Certainifying Uncertainty:

Bayesian parameter and truncation error estimation in EFTs

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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

This must be accomplished in the model calibration.

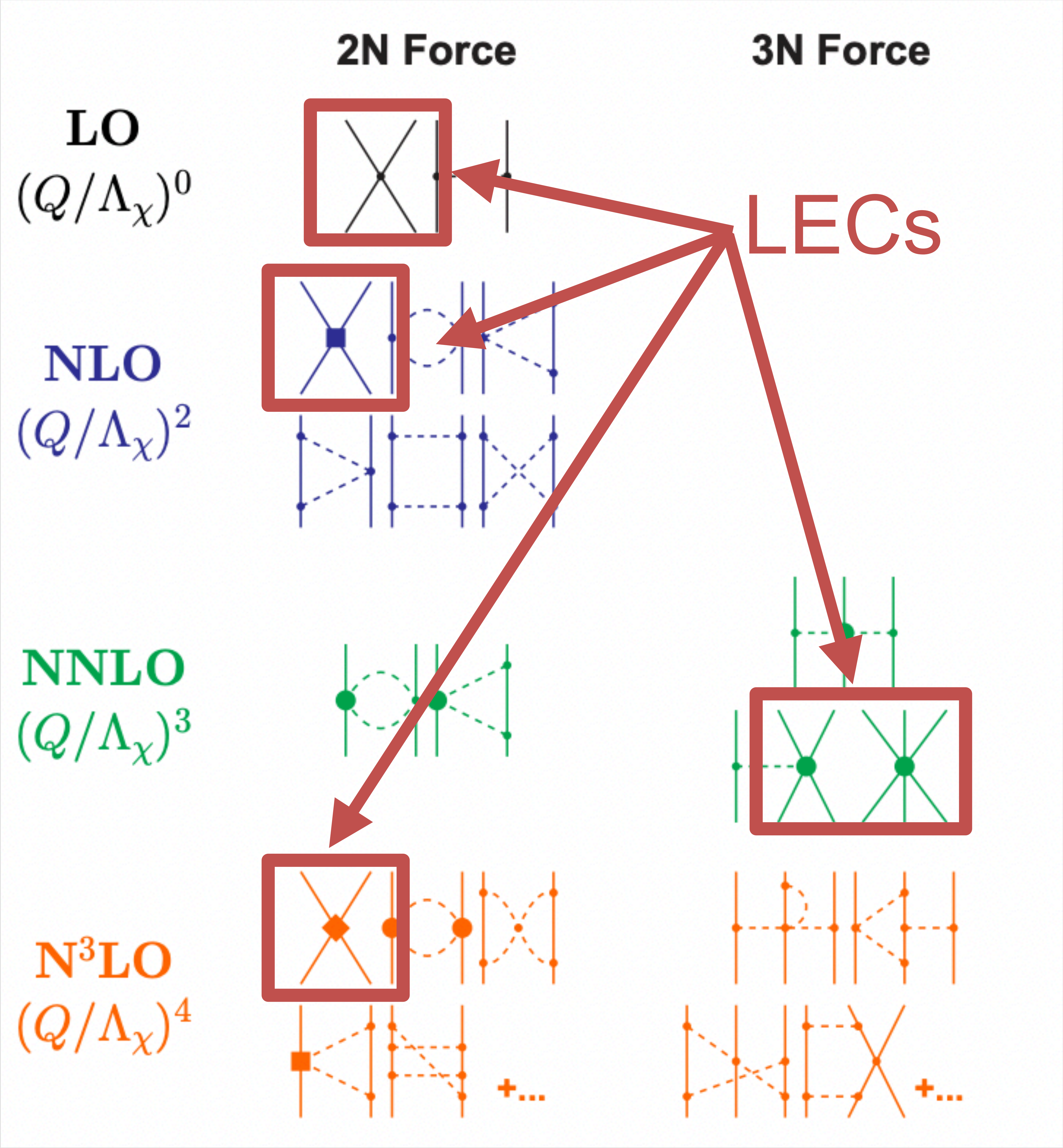
Effective Field Theory

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_χ

- p is a momentum or pion mass
- Λ_χ 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 take the form it uses in normal model fitting

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

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?

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

Theory Uncertainty in Calibration

Why are theory errors necessary in calibration?

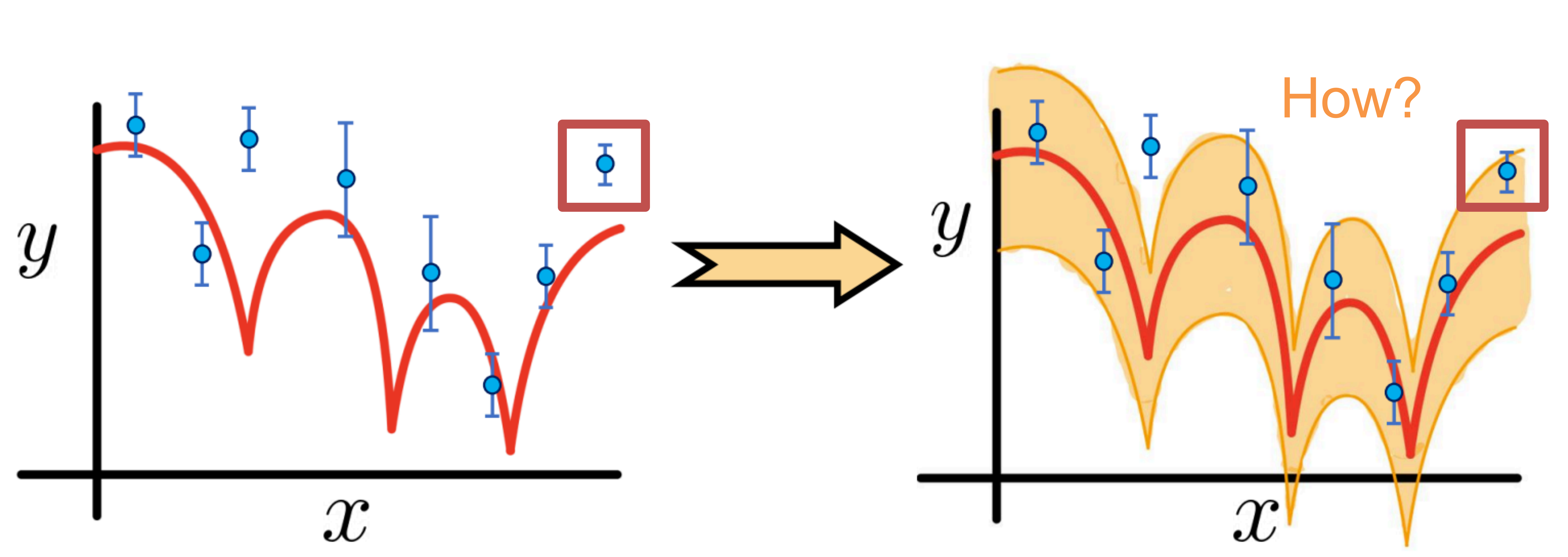


Figure courtesy of Pablo Giuliani

Modeling the Model

Since our model is a perturbative series, we can model it as such*:

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

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

This series follows the truncation scheme of the EFT:

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

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

Truncation Errors

From the neglected terms, we have

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

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,

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

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

Correlated Likelihood

We can build a total covariance,

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

And our correlated likelihood is now

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

where we define the Mahalanobis distance

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

Correlated version of χ^2

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 $\mathrm{pr}(\Lambda_b \,|\, \vec{a}, I)$.

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

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

Where we have hyperparameters:

$$\nu = \nu_0 + N_\mathrm{obs} n_\mathrm{orders}, \text{ degrees of freedom}$$

$$c_{n,i} = \frac{y_i^n - y_i^{(n-1)}}{y_{\mathrm{ref},i} Q_i^n}$$

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

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

Posterior for Λ_b

Our posterior for the breakdown scale also uses these hyperparameters:

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

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.

Pionless EFT

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

Our interaction takes the form:

$$y_{\text{th}}(x) = \sout{y_{\text{ref}}(x)} \sum_{n=0}^{\infty} c_{2n}(x) Q^{2n}(x)$$

$y_{\text{exp}}(x)$

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

$$v_{\text{NLO}}^{\text{CI}}(\vec{k}, \vec{K}) = C_1 k^2 + C_2 k^2 \sigma_1 \cdot \sigma_2 + C_3 S_{12}(k) + C_4 k^2 \tau_1 \cdot \tau_2$$
$$+ i C_5 \vec{S} \cdot (\vec{K} \times \vec{k}) + C_6 k^2 \tau_1 \cdot \tau_2 \sigma_1 \cdot \sigma_2 + C_7 S_{12}(k) \tau_2 \cdot \tau_2$$

$$v_{\text{NLO}}^{\text{CD}} = C_0^{\text{IT}} T_{12} + C_0^{\text{IV}} (\tau_{1z} + \tau_{2z})$$

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 $\sim \frac{400}{R_s}$ MeV in momentum space.

Parameter Estimation Algorithm

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

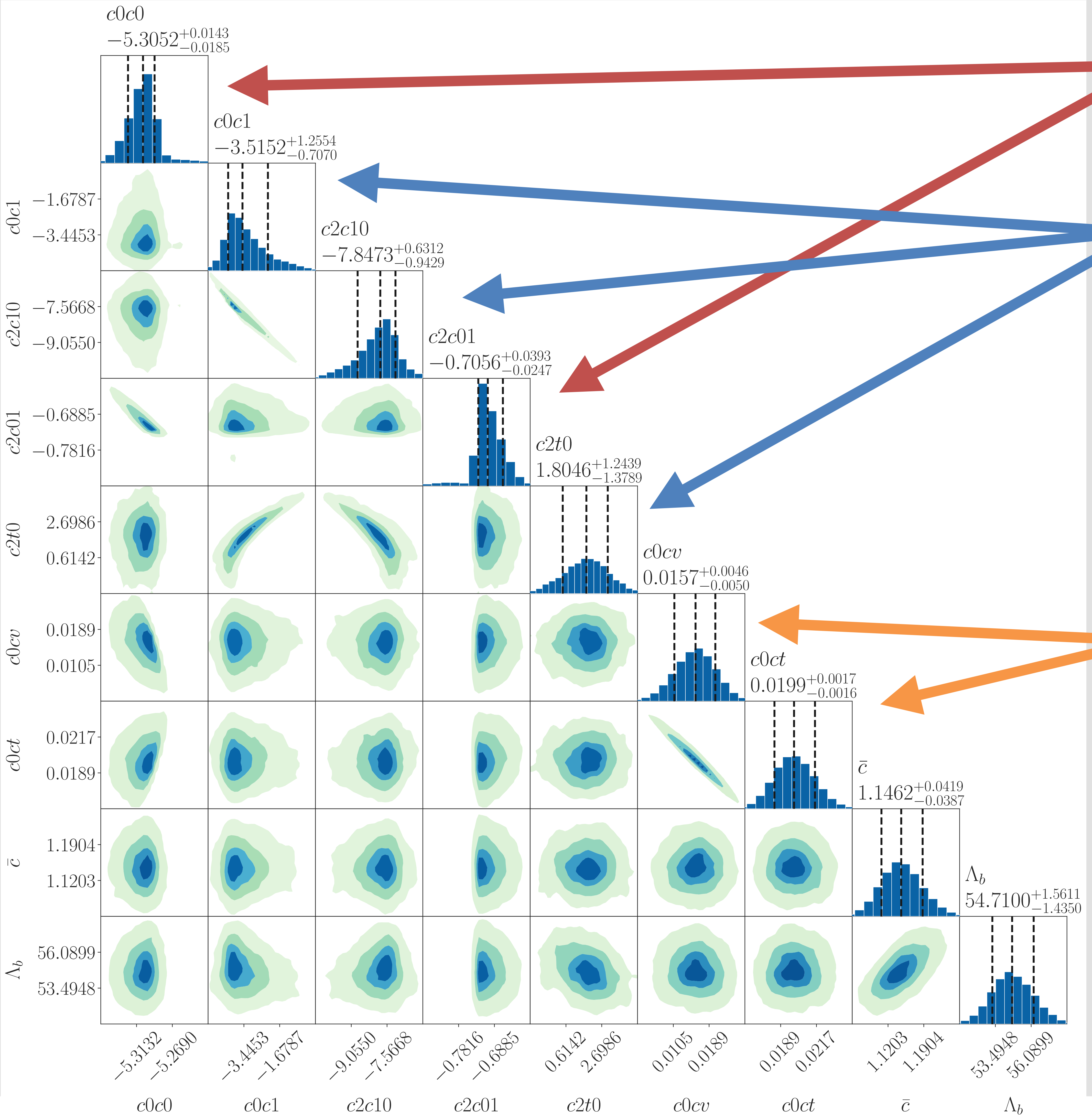
Our choice of data is the pp and np Granada database (differential cross sections, total cross sections) up to 5 MeV + deuteron binding energy + nn scattering length.

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.

Prior Choices

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

NLO Posterior

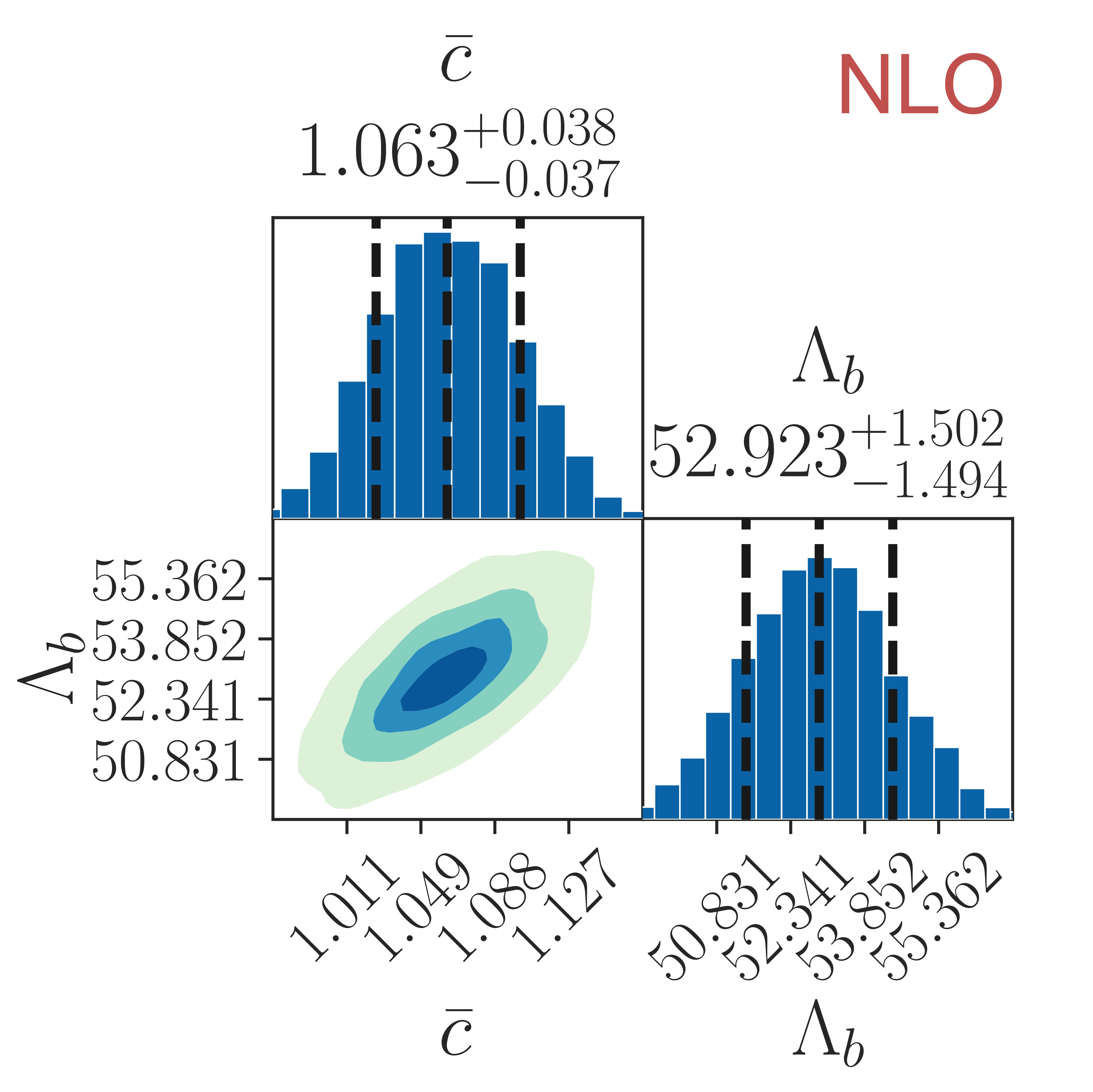


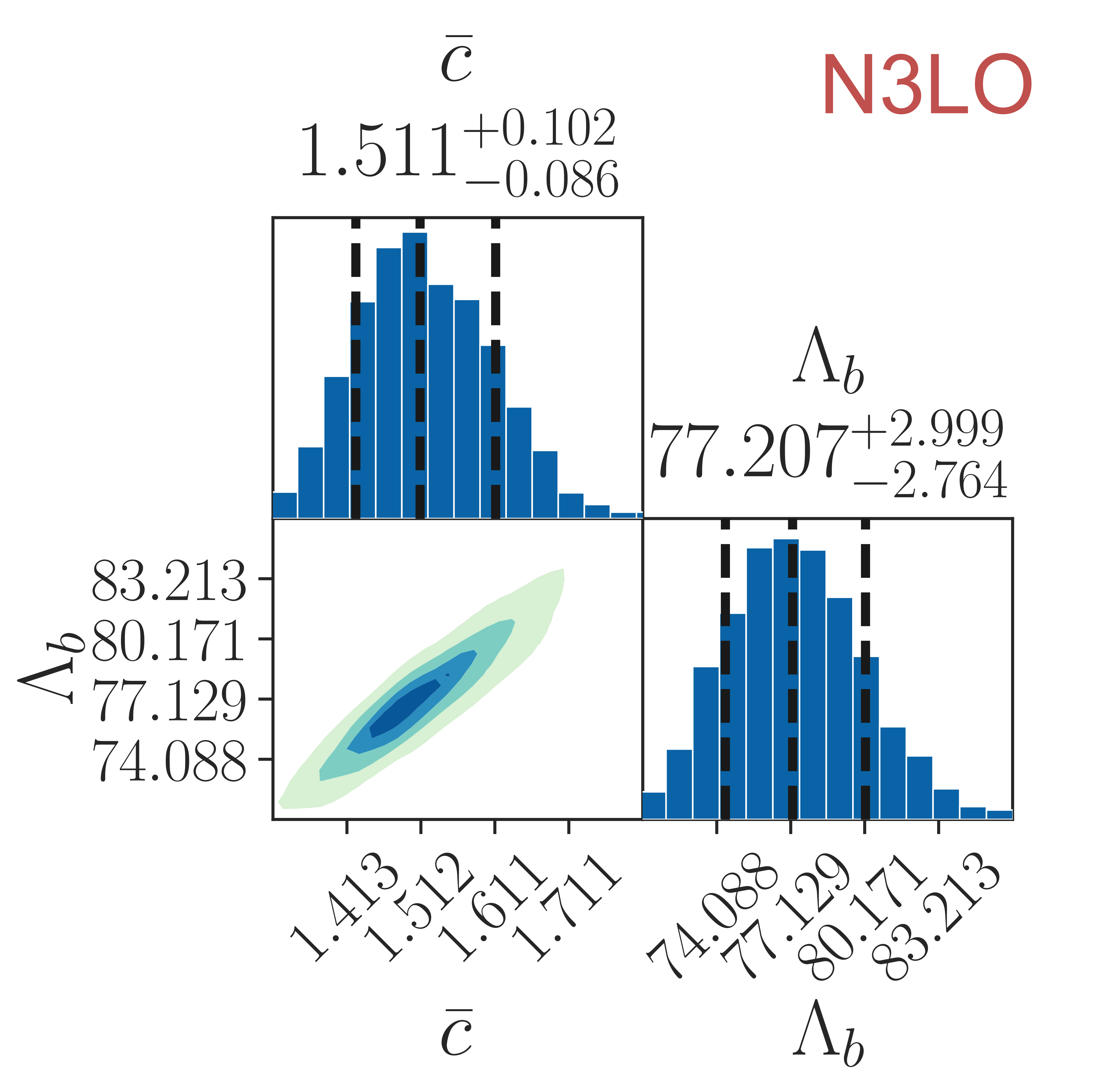
$(S, T) = (0,1)$

$(S, T) = (1,0)$

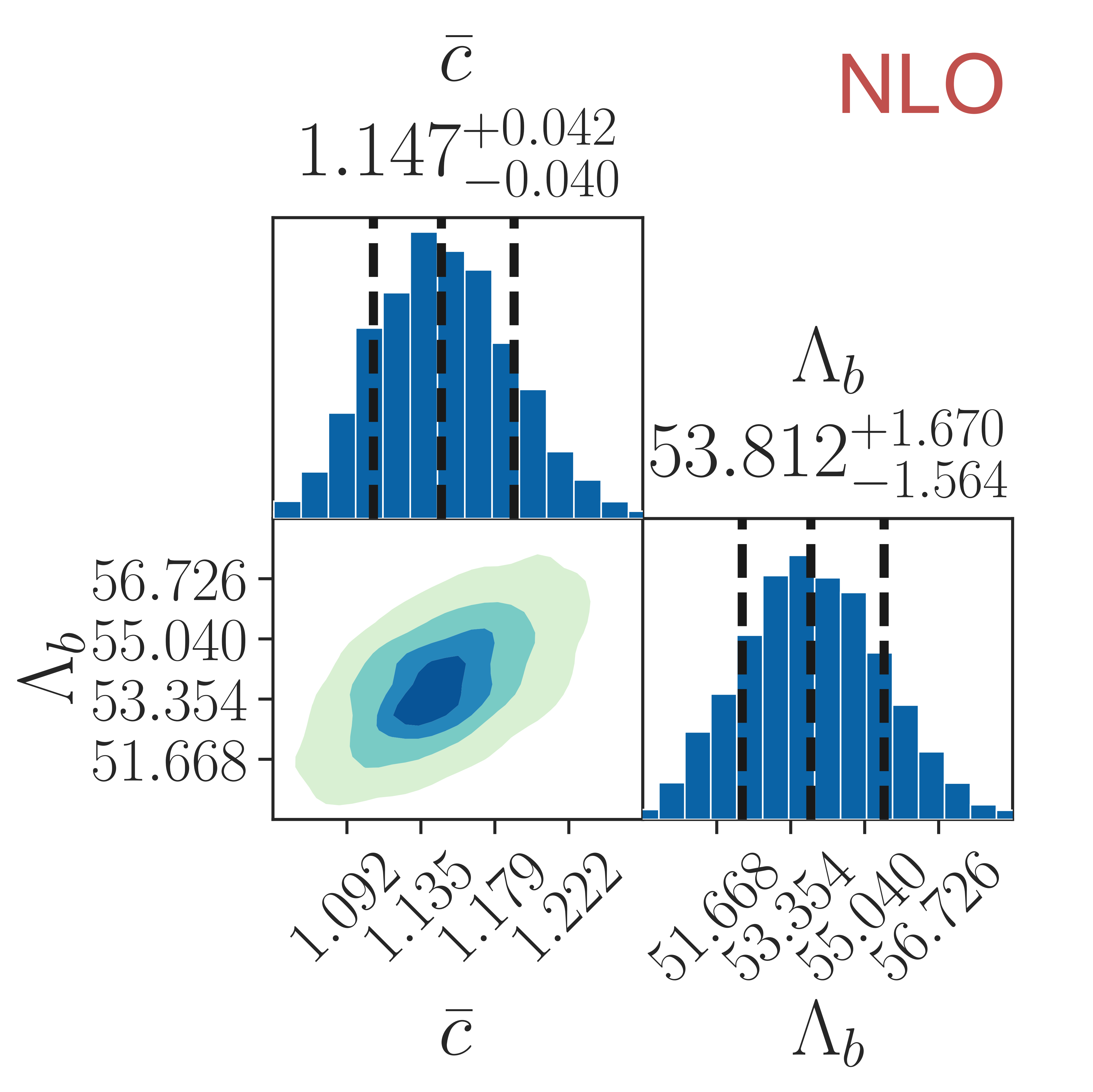
C^{CD}

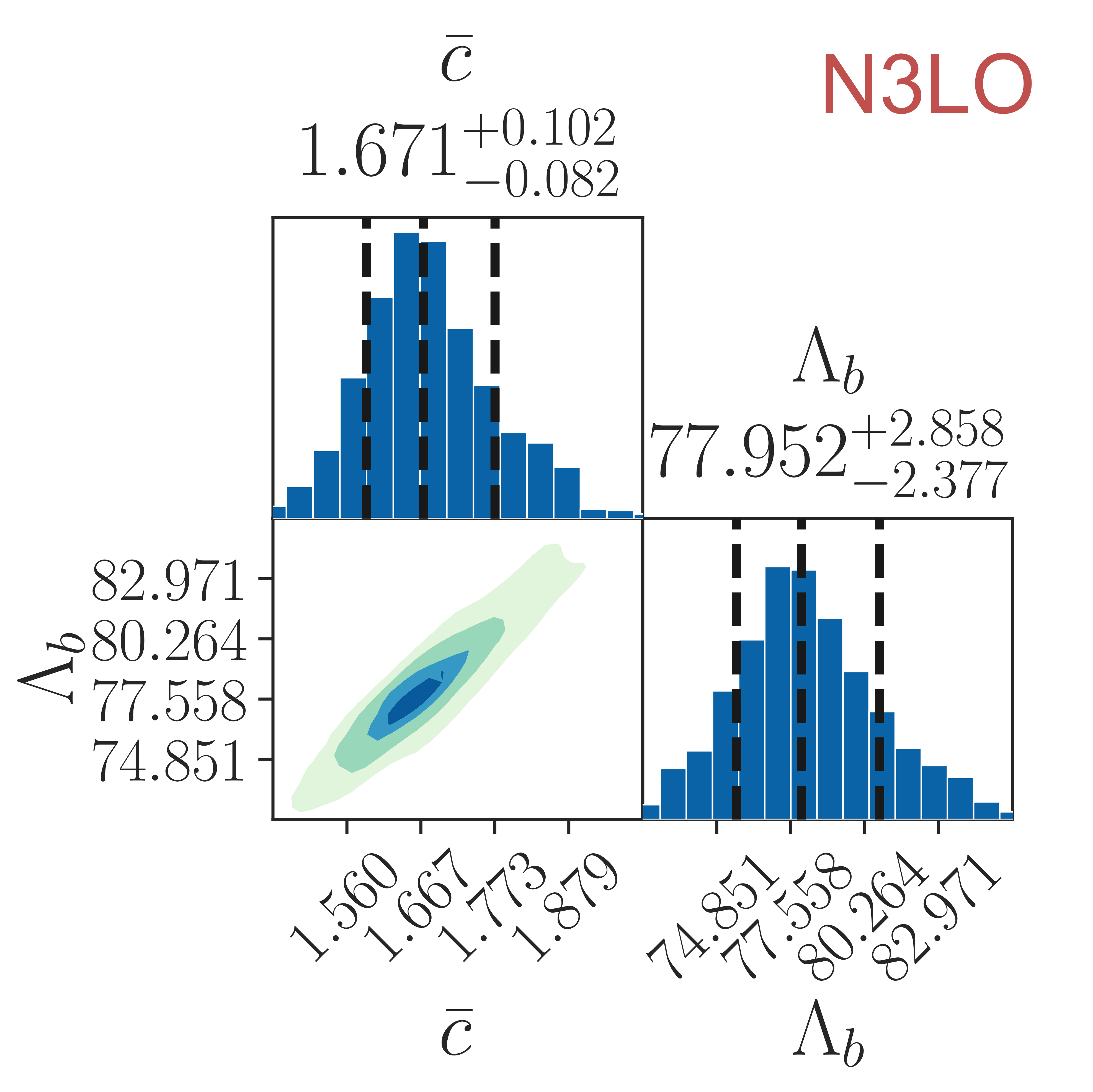
2.5 fm $\bar{c}$ and Λ_b Posteriors



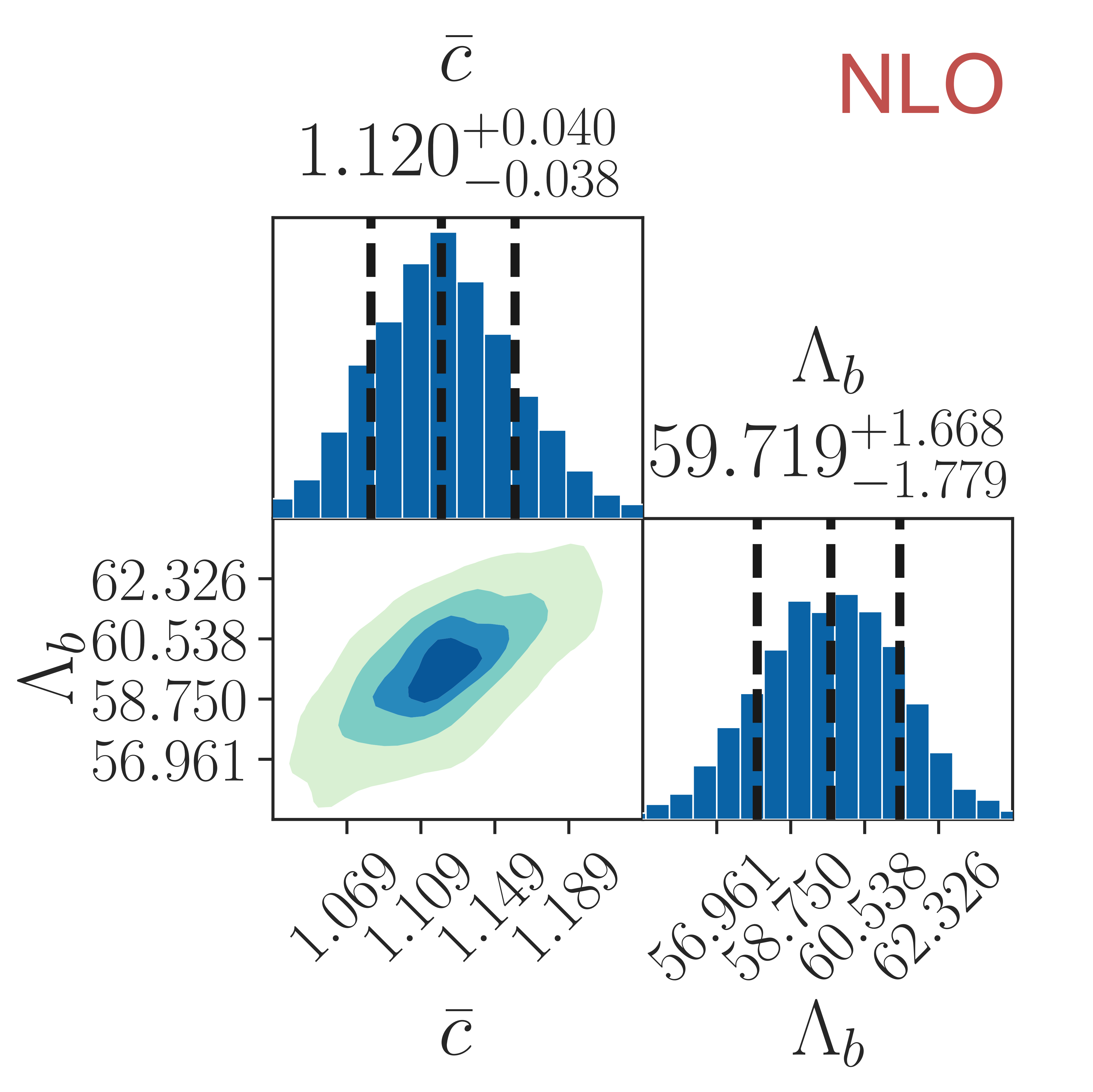


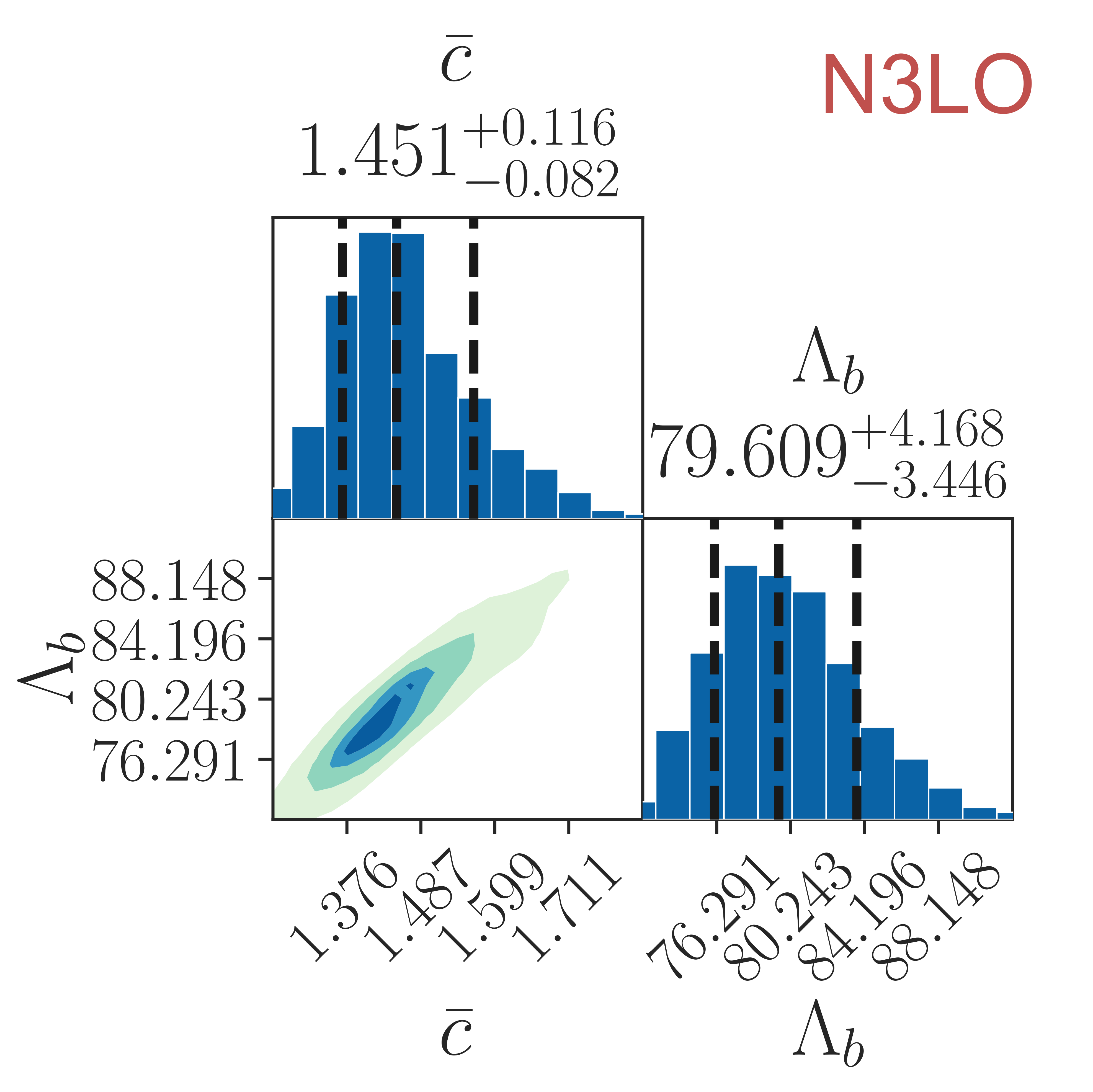
2.0 fm $\bar{c}$ and Λ_b Posteriors



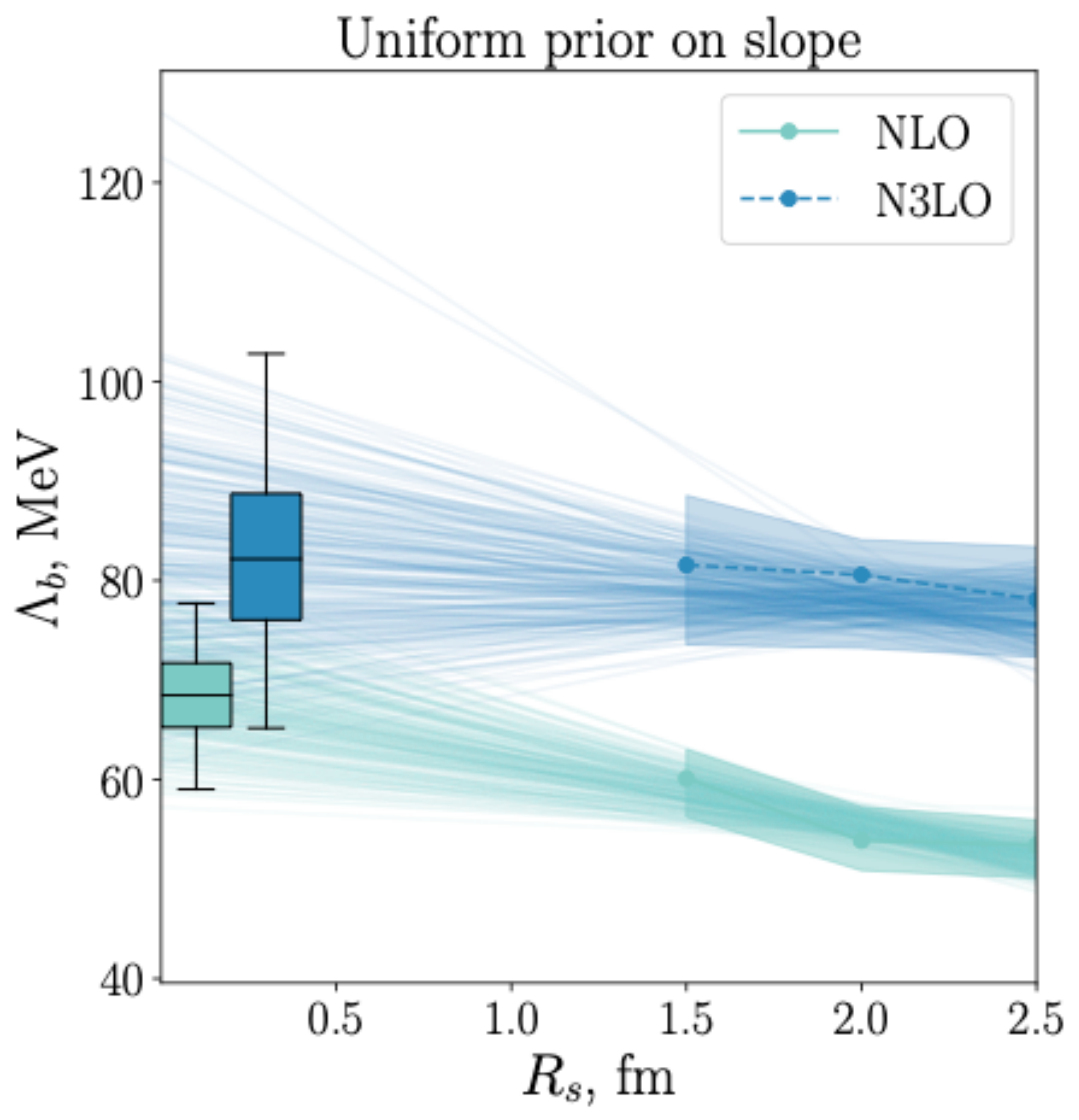


1.5 fm $\bar{c}$ and Λ_b Posteriors





Extrapolation to Remove Artifacts

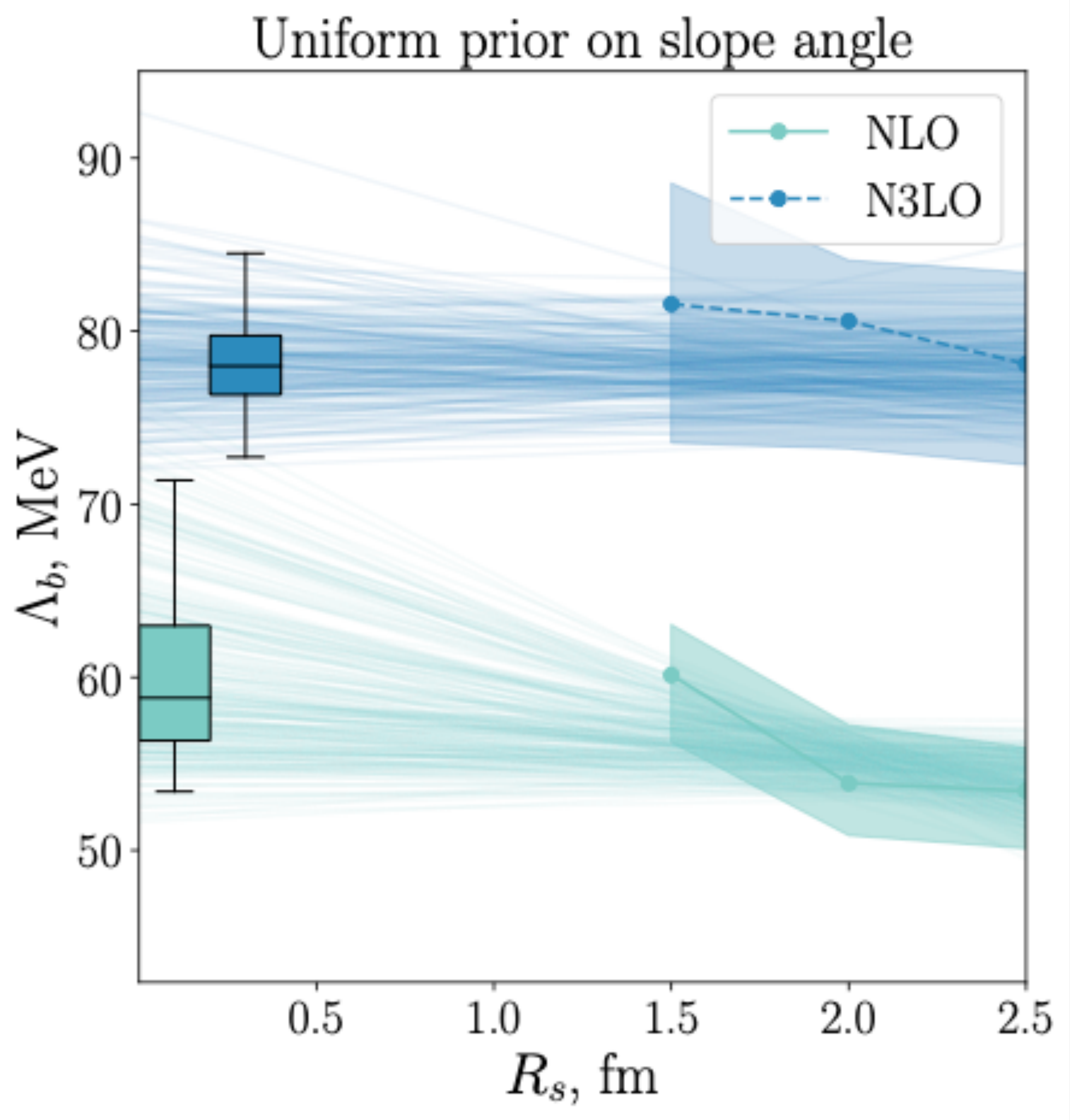


Why is there dependence on the order?

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

Extrapolation to Remove Artifacts

Proper choice of prior!!!



Why is there dependence on the order?

- Power counting?
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- ~~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.

We can explore removing p-wave interactions from our models.

Posterior Predictive Density

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

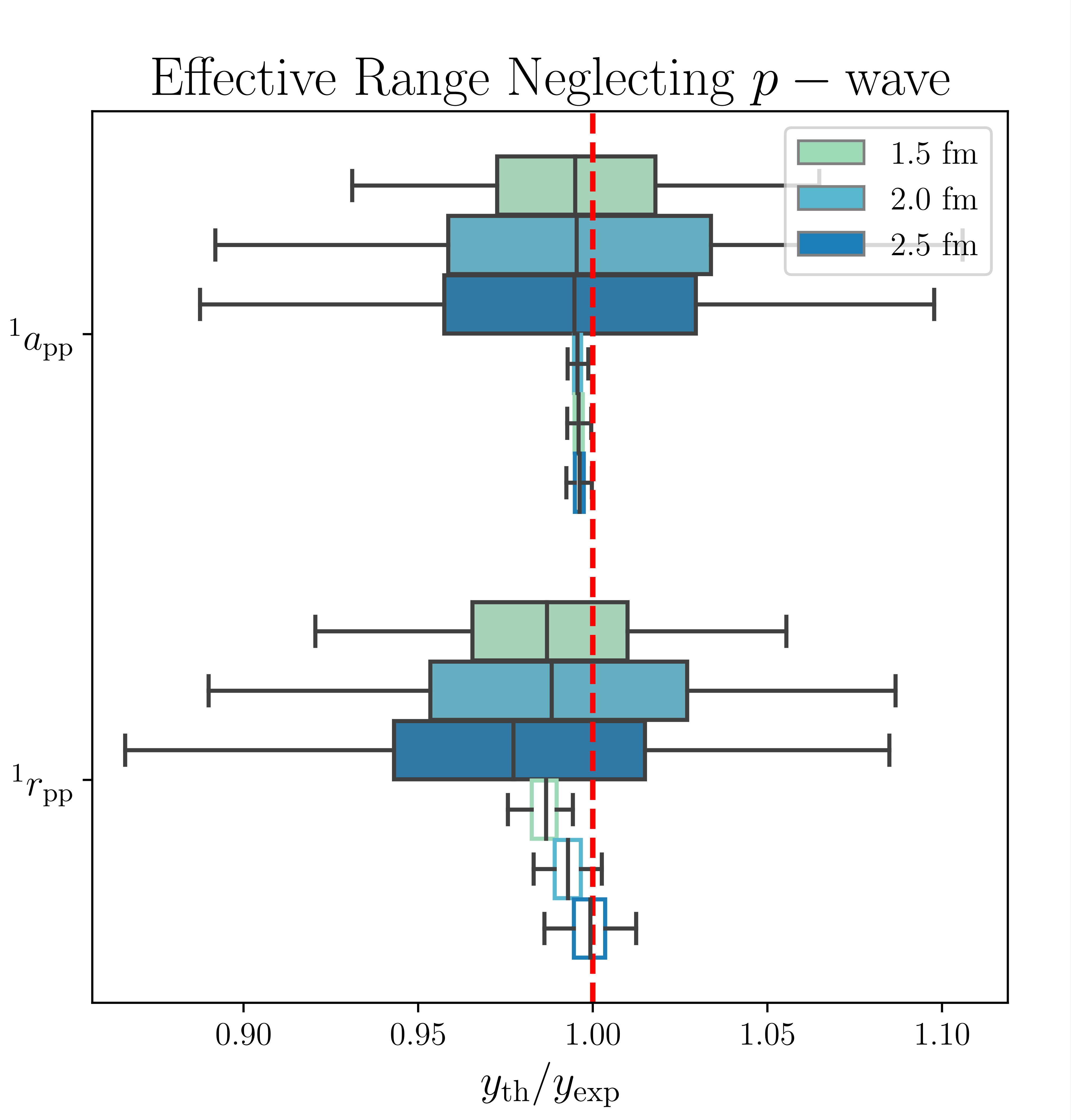
We calculate a posterior predictive distribution (p.p.d.) for the observables

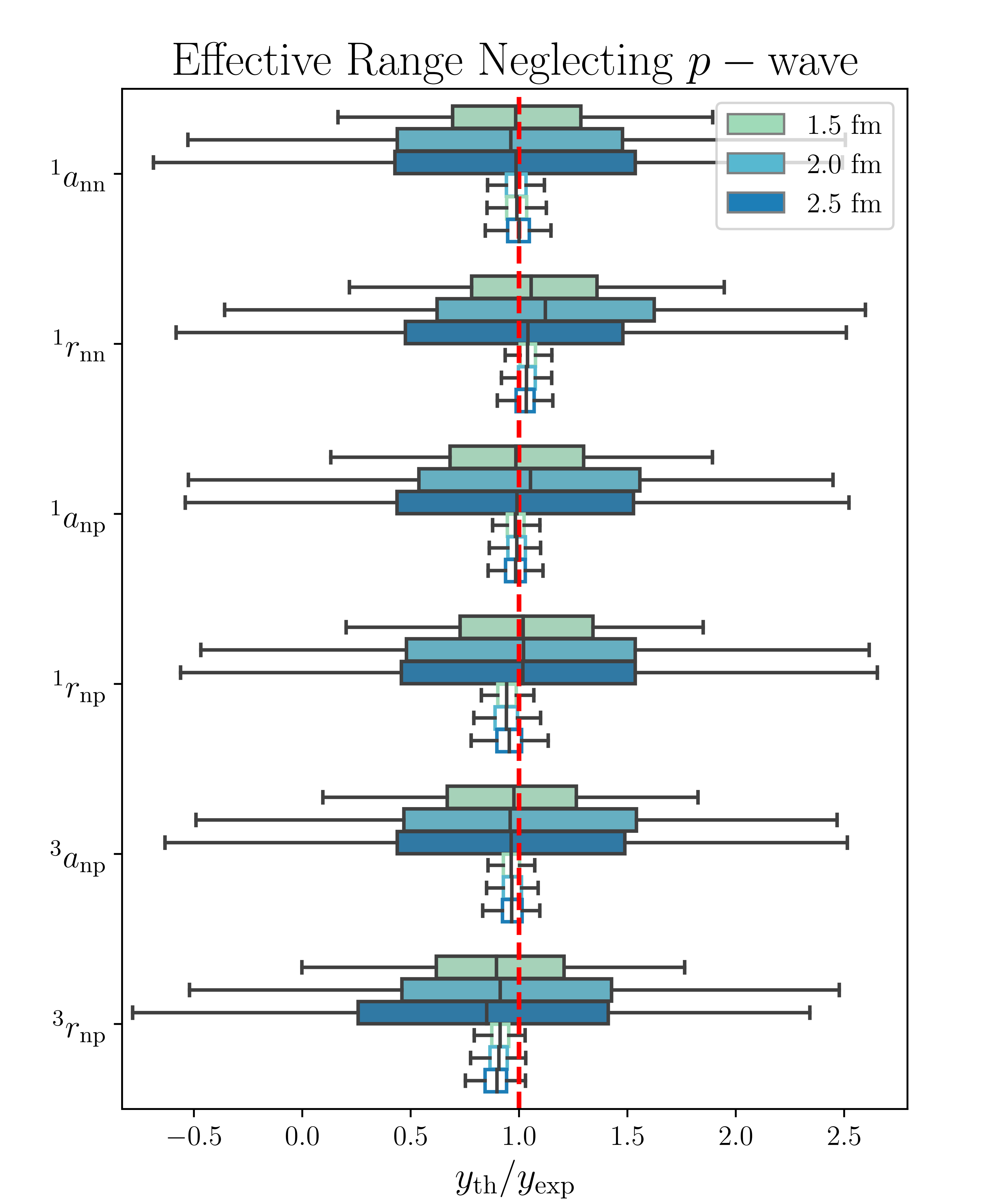
$$\mathrm{pr}(\vec{y}_{\mathrm{th}} \,|\, \vec{y}, \vec{x}, I) = \int d\vec{a}\, d\bar{c}^2\, d\Lambda_b\, \mathcal{N}\left(\vec{y}_{\mathrm{th}}, \Sigma_{\mathrm{th}}\right) \mathrm{pr}(\vec{\mathrm{a}}, \bar{\mathrm{c}}^2, \Lambda_{\mathrm{b}} \,|\, \vec{\mathrm{y}}_{\mathrm{exp}}, \mathrm{I})$$

which is done via sampling the posterior.

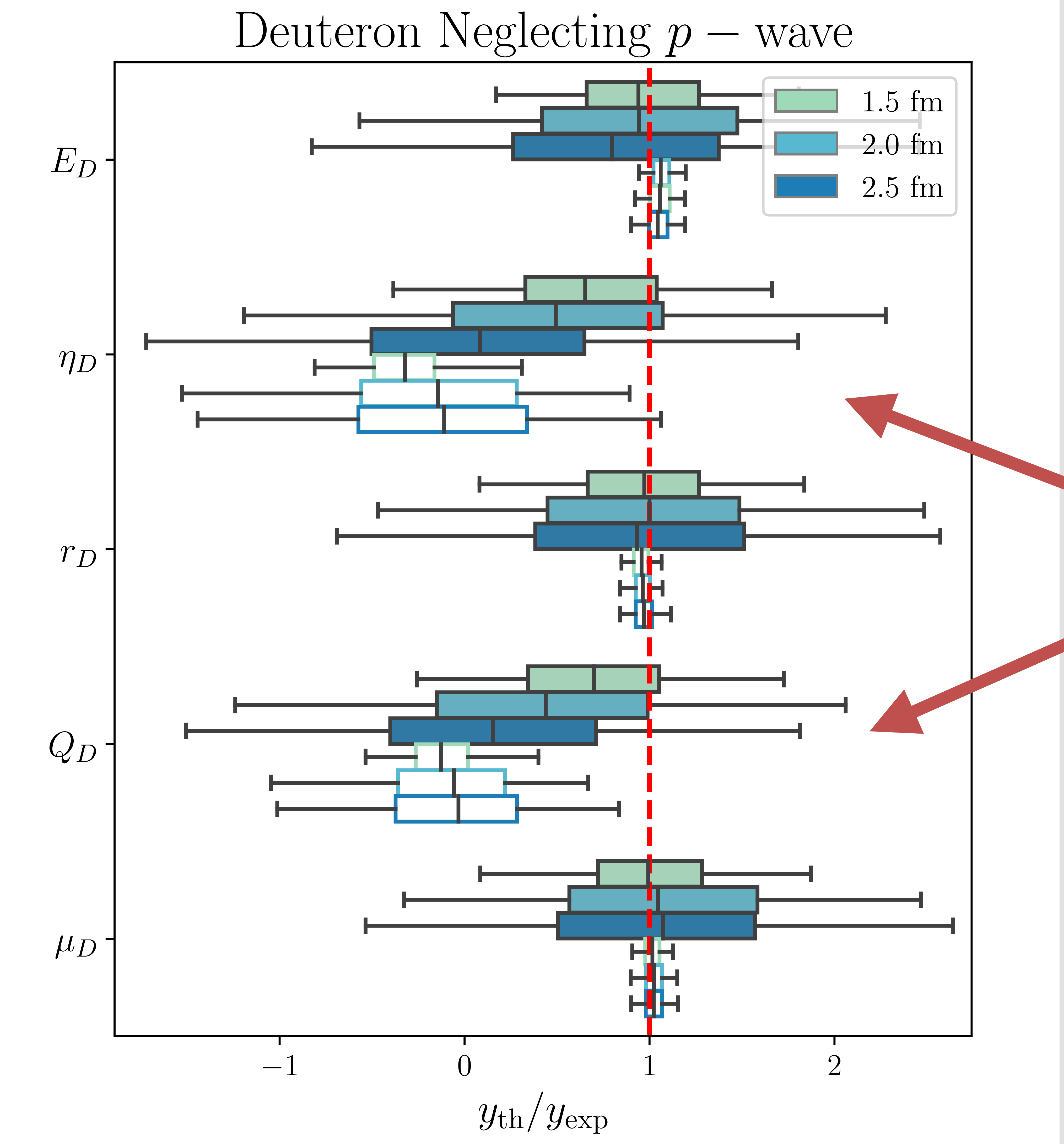
This can be done for **any** calculation of nuclear observables.

Propagation of Errors for ERPs





Propagation of Errors for Deuteron



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

Long-term Goals

- 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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Amazon

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MSU/FRIB

Daniel Odell
SRNL

Gaussian Process Emulation

Reduced Basis Methods via Galerkin Projection

Open Questions

- 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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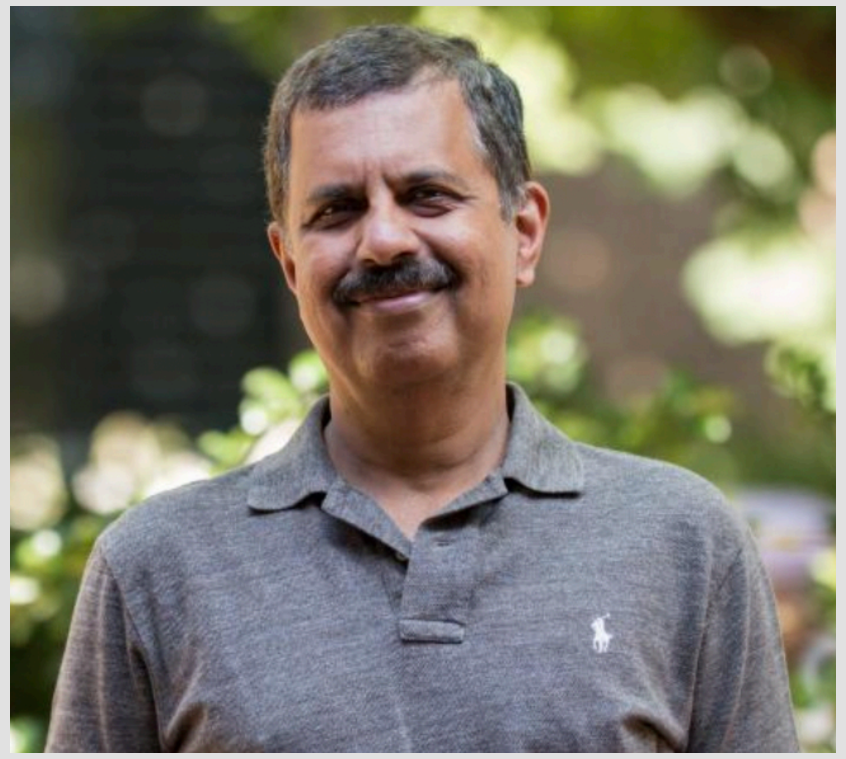

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