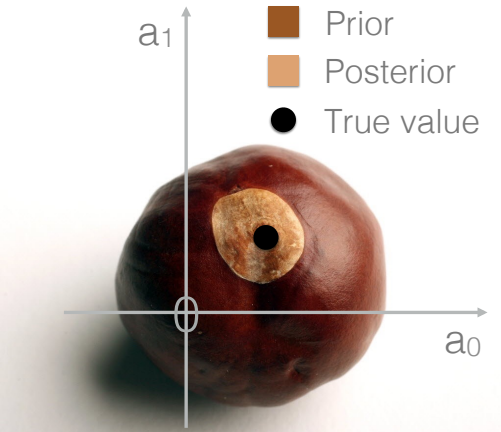
Application of Bayesian methods in effective field theory (EFT)

Dick Furnstahl

APS/DNP meeting, October, 2019

THE OHIO STATE UNIVERSITY



BUQEYE Collaboration

Special thanks to my BUQEYE collaborators!

NSF
U.S. DEPARTMENT OF ENERGY
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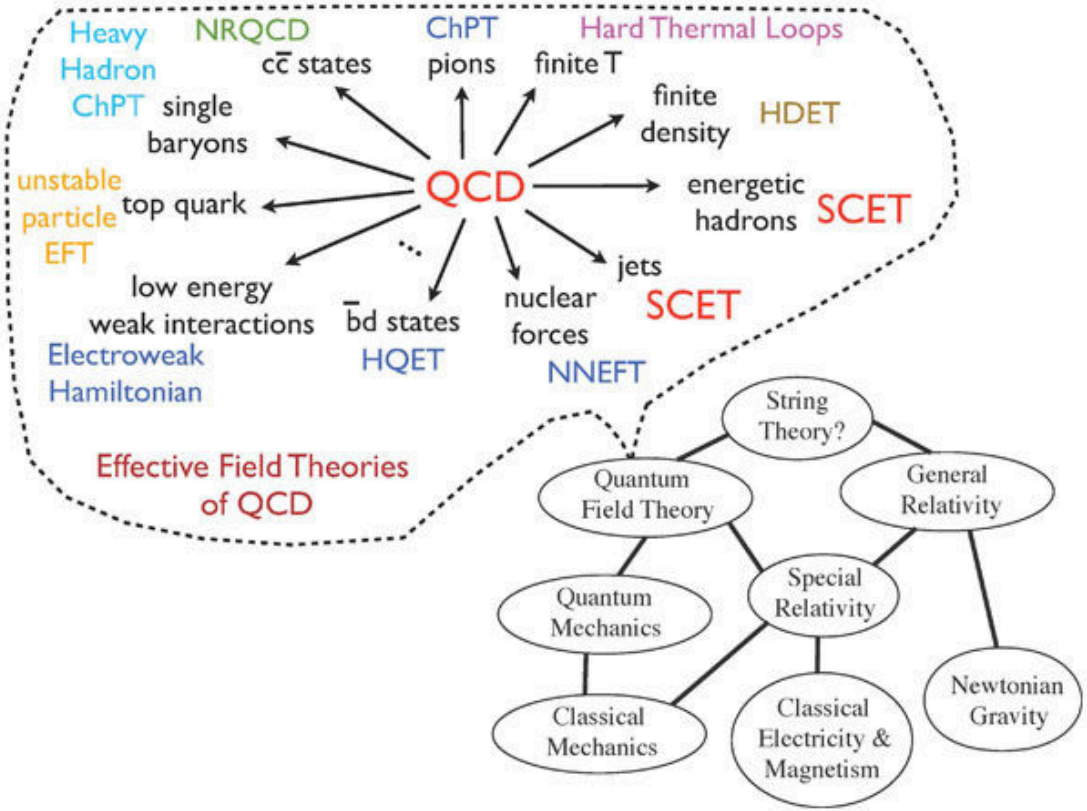
Nuclear Computational Low-Energy Initiative

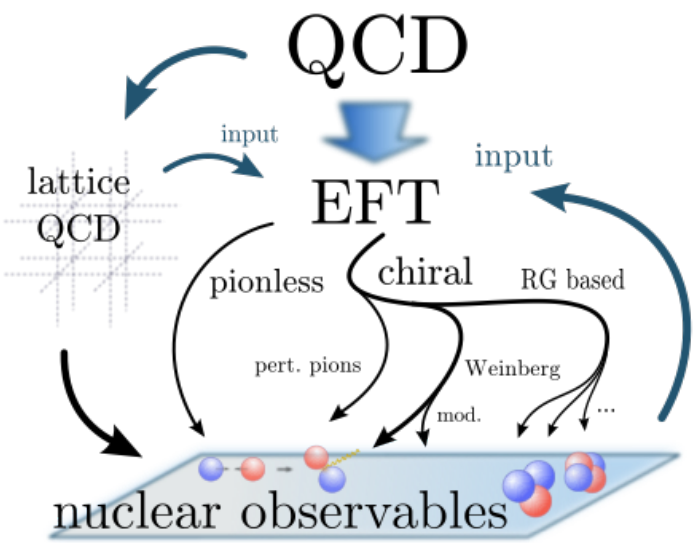
Outline

- Overview of Bayesian methods for EFT
- Truncation errors and model checking
- Aspects of EFT parameter estimation
- Snapshots of Bayesian EFT applications
- Take-away points and advertisements

Quantum chromodynamics has many EFTs!

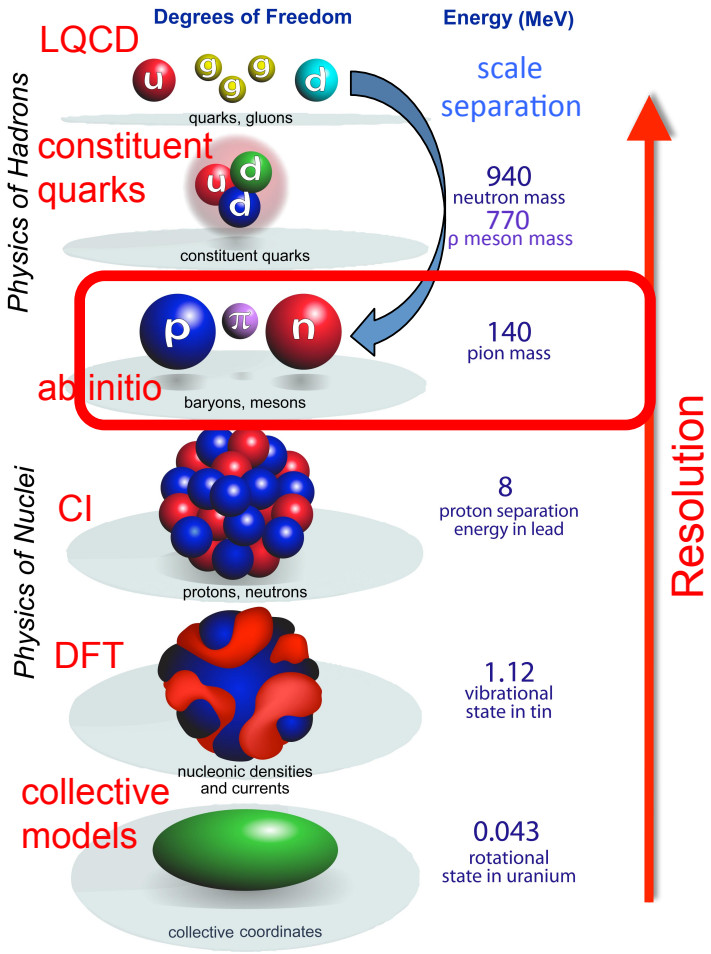


[From Iain Stewart]



[From Sebastian König]

Ingredients of EFTs that invite Bayesian statistics



- *Choice* of degrees of freedom and organization ("power counting")
- Well-defined order-by-order construction used to predict observables ⇒ *truncation error*
- Short distance physics is encoded in low-energy constants (LECs) that need to be *fitted*
- *Expectation* is that observables improve as powers of a small parameter (e.g., ratios of scales) that may not be well determined
- Need to *validate* the EFT and provide robust theory error bars

Ingredients of EFTs that invite Bayesian statistics

Bayesian approach: (almost) *everything* is a probability density function (pdf)!

$\mathrm{pr}(\mathrm{EFT}_1 \mid \boldsymbol{y}_{exp}, I)/\mathrm{pr}(\mathrm{EFT}_2 \mid \boldsymbol{y}_{exp}, I)$

$\Longrightarrow$ evidence ratio given data

$\mathrm{pr}(c_n(\boldsymbol{x}) \mid \vec{\boldsymbol{c}}_{\boldsymbol{k}}, I) \Longrightarrow$ pdf of expansion coefficients

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

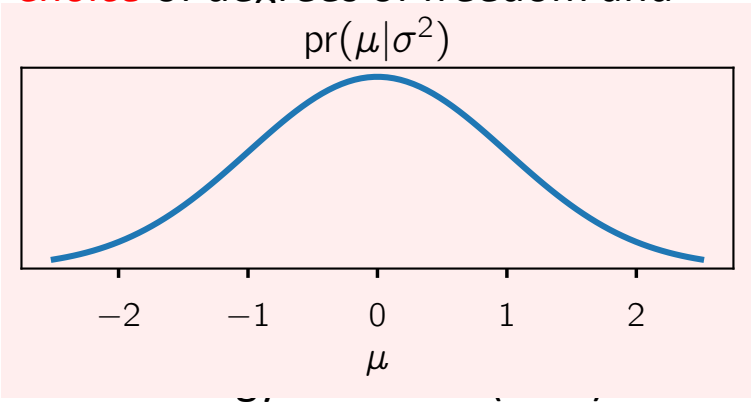
$\Longrightarrow$ pdf of LECs given data $\boldsymbol{y}_{exp}, \Sigma_{\mathrm{exp}}$ (and Σ_{th}!)

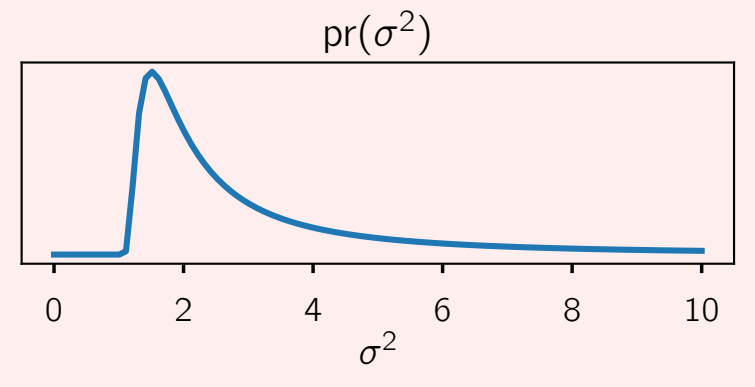
$\mathrm{pr}(\Lambda_b \mid \boldsymbol{\theta}, I) \Longrightarrow$ pdf of EFT breakdown scale

$\mathrm{pr}(\mu, \sigma \mid I) \Longrightarrow$ pdf of hyperparameters

Use rules of probability to manipulate
Marginalize over nuisance parameters

- *Choice* of degrees of freedom and

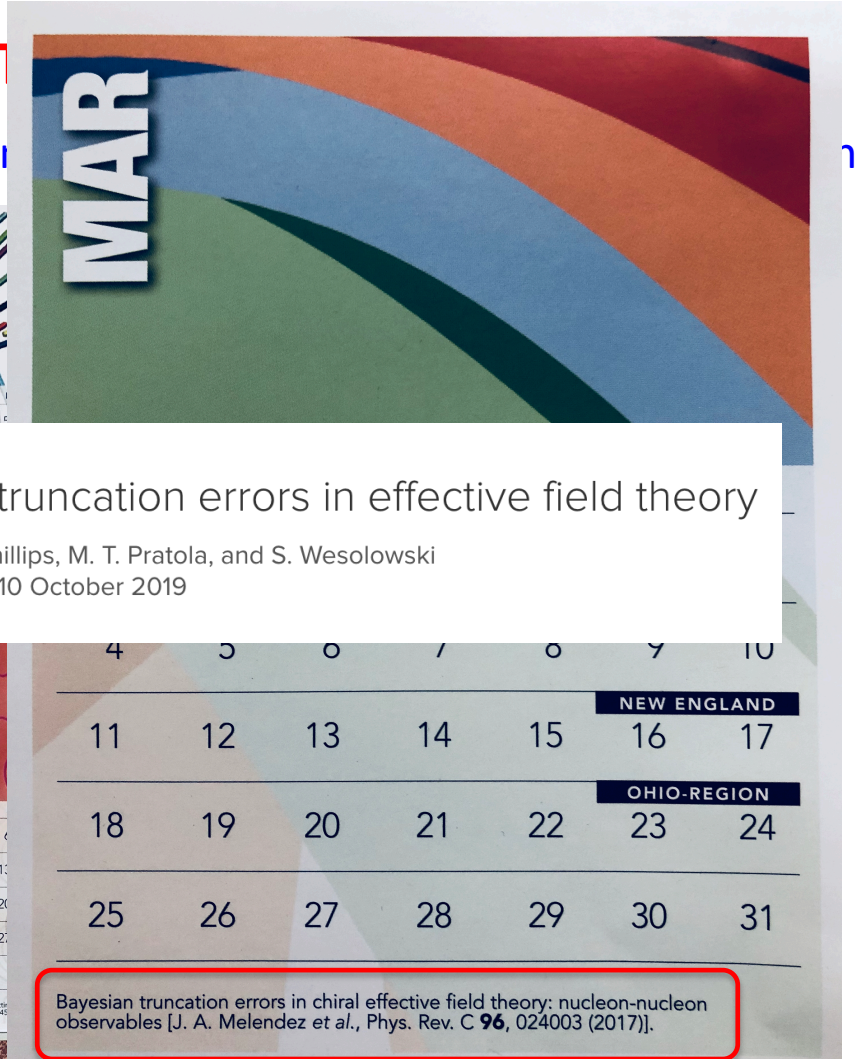




- provide robust theory error bars

Example: chiral EFT

How do we apply Bayesian ur ng?



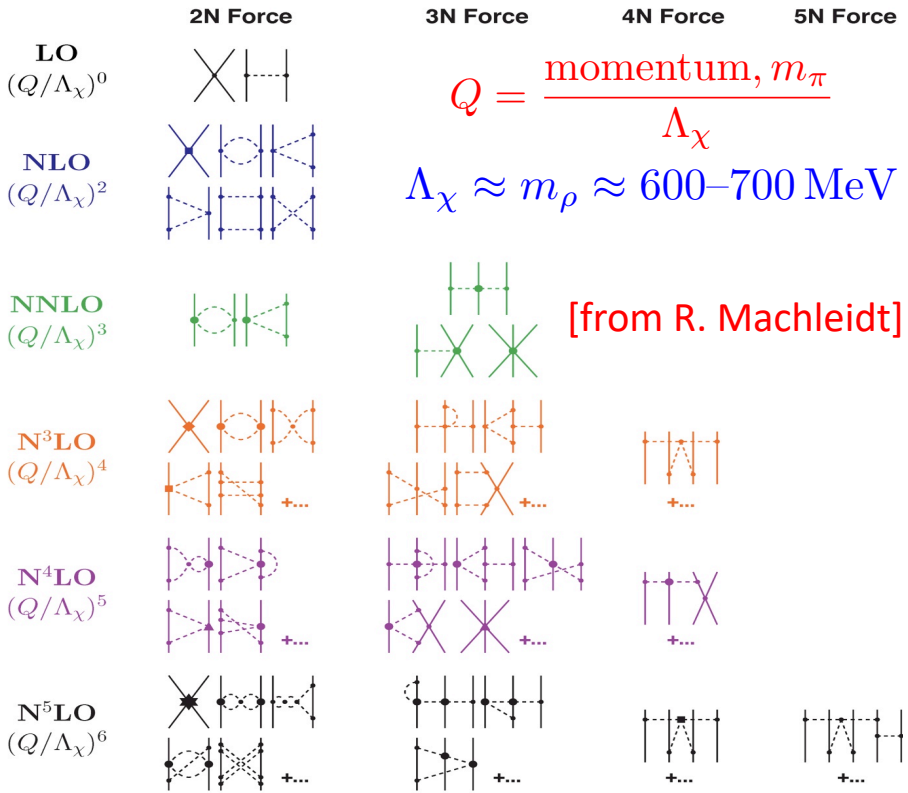
Quantifying correlated truncation errors in effective field theory

J. A. Melendez, R. J. Furnstahl, D. R. Phillips, M. T. Pratola, and S. Wesolowski
Phys. Rev. C **100**, 044001 – Published 10 October 2019

Bayesian truncation errors in chiral effective field theory: nucleon-nucleon observables [J. A. Melendez *et al.*, Phys. Rev. C **96**, 024003 (2017)].

Example: chiral EFT expansion for NN observables

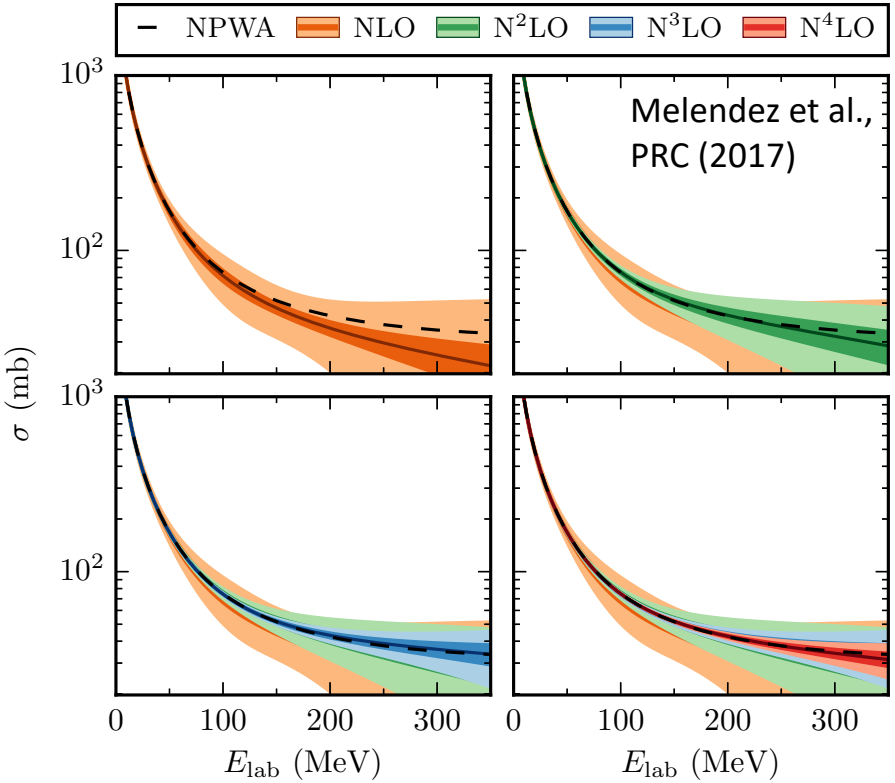
How do we apply Bayesian uncertainty quantification and model checking?



$$Q = \frac{\text{momentum}, m_\pi}{\Lambda_\chi}$$

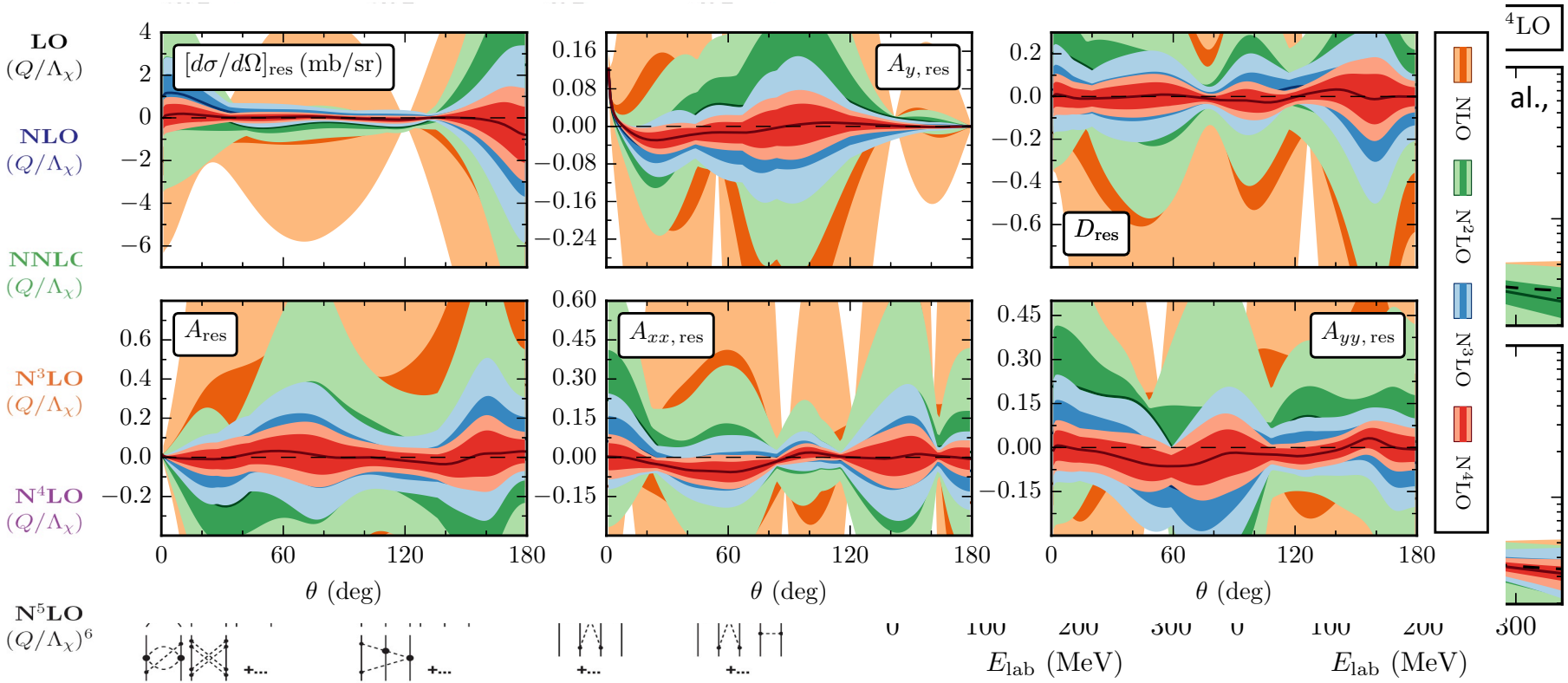
$$\Lambda_\chi \approx m_\rho \approx 600\text{–}700\,\text{MeV}$$

[from R. Machleidt]



Example: chiral EFT expansion for NN observables

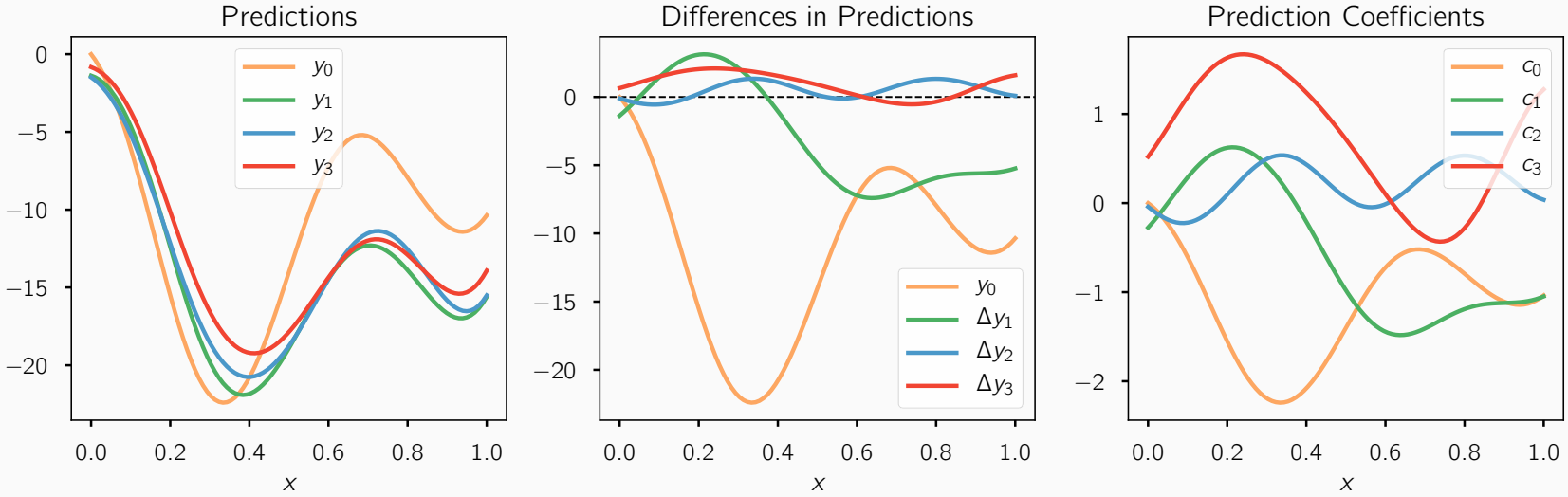
How do we apply Bayesian uncertainty quantification and model checking?



Generic example of EFT expansion (based on NN analysis)

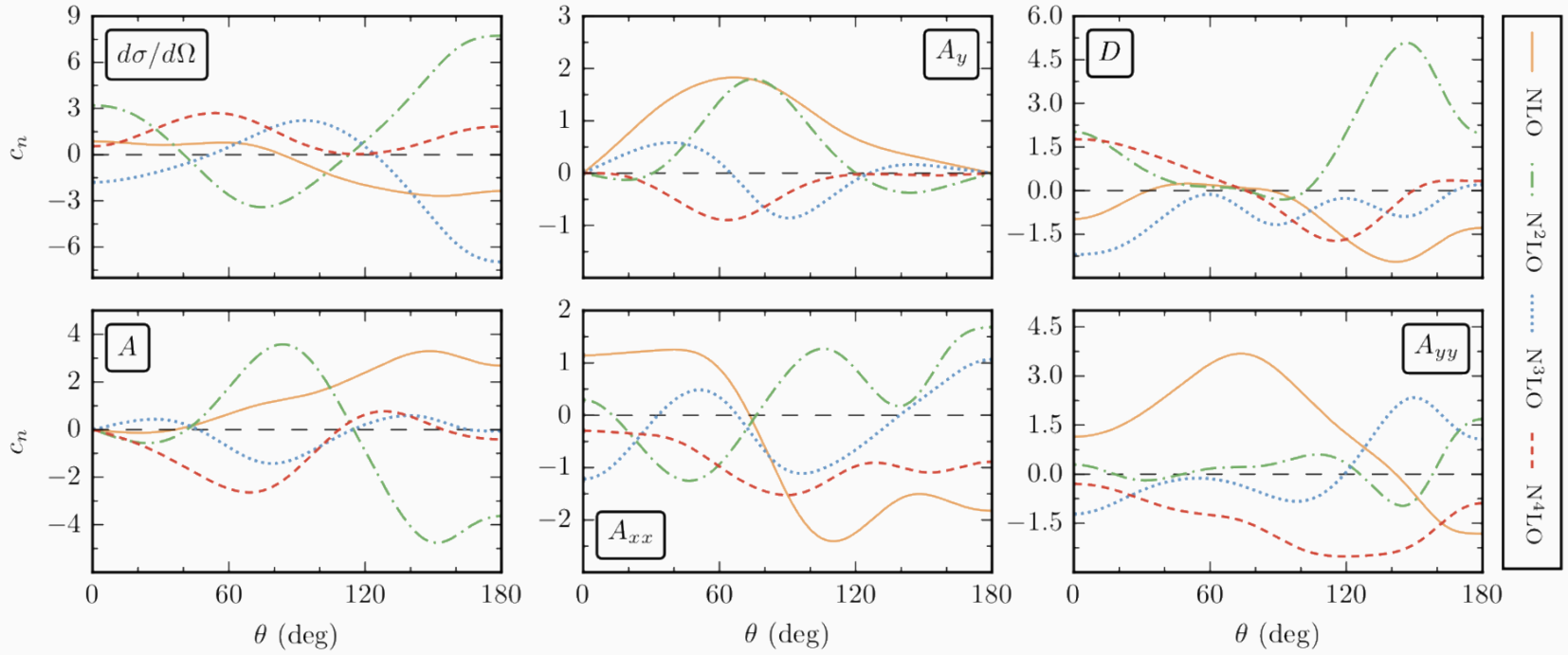
- $V_{NN}(\vec{a}) = V_{LO} + V_{NLO} + \cdots + V_{N^kLO} \Longrightarrow$ $\boxed{\text{Schrödinger Eq.}}$ $\Longrightarrow y_k(x;\vec{a})$
- One can change variables for convenience/insight.
- $\Delta y_n = y_{\text{ref}} c_n Q^n$

$$y_3 = y_{\text{ref}}\left[c_0 Q^0 + c_1 Q^1 + c_2 Q^2 + c_3 Q^3\right]$$



Generic example of EFT expansion (based on NN analysis)

Coefficients from NN scattering look like the example on the previous slide!



Model discrepancy: EFT theory errors

- Statistical model relating experiment and theory (all are functions of *x*):

$$\boldsymbol{y}_{\rm exp} = \boldsymbol{y}_{\rm th} + \boxed{\delta \boldsymbol{y}_{\rm th}} + \boxed{\delta \boldsymbol{y}_{\rm exp}}$$

- Experimental discrepancy: usually normally distributed, can be correlated
- Theoretical discrepancy: systematic, often difficult to quantify, often correlated
- EFTs: specific expectations for theory error
- Theory prediction at a certain order: [Q < 1: expansion parameter (e.g., p/Λ_b)]

$$\boldsymbol{y}_k = \boldsymbol{y}_{\rm ref} \sum_{n=0}^{k} c_n Q^n \quad \boxed{+\ \boldsymbol{y}_{\rm ref} \sum_{n=k+1}^{\infty} c_n Q^n}$$

Theory prediction at order k Omitted terms from truncation

Bayesian: treat the c_ns as random variables, depending on x; train on c_n for $n \leq k$

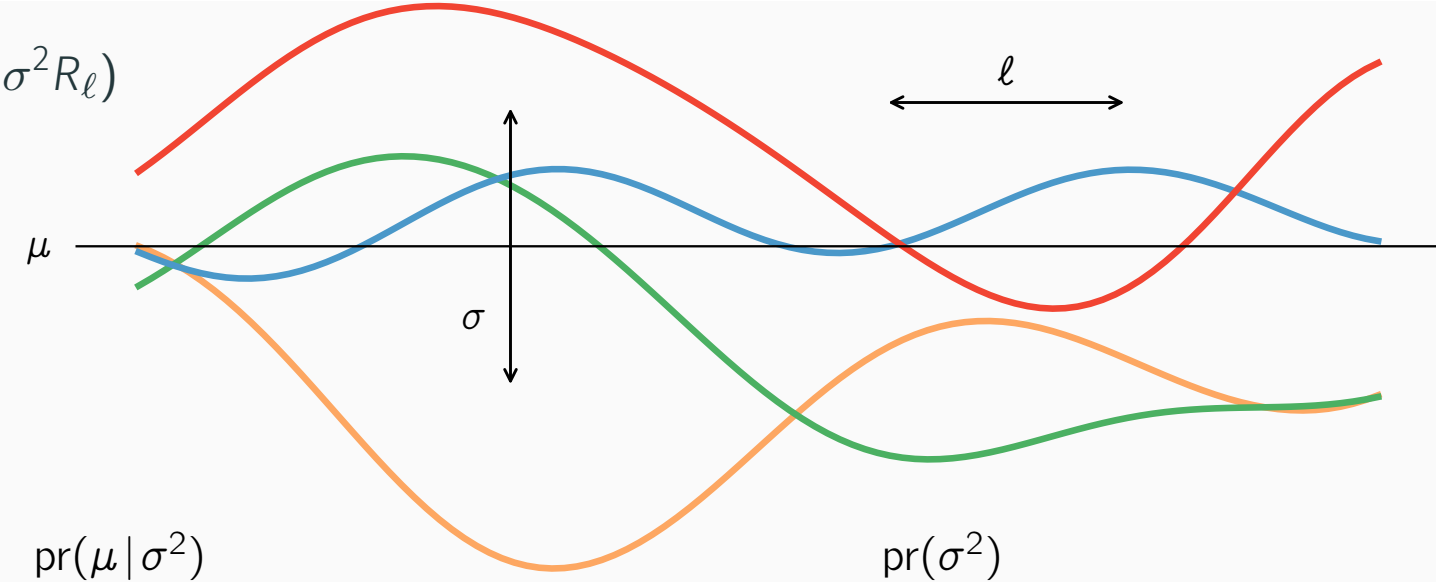
Gaussian process model of the coefficients

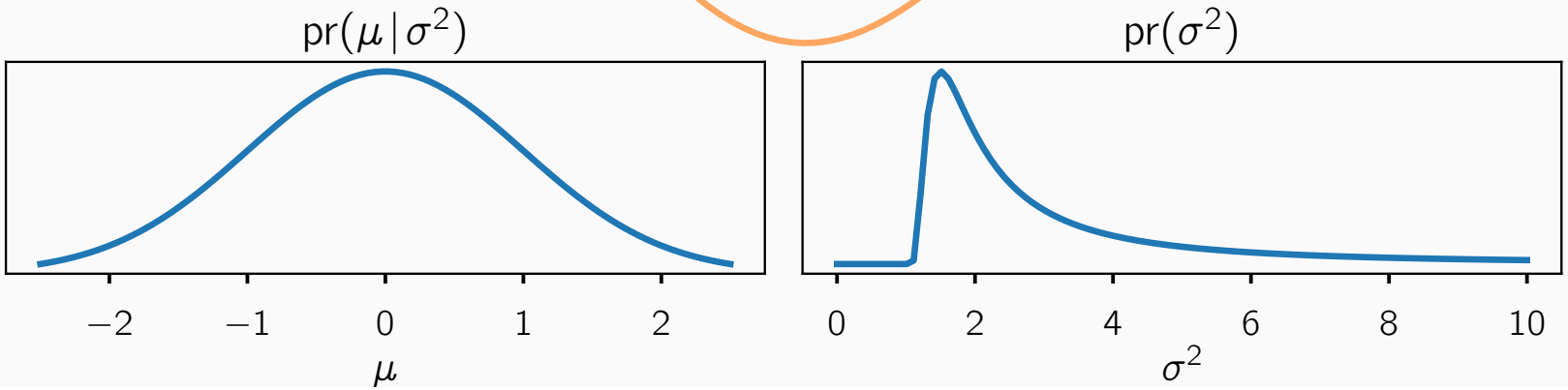
$$\mathrm{pr}(c_n \mid \boldsymbol{\theta}) \overset{\text{iid}}{\sim} \mathcal{GP}(\mu, \sigma^2 R_\ell)$$

Conjugate priors:

$$\mu \mid \sigma^2 \sim \mathcal{N}(\eta, \sigma^2 V)$$

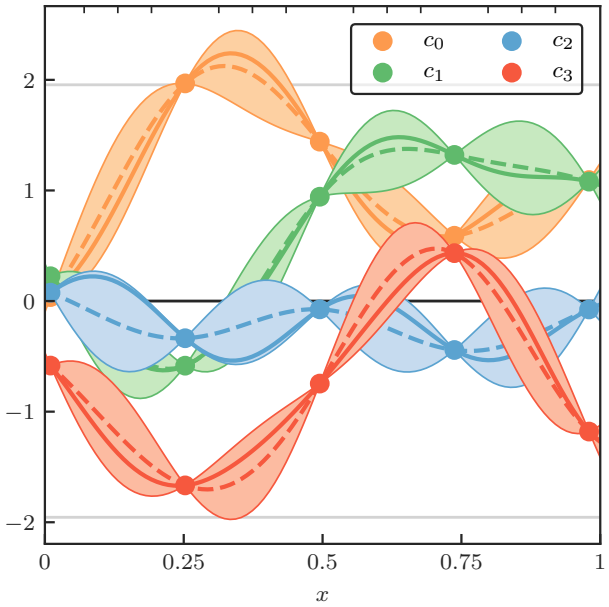
$$\sigma^2 \sim \chi^{-2}(\nu, \tau^2)$$

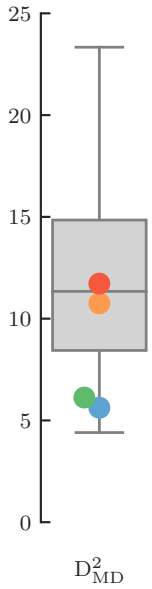


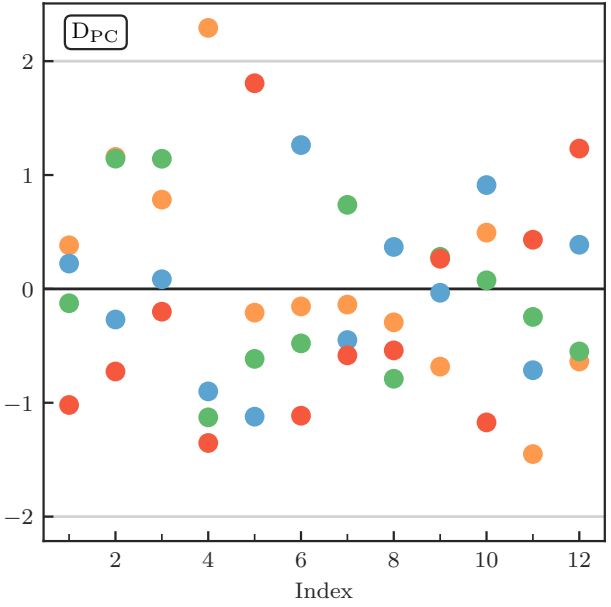


Model checking: Does our model refer to reality?

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





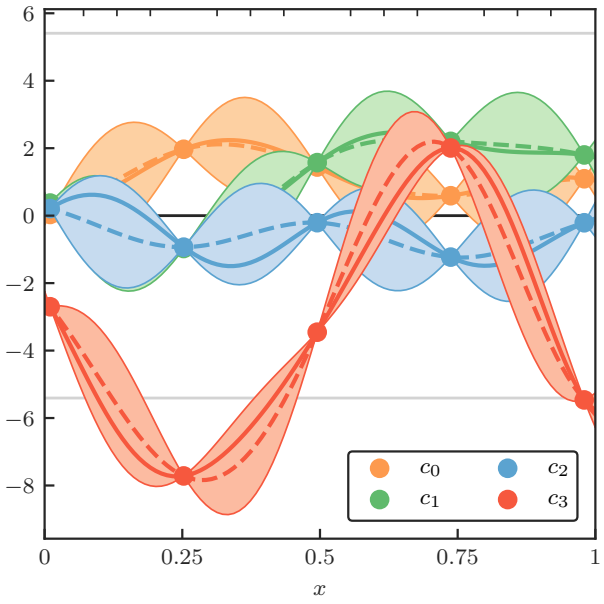


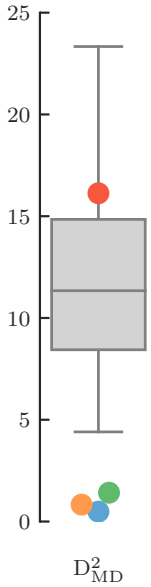
This is what success looks like!

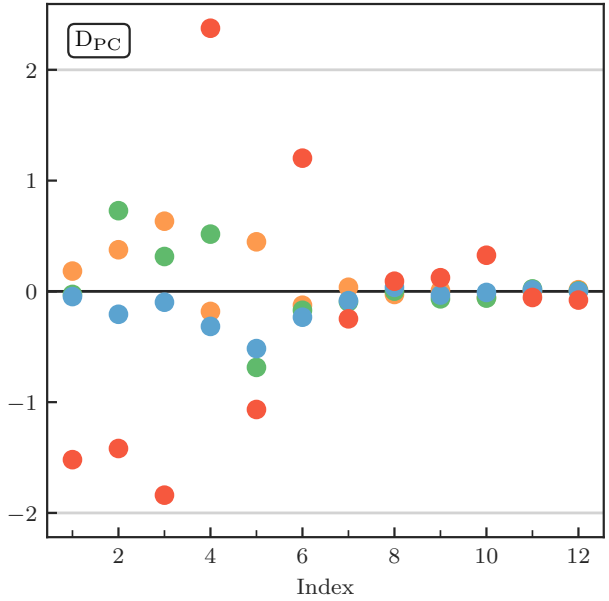
Melendez et al., PRC (2019)

Model checking: Does our model refer to reality?

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





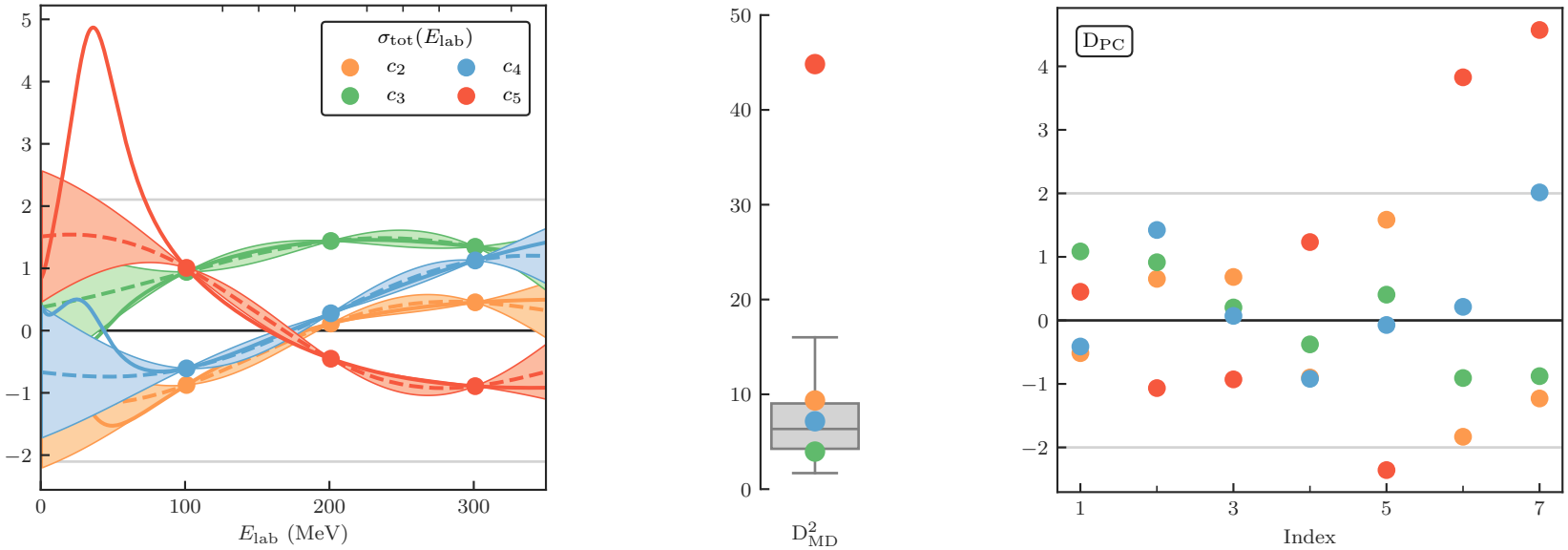


This is what failure looks like!

Melendez et al., PRC (2019)

Model checking: Does our model refer to reality?

EKM semi-local NN potential (R = 0.9 fm). Results for total *np* cross section.

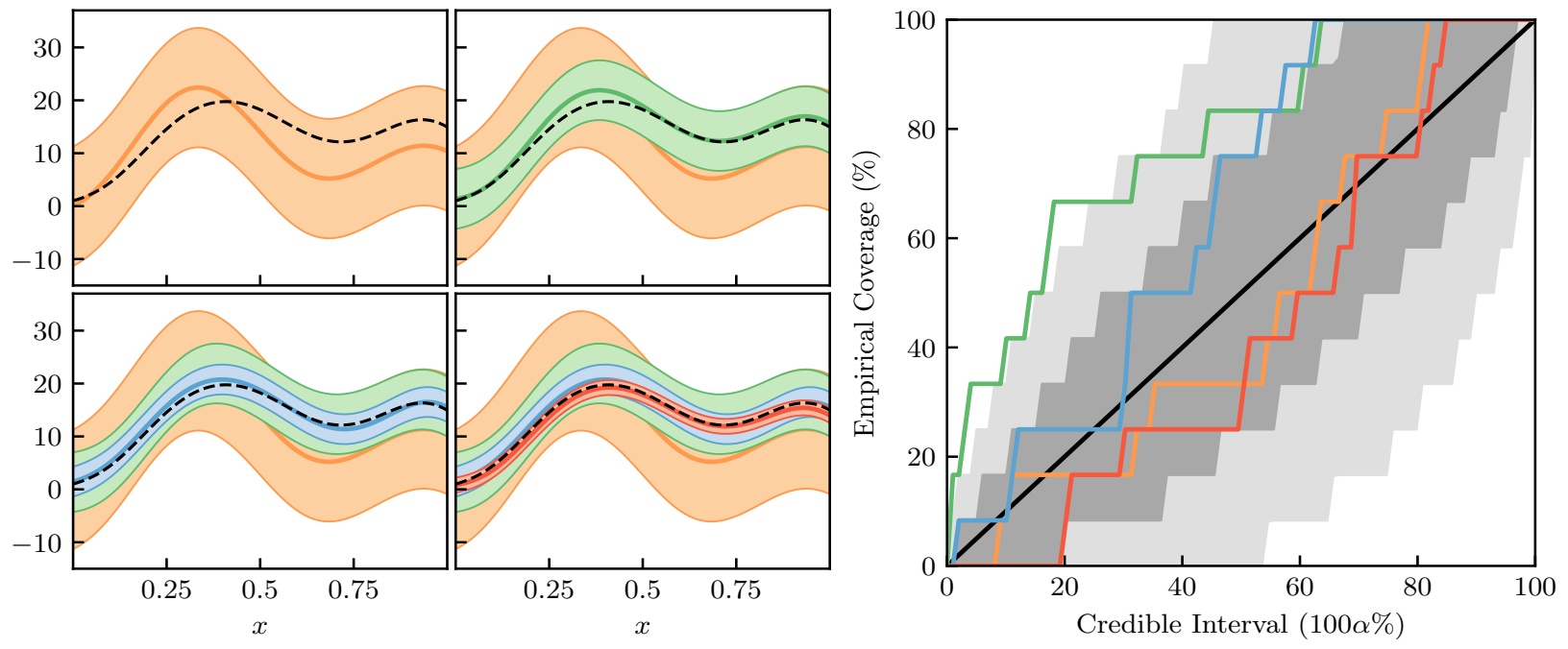


Ok for low orders but a problem at the highest order.

Melendez et al., PRC (2019)

Model checking: Do our error bands have statistical meaning?

Credible interval diagnostic



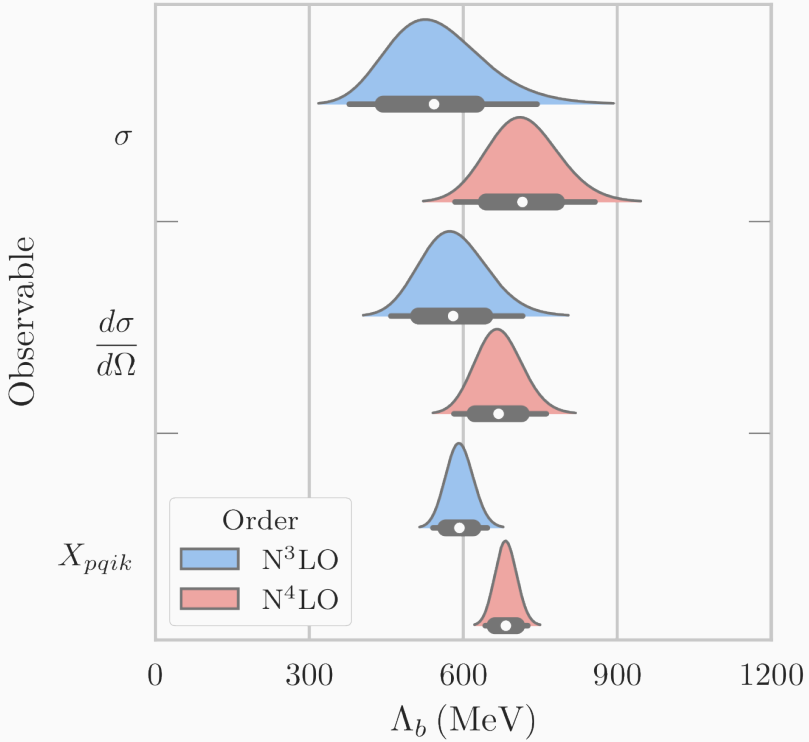
Melendez et al., PRC (2019)

What is the breakdown scale of our EFT?

- The breakdown scale of the EFT Λ_b:

$$Q \approx \frac{f(p, m_\pi)}{\Lambda_b}$$

- Once energies approach Λ_b, the EFT no longer works.
- By promoting Λ_b to a random variable, its posterior can be produced as a byproduct of δy_{th} estimation.

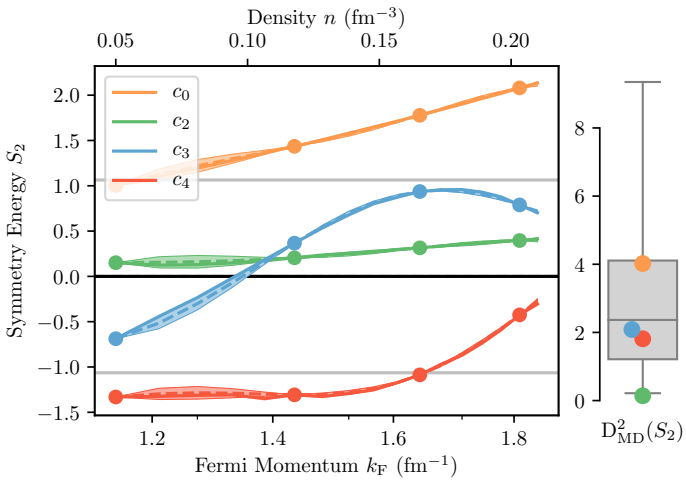


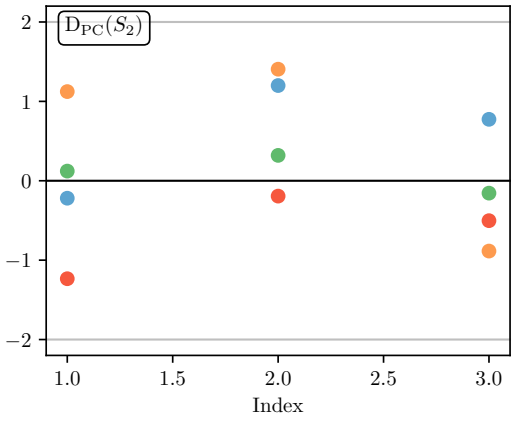
Melendez et al., in preparation (2019)

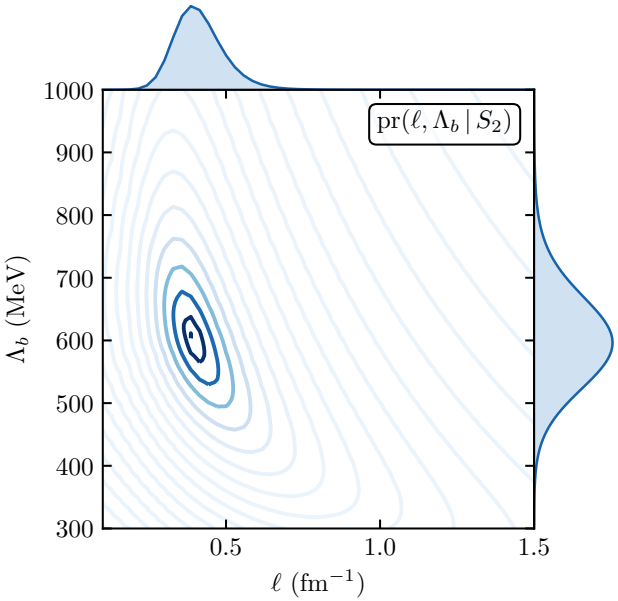
Symmetry energy in infinite matter (preliminary!)

Christian Drischler, Jordan Melendez, et al., in preparation

NN potential: Entem-Machleidt-Nosyk (450 MeV) with fitted 3N LECs







Many interesting questions to investigate and comparisons to make!

Parameter estimation: Exploring projected posteriors

- First without the model discrepancy (theory error) term:

$$\boldsymbol{y}_{\rm exp} = \boldsymbol{y}_{\rm th} \qquad\qquad + \delta \boldsymbol{y}_{\rm exp}$$

- Consider high-enough order so that truncation error is small
- Regular least-squares (χ^2) likelihood times Gaussian prior for natural LECs:

$$\mathrm{pr}(\vec{a}_k|\boldsymbol{y}_{\rm exp}, \Sigma_{\rm exp}) \propto \mathrm{pr}(\boldsymbol{y}_{\rm exp}|\vec{a}_k, \Sigma_{\rm exp})\ \mathrm{pr}(\vec{a}_k)$$

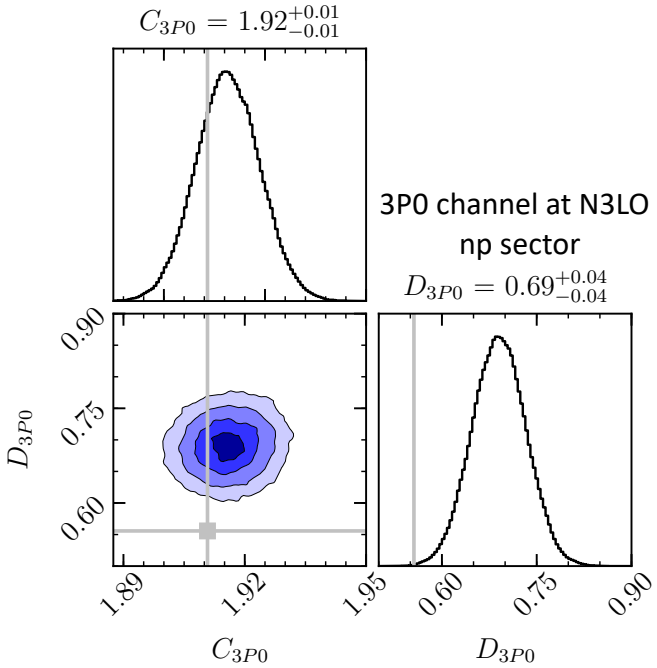
$$\propto e^{-\frac{1}{2}\mathbf{r}^T \Sigma_{\rm exp}^{-1}\mathbf{r}} \times e^{-(\vec{a}_k)^2/2\bar{a}^2}$$

Residual: $\boldsymbol{r} \equiv \boldsymbol{y}_{\rm exp} - \boldsymbol{y}_{\rm th}$

Discourages large LECs (naturalness)

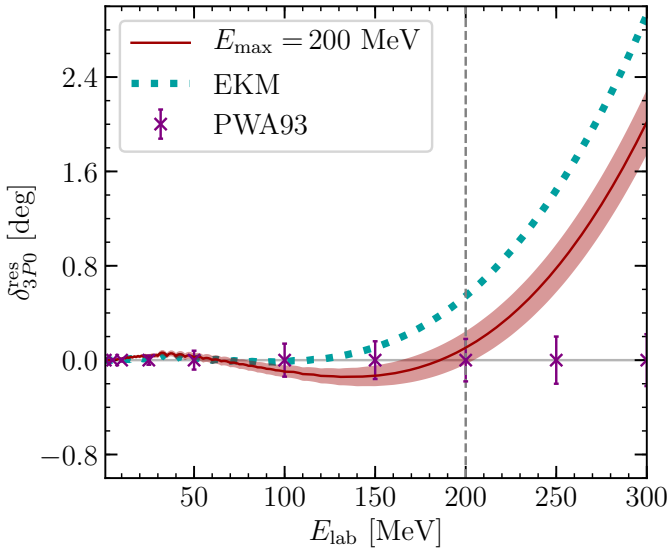
Projected posteriors as a diagnostic tool

$$\mathrm{pr}(\vec{a}|\boldsymbol{y}_{\mathrm{exp}}, \Sigma_{\mathrm{exp}}) \propto \exp\left[-\frac{1}{2}\sum_{i=1}^{N_d}\frac{r_i^2}{\sigma_i^2}\right] \times e^{-(\vec{a}_k)^2/2\bar{a}^2}$$



- Projected posteriors give:
  - info on correlations
  - "best" parameter values
  - indication of normality

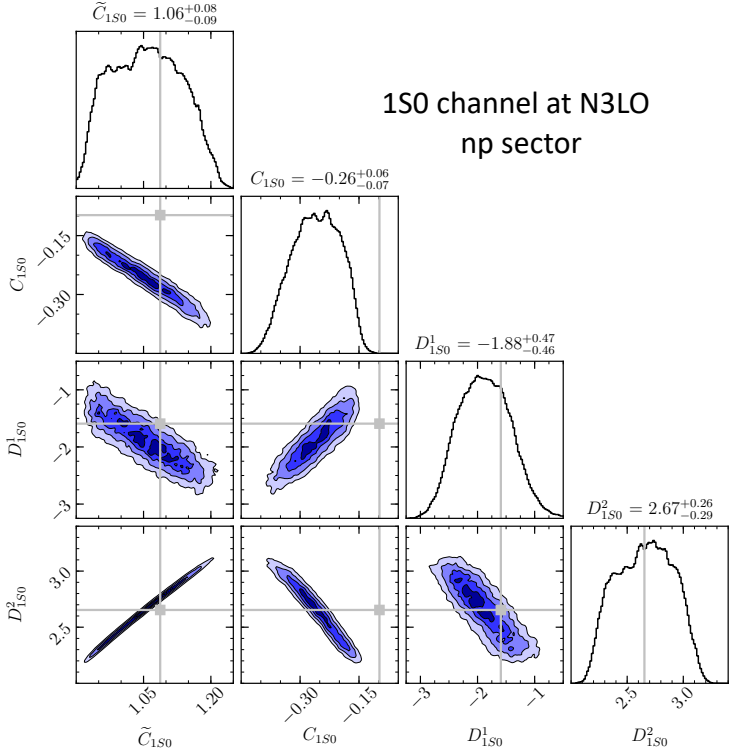
- Uncorrelated and Gaussian
- Also: Comparison to EKM's values from optimization (need not match!)



$$\delta^{\mathrm{res}}_{\mathrm{p.w.}} = \delta^{\mathrm{pred}}_{\mathrm{p.w.}} - \delta^{\mathrm{PWA93}}_{\mathrm{p.w.}}$$

Projected posteriors as a diagnostic tool

$$\mathrm{pr}(\vec{a}|\boldsymbol{y}_{\mathrm{exp}}, \Sigma_{\mathrm{exp}}) \propto \exp\left[-\frac{1}{2}\sum_{i=1}^{N_d}\frac{r_i^2}{\sigma_i^2}\right] \times e^{-(\vec{a}_k)^2/2\bar{a}^2}$$



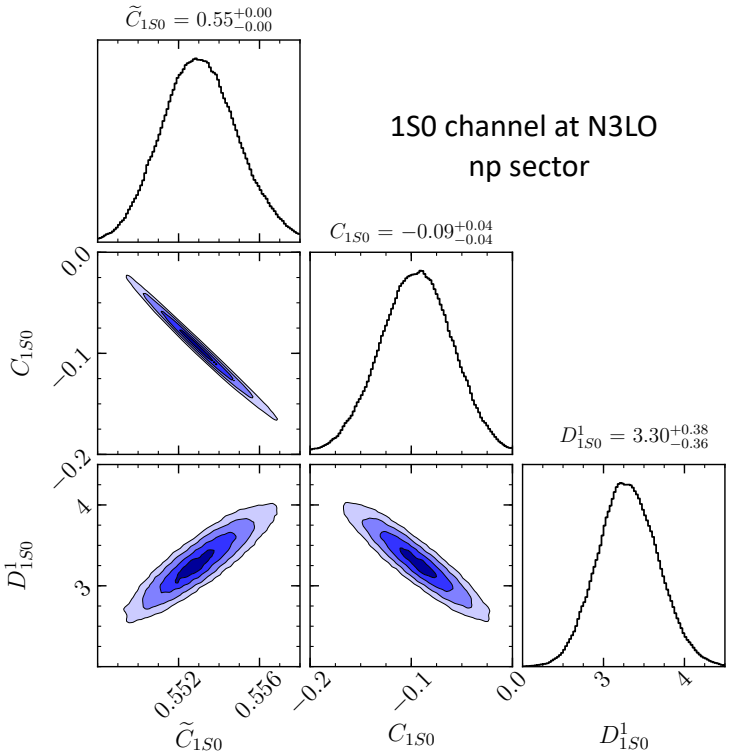
1S0 channel at N3LO
np sector

- Irregular structure of posterior
- Nothing *necessarily* wrong, but a clue
- Here: a physics issue actually explains the distorted structure
- Parameter redundancy at N3LO, an operator can be eliminated
- True in 3S1-3D1 channel as well

Wesolowski et al., J. Phys. G (2019)

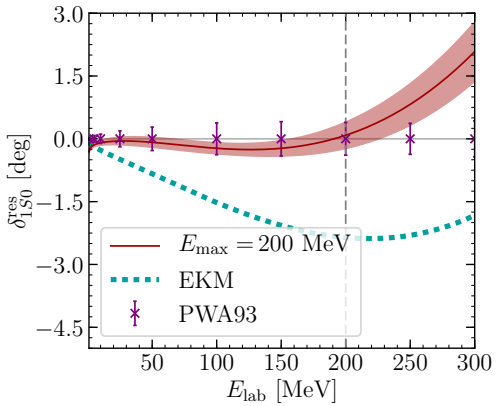
Projected posteriors as a diagnostic tool

$$\mathrm{pr}(\vec{a}|\boldsymbol{y}_{\mathrm{exp}}, \Sigma_{\mathrm{exp}}) \propto \exp\left[-\frac{1}{2}\sum_{i=1}^{N_d}\frac{r_i^2}{\sigma_i^2}\right] \times e^{-(\vec{a}_k)^2/2\bar{a}^2}$$



1S0 channel at N3LO
np sector

- Set D^2_{1S0} to 0 and use only 3 parameters
- Description of data still good (and potential softer)
- Reinert et al., EPJA (2018) improved potential



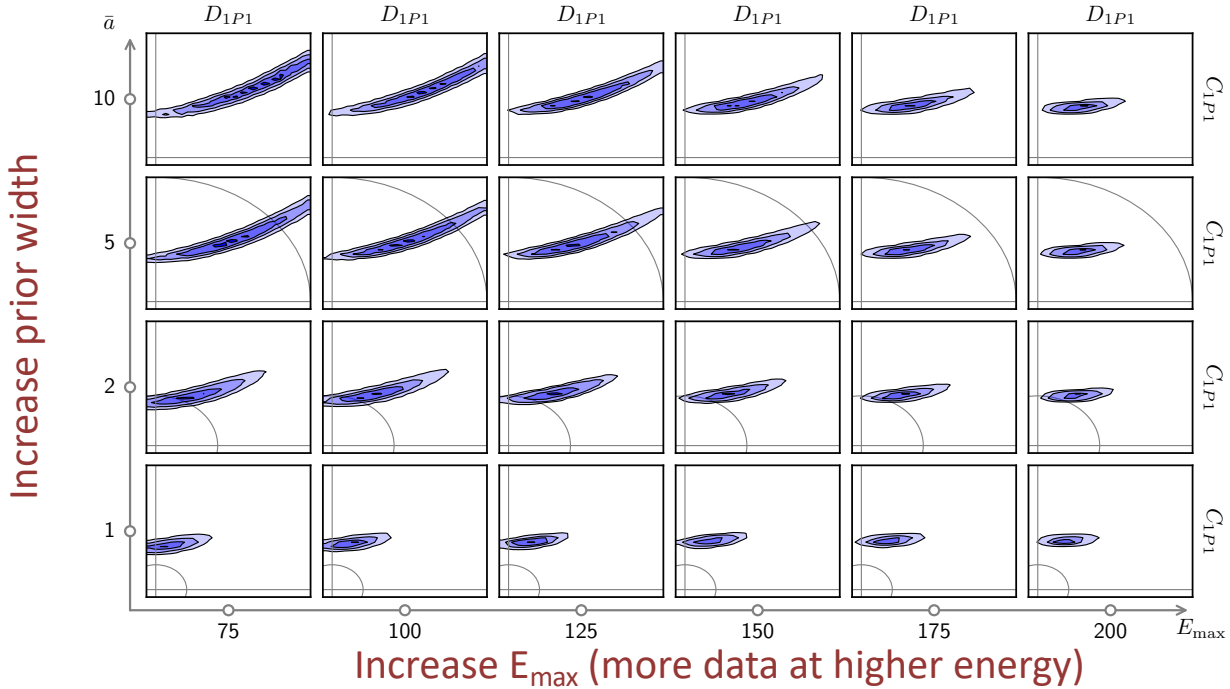
Wesolowski et al., J. Phys. G (2019)

Effect of the prior with less data

$$\mathrm{pr}(\vec{a}|\boldsymbol{y}_{\mathrm{exp}}, \Sigma_{\mathrm{exp}}) \propto \exp\left[-\frac{1}{2}\sum_{i=1}^{N_d}\frac{r_i^2}{\sigma_i^2}\right] \times e^{-(\vec{a}_k)^2/2\bar{a}^2}$$

Wesolowski et al., J. Phys. G (2019)

Repeat same problem, vary givens



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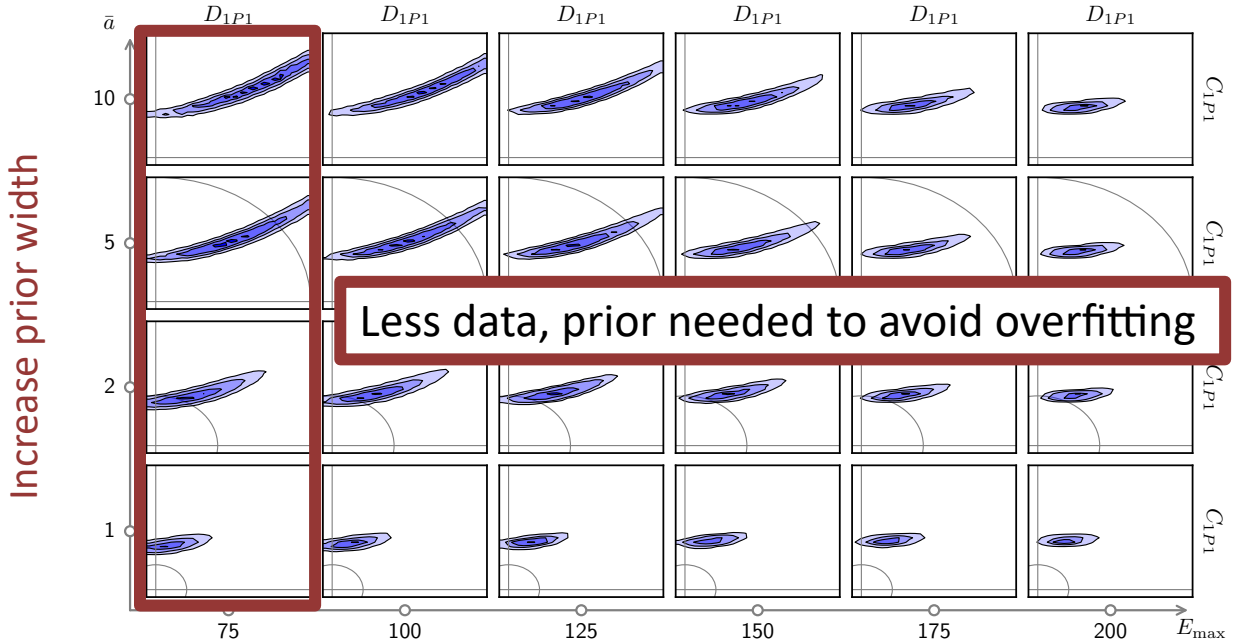
Wesolowski et al., J. Phys. G (2019)

Repeat same problem, vary givens



Less data, prior needed to avoid overfitting

Increase prior width

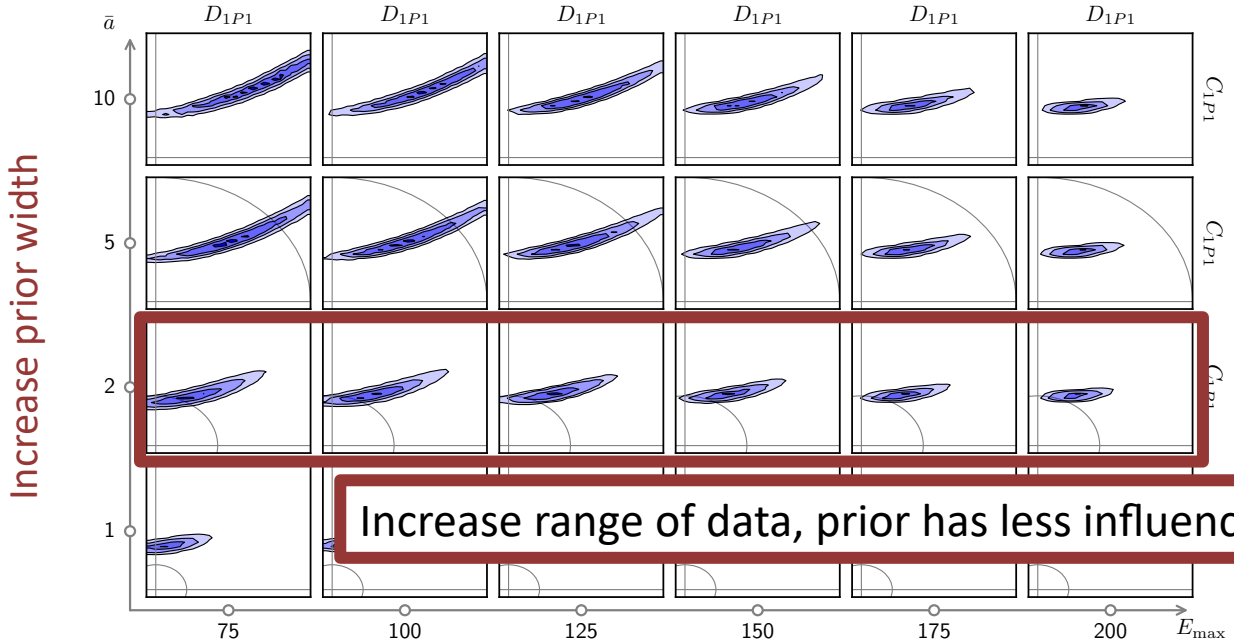
Increase E_{max} (more data at higher energy)

Effect of the prior with less data

$$\mathrm{pr}(\vec{a}|\boldsymbol{y}_{\mathrm{exp}}, \Sigma_{\mathrm{exp}}) \propto \exp\left[-\frac{1}{2}\sum_{i=1}^{N_d}\frac{r_i^2}{\sigma_i^2}\right] \times e^{-(\vec{a}_k)^2/2\bar{a}^2}$$

Wesolowski et al., J. Phys. G (2019)

Repeat same problem, vary givens



Increase range of data, prior has less influence

Increase prior width

Increase E_{max} (more data at higher energy)

Parameter estimation including truncation errors

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

We can put a prior on the unknown higher-order coefficients: $\mathbf{c}_n | \bar{c} \sim \mathcal{N}(0, \bar{c}^2)$

Just a sum of Gaussian random variables using this prior (which we have validated)

Two extreme assumptions about correlations

1. Theory error at each kinematic point (Q) is completely uncorrelated:

$$[\delta y_{\rm th}]_i = [y_{\rm ref}]_i \sum_{n=k+1}^{\infty} [c_n]_i Q_i^n$$

2. Theory error at each kinematic point (Q) is fully correlated, with same coefficients:

$$[\delta y_{\rm th}]_i = [y_{\rm ref}]_i \sum_{n=k+1}^{\infty} c_n Q_i^n$$

Parameter estimation including truncation errors

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

Full posterior pdf including theory error:

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

Covariance matrix for assuming uncorrelated *Q* points:

$$(\Sigma_{\rm th,uncorr.})_{ij} = (\boldsymbol{y}_{\rm ref})_i^2\, \bar{c}^2 \sum_{n=k+1}^{k_{\rm max}} Q_i^{2n} \delta_{ij} \xrightarrow[k_{\rm max}\to\infty]{} \frac{(\boldsymbol{y}_{\rm ref})_i^2\, \bar{c}^2\, Q_i^{2k+2}}{1-Q_i^2}\, \delta_{ij}$$

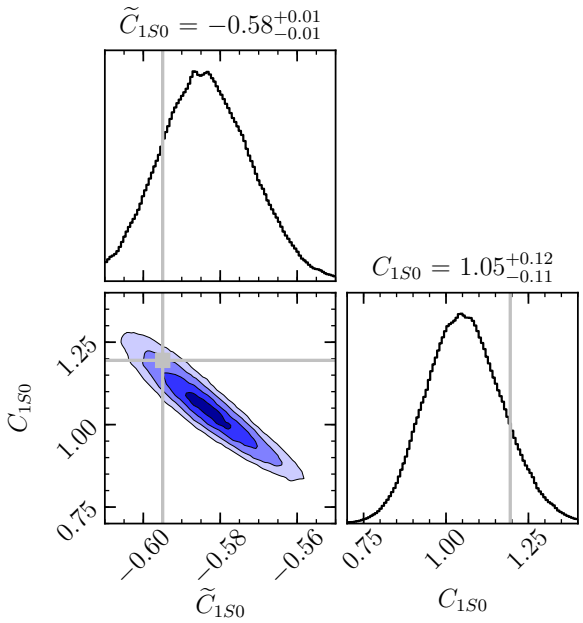
Covariance matrix assuming fully correlated *Q* points:

$$(\Sigma_{\rm th,corr.})_{ij} = (\boldsymbol{y}_{\rm ref})_i (\boldsymbol{y}_{\rm ref})_j\, \bar{c}^2 \sum_{n=k+1}^{k_{\rm max}} Q_i^n Q_j^n \xrightarrow[k_{\rm max}\to\infty]{} \frac{(\boldsymbol{y}_{\rm ref})_i (\boldsymbol{y}_{\rm ref})_j\, \bar{c}^2\, Q_i^{k+1} Q_j^{k+1}}{1-Q_i Q_j}$$

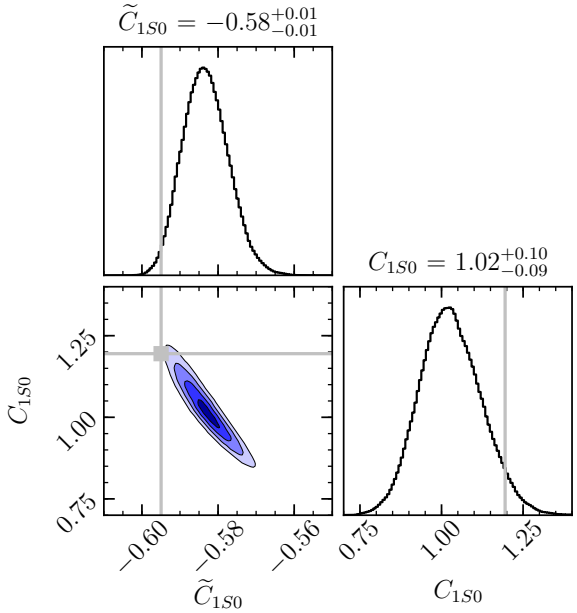
Wesolowski et al., J. Phys. G (2019)

Effect of including truncation errors

Use partial-wave cross sections extracted from PWA phase shifts



Uncorrelated assumption



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Wesolowski et al., J. Phys. G (2019)

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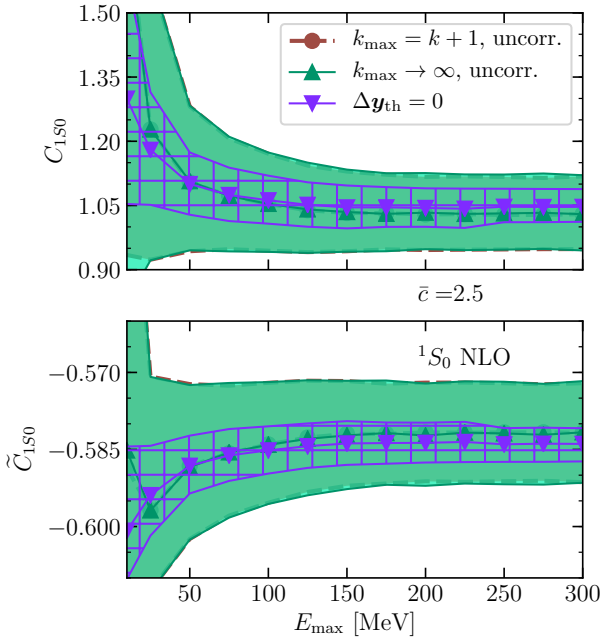

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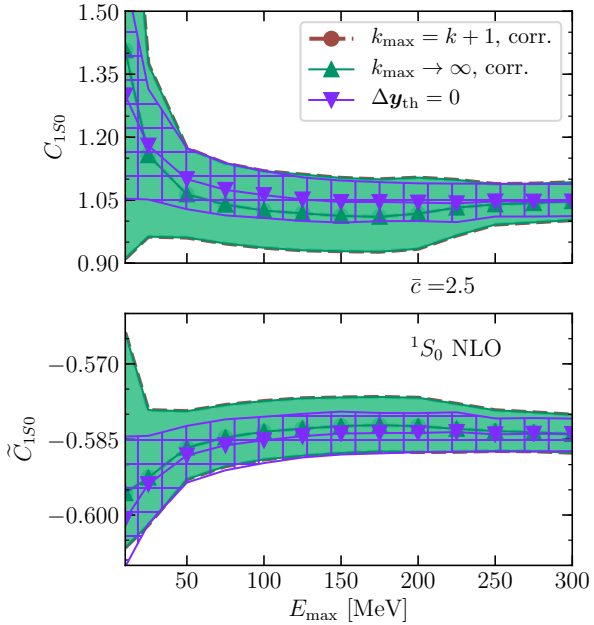

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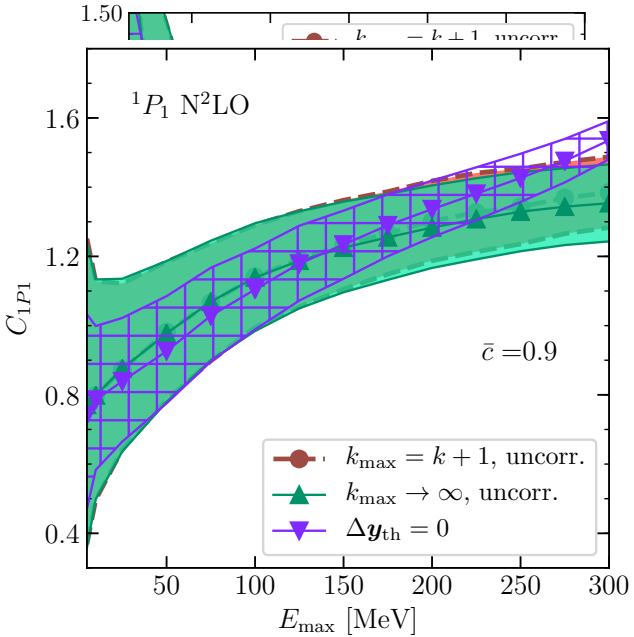

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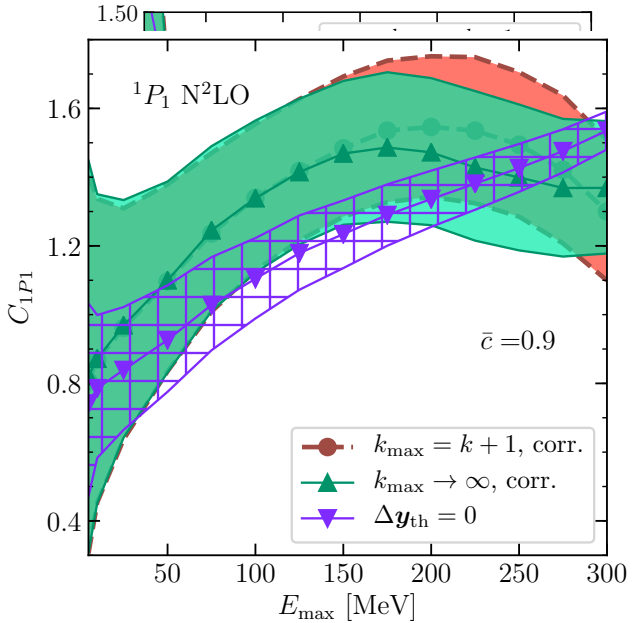

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Wesolowski et al., J. Phys. G (2019)

But won't the Bayesian sampling calculations take too long?

Eigenvector Continuation as an Efficient and Accurate Emulator for Uncertainty Quantification

arXiv:1909.08446

S. König,[1,2,*] A. Ekström,[3,†] K. Hebeler,[1,2,‡] D. Lee,[4,§] and A. Schwenk[1,2,5,¶]

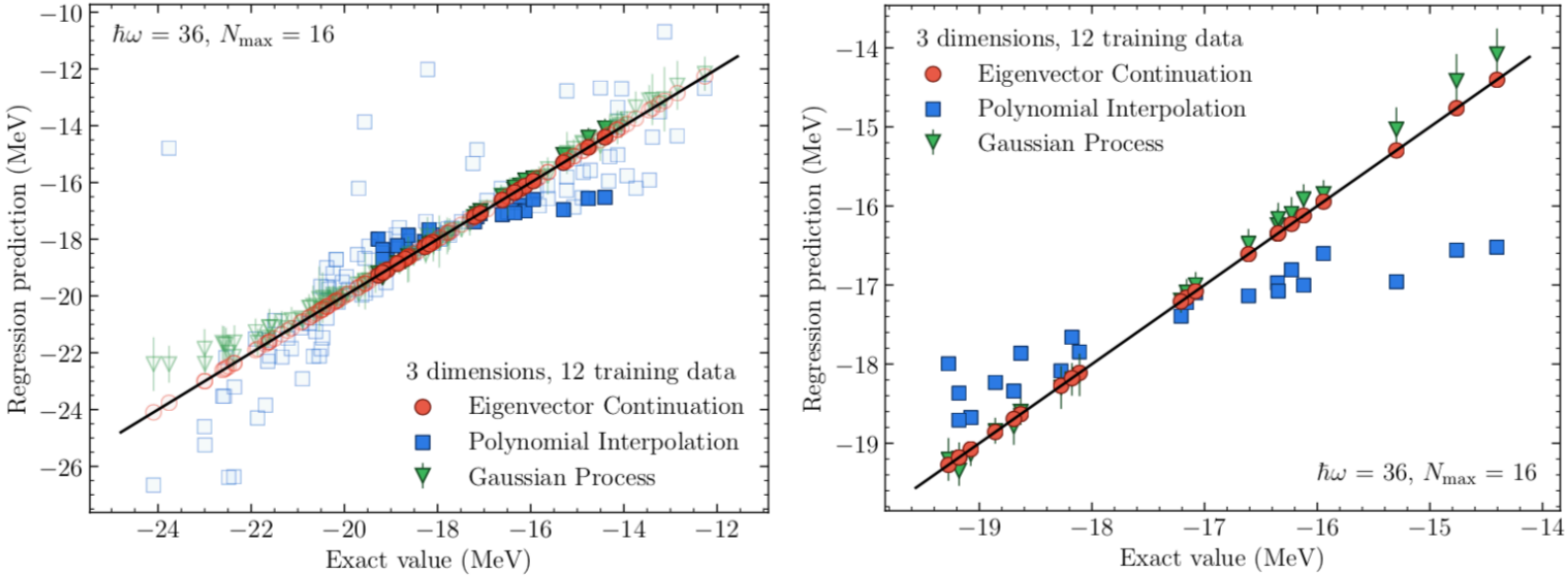


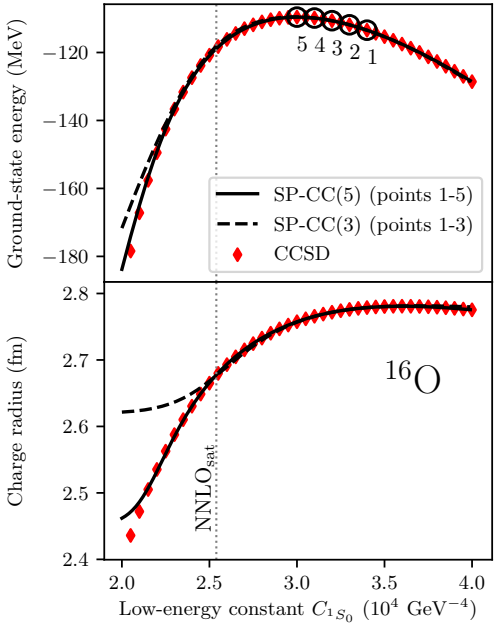
Figure 1. Comparison of different emulators for the ^{4}He ground-state energy using 12 training data points to explore a space where three LECs are varied. The left panel includes samples for both interpolation (solid symbols) and extrapolation (semi-transparent symbols). See main text on how these are defined. The right panel shows the same data restricted to interpolation samples (note the smaller axis range).

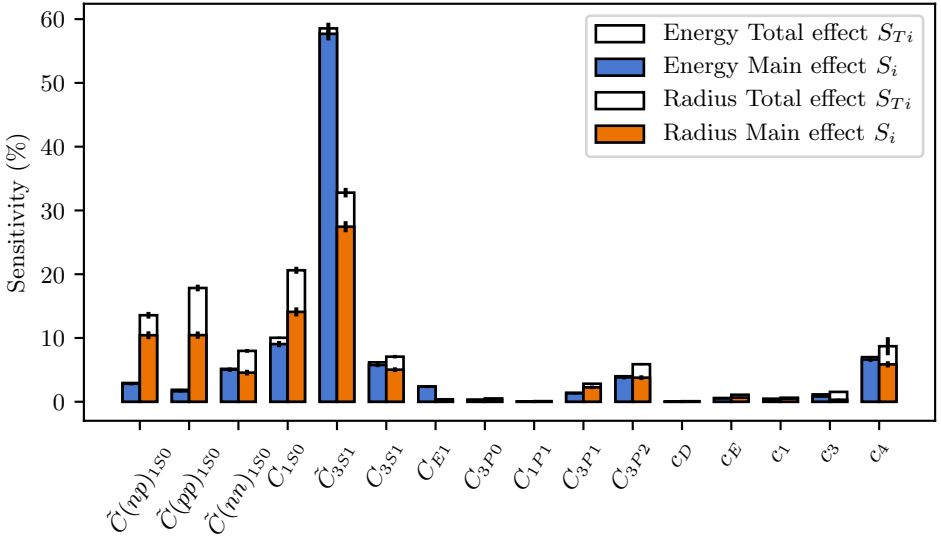
But won't all of these Bayesian sampling calculations take too long?

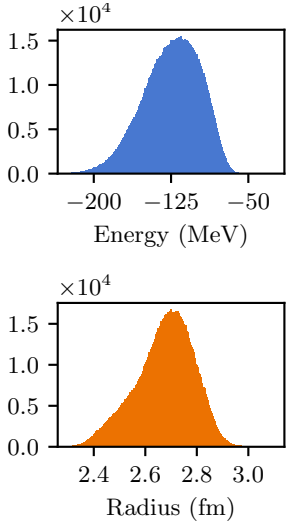
Global sensitivity analysis of bulk properties of an atomic nucleus

arXiv: 1910.02922

Andreas Ekström[1] and Gaute Hagen[2,3]







"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."

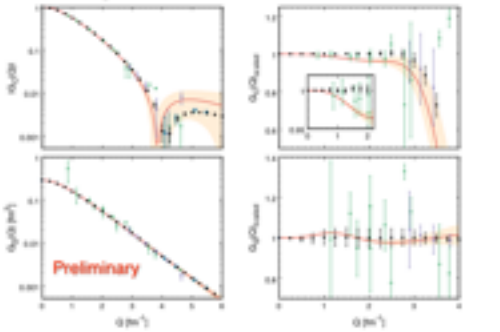
Snapshots of Bayesian methods for EFT

Form factors of deuteron with *consistent* chiral EFT current operators

Hermann Krebs and Evgeny Epelbaum (from HK talk at INT, July 2019)

http://www.lenpic.org/

- A major advantage of EFT: consistent current operators
- Here: new developments by HK and EE for chiral EFT
- Colored band is 68% Bayes credible interval for truncation error from convergence pattern



Truncation error band from Bayesian analysis: 68% DoB, Λ_b = 600 MeV Furnstahl et al. '15

EFT for nuclear vibrations with quantified uncertainties

E. A. Coello Pérez and Thomas Papenbrock, PRC (2015, 2016)

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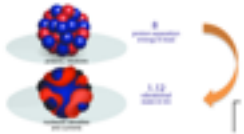

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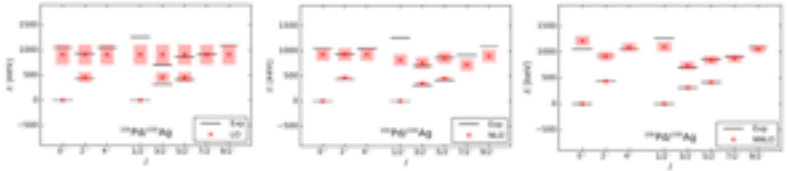

"The systematic improvement inherent to EFT approaches is evident."

EFT + Bayes for nuclear reactions: $^3He(\alpha,\gamma)^7Be$

Xilin Zhang, Ken Nollett, Daniel Phillips, arXiv:1909.07287

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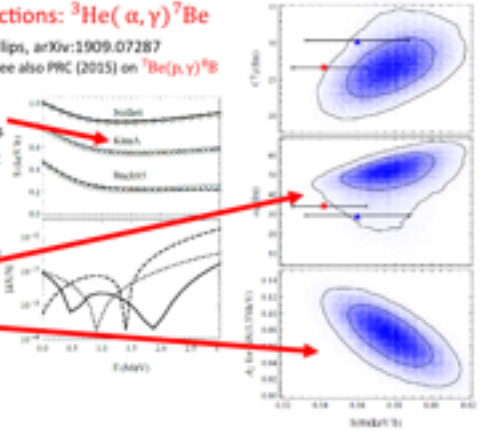

Bayesian model selection: Two competing EFT power countings

Pradeepa Premarathna and Gautam Rupak; arXiv:1906.04143

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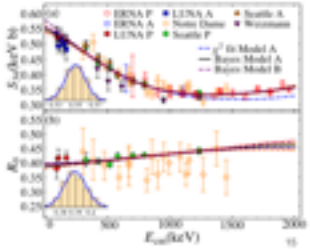

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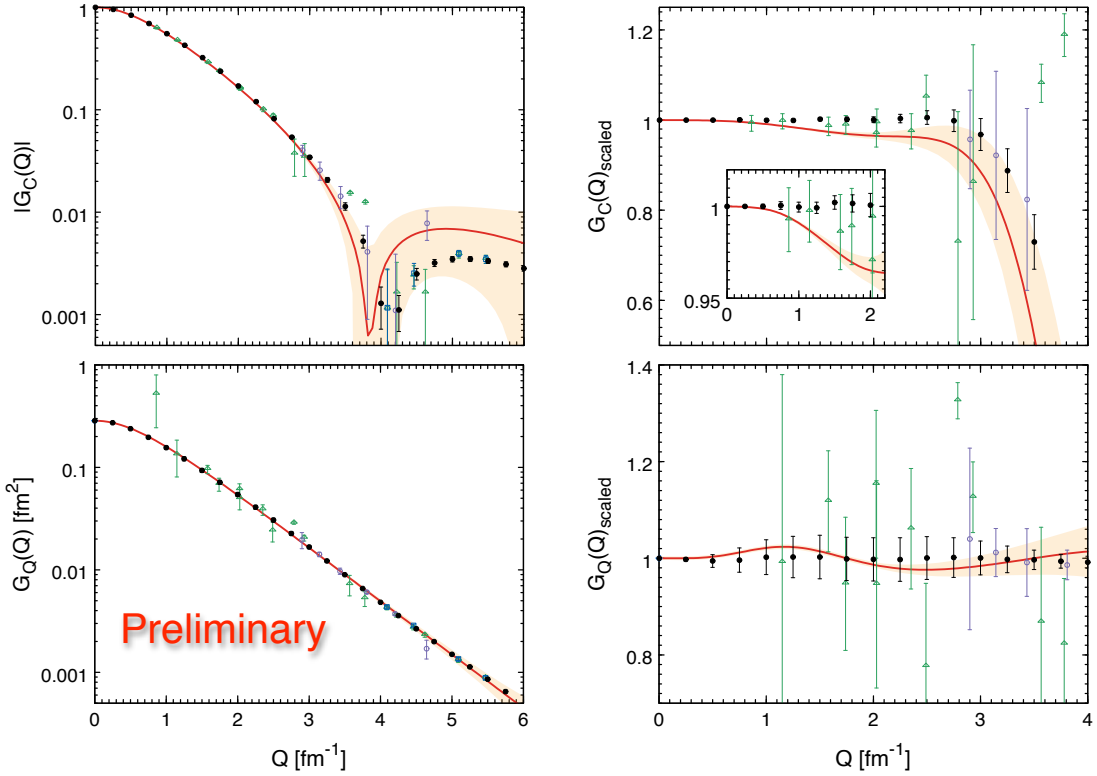

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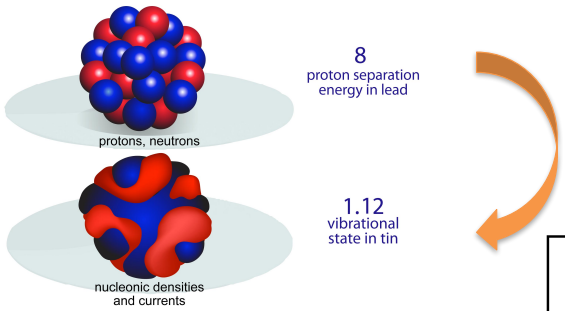

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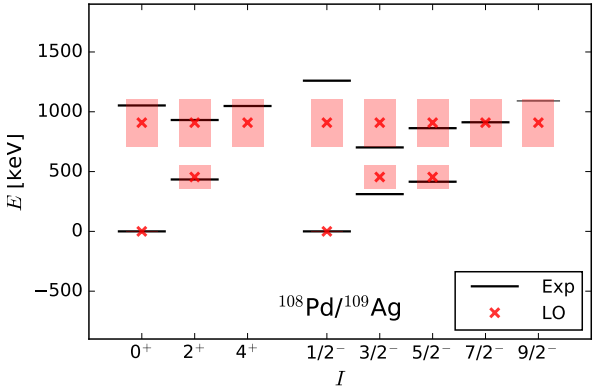

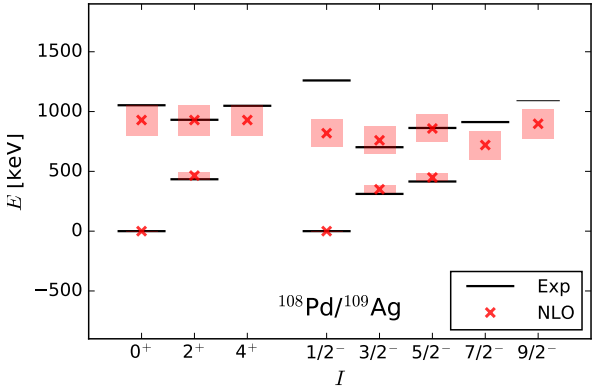

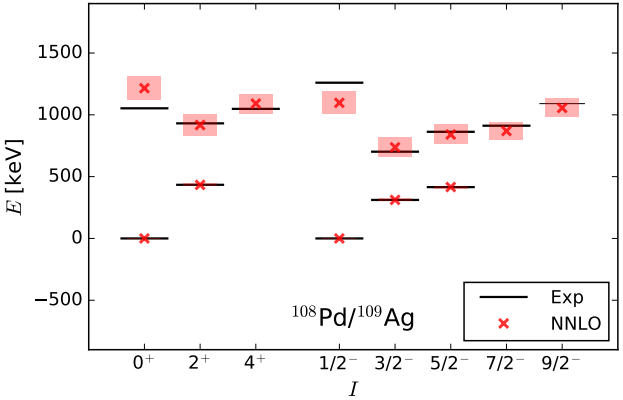

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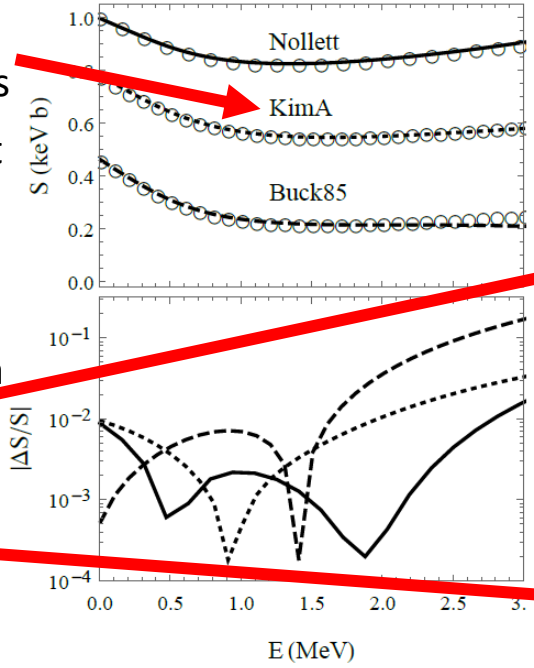

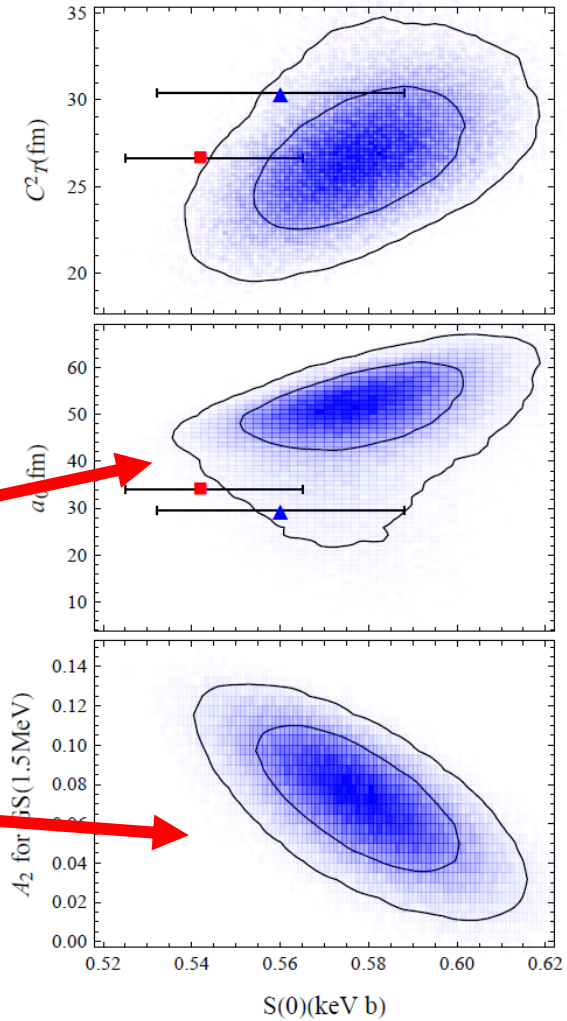

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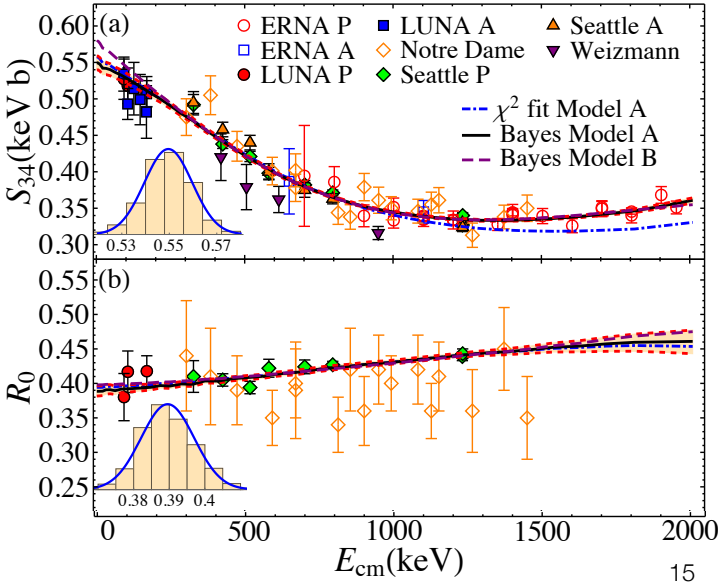

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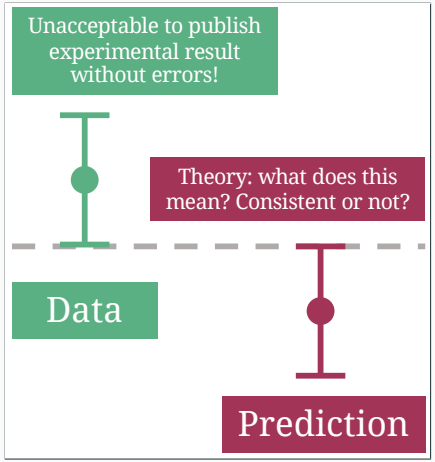
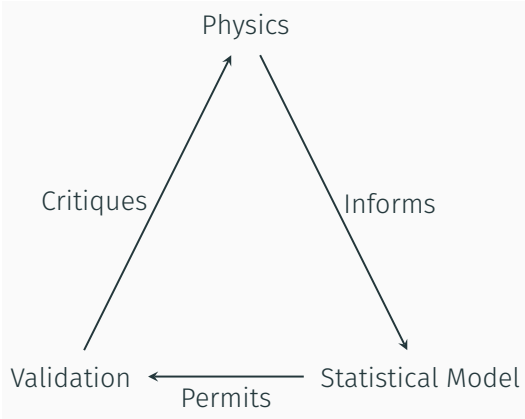
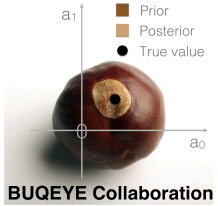
Take-away Points

- Bayesian statistics is an ideal framework for EFT uncertainty quantification.
- Theory discrepancy model based on convergence pattern and naturalness priors; GP truncation error model accounts for correlations; Λ_b estimates.
- Model checking is an essential part of Bayesian UQ.
- Parameter estimation with LEC priors and model discrepancy minimizes dependence on how much data is used; posterior diagnostics point to physics issues.
- Need to sample for parameter estimation and the propagation of uncertainties: Eigenvector continuation is very promising solution to computational load!
- Model selection is a frontier for EFT Bayesian statistics.





BUQEYE Collaboration ("Bayesian Uncertainty Quantification: Errors for Your EFT")



https://buqeye.github.io

gsum: A Bayesian model of series convergence using Gaussian sums.
The gsum package provides convenient classes that allow one to analyze the convergence pattern of Effective Field Theory (EFT) observables. Specifically, this is a conjugacy-based implementation of the statistical model described in arXiv:1904.10581.

Correlated truncation errors in effective field theory: The code behind the manuscript.
This Jupyter notebook provides the Python code to reproduce *all* of the plots from Melendez et al., Phys. Rev. C **100**, 044001 (2019), arXiv:1904.10581.

Journal of Physics G Special Focus Issue

Focus on further enhancing the interaction between nuclear experiment and theory through information and statistics (ISNET 2.0)

Guest Editors

Dick Furnstahl Ohio State University
David Ireland University of Glasgow
Daniel Philips Ohio University

"Following on from the hugely successful first edition in 2015, Journal of Physics G: Nuclear and Particle Physics is delighted to announce a second focus issue inspired by the ISNET workshops (Information and Statistics in Nuclear Experiment and Theory."

Two articles already published!
Please consider contributing!

https://iopscience.iop.org/journal/0954-3899/page/ISNET2

TALENT: Training in Advanced Low-Energy Nuclear Theory

The TALENT initiative aims at providing advanced training to graduate students and young researchers in low-energy nuclear theory. TALENT offers intensive three-week courses on a rotating set of topics.

Bayes2019. Learning from Data: Bayesian Methods and Machine Learning, at the University of York, UK, June 10-28, 2019. See the github site for many Jupyter notebooks and lecture notes: https://nucleartalent.github.io/Bayes2019/

TALENT courses scheduled for 2020 (see http://nucleartalent.org for more info):

- **Atomic Nuclei as Open Quantum Systems: Unifying Nuclear Structure and Reactions** will be held at the INT in Seattle, WA from June 22 to July 10, 2020.
  Contact: Christian Forssén (christian.forssen@chalmers.se).
- **Density Functional Theory and Self-Consistent Methods** will be held at LBNL, in Berkeley, CA. The (tentative) dates are July 6 to July 24, 2020. **Contact:** Nicolas Schunck (schunck1@llnl.gov).
- **Machine Learning and Data Analysis for Nuclear Physics** will be held at the ECT* in Trento, Italy. The (tentative) dates are June 29 to July 17, 2020. **Contact:** Morten Hjorth-Jensen (hjensen@msu.edu).