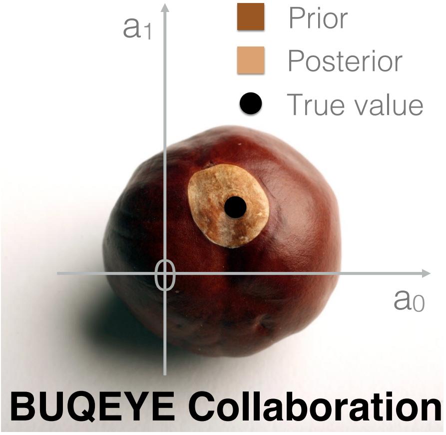
Frontiers of Uncertainty Quantification for EFTs

Dick Furnstahl

EMMI Hirschegg Meeting, January 2023

The Ohio State University

Slides: http://bit.ly/3vTc0IW



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

See also later talks and Frontiers in Physics volume on *Uncertainty Quantification in Nuclear Physics*

Questions for the Hirschegg meeting

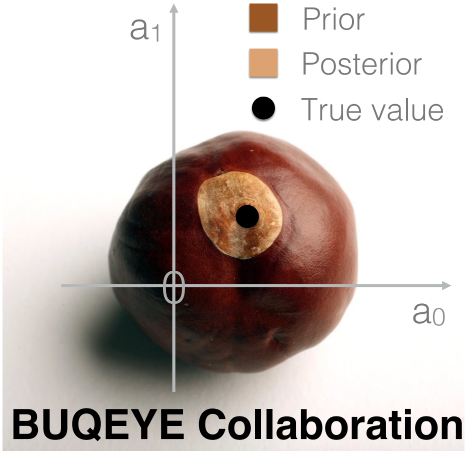
- What are the limits of EFT for nuclei and for matter? What should be the priority developments and improvements for EFTs, including the exploration of alternative power counting schemes?
- What are systems where more effective EFTs, such as pionless or halo EFT, are particularly promising? What are priorities for improving nuclear energy density functionals in the spirit of EFT?
- What are the priorities for developments and applications in **uncertainty quantification**? What are new opportunities for nuclear structure from emerging technologies?
- What should be EFT and many-body priorities in nuclear structure research in light of the advent of new experimental facilities for the study of exotic nuclei?

Uncertainty quantification (UQ) is explicitly called out in one of these questions, but (Bayesian) statistical analysis can play an important role in addressing all questions!

Frontier UQ topics: validation of models for truncation errors; limits of EFTs from statistical analysis; calibration of EFTs; accounting for and exploiting correlations; Bayesian model mixing; experimental design; development of emulators.

Checklist for statistically sound Bayesian inference for EFTs

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



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

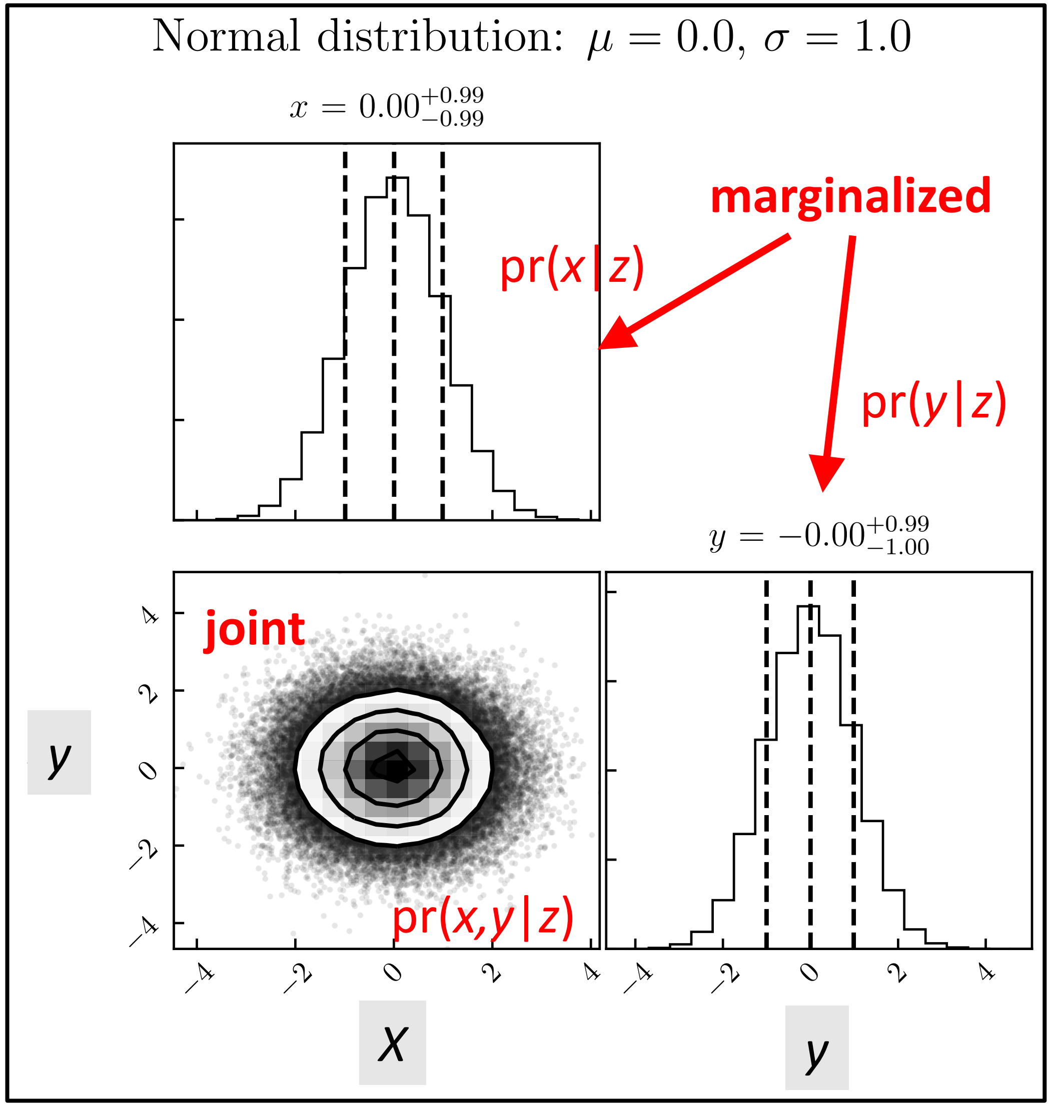
Jupyter notebooks also!

Bayesian updating of knowledge ←

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

Reminder about statistical correlations

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



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

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

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

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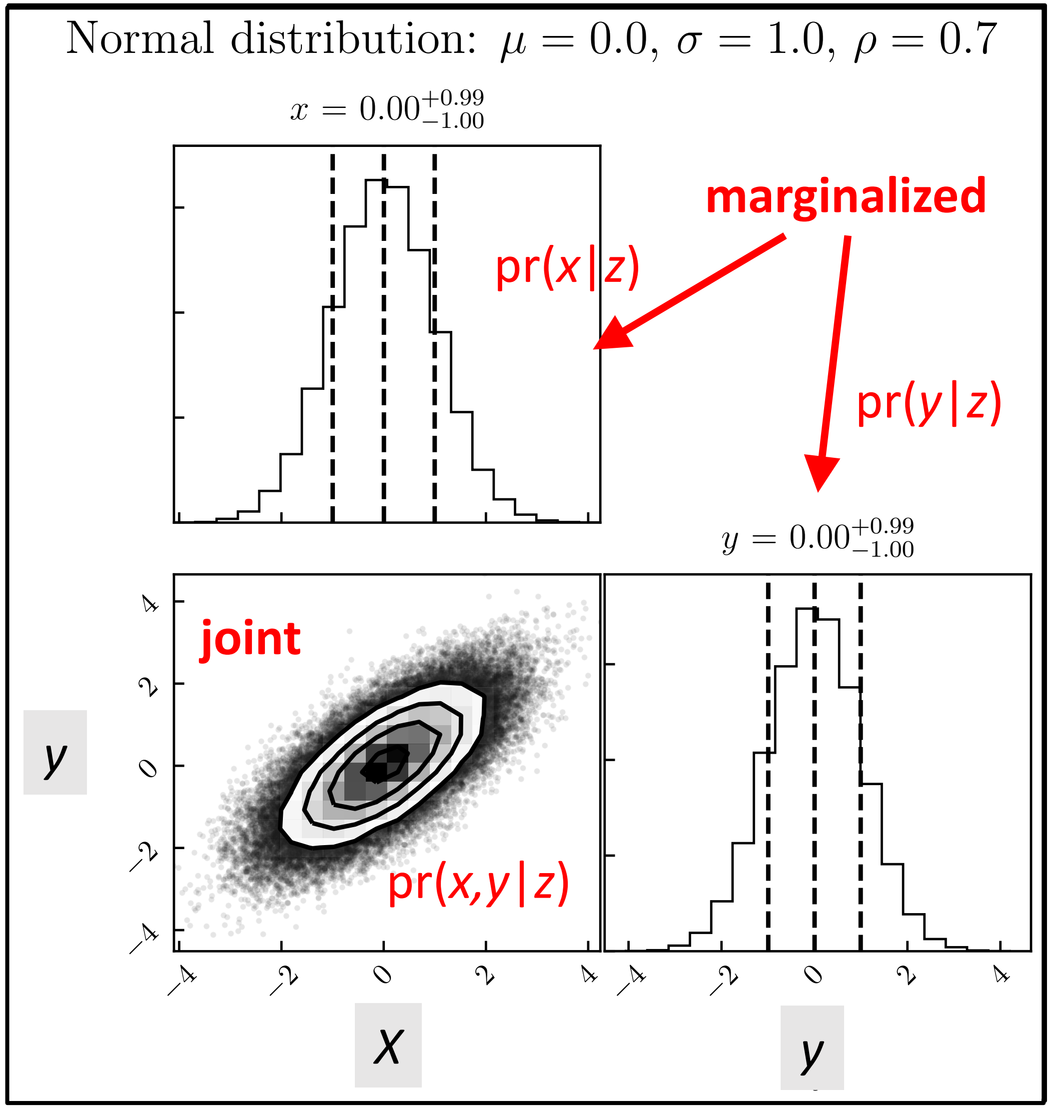


$$\mathcal{N} e^{-\frac{1}{2}\mathbf{r}^\intercal \Sigma^{-1} \mathbf{r}} = \text{correlated gaussian}$$

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

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

With two, e.g., *x* and *y*, $-1 \le \rho \le 1$ → correlation. With many $x_1, x_2, \ldots x_N$, all pairs have a ρ_{ij} correlation to be learned. A *gaussian process* parametrizes the ρ_{ij} (and σ_i) via hyperparameters.

Two ways to treat 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 *learn* it (train and test; correlated → GP).

2. For EFTs, can learn from *convergence pattern* (cutoff dependence?)

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

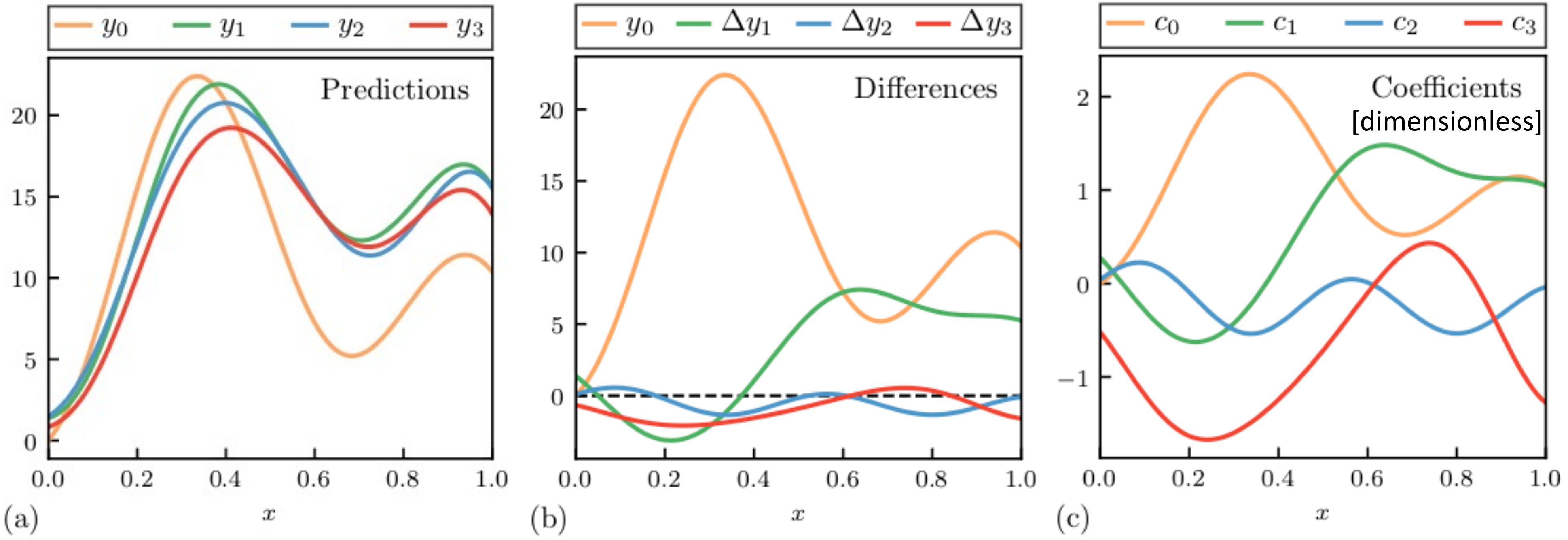
Theory at order k: $\boldsymbol{y}_k = \boldsymbol{y}_{\rm ref} \sum_{n=0}^{k} c_n Q^n$ Omitted orders: $\delta\boldsymbol{y}_{\rm th} = \boldsymbol{y}_{\rm ref} \sum_{n=k+1}^{\infty} c_n Q^n$

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

$$\boldsymbol{y}_k = \boldsymbol{y}_{\text{ref}} \sum_{n=0}^{k} c_n Q^n \rightarrow \delta \boldsymbol{y}_{\text{th}} = \boldsymbol{y}_{\text{ref}} \sum_{n=k+1}^{\infty} c_n Q^n \quad \Rightarrow Q = \frac{\{p, m_{\text{low}}\}}{\Lambda_b}, \quad \Lambda_b \Rightarrow \text{breakdown}$$

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

Choices of parametrization

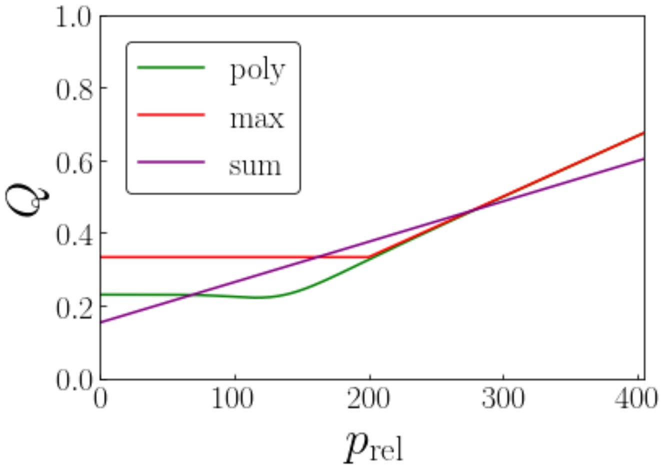
- Many choices of how to parametrize Q, p, and x

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

dimensionless expansion parameter

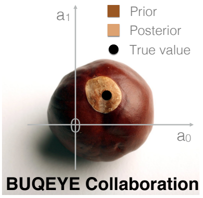
characteristic momentum

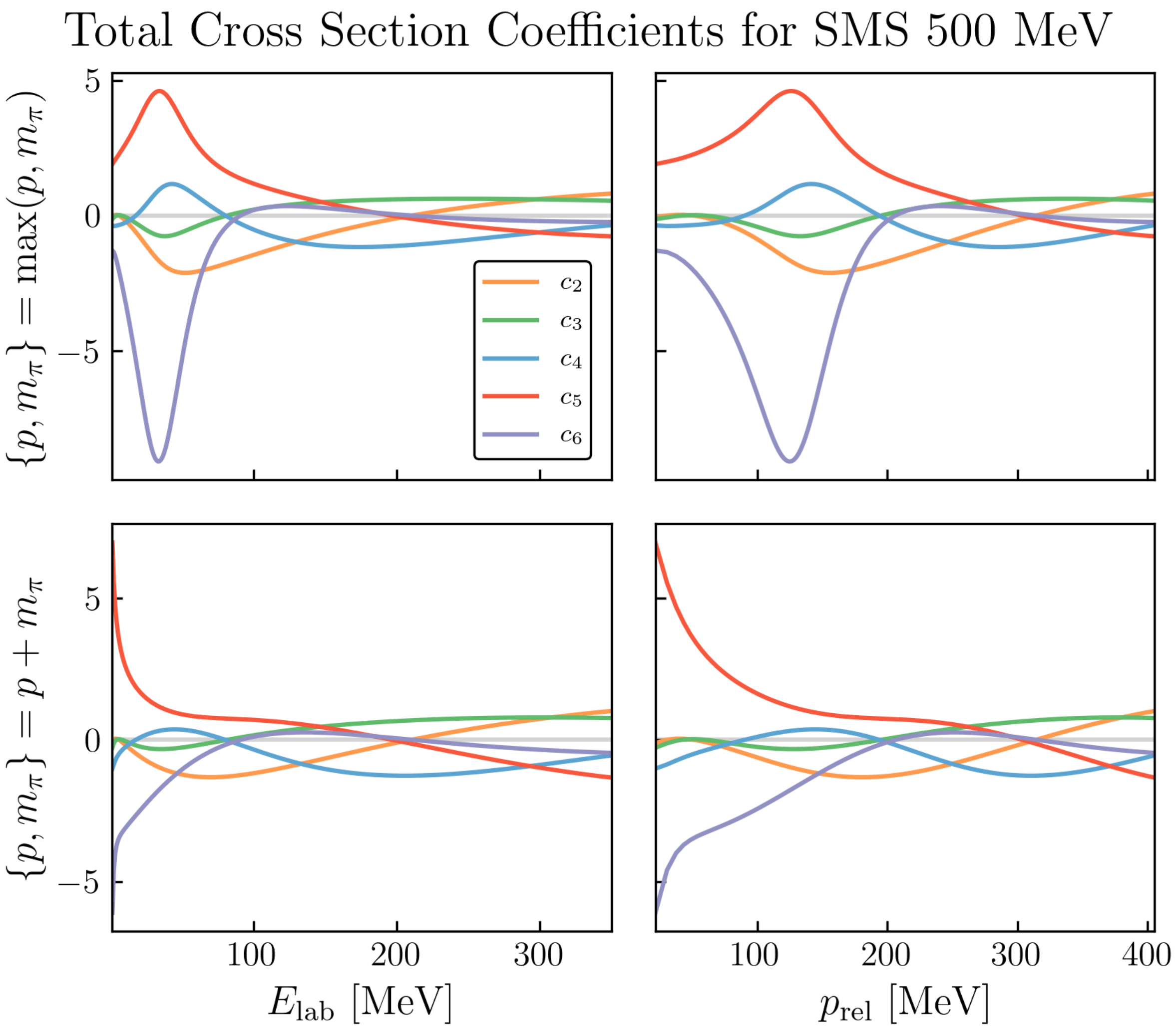
input space



- Use diagnostics to check stationarity ("Do c_n behave the same way across x?")

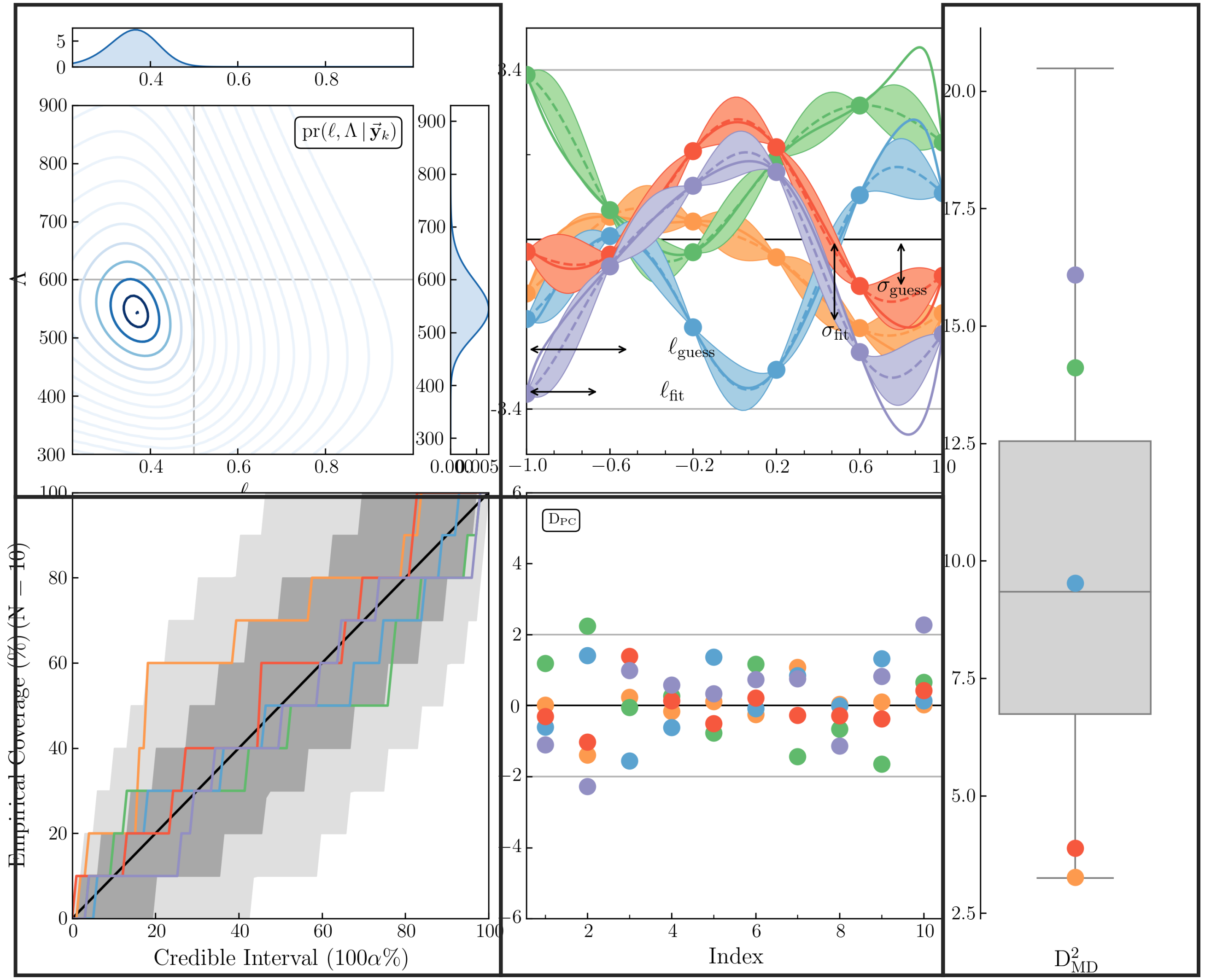
From P. Millican et al., *Effective Field Theory Convergence Pattern of Modern Nucleon-Nucleon Potentials* (in prep., 2023)





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

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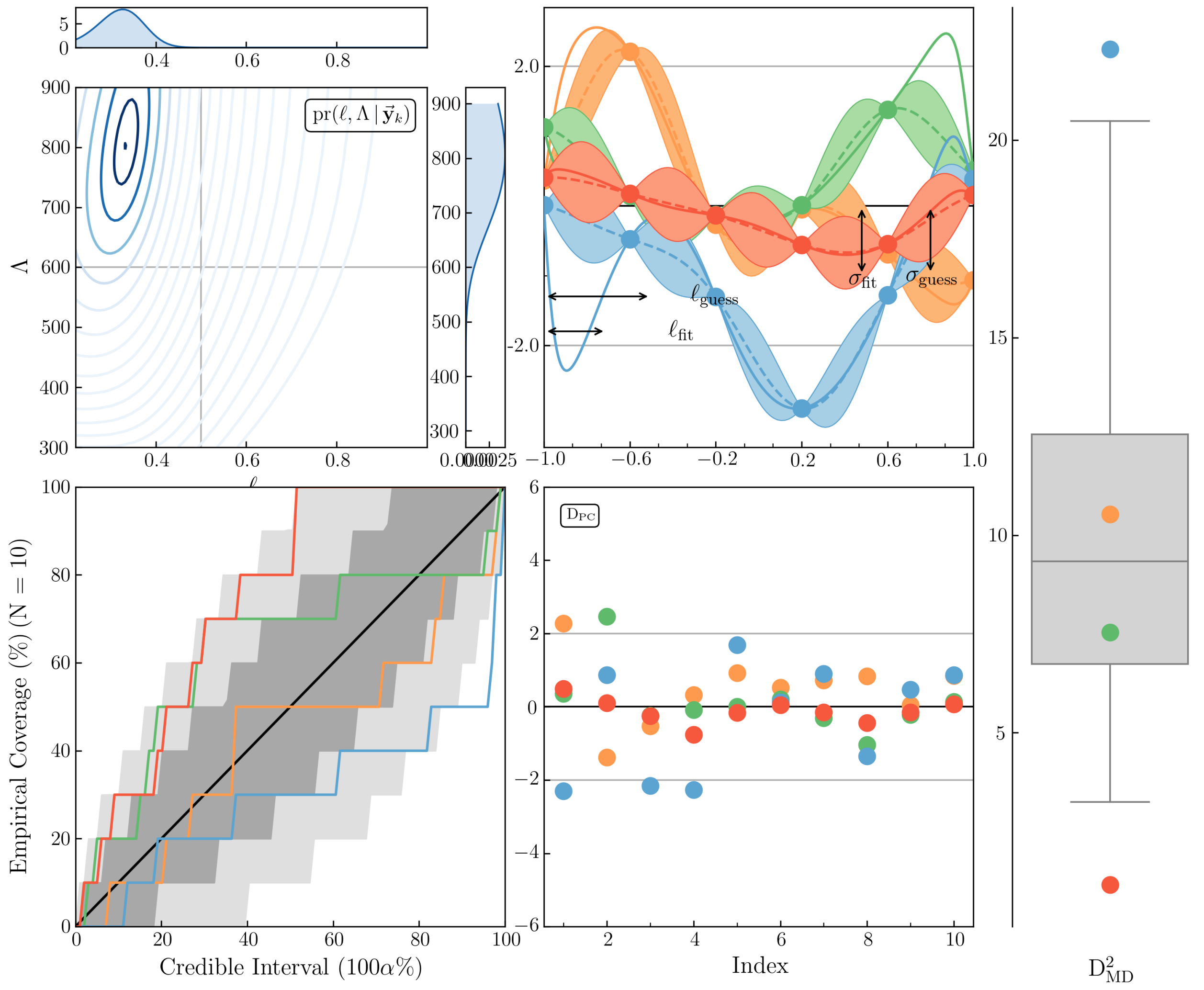
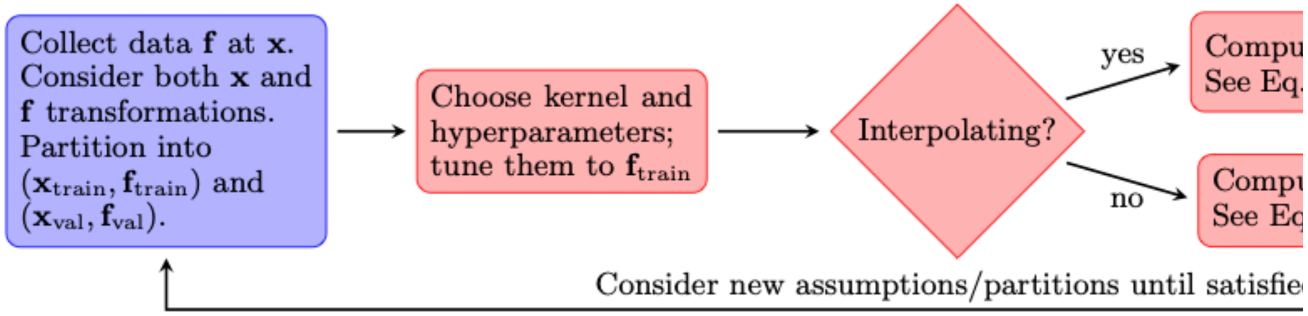
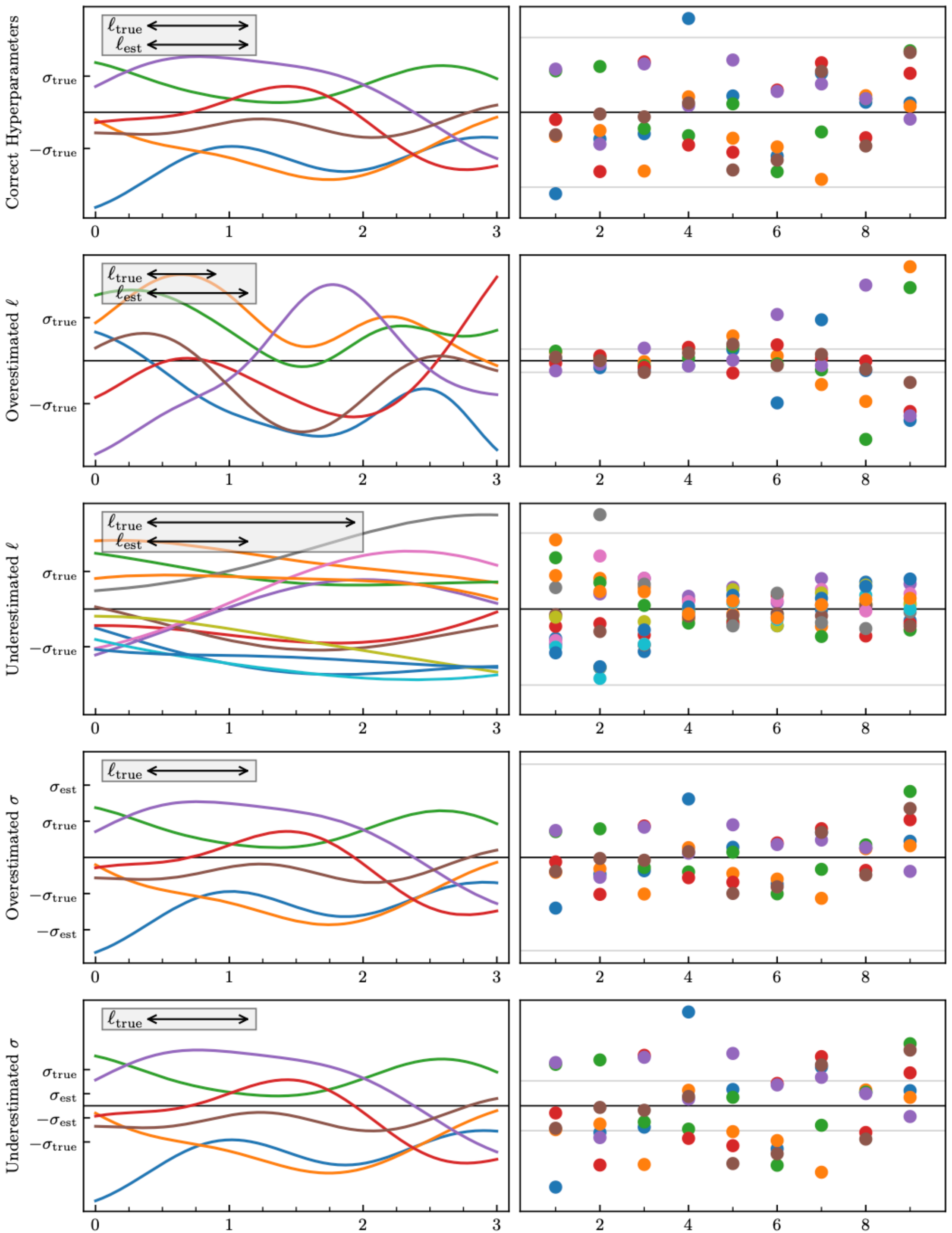


Spin observable D (150 MeV) for SCS 1.2 fm potential



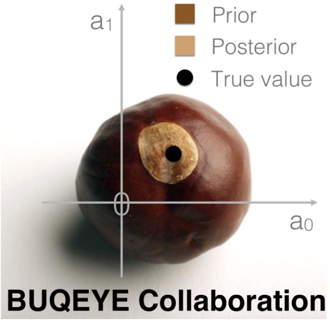
Diagnostic	Formula	Motivation
Visualize the function	—	Does $\mathbf{f}_{\text{val}}$ look like a draw from a GP? What kind of GP?
Mahalanobis Distance $\mathrm{D}^2_{\mathrm{MD}}$	$(\mathbf{f}_{\text{val}} - \mathbf{m})^\intercal K^{-1}(\mathbf{f}_{\text{val}} - \mathbf{m})$	Can we *quantify* how much 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 $p \in [0,1]$	$\frac{1}{M}\sum_{i=1}^{M} \mathbf{1}[\mathbf{f}_{\text{val},i} \in \mathrm{CI}_i(p)]$	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



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, arXiv:2104.04441 PRC **104**, 064001 (2021)



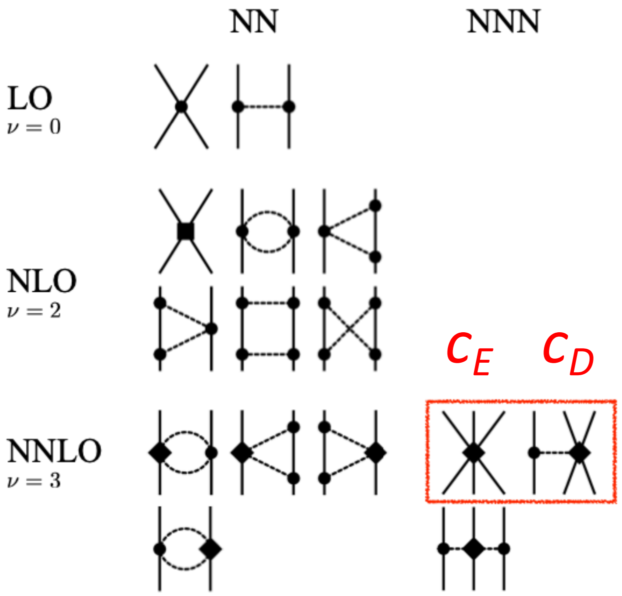
BUQEYE Collaboration

Notebook with all figures at

https://buqeye.github.io

See also: Djärv et al., PRC (2022) on A=6 nuclei, Svensson et al., arXiv:2206.08250 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

(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

Individual posteriors; everything has priors!

All experiment and theory errors

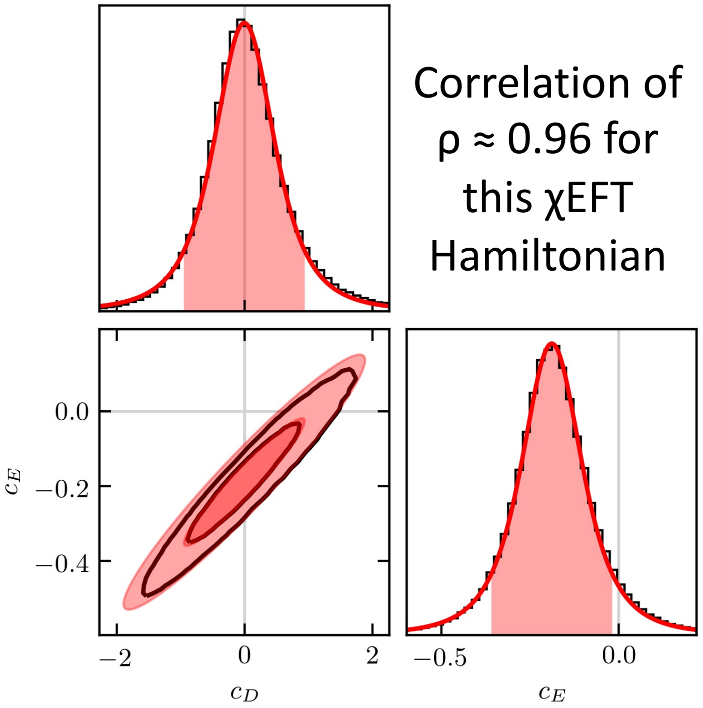
Likelihood: $\mathrm{pr}(\mathbf{y}_{\mathrm{exp}} \,|\, \vec{a}, \Sigma, I) \sim \mathcal{N}(\mathbf{y}_{\mathrm{th}}(\vec{a}),\; \Sigma_{\mathrm{exp}} + \Sigma_{\mathrm{method}} + \Sigma_{\mathrm{th}})$

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*" [PRC 104, 064001 (2021)]

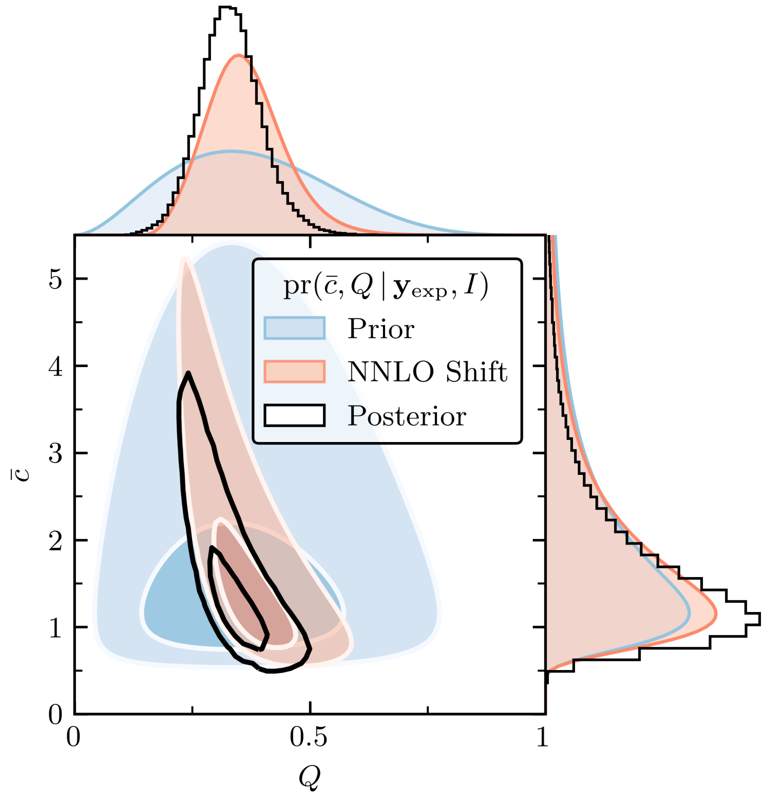
Posterior for c_D and c_E



Correlation of ρ ≈ 0.96 for this χEFT Hamiltonian

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

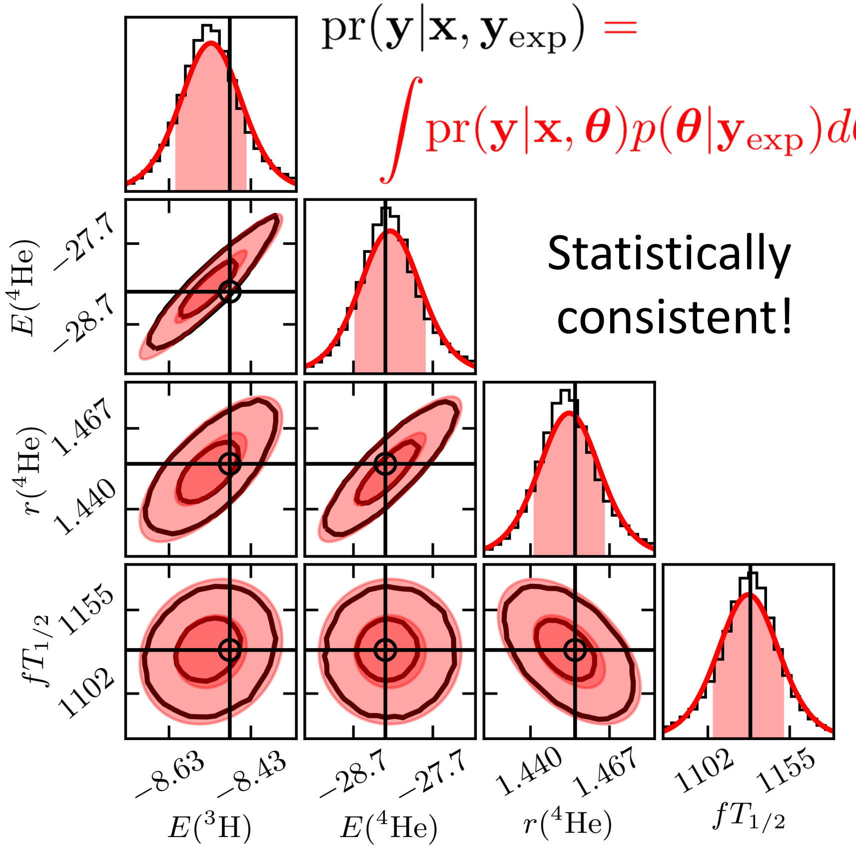
Posterior for Q and $\bar{c}$



Truncation error for observables:

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!

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

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

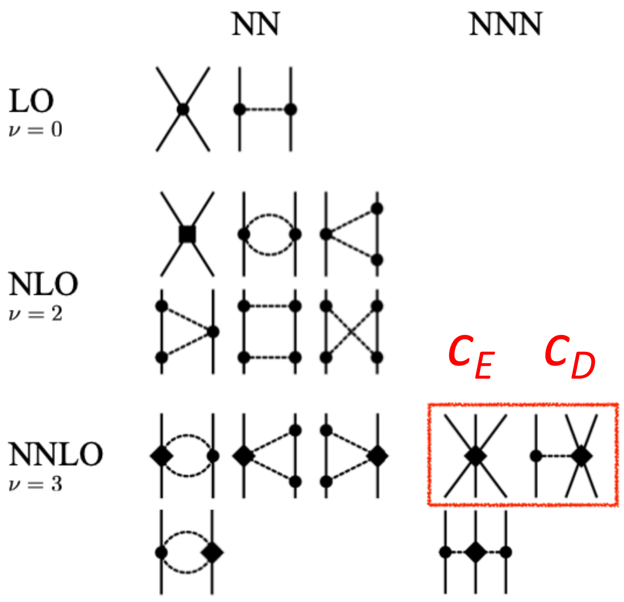
Light nuclei with semilocal momentum-space regularized chiral interactions up to [and beyond] N^2LO

LENPIC Collaboration

https://www.lenpic.org/

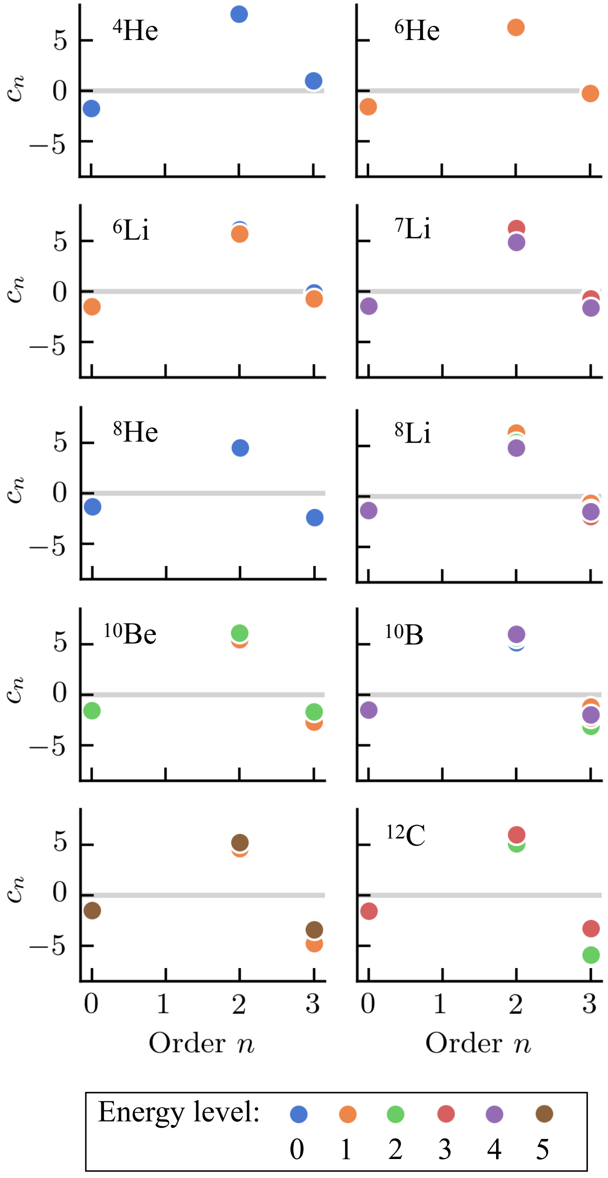
P. Maris et al., PRC **103**, 054001 (2021) arXiv:2104.04441

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

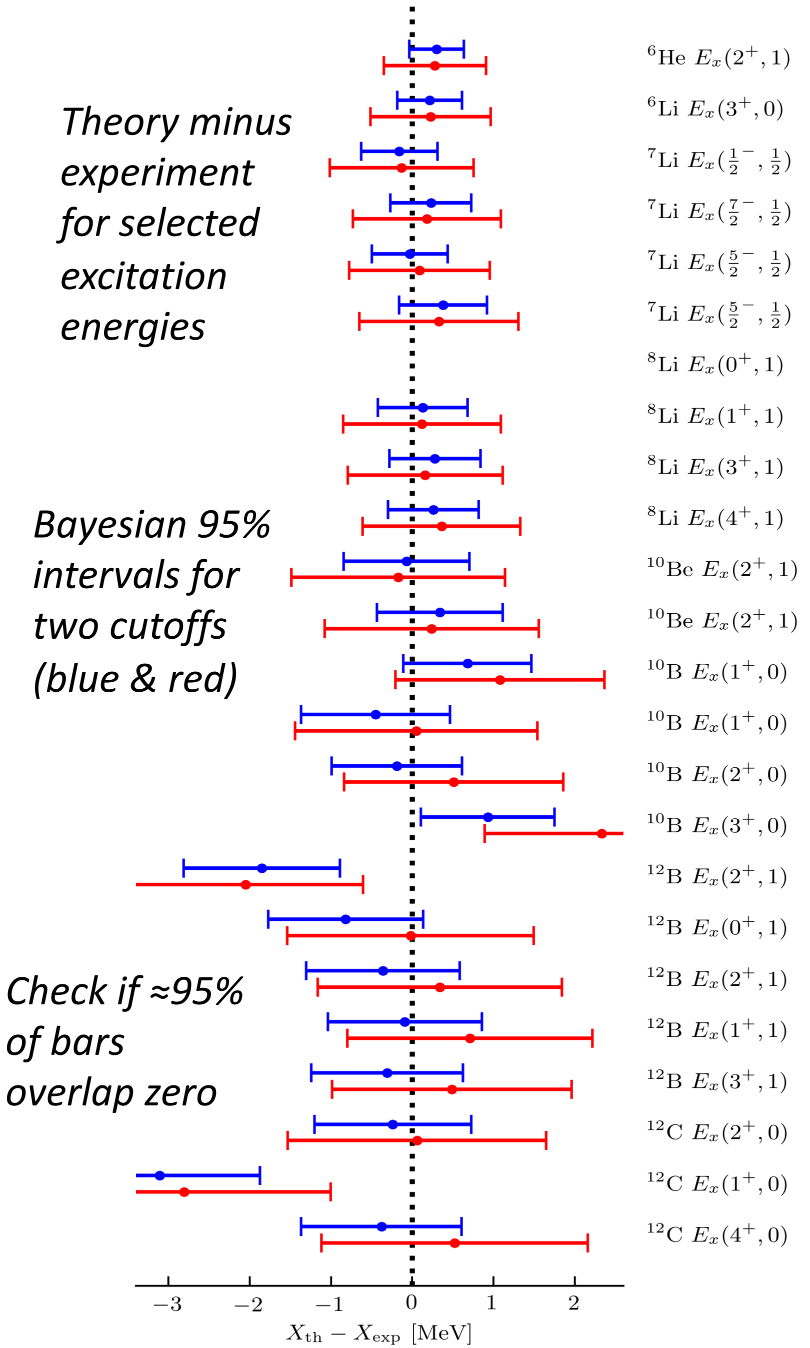


Coefficients for all the levels

- Empirically: calculated excitation energies are better determined than each level.
- Why? If E_1 and E_2 have $\delta \boldsymbol{y}_{\text{th}}$ 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.
- **Higher order:** >N^{2}LO enables better estimates of correlations → more insight



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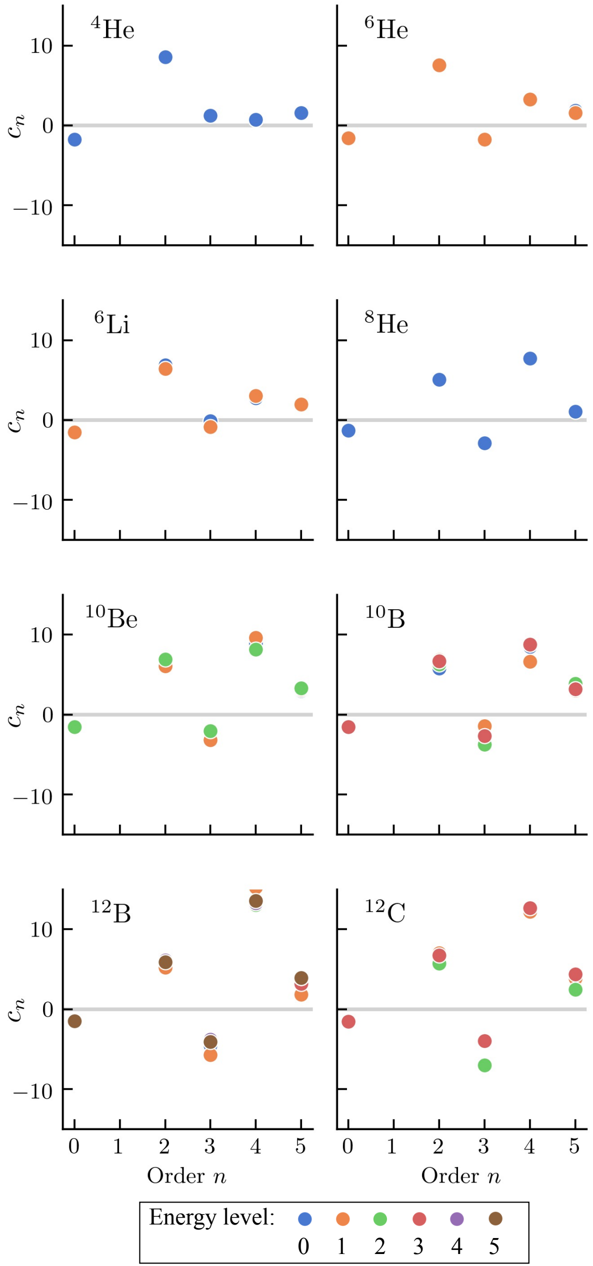

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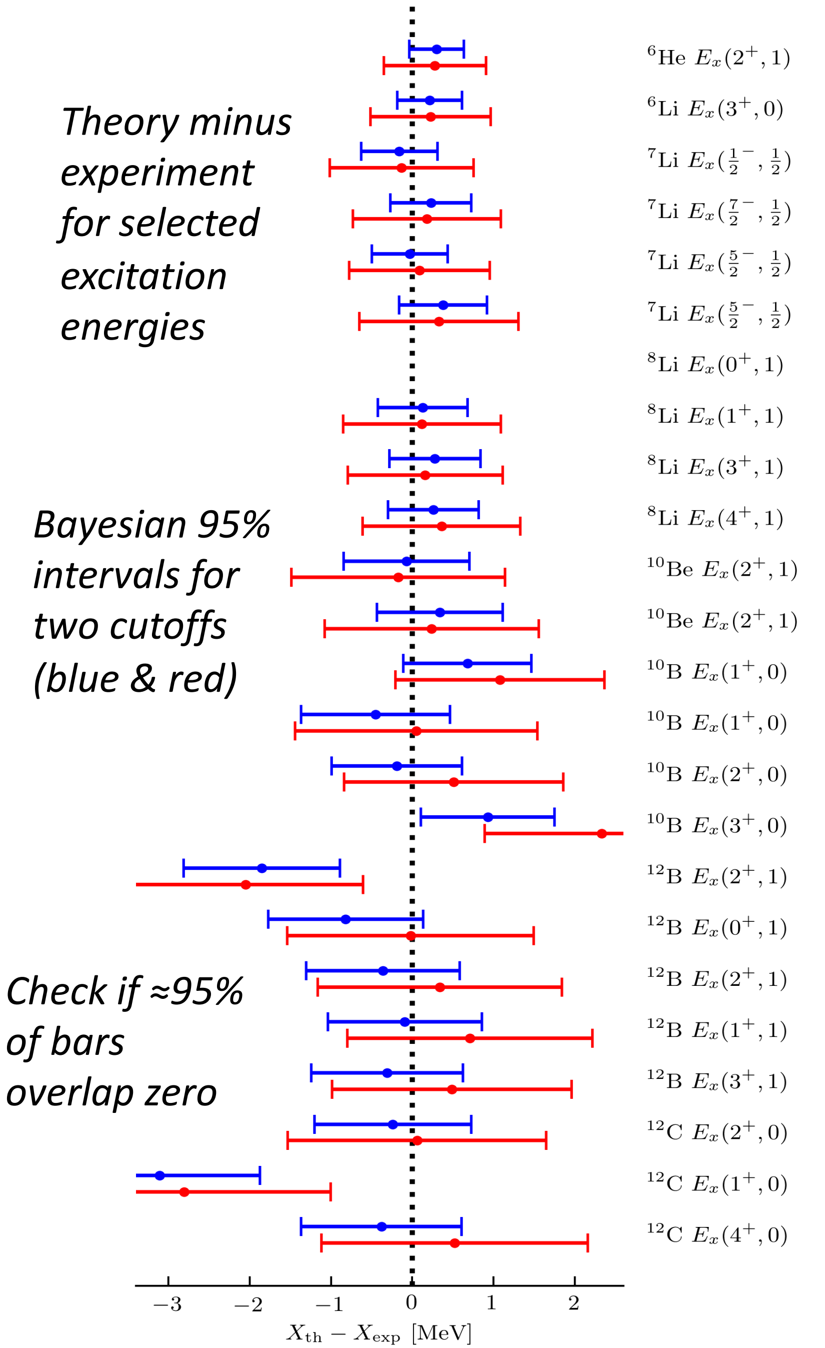
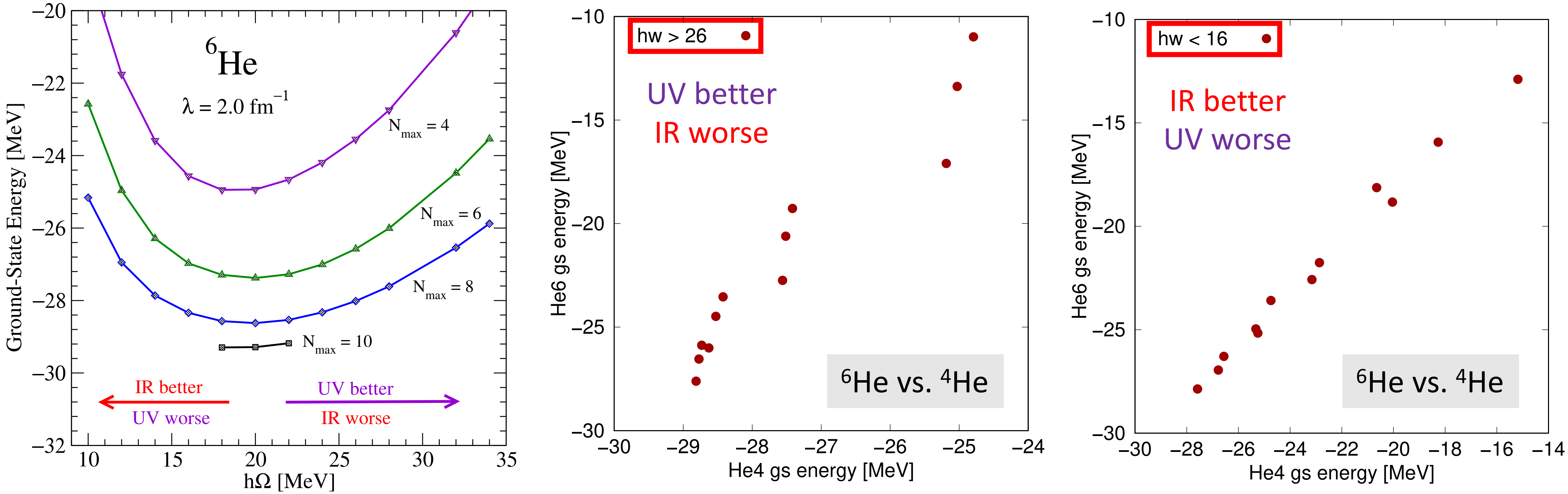


More correlations . . .

- **UQ for infinite matter** [see C. Forssén talk]
  - Truncation-error correlations between different densities and observables is crucial for reliable UQ!
  - C. Drischler et al., *Quantifying uncertainties and correlations in the nuclear-matter equation of state*
  - W.G. Jiang et al., *Emulating ab initio computations of infinite nucleonic matter* and *Emergence of nuclear saturation within Δ-full chiral effective field theory*

- **Model space extrapolations: correlations between observables** (machine learning?)

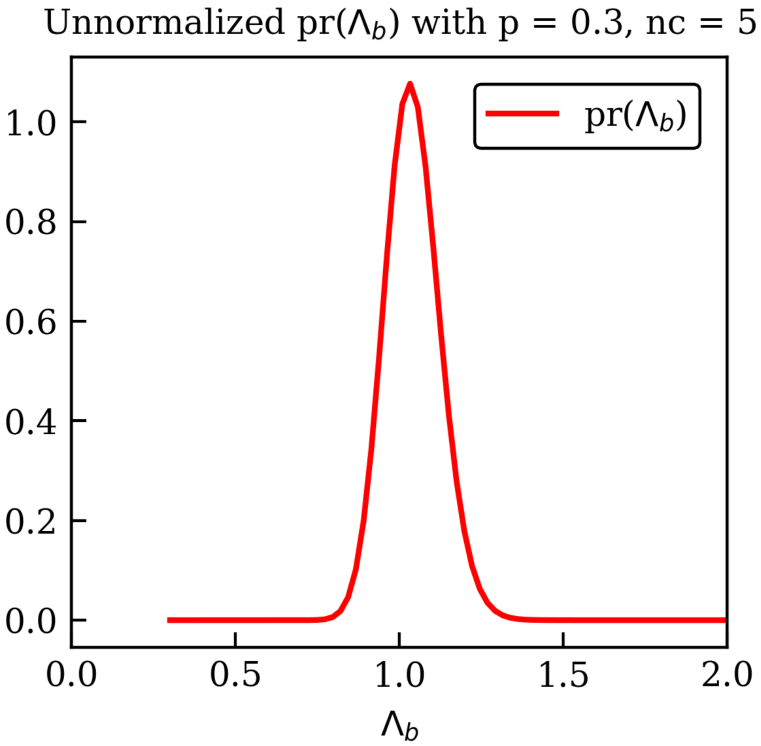


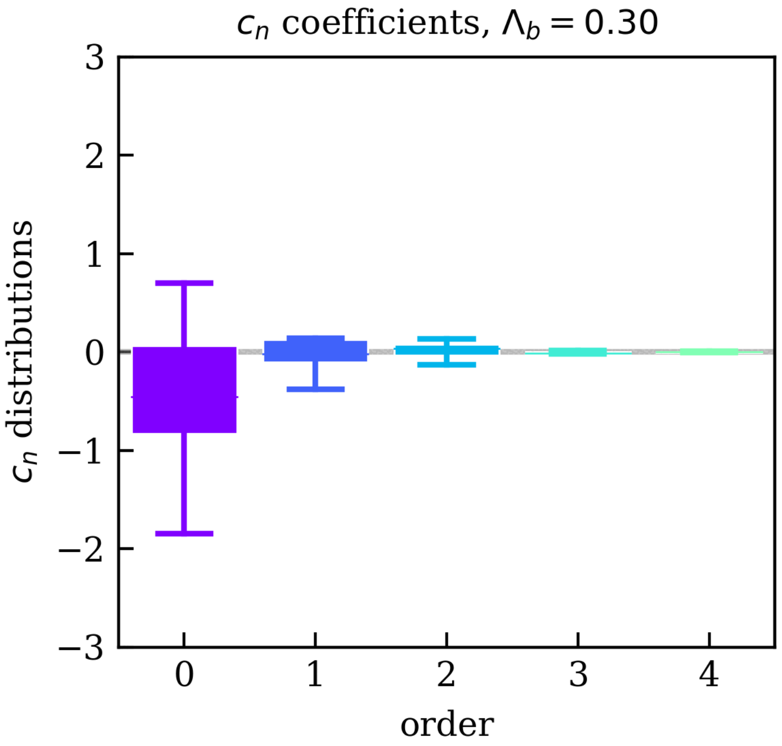
- cf., Sun et al., *How to renormalize coupled cluster theory*, PRC **106** (2022)

Limits of EFTs: Learning the expansion parameter

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

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





Melendez et al. (2019):

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

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

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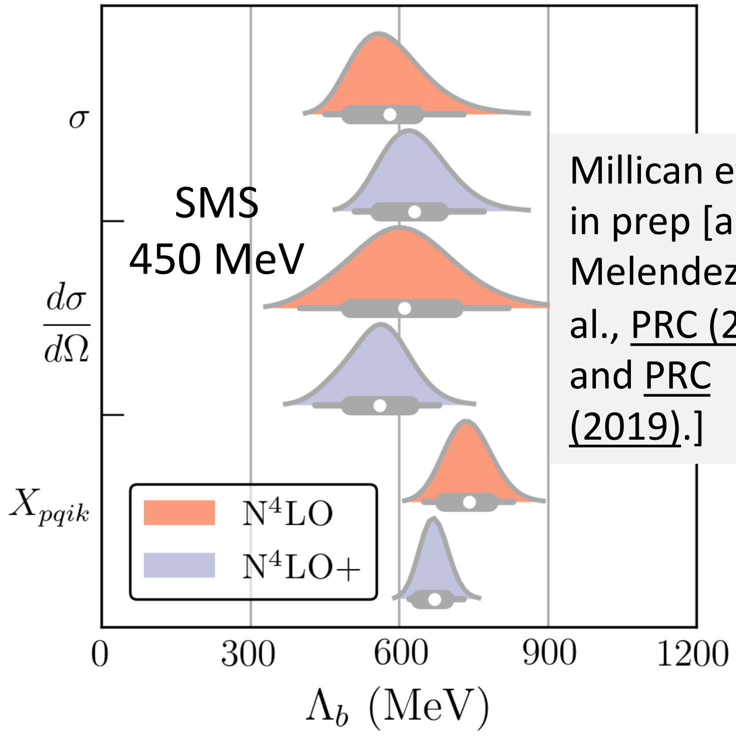
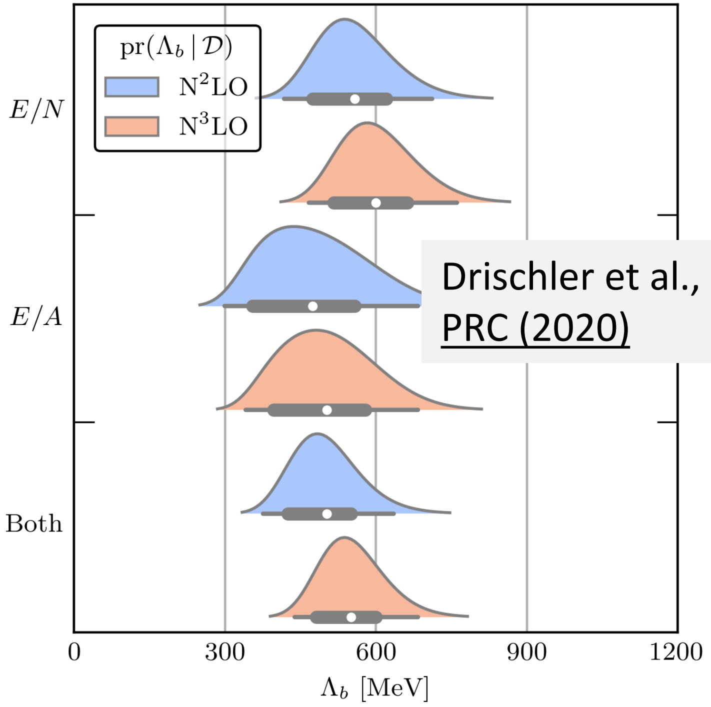
Λ_b from NN observables



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

Λ_b from infinite matter



Drischler et al., PRC (2020)

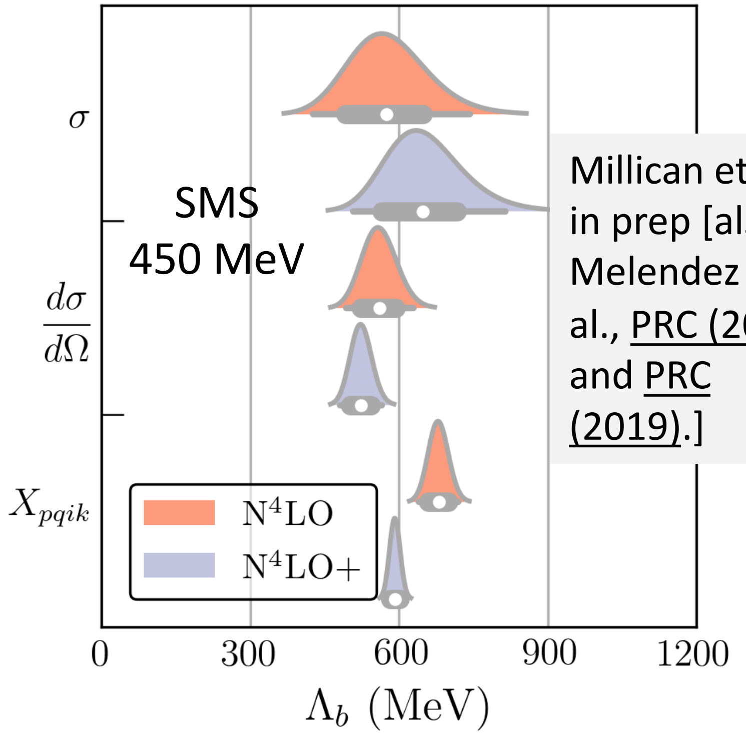
- Are different Λ_b posteriors consistent? Other ways?
- How do correlations affect the estimation of the breakdown scale?
- …

Limits of EFTs: Learning the expansion parameter

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

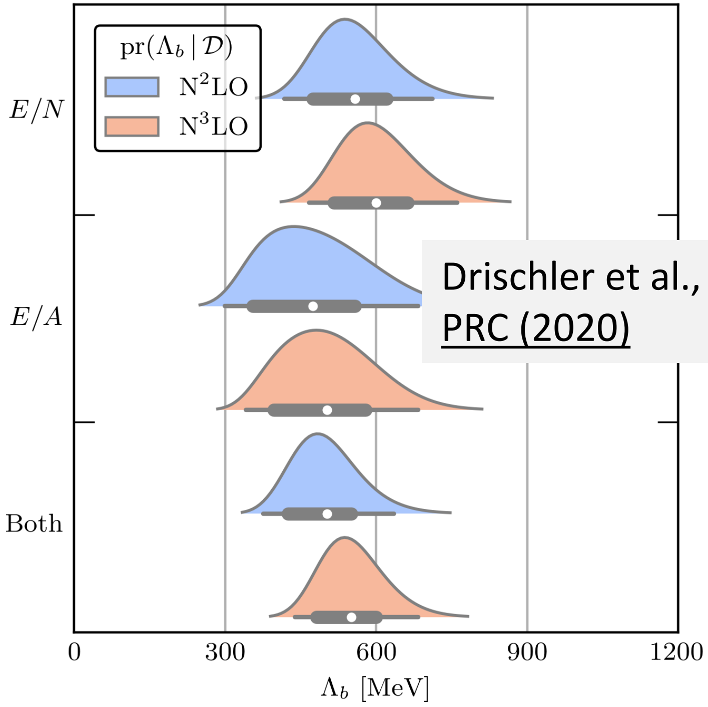
Expectation: $\chi{\rm EFT} \Rightarrow Q = \dfrac{\{p, m_\pi\}}{\Lambda_b}, \quad \Lambda_b \approx 600\,{\rm MeV}$

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)

Melendez et al. (2019):

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

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

- Are different $\Lambda_{\rm b}$ posteriors consistent? Other ways?
- How do correlations affect the estimation of the breakdown scale?
- …

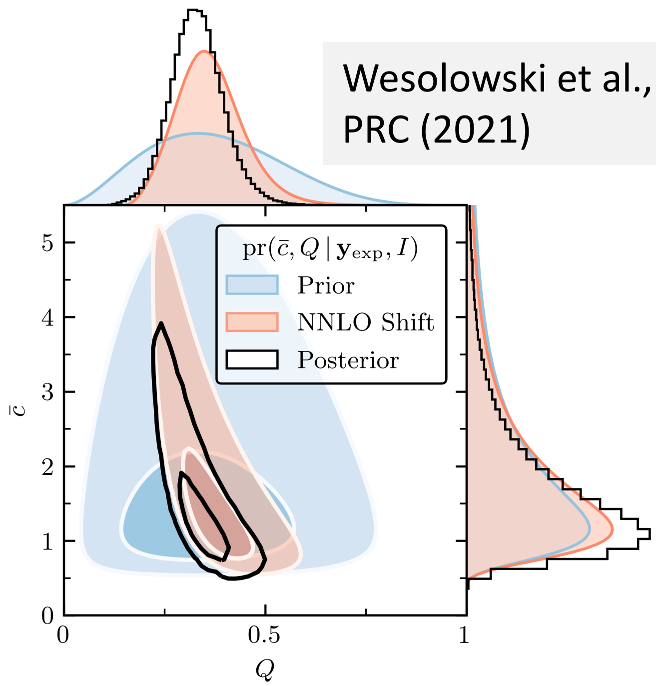
Limits of EFTs: Learning the expansion parameter

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

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

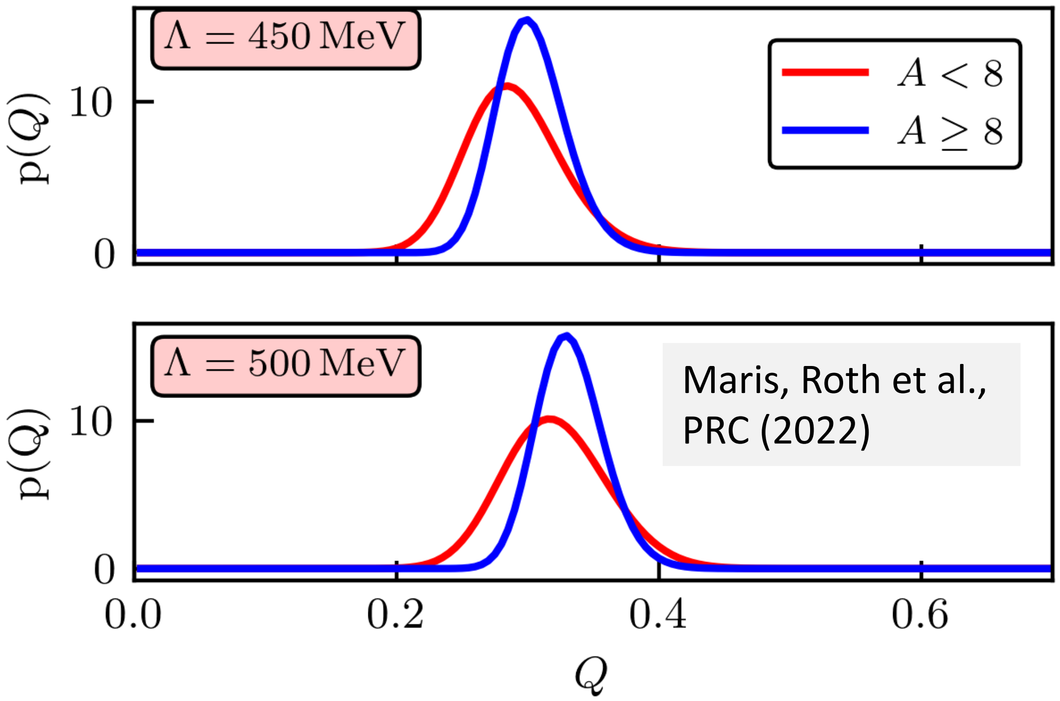
What about spectra of light nuclei?
Convergence pattern obscured at low order by KE vs. PE cancellation.
→ only use higher orders → Q ≈ 0.3
[consistent with $(m_\pi)^{\mathrm{eff.}}/\Lambda_b$ (see Ref.)]

Q from few-body observables



Wesolowski et al., PRC (2021)

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

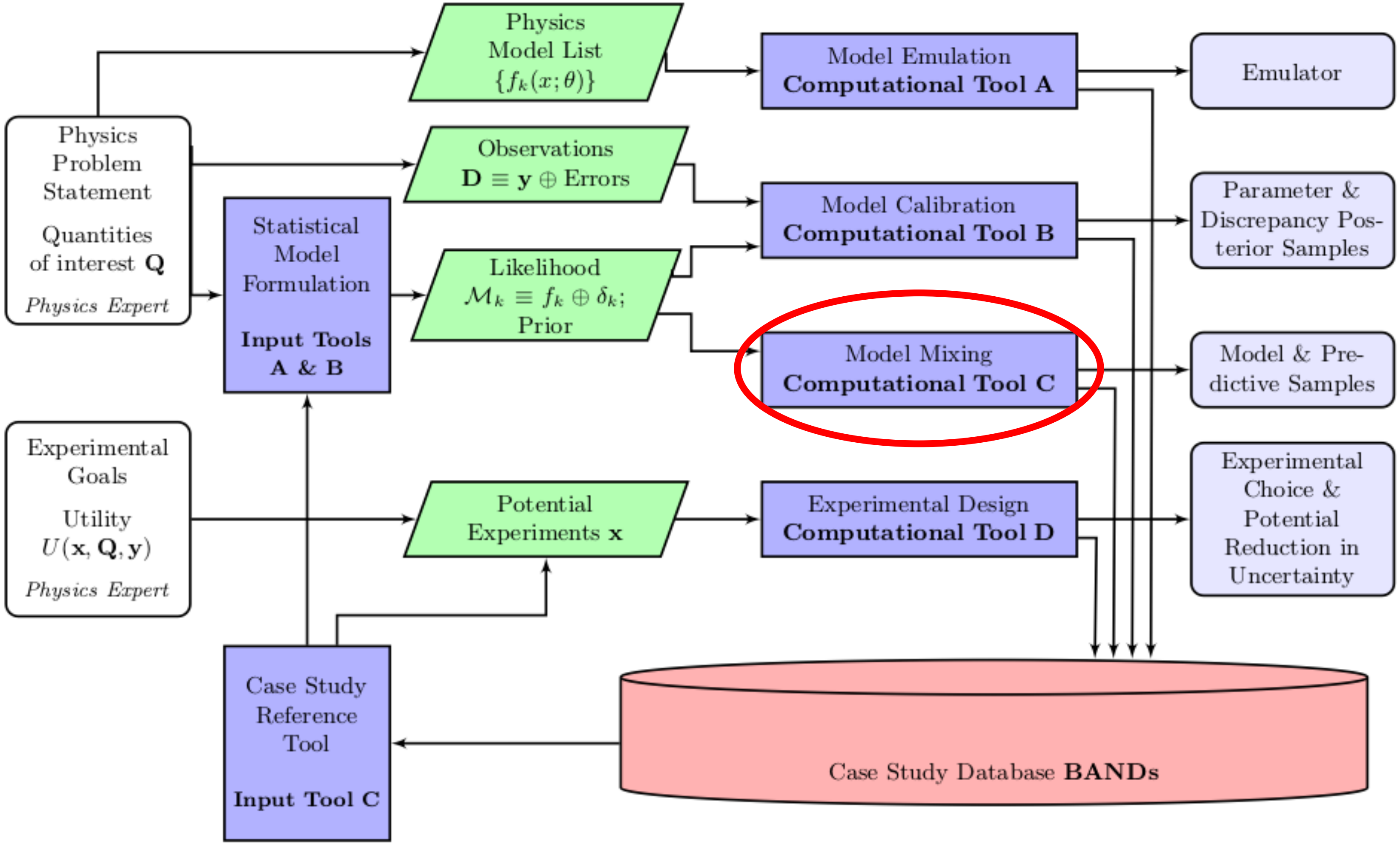


Maris, Roth et al., PRC (2022)

BAND (Bayesian Analysis of Nuclear Dynamics)

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

Look to https://bandframework.github.io/ for manifeso and developments!



Model-mixing examples:
Semposki et al., PRC (2022); Yannotty et al, 2301.02296. Matching expansions of a toy model at small and large coupling; different BMMs.
Future: mixing nuclear EOS across ρ; mixing pionless + chiral EFT; …

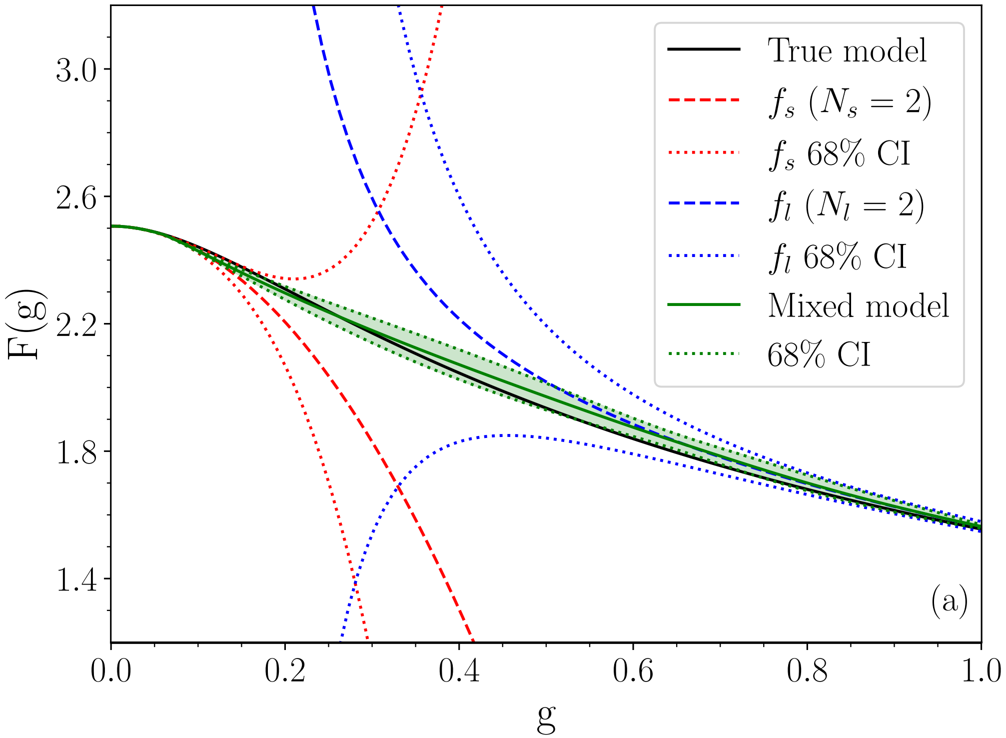
Toy Bayesian model mixing (BMM) example

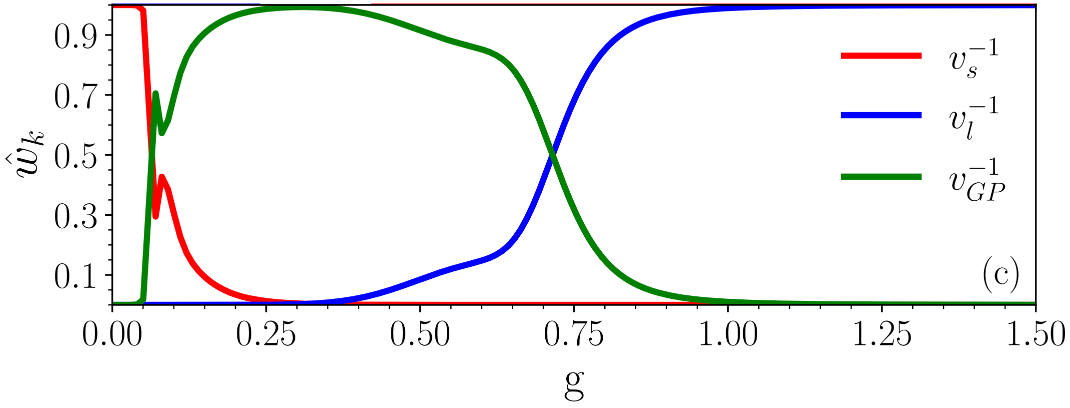
Semposki et al., PRC (2022);

- 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.





A. Semposki J. Yanotty

Test strategies with expansions of:

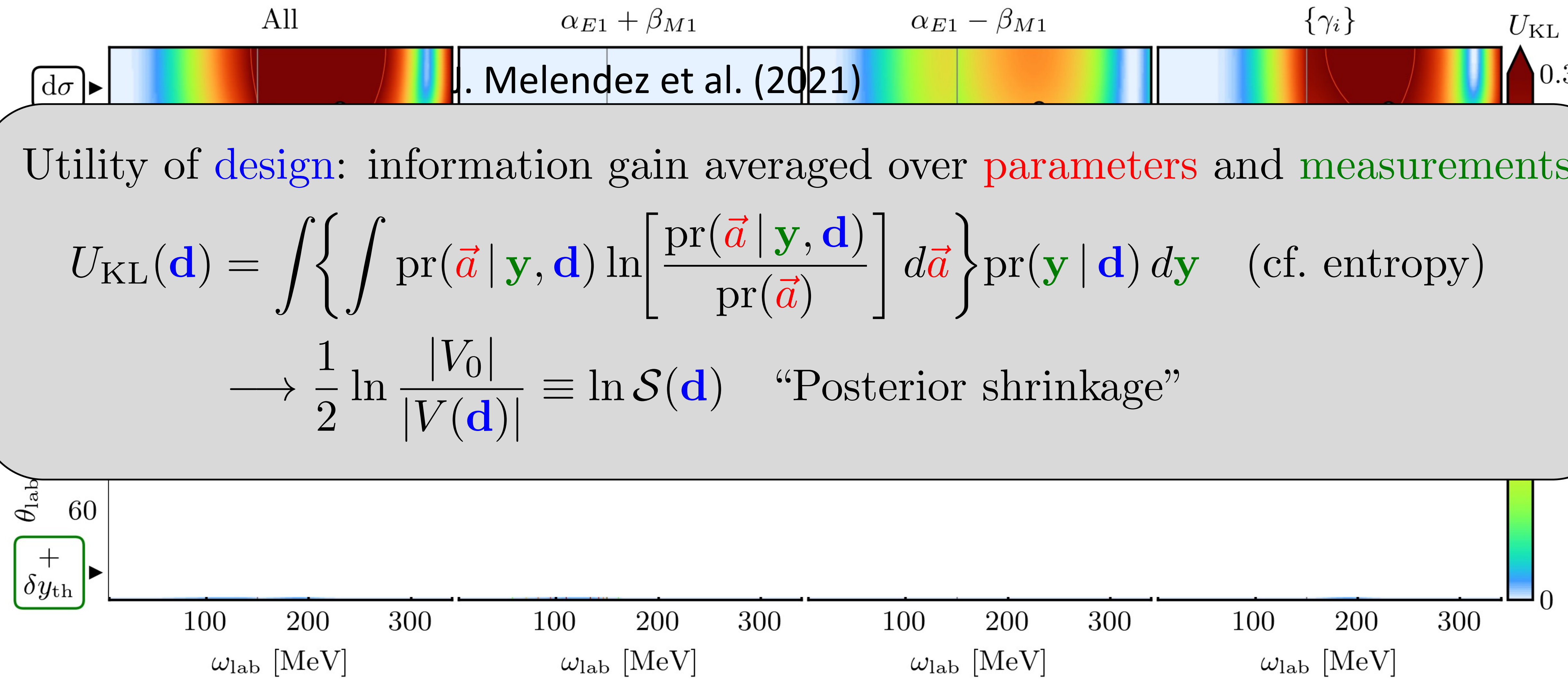
$$F(g) = \int_{-\infty}^{\infty} dx\ e^{-\frac{x^2}{2} - g^2 x^4}$$

and truncation error models.

Experimental design: Future Compton scattering experiments

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

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



Utility of design: information gain averaged over parameters and measurements

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

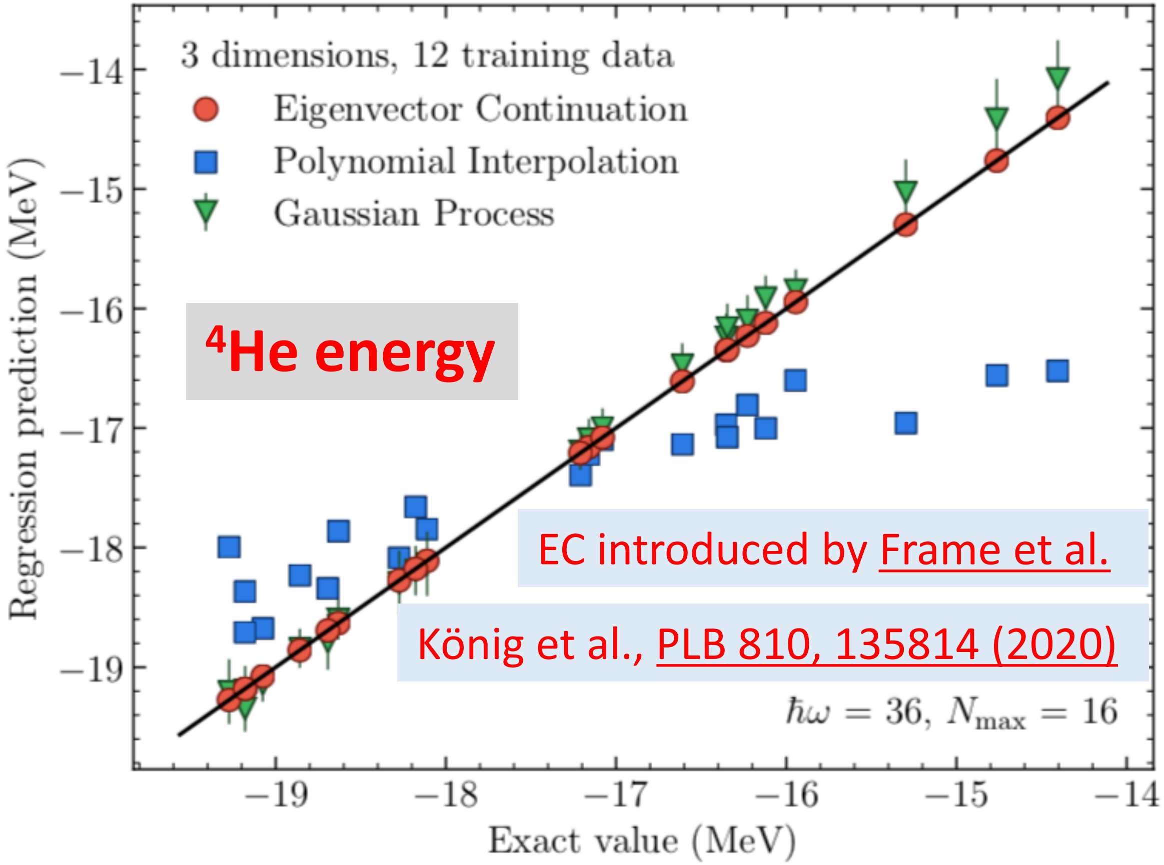
$$\longrightarrow \frac{1}{2}\ln\frac{|V_0|}{|V(\mathbf{d})|} \equiv \ln\mathcal{S}(\mathbf{d}) \quad \text{“Posterior shrinkage”}$$

Compare utility with and without truncation error included ⇒ very different implications!

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.

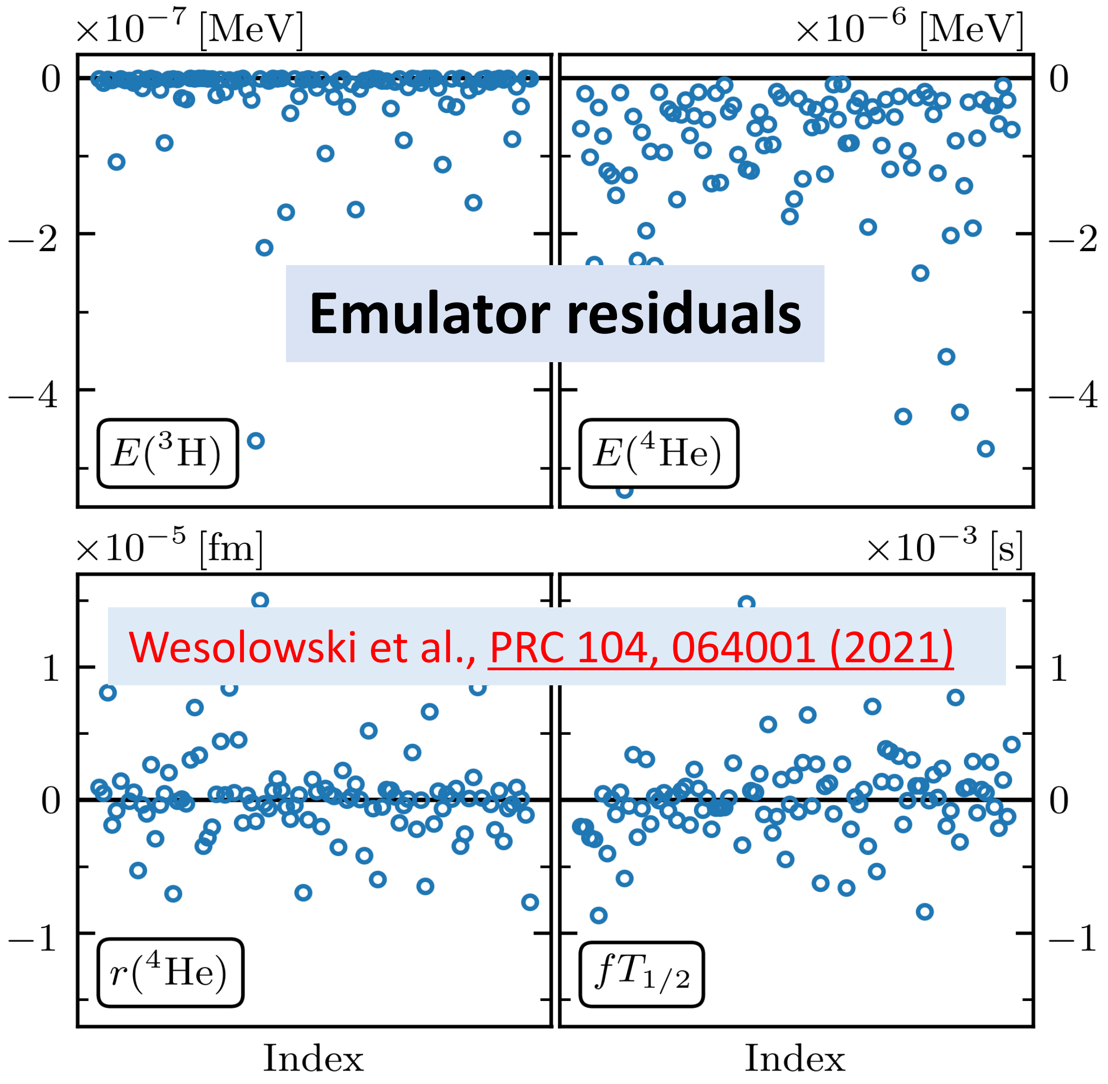
Characteristics: fast and accurate!



^{4}He energy

EC introduced by Frame et al.

König et al., PLB 810, 135814 (2020)



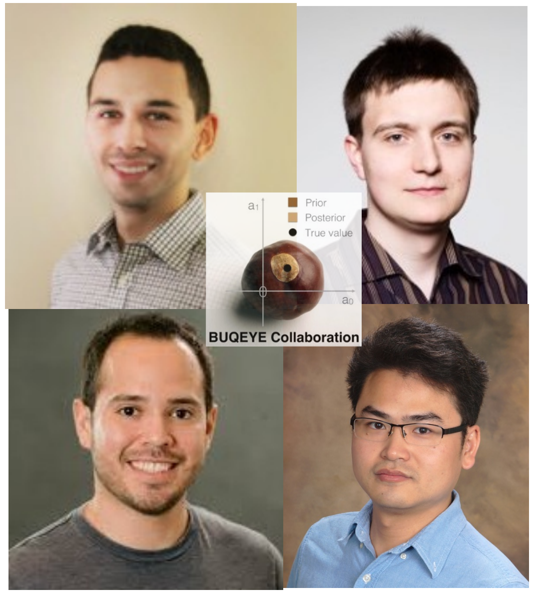
Emulator residuals

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

Emulator doesn't require specialized calculations!

Model reduction methods for nuclear emulators

Melendez, Drischler, rjf, Garcia, Zhang, J. Phys. G (2022) → **many references**



BUQEYE Guide to Projection-Based Emulators in Nuclear Physics

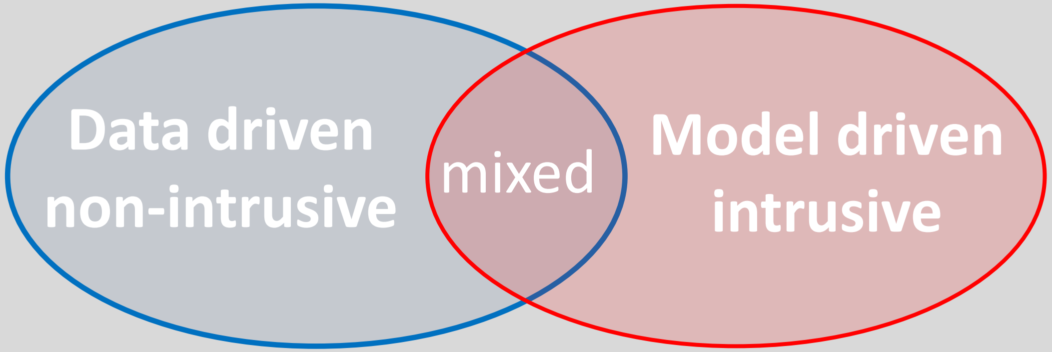
→ Pedagogical guide in Front. Physics; all examples available as interactive, Python code [format: Quarto book]

Need: to vary parameters for design, control, optimization, UQ.

Exploit: much information in high-fidelity models is superfluous.

Solution: reduced-order model (ROM) → emulator (fast & accurate™).

General classification of ROMs



Model reduction methods for nuclear emulators

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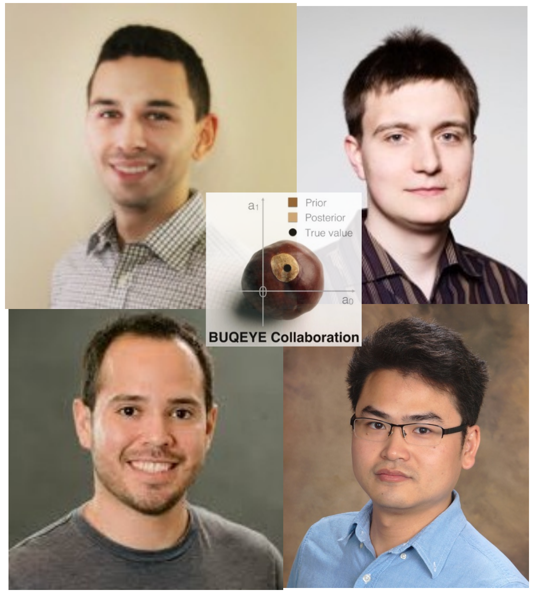

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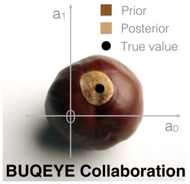
[Parametric] MOR (model order reduction)

- …
- …
- RB (reduced basis) method
  - EC (eigenvector continuation)
  - *E. Bonilla, P. Giuliani et al., Phys. Rev. C 106, 054322*
- …
- …

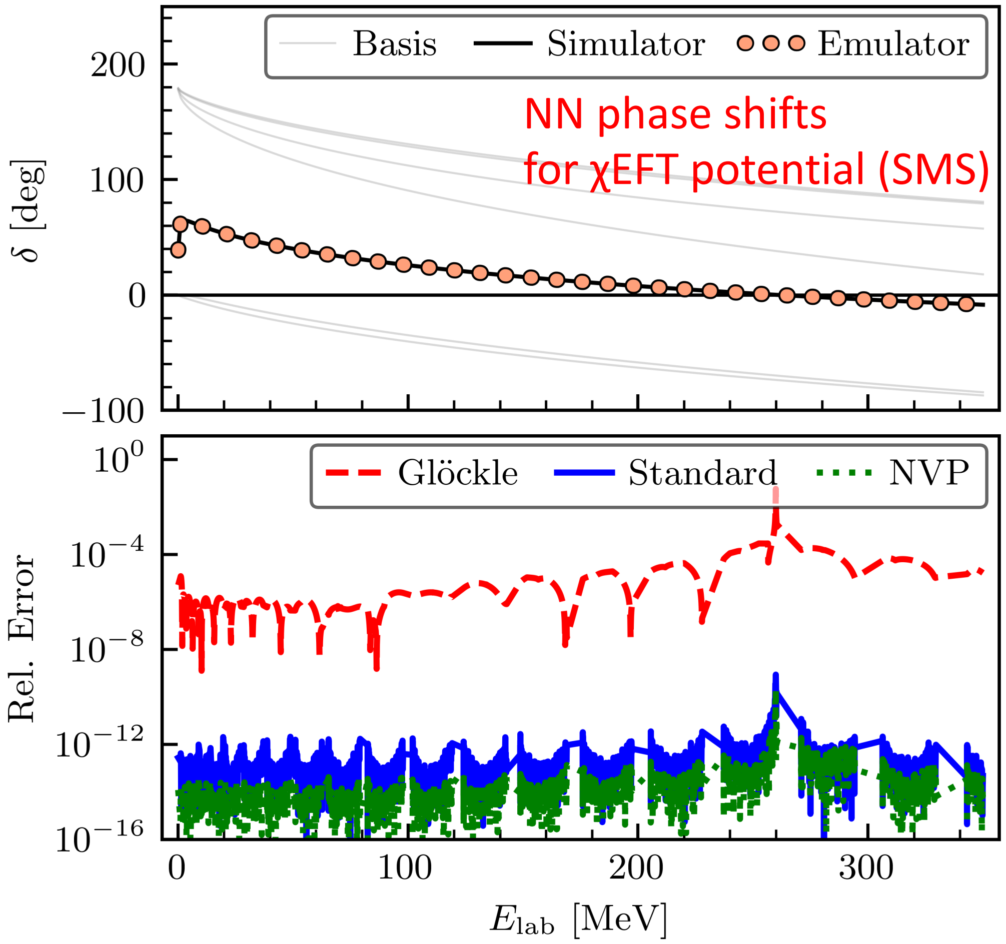
P. Giuliani, K. Godbey et al., arXiv:2209.13039.

Overall message: ROMs from variational principles relate to a vast literature (plus software!) on the Galerkin method, which is even more general. Many alternative implementations are possible and many technical aspects to adapt (e.g., non-affine treatments).

EC-like emulators for NN and 3N scattering



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



Latest from Alberto Garcia et al. (arXiv:2301.05093)

- Here: χEFT SMS potential from Reinert et al.
- Partial waves up to $j = 20$
- Used LHS to sample 500 parameter sets in an interval of [-5, 5]

- Errors essentially negligible
- Here: # of basis states = 2 × # LECs
- Speed-up is implementation-dependent!
- Consistent for $\Lambda = 400 - 550\,\mathrm{MeV}$

- Kohn anomalies mitigated!

EC emulators for NN and 3N scattering

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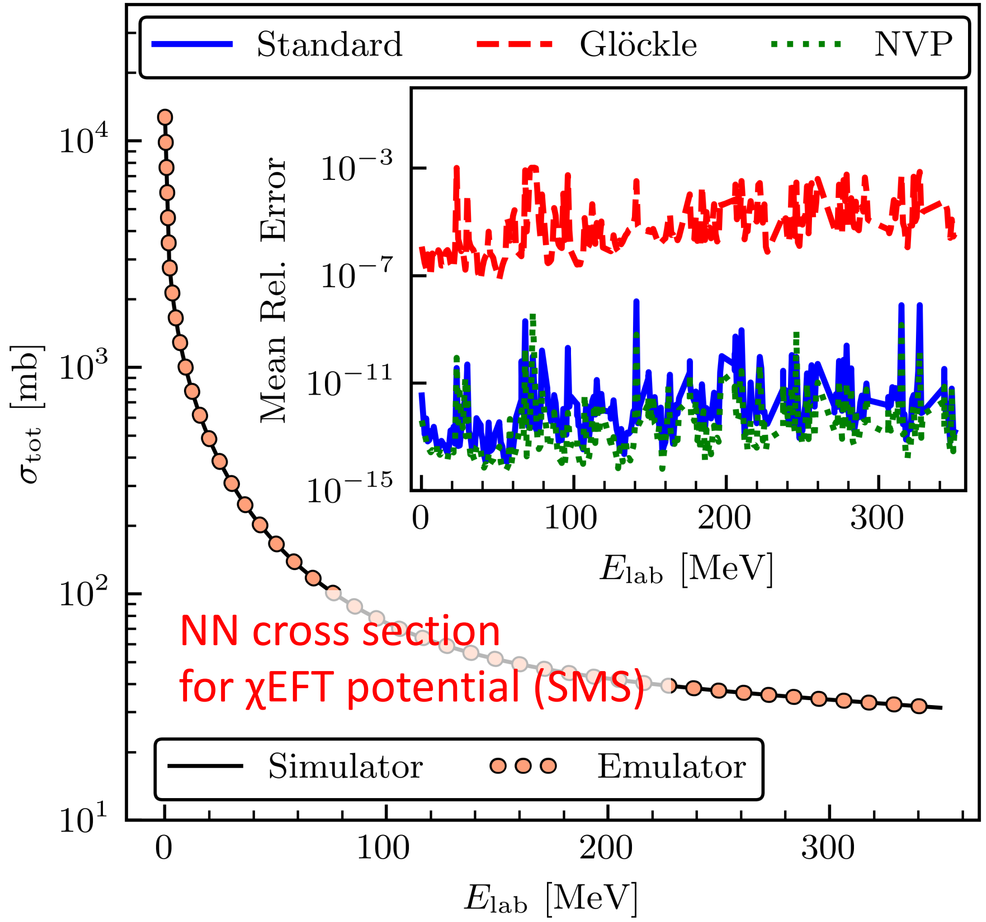

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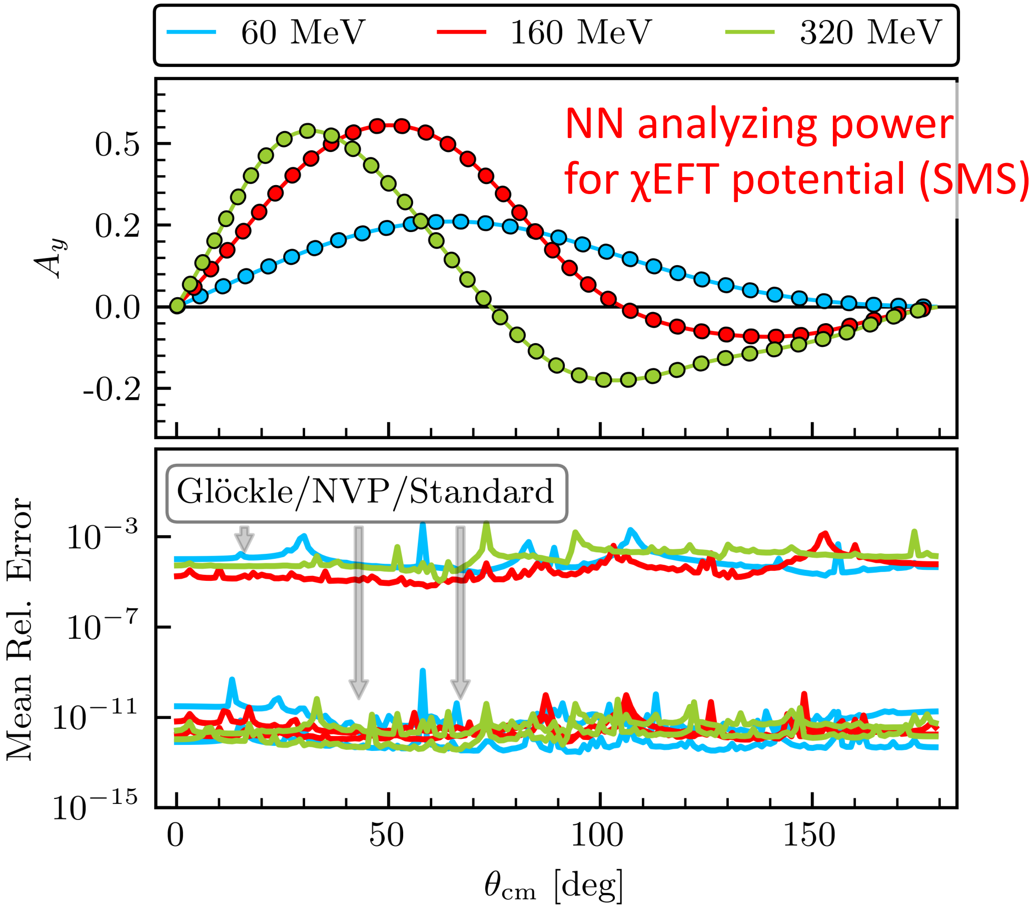

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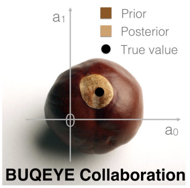

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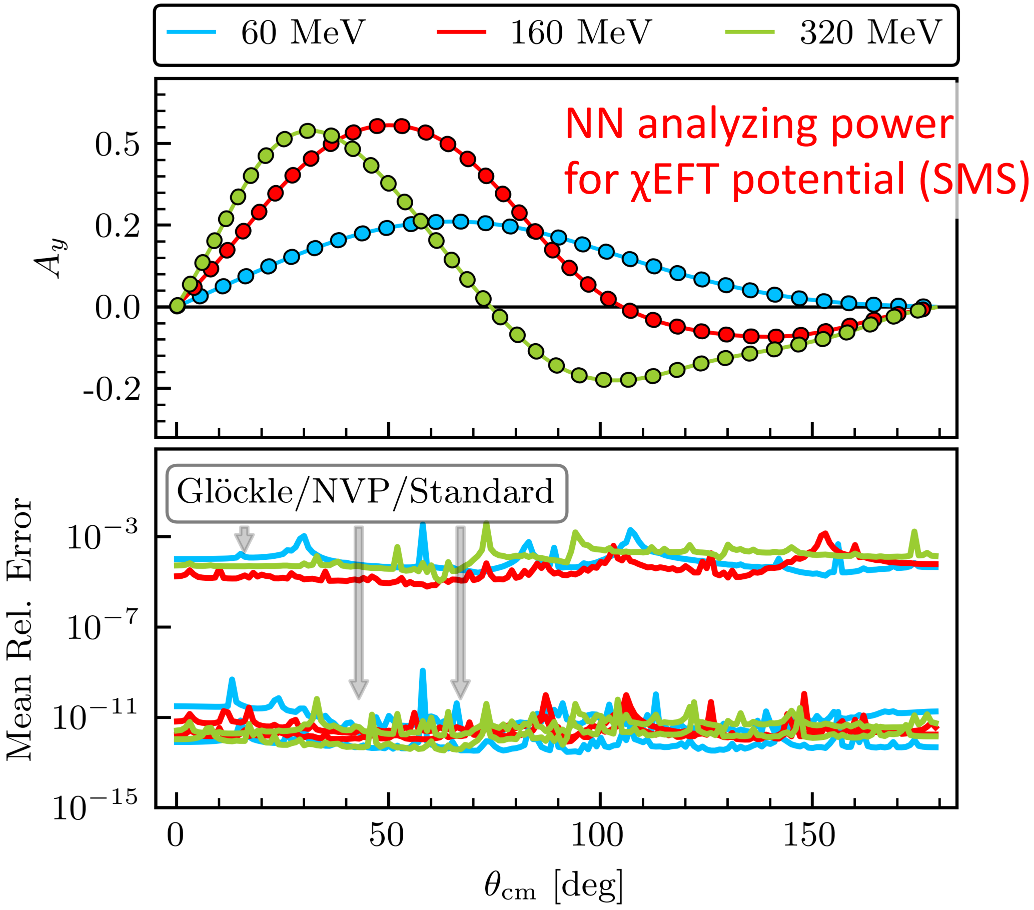
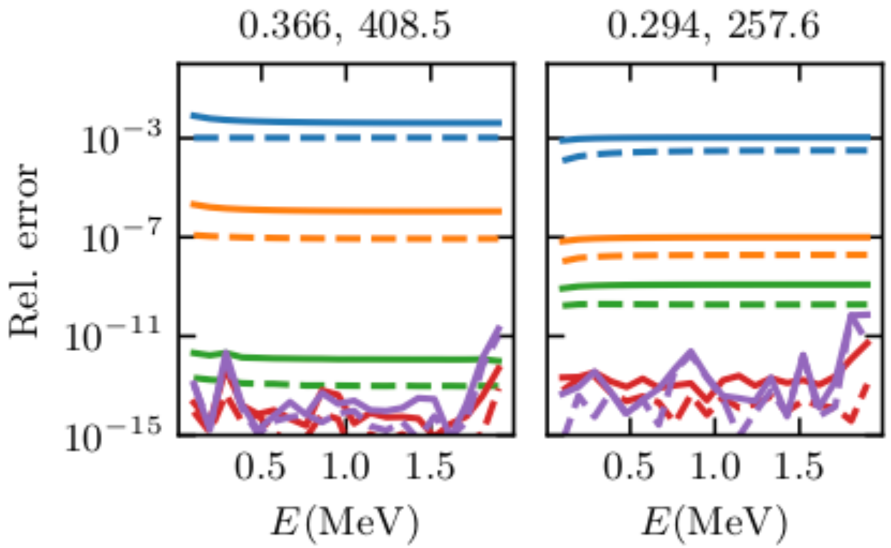


What about 3-body scattering emulators?
E.g, for Bayesian χEFT LEC estimation.
→ X. Zhang, rjf proof of principle w/KVP (2022).



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 PR Res. 4 (2022) and Krakow group for Faddeev emulator, EPJA 57 (2021).

Opportunities at the frontiers of UQ for EFTs

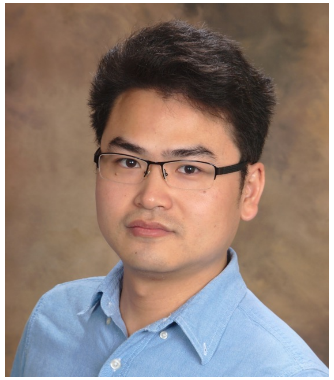
- Extend full Bayesian treatments. Do calculations with different regularized Weinberg counting agree within expectations? Analysis of other power countings.
- Power counting / EFT truncation model at finite density –> use statistics to uncover power counting? Modeling convergence pattern when there is fine-tuning.
- Applications to external currents [e.g., Acharya and Bacca, arxiv:2109.13972]
- Exploiting statistical correlations using Bayesian tools, e.g., in nuclear spectra
- Using RG for UQ (combine with convergence pattern?)
- UQ technologies to develop and apply: model mixing; experimental design, …
- Emulators: 3N scattering; infinite matter; new technologies (e.g., active learning)
- Making increased use of AI/machine learning
- And much more . . . **See other talks!!**

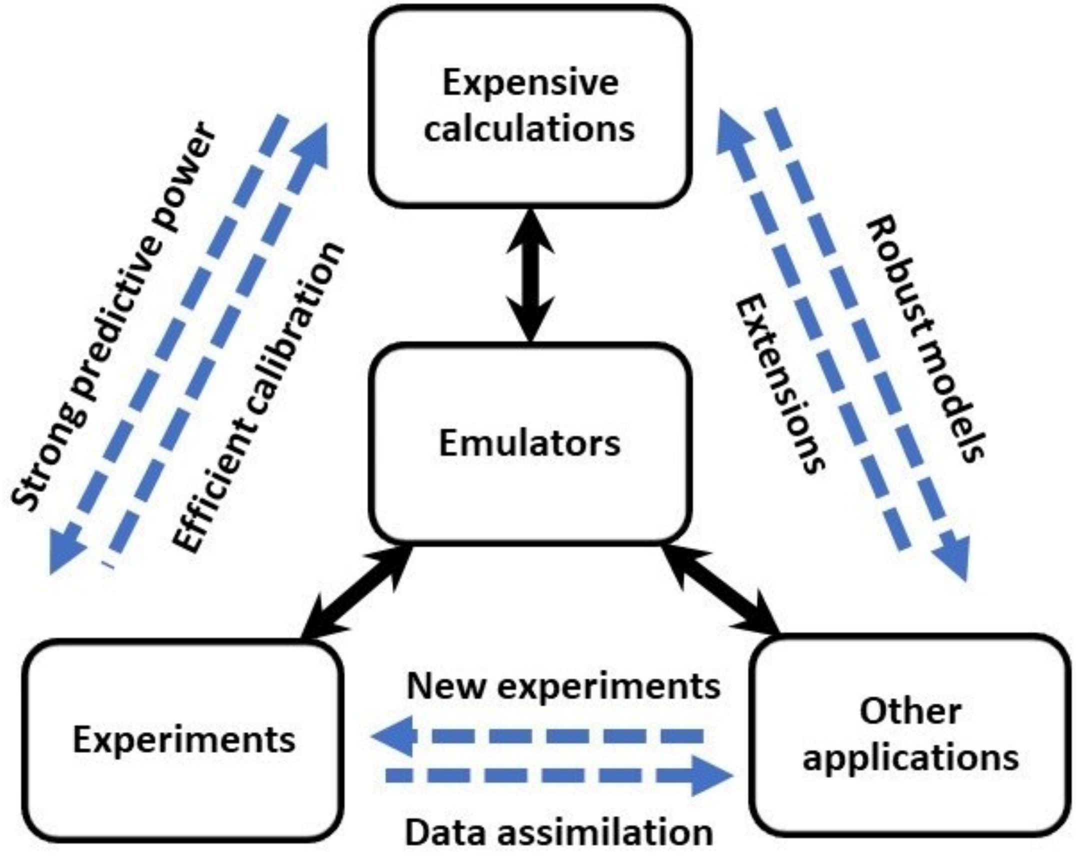
Thank you!

Extra slides

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!

Some of the applications of Bayesian inference

In order of complexity . . .

1. Forward UQ (e.g., propagate errors using already-sampled posteriors)

2. Inverse UQ (e.g., parameter estimation including theory errors)

3. Experimental Design (guide to experiment: which data are most likely to provide the largest information gain; both theory uncertainty *and* the expected pattern of experimental errors must be considered)

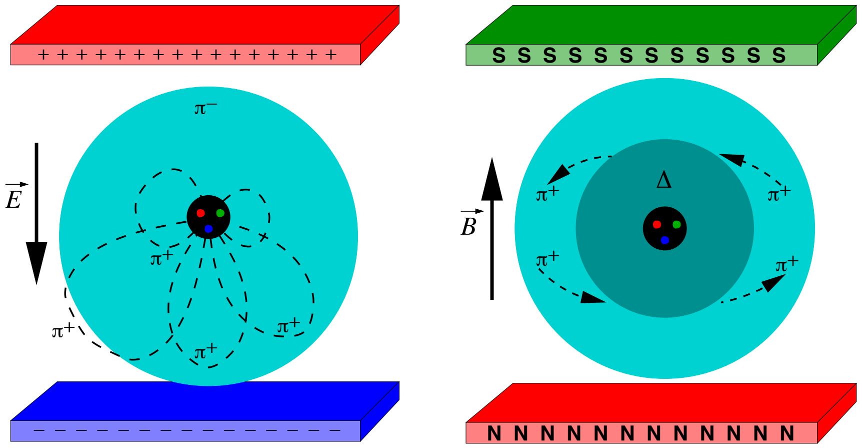
Experimental design: A case study

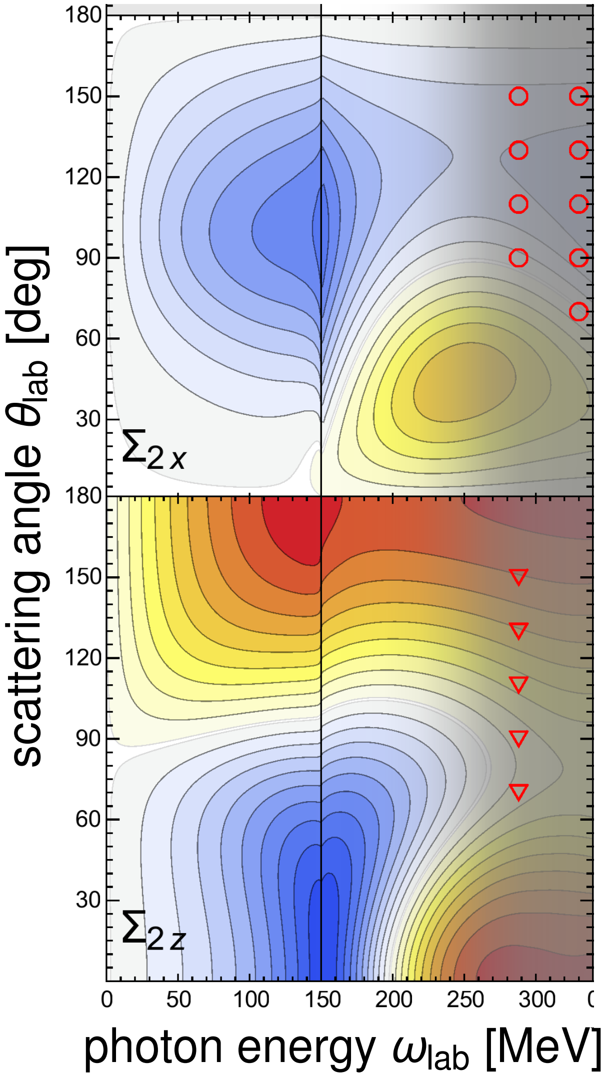
Maximize benefits – minimize cost (time, money, workforce)

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?





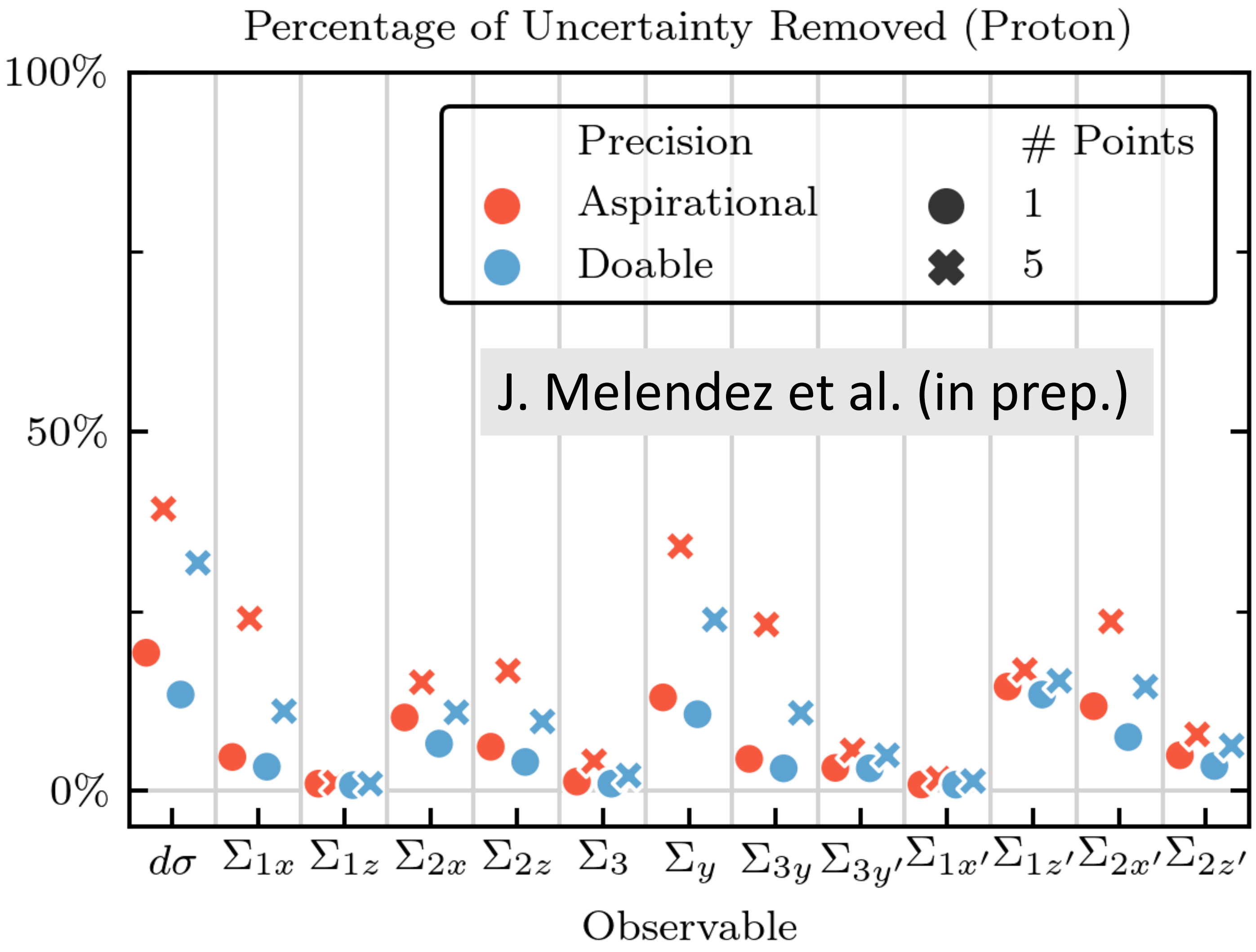
$$2\pi \Big[\underbrace{\alpha_{E1}\,\vec{E}^2 + \beta_{M1}\,\vec{B}^2}_{\text{electric, magnetic scalar dipole}} + \underbrace{\gamma_{E1E1}\vec{\sigma}\cdot(\vec{E}\times\dot{\vec{E}}) + \gamma_{M1M1}\vec{\sigma}\cdot(\vec{B}\times\dot{\vec{B}}) + 2\gamma_{M1E2}\sigma^i B^j E_{ij} + 2\gamma_{E1M2}\sigma^i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

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?

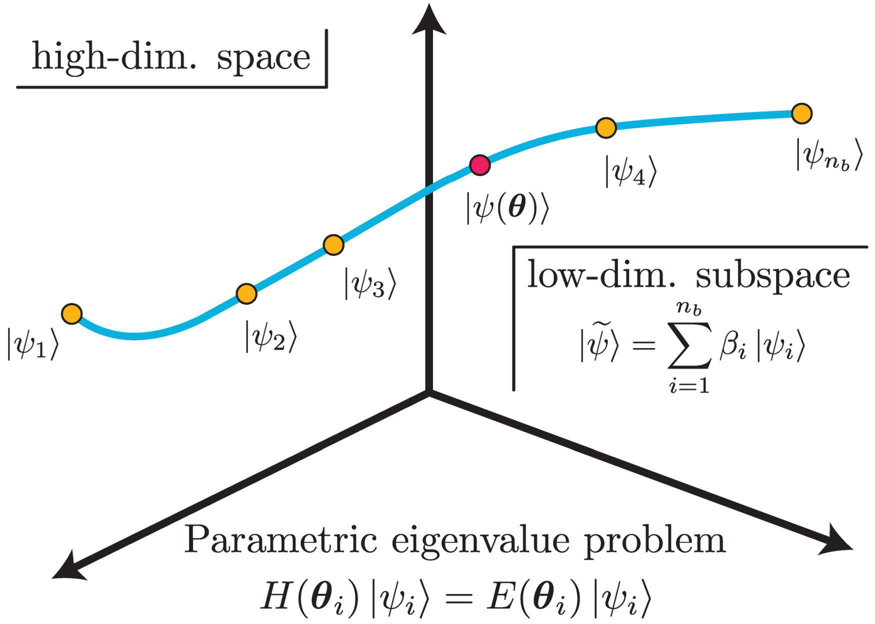
Ingredient: Calculate a utility function for sum of variances for each kinematic point on a grid.

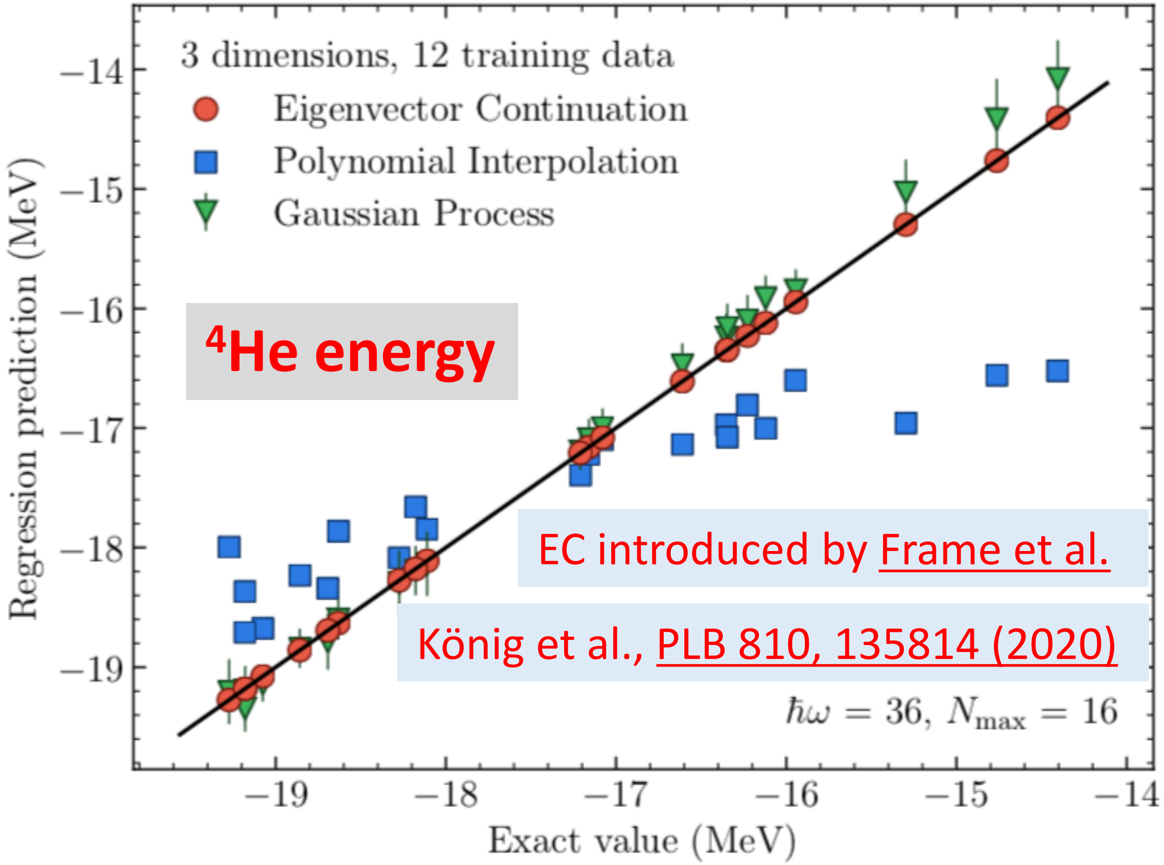


- Apply to decide on trade-off between different allocations of experimental resources (exploration vs. exploitation).
- 1-point vs 5-point?
- Increase precision or more points?

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!

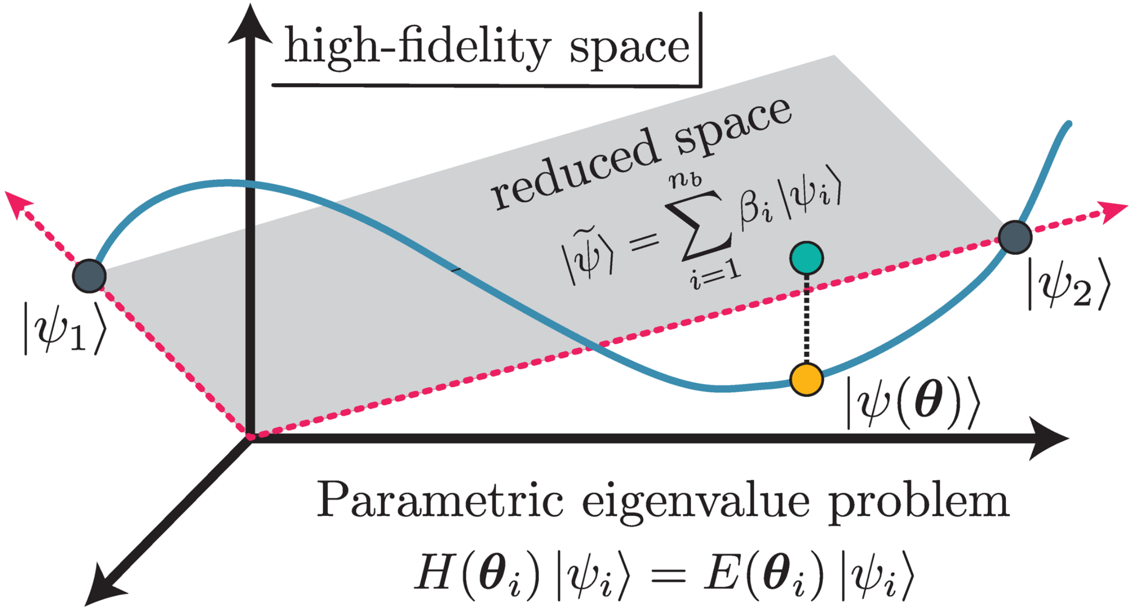




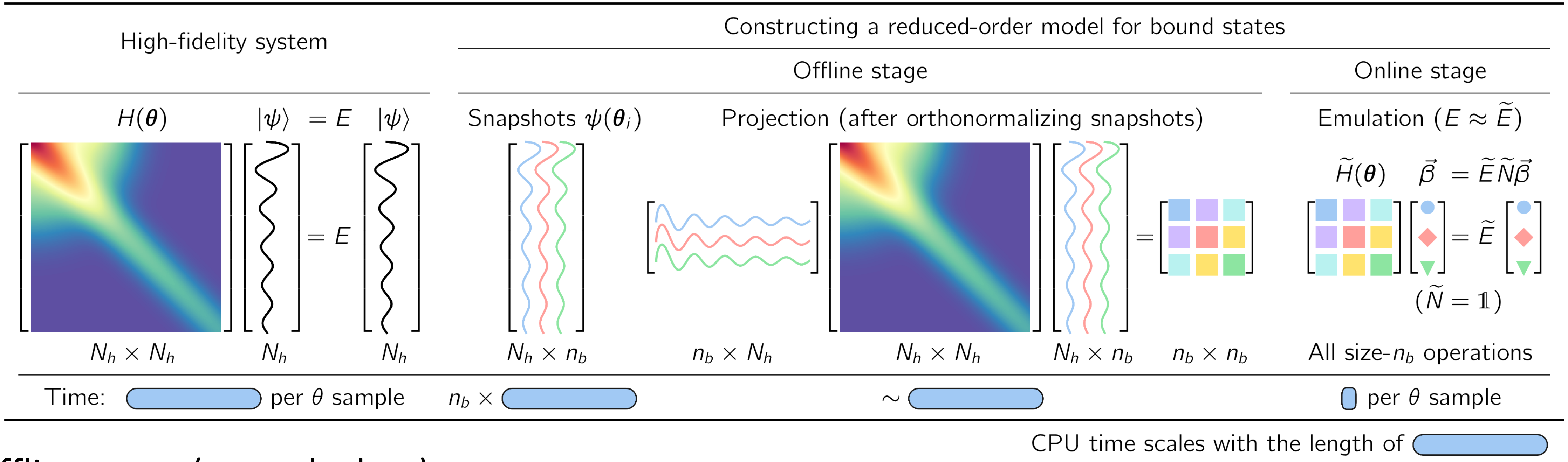
^{4}He energy

EC introduced by Frame et al.

König et al., PLB 810, 135814 (2020)



Constructing a reduced-order model (ROM)



- Offline stage (pre-calculate):
  - Parameter sets using a greedy algorithm, Latin-hypercube sampling, etc.
  - Construct basis using snapshots from high-fidelity system (simulator)
  - Project high-fidelity system to small-space using snapshots
  - Exploit affine dependence on the low-energy couplings (LECs):

$$V(\boldsymbol{\theta}) = V^0 + \boldsymbol{\theta} \cdot \boldsymbol{V}^1$$

- Online stage:
  - 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

Parametric MOR emulator workflow

Bird's eye view but still for projection-based PMOR only (i.e., not an exhaustive set!)

(1) Sampling across range of parameters θ for N_{sample} candidate snapshots → {θ_i}

- E.g., space-filling design (like latin hypercube) or center near emulated values.
- Want $N_b \le N_{sample}$ snapshots; locate wisely based on basis construction method.

(2) Generating a basis *X* from the snapshots to create. Multiple options, including:

- *Proper Orthogonal Decomposition* (POD) [cf. PCA] → extract most important basis vectors. Compute all N_{sample} snapshots $\psi(\boldsymbol{\theta}_i)$ but keep N_b based on SVD.
- *Greedy algorithm* is an iterative approach: next location $\boldsymbol{\theta}_i$ from *fast* estimated emulator error at N_{sample} values and choose value with largest expected error.
- For time-dependent case, sample also in time or frequency. Many options here!

(3) Construct the reduced system. Single basis ***X*** or multiple bases across **θ**

- Linear system and affine operators → projecting to single basis works well.
- If non-linear or non-affine → *hyper-reduction* approaches: e.g., empirical interpolation method EIM or DEIM, which finds an affine (separable) expansion.

Variational and Galerkin emulators by concrete example

Emulator → $\psi(\boldsymbol{\theta}) \approx \widetilde{\psi}(\boldsymbol{\theta}) = X\vec{\beta}_*, \quad X \equiv [\psi_1\, \psi_2\, \cdots\, \psi_{N_b}]$ find optimal $\vec{\beta}_*$ cheaply online

E.g., Poisson equation with Neumann BCs → $[-\nabla^2\psi = g(\boldsymbol{\theta})]_\Omega$ with $[\frac{\partial\psi}{\partial n} = f(\boldsymbol{\theta})]_\Gamma$

Variational (Ritz)

$$S[\psi] = \int_\Omega d\Omega\, (\tfrac{1}{2}\nabla\psi\cdot\nabla\psi - g\psi) - \int_\Gamma d\Gamma\, f\psi$$

$$\Longrightarrow \delta S = \int_\Omega d\Omega\, \delta\psi(-\nabla^2\psi - g) + \int_\Gamma d\Gamma\, \delta\psi\Big(\frac{\partial\psi}{\partial n} - f\Big)$$

So δS = 0 gives the Poisson eq. and BCs. Emulate $\psi(\boldsymbol{\theta})$:

$$S[\widetilde{\psi}] \to \delta S[\widetilde{\psi}] = \sum_{i=1}^{N_b} \frac{\partial S}{\partial \beta_i}\delta\beta_i = 0$$ → N_b equations for $\vec{\beta}_*$

If linear (as here) → $\widetilde{A}\vec{\beta}_* = \vec{g} + \vec{f}, \quad \widetilde{A}_{ij} = \int_\Omega \nabla\psi_i\cdot\nabla\psi_j,$
$g_i = \int_\Omega g(\boldsymbol{\theta})\psi_i, \quad f_i = \int_\Gamma f(\boldsymbol{\theta})\psi_i$

If affine g(**θ**), f(**θ**) → calculate high-fidelity offline.
If nonlinear or nonaffine → hyper-reduction, etc.

Ritz-Galerkin

Weak formulation rather than variational
→ multiply each equation by *test function*

$$\int_\Omega d\Omega\, \phi(-\nabla^2\psi - g) + \int_\Gamma d\Gamma\, \phi\Big(\frac{\partial\psi}{\partial n} - f\Big) = 0$$

$$\Longrightarrow \int_\Omega d\Omega\, (\nabla\phi\cdot\nabla\psi - g\phi) - \int_\Gamma d\Gamma\, f\phi = 0$$

Assert holds for $\psi \to \widetilde{\psi} = X\vec{\beta}$ and $\phi = \sum_{i=1}^{N_b}\delta\beta_i\psi_i$

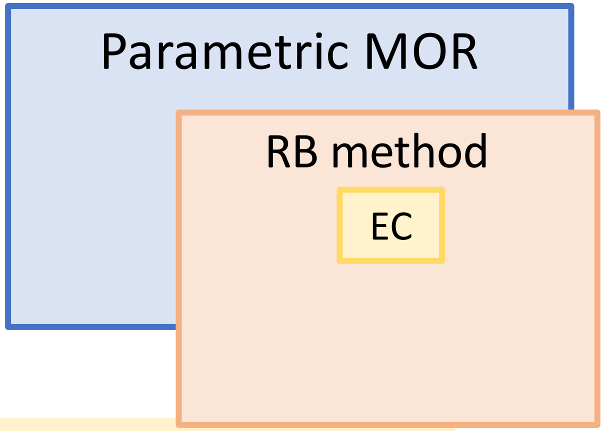
$$\delta\beta_i\Big[\int_\Omega d\Omega\, (\nabla\psi_i\cdot\nabla\psi_j\beta_j - g\psi_i) - \int_\Gamma d\Gamma\, f\psi_i\Big] = 0$$

Same result as variational here (but Galerkin is more general). If $\varphi_i \neq \psi_i$, then *Petrov-Galerkin*.

Some model reduction methods in context

Reduced Basis method (1980) widely used to emulate PDEs in reduced-order approach. Specific choices in MOR framework:

- Parameter set chosen using greedy algorithm (or POD)
- Single basis *X* constructed from snapshots
- RB model built from global basis projection



Eigenvector continuation (EC) is a particular implementation of the RB method
→ parametric reduced-order model for an eigenvalue problem (lots of prior art)

- Global basis constructed with snapshot-based POD approach
- "Active learning" by Sarkar and Lee adds greedy sampling algorithm for next $\boldsymbol{\theta}_i$

Summary: general features of *good* reduced-order emulators

- System dependent → works best when QOI lies in low-D manifold and operations on ψ can be avoided during online phase
- Relative smoothness of parameter dependence
- Affine parameter dependence (or effective hyper-reduction or other approach)

Reduced-order model (ROM) for scattering w/ NVP

LS equation:

$$K(\vec{a}) = V(\vec{a}) + V(\vec{a})\, G_0(E_q)\, K(\vec{a})$$

→ Training set: $\{\vec{a}_i\}$

K-matrix formulation:

$$K_\ell(E_q) = -\tan\delta_\ell(E_q)$$

$$E_q = q^2/2\mu$$

Newton variational principle (NVP):

$$\mathcal{K}[\tilde{K}] = V + VG_0\tilde{K} + \tilde{K}G_0V - \tilde{K}G_0\tilde{K} + \tilde{K}G_0VG_0\tilde{K}$$

$$\mathcal{K}[K_{\text{exact}} + \delta K] = K_{\text{exact}} + (\delta K)^2$$

Implementation:

$$\tilde{K}(\vec{\beta}) = \sum_{i=1}^{n_t} \beta_i K_i$$

Snapshots (K_i)

Basis weights (β_i)

$$\langle\phi'|\mathcal{K}(\vec{a},\vec{\beta})|\phi\rangle \approx \langle\phi'|V(\vec{a})|\phi\rangle + \frac{1}{2}\vec{m}^T M^{-1}(\vec{a})\,\vec{m}$$

→ Linear algebra in small-space!

J. A. Melendez et al., Phys. Lett. B 821, 136608 (2021)

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Reduced-order model (ROM) for scattering w/ KVP

Hamiltonian:

$$\widehat{H}(\boldsymbol{\theta}) = \widehat{T} + \widehat{V}(\boldsymbol{\theta}) \rightarrow$$

Training set:

$$\{(\boldsymbol{\theta})_i\}$$

K-matrix formulation:

$$K_s(E) = \tan \delta_s(E)$$

$$E = k_0^2/2\mu$$

Generalized Kohn variational principle (KVP):

$$\mathcal{L}[\widetilde{\psi}] = L^{ss'}(E) - \frac{2\mu}{\det \boldsymbol{u}} \langle \widetilde{\psi}^{st} | [\widehat{H}(\boldsymbol{\theta}) - E]^{tt'} | \widetilde{\psi}^{t's'} \rangle$$

$$\mathcal{L}[\psi_{\text{exact}}] = L_{\text{exact}} + \mathcal{O}(\delta L^2)$$

Here momentum space implementation.
For coordinate space implementation:
Furnstahl et al., Phys. Lett. B 809, 135719 (2020)
Drischler et al., Phys. Lett. B 823, 136777 (2021)

Implementation:

Snapshots

$$|\widetilde{\psi}^{tt'}\rangle \equiv \sum_{i=1}^{N_b} \beta_i |(\psi_i)^{tt'}\rangle$$

Basis weights

$$\Delta\tilde{U}_{ij}(\boldsymbol{\theta}) = \frac{2\mu}{\det \boldsymbol{u}} \left[\langle (\psi_i)^{st} | [V(\boldsymbol{\theta}) - V_j]^{tt'} | (\psi_j)^{t's'} \rangle + (i \leftrightarrow j) \right]$$

$$\mathcal{L}[\vec{\beta}] = \beta_i L_i^{ss'} - \frac{k_0}{2} \beta_i \Delta\tilde{U}_{ij} \beta_j$$

→ Linear algebra in small-space!

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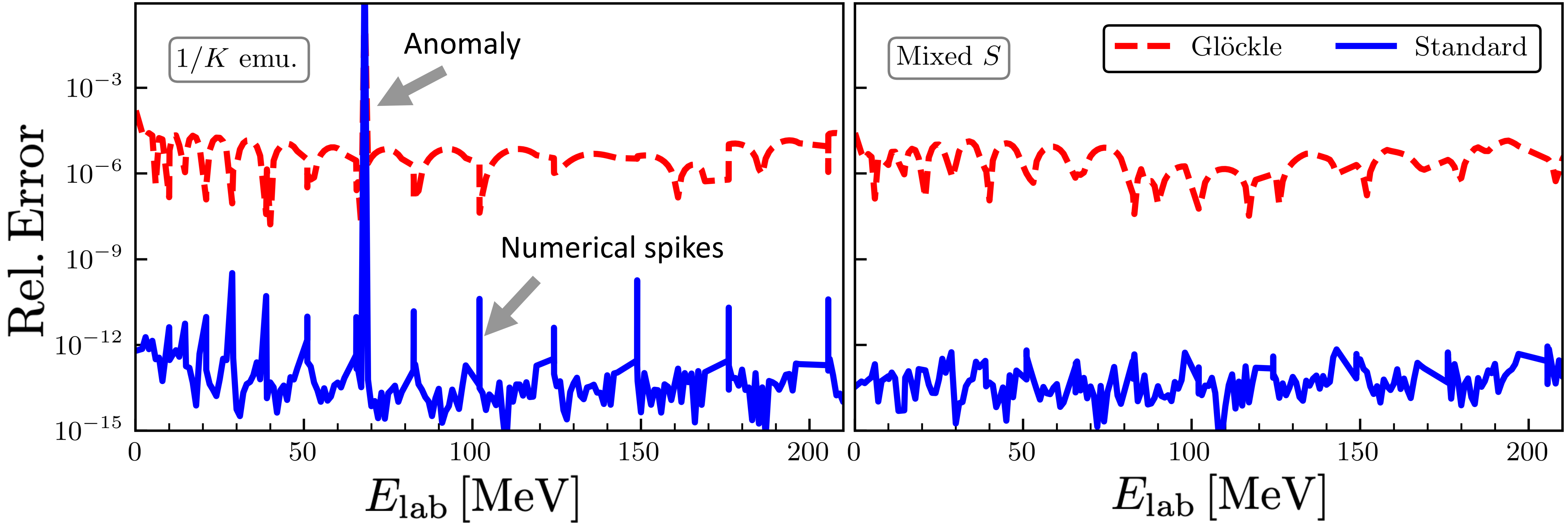
Anomalies example

- Kohn anomalies mitigated!
- Mesh-induced spikes in high-fidelity LS equation detected and removed



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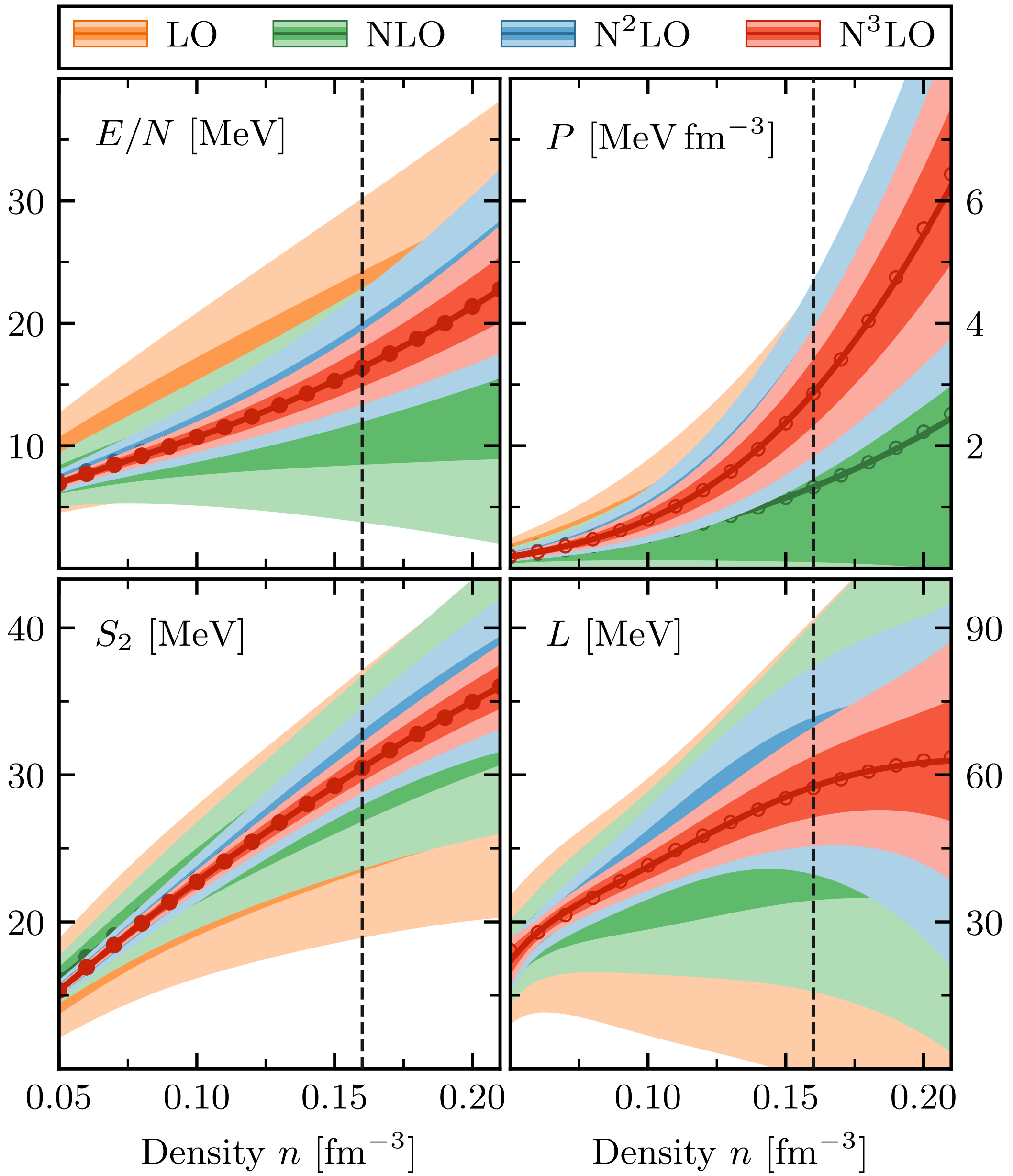
Correlated theory errors for EOS properties



C. Drischler et al. (in prep.)

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