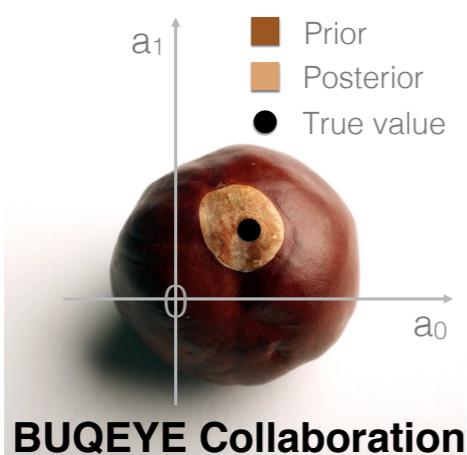


Bayesian statistical models for truncation errors

Dick Furnstahl
ISNET-5 in York, November, 2017



THE OHIO STATE UNIVERSITY



U.S. DEPARTMENT OF
ENERGY



Jordan Melendez (OSU)
Daniel Phillips (OU)
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Harald Grießhammer (GWU)
Sarah Wesolowski (Salisbury U.)

NUCLEI
Nuclear Computational Low-Energy Initiative

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BUQEYE Collaboration



VERSITY

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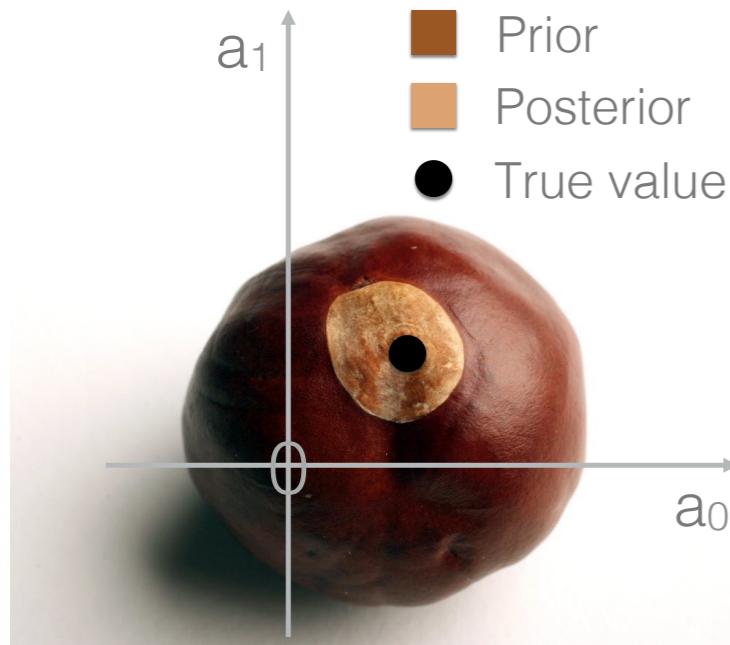


U.S. DEPARTMENT OF
ENERGY



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Nuclear Computational Low-Energy Initiative

Bayesian Uncertainty Quantification: Errors for Your EFT



BUQEYE Collaboration

Goal:

Full uncertainty quantification (UQ)
for effective field theory (EFT)
predictions using Bayesian statistics

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)
- “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) [Editors’ Suggestion]

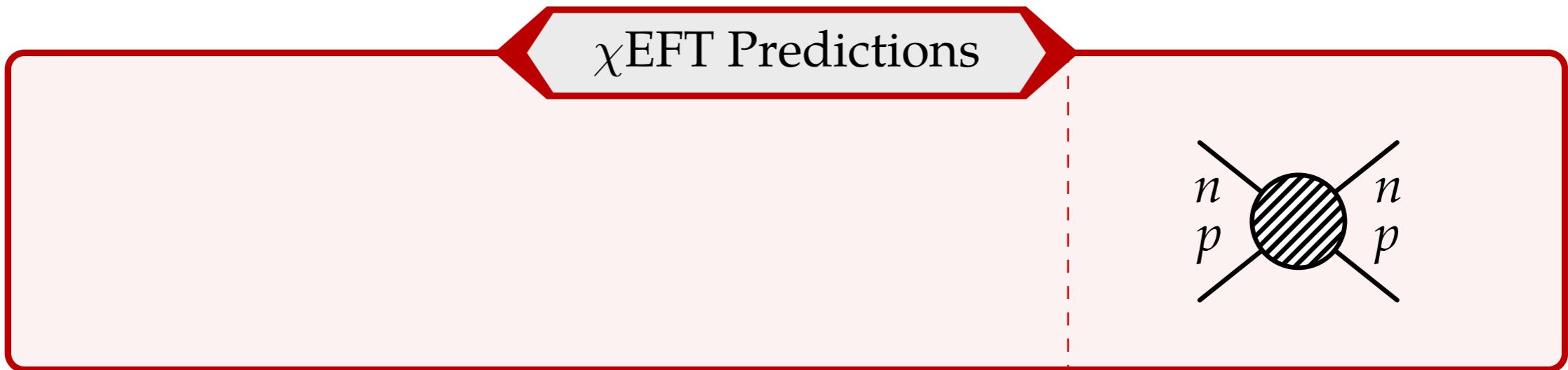
Themes using EFT truncation error example

- ★ Building a statistical model (Bayes!)
 - How do we exploit an EFT expansion?
- ★ Model checking and validation
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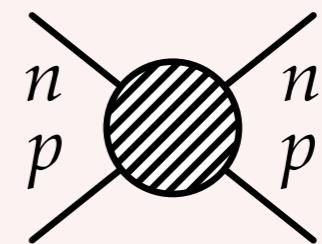
EXAMPLE: NN SCATTERING (AT A GIVEN ENERGY)



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χ EFT Predictions

$$\sigma = 50 \text{ mb} + 20 \text{ mb} - 9 \text{ mb} + 4 \text{ mb} + \dots$$

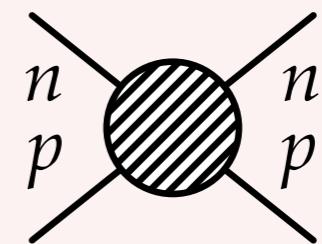


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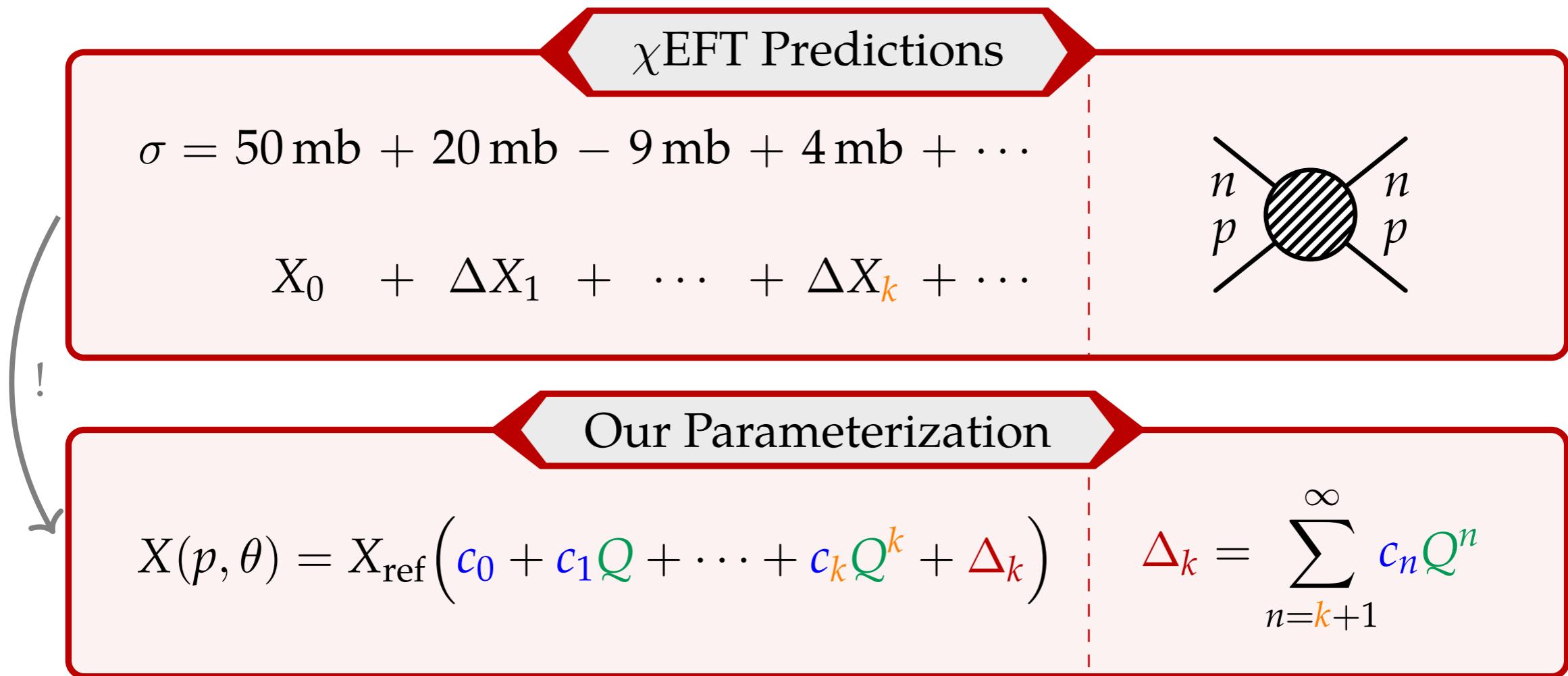
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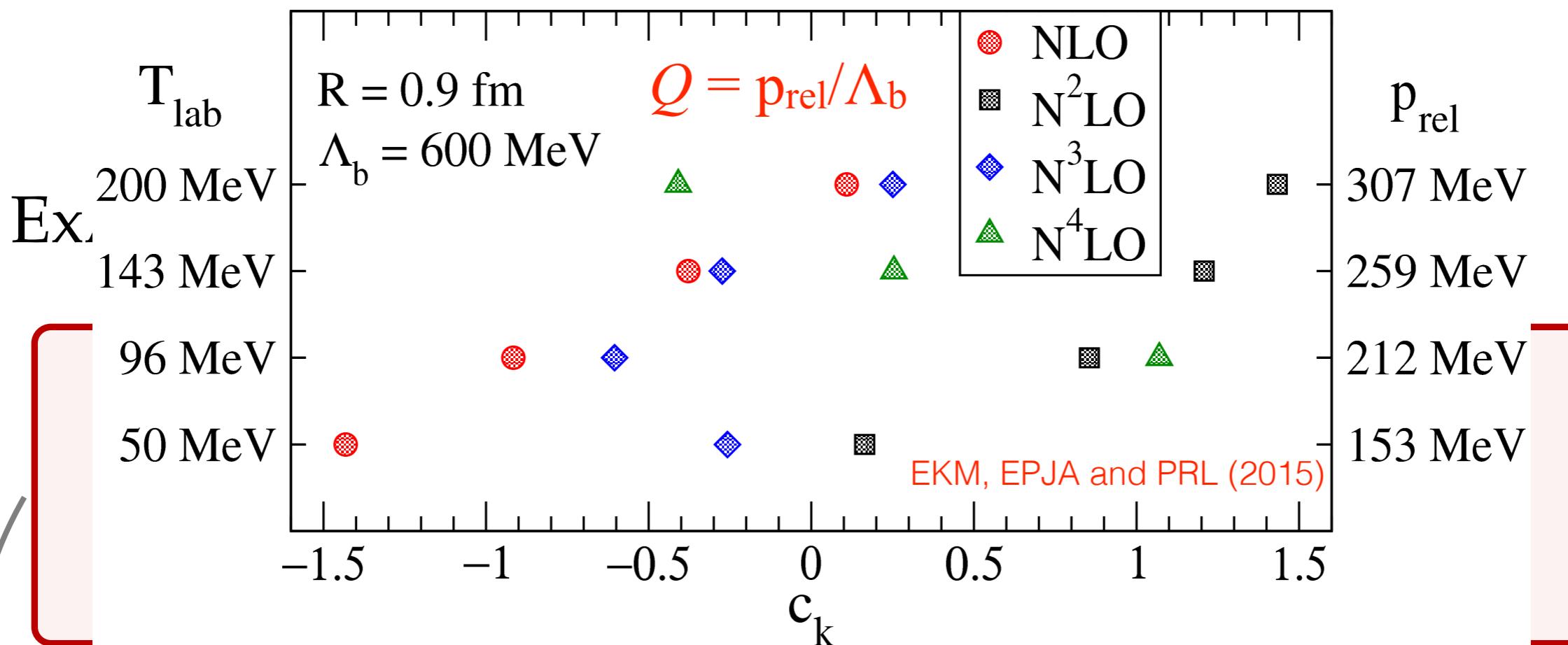
$$X_0 + \Delta X_1 + \dots + \Delta X_k + \dots$$



EXAMPLE: NN SCATTERING (AT A GIVEN ENERGY)



- X_{ref} : Dimensionful scale
- k : Truncation order
- Q : Expansion parameter
- c_n : *Natural* coefficients
- Δ_k : Truncation error
- Λ_b : Breakdown scale



Our Parameterization

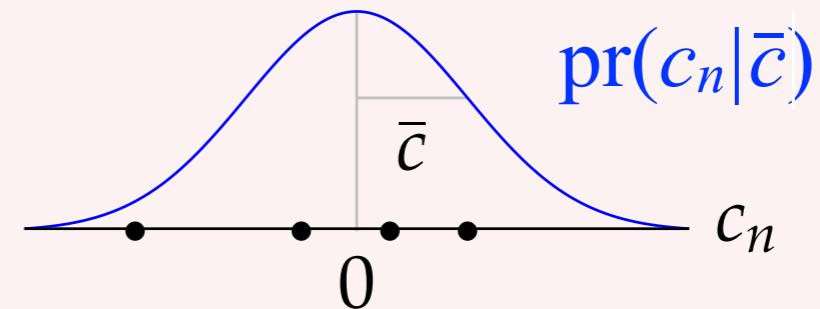
$$X(p, \theta) = X_{\text{ref}} \left(c_0 + c_1 Q + \cdots + c_k Q^k + \Delta_k \right)$$

$$\Delta_k = \sum_{n=k+1}^{\infty} c_n Q^n$$

- X_{ref} : Dimensionful scale
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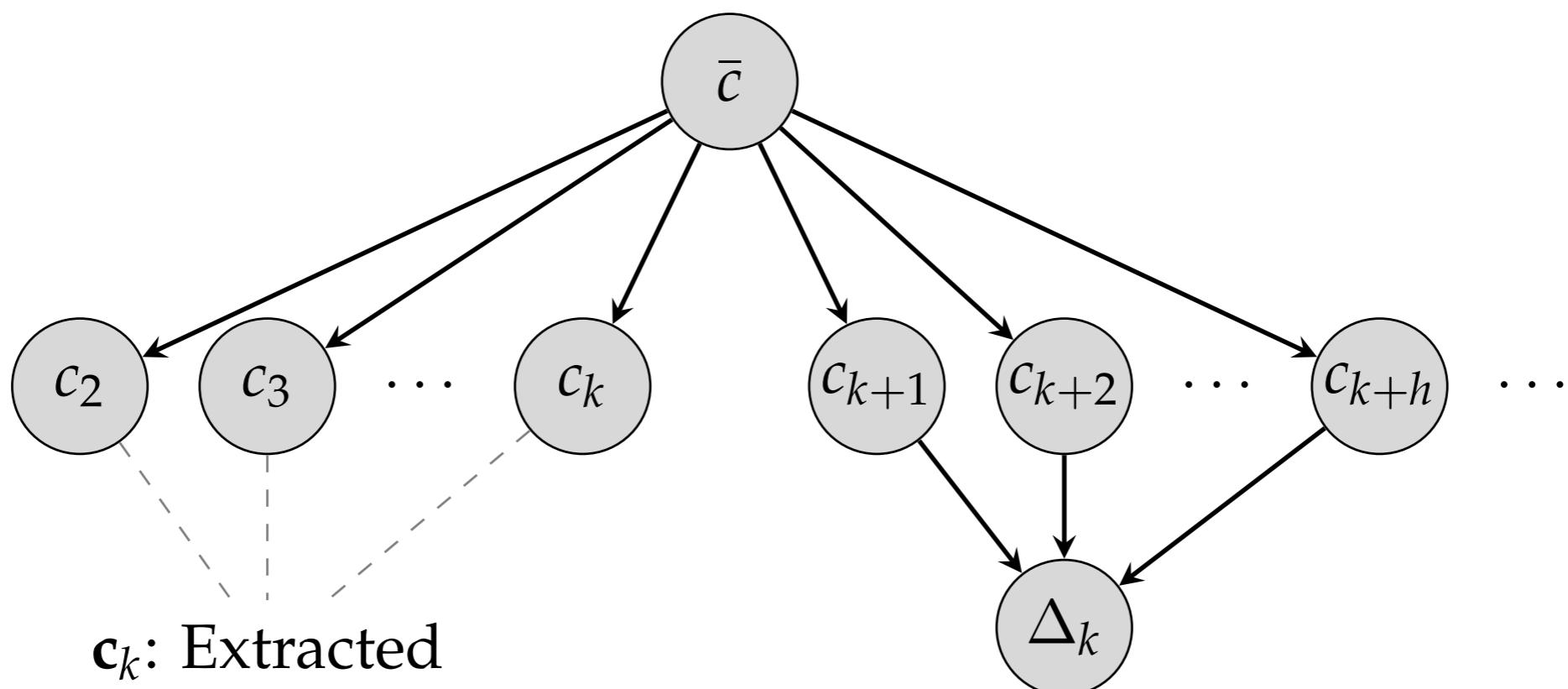
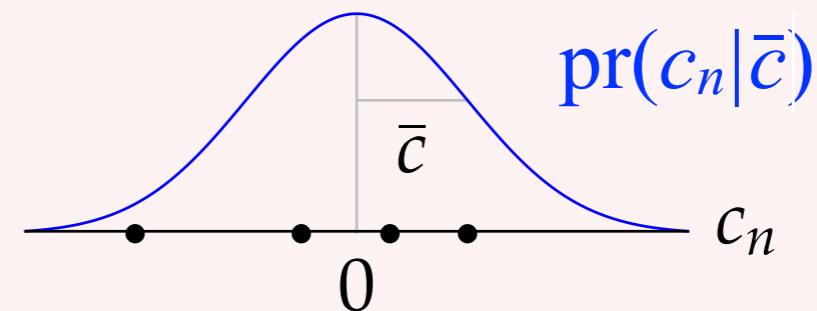
Key Assumption: Naturalness bound

All c_n are drawn from the *same* distribution with a natural size \bar{c}



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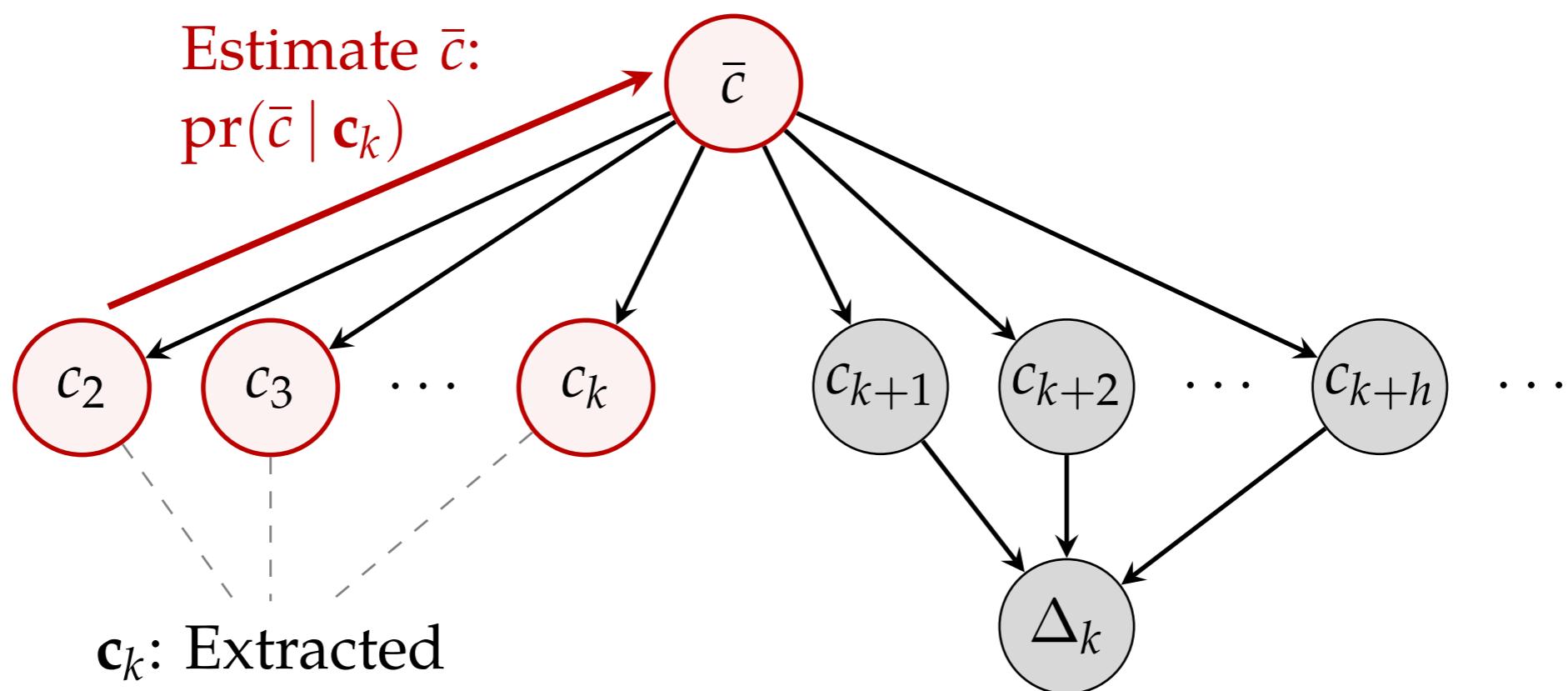
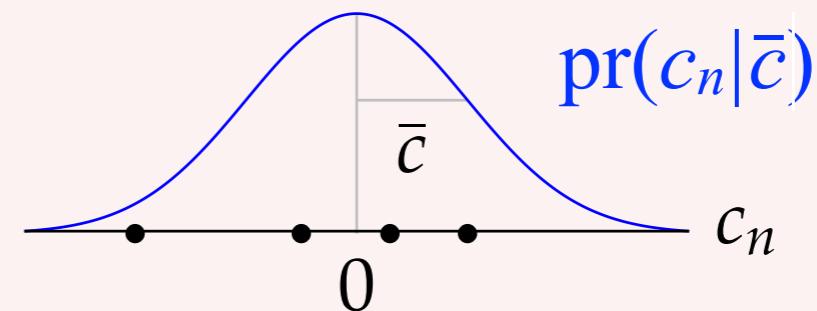
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$$pr(\Delta_k | c_k) \propto$$

Key Assumption: Naturalness bound

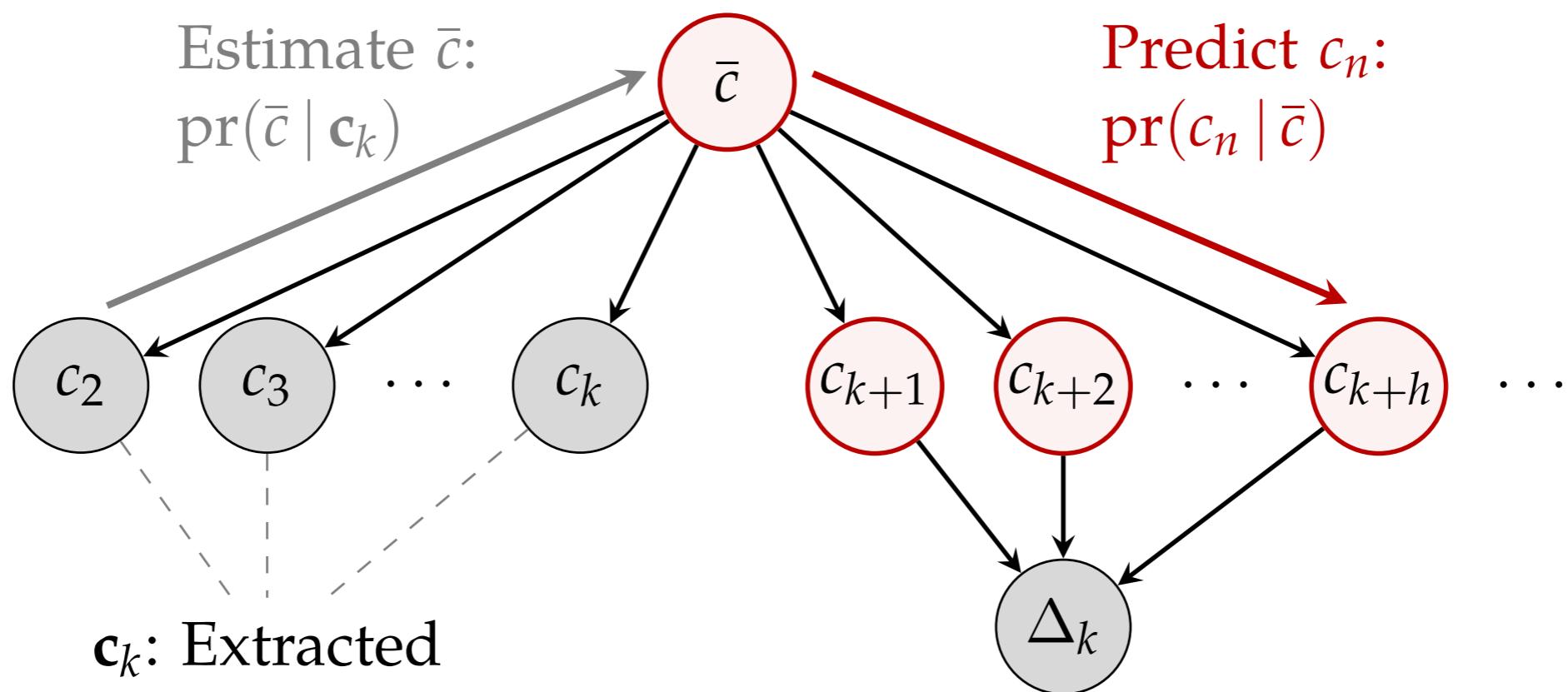
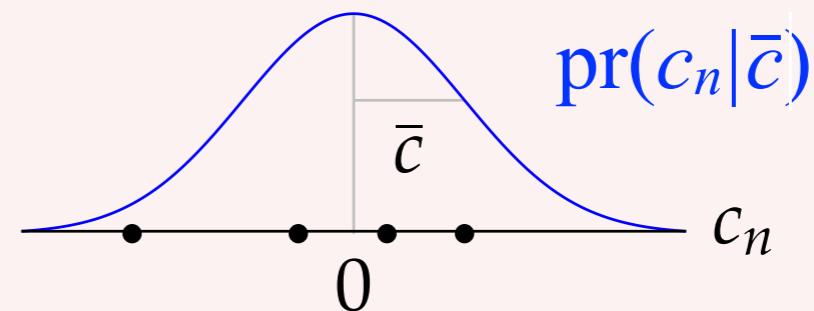
All c_n are drawn from the *same* distribution with a natural size \bar{c}



$$\text{pr}(\Delta | \mathbf{c}_k) \propto \int d\bar{c} \text{pr}(\bar{c} | \mathbf{c}_k)$$

Key Assumption: Naturalness bound

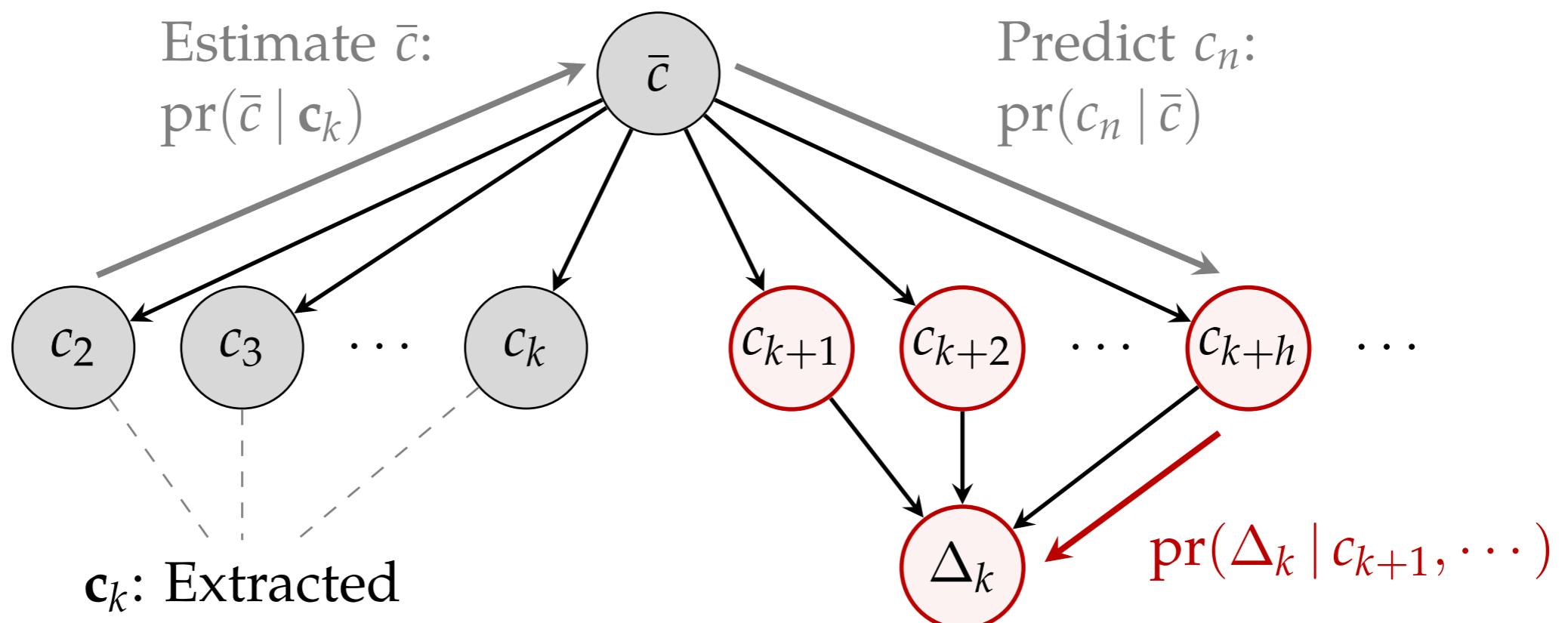
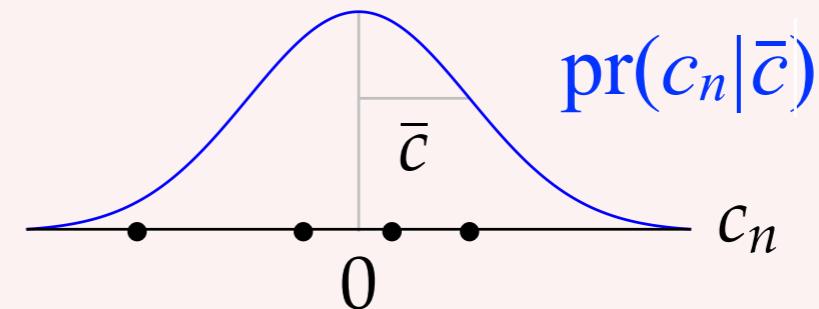
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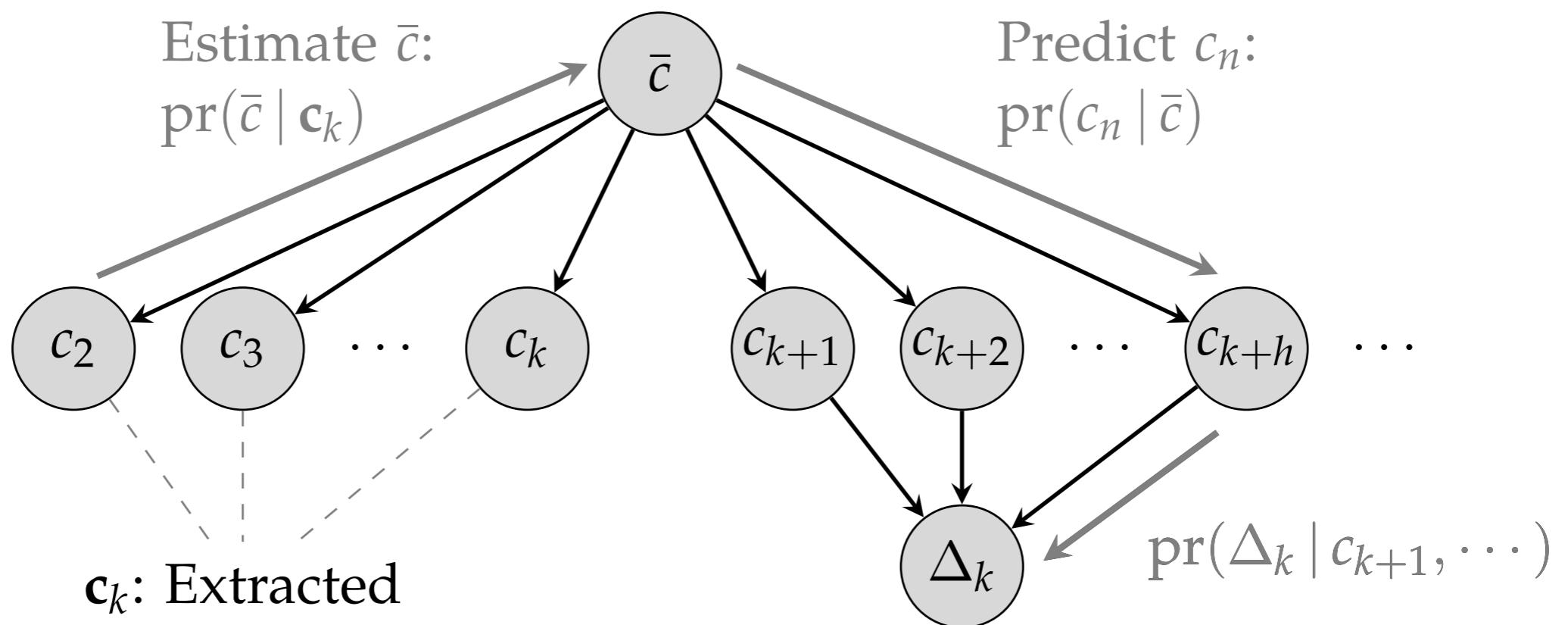
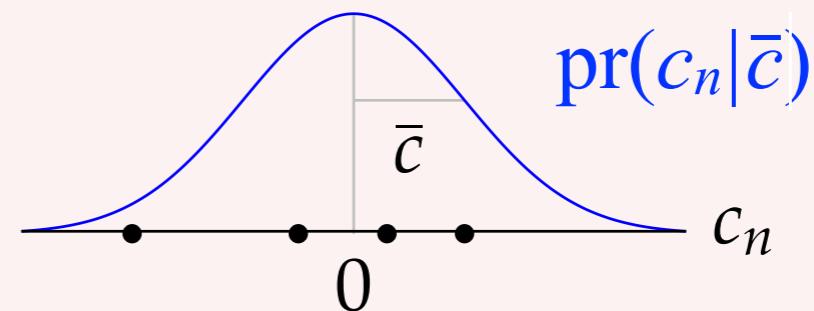
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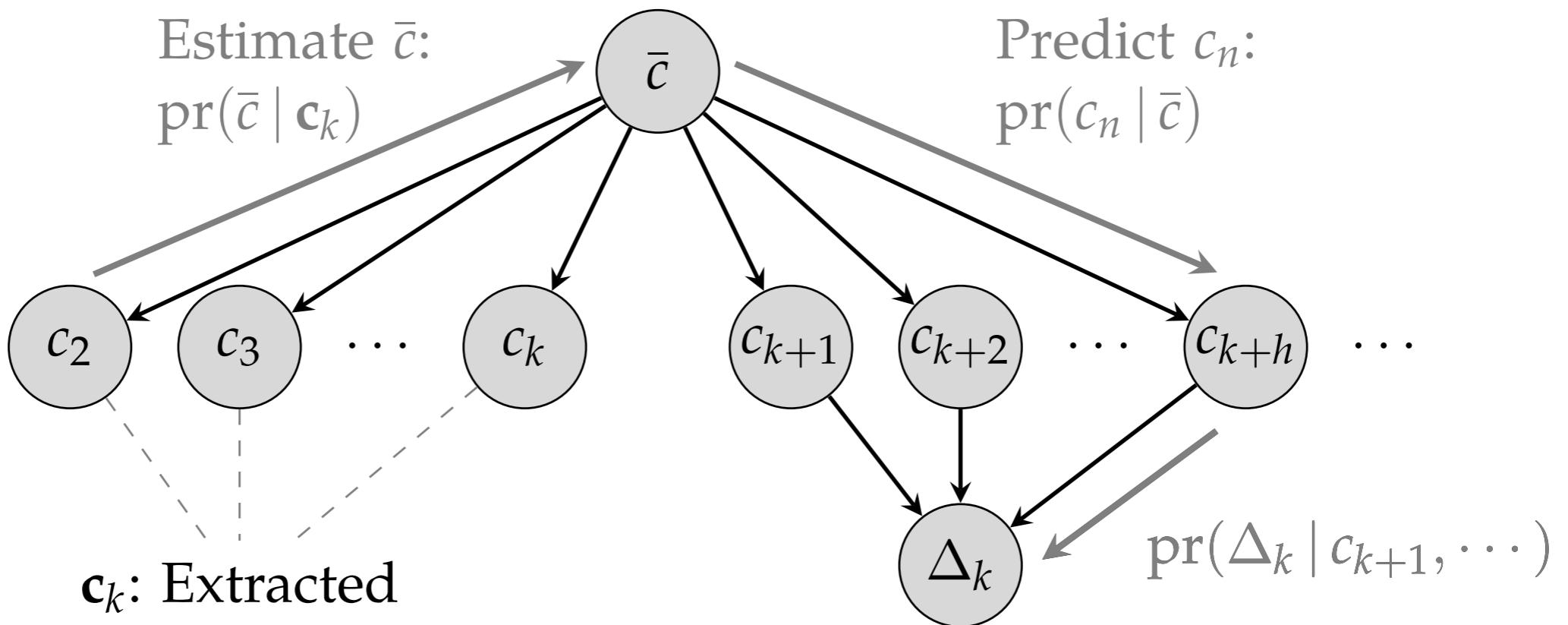
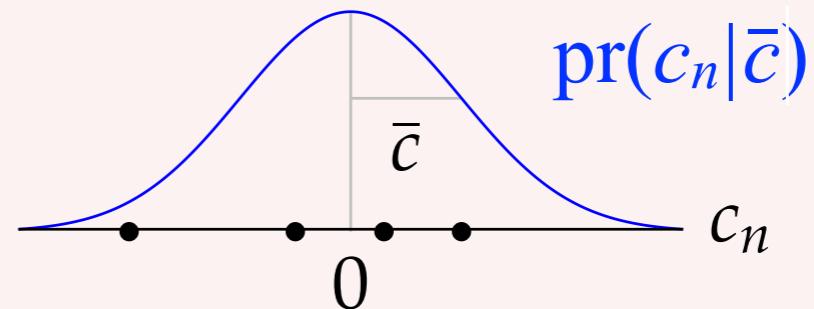
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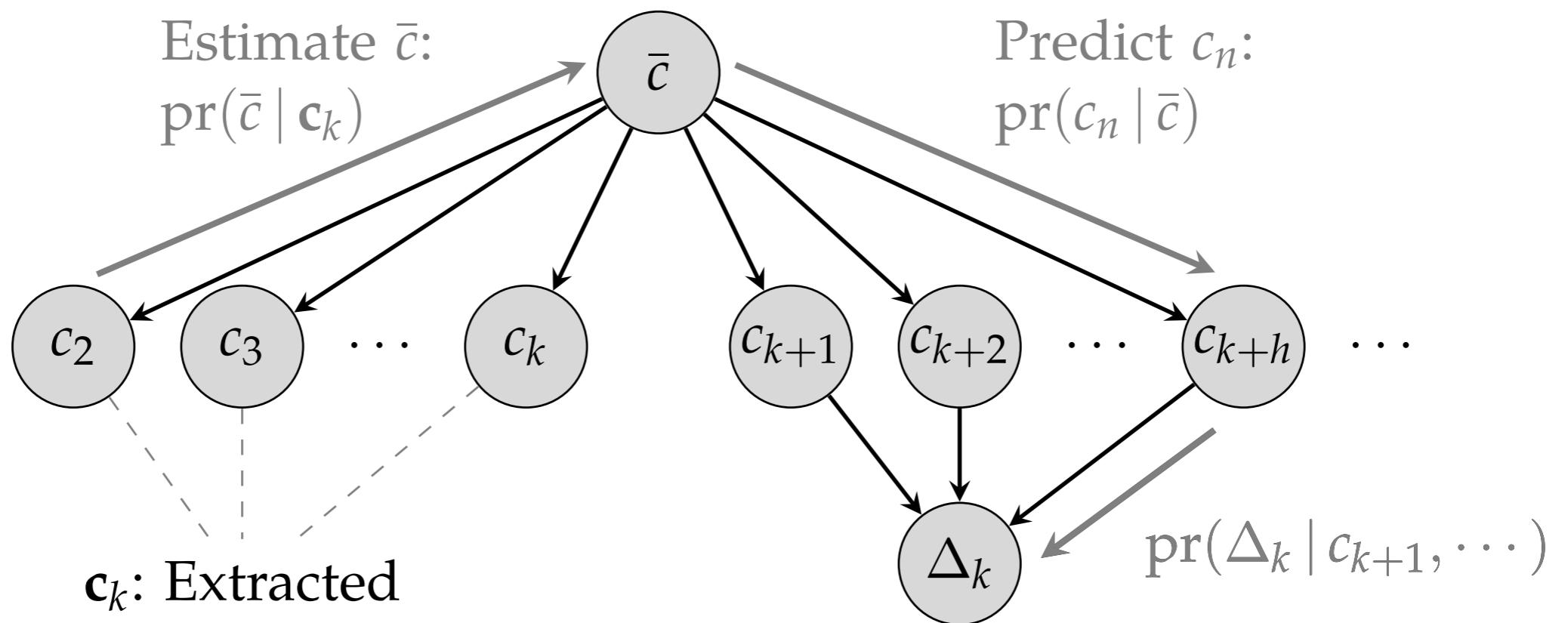
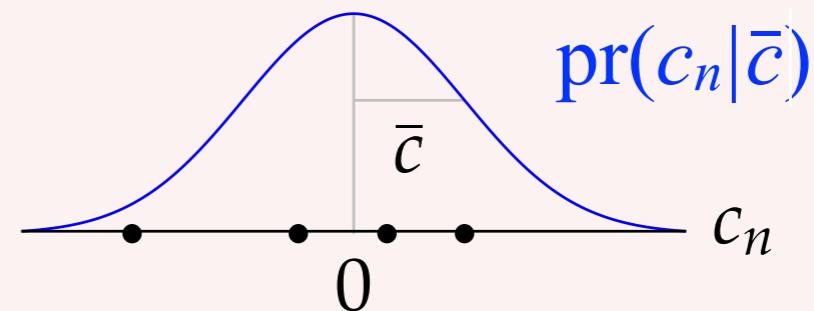
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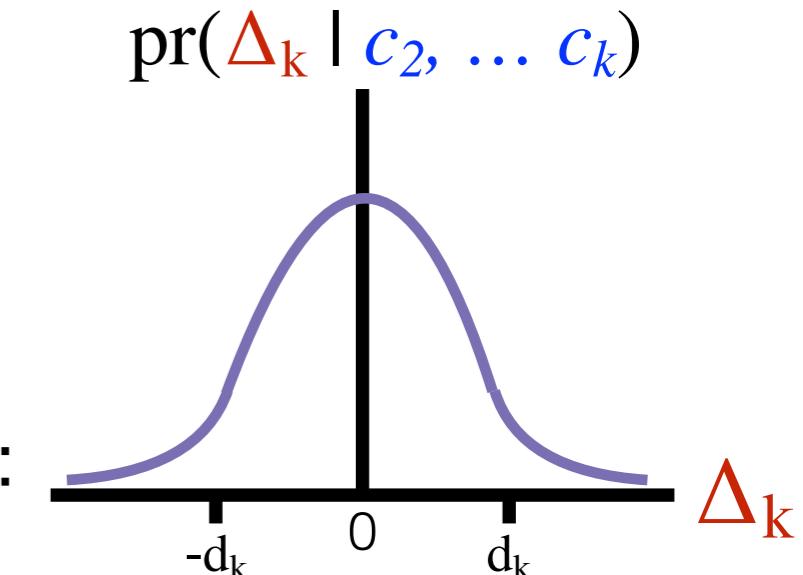


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If the first omitted term dominates, the posterior is

$$\text{pr}(\Delta | \mathbf{c}_k) \propto \int_0^\infty d\bar{c} \text{pr}(\Delta / Q^{k+1} | \bar{c}) \left[\prod_{n=2}^k \text{pr}(c_n | \bar{c}) \right] \text{pr}(\bar{c})$$

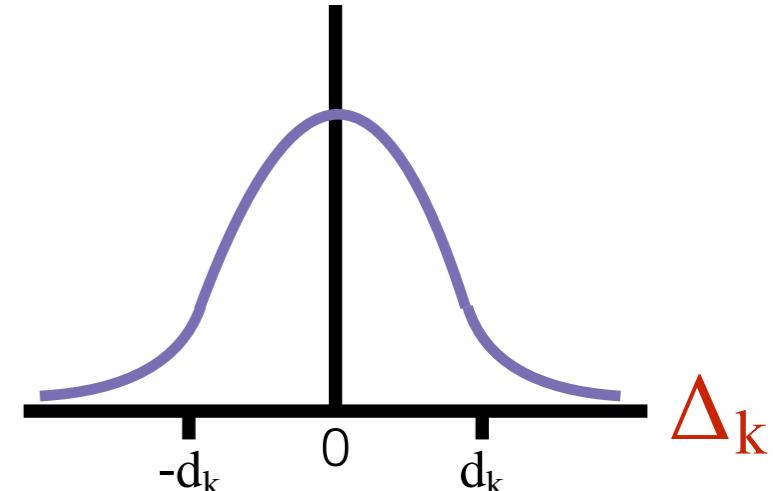
Integrate posterior to find degree of belief (DoB) intervals:



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$$\text{pr}(\Delta_k | c_2, \dots, c_k)$$



Integrate posterior to find degree of belief (DoB) intervals:

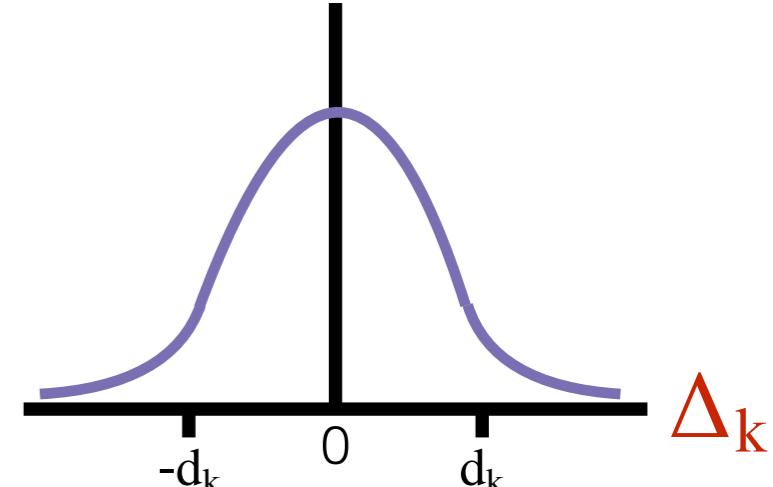
What priors should we choose?

Set	$\text{pr}(c_n \bar{c})$	$\text{pr}(\bar{c})$	
A	$\frac{1}{2\bar{c}} \theta(\bar{c} - c_n)$	$\frac{1}{\ln \bar{c}_>/\bar{c}_<} \frac{1}{\bar{c}} \theta(\bar{c} - \bar{c}_<) \theta(\bar{c}_> - \bar{c})$	Uniform from $\bar{c}_<$ to $\bar{c}_>$
B	$\frac{1}{2\bar{c}} \theta(\bar{c} - c_n)$	$\frac{1}{\sqrt{2\pi}\bar{c}\sigma} e^{-(\ln \bar{c})^2/2\sigma^2}$	Log normal
C	$\frac{1}{\sqrt{2\pi}\bar{c}} e^{-c_n^2/2\bar{c}^2}$	$\frac{1}{\ln \bar{c}_>/\bar{c}_<} \frac{1}{\bar{c}} \theta(\bar{c} - \bar{c}_<) \theta(\bar{c}_> - \bar{c})$	Uniform from $\bar{c}_<$ to $\bar{c}_>$

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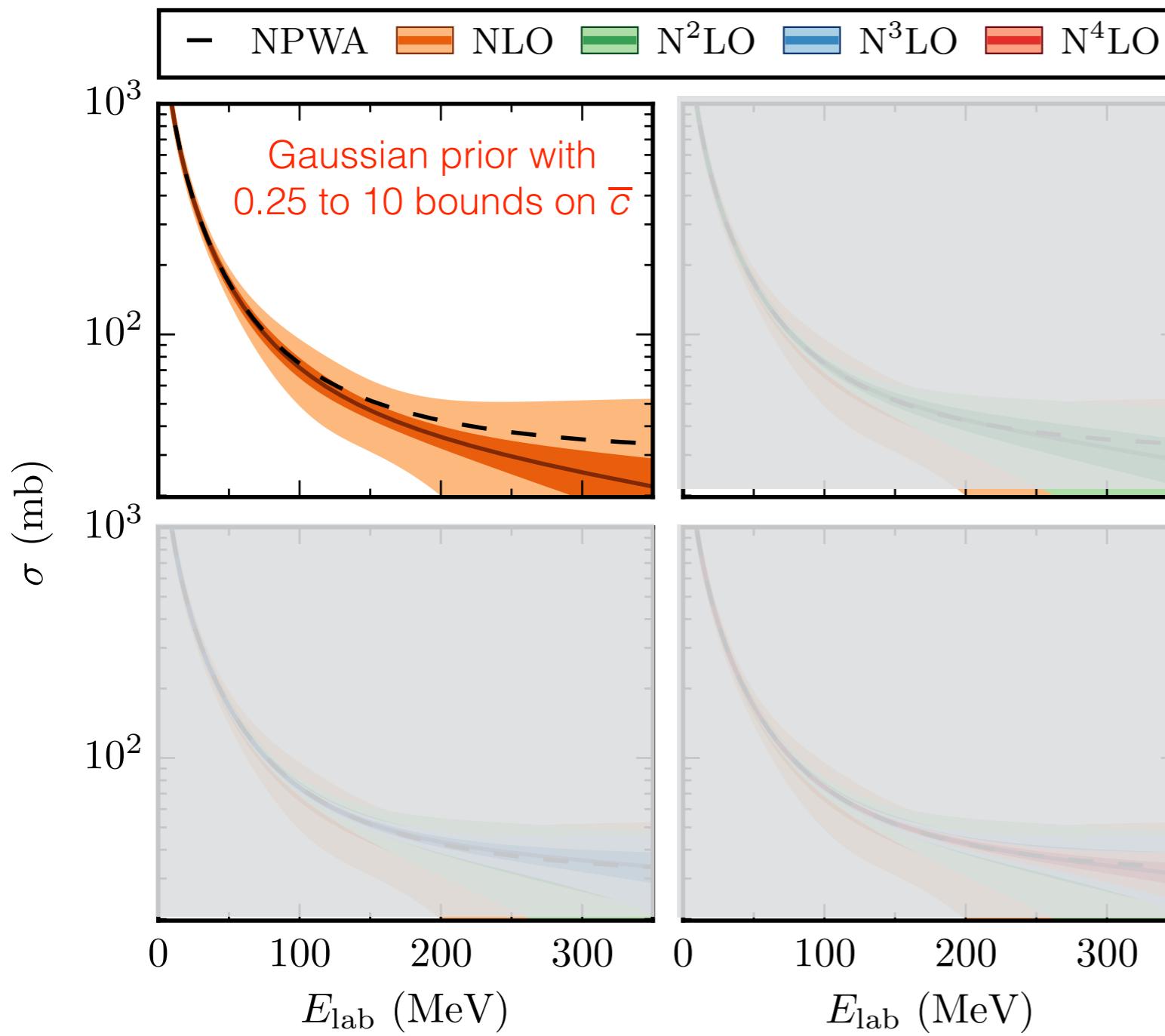
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- Maximum entropy motivates uniform or Gaussian c_n prior
- EKM prescription is set A with no bounds on \bar{c}
- We need to check sensitivity of error bands to details of the priors!

Truncation error estimates

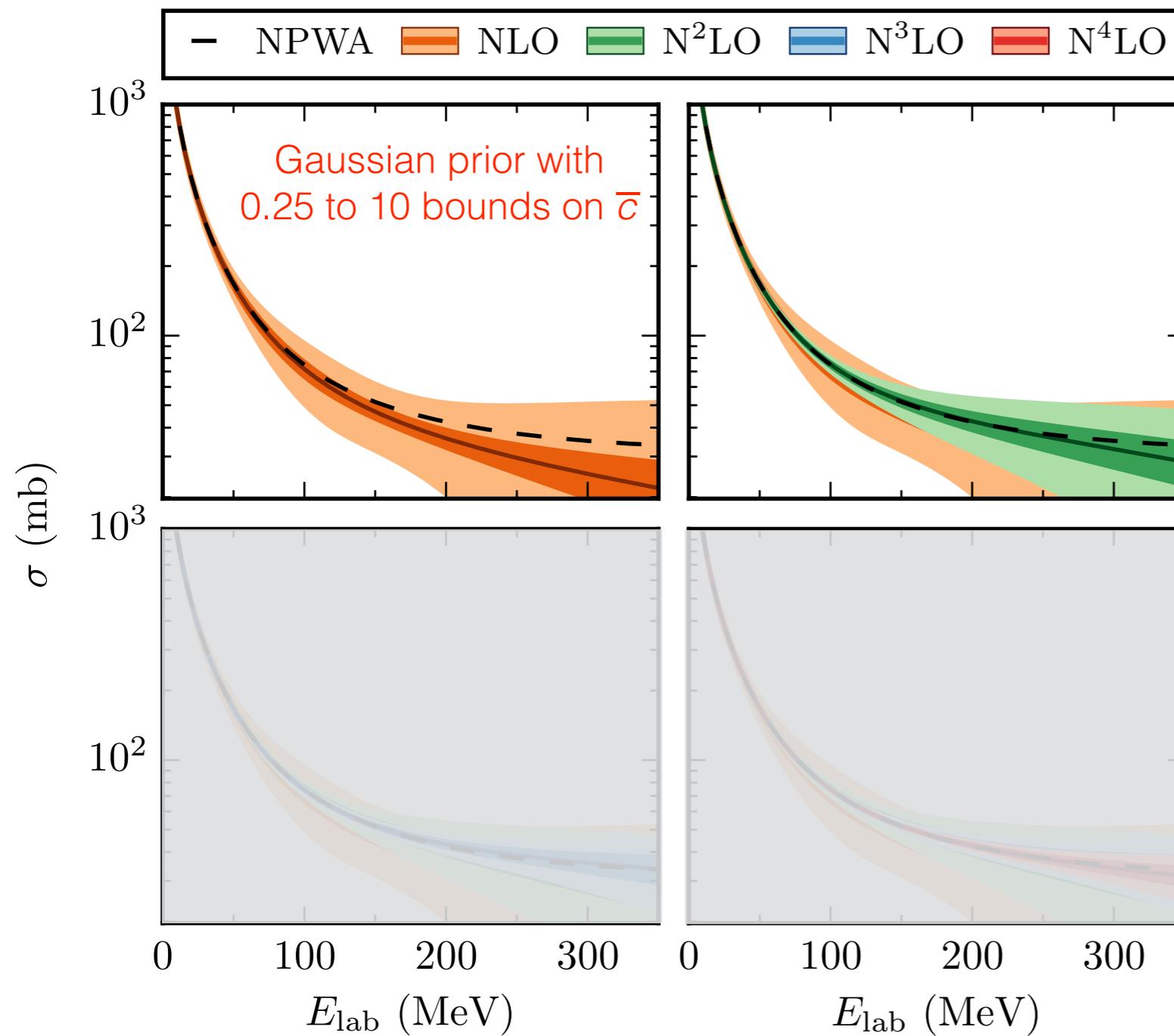
Use the pattern of lower-order corrections to inform estimates for size of higher-order terms



- Total np cross section
- EKM semi-local interaction with $R=0.9$ fm regulator
- NLO through N4LO with error bands (68% and 95% DoBs)
- Compare to Nijmegen PWA93
- Better to look at *residuals* for detailed comparisons

Truncation error estimates

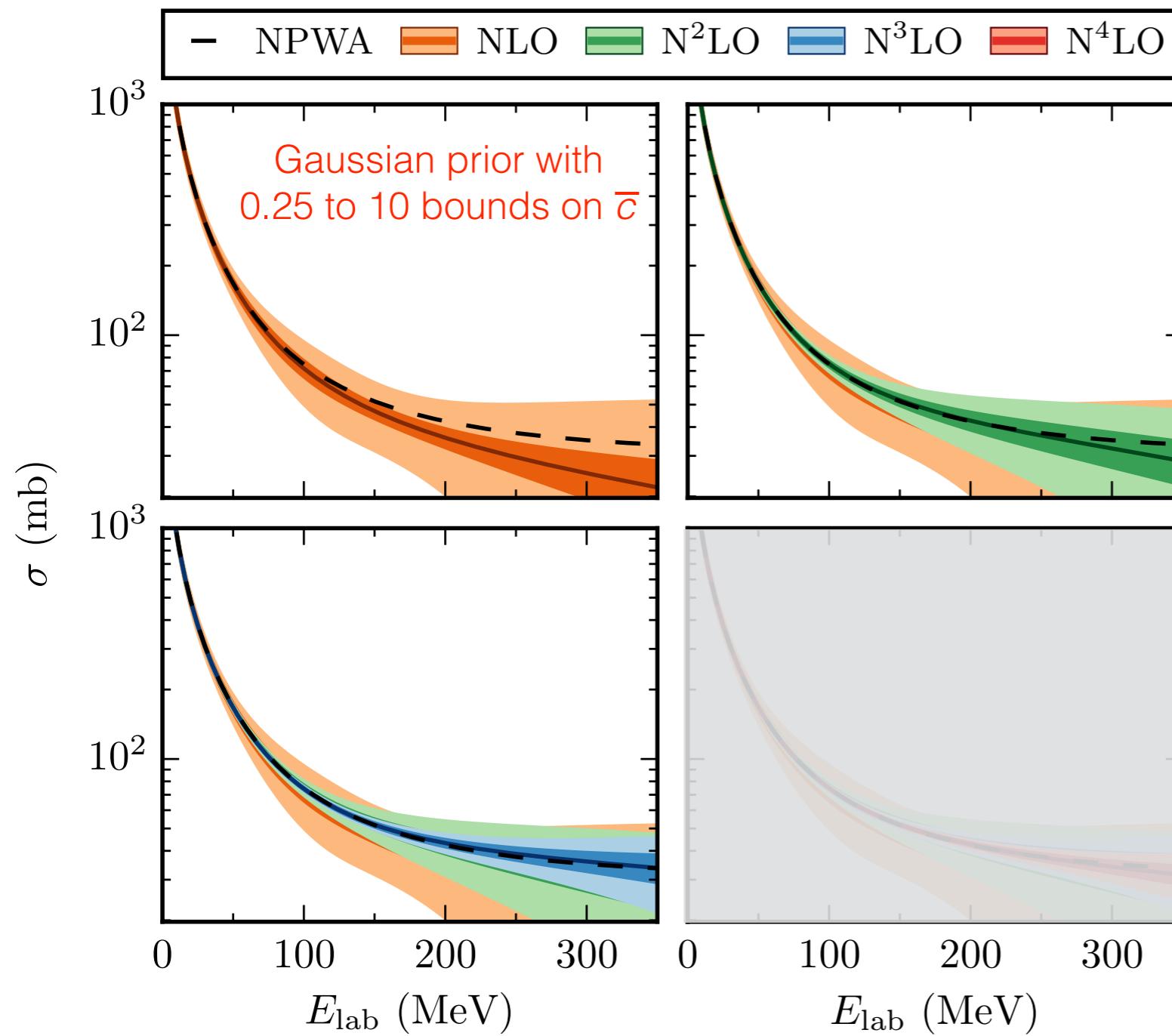
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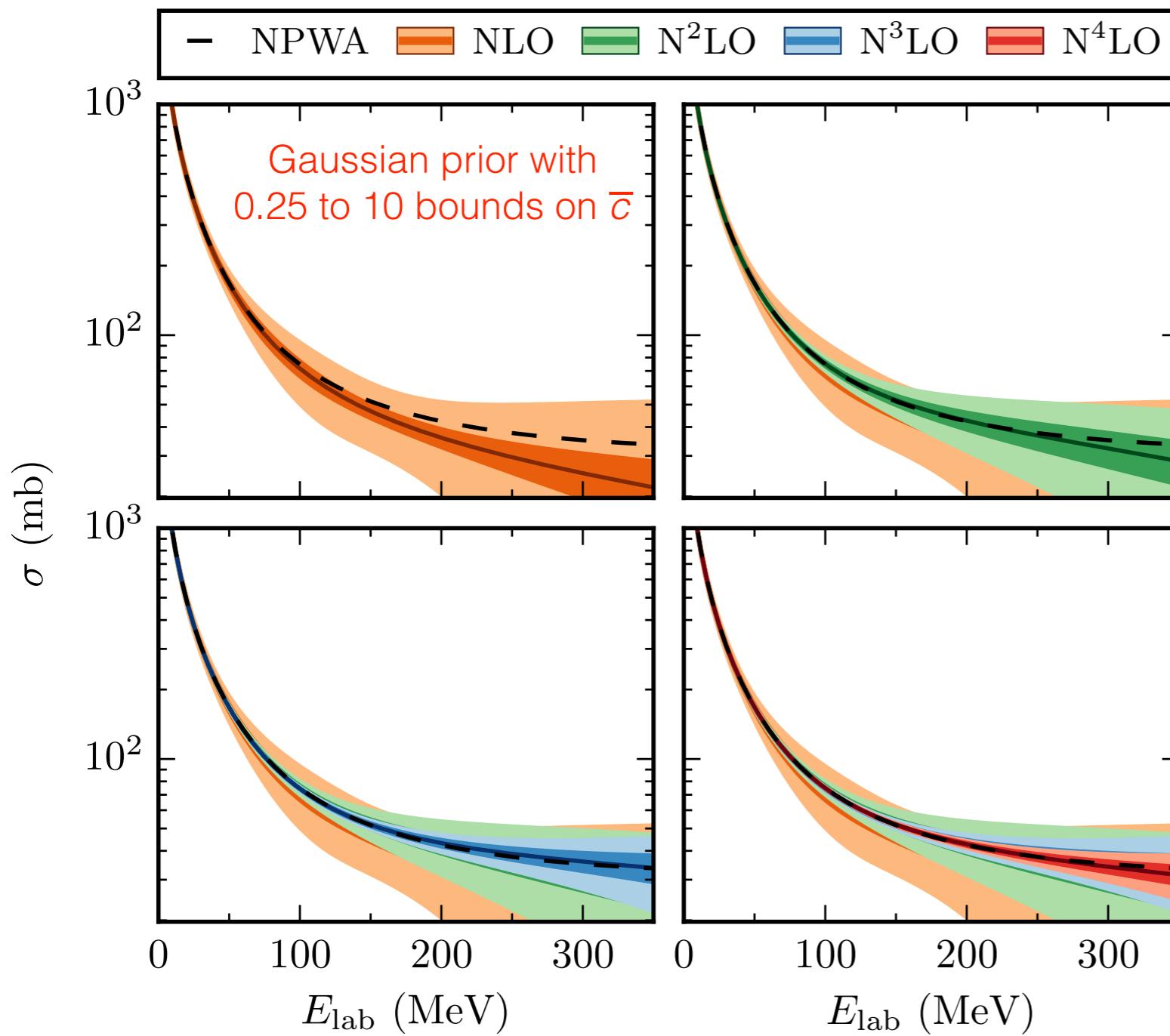
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Truncation error estimates

Use the pattern of lower-order corrections to inform estimates for size of higher-order terms



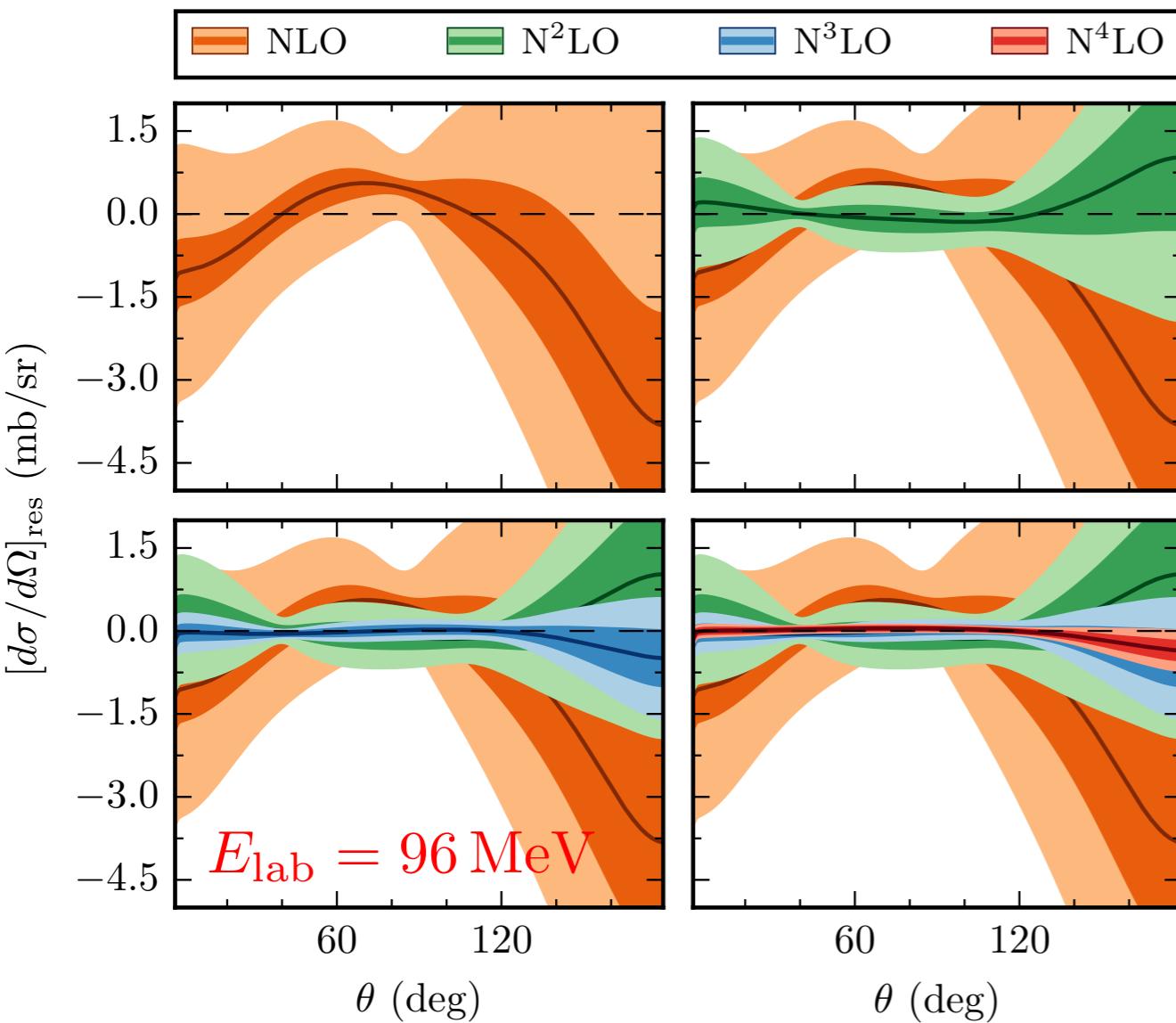
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More truncation error estimates

Use EKM semi-local NN interactions as example.

[V_{NN} from Eur. Phys. J. A **51**, 53 (2015) and Phys. Rev. Lett. **115**, 122301 (2015)]

Differential cross section



- Plotted as a function of angle
- Generate DoB intervals (error bands) and compare to PWA93 (*plotting residuals here*)
- 68% and 95% DoB bands

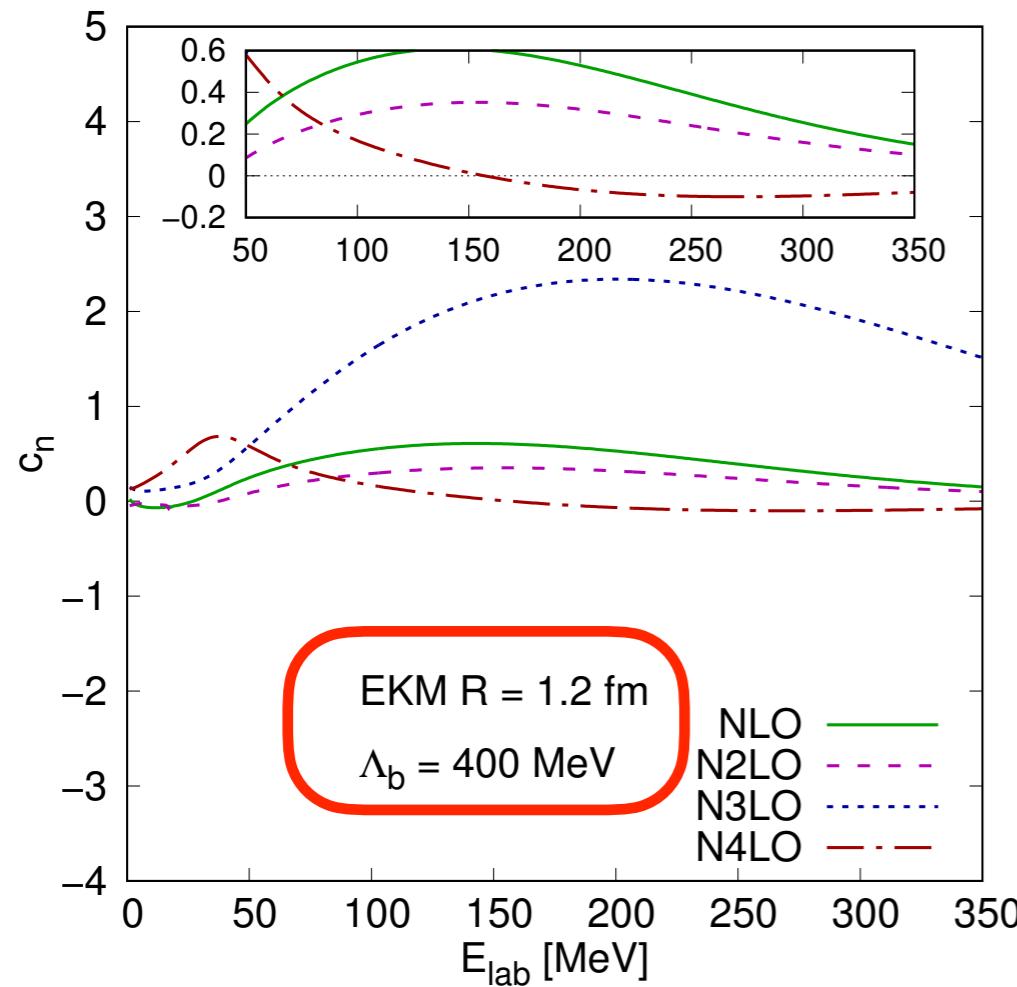
For many more examples:
see [arXiv:1704.03308]

Themes using EFT truncation error example

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Bayesian model checking

- Must check our truncation error model for statistical consistency
- Are the prior assumptions causing issues? Check sensitivity
- We assumed a fixed EFT breakdown scale Λ_b – is it correct?
- What about other regulator values? E.g., for soft EKM R=1.2 fm, do draws from the model posterior look like the “data”?

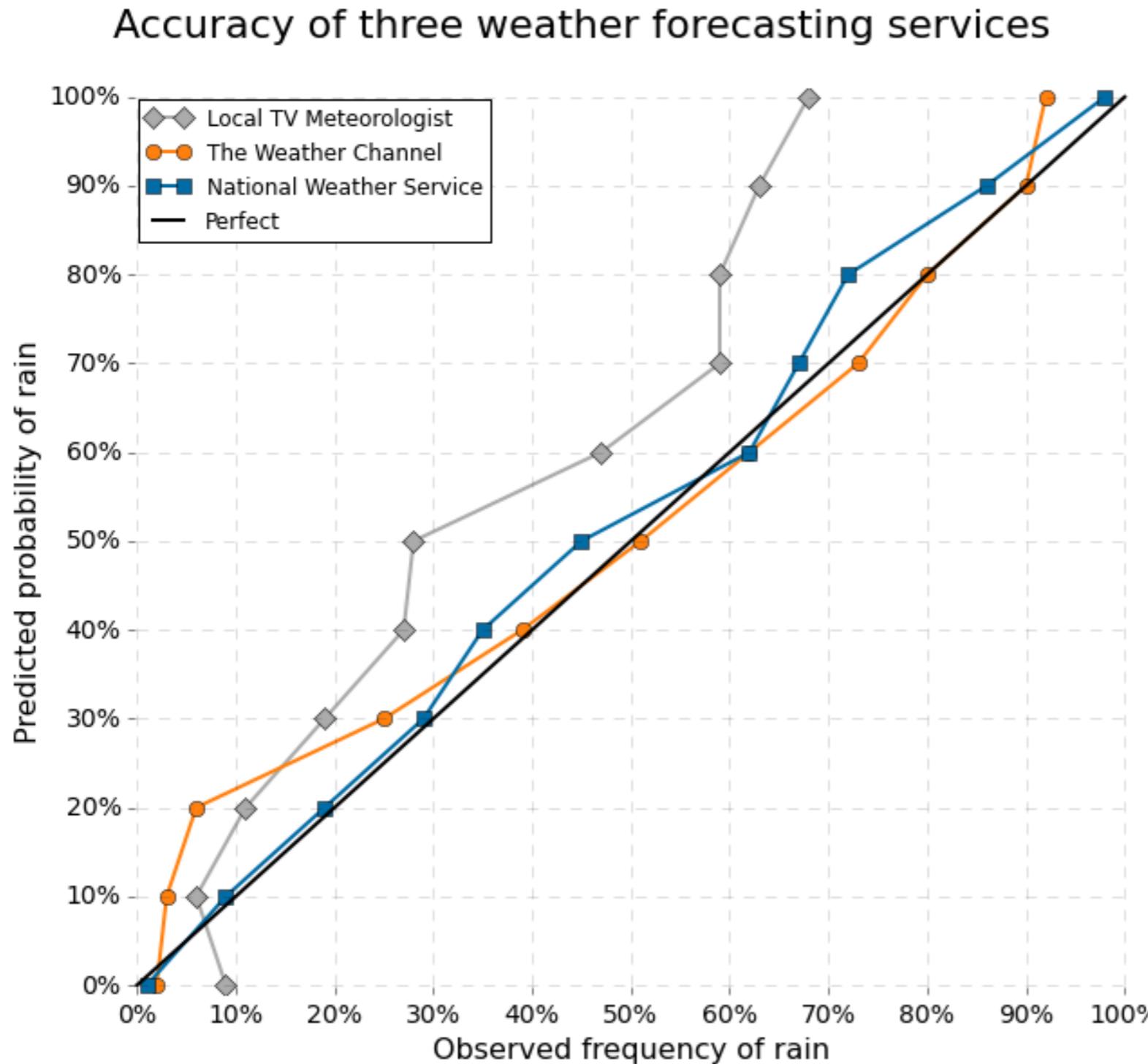


Checks for *statistical* consistency
but also gives insight into physics issues,
e.g., regulator artifacts, etc.

More on Bayesian model checking
see Bayesian Data Analysis by Gelman et al.

Bayesian model checking

Weather forecasting example from Nate Silver's book



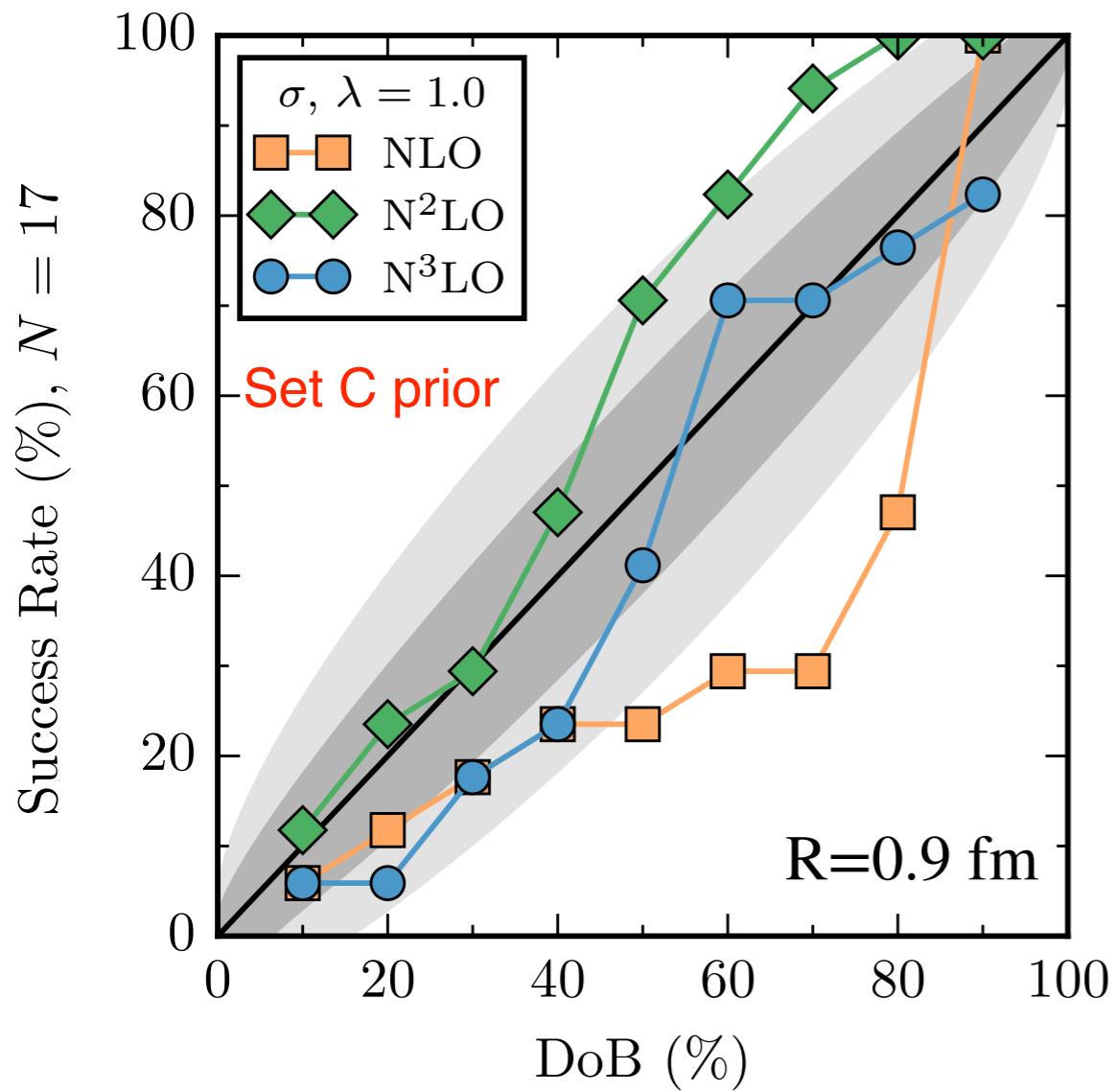
Use a “calibration plot” (or “graph”) to validate the model

Check our EFT
“forecast” the
same way!

Bayesian model checking

“Consistency plots”

details: see [arXiv:1704.03308]

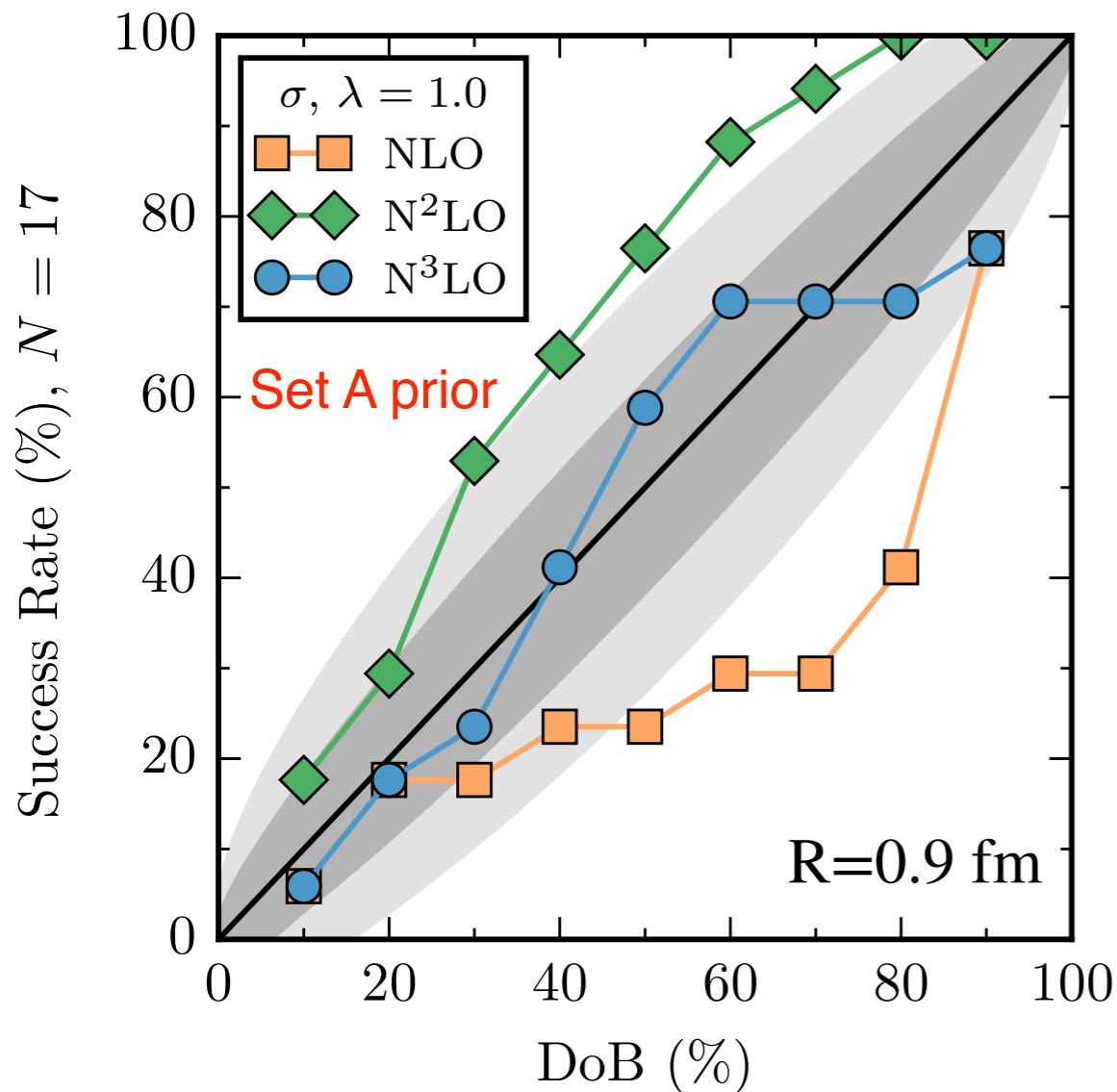


- Choose N predictions of observables
- Here: total cross section at many energies
- How often does the $(k+1)^{\text{th}}$ prediction lie in the $p\%$ error band for prediction at k^{th} order?
- Gray bands are 68% / 95% from finite N
 - First check: Look order-by-order
 - Do any orders have deviant behavior?
 - For this regulator $R=0.9 \text{ fm}$, looks ok

Bayesian model checking

“Consistency plots”

details: see [arXiv:1704.03308]

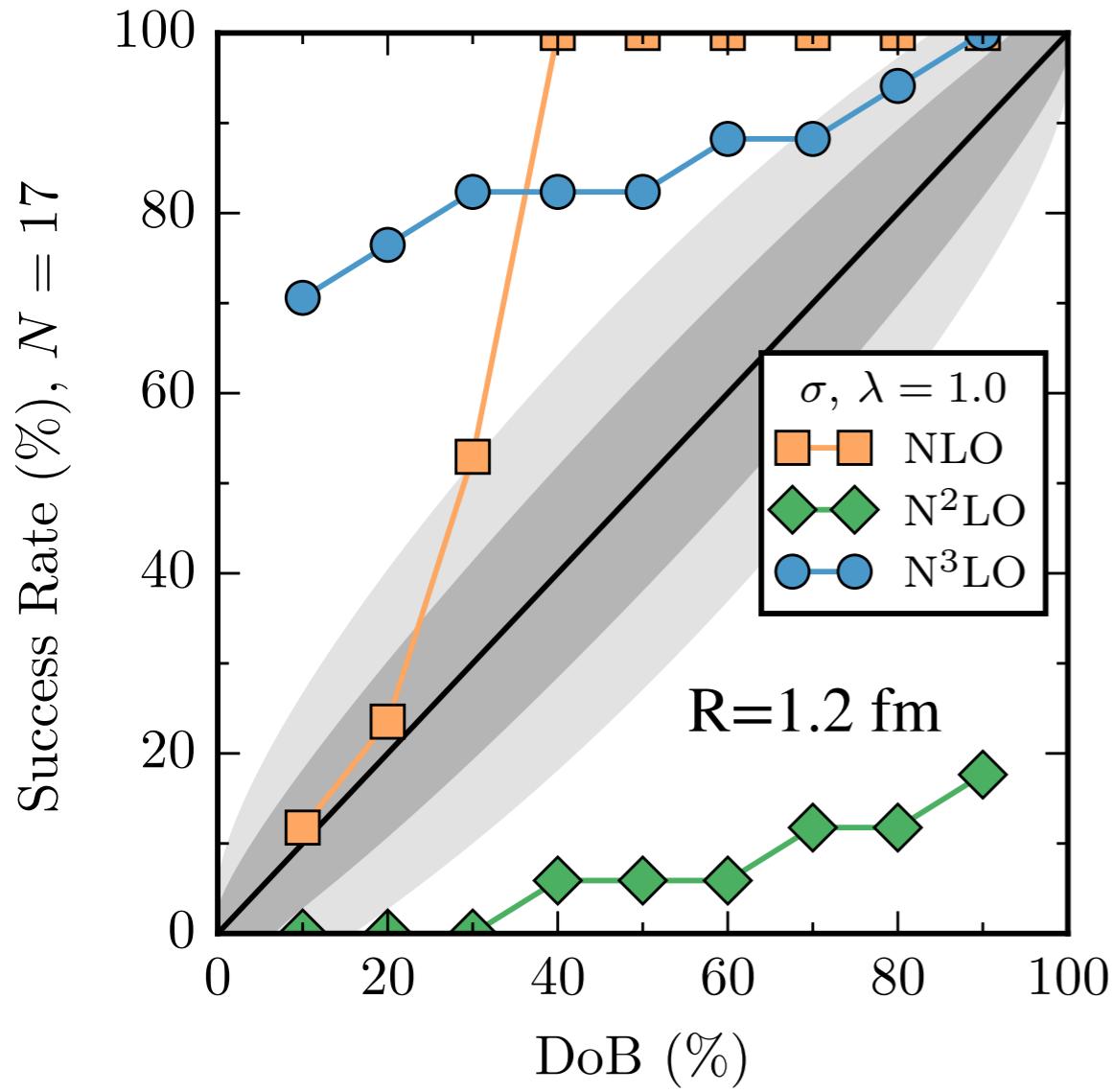


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- First check: Look order-by-order
- Do any orders have deviant behavior?
- For this regulator $R=0.9$ fm, looks ok
- Check sensitivity to prior (here C vs. A)

Bayesian model checking

“Consistency plots”

details: see [arXiv:1704.03308]



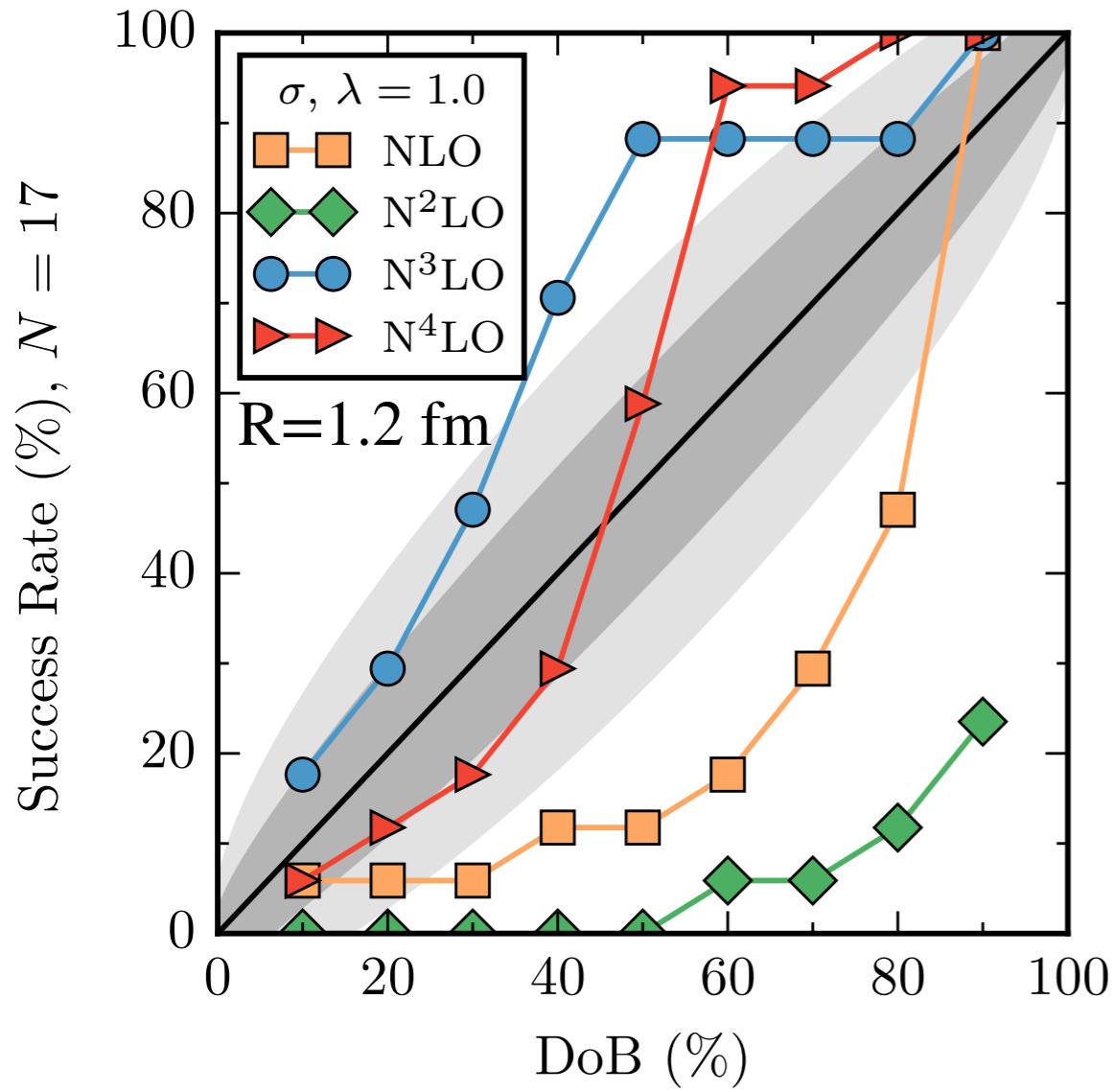
- Total cross section again but R=1.2 fm
- Again look order-by-order
- Do any orders have deviant behavior?
- This regulator does not look so good!
- **Consistent under- and over- prediction!**

For angular observables, other regulators, and more
see [arXiv:1704.03308] and Supplemental material

Bayesian model checking

“Consistency plots”

details: see [arXiv:1704.03308]



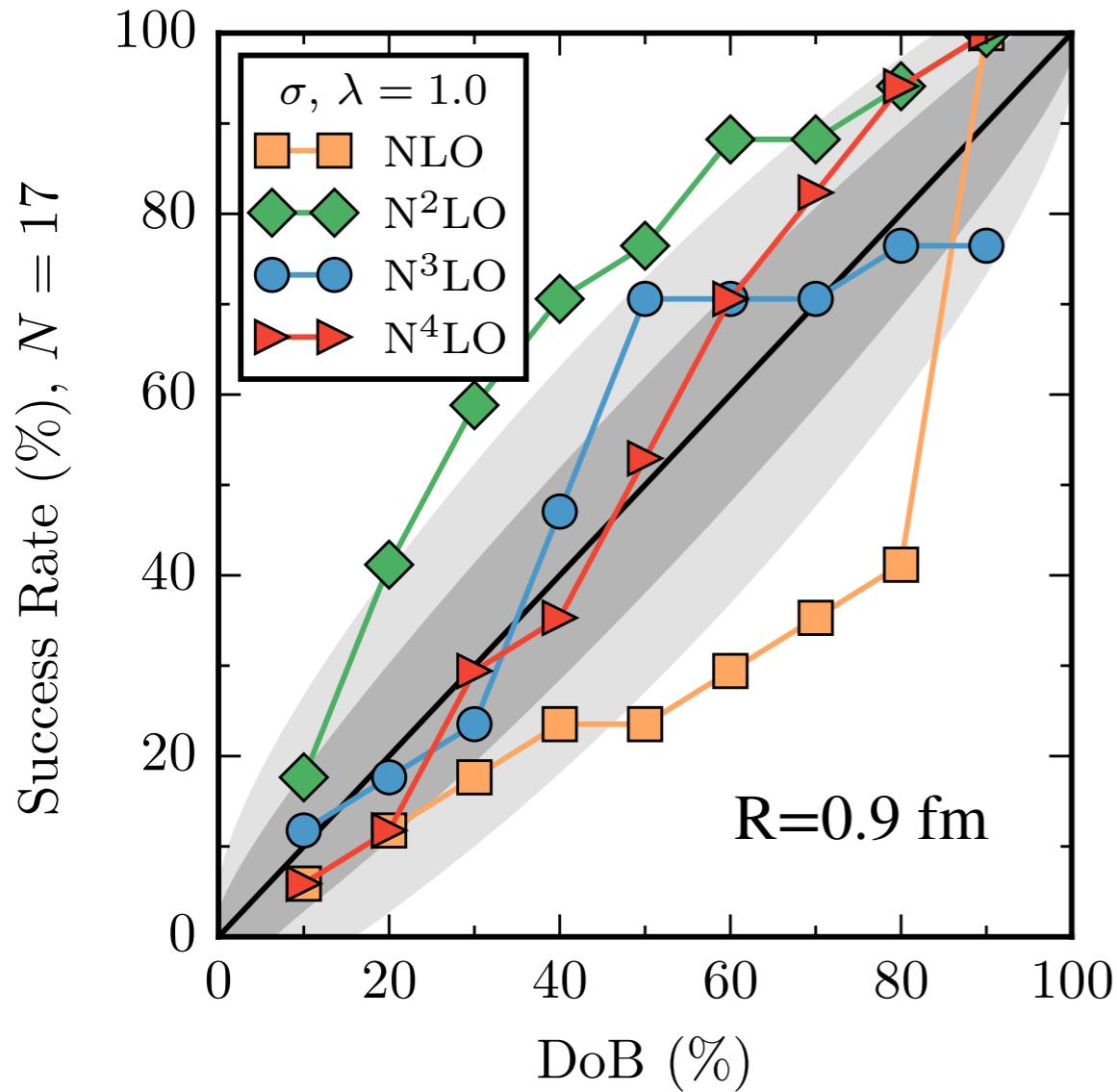
- Total cross section again but $R=1.2$ fm
- Again look order-by-order
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- Consistent under- and over- prediction!
- Ok... but how does it compare to data?

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Bayesian model checking

“Consistency plots”

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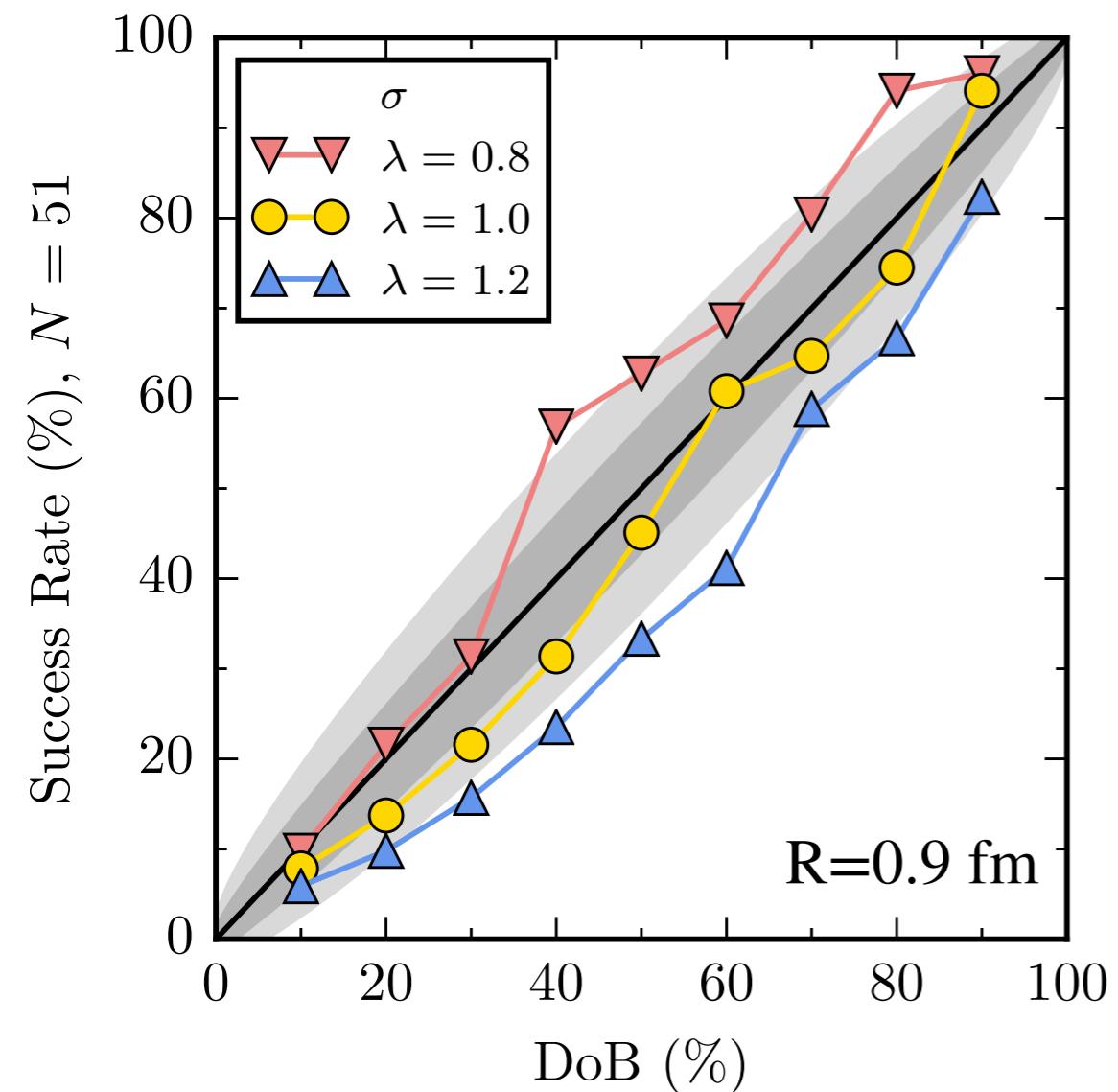
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- Again look order-by-order
- Do any orders have deviant behavior?
- This regulator does not look so good!
- Consistent under- and over- prediction!
- Ok... but how does it compare to data?
- Now check how R=0.9 fm compares ...

For angular observables, other regulators, and more
see [arXiv:1704.03308] and Supplemental material

More Bayesian model checking

“Consistency plots”
details: see [arXiv:1704.03308]

$$X(p) = X_0 \sum_{n=0}^k c_n \lambda^n \left(\frac{p}{\lambda \times \Lambda_b} \right)^n$$



- Choose N predictions of observable (N=51)
- Here: total cross section at many energies
- How often does the $(k+1)^{\text{th}}$ prediction lie in the $p\%$ error band for prediction at k^{th} order?
- Another check: vary expansion parameter
- $\lambda > 1$ indicates larger breakdown favored

Gaussian prior on c_n with
0.25 to 10 bounds on \bar{c}

Themes using EFT truncation error example

- ★ Building a statistical model (Bayes!)
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Extracting the breakdown scale

Our Parameterization

$$\begin{aligned} X(p, \theta) &= X_0 + \Delta X_1 + \cdots + \Delta X_k \\ &= X_{\text{ref}} \left(c_0 + c_1 Q + \cdots + c_k Q^k + \Delta_k \right) \end{aligned}$$

$$\Delta_k = \sum_{n=k+1}^{\infty} c_n Q^n$$

“Data”

$$c_n Q^n = \frac{\Delta X_n}{X_{\text{ref}}} \text{ at } (p, \theta)_i$$

Learned Parameters

$$\begin{aligned} c_n &\sim \text{natural} \\ Q &= \frac{\{p, m_\pi\}}{\Lambda_b} \end{aligned}$$

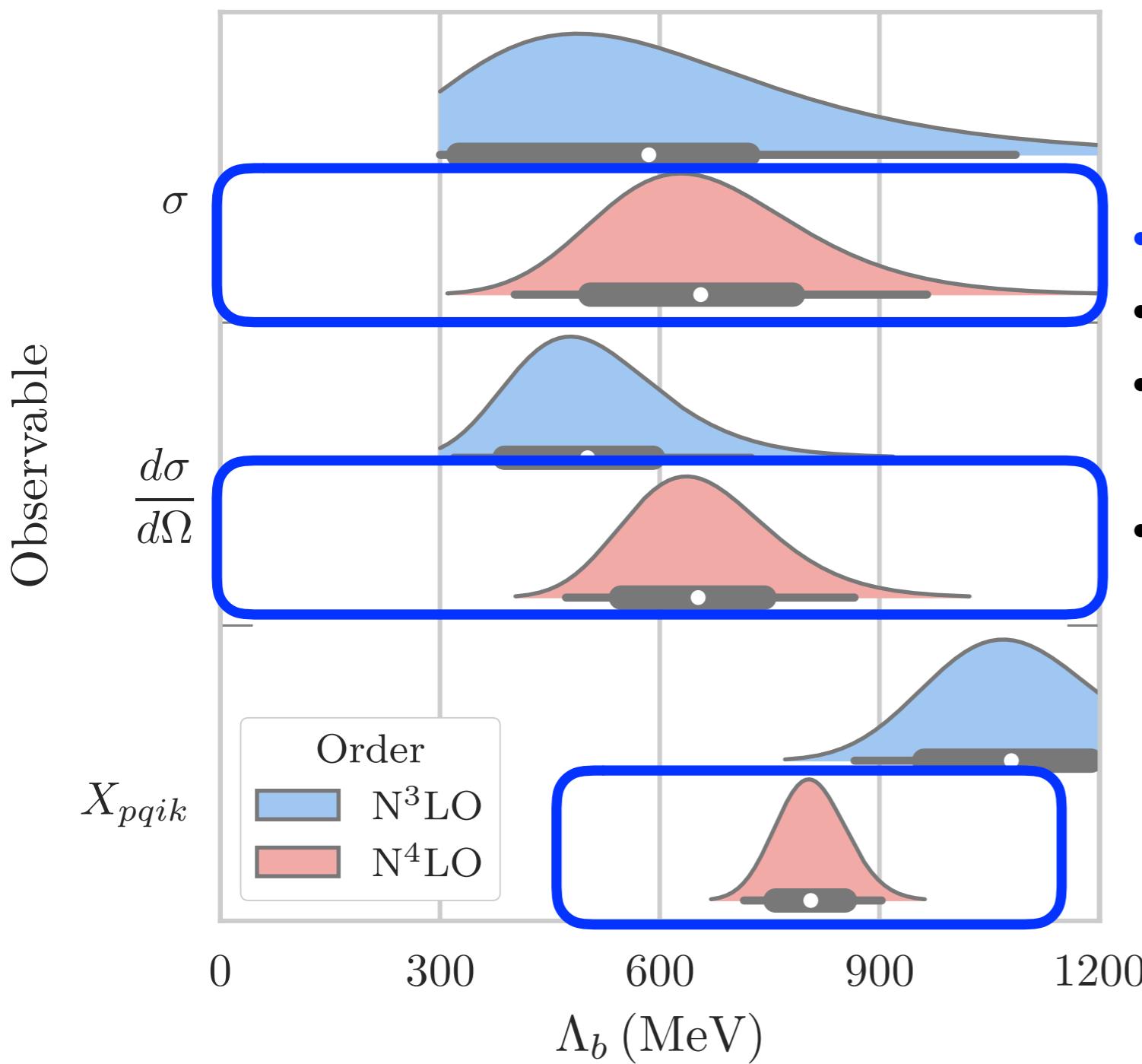
Can we learn Q directly from the expansion?

E.g., find $\text{pr}(\Lambda_b | X_{\text{ref}}, \Delta X_n)$?

Derivation and more details:
see [arXiv:1704.03308]

Posterior for the breakdown scale

Compute the pdf: $\text{pr}(\Lambda_b | X_{\text{ref}}, \Delta X_n)$

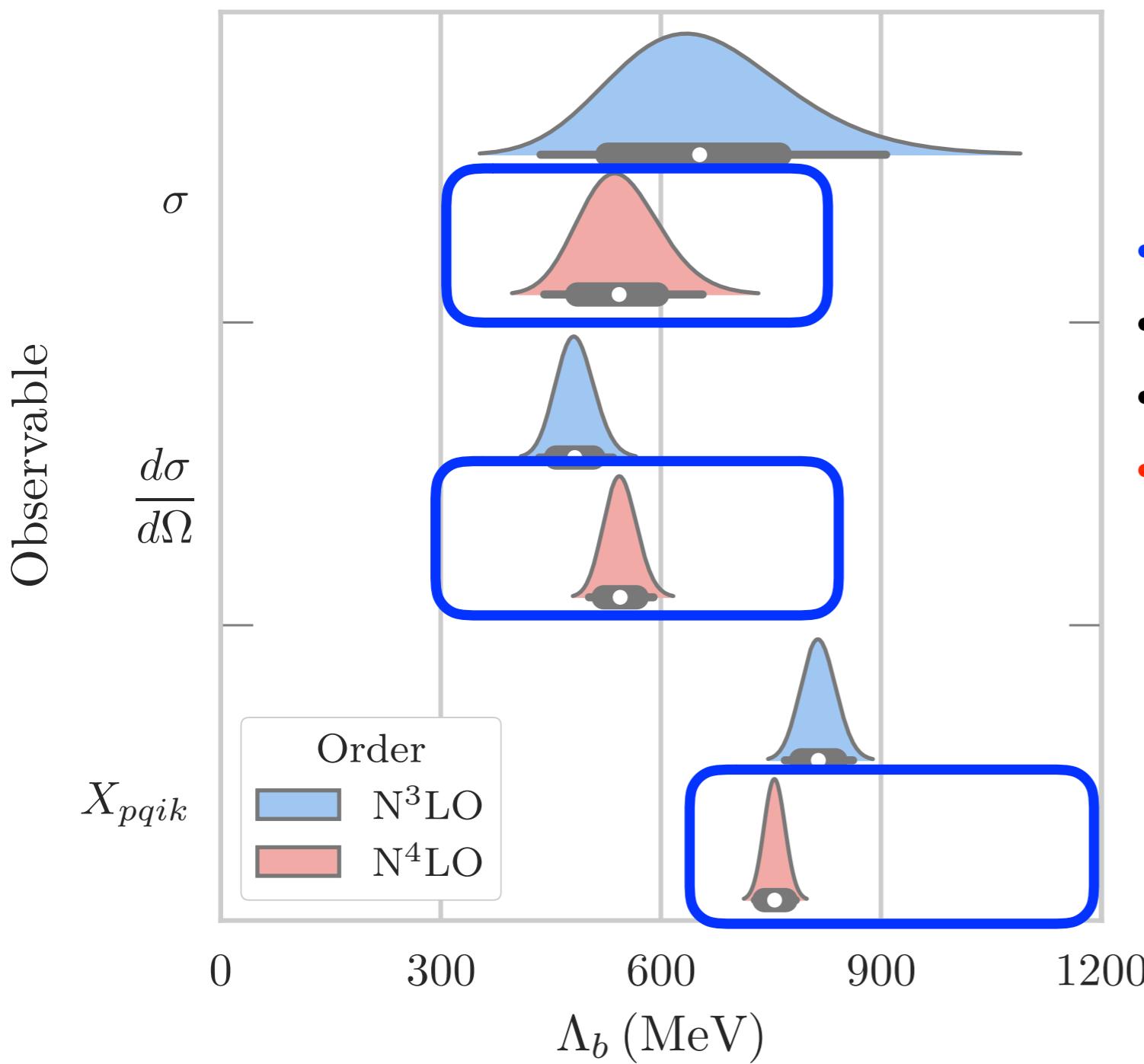


- Focus on results using NLO to N4LO
- $R = 0.9$ fm potential; independent(?)
- Different observables, different breakdown? cf. consistency plots
- Connection to underlying EFT?

EKM extracted: $\Lambda_b = 600$ MeV

Posterior for the breakdown scale

Compute the pdf: $\text{pr}(\Lambda_b | X_{\text{ref}}, \Delta X_n)$

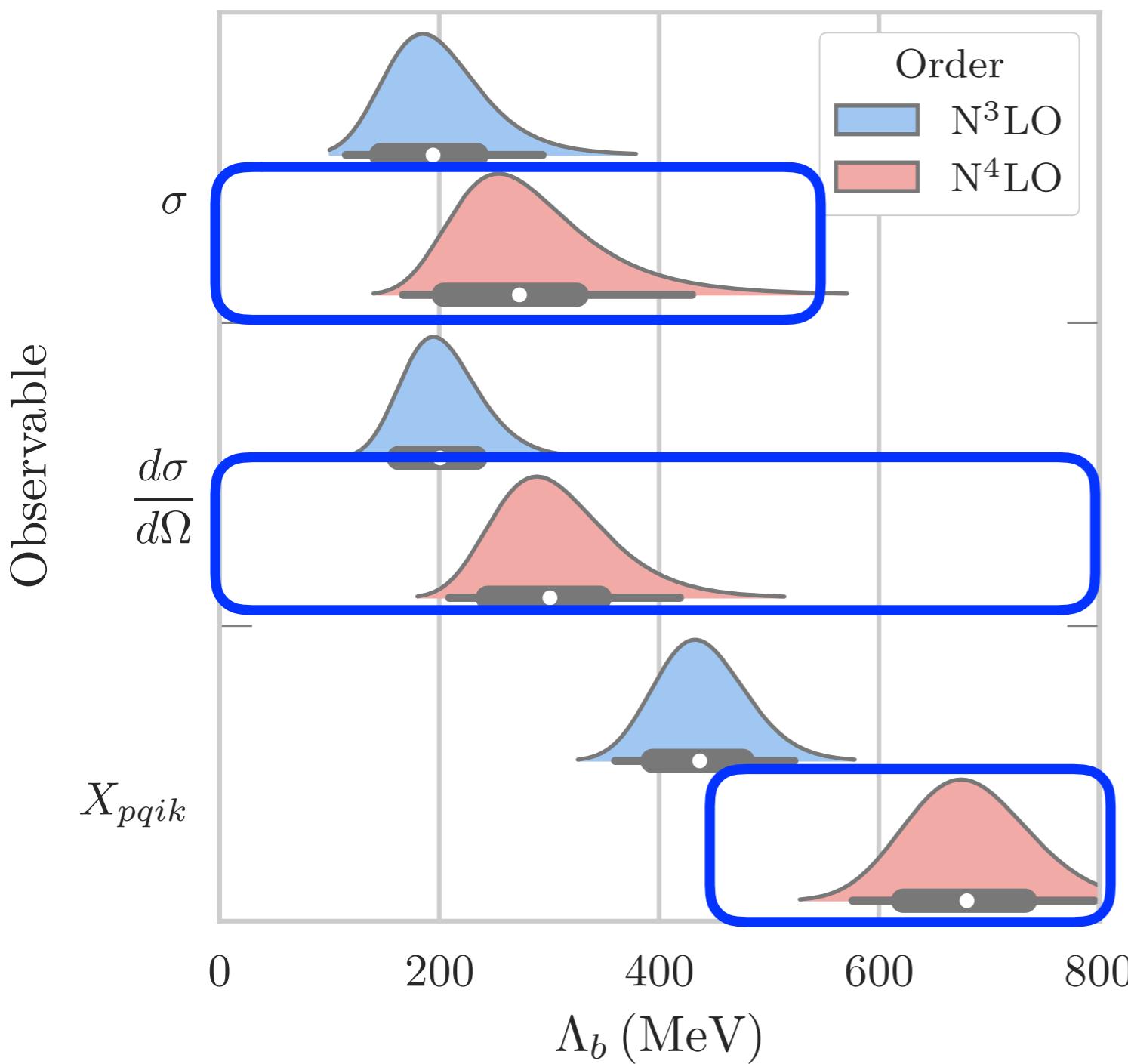


- Focus on results using NLO to N4LO
- R=0.9 fm, more energies and angles
- Smaller width; are they consistent?
- Possibly using redundant information:
How can we account for correlations?

EKM extracted: $\Lambda_b = 600$ MeV

Posterior for the breakdown scale

Compute the pdf: $\text{pr}(\Lambda_b | X_{\text{ref}}, \Delta X_n)$



- Focus on results using NLO to N4LO
- R=1.2 fm, indicates $x > 1$ expansion
- Inconsistent with statistical model

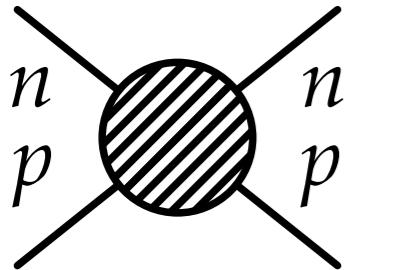
EKM extracted: $\Lambda_b = 400$ MeV

Themes using EFT truncation error example

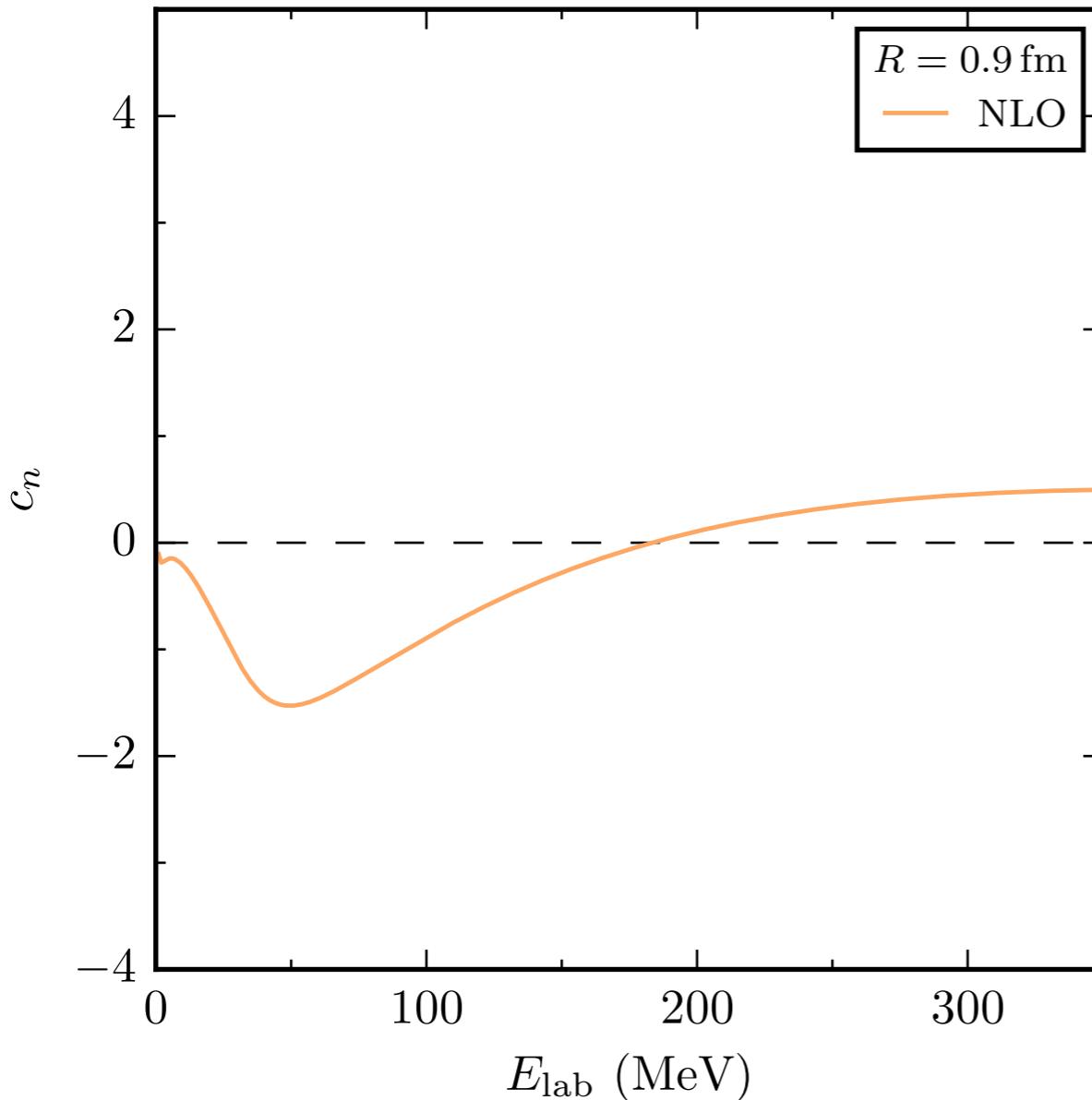
- ★ Building a statistical model (Bayes!)
 - How do we exploit an EFT expansion?
- ★ Model checking and validation
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 - Can we *extract* the EFT expansion parameter?
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 - Using Gaussian processes in our model
- ★ Combining with other errors
 - Parameter estimation and truncation errors

COEFFICIENT FUNCTIONS

(Note: $c_1 = 0$ in χ EFT!)



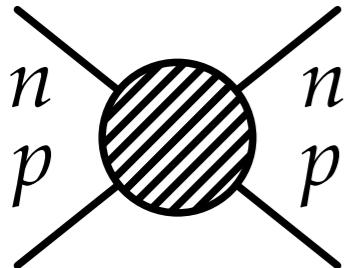
$$\sigma_{\text{tot}}(E) = \sigma_{\text{ref}}(E) \left(c_0(E) + c_2(E) Q^2 \right)$$



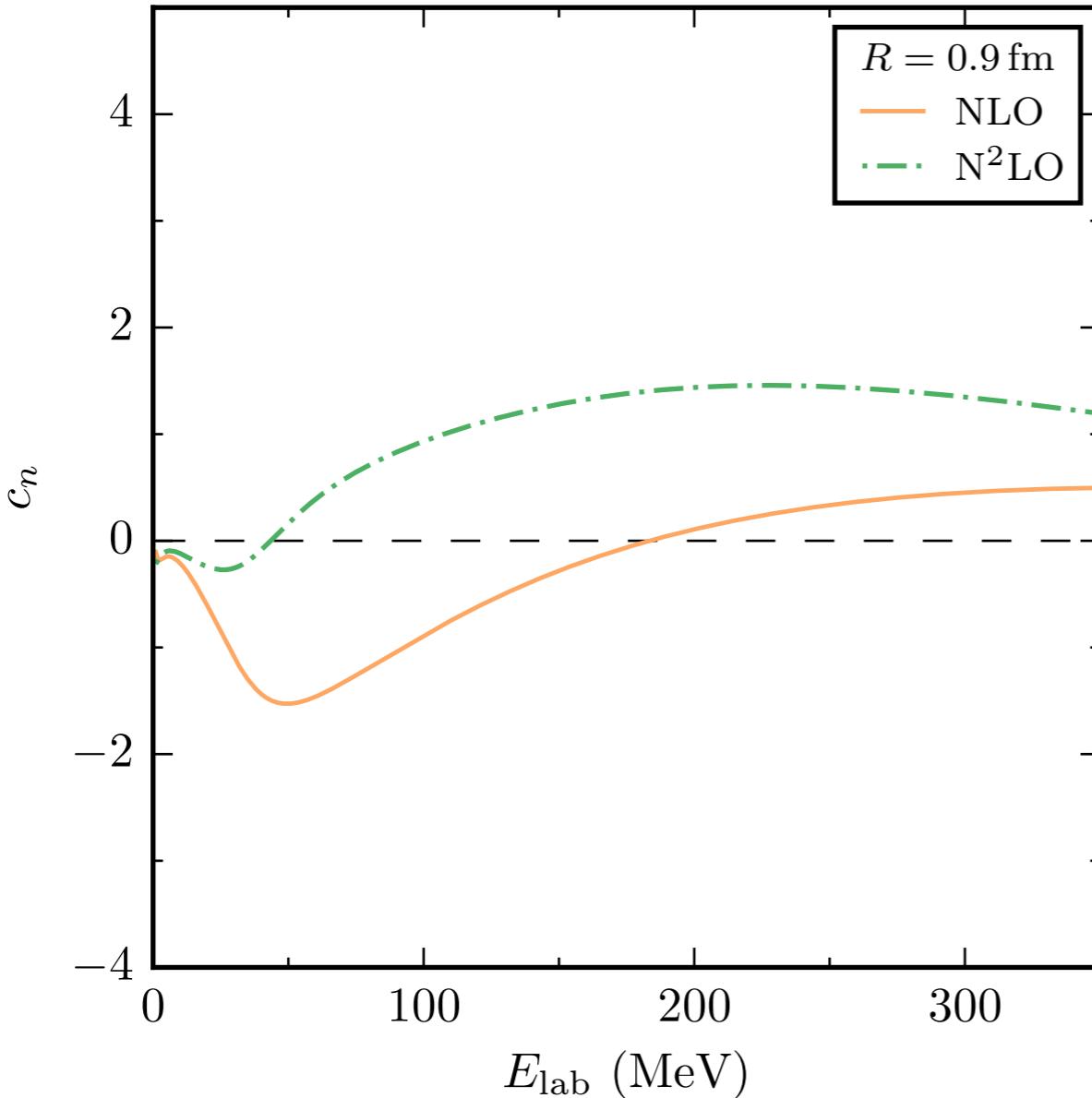
- This is a double expansion:
$$Q = \frac{\{p, m_\pi\}}{\Lambda_b}$$
- Smooth crossover assumed

COEFFICIENT FUNCTIONS

(Note: $c_1 = 0$ in χ EFT!)



$$\sigma_{\text{tot}}(E) = \sigma_{\text{ref}}(E) \left(c_0(E) + c_2(E)Q^2 + c_3(E)Q^3 \right)$$



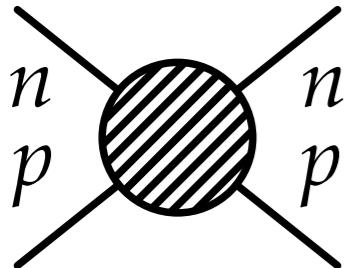
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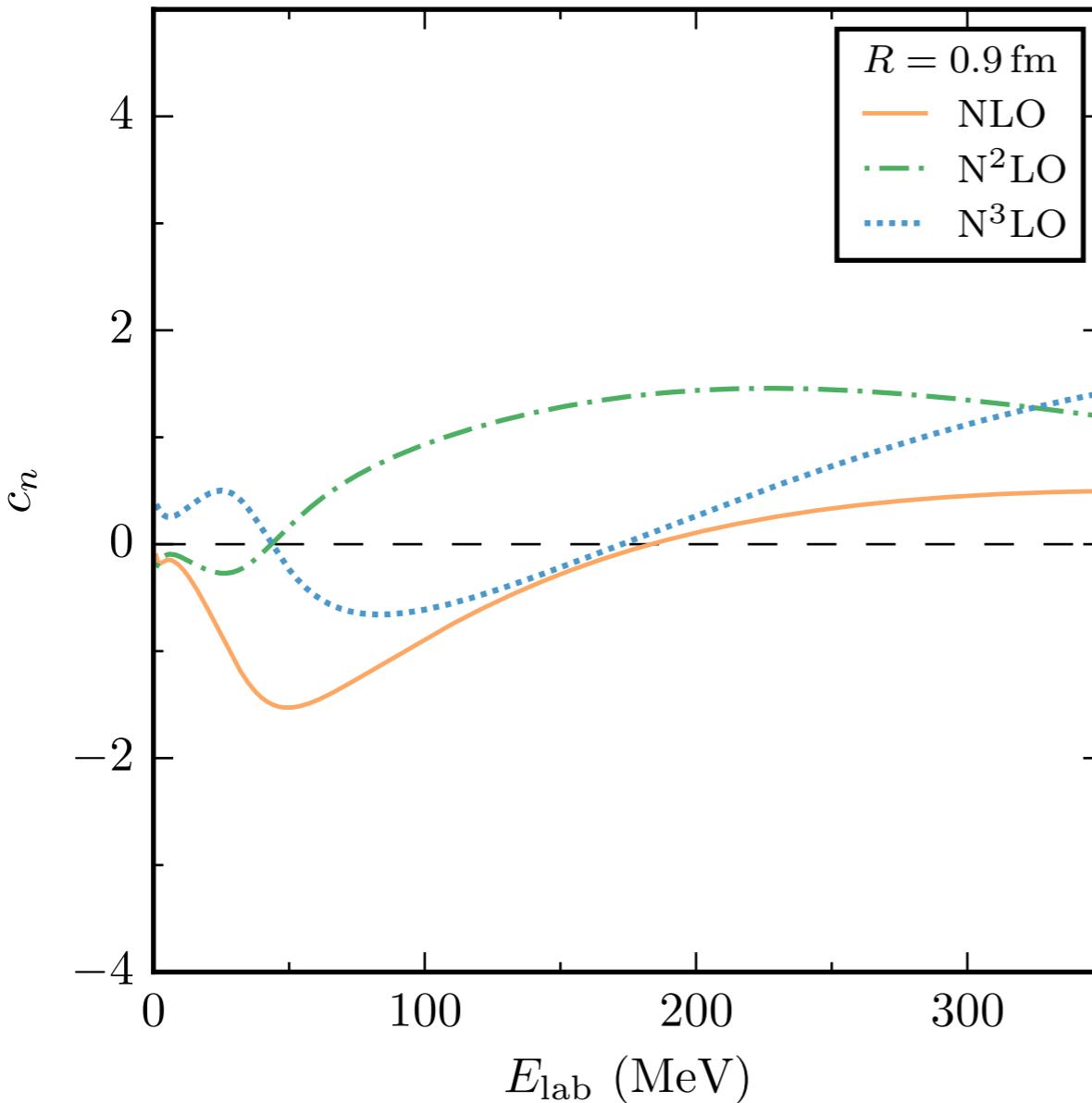
COEFFICIENT FUNCTIONS

(Note: $c_1 = 0$ in χ EFT!)



$$X_0 + \Delta X_2 + \Delta X_3 + \Delta X_4$$

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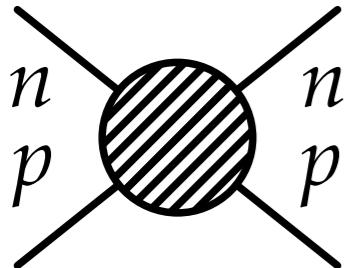
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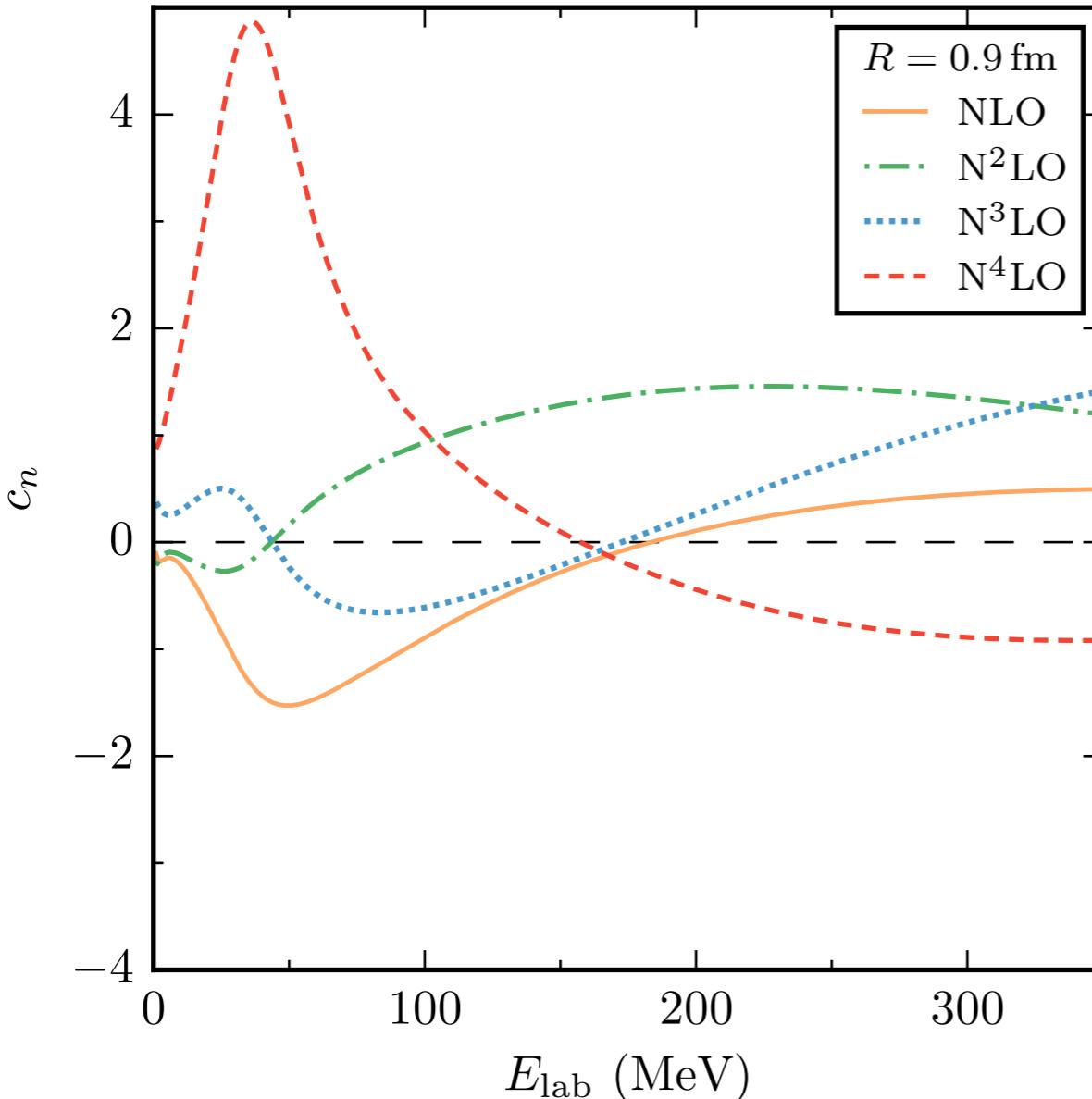
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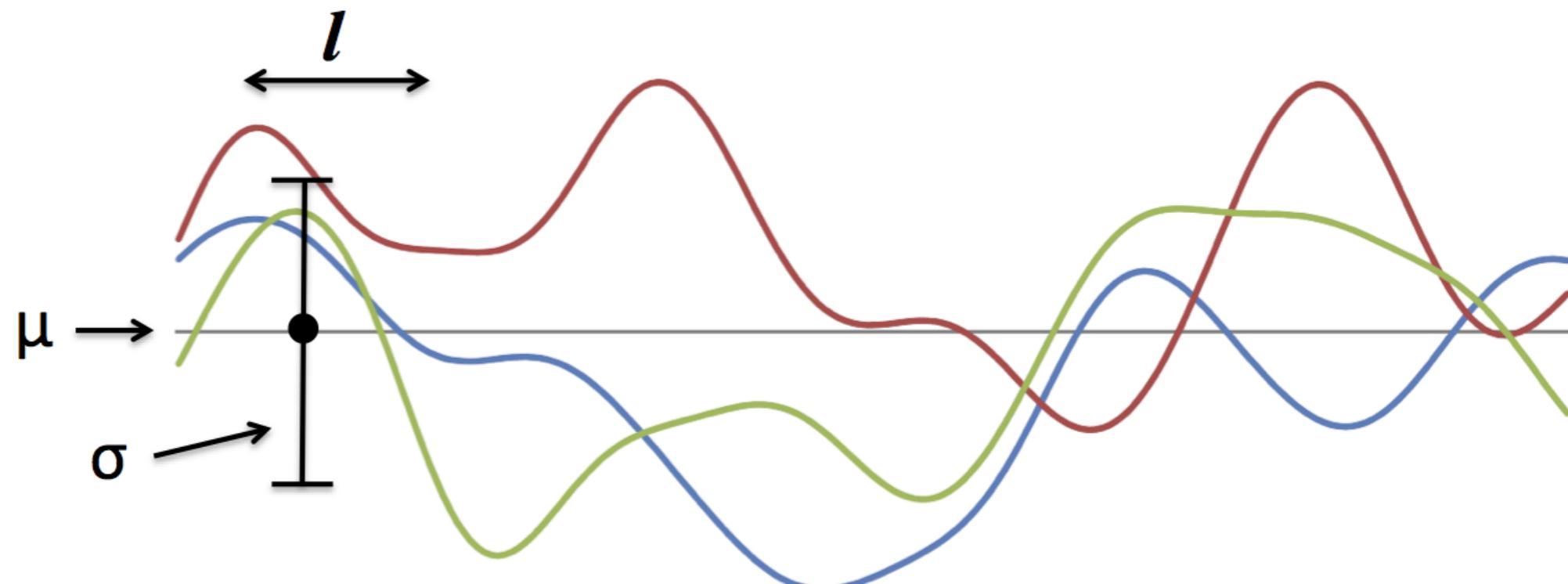


- This is a double expansion:
$$Q = \frac{\{p, m_\pi\}}{\Lambda_b}$$
- Smooth crossover assumed
- Large scattering length physics at small E_{lab} !

Gaussian Process (GPs)

Natural generalization of multivariate Gaussian random variables to infinite (countably or continuous) index sets

Random draws from a GP:



GP specified by hyperparameters for mean, std dev, correlation length

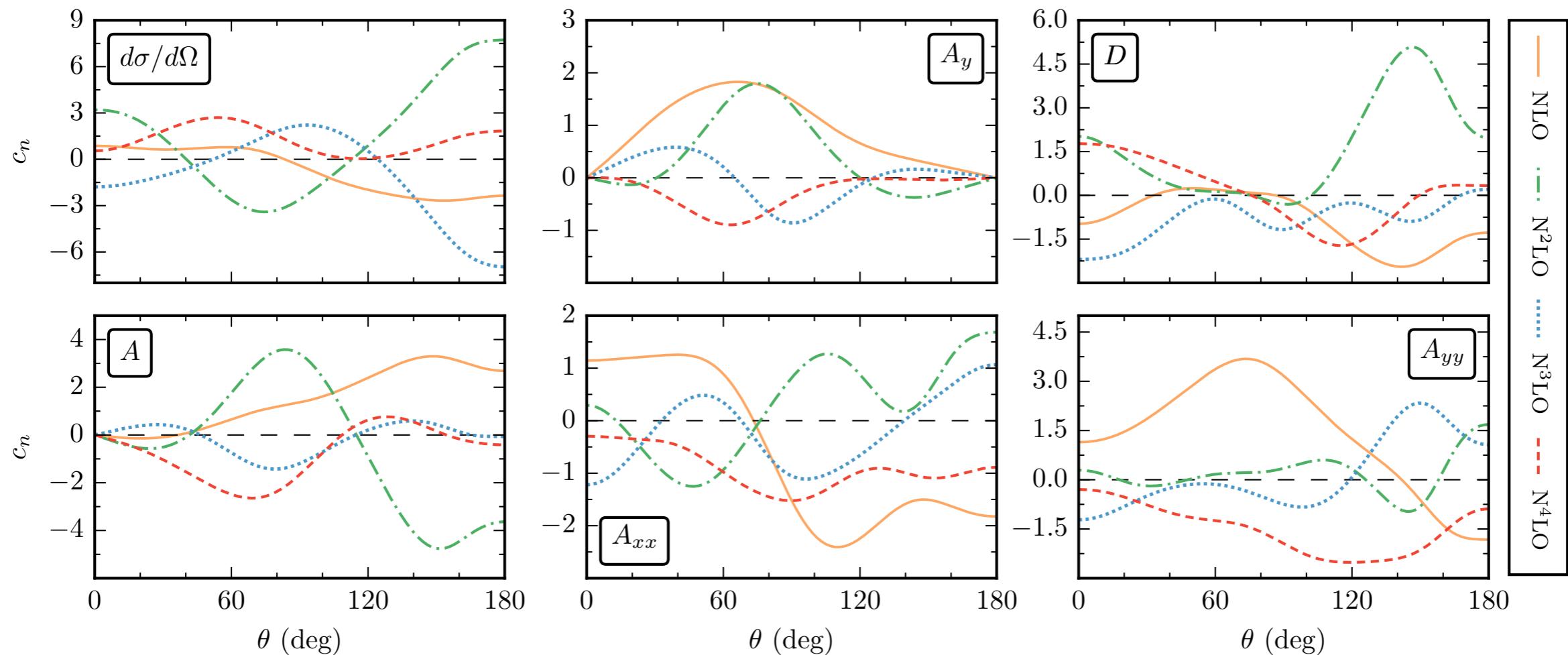
$$\text{pr}(c(\mathbf{x})|\mu(\mathbf{x}), k) = \frac{1}{Z} e^{-\frac{1}{2} (c(\mathbf{x}) - \mu(\mathbf{x}))^T k^{-1} (c(\mathbf{x}') - \mu(\mathbf{x}'))}$$

$$\text{where (e.g.) } k(\mathbf{x}, \mathbf{x}'; \theta) = \bar{c}^2 e^{-\frac{1}{2} \sum_i (x_i - x'_i)^2 / l_i^2}$$

Gaussian Process (GPs)

Natural generalization of multivariate Gaussian random variables to infinite (countably or continuous) index sets

Our coefficient data:

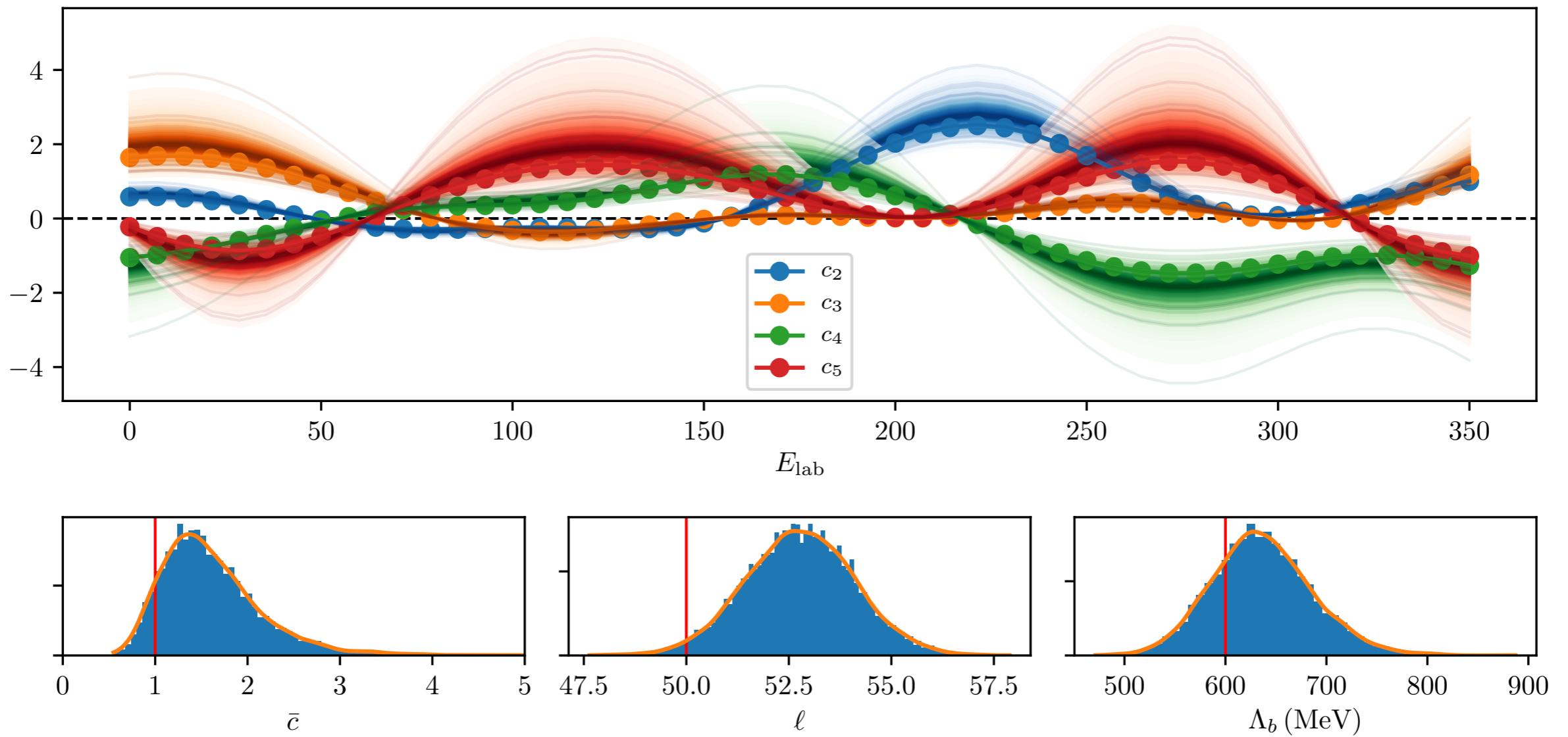


For coefficient functions of energy, other regulators, and more
see [arXiv:1704.03308] and Supplemental material

Non-parametric stochastic model using Gaussian process

Knowledge of correlations → better estimates of error, Λ_b , etc.

Test problem with synthetic data: Can we recover \bar{c} , l , and Λ_b ?



MCMC sampling recovers input parameters. Real-data tests in progress.

Themes using EFT truncation error example

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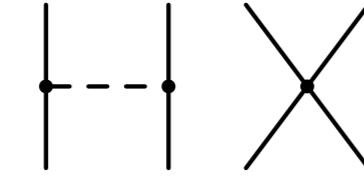
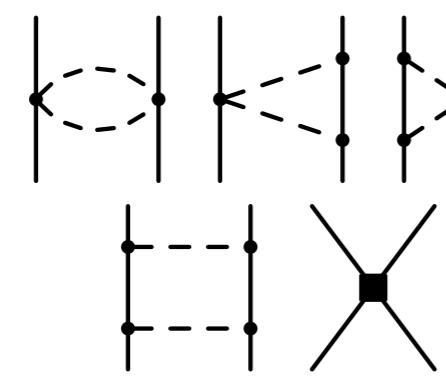
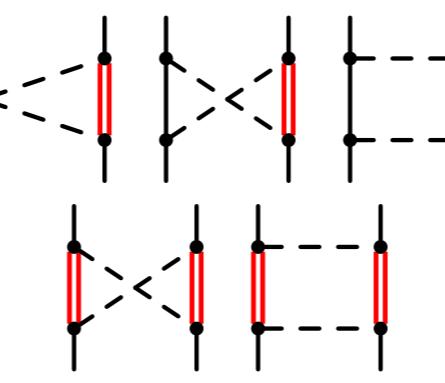
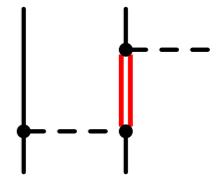
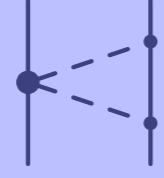
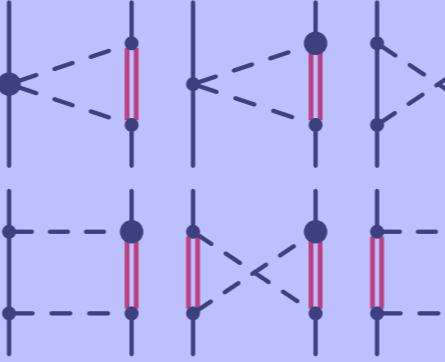
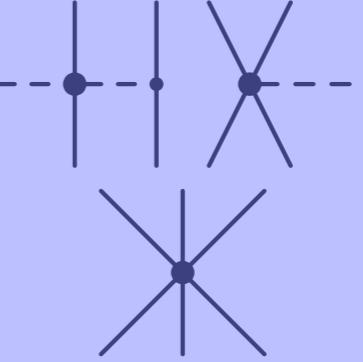
Effective field theories as expansions

Example: chiral EFT NN + 3N *potential* with
Weinberg power-counting

		NN force		$3N$ force	
		Δ -less EFT	Δ contributions	Δ -less EFT	Δ contributions
		LO		NLO	
	Δ -less EFT		—	—	—
LO	Δ contributions		—		—
NLO	Δ -less EFT			—	
N ² LO	Δ -less EFT				—

Effective field theories as expansions

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		Δ -less EFT	Δ contributions	Δ -less EFT	Δ contributions
LO			—	—	—
NLO				—	
$N^2\text{LO}$					—

Truncation error: omitted higher-order diagrams

Effective field theories as expansions

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NLO	 	—	—	
N^2LO	 	—	 	—

Parameter estimation: e.g. NN and NNN contacts

Effective field theories as expansions

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		LO		NLO	
			—	—	—
				—	
					—

“Bayesian model selection”: What are the optimal degrees of freedom?

Parameter estimation including truncation error

See “Bayesian parameter estimation for effective field theories”,
J. Phys. G 43, 074001 (2016) for extensive framework including diagnostics

- Bayesian framework ideal for combining errors with transparent assumptions
 - Basic parameter estimation problem: find the posterior for a parameter vector \mathbf{a} given some data D and information I , which includes EFT details.
 - That is, find $\text{pr}(\mathbf{a}|D, I)$ and also posteriors for observables X : $\text{pr}(X|D, I)$

$$\text{pr}(\mathbf{a}|D, k, k_{\max}, I) \propto \underbrace{\text{pr}(D|\mathbf{a}, k, k_{\max}, I)}_{\text{likelihood}} \underbrace{\text{pr}(\mathbf{a}|k, k_{\max}, I)}_{\text{prior}}$$

chiral order

truncation order

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chiral order

truncation order

Marginalize over higher-order observable coefficients (first omitted here):

$$\begin{aligned} \text{pr}(D|\mathbf{a}, I') &= \int dc_{k+1} \text{pr}(D, c_{k+1}|\mathbf{a}, I') \\ &= \int dc_{k+1} \text{pr}(D|c_{k+1}, \mathbf{a}, I') \text{pr}(c_{k+1}|\mathbf{a}, I') \end{aligned}$$

and so on ... (straightforward but too many details for here)

Implications of truncation errors for parameter estimation

Example: fitting an NN potential in chiral EFT

[S. Wesolowski, rjf, D. Phillips, in preparation]

NN-only fits have many data up to high energies with rather small errors, so differences between our Bayesian machinery and standard fitting protocols are subtle.

- Little impact on LECs for high orders in the expansion because truncation error is small
[Note: projected posterior plots clearly reveal redundancies at high order!]

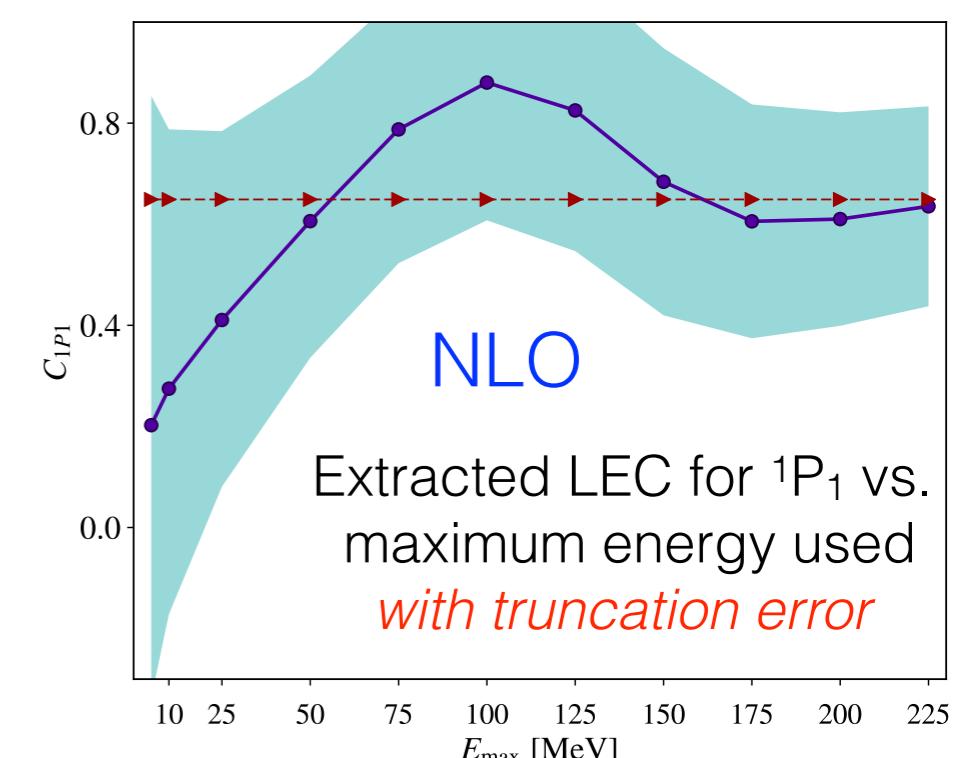
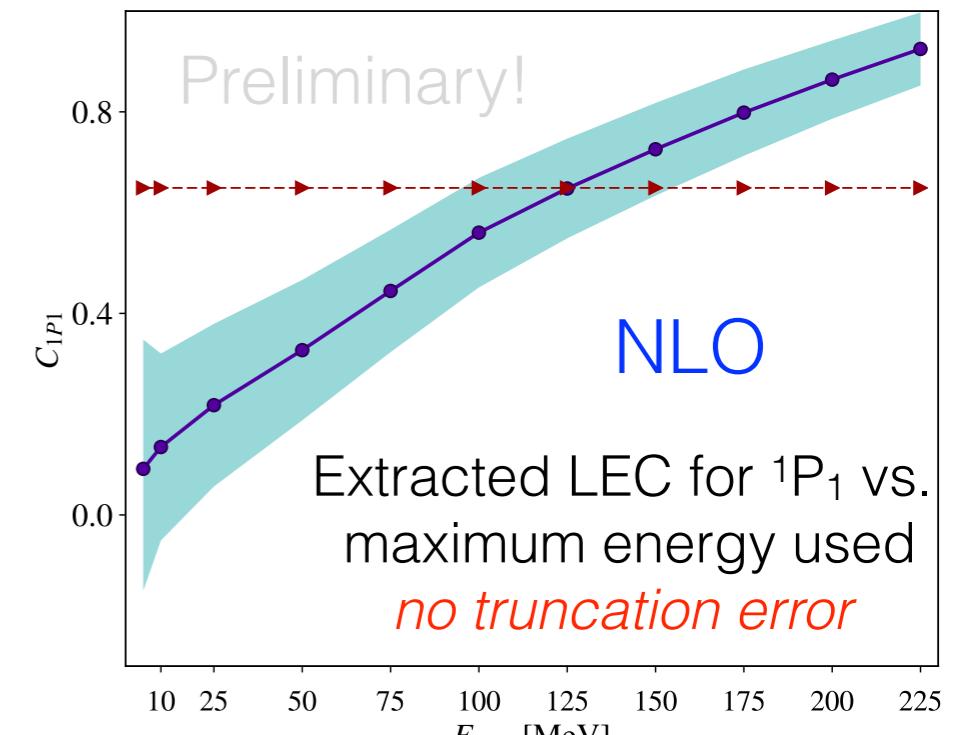
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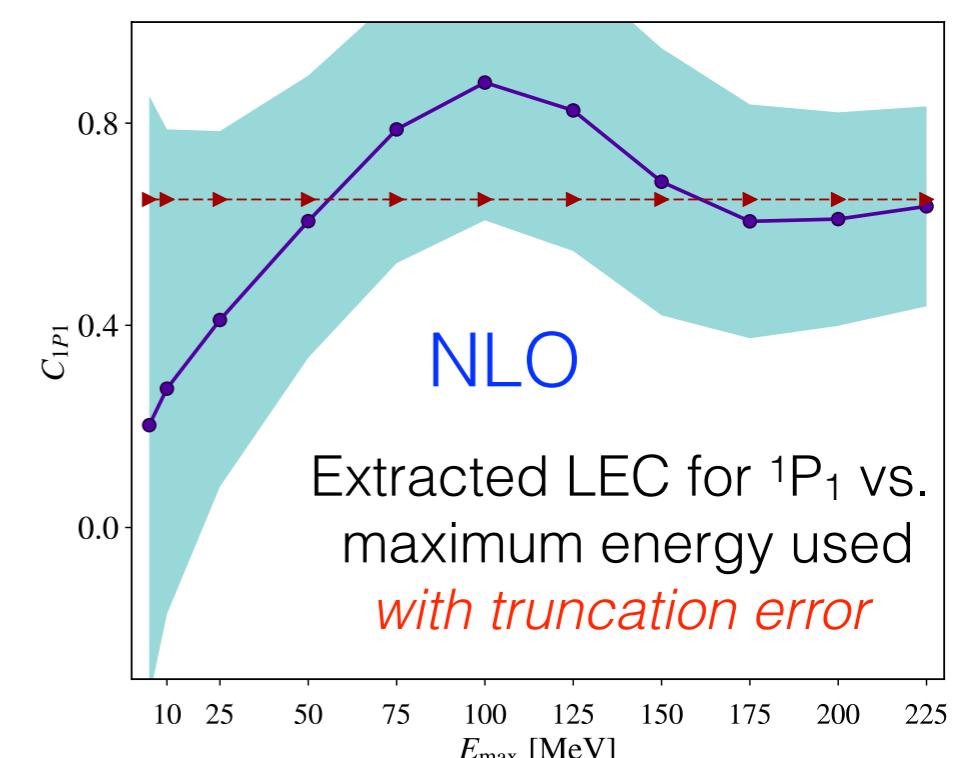
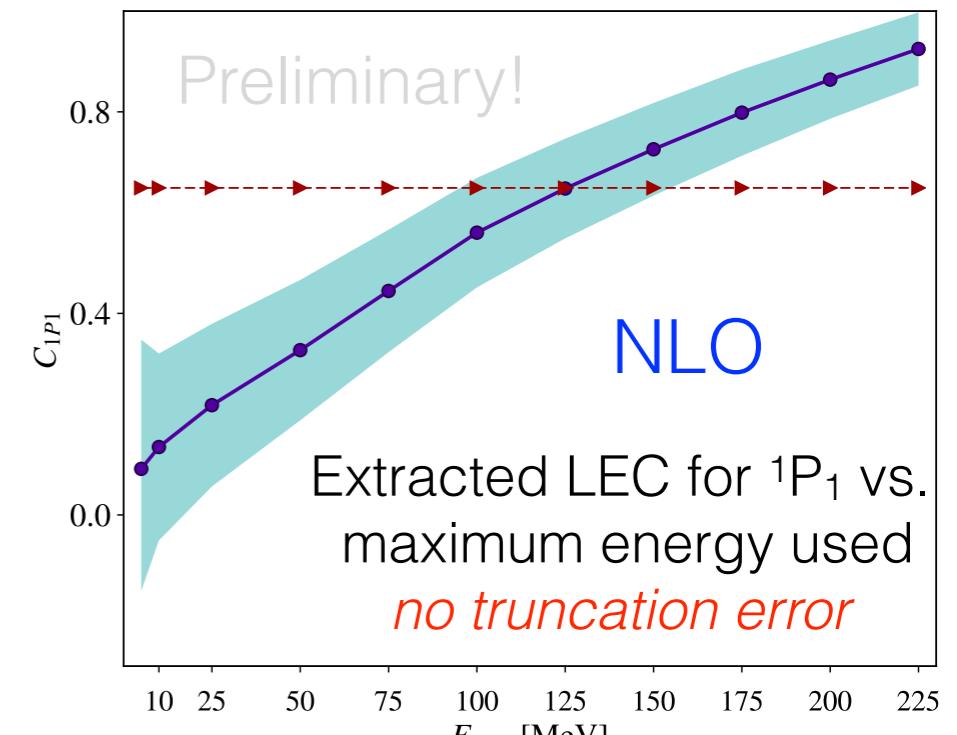
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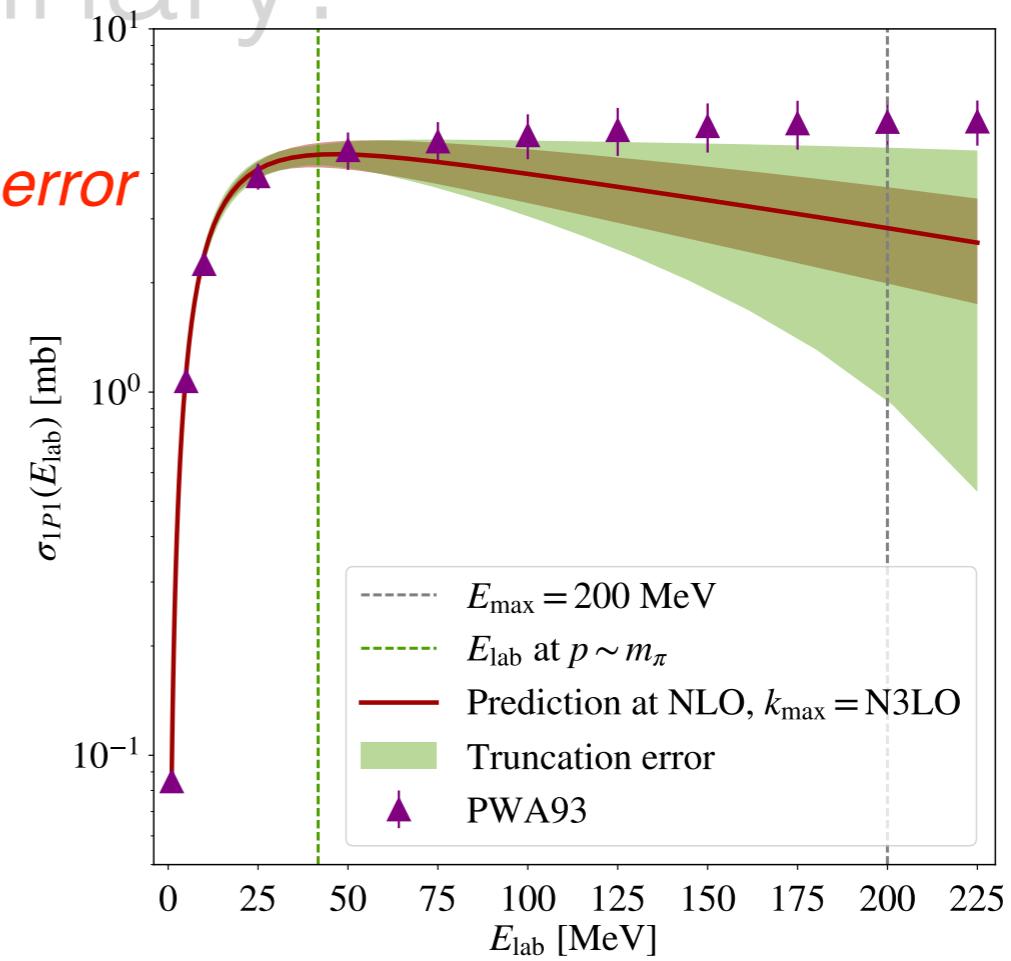
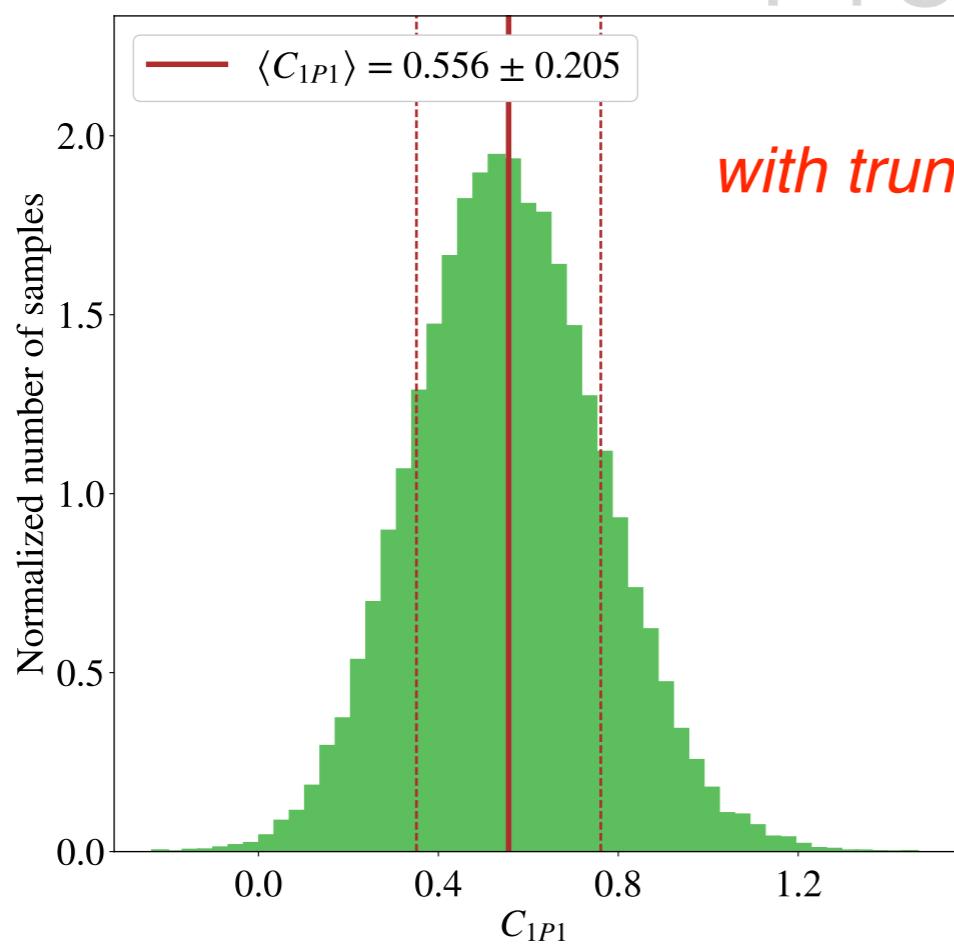
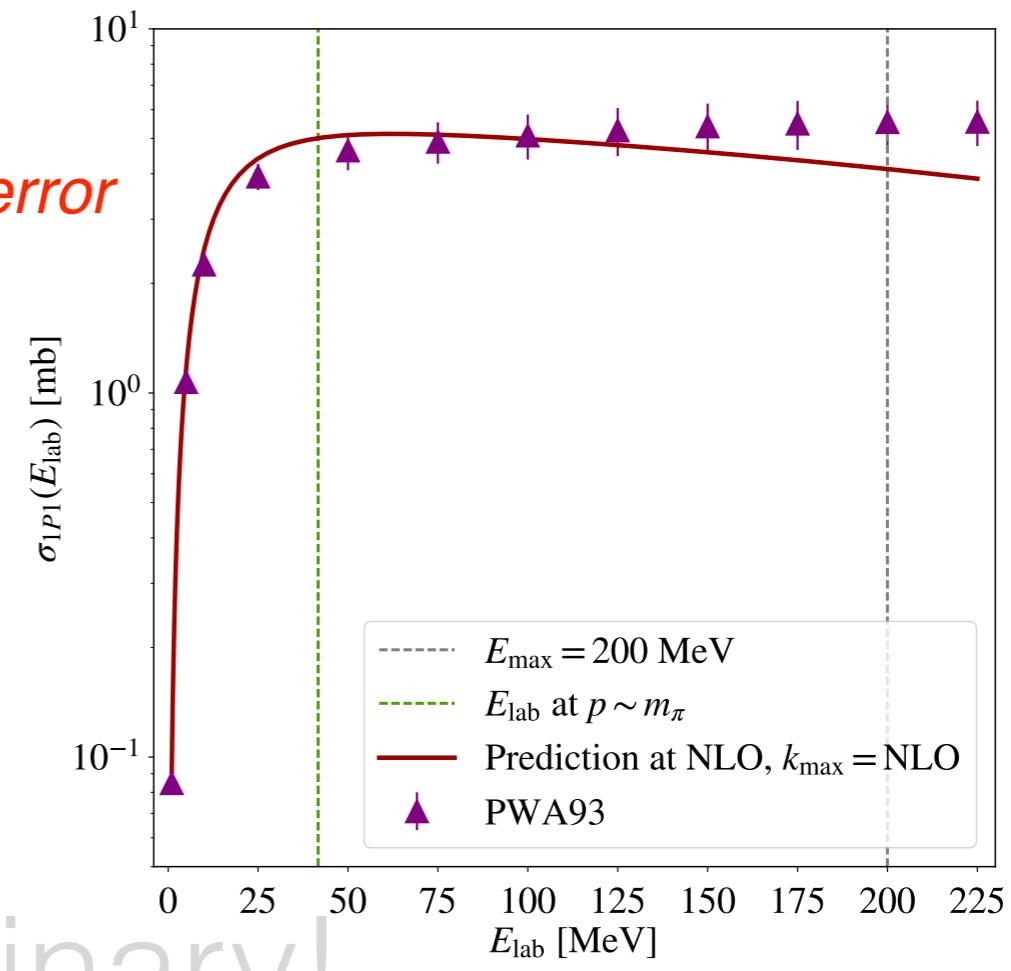
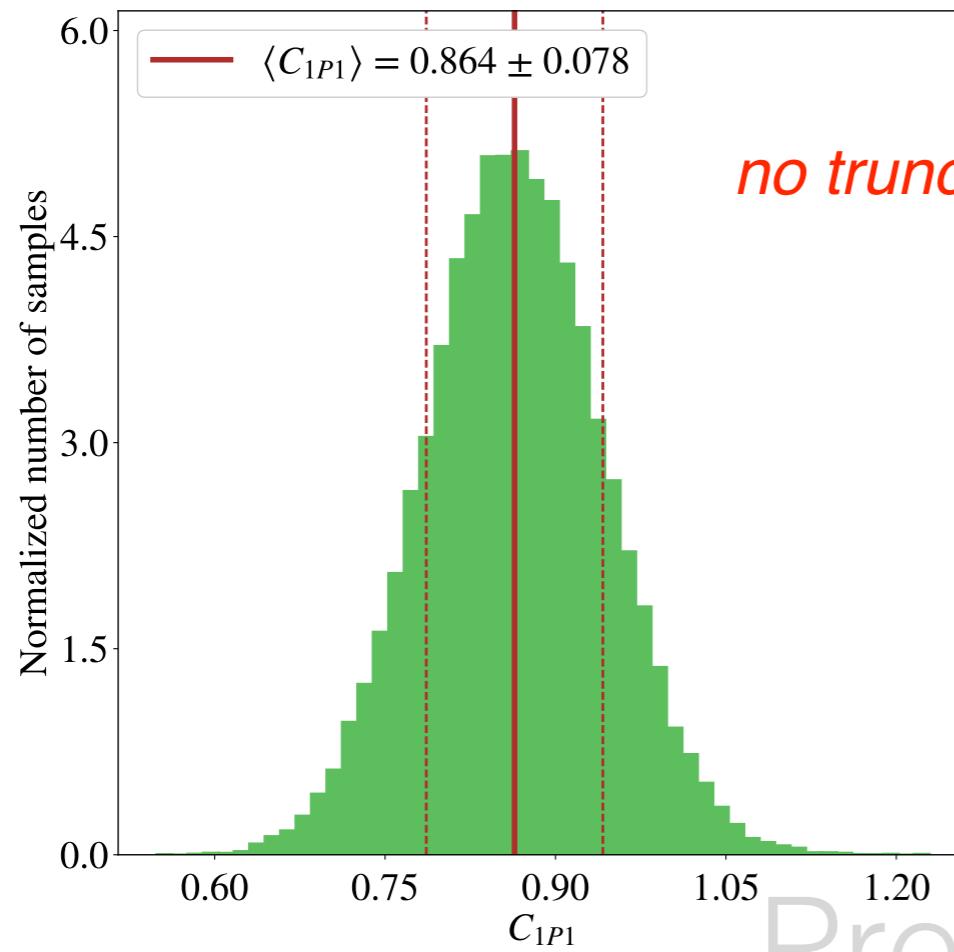
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Summary

- Statistical models let EFT truncation error be quantified
- Assumptions → Bayesian network → explicit priors
- NN observable coefficients from EFT (generally!) behave as random bounded functions in both energy and angle *except* when regulator artifacts disrupt pattern
- Bayesian model checking for many consistency checks
- Gaussian processes to include correlations in model
- Bayesian framework shows how to combine errors

Ongoing and future

- Test for other potentials (e.g., new EMN results)
- Using the truncation error model for fitting LECs
- Other consistency checks for EFT convergence
- Few- and many-body observables!
- Model selection: compare different EFT implementations
- ...

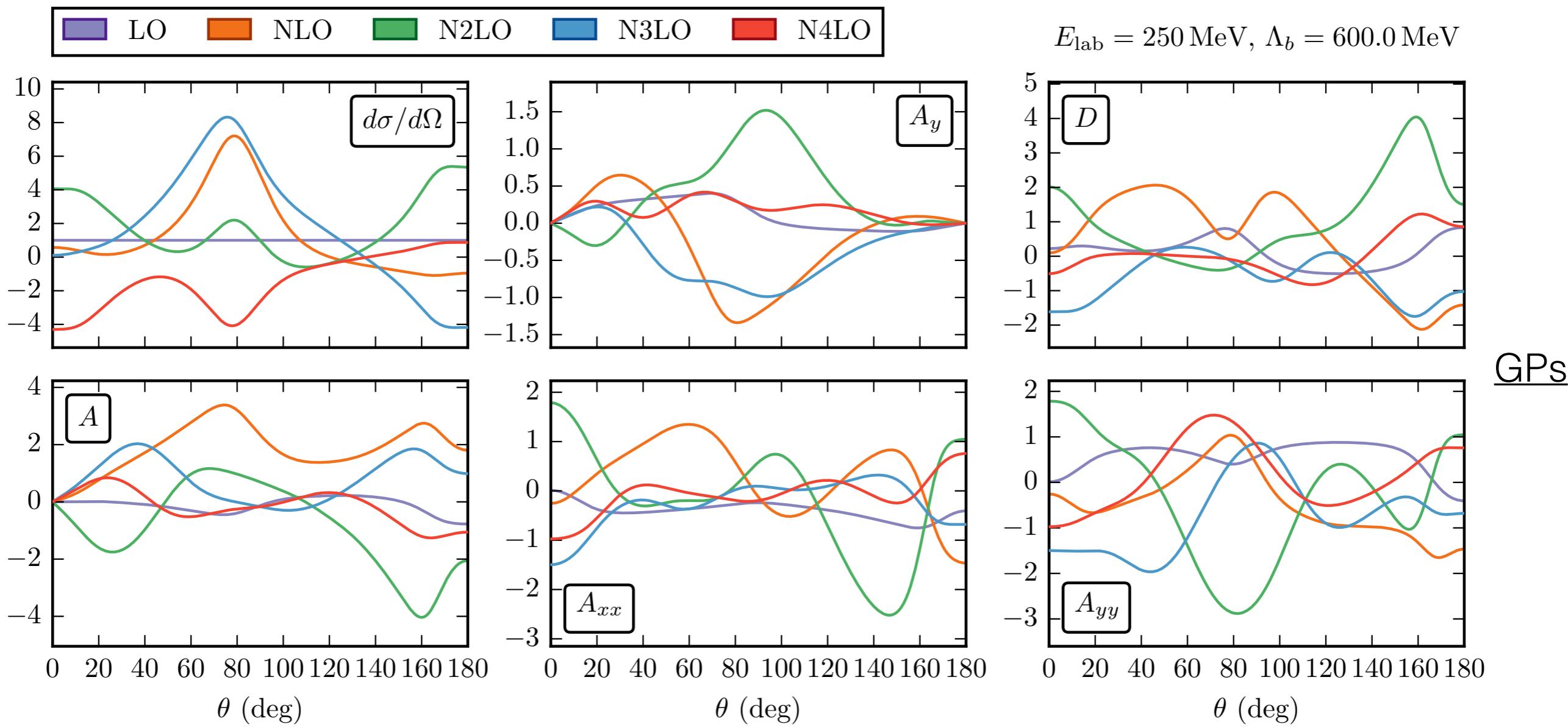
Extra slides

Errors on NN observables in chiral EFT

Use EKM semi-local NN interactions as example.

Eur. Phys. J. A **51**, 53 (2015) and Phys. Rev. Lett. **115**, 122301 (2015)

Angular observables overall: as a function of angle at single energy

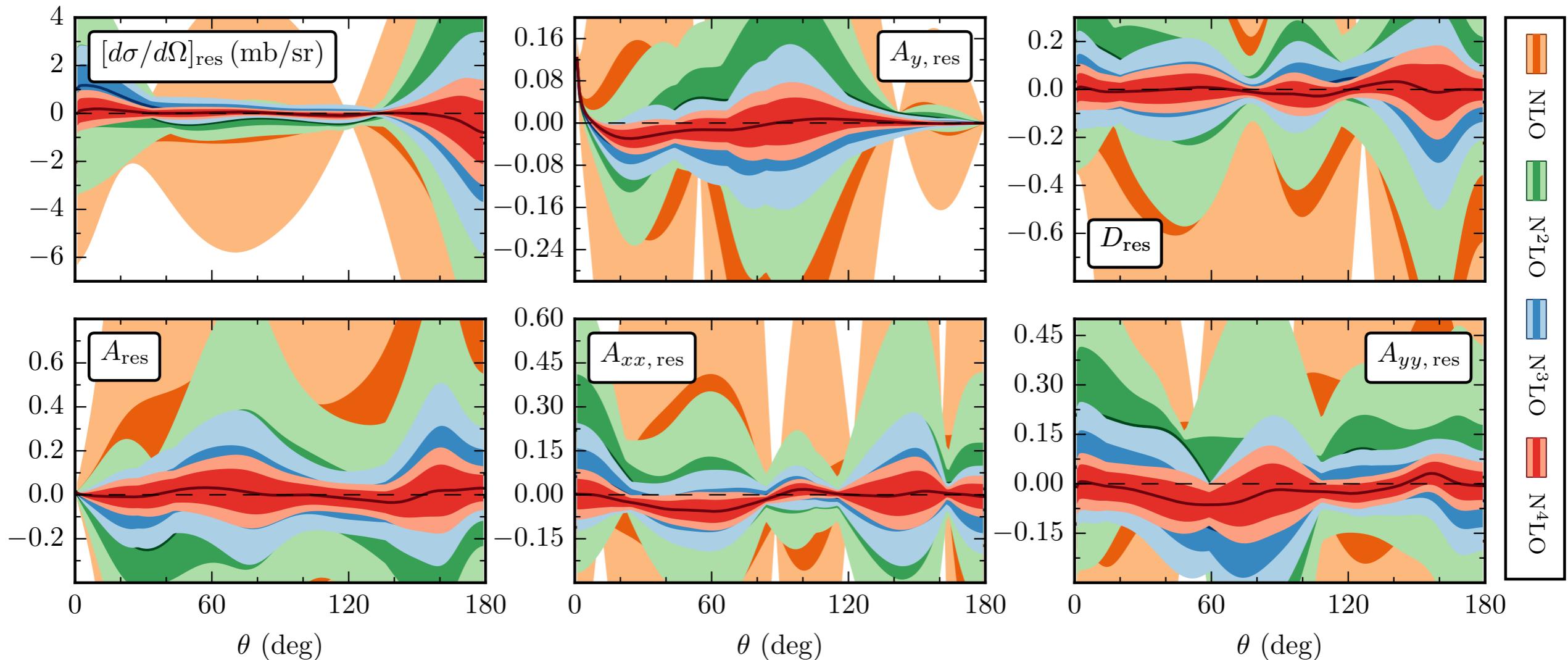


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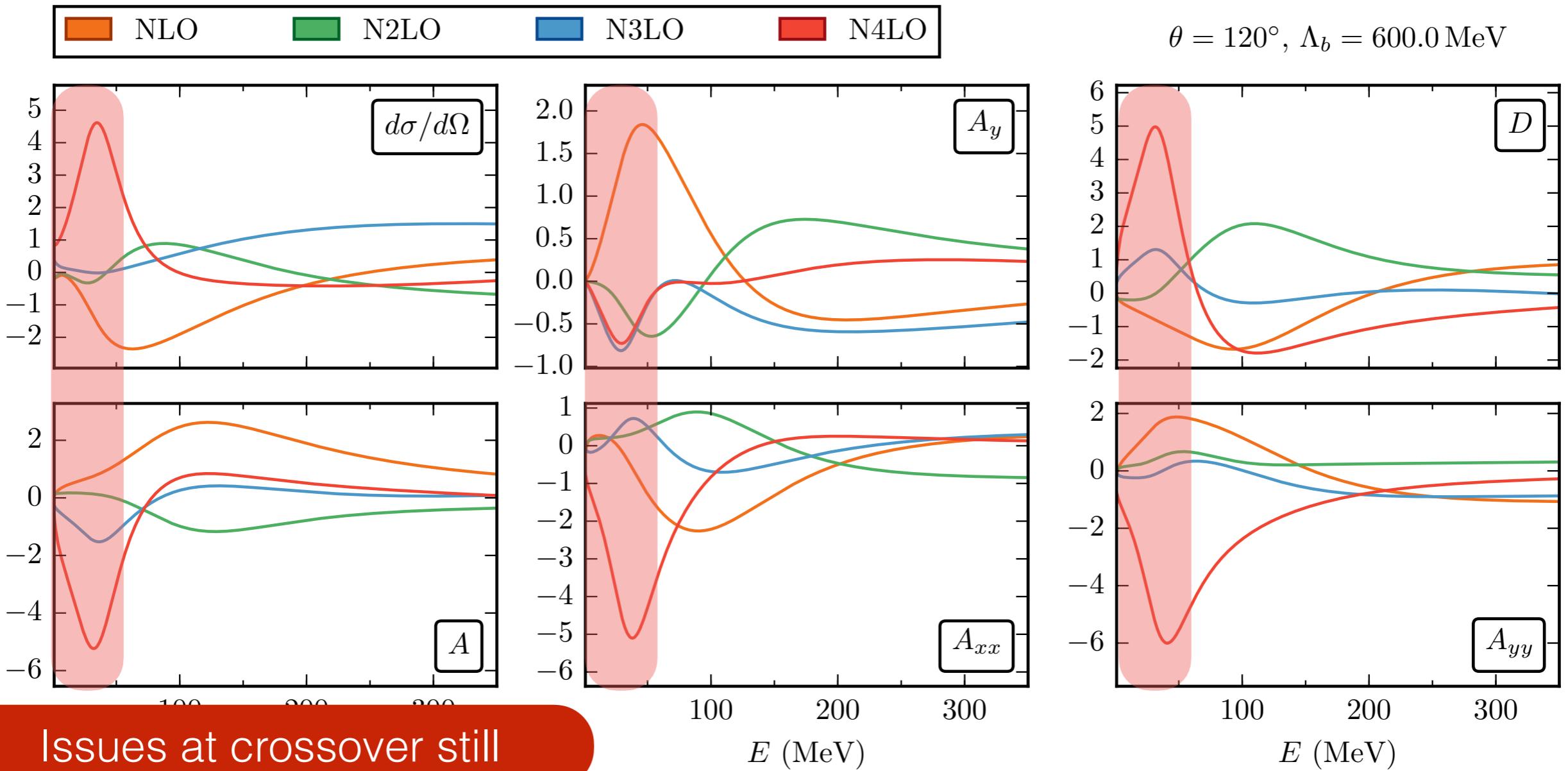


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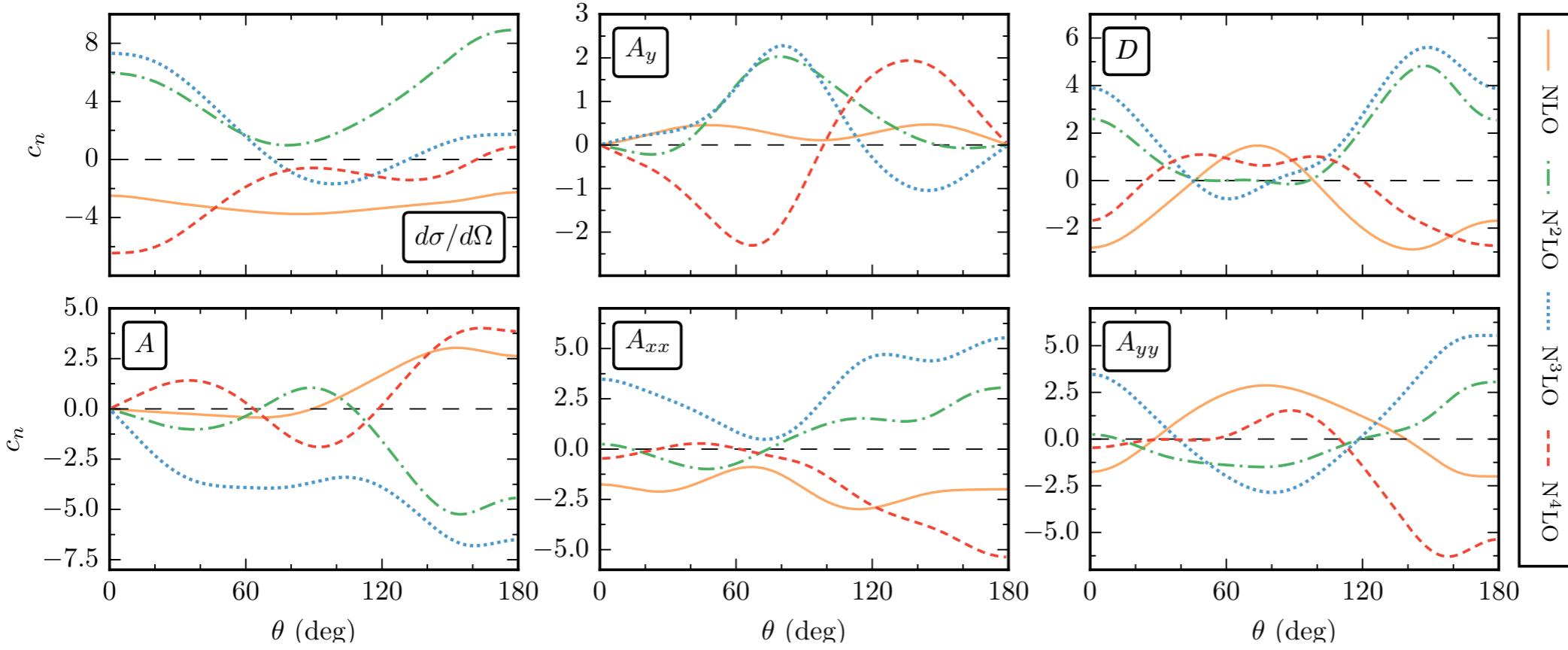
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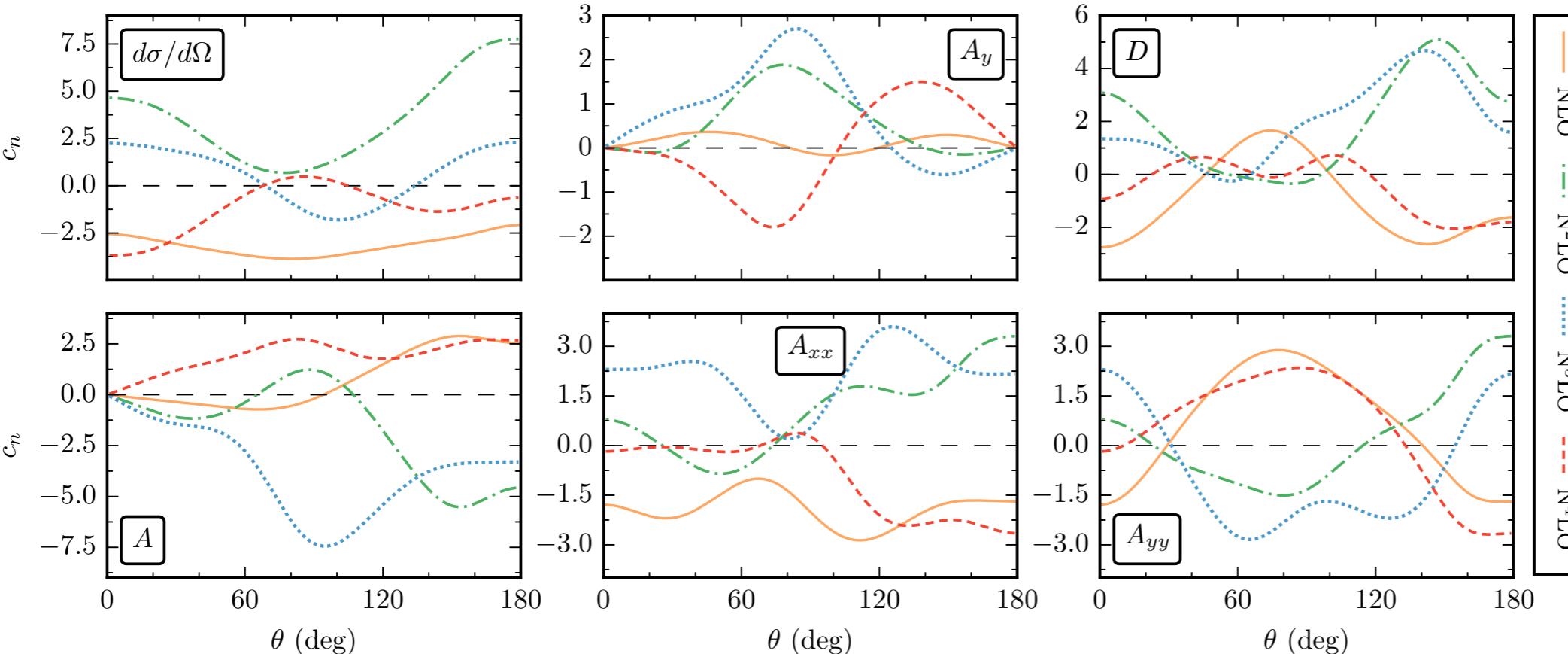
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Update: New potentials from EMN

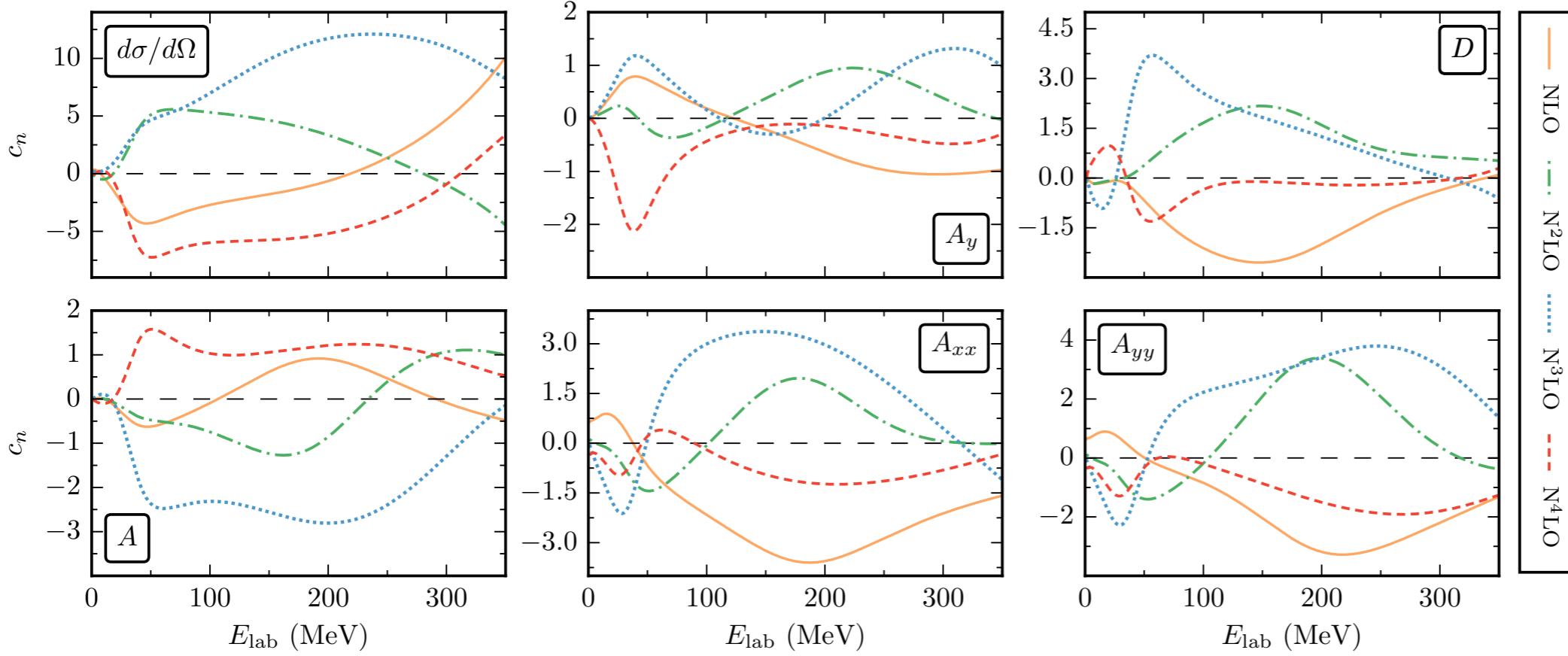


$\Lambda_b = 600 \text{ MeV}$

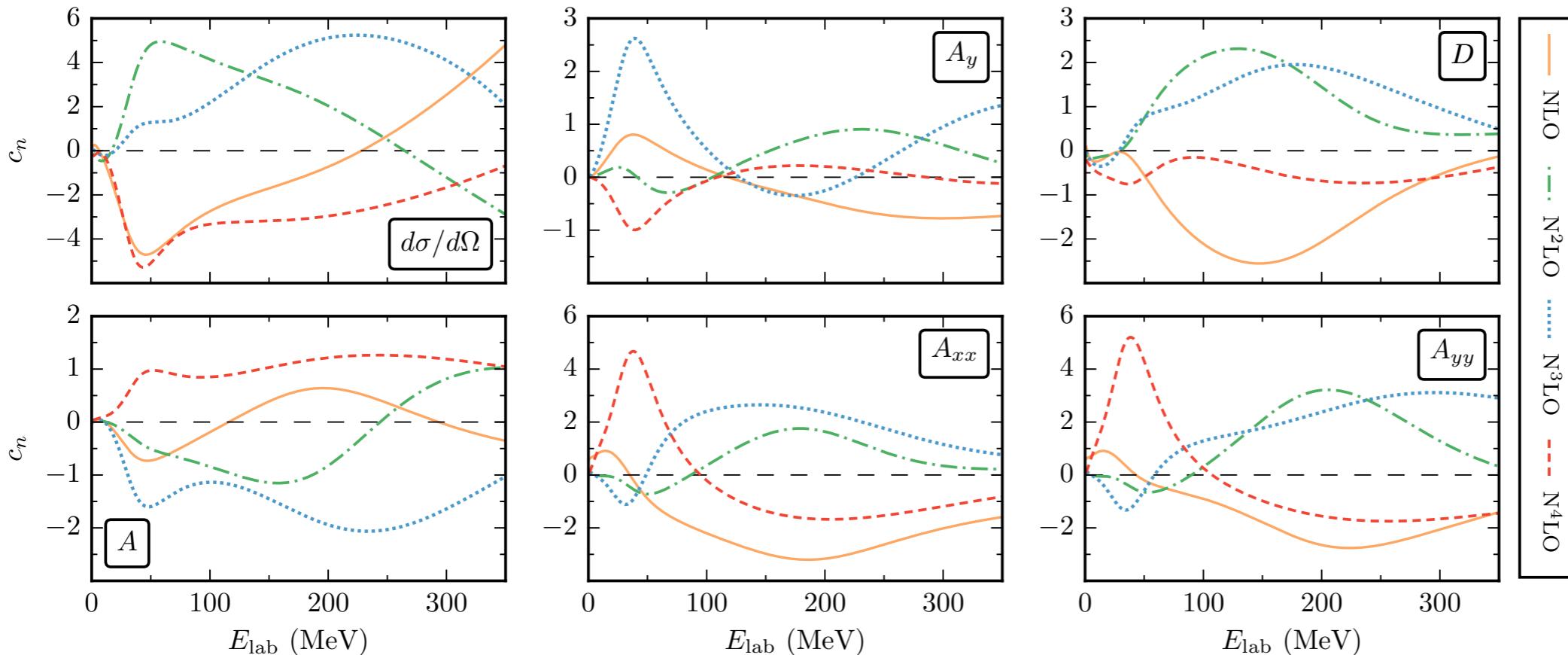


Entem, Machleidt, Nosyk,
arXiv:1703.05454

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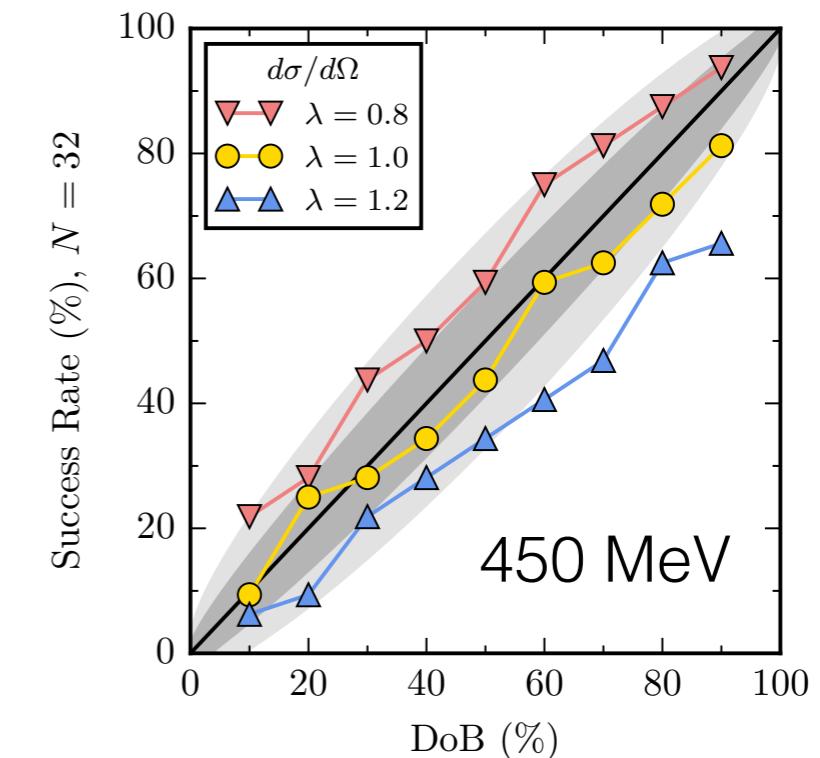
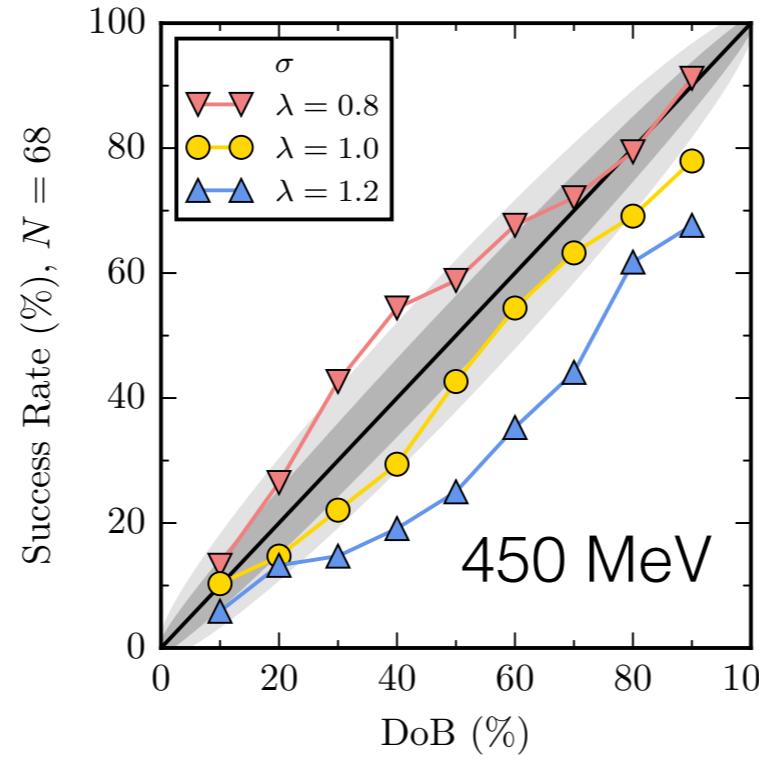
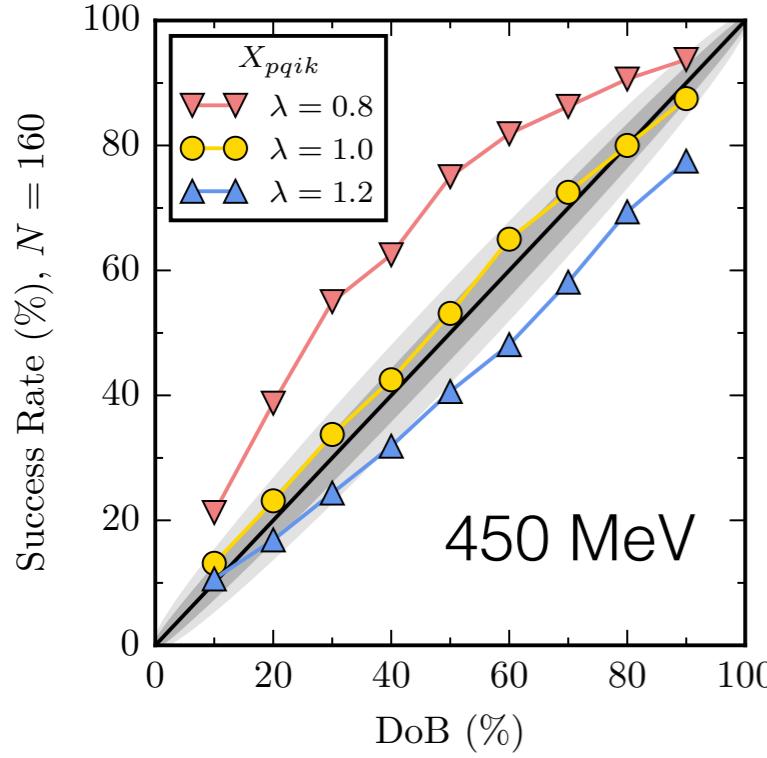


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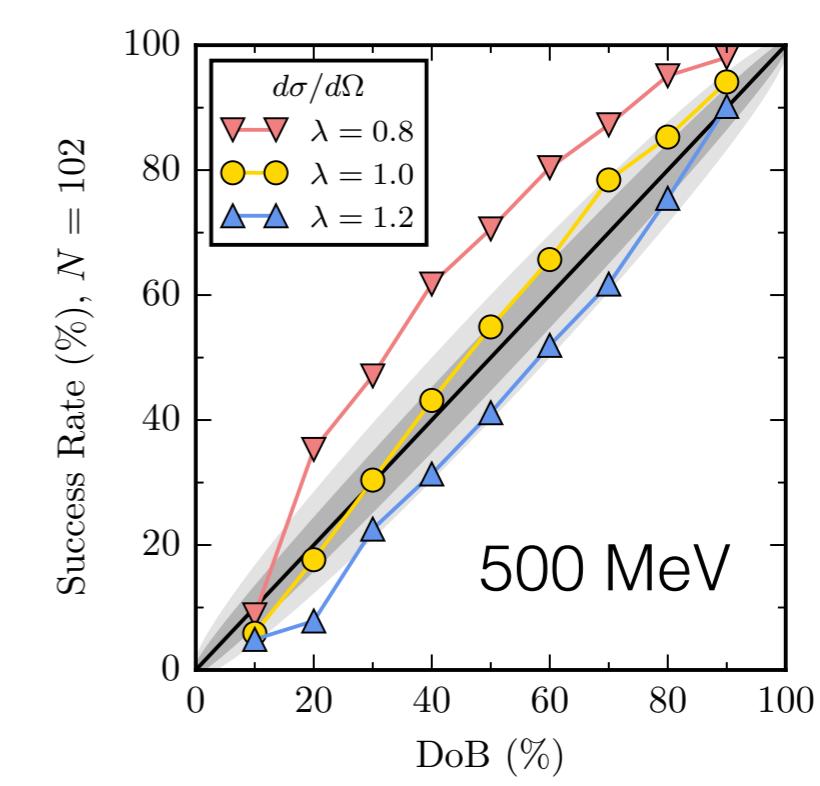
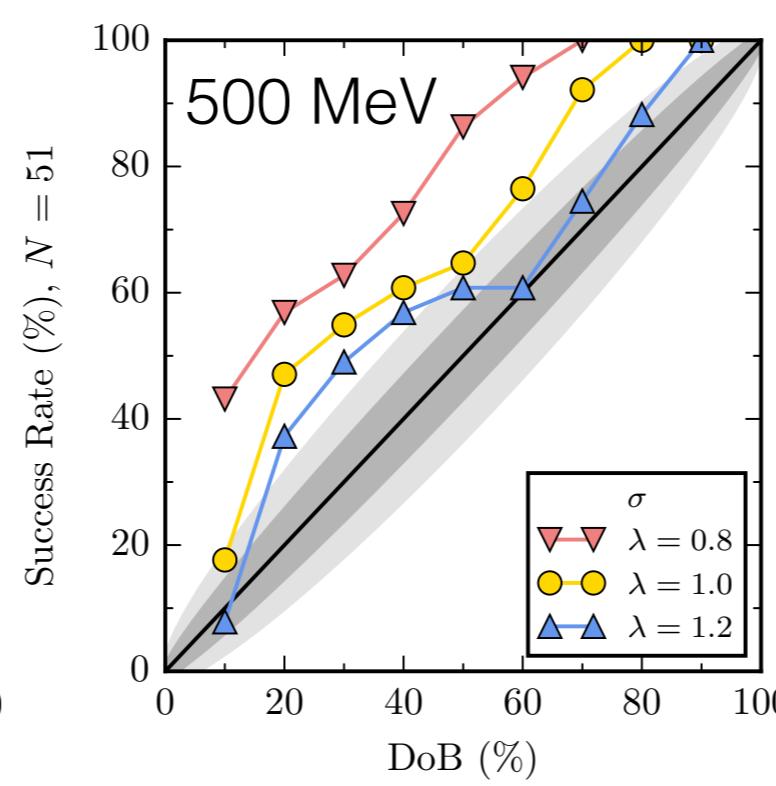
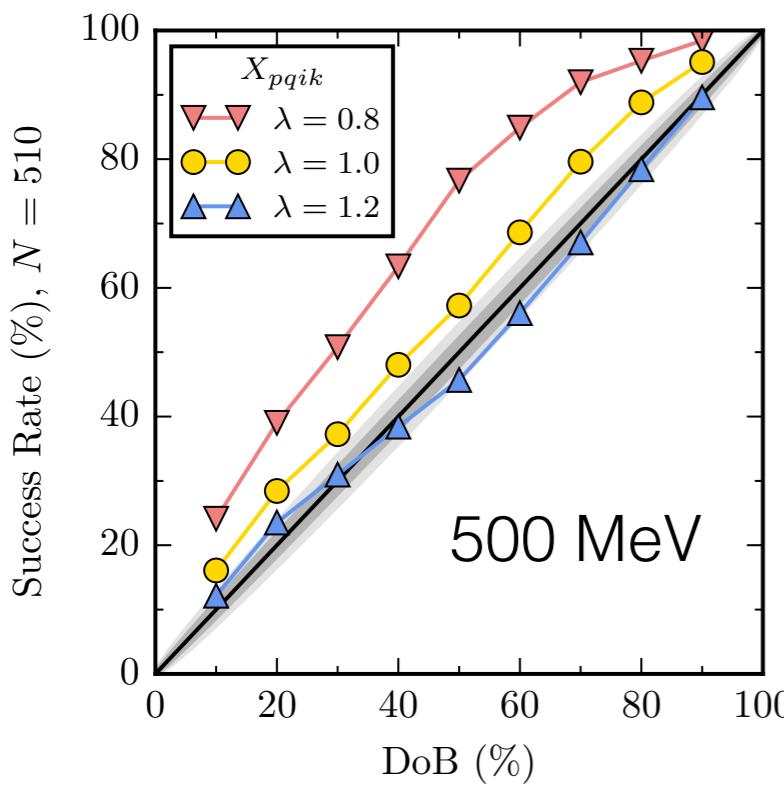


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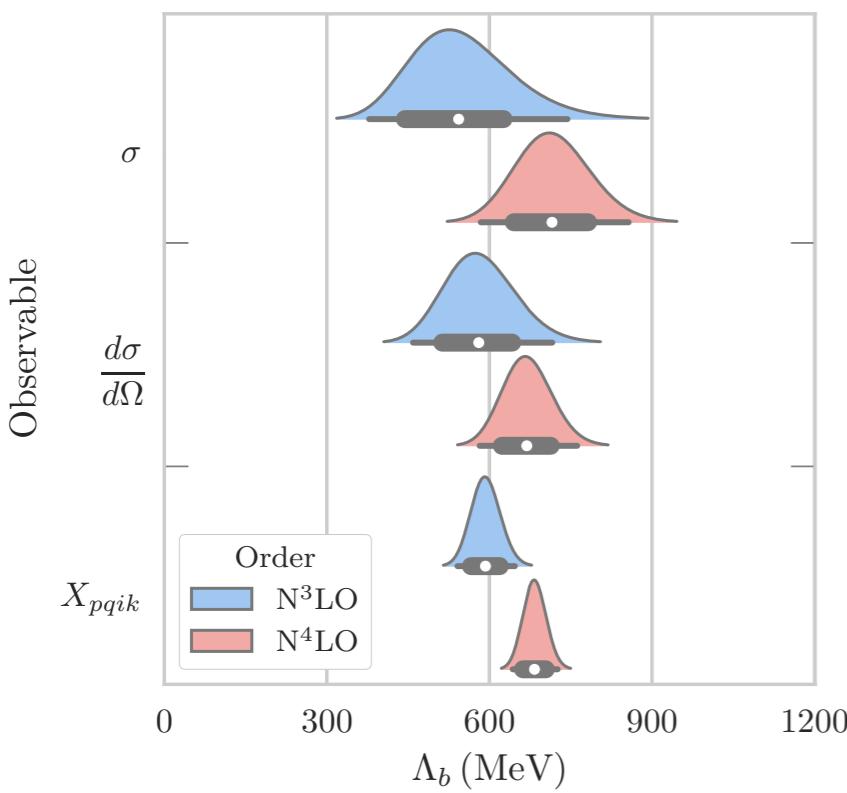


Bayesian model checking for new EMN

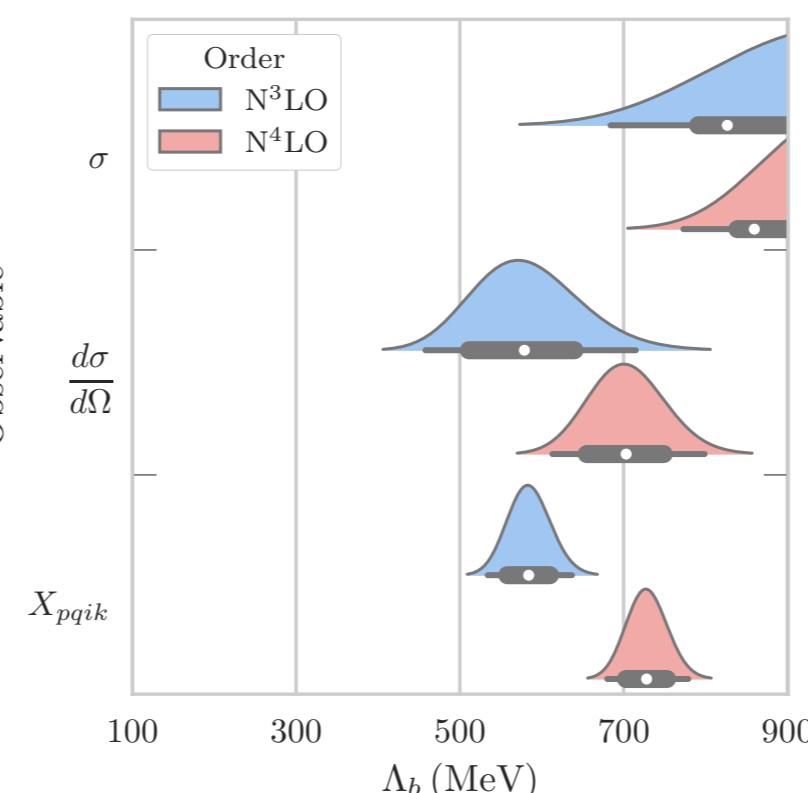
Compute a pdf for the breakdown scale:

$$\text{pr}(\Lambda_b | b_2, \dots, b_k)$$

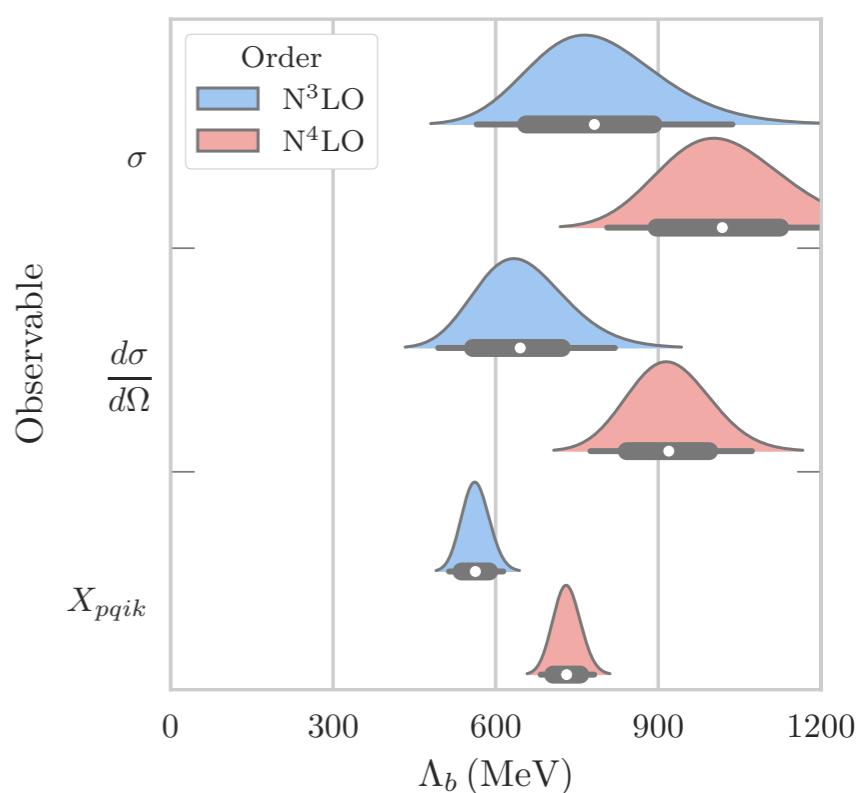
450 MeV



500 MeV



600 MeV

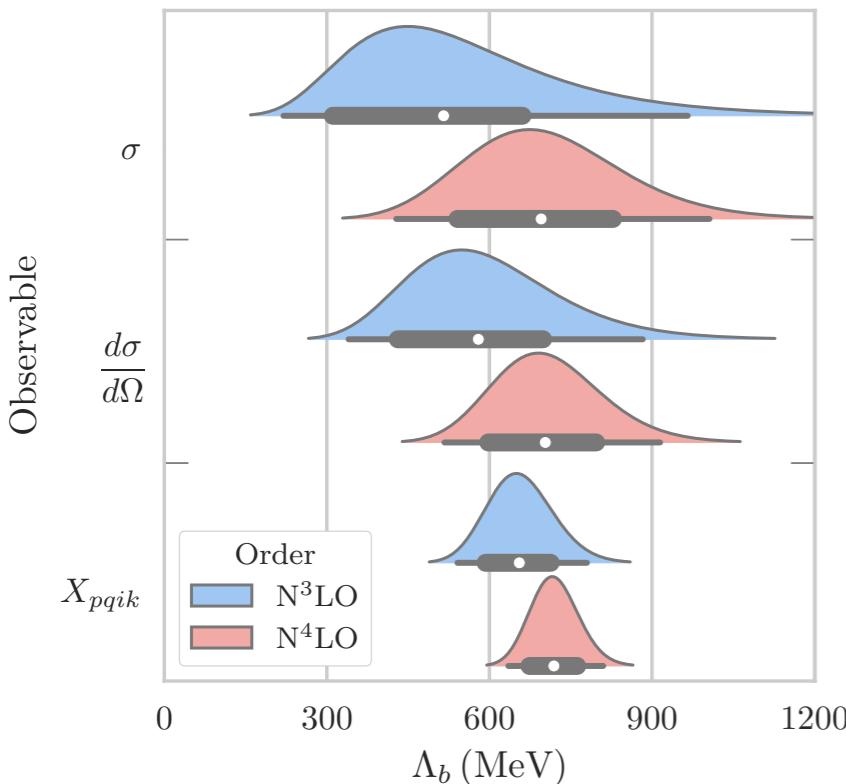


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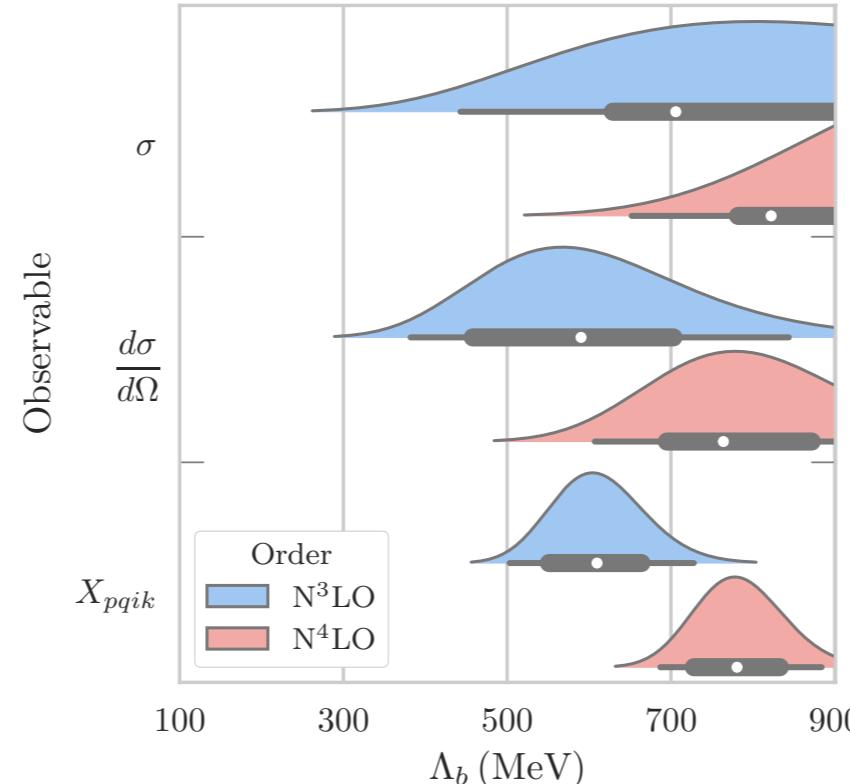
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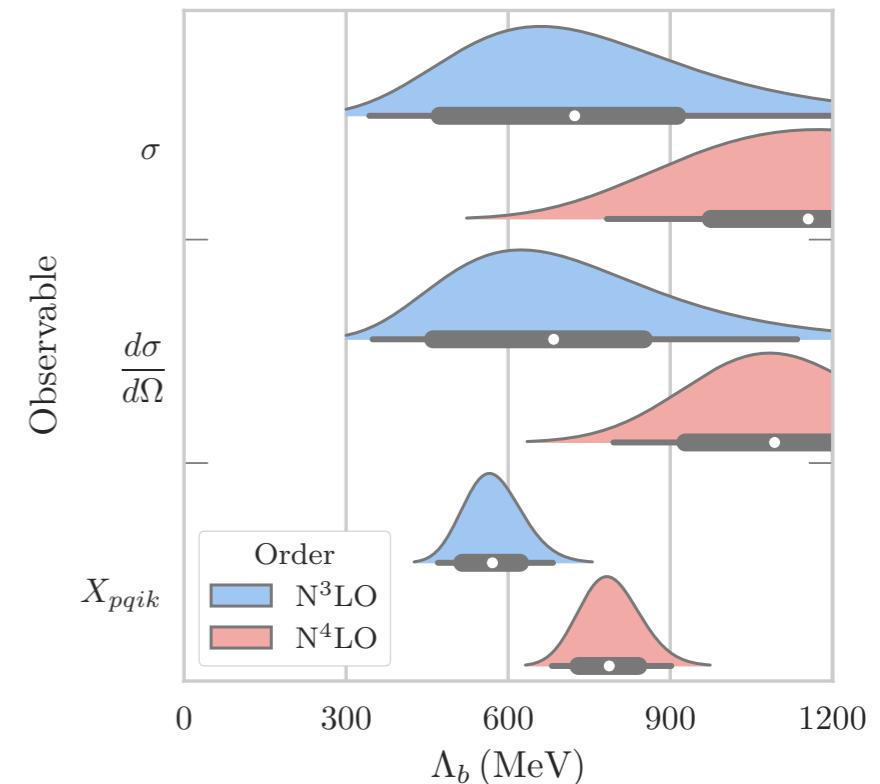
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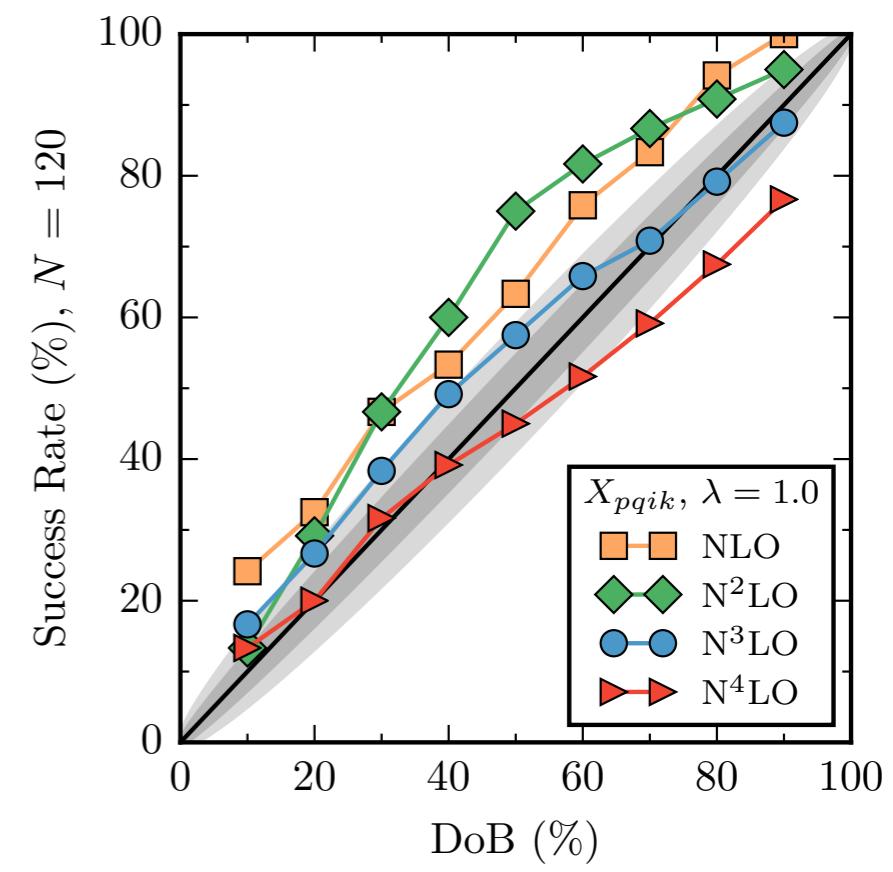
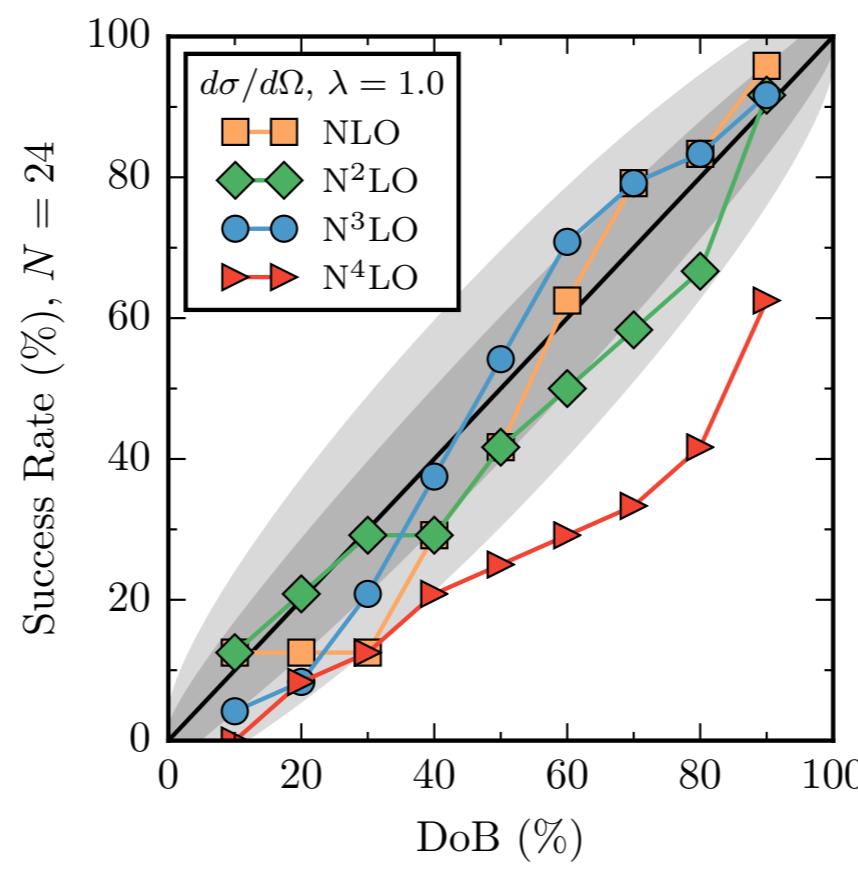
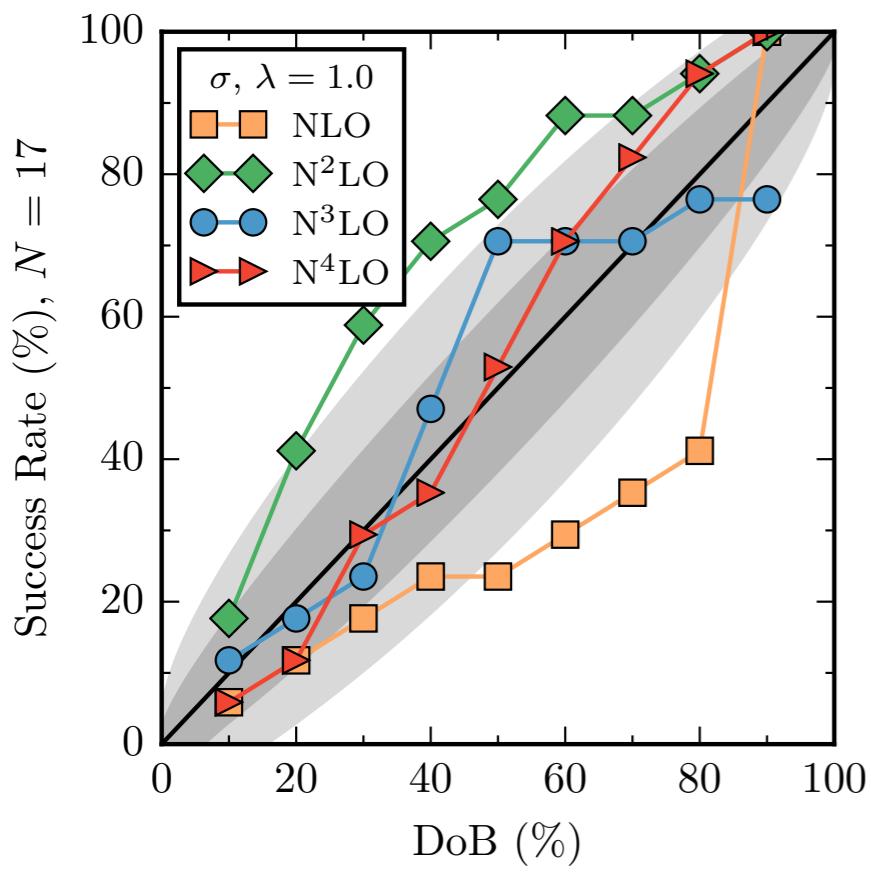


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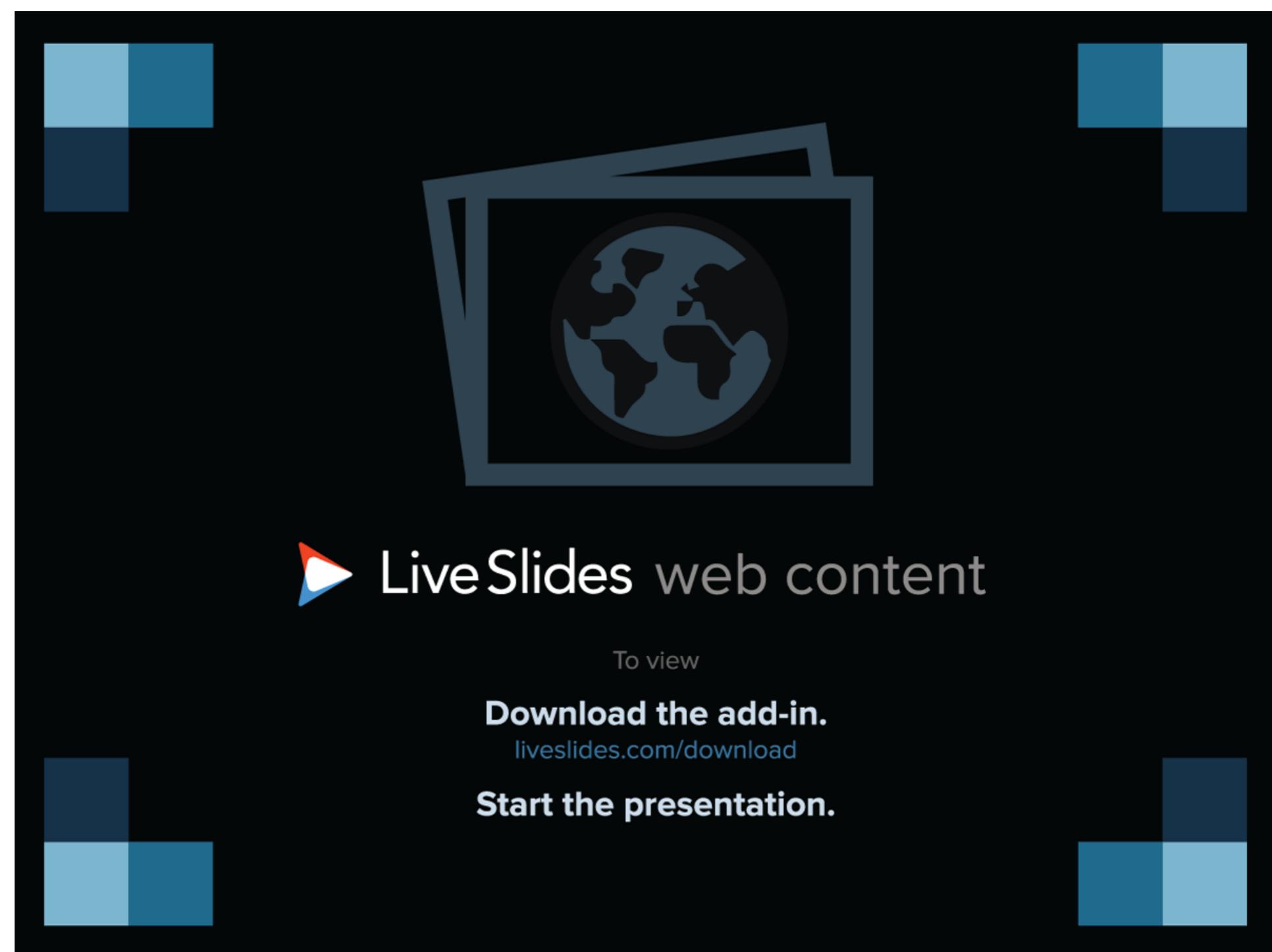
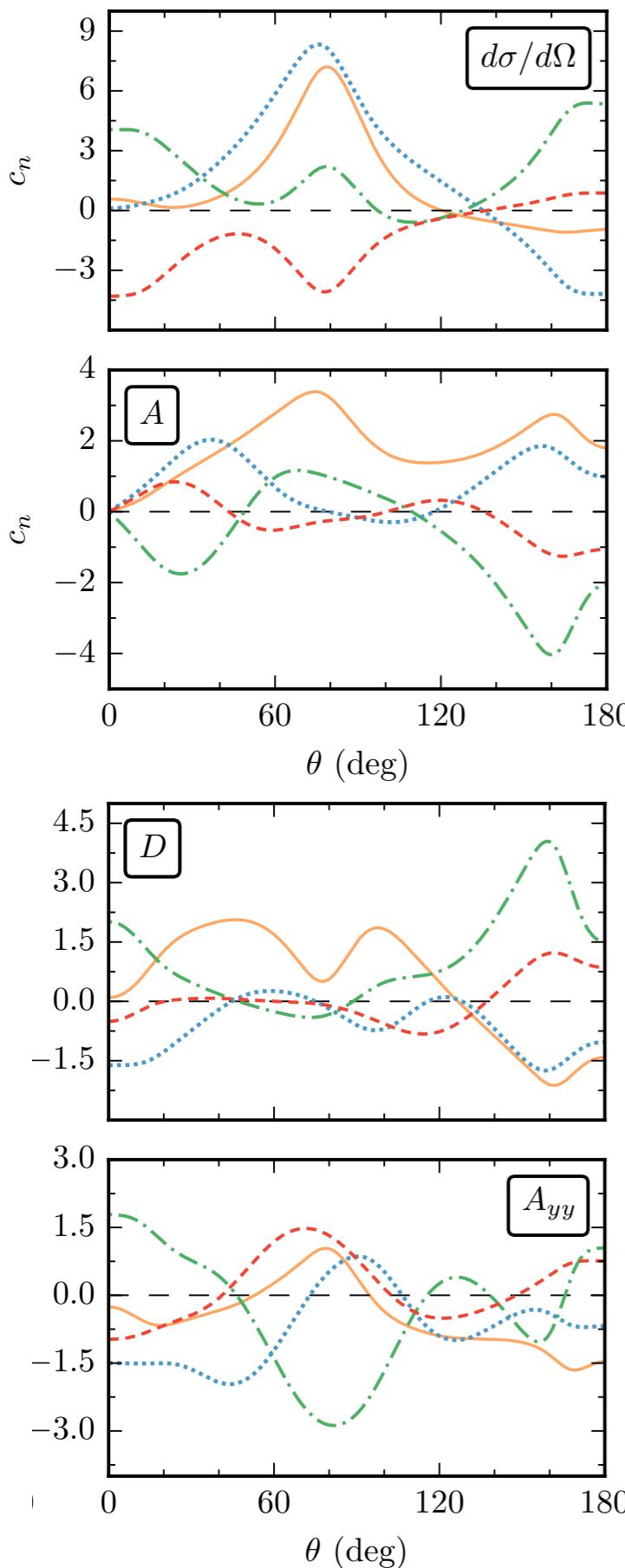


Comparison to NPWA data

Using many (correlated?) energies and angles



Can we model coefficients with Gaussian Processes?



[Go back!](#)