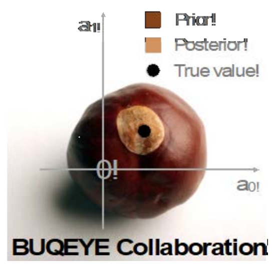
Bayesian parameter estimation for chiral interactions: NN sector

Sarah Wesolowski

New Ideas in Constraining Nuclear Forces, ECT* 2018



Dick Furnstahl (OSU)
Jordan Melendez (OSU)
Matt Pratola (OSU statistics)
Daniel Phillips (OU)

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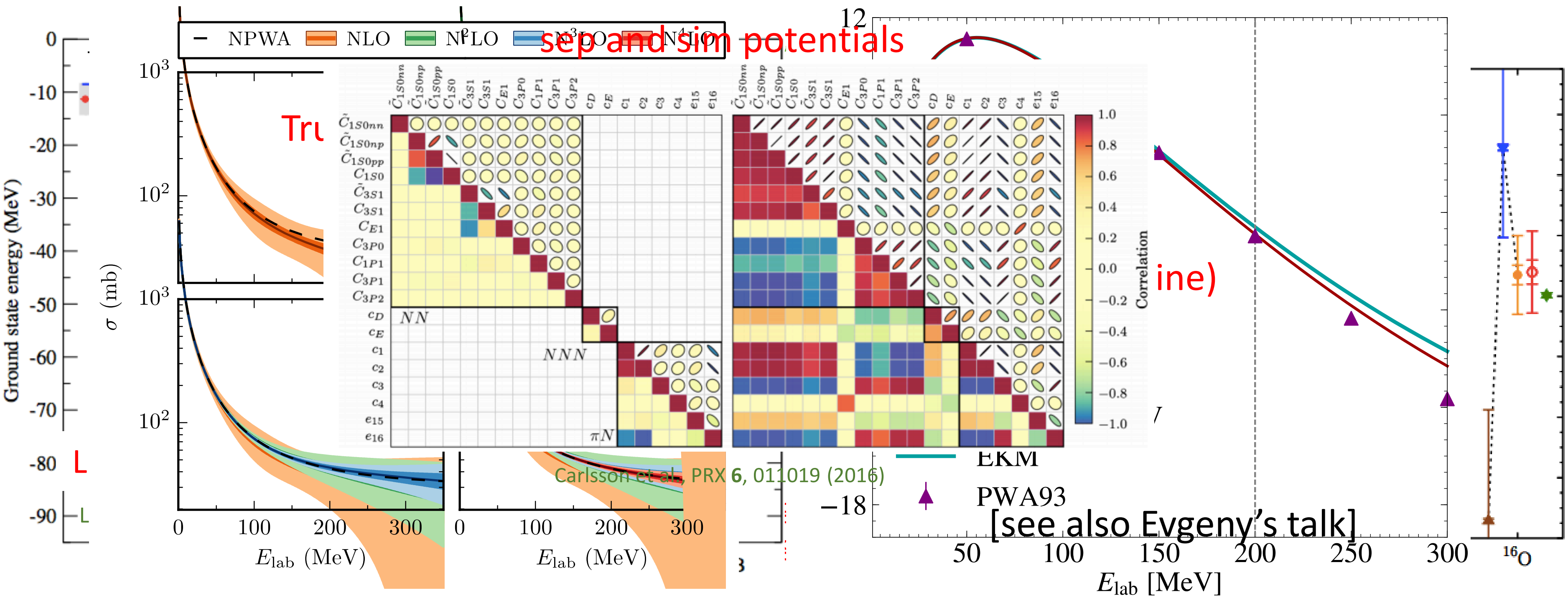
Motivation

Current landscape of uncertainty quantification for interactions

- **Covariance methods**: uncertainty from fitting to data
- **Bootstrapping**: uncertainty from fitting or numerics
- **Truncation error estimates for EFTs**: codifying standard EFT protocols
- **Bayesian**: can fit the above methods into this framework



Outline

GOAL: estimate the low-energy constants (LECs) of nuclear interactions, include all information consistently, and provide statistically meaningful uncertainty estimates

E.g. overestimating error bands:
"We're going to win so much, you're going to be so sick and tired of winning."

- Case study 1: usefulness of projected posterior plots
- Case study 2: LEC stability with maximum energy for fit

- **Part 2:** modeling truncation errors using Gaussian processes
  - Brief motivation of the GP model
  - Point-wise versus curve-wise implementation
  - Posterior for the EFT breakdown scale

Recent explosion of chiral EFT interactions

Interactions from 2003-4: EM(500, 600 MeV) or family of EGM potentials; used similar non-local regulators and similar fits to NN, 3N

New generation NN+3N interactions **[references at end]**

- **Non-local:** updated EMN and new soft; Ekstrom et al. sim, sat, and with Δs
- **Local** (for QMC): Gezerlis et al. nucleons only; Piarulli et al. with Δs
- **Semi-local:** Bochum-Julich group, SCS (x-space) and SMS (p-space)

Issues: power counting, regulator artifacts, EFT convergence, fitting protocols, fine-tuning, over/under-fitting, parameter redundancies, how to do UQ?

Parameter estimation issues repeat with LECs for currents and for other EFTs

Propaganda: Follow the Bayes Way

$$\mathrm{pr}(A|B,I) = \frac{\mathrm{pr}(B|A,I)\mathrm{pr}(A|I)}{\mathrm{pr}(B|I)} \Longrightarrow \underbrace{\mathrm{pr}(x|\mathrm{data},I)}_{\text{posterior}} \propto \underbrace{\mathrm{pr}(\mathrm{data}|x,I)}_{\text{likelihood}} \times \underbrace{\mathrm{pr}(x|I)}_{\text{prior}}$$

Why use Bayesian statistics?

- Parameter estimation: conventional optimization recovered as special case
- Update expectations using Bayes' theorem when have more information
- *Assumptions are made explicit* (e.g. naturalness of LECs)
- Clear prescriptions for combining errors
- Statistics as diagnostics for *physics*
- Model checking: we can *test* if our UQ model works and study sensitivities
- Model selection: Is the Δ needed? Pionless vs. pionful formulations, …
- Particularly well suited for (any) EFT, but generally suited for theory errors

Bayesian framework for parameter estimation in EFTs

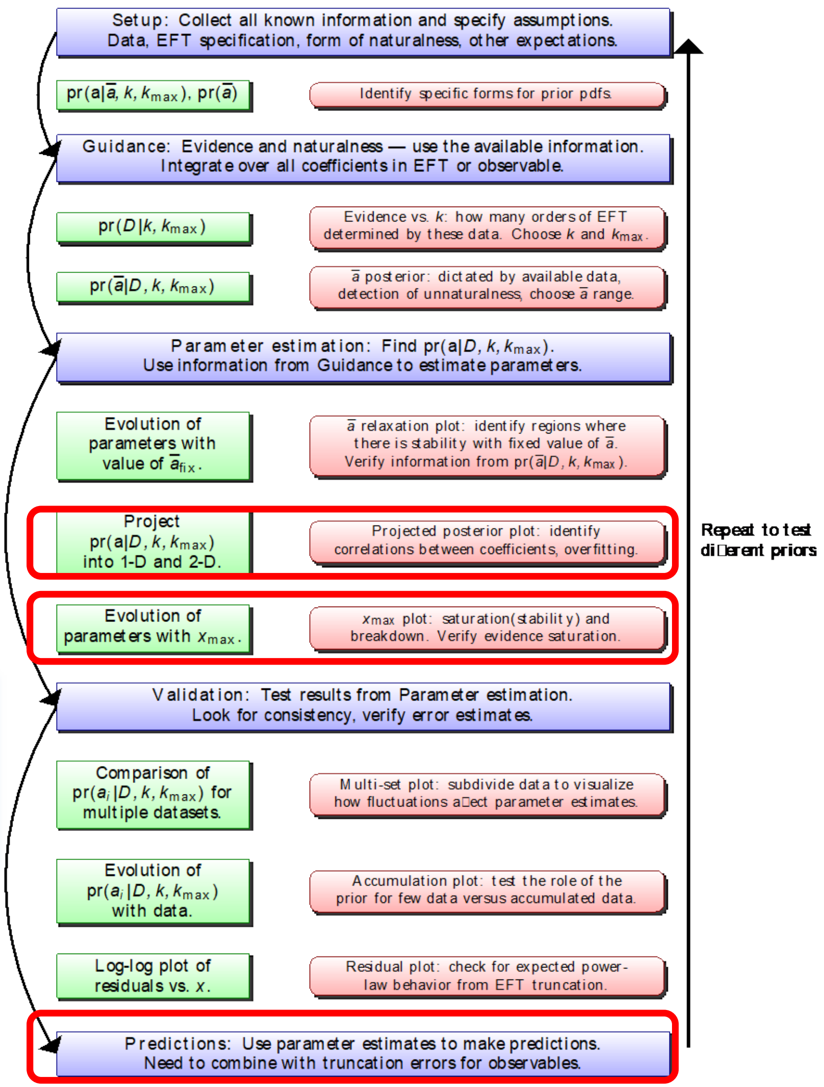
[See sw et al., J. Phys. G 43, 074001 (2016)]

Here: Use parameter estimation for NN phase shifts as test case (SCS potential of EKM)

- Good news: well studied, clear example for comparison, fairly easy computation
- Bad news: numerous and precise data ➔ differences from conventional approach are subtle. Plan: focus on illuminating cases.

1. The usefulness of projected posterior plots
2. LEC stability with maximum energy for fit
3. Combining theory uncertainties (in progress)

Based on: *Exploring Bayesian parameter estimation for chiral effective field theory using nucleon-nucleon phase shifts,* sw, R.J. Furnstahl, D. Phillips (posted soon)



Case study 1: The usefulness of projected posteriors

$$\underbrace{\mathrm{pr}(\mathbf{a}|D,I)}_{\text{posterior}} \propto \underbrace{\mathrm{pr}(D|\mathbf{a},I)}_{\text{likelihood}} \times \underbrace{\mathrm{pr}(\mathbf{a}|I)}_{\text{prior}}$$

D = data, I = background info.

Posterior pdf for vector of k^{th} order LECs $\mathbf{a}^{(k)}$ with naturalness assumption

$$\mathrm{pr}(\mathbf{a}^{(k)}|k, k_{\max}, D(E_{\max})) \propto e^{-\chi^2_{\mathrm{aug}}/2}\, e^{\mathbf{B}^T\mathbf{A}^{-1}\mathbf{B}/2}$$

account for omitted terms up to k_{max}

use data up to energy E_{max}

Case study 1: The usefulness of projected posteriors

$$\underbrace{\mathrm{pr}(\mathbf{a}|D,I)}_{\text{posterior}} \propto \underbrace{\mathrm{pr}(D|\mathbf{a},I)}_{\text{likelihood}} \times \underbrace{\mathrm{pr}(\mathbf{a}|I)}_{\text{prior}} \qquad D = \text{data}, \quad I = \text{background info.}$$

Posterior pdf for vector of k^{th} order LECs $\mathbf{a}^{(k)}$ with naturalness assumption

$$\mathrm{pr}(\mathbf{a}^{(k)}|k, k_{\max}, D(E_{\max})) \propto \boxed{e^{-\chi^2_{\text{aug}}/2}} e^{\mathbf{B}^T\mathbf{A}^{-1}\mathbf{B}/2}$$

data EFT prediction at k^{th} order

$$\boxed{\chi^2_{\text{aug}} = \sum_{i=1}^{N} \left(\frac{d_i - t^{(k)}(p_i; \mathbf{a}^{(k)})}{\sigma_i} \right)^2 + \frac{\left(\mathbf{a}^{(k)}\right)^2}{2\bar{a}^2_{\text{fix}}}}$$

Augmented χ^2 accounts for data errors σ_i *and* bounded (natural) LECs, here with simple δ-function prior at $\bar{a}_{\text{fix}}$

Case study 1: The usefulness of projected posteriors

$$\underbrace{\mathrm{pr}(\mathbf{a}|D,I)}_{\text{posterior}} \propto \underbrace{\mathrm{pr}(D|\mathbf{a},I)}_{\text{likelihood}} \times \underbrace{\mathrm{pr}(\mathbf{a}|I)}_{\text{prior}} \qquad D = \text{data}, \quad I = \text{background info.}$$

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$$A_{jj'} = \frac{\delta_{j,j'}}{\bar{c}_{\text{fix}}{}^2} + \sum_{i=1}^{N}\frac{X_0(p_i)^2\; Q_i^{j+j'}}{\sigma_i^2}$$

$$B_j = \sum_{i=1}^{N} X_0(p_i)\, Q_i^j\; \frac{d_i - t^{(k)}(p_i;\mathbf{a}^{(k)})}{\sigma_i^2}$$

Accounts for *truncation error* from omitted higher-order terms

Ref: Stump et al., PRD 65 **014012 (appendix B)**

- Consistently include higher-order correlated errors
- Assumed to be same set of coefficients for each datum
- Minimally informative assumptions
- Easy to implement! (more consistent alternatives in progress)

Case study 1: The usefulness of projected posteriors

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Posterior pdf for vector of k^{th} order LECs $\mathbf{a}^{(k)}$ with naturalness assumption

$$\mathrm{pr}(\mathbf{a}^{(k)}|k, k_{\max}, D(E_{\max})) \propto \; e^{-\chi^2_{\text{aug}}/2} \, e^{\mathbf{B}^T\mathbf{A}^{-1}\mathbf{B}/2}$$

$$\chi^2_{\text{aug}} = \sum_{i=1}^{N}\left(\frac{d_i - t^{(k)}(p_i;\mathbf{a}^{(k)})}{\sigma_i}\right)^2 + \frac{\left(\mathbf{a}^{(k)}\right)^2}{2\bar{a}^2_{\text{fix}}}$$

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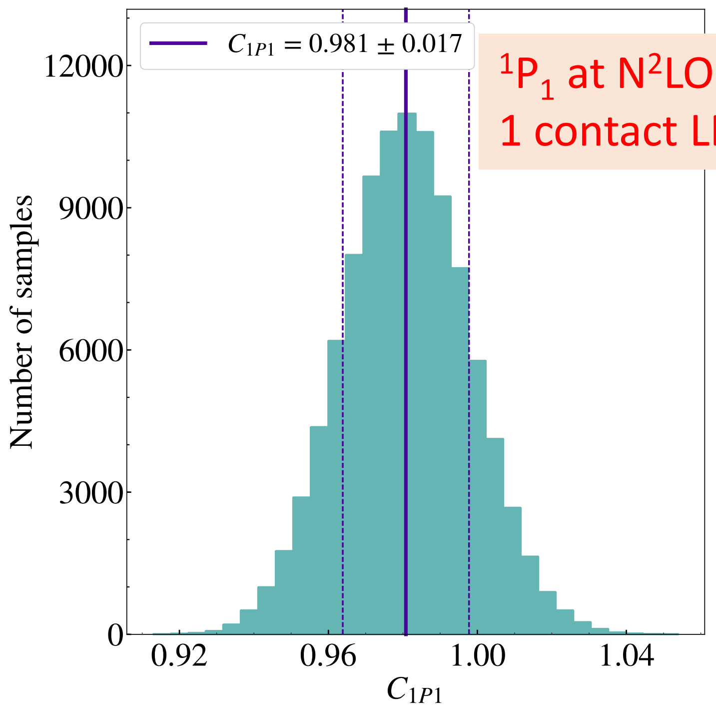
$$B_j = \sum_{i=1}^{N} X_0(p_i)\, Q_i^j\, \frac{d_i - t^{(k)}(p_i;\mathbf{a}^{(k)})}{\sigma_i^2}$$

For case study 1, we won't include truncation errors, so $k = k_{\max}$

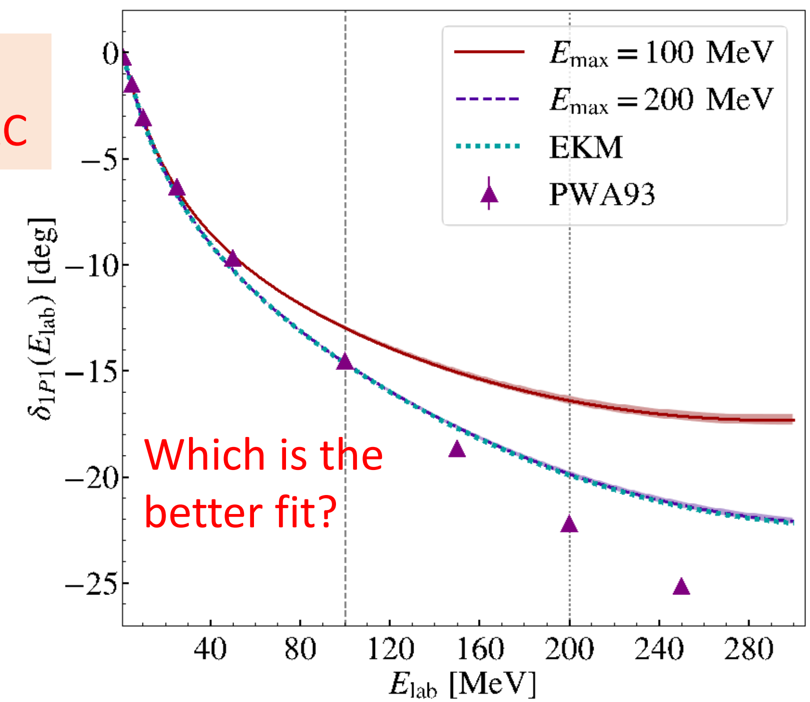
Case study 1: The usefulness of projected posteriors

$$\mathrm{pr}(\mathbf{a}^{(k)}|k, k_{\max} = k, D(E_{\max})) \propto e^{-\chi^2_{\mathrm{aug}}/2}$$

$$\chi^2_{\mathrm{aug}} = \sum_{i=1}^{N} \left(\frac{d_i - t^{(k)}(p_i; \mathbf{a}^{(k)})}{\sigma_i} \right)^2 + \frac{\left(\mathbf{a}^{(k)}\right)^2}{2\bar{a}^2_{\mathrm{fix}}}$$



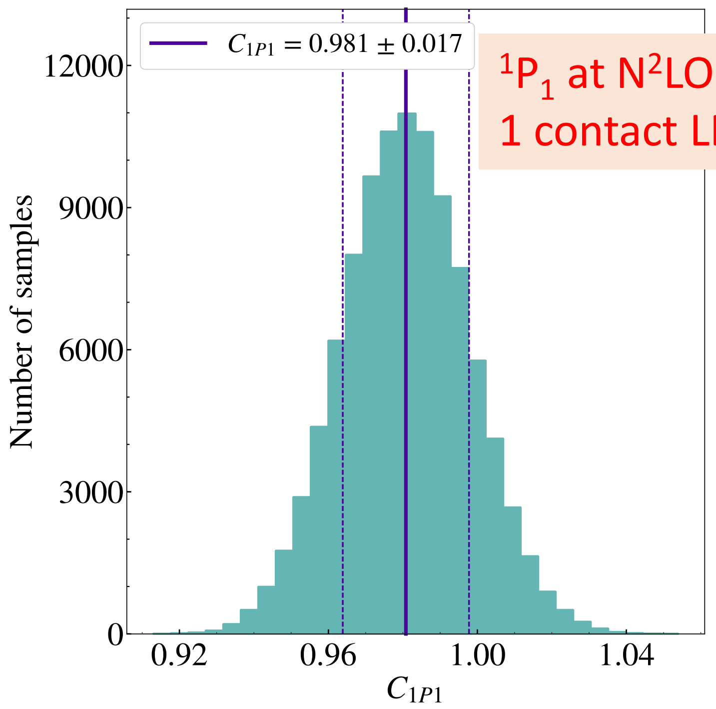
$^1P_1$ at N^2LO
1 contact LEC



Which is the better fit?

Case study 1: The usefulness of projected posteriors

$$\mathrm{pr}(\mathbf{a}^{(k)}|k, k_{\max}=k, D(E_{\max})) \propto e^{-\chi^2_{\mathrm{aug}}/2} \qquad \chi^2_{\mathrm{aug}} = \sum_{i=1}^{N}\left(\frac{d_i - t^{(k)}(p_i;\mathbf{a}^{(k)})}{\sigma_i}\right)^2 + \frac{\left(\mathbf{a}^{(k)}\right)^2}{2\bar{a}^2_{\mathrm{fix}}}$$



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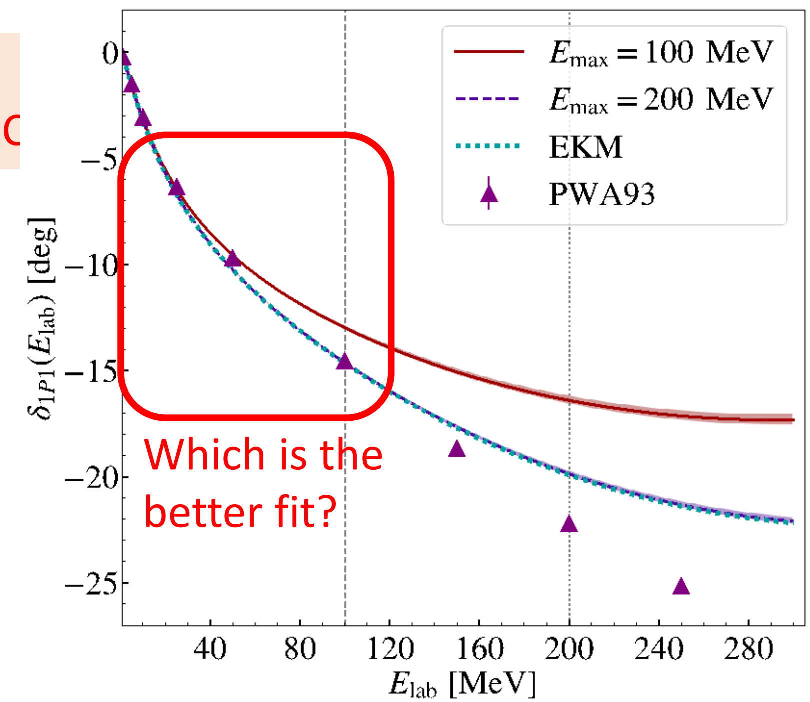
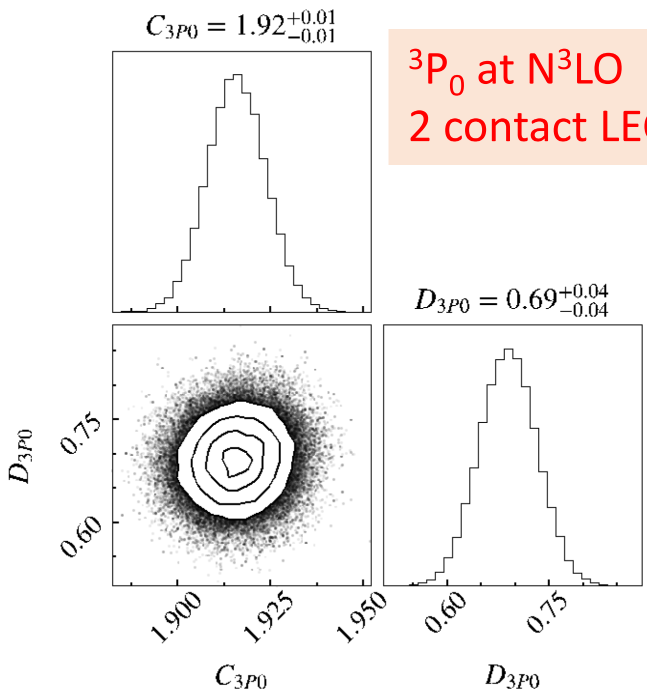


Which is the better fit?

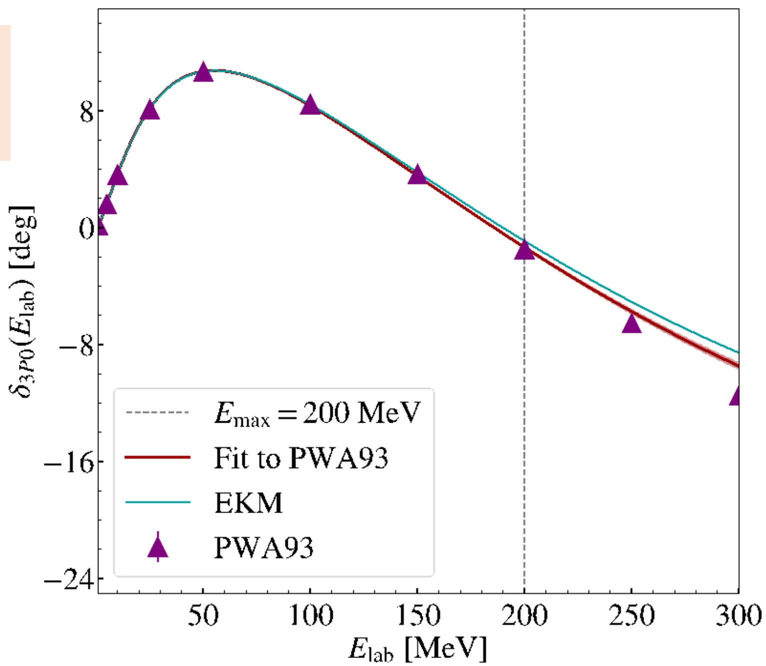
Case study 1: The usefulness of projected posteriors

$$\mathrm{pr}(\mathbf{a}^{(k)}|k, k_{\max}=k, D(E_{\max})) \propto e^{-\chi^2_{\mathrm{aug}}/2}$$

$$\chi^2_{\mathrm{aug}} = \sum_{i=1}^{N}\left(\frac{d_i - t^{(k)}(p_i;\mathbf{a}^{(k)})}{\sigma_i}\right)^2 + \frac{\left(\mathbf{a}^{(k)}\right)^2}{2\bar{a}^2_{\mathrm{fix}}}$$

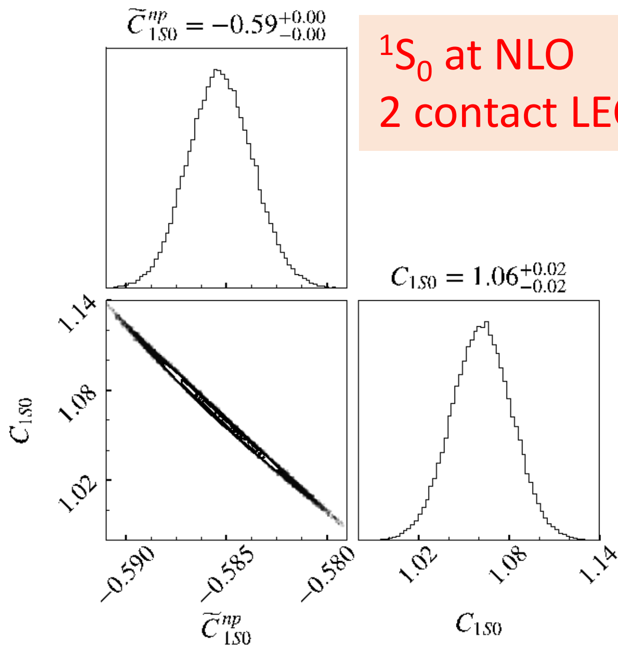


$^3P_0$ at N^3LO
2 contact LECs

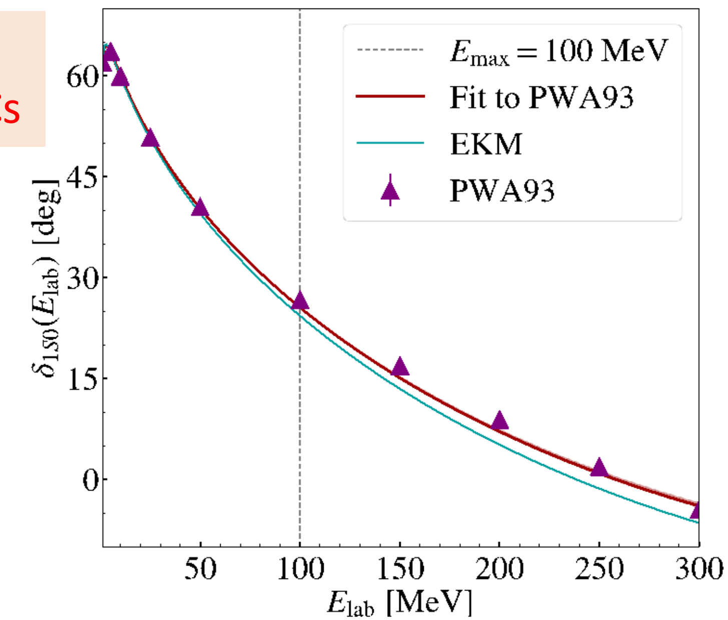


Case study 1: The usefulness of projected posteriors

$$\mathrm{pr}(\mathbf{a}^{(k)}|k, k_{\max} = k, D(E_{\max})) \propto e^{-\chi^2_{\mathrm{aug}}/2} \qquad \chi^2_{\mathrm{aug}} = \sum_{i=1}^{N} \left(\frac{d_i - t^{(k)}(p_i; \mathbf{a}^{(k)})}{\sigma_i} \right)^2 + \frac{\left(\mathbf{a}^{(k)}\right)^2}{2\bar{a}^2_{\mathrm{fix}}}$$

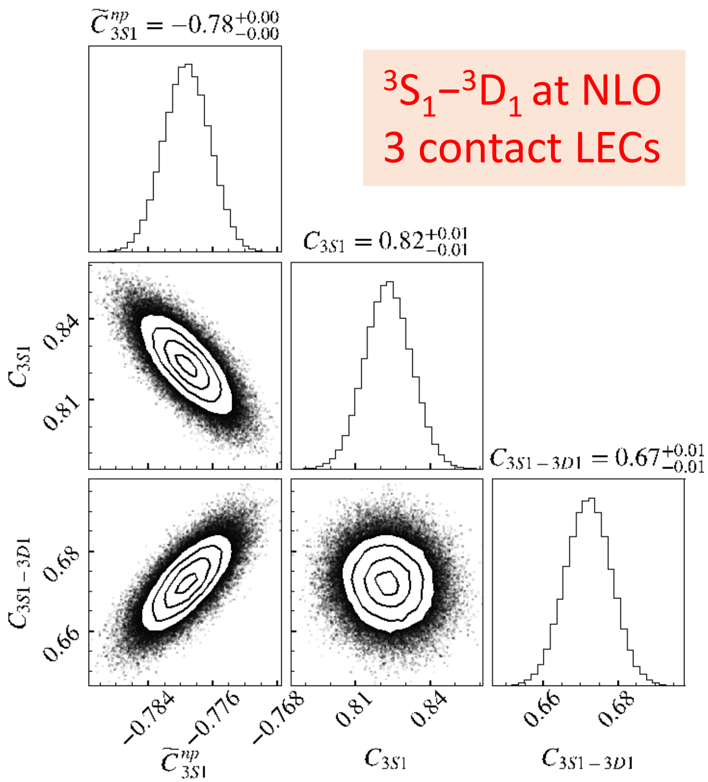


$^1S_0$ at NLO
2 contact LECs

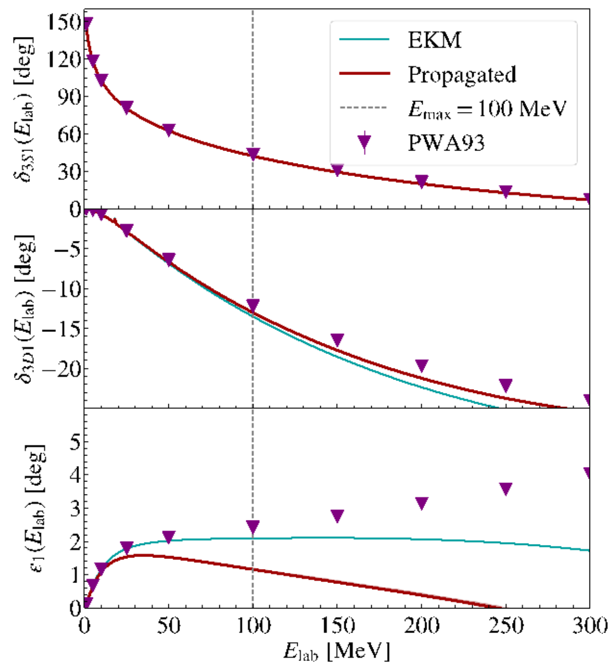


Case study 1: The usefulness of projected posteriors

$$\mathrm{pr}(\mathbf{a}^{(k)}|k, k_{\max} = k, D(E_{\max})) \propto e^{-\chi^2_{\mathrm{aug}}/2} \qquad \chi^2_{\mathrm{aug}} = \sum_{i=1}^{N}\left(\frac{d_i - t^{(k)}(p_i;\mathbf{a}^{(k)})}{\sigma_i}\right)^2 + \frac{\left(\mathbf{a}^{(k)}\right)^2}{2\bar{a}^2_{\mathrm{fix}}}$$



$^3S_1$–$^3D_1$ at NLO
3 contact LECs

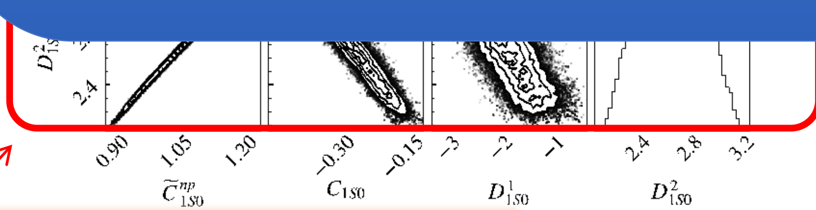


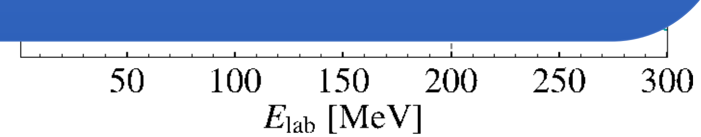
Case study 1: The usefulness of projected posteriors

$\mathrm{pr}(\mathbf{a}^{(k)}| \ldots \qquad \chi^2 = \sum^{N} \Big(d_i - t^{(k)}(p_i;\mathbf{a}^{(k)}) \Big)^2 + (\mathbf{a}^{(k)})^2$

S-wave potentials at N^{3}LO have off-shell pieces → redundancy!

$$
\begin{aligned}
D^1_{(1S0)} p^2 p'^2 + D^2_{(1S0)}(p^4 + p'^4)
&= \frac{1}{4}(D^1_{(1S0)} + 2D^2_{(1S0)})(p^2 + p'^2)^2 \\
&\quad - \frac{1}{4}(D^1_{(1S0)} - 2D^2_{(1S0)})(p^2 - p'^2)^2 \\
&= (D^1_{(1S0)} + 2D^2_{(1S0)}) p^2 p'^2 + D^2_{(1S0)}(p^2 - p'^2)^2
\end{aligned}
$$



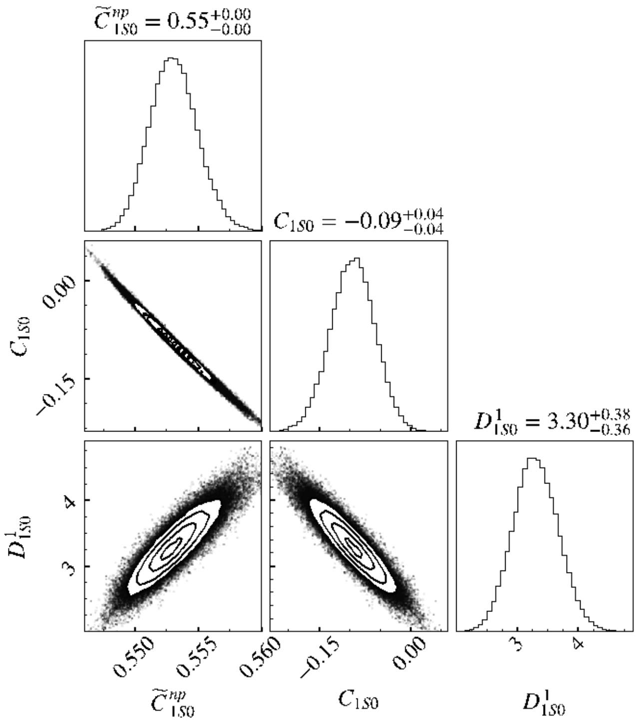


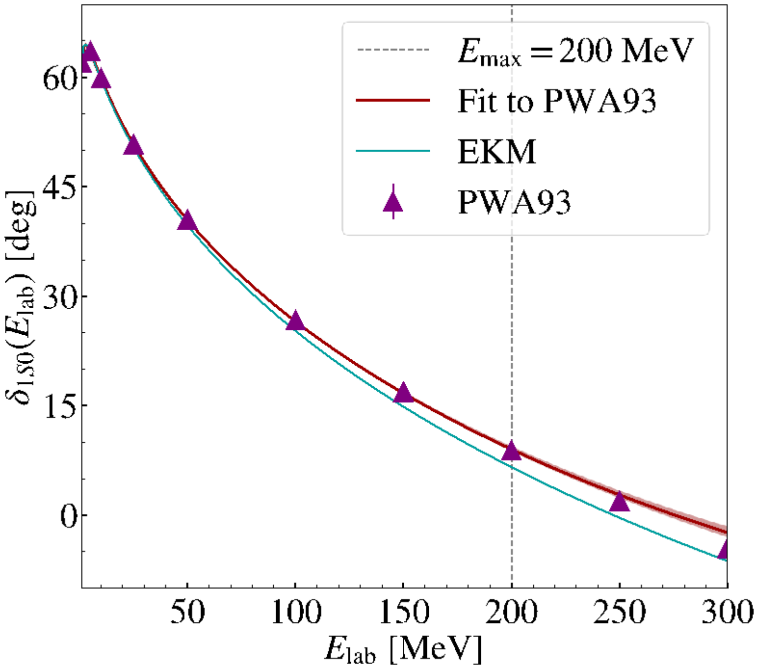
Freeze redundant operator LEC

Case study 1: The usefulness of projected posteriors

$$\mathrm{pr}(\mathbf{a}^{(k)}|k, k_{\max} = k, D(E_{\max})) \propto e^{-\chi^2_{\mathrm{aug}}/2}$$

$$\chi^2_{\mathrm{aug}} = \sum_{i=1}^{N} \left(\frac{d_i - t^{(k)}(p_i; \mathbf{a}^{(k)})}{\sigma_i} \right)^2 + \frac{\left(\mathbf{a}^{(k)}\right)^2}{2\bar{a}^2_{\mathrm{fix}}}$$





Reinert et al. find much better behaved SMS fit with three fewer parameters!

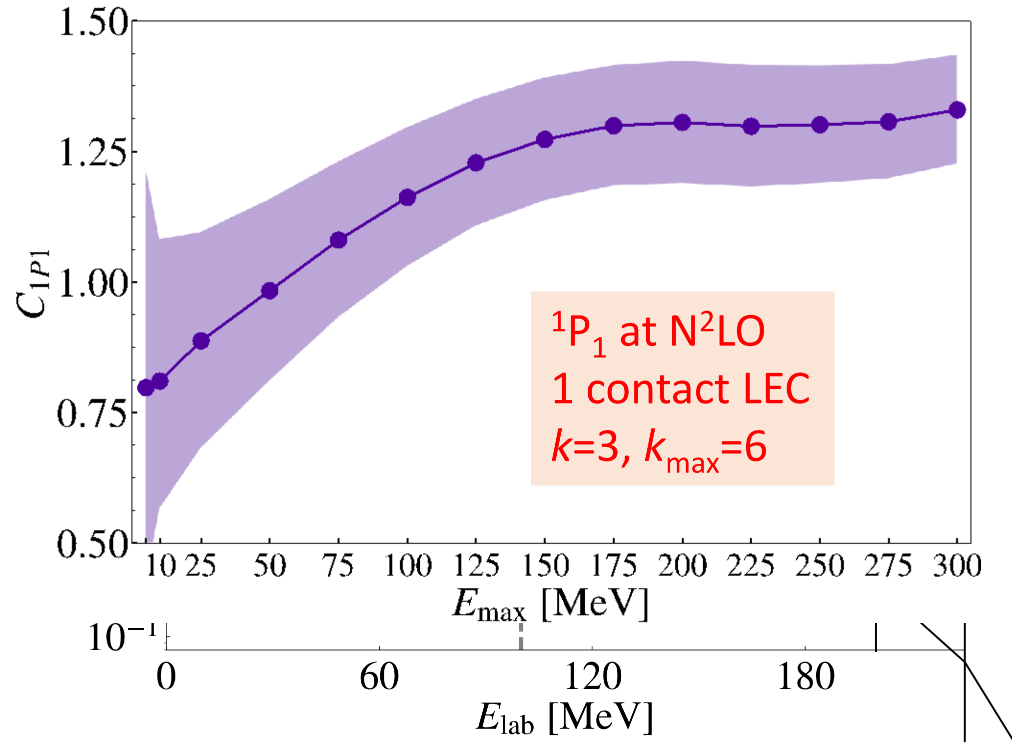
Case study 2: LEC stability with maximum energy for fit

EFT convergence

$$X(p) = X_0 \sum_{n=0}^{k} c_n Q^n, \quad \Delta_k = \sum_{n=k+1}^{k_{\max}} c_n Q^n$$

$$Q = \max(p, m_\pi)/\Lambda_b$$

- How should we choose $E_{\max}$ to fit?
- Operator expansion, so LECs should be independent of data used
- *Could distort observables* (e.g., energies work but not radii)
- Solution: account for EFT truncation
- $E_{\max}$ plots are simple proxy for Bayesian model selection
- Generally relevant for fitting!



Note: fit is to partial-wave cross section with larger uncertainty

Outline

GOAL: estimate the low-energy constants (LECs) of nuclear interactions, include all information consistently, and provide statistically meaningful uncertainty estimates

- **Part I:** parameter estimation for chiral EFT using NN phaseshifts
  - Setup: Bayesian propaganda and framework
  - How to incorporate truncation errors in parameter estimation
  - Case study 1: usefulness of projected posterior plots
  - Case study 2: LEC stability with maximum energy for fit
- **Part 2:** modeling truncation errors using Gaussian processes
  - Brief motivation of the GP model
  - Point-wise versus curve-wise implementation
  - Posterior for the EFT breakdown scale

Statistical model for truncation errors

Previous work: Furnstahl, Phillips, Klco, sw, PRC **92**, 024005 (2015)

- Previous work: used a Bayesian interpretation to develop a statistically meaningful model for truncation errors in EFTs
- Order-by-order convergence predicts size of truncation
- Can validate our predictions, diagnose convergence issues, etc.

Wondering how you can do it?

- Eq.(25) in above reference
- Generalizes common prescription
- Error bands are NOT Gaussian
- Model-checking diagnostics:
  - Furnstahl, Phillips, Klco, sw, PRC **92**, 024005 (2015)
  - Melendez, Furnstahl, sw PRC **96**, 024003 (2017)

In the limiting case of prior Set $A_\epsilon^{(1)}$, this integral can be evaluated explicitly [6],

$$\boxed{d_k^{(p)} = \bar{c}_{(k)}\, Q^{k+1} \times \begin{cases} \frac{n_c+1}{n_c}\, p\% & \text{if } p \leqslant \frac{n_c}{n_c+1}, \\ \left[\frac{1}{(n_c+1)(1-p\%)}\right]^{1/n_c} & \text{if } p > \frac{n_c}{n_c+1}, \end{cases} \quad (25)}$$

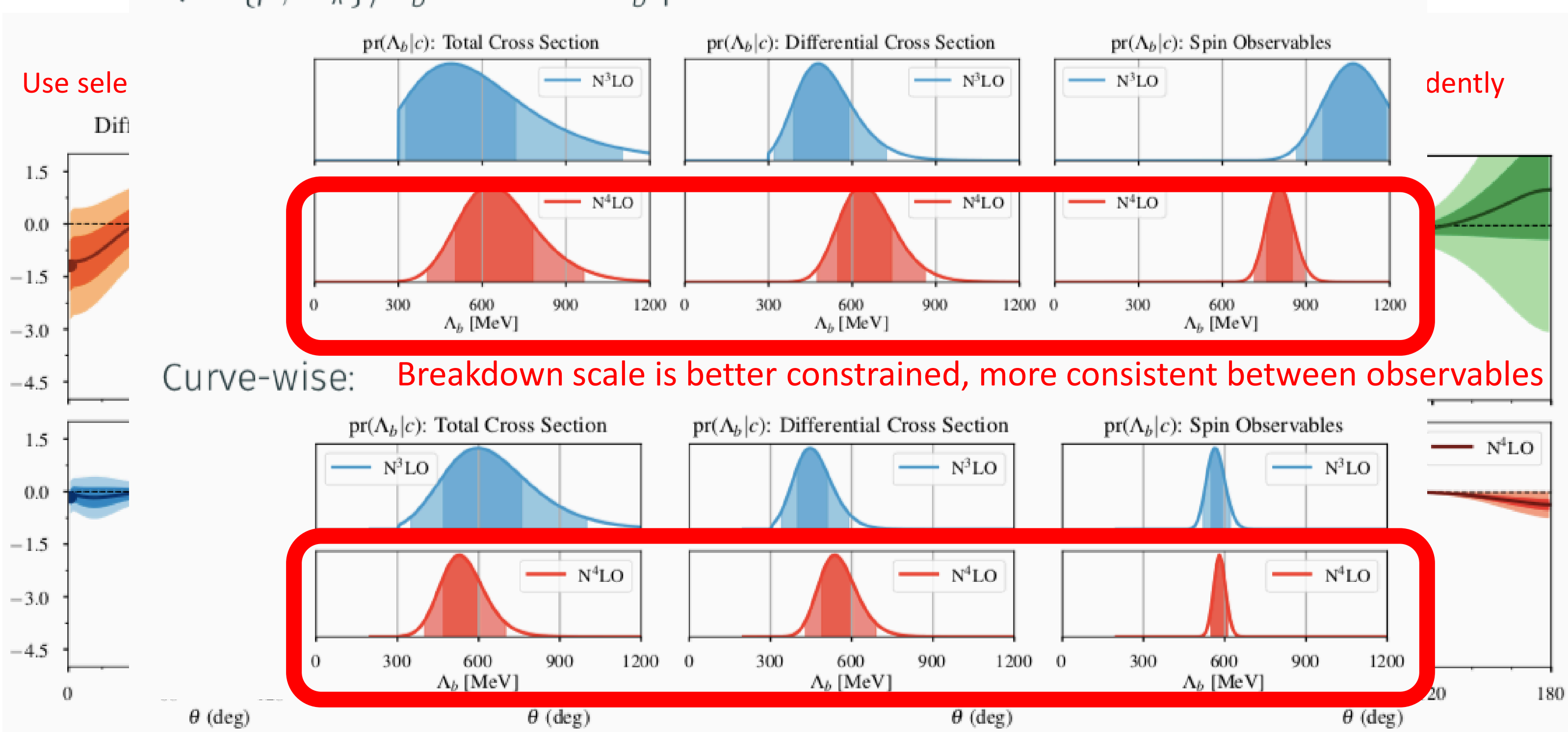
where n_c is again the number of nonzero known coefficients. Thus, with these priors, the interval of width $\bar{c}_{(k)} Q^{k+1}$ about the EFT prediction at order k is a $n_c/(n_c+1) * 100\%$ DOB interval, cf. Ref. [6]. Such a theory error bar has often been assigned in previous EFT calculations, and—as we discuss further in Sec. III—corresponds to the prescription formalized in Refs. [10,11]. It is important—e.g., in the context of error propagation—to keep in mind that this prior leads to a distribution of probability for the truncation error that is not Gaussian.

Improving the model: Gaussian processes

Gaussian process model for truncation errors:

- Predictions at nearby kinematics are not independent
- Use correlation information to improve truncation predictions
- Learn physics! diagnose breakdown scale + correlation length

$Q = \{p, m_\pi\}/\Lambda_b$. Estimate Λ_b point-wise:



Using EKM SCS R=0.9fm interaction

PRELIMINARY

Lessons from Bayesian methods in the NN sector

Tested by “fitting” (sampling posteriors) of NN LECs in partial waves; lessons are general

Case study 1: The usefulness of projected posterior plots

- Important for understanding the full information content of the data
- Most channels look Gaussian, but do statistical test before approximations!
- Use of projected posterior plots as a *physics diagnostic* illustrated by the fourth-order s-wave LECs ➔parameter degeneracy

Case study 2: LEC stability with maximum energy for fit

- What is optimal trade-off between more data to determine LECs more precisely and fit contamination at higher energies of omitted higher-order EFT terms?
- Sensitivity to E_{max} removed with Bayesian UQ ➔LECs should be independent
- Accounting for truncation errors; verify with E_{max} plots

Gaussian processes: Improving truncation error model using correlation information

- Nearby kinematics do not contain independent information
- Correlation information can be used to learn about the interaction
- The EFT breakdown can be statistically determined by examining convergence

Future Bayesian Plans (Collaborators wanted!)

- Use scattering observables directly for parameter estimation
- Identify appropriate priors for other theoretical expectations such as Wigner symmetry
- Propagate all sources of error, including from LECs, to few- and many-body observables
- Estimate the EFT expansion parameter from the expected convergence pattern of additional observable predictions (uniform matter in progress)
- Account for correlations between LECs from the πN, NN, and few-body sectors
- Assess the impact of available experimental data on the number of orders of the EFT that can be constrained via Bayesian model selection
- Employ Bayesian model checking techniques to verify for observable calculations that the EFT expansion is working ``as advertised"
- Model selection problems (which degrees of freedom to use)?

References

Some BUQEYE publications on UQ for EFT

- “A recipe for EFT uncertainty quantification in nuclear physics”, J. Phys. G 42, 034028 (2015)
- “Quantifying truncation errors in effective field theory”, Phys. Rev. C 92, 024005 (2015) [with Natalie Klco]
- “Bayesian parameter estimation for effective field theories”, J. Phys. G 43, 074001 (2016)
- “Bayesian truncation errors in chiral EFT: nucleon-nucleon observables”, Phys. Rev. C 96, 024003 (2017)

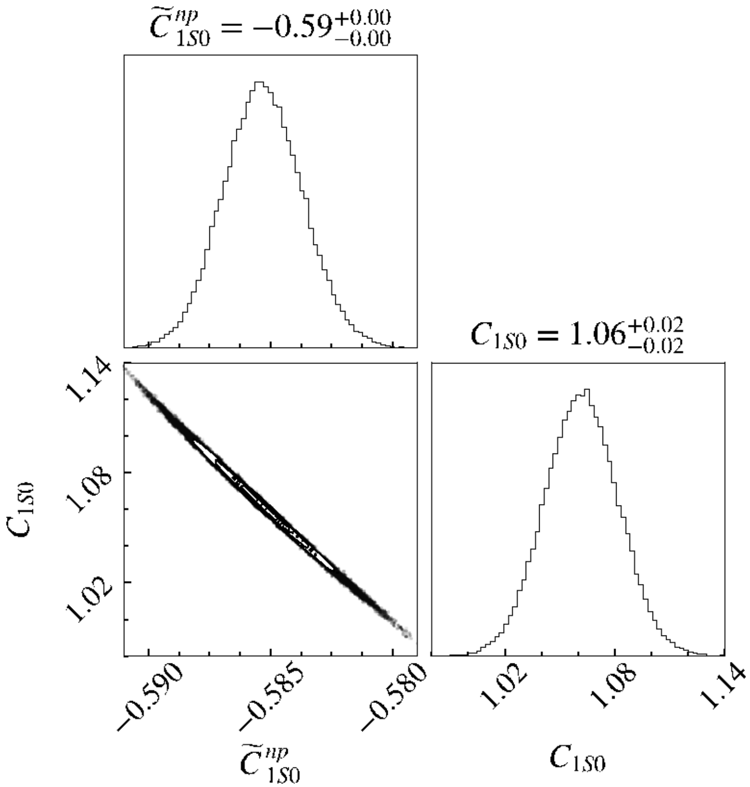
Recent publications on fitting chiral EFT interactions

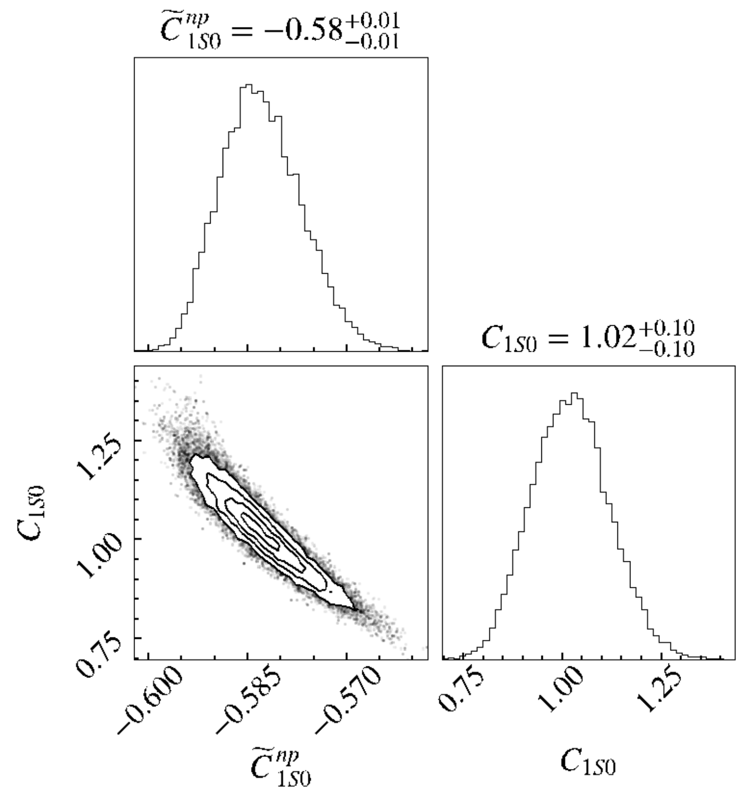
- D. R. Entem, R. Machleidt, and Y. Nosyk. “High-quality two-nucleon potentials up to fifth order of the chiral expansion,” Phys. Rev. C 96, 024004, 2017.
- B. Carlsson, A. Ekström, C. Forssén, D. F. Strömberg, O. Lilja, et al. “Uncertainty analysis and order-by-order optimization of chiral nuclear interactions,” Phys. Rev. X, 011019, 2015.
- A. Gezerlis, I. Tews, E. Epelbaum, M. Freunek , S. Gandolfi , K. Hebeler, A. Nogga, A. Schwenk. “Local chiral effective field theory interactions and quantum Monte Carlo applications,” Phys.Rev. C 90, 054323 (2014).
- M. Piarulli, L. Girlanda, R. Schiavilla, R. Navarro Ṕerez, J. E. Amaro, and E. Ruiz Arriola. “Minimally nonlocal nucleon-nucleon potentials with chiral two-pion exchange including resonances,” Phys. Rev. C, 024003, 2015.
- E. Epelbaum, H. Krebs, and U. G. Meißner. “Improved chiral nucleon-nucleon potential up to next-to-next-to-next-to-leading order,” Eur. Phys. J. A 51, 53, 2015.
- P. Reinert, H. Krebs, and E. Epelbaum. “Semilocal momentum-space regularized chiral two-nucleon potentials up to fifth order,” arXiv:1711.08821 2017.

Back-up Slides

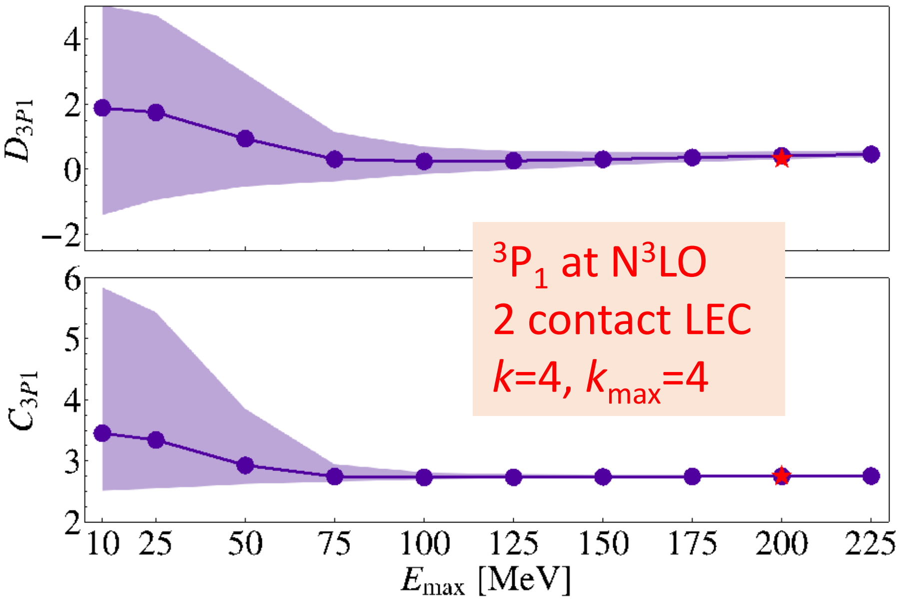
Case study 2: LEC stability with maximum energy for fit

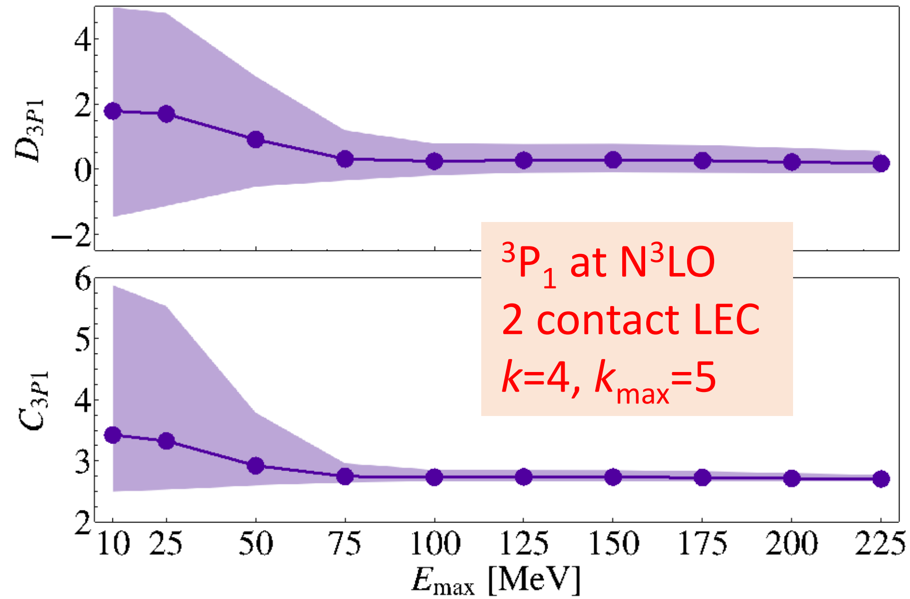
Now fitting to partial-wave *cross section:* Not completely Gaussian, but close





Case study 2: LEC stability with maximum energy for fit

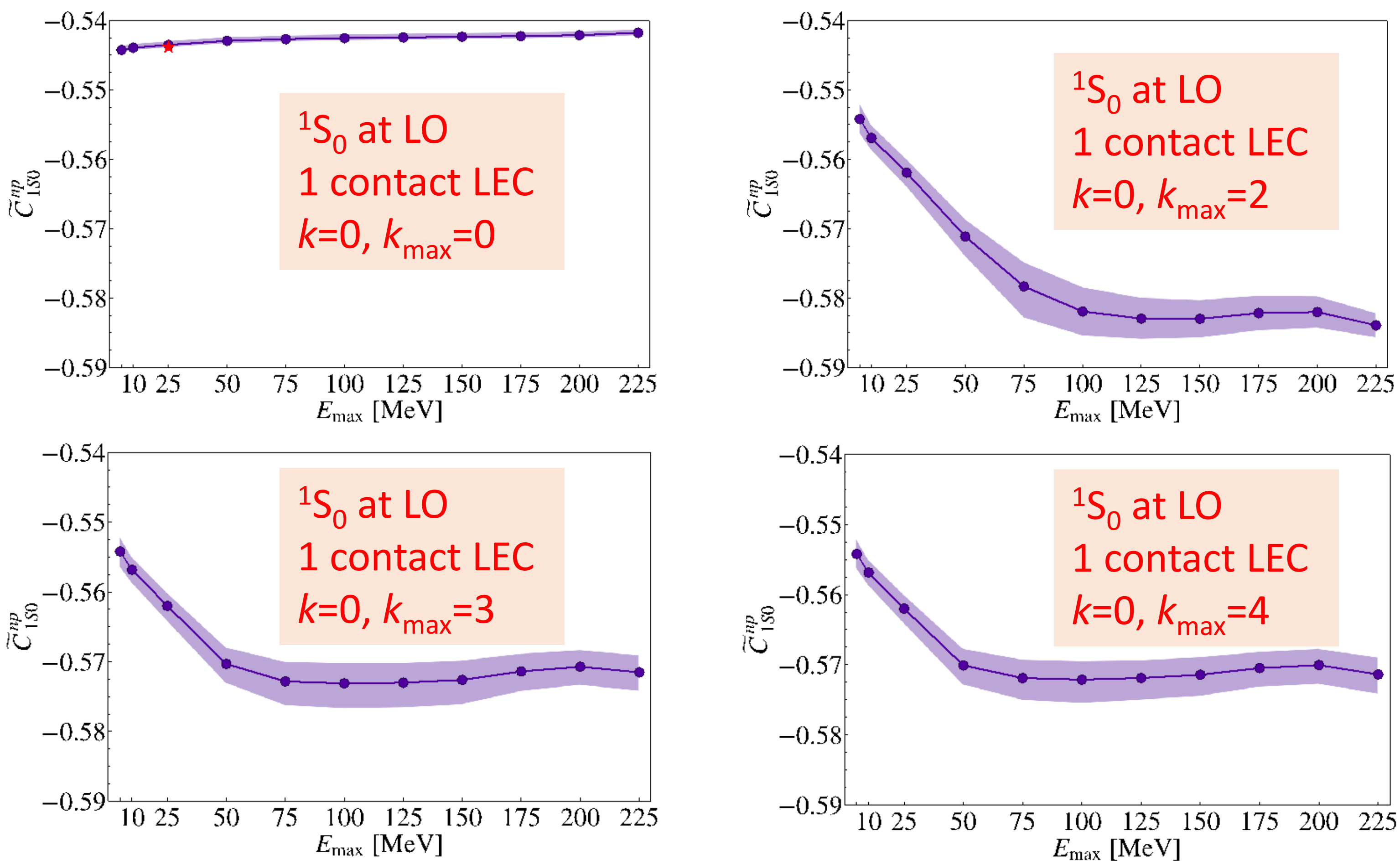




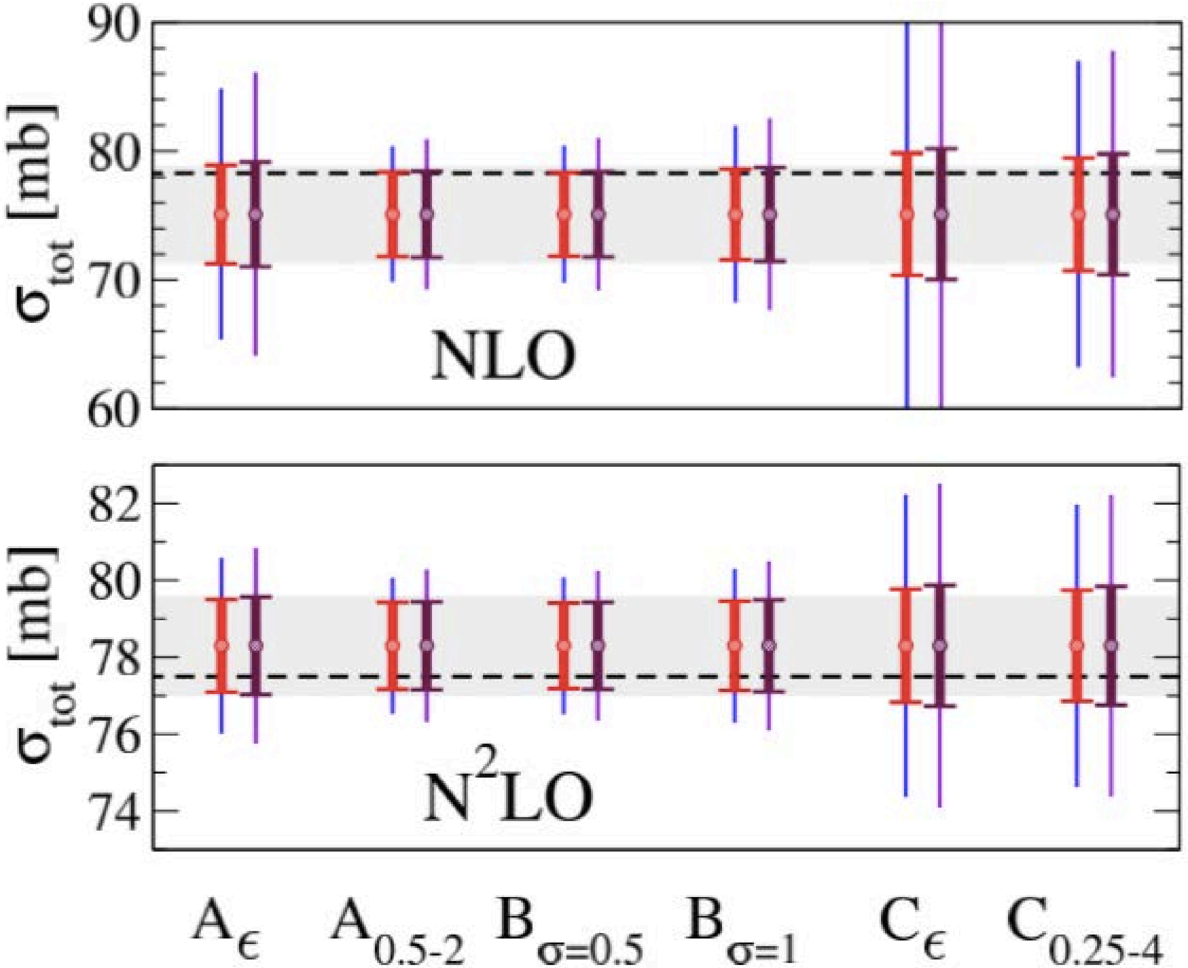
Less impact from neglected higher-order terms at higher EFT orders (larger *k*)

Here including truncation error for $^3P_1$ at N^{3}LO makes parameter estimates less E_{max} dependent and gives larger uncertainty (blow up to see details)

Case study 2: LEC stability with maximum energy for fit



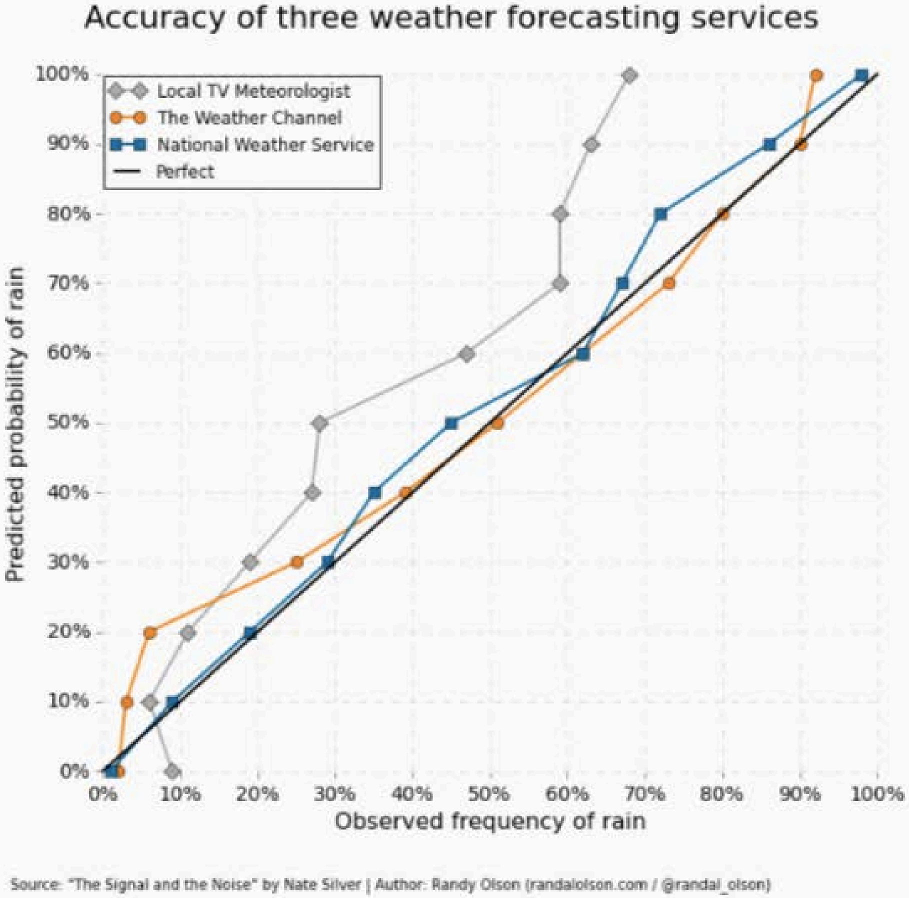
Different prior assumptions for truncation errors



EKM SCS
R=0.9fm
E_{lab} = 96MeV

Furnstahl, Phillips, Klco, sw, PRC **92**, 024005 (2015)

Credible Interval Diagnostic



- Tests model against reality
- Generalized to GPs in Bastos and O'Hagan (2009)
- Called "consistency plots" in Melendez et al. (2017)

Nuclear Matter [PRELIMINARY]

- First application to 3-body forces
- Uncertainty helps compare to empirical saturation