







"We have to use (16 + 1) · 216 = 1,114,112 quasi MC samples to extract statistically significant main and total effects of the energy and radius for all LECs. With SP-CC(64) this took about 1 hour on a standard laptop, while an equivalent set of exact CCSD computations would require 20 years."