Bayesian analysis of NN scattering data in pionless effective field theory

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Next-Generation χEFT Interactions

We are interested in calibrating the next generation of EFT nucleon-nucleon interactions.

These models should have robust uncertainty quantification:

- Parametric uncertainty
- Truncation uncertainty

Incorporating these uncertainties into our model calibration we aim to better understand and predict nuclear phenomena based on microscopic interactions of nucleons.

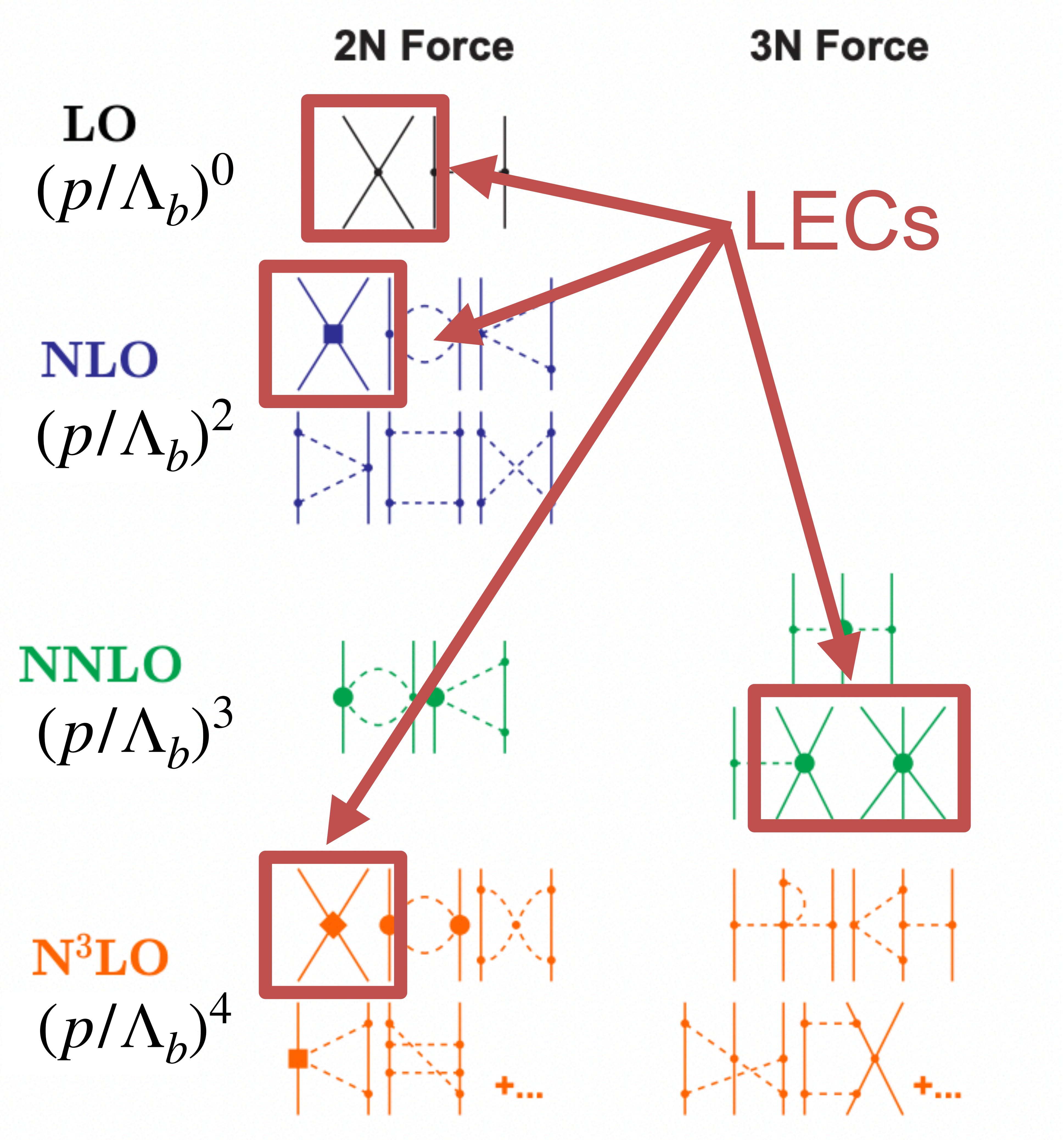
Effective Field Theory

We take an effective expansion of QCD preserving chiral symmetry with N and π d.o.f.

The interaction can be ordered in terms of powers of p/Λ_b

- p is a momentum or pion mass
- Λ_b is the symmetry breaking scale

Gives a systematic ordering to improve the interaction.



Bayes' Theorem

For a model calibration problem in a Bayesian approach, we have

$$\underbrace{\mathrm{pr}(\vec{\mathrm{a}}\,|\,\vec{\mathrm{y}},\mathrm{I})}_{\text{Posterior}} \propto \underbrace{\mathrm{pr}(\vec{\mathrm{y}}\,|\,\vec{\mathrm{a}})}_{\text{Likelihood}}\;\underbrace{\mathrm{pr}(\vec{\mathrm{a}}\,|\,\mathrm{I})}_{\text{Prior}}$$

The likelihood can be formulated as it is in standard model fitting for uncorrelated data

$$\mathrm{pr}(\vec{\mathrm{y}}\,|\,\vec{\mathrm{a}}) \sim e^{-\sum_i \left(y^{(i)}_{\mathrm{exp}} - y^{(i)}_{\mathrm{th}}(\vec{a})\right)^2/2\sigma_i^2} = e^{-\chi^2/2}$$

What the prior does for us is encode any previous information that we may know.

- Ex: LECs are natural, i.e., order 1 $\rightarrow \mathrm{pr}(\vec{\mathrm{a}}\,|\,\mathrm{I}) \sim \mathcal{N}\left(\vec{0}, \Sigma_{\mathrm{pr}}\right)$

Likelihood Improvement

In the simple likelihood, we had the χ^2, $\left(e^{-\chi^2/2}\right)$, but we can improve this.

We can inform the model calibration with information about the model *itself*.

In what way? If we assume that the exp and th errors are normally distributed:

$$\chi^2 = \sum_i \frac{\left(y_{\mathrm{exp}}^{(i)} - y_{\mathrm{th}}^{(i)}(\vec{a})\right)^2}{\sigma_i^2} \longrightarrow \sigma_i^2 \to \sigma_i^2 + \sigma_{\mathrm{th},i}^2$$

Modeling the Model

Since our model is a perturbative series, we can write an observable as such (BUQEYE framework)*:

$$y_{\mathrm{th}}(x) = y_{\mathrm{ref}}(x) \sum_{n=0}^{\infty} c_n(x) Q^n(x), \quad Q \equiv \frac{\max[p_{soft}, p]}{\Lambda_b},$$

where $y_{\mathrm{ref}}(x)$ sets a reference scale for the observable y_{th}, Λ_b is the EFT breakdown scale, and c_n are the natural coefficients.

This series follows the truncation scheme of the EFT:

$$y_{\mathrm{th}}(x) = y_{\mathrm{ref}}(x) \sum_{n=0}^{k} c_n(x) Q^n(x) + y_{\mathrm{ref}}(x) \sum_{n=k+1}^{\infty} c_n(x) Q^n(x) = y_{\mathrm{th}}^{(k)}(x) + \delta y_{\mathrm{th}}^{(k)}(x).$$

*R. J. Furnstahl et. al. Phys. Rev. C **92**, 024005

Truncation Errors

From the neglected terms, we have

$$\delta y_{\mathrm{th}}^{(k)}(x) = y_{\mathrm{ref}}(x) \sum_{n=k+1}^{\infty} c_n(x) Q^n(x).$$

Under the assumption that the truncation error is uncorrelated across orders, this is a geometric series in Q, so we can find*

$$\delta y_{\mathrm{th}}^{(k)}(x) = \frac{y_{\mathrm{ref}}\, \bar{c}\, Q^{(k+1)}}{1 - Q},$$

Where we assume that $c_n \,|\, \bar{c} \sim \mathcal{N}\left(0, \bar{c}^2\right)$.

*J. A. Melendez et. al. Phys. Rev. C **100**, 044001

Theoretical Covariance

From the truncation uncertainty, we can construct a covariance matrix*, assuming δy_{th} is normally distributed,

$$\Sigma_{ij}^{\mathrm{th}} = \frac{\left(y_{\mathrm{ref},i}\, \bar{c}\, Q_i^{(k+1)}\right)\left(y_{\mathrm{ref},j}\, \bar{c}\, Q_j^{(k+1)}\right)}{1 - Q_i Q_j} r(x_i, x_j; \vec{l}),$$

were we introduce a kernel $r(x_i, x_j; \vec{l})$ to smooth and handle correlations.

*S. Wesolowski et al. J. Phys. G **46**, 045102

Correlated Likelihood

We can build a total covariance,

$$\Sigma_{ij} = \Sigma_{ij}^{\exp}\delta_{ij} + \Sigma_{ij}^{\mathrm{th}}.$$

And our correlated likelihood is now

$$\mathrm{pr}(\vec{\mathrm{y}}\,|\,\vec{\mathrm{a}}, \mathrm{I}) \propto \mathrm{e}^{-\left(\vec{\mathrm{y}}_{\exp} - \vec{\mathrm{y}}_{\mathrm{th}}\right)^{\mathrm{T}}\Sigma^{-1}\left(\vec{\mathrm{y}}_{\exp} - \vec{\mathrm{y}}_{\mathrm{th}}\right)} = \mathrm{e}^{-\mathrm{d}_{\mathrm{M}}(\vec{\mathrm{a}})}$$

where we define the Mahalanobis distance

$$d_M(\vec{a}) = \left(\vec{y}_{\exp} - \vec{y}_{\mathrm{th}}\right)^{\mathrm{T}} \Sigma^{-1} \left(\vec{y}_{\exp} - \vec{y}_{\mathrm{th}}\right).$$

Additional Parameters

In this process, we have introduced two new parameters: $\bar{c}$ and Λ_b.

This changes the posterior we need to find:

$$\underbrace{\mathrm{pr}(\vec{a}, \bar{c}^2, \Lambda_b \,|\, \vec{y}_{exp}, I)}_{\text{Total posterior}} \propto \underbrace{\mathrm{pr}(\vec{y}_{exp} \,|\, \vec{a}, \Sigma, I)}_{\text{Likelihood for } \vec{a}} \; \underbrace{\mathrm{pr}(\vec{a} \,|\, I)}_{\text{Prior for } \vec{a}} \; \underbrace{\mathrm{pr}(\bar{c}^2 \,|\, \Lambda_b, \vec{a}, I)}_{\text{Posterior for } \bar{c}^2} \; \underbrace{\mathrm{pr}(\Lambda_b \,|\, \vec{a}, I)}_{\text{Posterior for } \Lambda_b} \;.$$

We can find a closed form of $\mathrm{pr}(\bar{c}^2 \,|\, \Lambda_b, \vec{a}, I)$ and $\mathrm{pr}(\Lambda_b \,|\, \vec{a}, I)$.

*J. A. Melendez et. al. Phys. Rev. C **100**, 044001

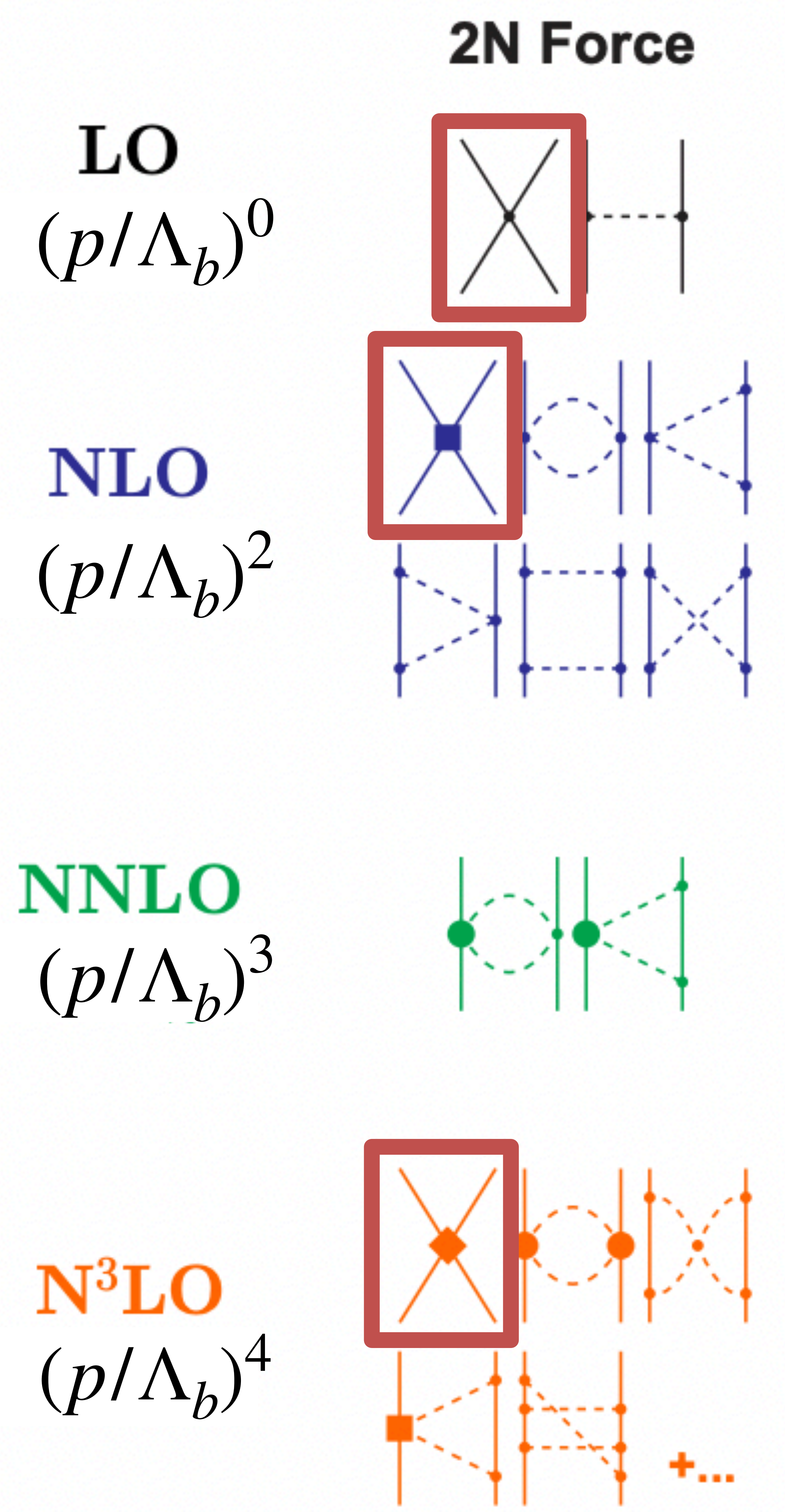
Pionless EFT

We are working in an EFT framework without pions in Weinberg PC

Our interaction takes the form:

$$v_{\mathrm{LO}} = C_S + C_T \sigma_1 \cdot \sigma_2$$

$$v^{\mathrm{CI}}_{\mathrm{NLO}}(\vec{k}, \vec{K}) = C_1 k^2 + C_2 k^2 \sigma_1 \cdot \sigma_2 + C_3 S_{12}(k) + C_4 k^2 \tau_1 \cdot \tau_2$$
$$+ i C_5 \vec{S} \cdot (\vec{K} \times \vec{k}) + C_6 k^2 \tau_1 \cdot \tau_2 \sigma_1 \cdot \sigma_2 + C_7 S_{12}(k) \tau_2 \cdot \tau_2$$
$$v^{\mathrm{CD}}_{\mathrm{NLO}} = C_0^{\mathrm{IT}} T_{12} + C_0^{\mathrm{IV}} (\tau_{1z} + \tau_{2z})$$



Regularization

To use these interactions, they must be regularized in some fashion and must be local in coordinate space (for QMC).

We employ a Gaussian cutoff in coordinate space, which smears δ-functions upon Fourier transformation

$$f(r) = \frac{1}{\pi^{3/2} R_s^3} e^{-\left(\frac{r}{R_s}\right)^2}$$

We choose $R_s \in [1.5, 2.0, 2.5]$ fm which are ~$\frac{400}{R_s} \sim [270, 200, 160]\,\mathrm{MeV}$ in momentum space.

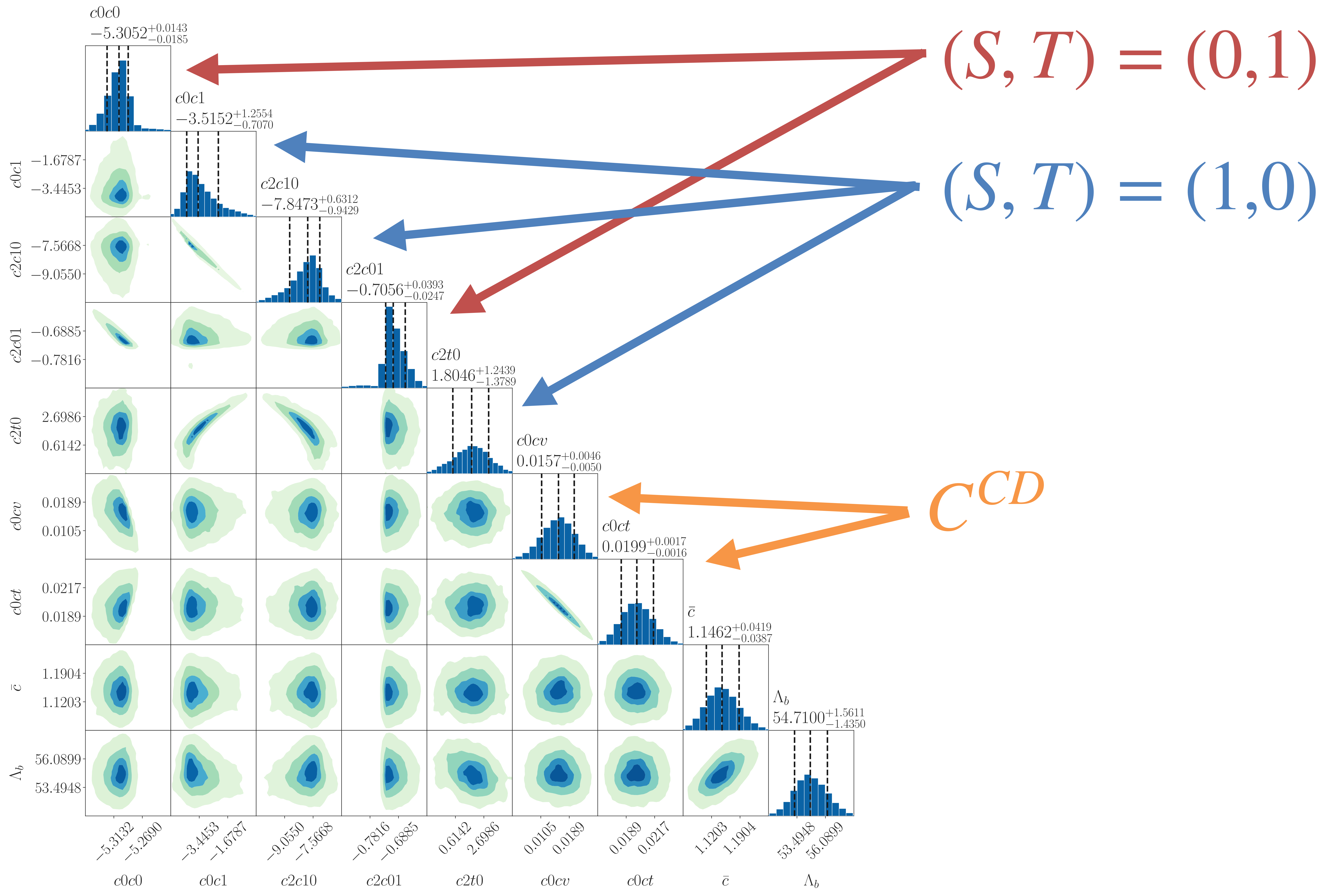
Parameter Estimation Algorithm

To estimate all of these parameters, we need data to calibrate to:

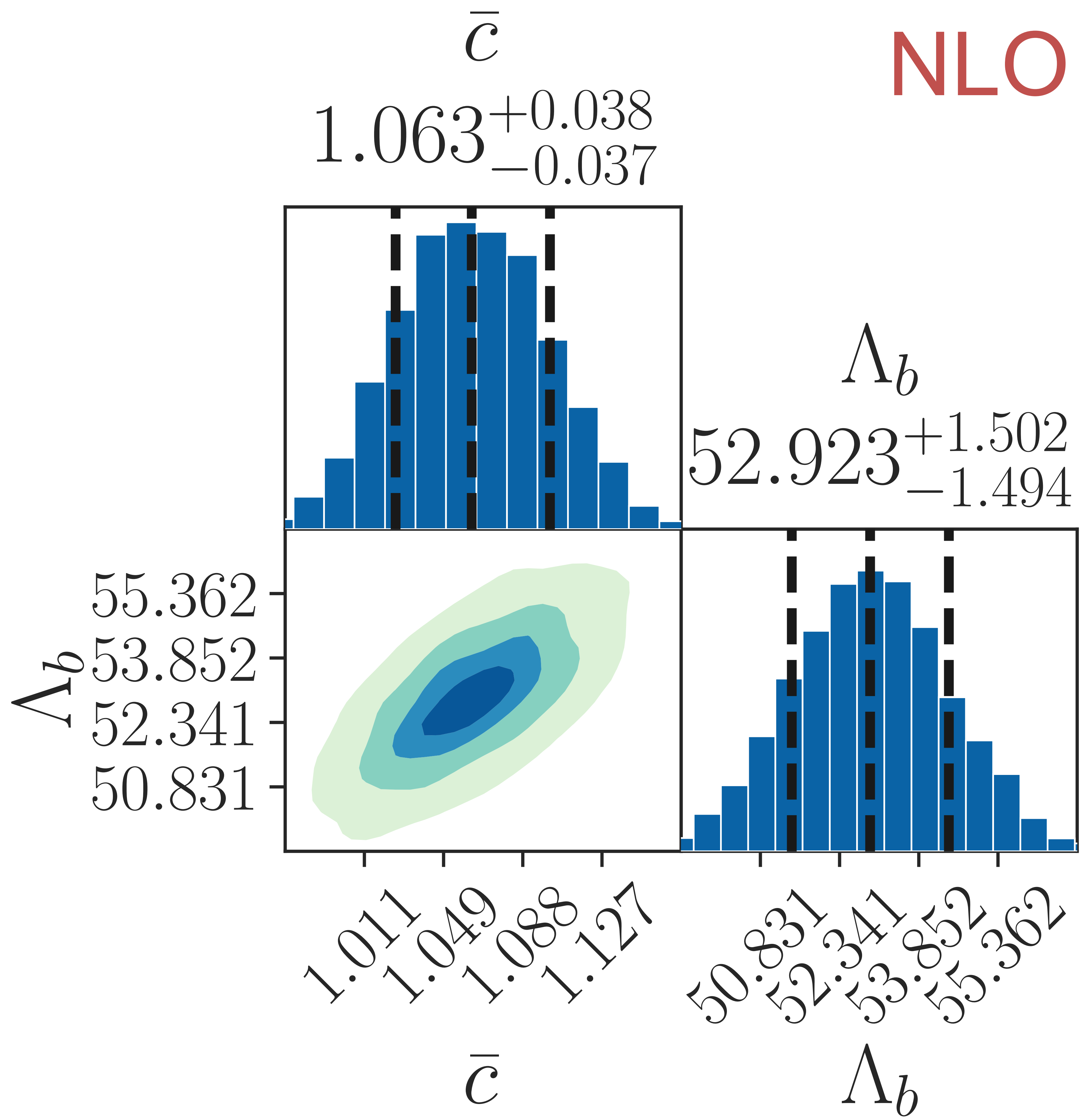
Our choice of data is the pp and np Granada database (differential cross sections, total cross sections) up to 5 MeV + deuteron binding energy + nn scattering length. Not phase shifts!

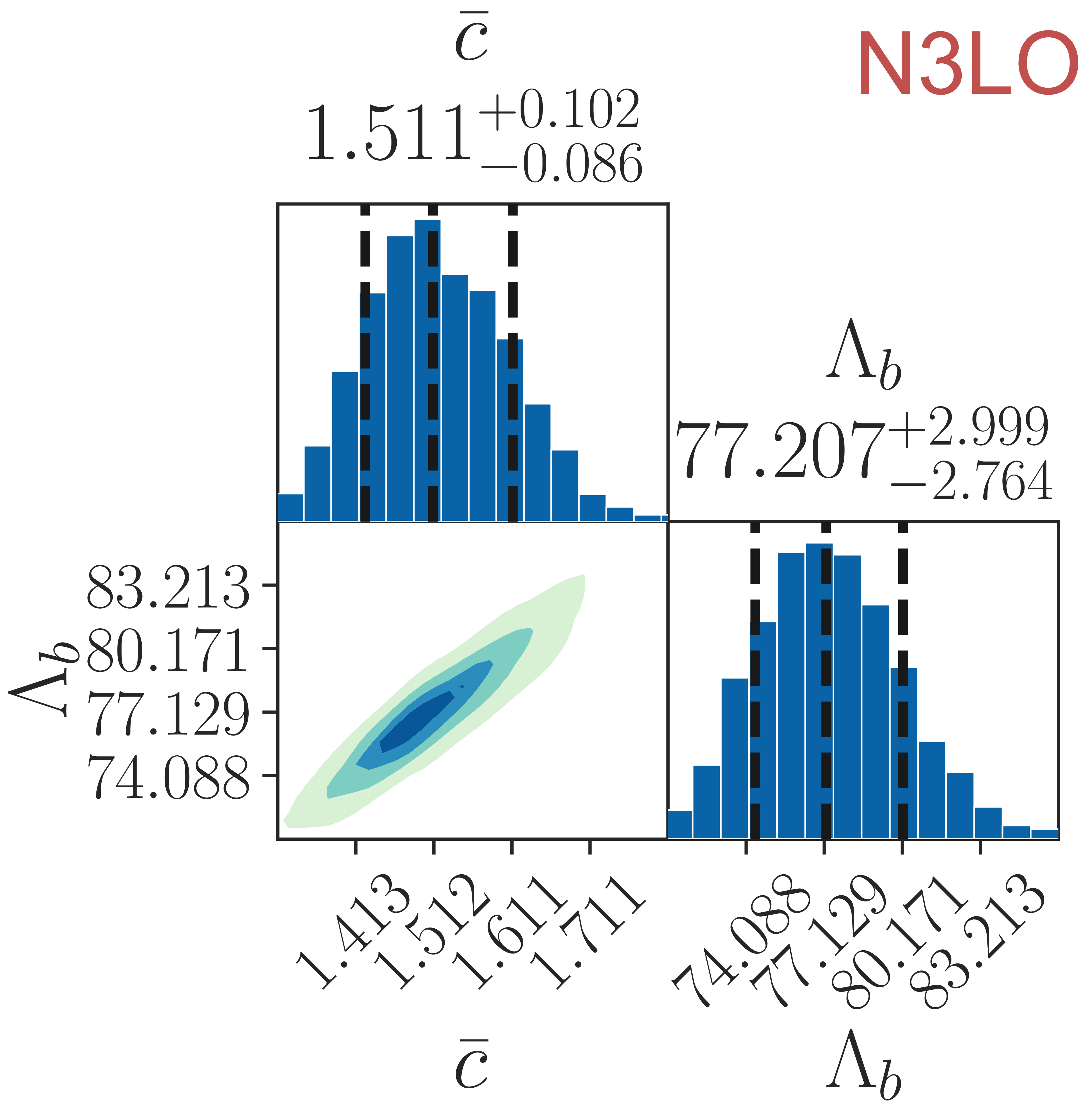
We then use Markov Chain Monte Carlo (MCMC) to sample the posteriors at LO $\left(Q^0\right)$, NLO $\left(Q^2\right)$, and N3LO $\left(Q^4\right)$, allowing for the order-by-order convergence analysis for LO→NLO and NLO→N3LO to estimate $\bar{c}$ and Λ_b.

NLO Posterior

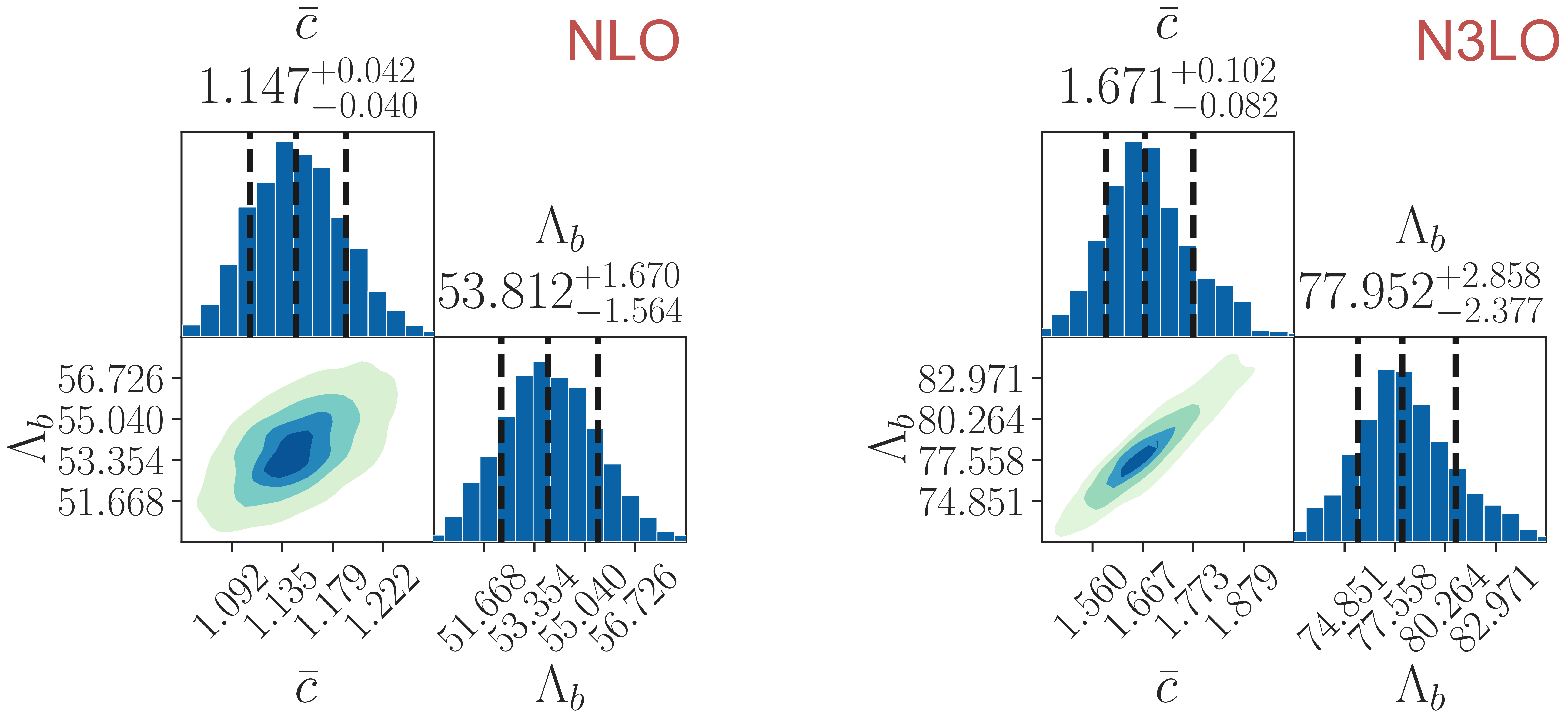


2.5 fm $\bar{c}$ and Λ_b Posteriors

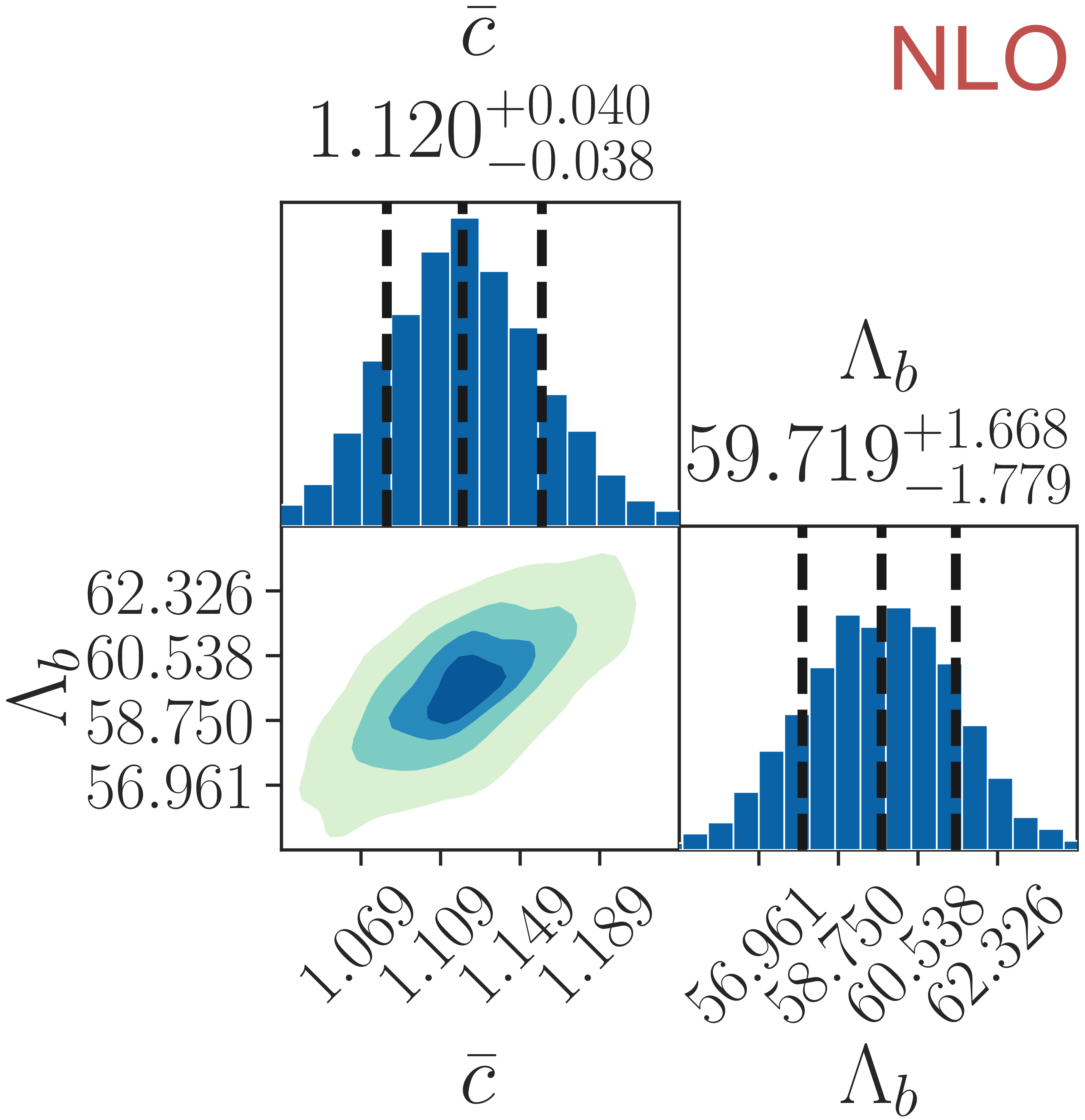


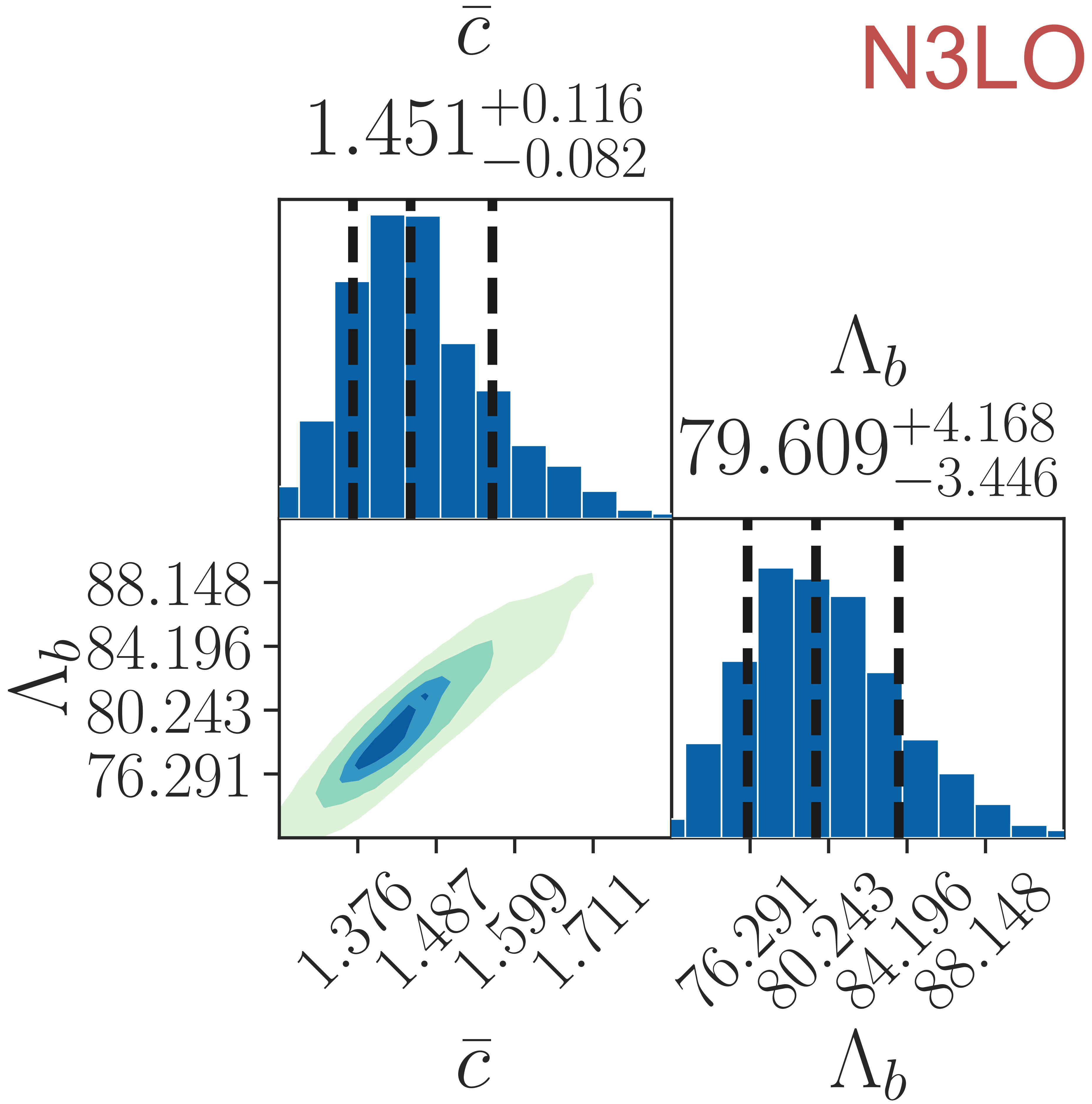


2.0 fm $\bar{c}$ and Λ_b Posteriors

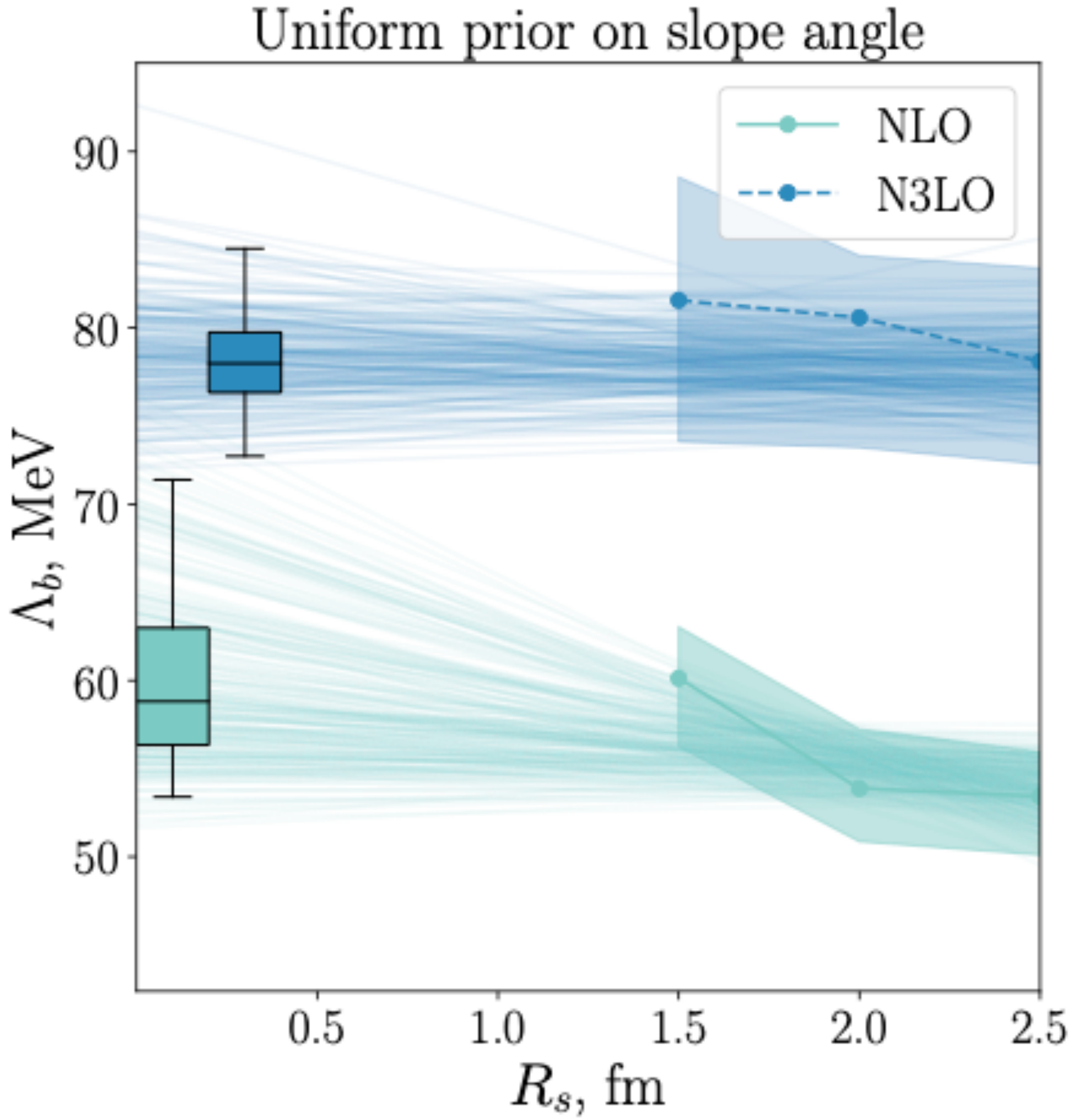


1.5 fm $\bar{c}$ and Λ_b Posteriors





Extrapolation to Remove Artifacts



Why is there dependence on the order?

- Power counting?
- Flawed assumption of geometric series?
- ~~Fierz transformation breaking?~~

Unconstrained p-waves

With Λ_b~50 MeV, the max lab energy is given by

$$\frac{p_{\text{c.m.}}^{(max)}}{\Lambda_b} = \frac{\sqrt{E_{\text{lab}}^{(max)}\mu}}{\Lambda_b} = 1 \Rightarrow E_{\text{lab}}^{(max)} = \frac{\Lambda_b^2}{\mu} \sim 5 \text{ MeV}$$

The Granada database has 4 data (polarized cross sections) up to 5 MeV that constrains ${}^1P_1$ and ${}^3P_0$ channels.

Thus the pionless models are constrained predominantly in s-waves, in agreement with expectations.

Posterior Predictive Density

We can now easily and rigorously propagate uncertainty to observable calculations.

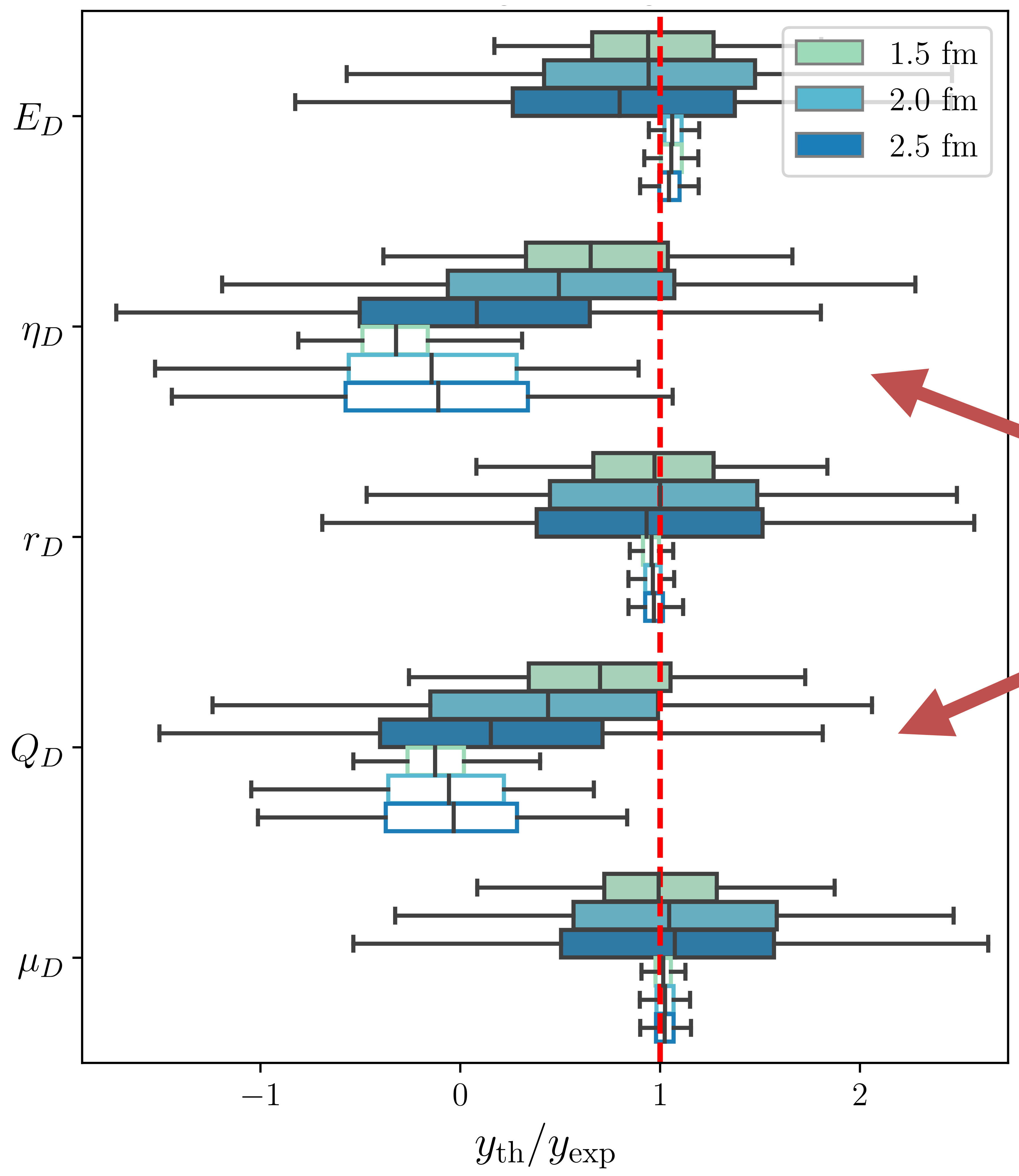
We calculate a posterior predictive distribution (p.p.d.) for the observables

$$\mathrm{pr}(\vec{y}_{\mathrm{th}} \,|\, \vec{y}, \vec{x}, I) = \int d\vec{a}\, d\bar{c}^2\, d\Lambda_b\, \mathcal{N}\left(\vec{y}_{\mathrm{th}}, \Sigma_{\mathrm{th}}\right) \mathrm{pr}(\vec{\mathrm{a}}, \bar{\mathrm{c}}^2, \Lambda_{\mathrm{b}} \,|\, \vec{\mathrm{y}}_{\mathrm{exp}}, \mathrm{I})$$

which is done via sampling the posterior.

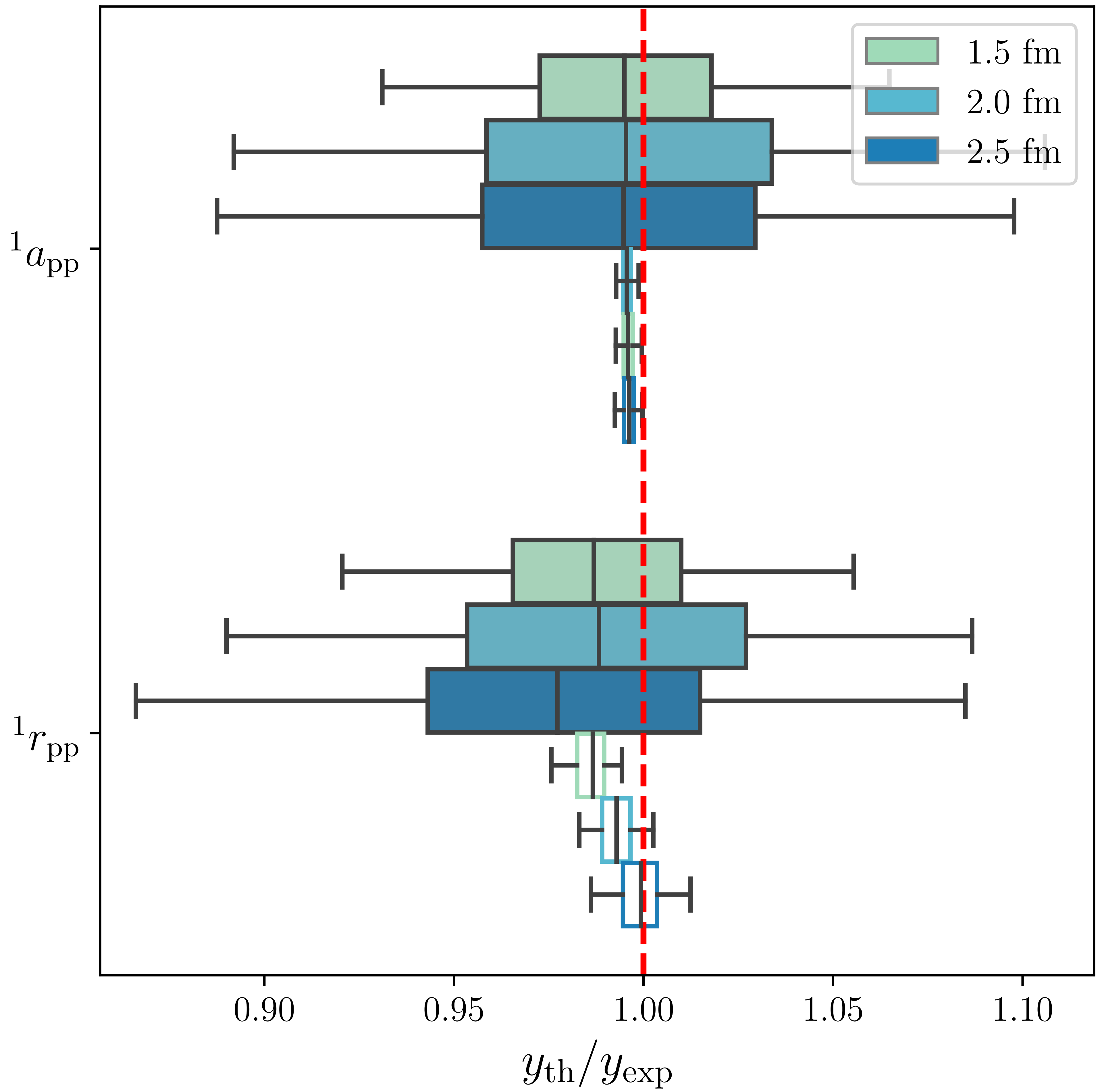
This can be done for **any** calculation of nuclear observables.

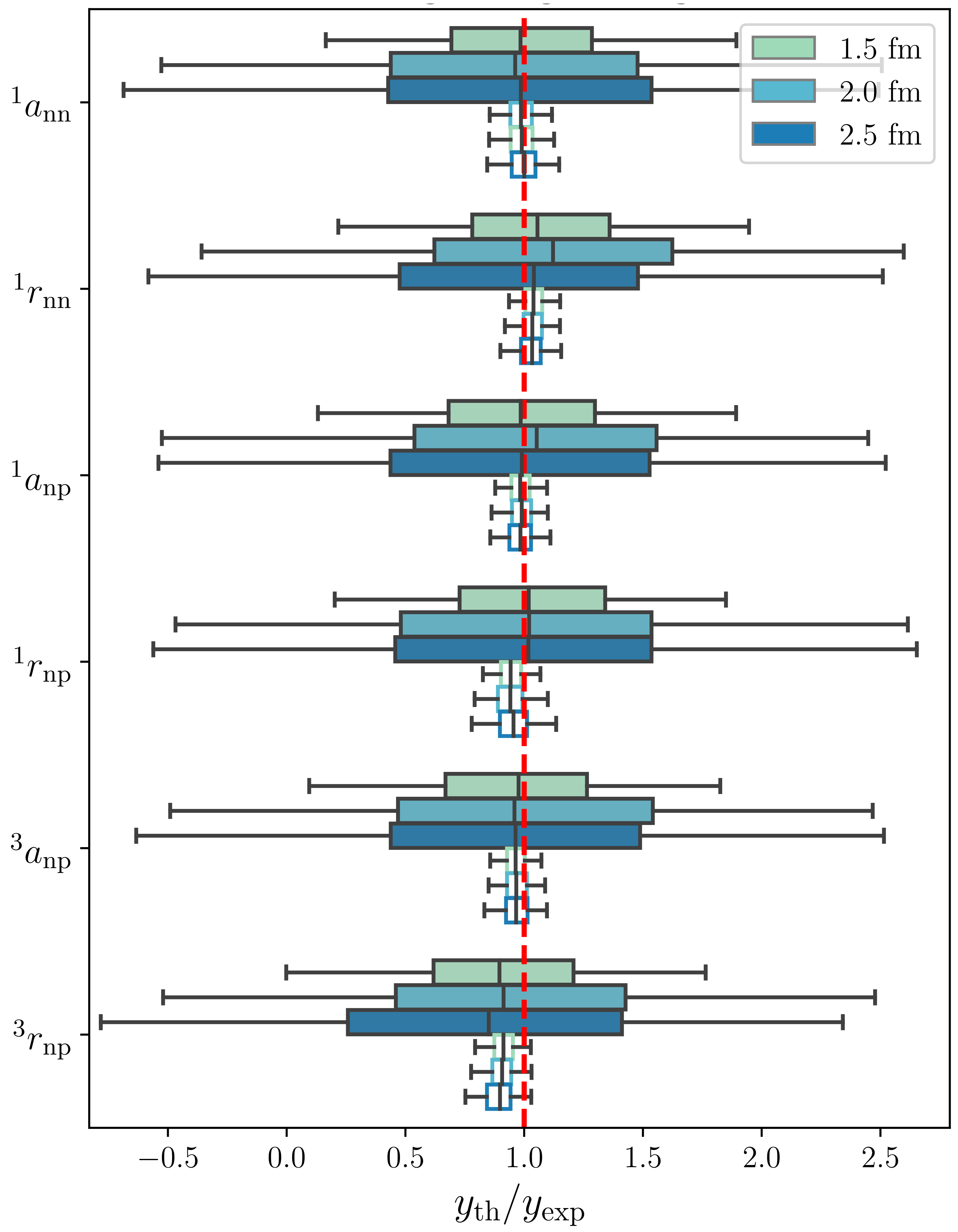
Propagation of Errors for Deuteron



- Poorly constrained d-waves
- 2b corrections at $O(Q^5)$

Propagation of Errors for ERPs





Long-term Goals

~10^5 parallel sample steps at ~4 min. per step

→280 days of wall time on an HPC

- For pion- and Δ-full interactions, we must look at higher energy data (~200 MeV)
- Emulation for calculation of scattering observables

Ozge Surer
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LBNL

Matt Plumlee
Amazon

Pablo Giuliani
MSU/FRIB

Daniel Odell
SRNL

Gaussian Process Emulation

Reduced Basis Methods via Galerkin Projection

Open Questions

- Application to different power counting
- Application to few- and many-body observables
  - How do we generate ppds using expensive many-body methods?
  - Estimation of the momentum to treat model discrepancy?

- Model mixing EFT model
  - Across degrees-of-freedom
  - Cutoffs
  - Regulators

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BAND Bayesian Analysis of Nuclear Dynamics

Jason Bub
Graduate Student

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Backup Slides

Posterior for $\bar{c}$

Since we had $c_n \,|\, \bar{c} \sim \mathcal{N}\left(0, \bar{c}^2\right)$, where $\bar{c}^2$ is a population variance, we make the standard choice of prior for an unknown variance:

$$\bar{c}^2 \sim \chi^{-2}\left(\nu_0, \tau_0^2\right)$$

This yields a conjugate posterior

$$\mathrm{pr}(\bar{\mathrm{c}}^2 \,|\, \mathrm{I}) \sim \chi^{-2}(\nu_0, \tau_0^2) \iff \mathrm{pr}(\bar{\mathrm{c}}^2 \,|\, \vec{\mathrm{a}}, \Lambda_\mathrm{b}, \mathrm{I}) \sim \chi^{-2}\left(\nu, \tau^2(\vec{\mathrm{a}}, \Lambda_\mathrm{b})\right).$$

Where we have hyperparameters:

$$\nu = \nu_0 + N_{\mathrm{obs}} n_{\mathrm{orders}}, \text{ degrees of freedom} \qquad c_{n,i} = \frac{y_i^n - y_i^{(n-1)}}{y_{\mathrm{ref},i}\, Q_i^n}$$

$$\tau^2\left(\vec{a}, \Lambda_b\right) = \frac{1}{\nu}\left(\nu_0 \tau_0 + \sum_{i,n} c_{n,i}^2(\vec{a}, \Lambda_b)\right), \text{ scale}$$

*J. A. Melendez et. al. Phys. Rev. C **100**, 044001

Posterior for Λ_b

Our posterior for the breakdown scale also uses these hyperparameters:

$$\mathrm{pr}(\Lambda_b \,|\, \vec{a}, I) \propto \frac{\mathrm{pr}(\Lambda_b \,|\, I)}{\tau^{\nu} \prod_{n,i} \left(\frac{p_i}{\Lambda_b} \right)^{n}}$$

This posterior needs to be numerically normalized as the normalization constant is dependent on $\vec{a}$.

With all our components, we can estimate our parameters.

Prior Choices

- $\mathrm{pr}(\vec{\mathrm{a}}\,|\,\mathrm{I}) \sim \mathcal{N}\left(\vec{\mathrm{a}}^{\mathrm{MAP}}_{\mathrm{p.s}}, \overrightarrow{10^2}\right)$
- $\mathrm{pr}(\Lambda_{\mathrm{b}}\,|\,\mathrm{I}) \sim \mathcal{N}\left(500\ \text{MeV}, 1000^2\ \text{MeV}\right)$
- $\mathrm{pr}(\bar{\mathrm{c}}^2\,|\,\mathrm{I}) \sim \chi^{-2}(\nu_0 = 1.5, \tau_0^2 = 1.5^2)$
- $r(x_i, x_j; \vec{l}) = e^{|p_i - p_j|/2l_p} e^{|\theta_i - \theta_j|/2l_\theta} \delta_{\mathrm{type}_i, \mathrm{type}_j}, \quad l_p = 0.3\ \text{MeV}, l_\theta = 20°$
- $p_{\mathrm{soft}} = \begin{cases} p_d \sim 45\ \text{MeV}/c, & \text{for } np \text{ and } nn \text{ scattering} \\ 1/{}^1a_{\mathrm{pp}} \sim 25\ \text{MeV}, & \text{for } pp \text{ scattering}. \end{cases}$