How Uncertain Am I?

Theoretical errors in Bayesian model calibration for EFTs

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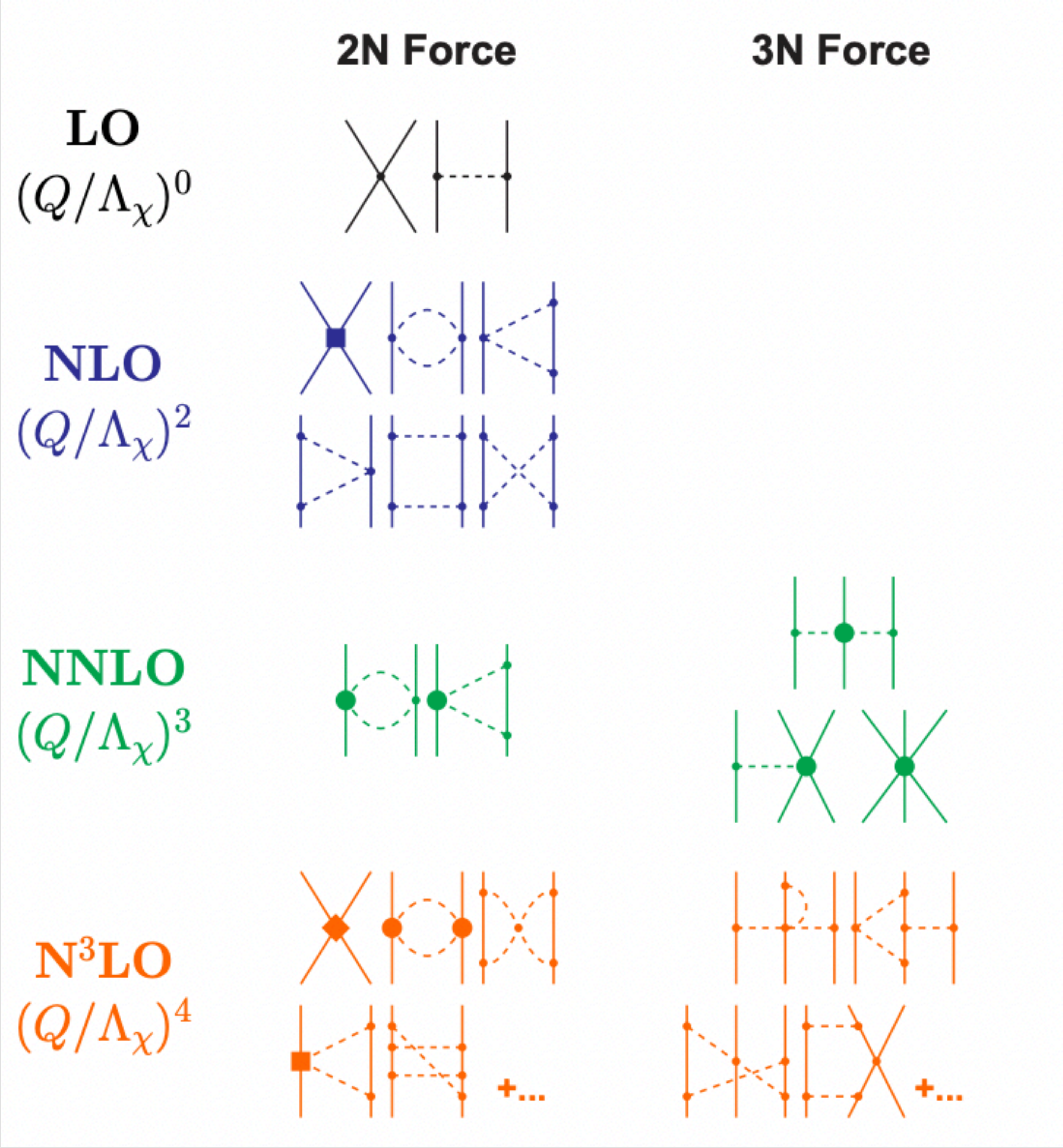
Effective Field Theory

We take an effective expansion of QCD preserving chiral symmetry.

The interaction can be ordered in terms of powers of Q/Λ_χ

- Q is a momentum or pion mass
- Λ_χ is the symmetry breaking scale

Gives a systematic ordering to improve the interaction.



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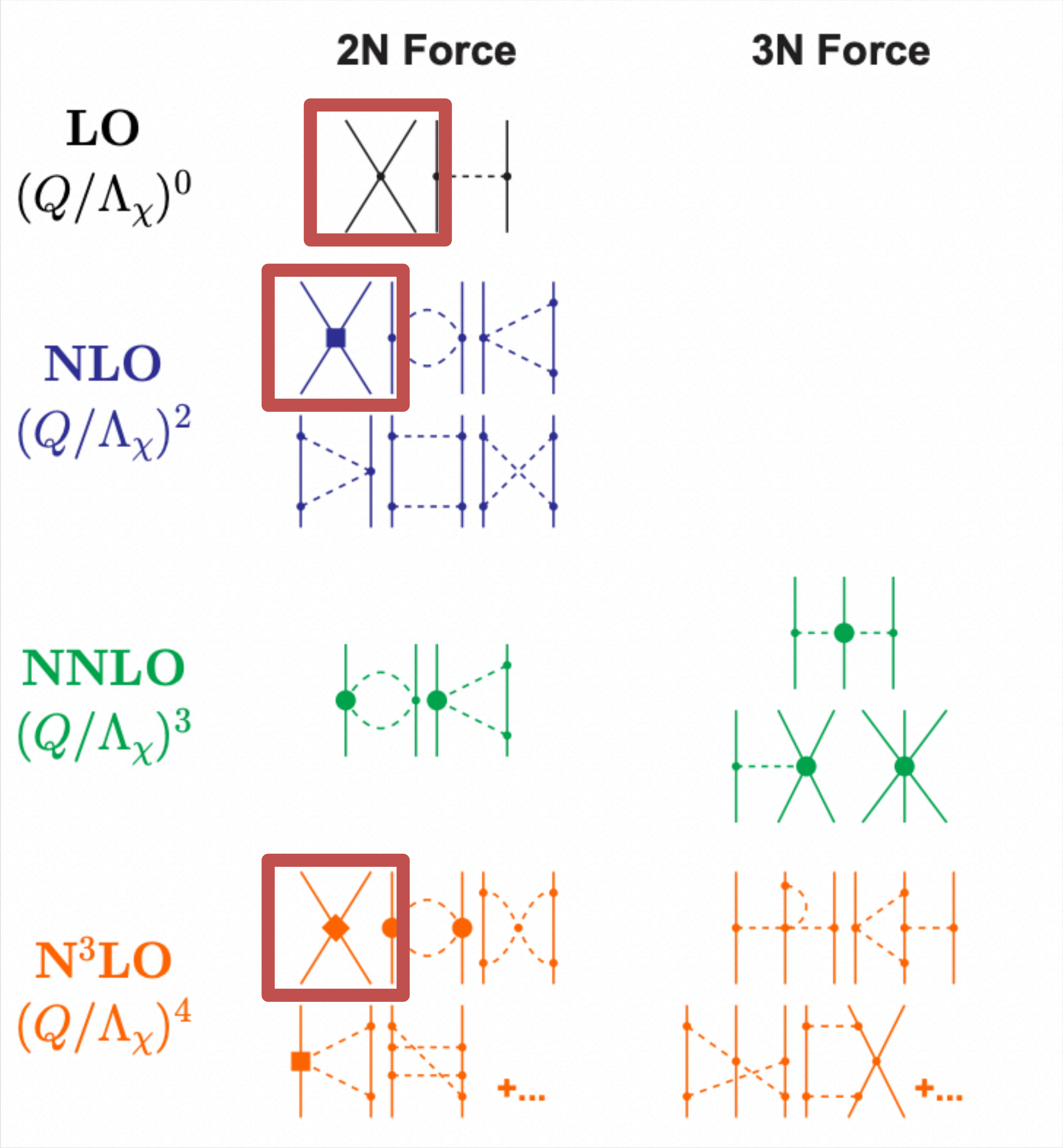

Pionless EFT

We are working in an EFT framework without pions

Our interaction takes the form:

$$v^{(LO)}(k) = C_S + C_T \sigma_1 \cdot \sigma_2$$

$$v^{(NLO)}(k) = C_1 k^2 + C_2 k^2 \sigma_1 \cdot \sigma_2 + C_3 S_{12}(k) + C_4 k^2 \tau_1 \cdot \tau_2$$
$$+ iC_5 S \cdot (K \times k) + C_6 k^2 \tau_1 \cdot \tau_2 \sigma_1 \cdot \sigma_2 + C_7 S_{12}(k) \tau_2 \cdot \tau_2$$

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Undetermined Low Energy Constants (LECs)

$$v^{(LO)}(k) = \boxed{C_S} + \boxed{C_T}\sigma_1 \cdot \sigma_2$$

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

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.

$$f(r) = \frac{1}{\pi^{3/2} R_0^3} e^{-\left(\frac{r}{R_0}\right)^2}$$

For this work, we choose $R_0 = 2.0 \text{ fm}$ corresponding to a momentum space cutoff of 200 MeV.

Model Calibration

To calibrate our EFT model, we use a Bayesian framework

$$\underbrace{\rho(\mathbf{a}\,|\,\mathbf{y},I)}_{\text{posterior}} \propto \underbrace{\rho(\mathbf{y}\,|\,\mathbf{a},I)}_{\text{likelihood}}\,\underbrace{\rho(\mathbf{a}\,|\,I)}_{\text{prior}}$$

$$\rho(\mathbf{y}\,|\,\mathbf{x},\sigma,\mathbf{a}) = \prod_i \left(\frac{1}{\sqrt{2\pi\sigma_i}}\right) e^{-\frac{\chi^2}{2}}$$

The posterior gives the distribution for a certain set of parameters, $\mathbf{a}$ (LECs), given data, $\mathbf{y}$ (scattering data), and any other information, I, which we maximize.

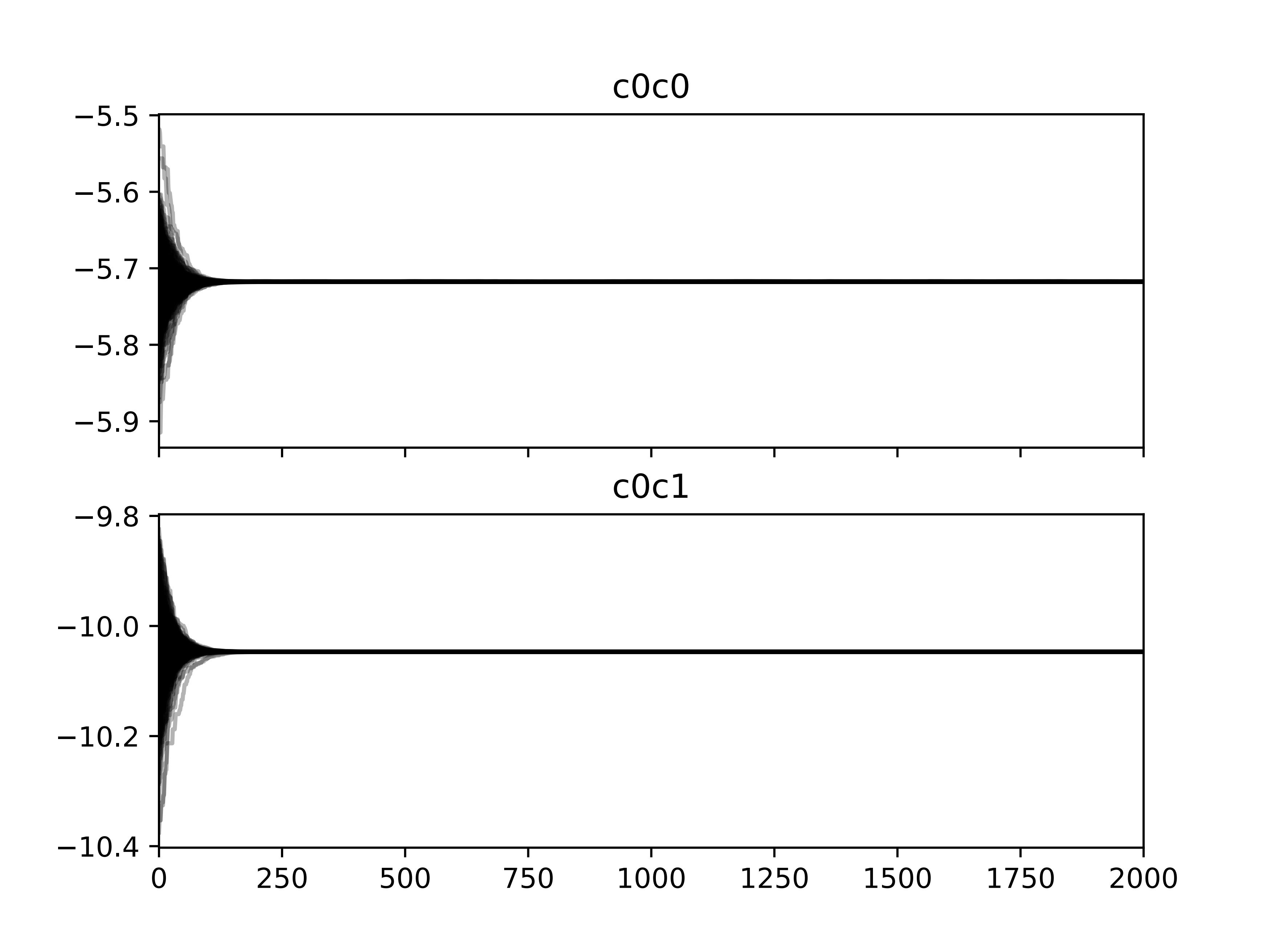
The likelihood gives the probability of scattering data for a given parameter set

- Find region of minimum χ^2

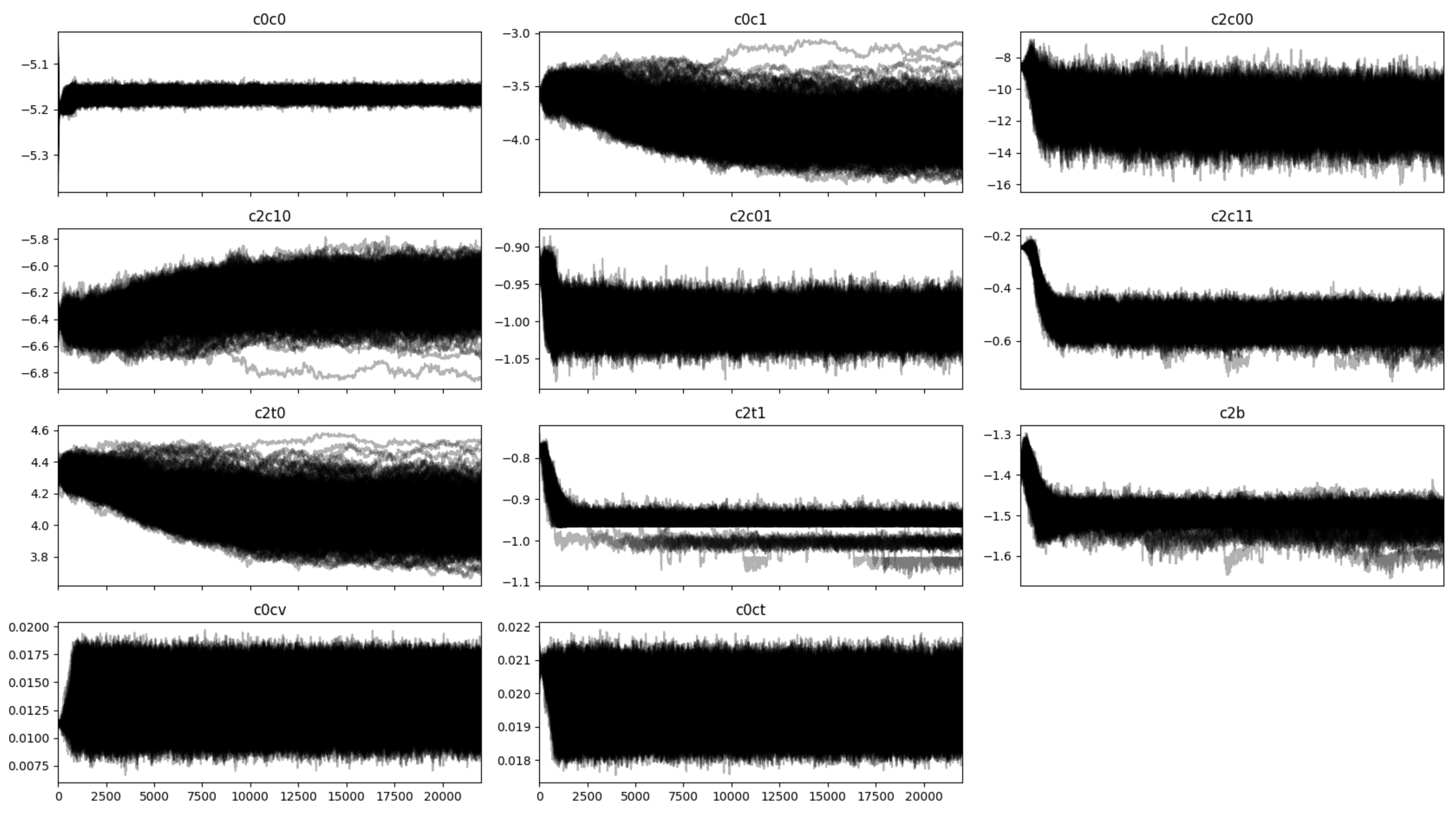
The prior encodes any external information we know about the parameters.

- Initial point/naturalness → ours is relatively uninformative

Proof of Concept Calibration

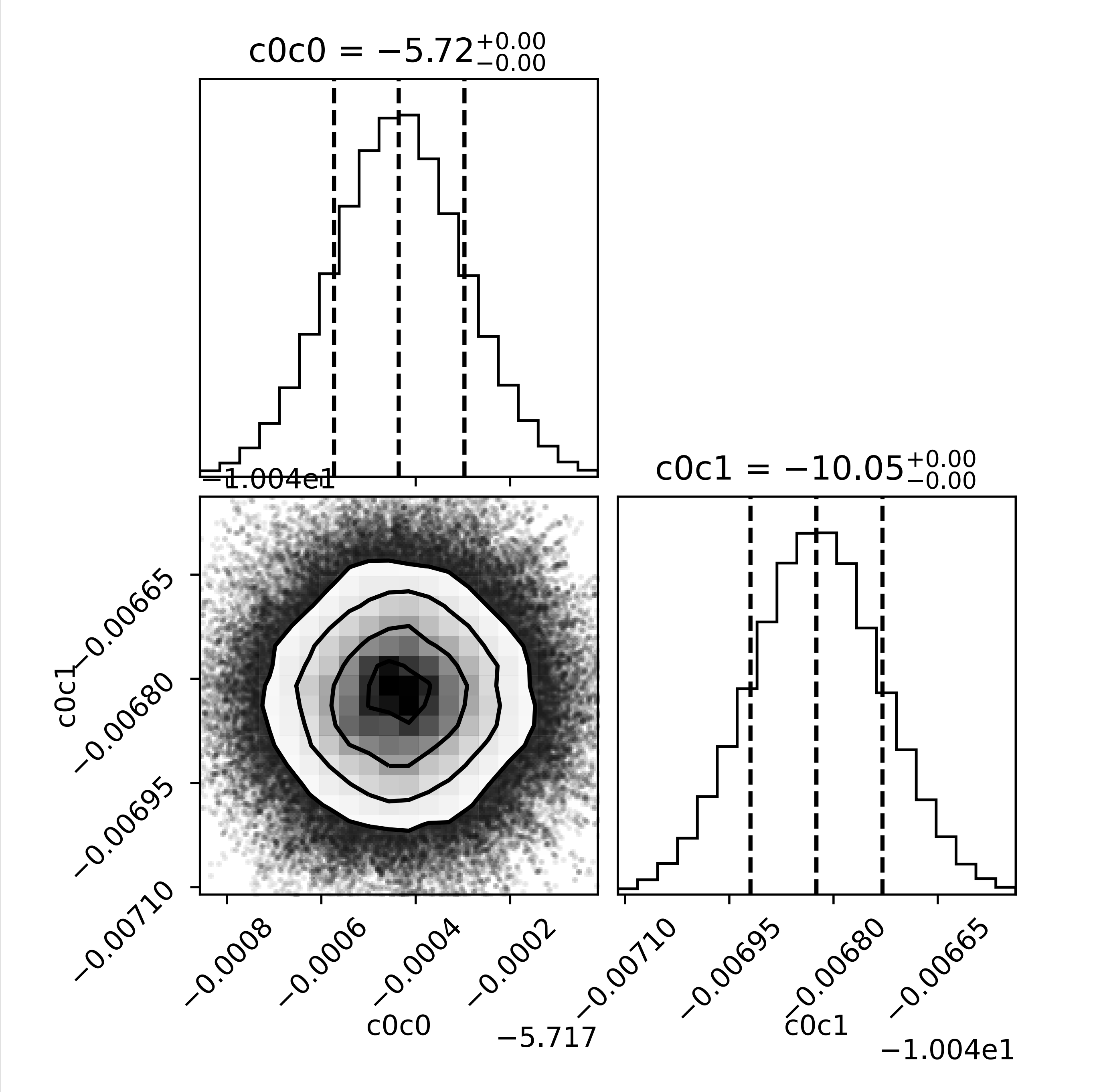


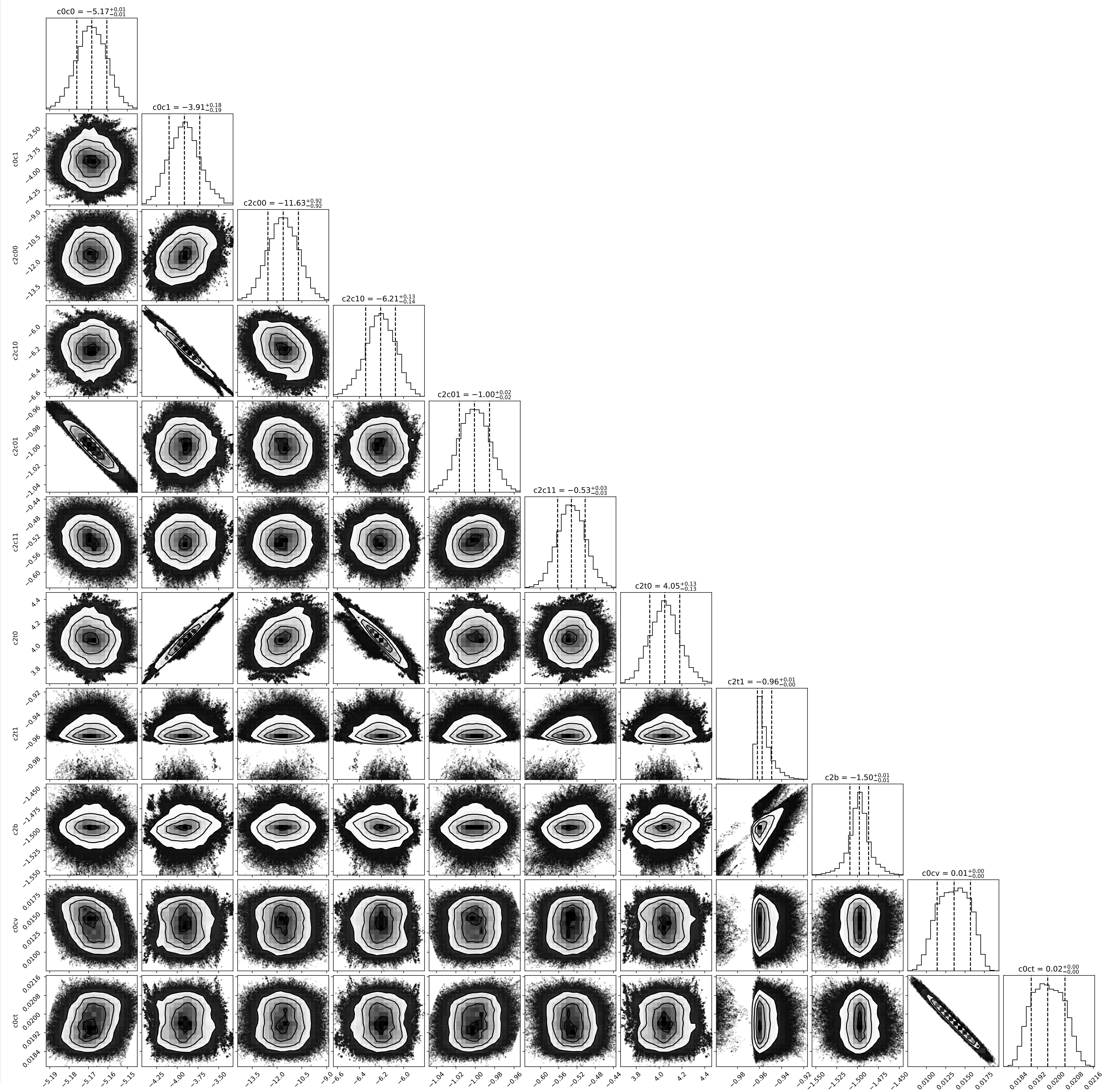
LO: 0.5 MeV, n_{data}=57 (np, E_d)



NLO: 15 MeV, n_{data}=773 (np, pp, E_d, np scatt. length)

2 fm Cutoff Fits





Full Bayesian model calibration

In our model calibration, we can include theory errors (Wesolowski et. al. Phys. Rev. C **104**, 064001)

$$\chi^2 = \sum_i \frac{(y_i - t_i)^2}{\sigma^2_{\exp,i}} \rightarrow \chi^2 = \sum_i \frac{(y_i - t_i)^2}{\sigma^2_{\exp,i} + \sigma^2_{\mathrm{ther},i}}$$

Where

$$\sigma^2_{\mathrm{ther},i} = \frac{(y_{\mathrm{ref},i}\, \bar{c}\, Q_i^{n+1})^2}{1 - Q_i^2}, \quad Q_i = \frac{\max[p_{\mathrm{soft}}, p_i]}{\Lambda_b \sim m_\pi}$$

and $y_{\mathrm{ref},i}$ sets the scale of the correction for observable y_i, and $\bar{c}$ sets the magnitude of the correction.

Dick Furnstahl

Daniel Phillips

Correlated theory errors

We can correlate our theory errors as well:

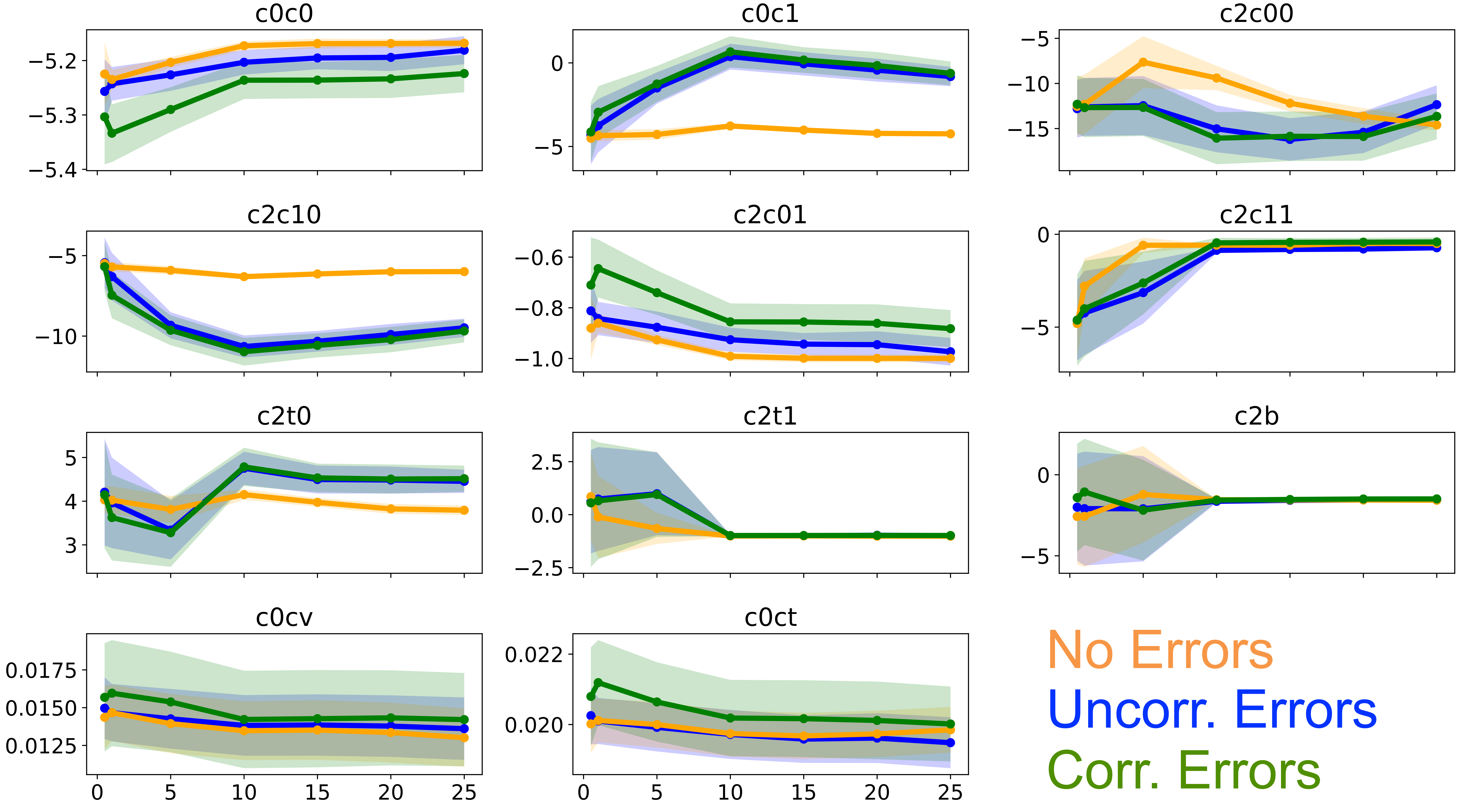
$$\sigma^2_{\text{ther},i} = \frac{(y_{\text{ref},i}\,\bar{c}\,Q_i^{n+1})^2}{1 - Q_i^2} \rightarrow \sigma^2_{\text{ther},ij} = \frac{y_{\text{ref},i}\,y_{\text{ref},j}\,\bar{c}^2\,Q_i^{n+1}Q_j^{n+1}}{1 - Q_i\,Q_j} e^{-|p_i - p_j|/2l_p} e^{-|\theta_i - \theta_j|/2l_\theta}$$

with the goodness of fit determined by the Mahalanobis distance ("modified" χ^2)

$$d_M(\overrightarrow{a}) = \left(\overrightarrow{y} - \vec{t}(\overrightarrow{a})\right)^T (\sigma^2_{\text{exp}} + \sigma^2_{\text{ther},ij})^{-1} \left(\overrightarrow{y} - \vec{t}(\overrightarrow{a})\right)$$

Correlations on data introduces strong degeneracies in the covariance matrix, so we use Gaussian processes to smooth the correlations.

"Wesolowski Plots" for Pionless EFT at NLO



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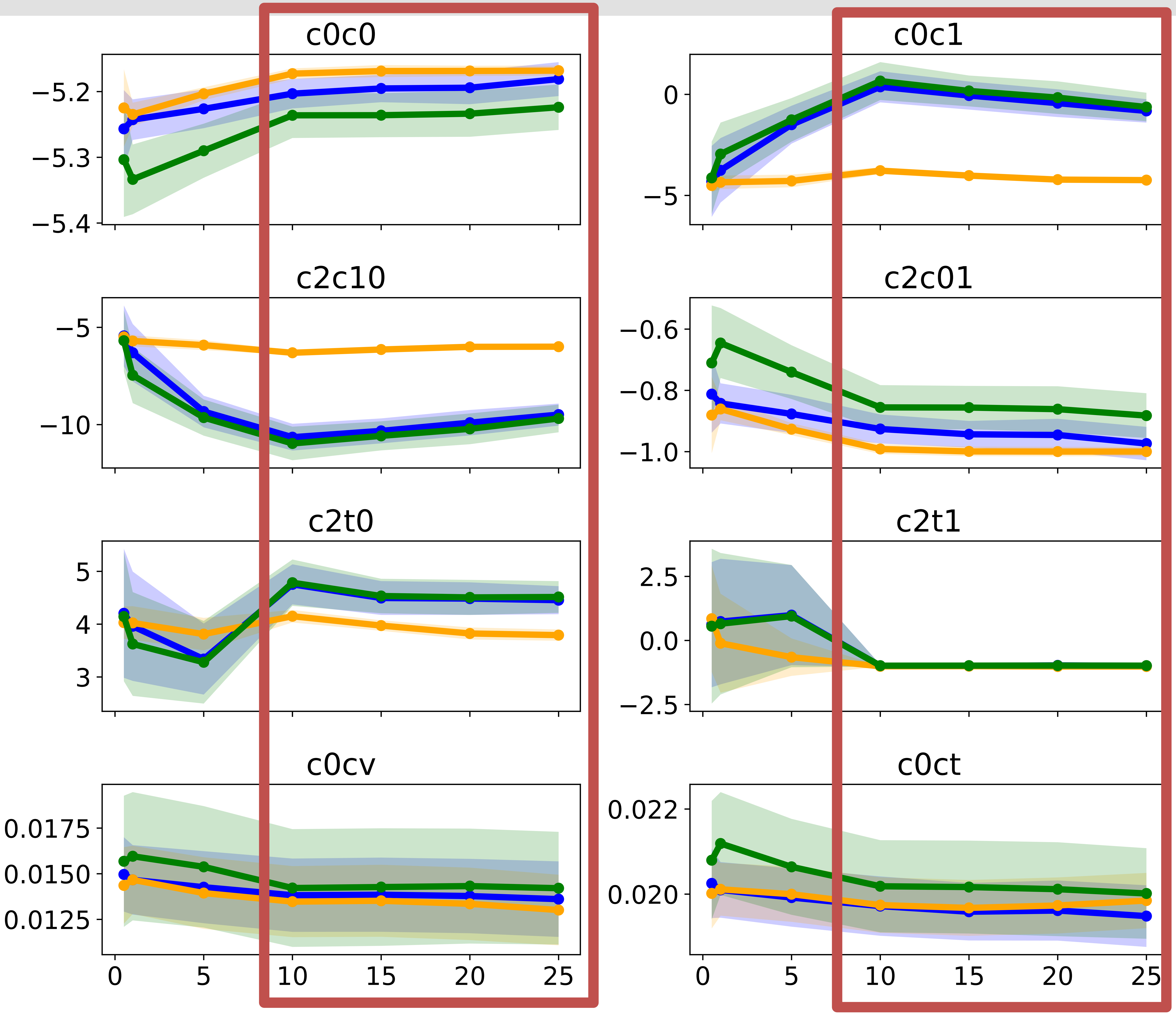


No Errors
Uncorr. Errors
Corr. Errors

Full posterior

We have two more parameters to estimate in a full Bayesian model calibration: $\bar{c}^2$ (scale of truncation error) and Λ_b (EFT breakdown scale).

Full posterior for our EFT:

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

The posterior is found via sampling of $\{\vec{a}, \bar{c}^2, \Lambda_b\}$.

Posterior for $\bar{c}^2$

For $\bar{c}^2$ we choose (following Melendez et. al. Phys. Rev. C **100**, 044001)

$$P(\bar{c}^2 \,|\, \overrightarrow{a}, \Lambda_b, I) \sim \chi^{-2}\left(\nu, \tau^2(\overrightarrow{a}, \Lambda_b)\right)$$

With hyper parameters:

$$\nu = \nu_0 + N_{\text{obs}} n_c$$

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

$$c_{n,i}\left(\overrightarrow{a}, \Lambda_b\right) = \frac{y_i^{(n)}\left(\overrightarrow{a}_{(n)}\right) - y_i^{(n-1)}\left(\overrightarrow{a}_{(n-1)}\right)}{y_{\text{ref}}\left(\frac{\max[p_{\text{soft}}, p_i]}{\Lambda_b}\right)^n}$$

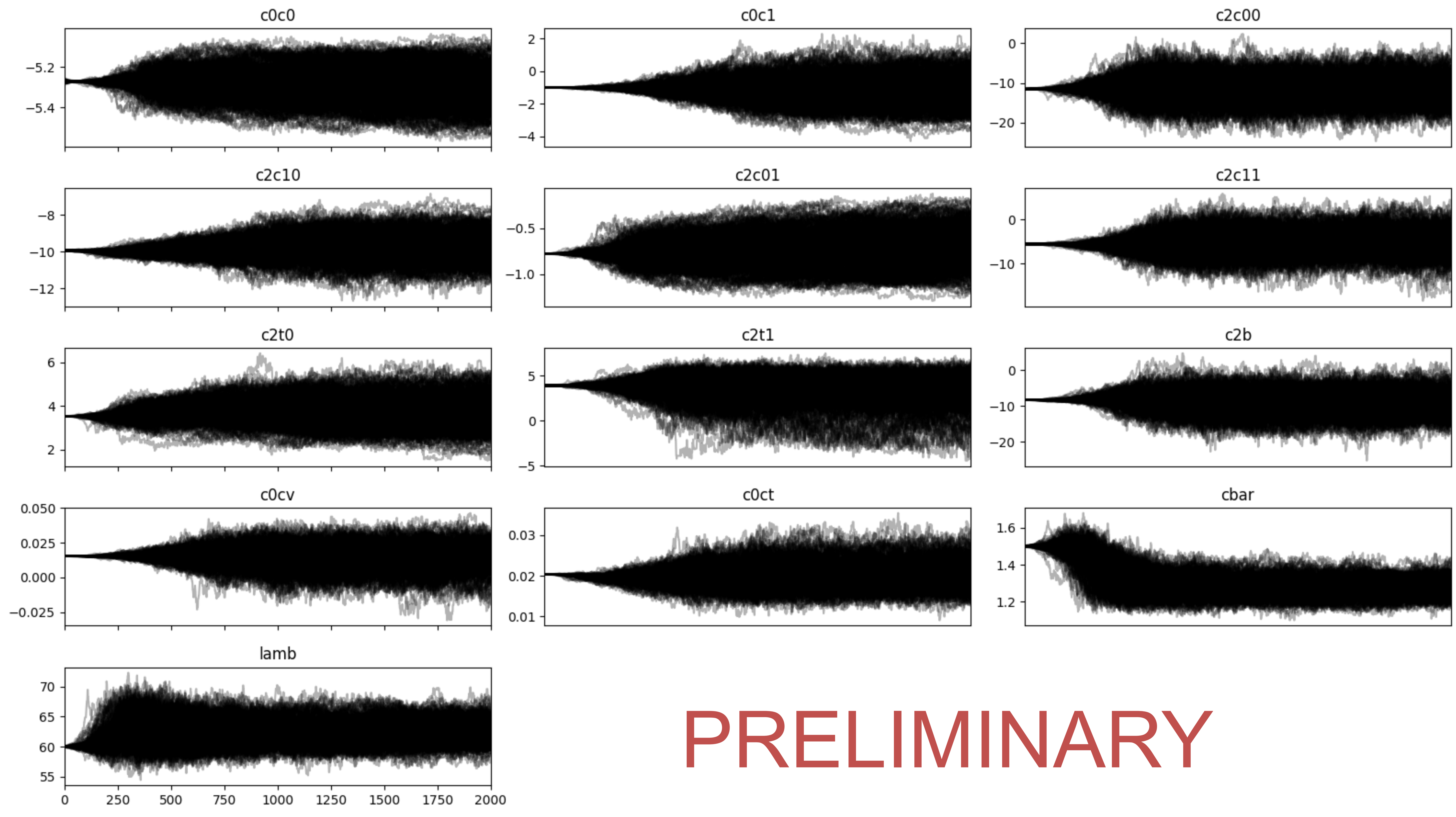
Posterior for Λ_b

Our posterior for the breakdown scale also uses these hyper parameters:

$$P(\Lambda_b \,|\, \vec{a}, I) \propto \frac{P(\Lambda_b \,|\, I)}{\tau^{\nu} \prod_{n,i} \left(\frac{\max[p_{\text{soft}}, p_i]}{\Lambda_b} \right)^{n}}$$

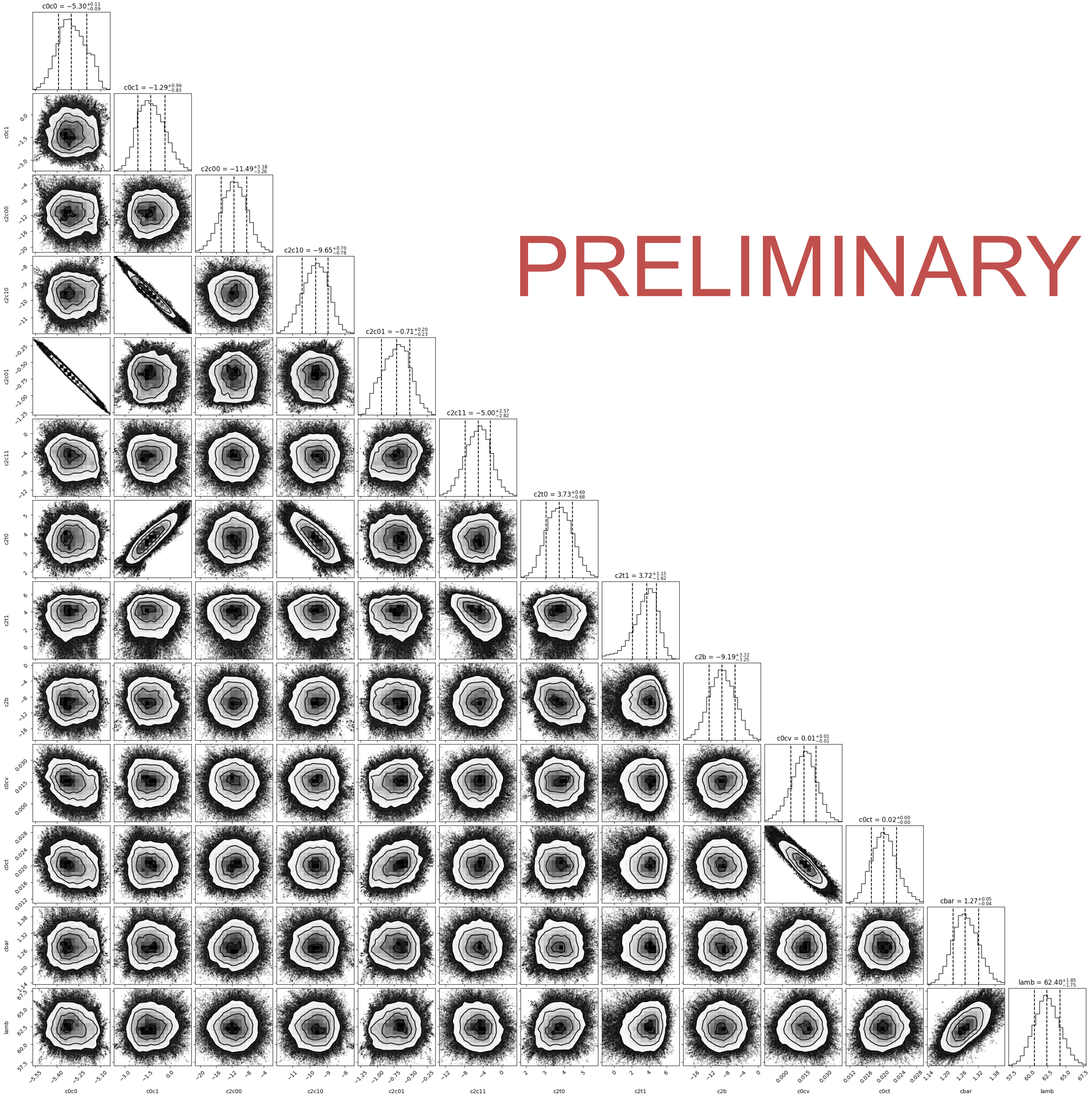
This posterior needs to be numerically normalized as the normalization constant is dependent on $\vec{a}$.

Full Model Calibration



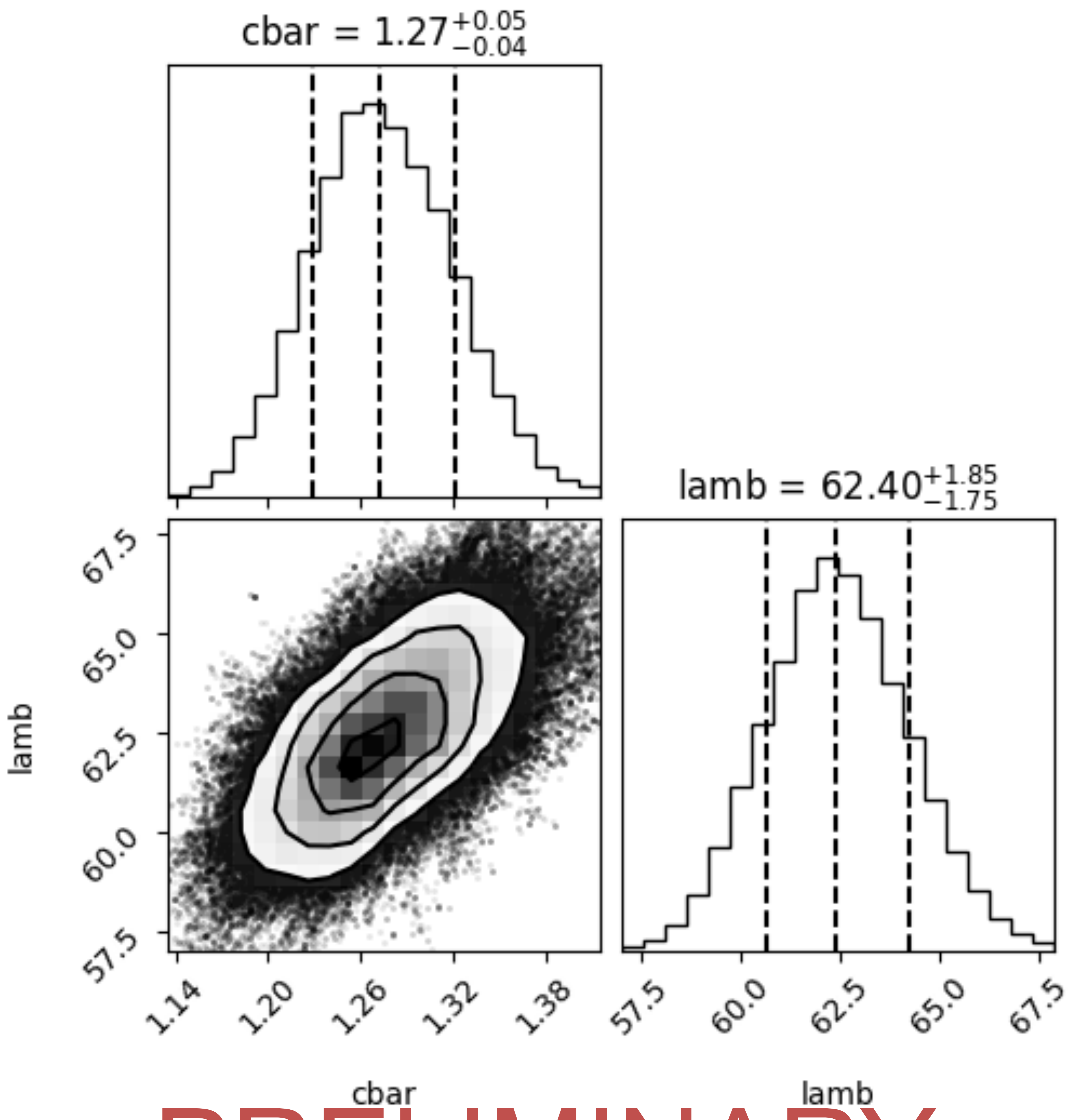
PRELIMINARY

Marginal Distributions



PRELIMINARY

Truncation Error Parameters



PRELIMINARY

Future Steps

- Investigate fits at N3LO in the pionless regime
- Emulation for calculation of scattering observables

Ozge Surer
Miami University

Stefan Wild
LBNL

Matt Plumlee
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- Include other degrees of freedom: π's and Δ's $\rightarrow$ A new set of interactions with uncertainty quantification in χEFTs

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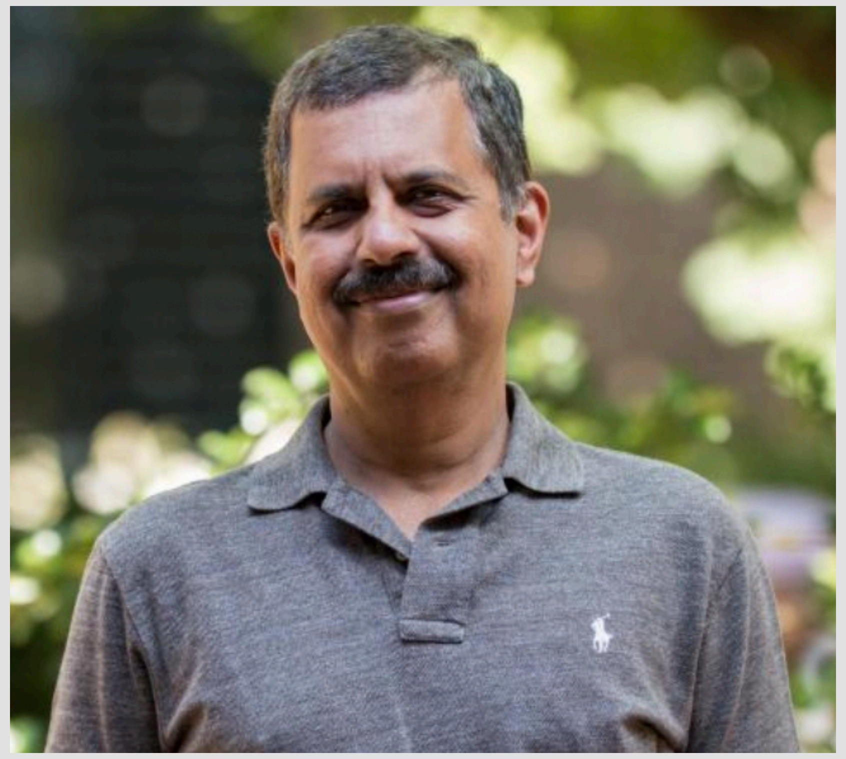
Fellowship/Travel

BAND Bayesian Analysis of Nuclear Dynamics



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