Acknowledging the existence of a higher power: how ‘discrepancy modeling' of truncation uncertainties in EFT expansions improves parameter estimation and uncovers underlying physics

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RESEARCH SUPPORTED BY THE DOE OFFICE OF SCIENCE THE NSF OFFICE OF ADVANCED CYBERINFRASTRUCTRE

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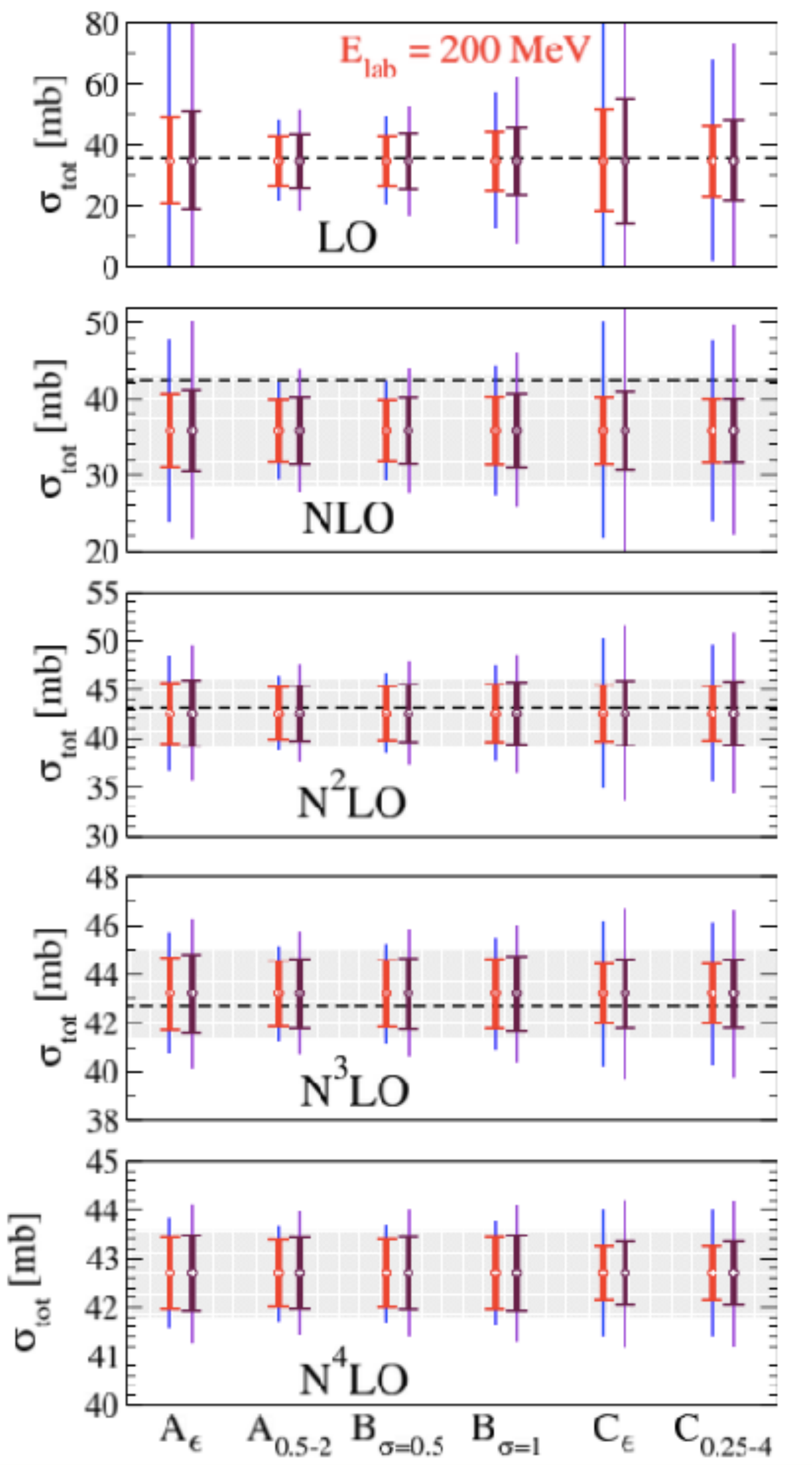

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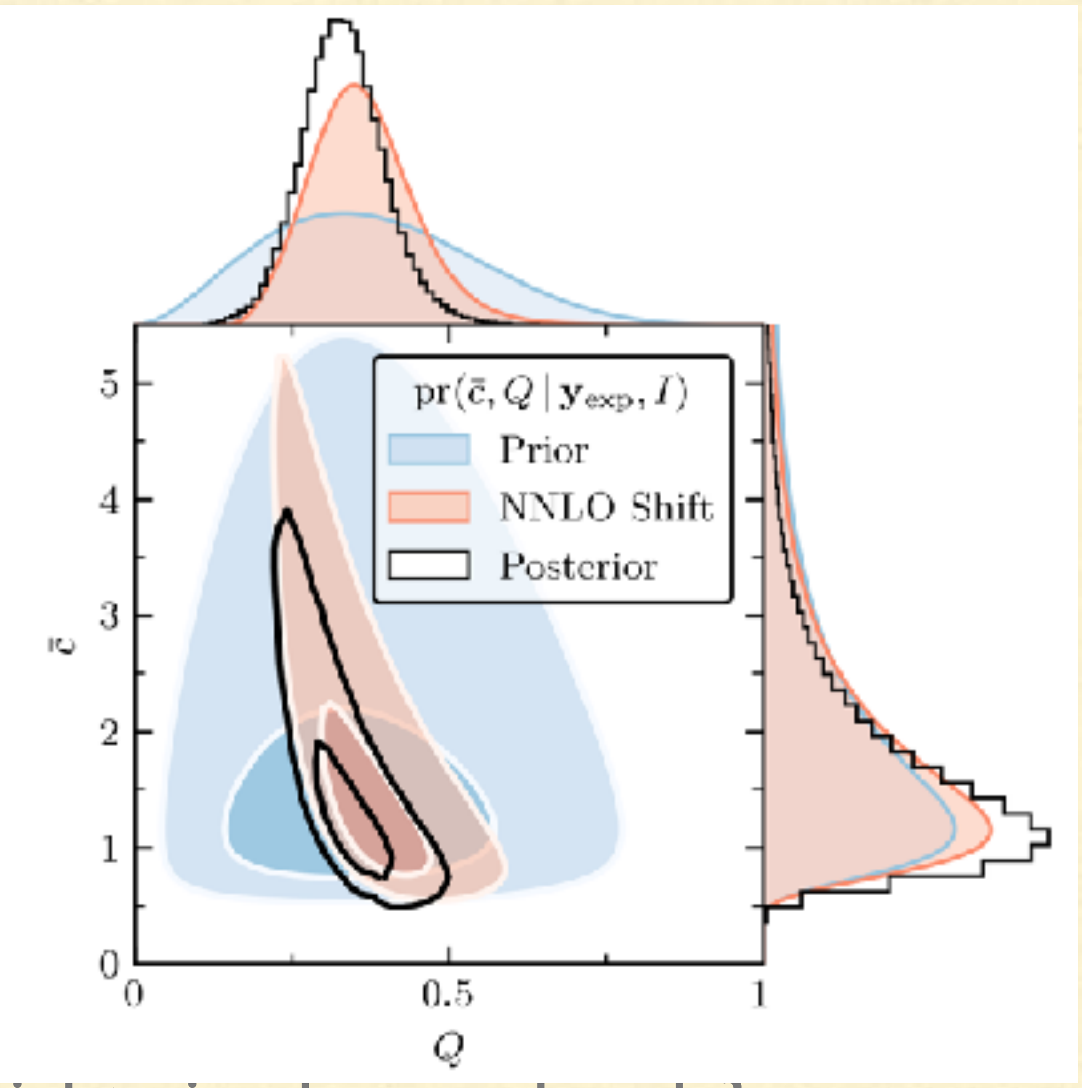

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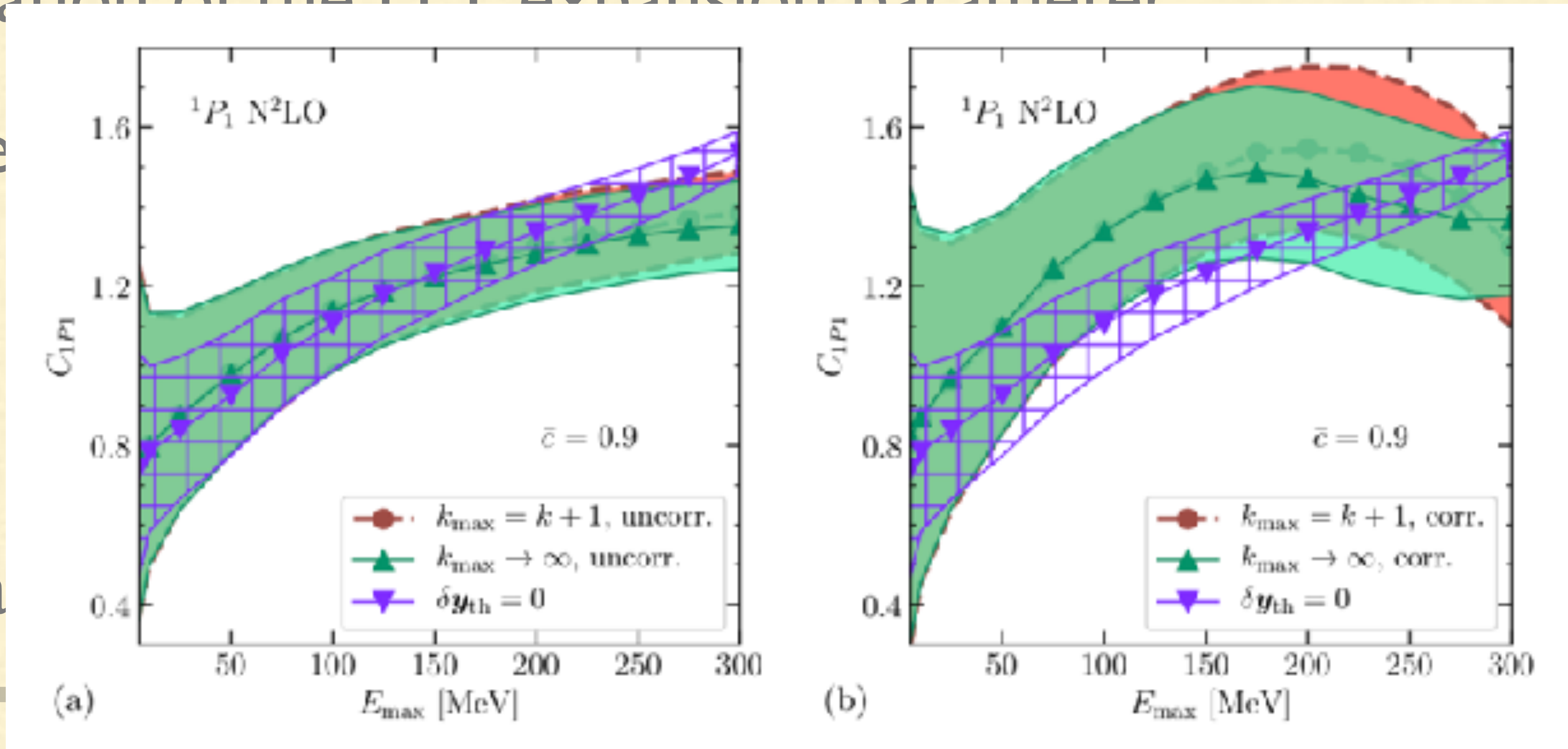

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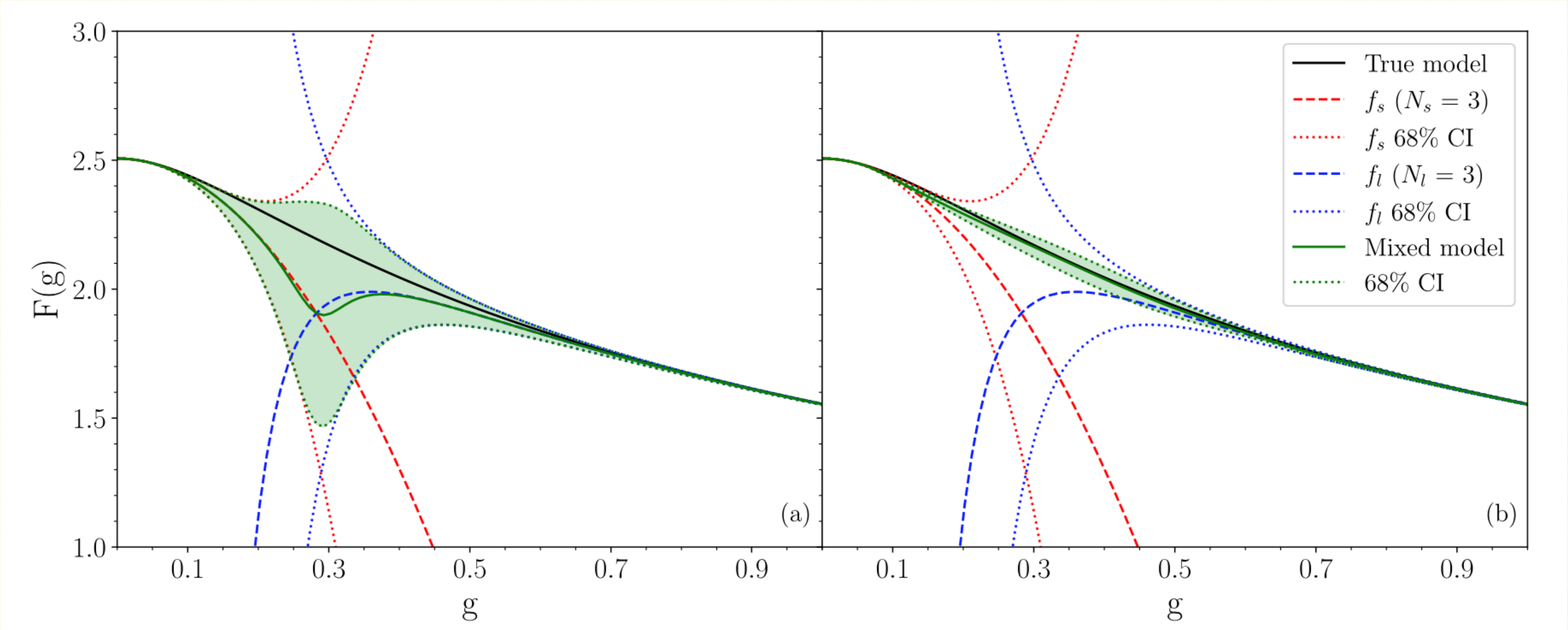

- Low-momentum EFTs with UQ can be combined with high-momentum approaches with UQ using Bayesian Model Mixing

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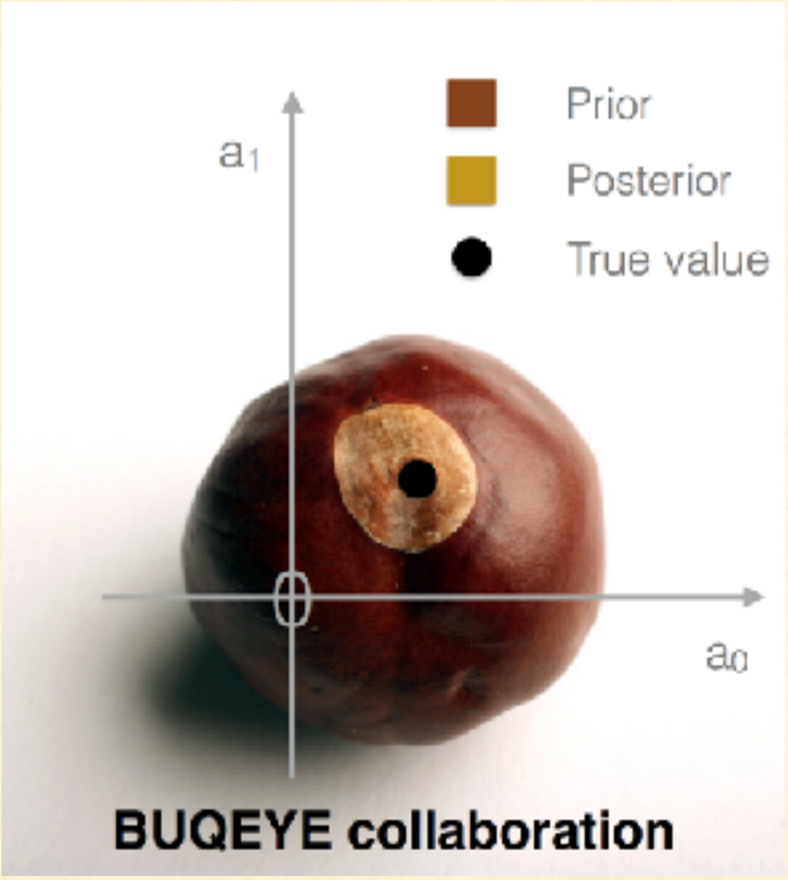
Outline

- How to calculate rigorous truncation errors
- LEC extraction with truncation errors
  - Getting LECs and the EFT expansion parameter simultaneously
  - Stabilizing LEC fits
- But what should I do about correlated theory uncertainty?
- The BAND Framework
  - Bayesian Model Mixing
- Future Work



Bayesian Analysis of Nuclear Dynamics

Truncation errors in χEFT

- General EFT series for observable to order k: $y = y_{\rm ref} \sum_{n=0}^{k} c_n(p/m_\pi) Q^n$
- In χEFT $Q = \dfrac{(p, m_\pi)}{\Lambda_b}; \quad \Lambda_b \approx 600\ \text{MeV}$

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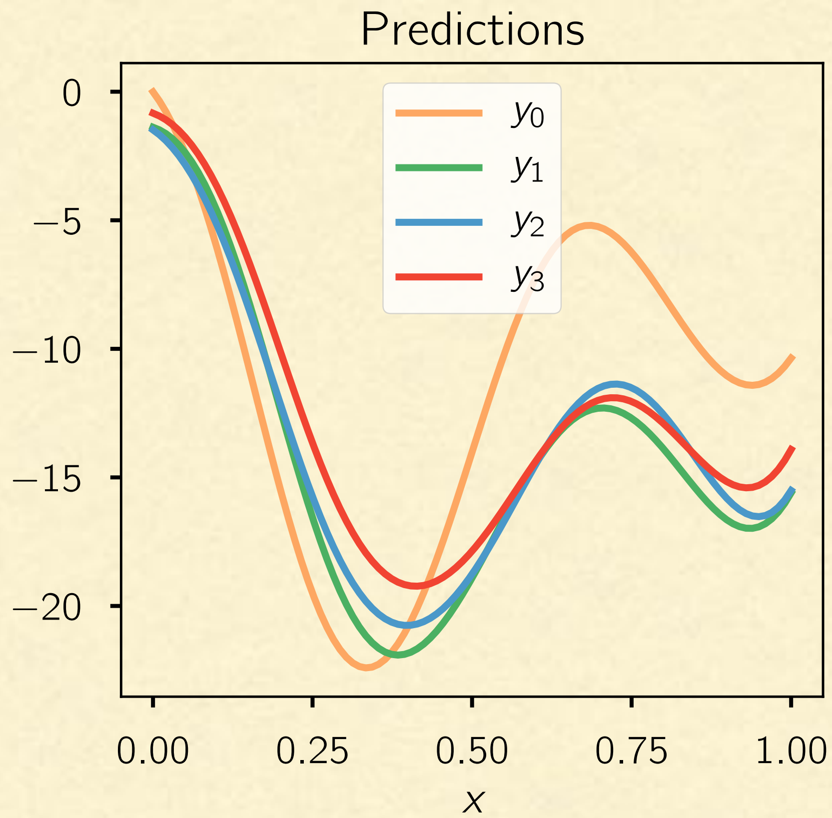

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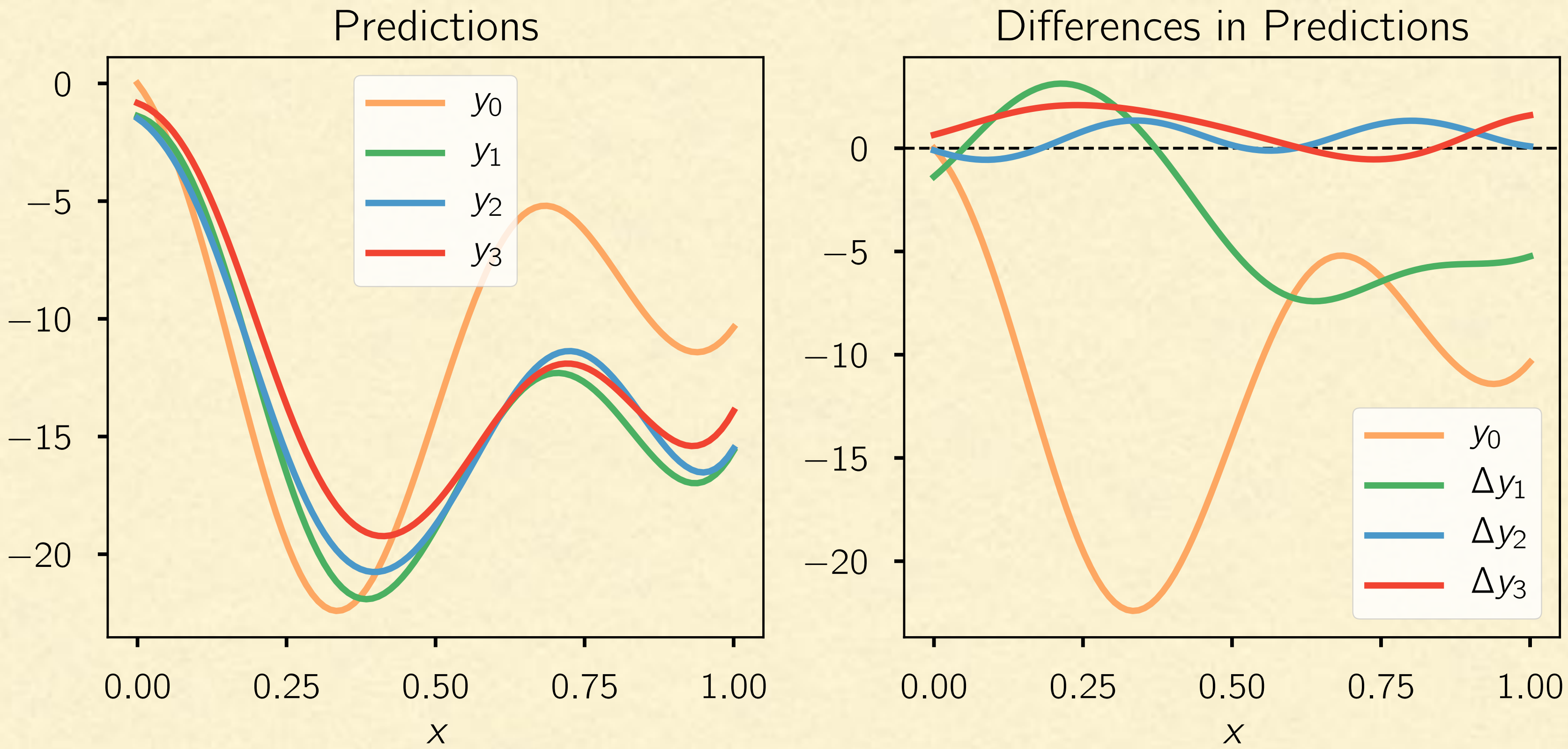

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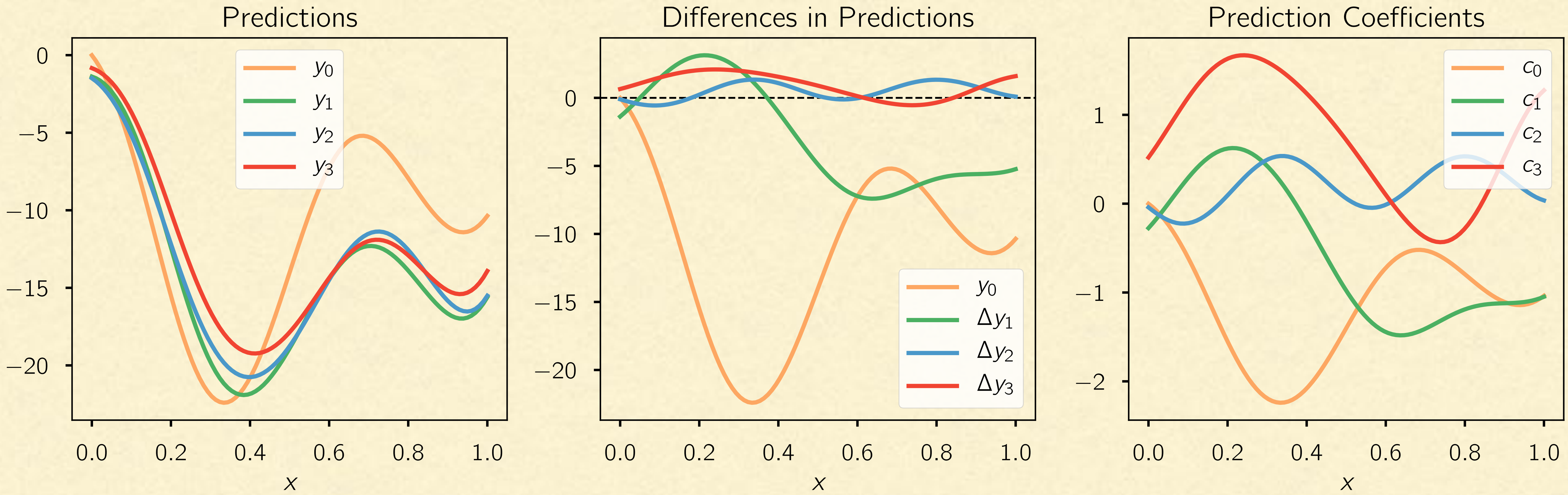

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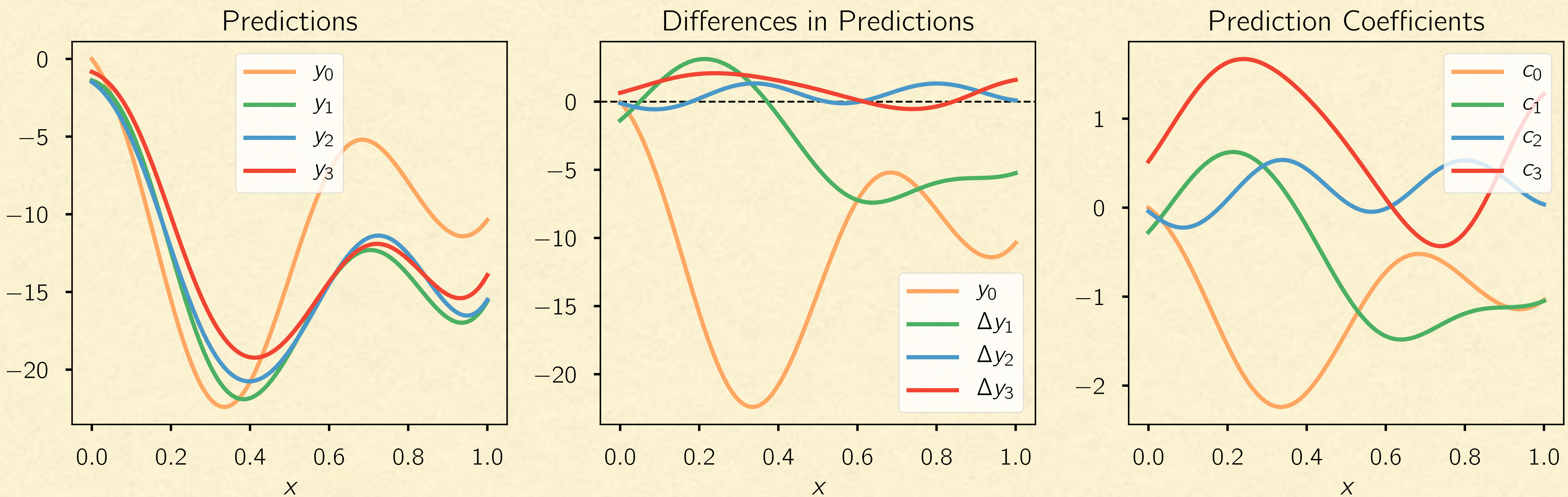

This is what a healthy observable expansion looks like: bounded coefficients, that do not grow or shrink with order.

Probability for EFT coefficients

Furnstahl, Klco, DP, Wesolowski, PRC, 2015 after Cacciari and Houdeau, JHEP, 2011

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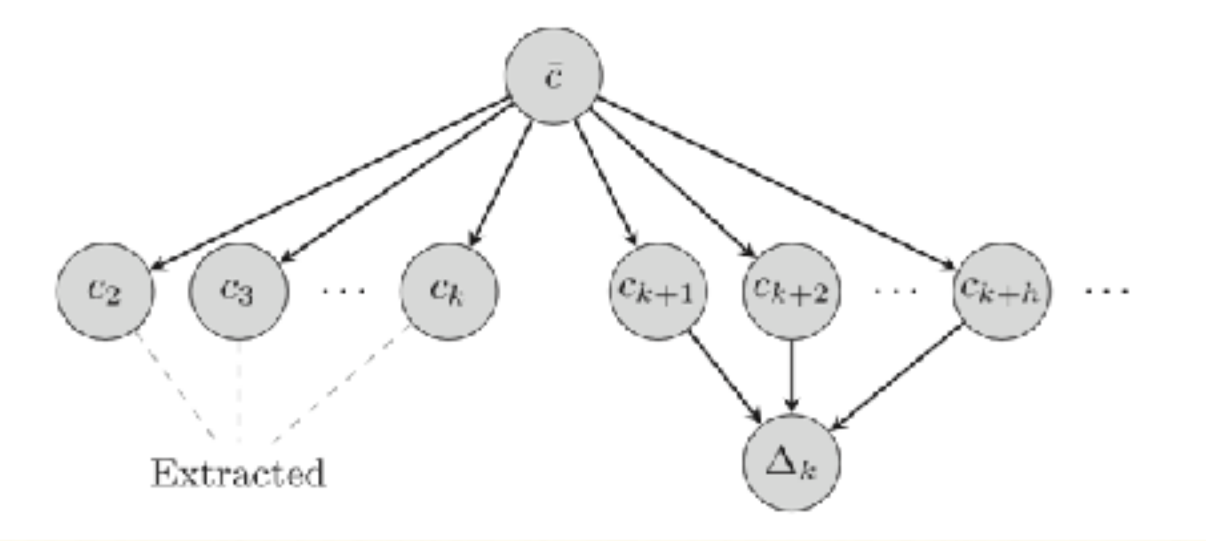
- Bayesian model:



Parameter cbar sets size of all dimensionless coefficients

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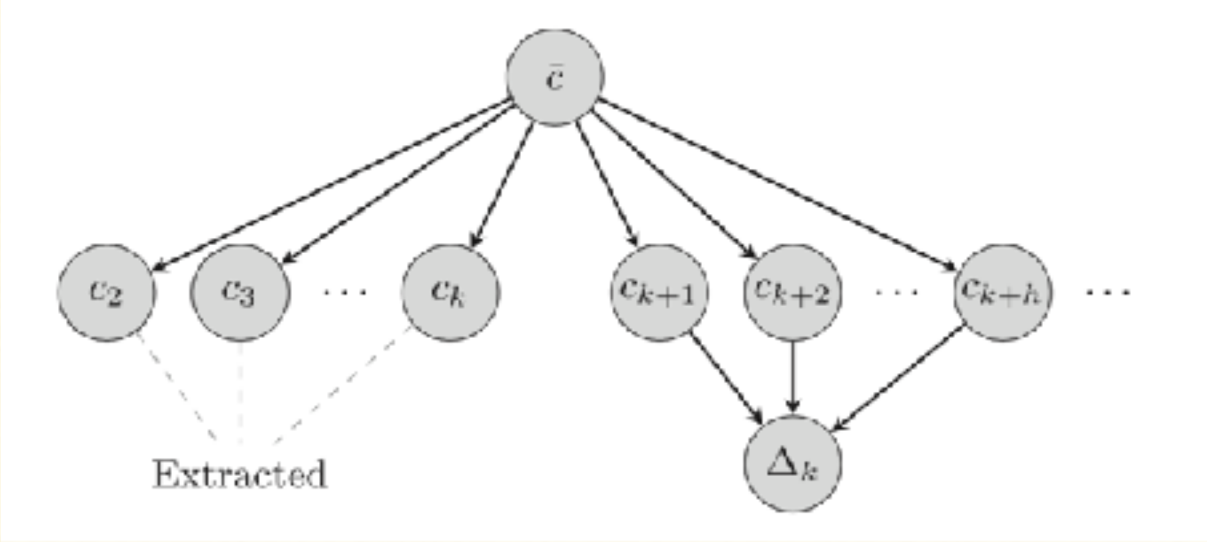

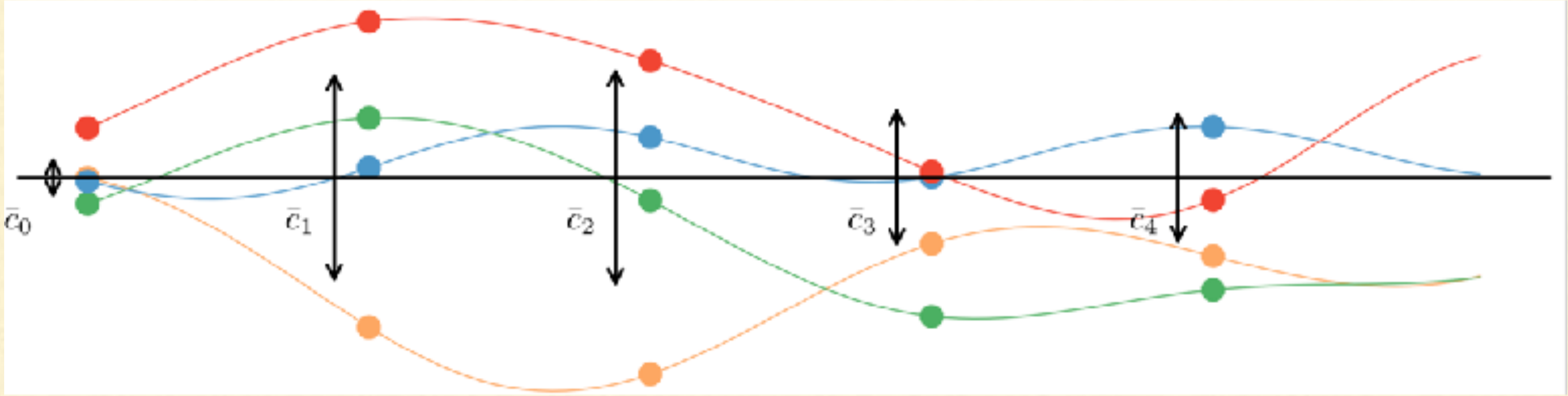

First shot: cbar can be different at different kinematic points: "uncorrelated model"

NN scattering

Epelbaum, Krebs, Meißner, PRC, 2015

Employ "semi-local" potentials of Epelbaum, Krebs, and Meißner

χEFT: $\mathcal{L}(N,\pi) \to V^{(k)} \to \delta \to \sigma_{np}$

$$\sigma_{np}(E_{\rm lab}) = \sigma_{\rm LO} \sum_{n=0}^{k} c_n(p_{\rm rel}) \left(\frac{p_{\rm rel}}{\Lambda_b}\right)^n$$

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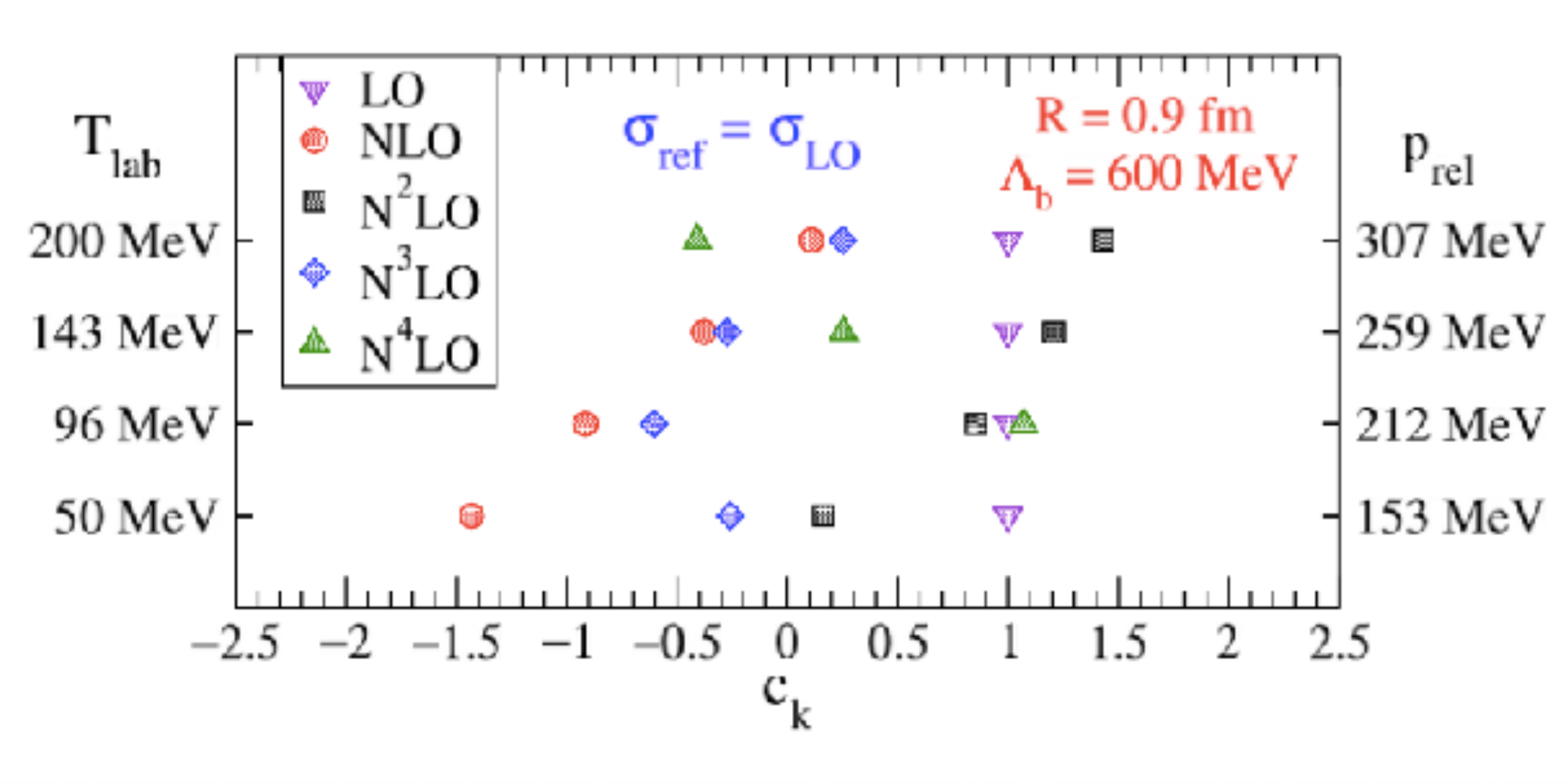
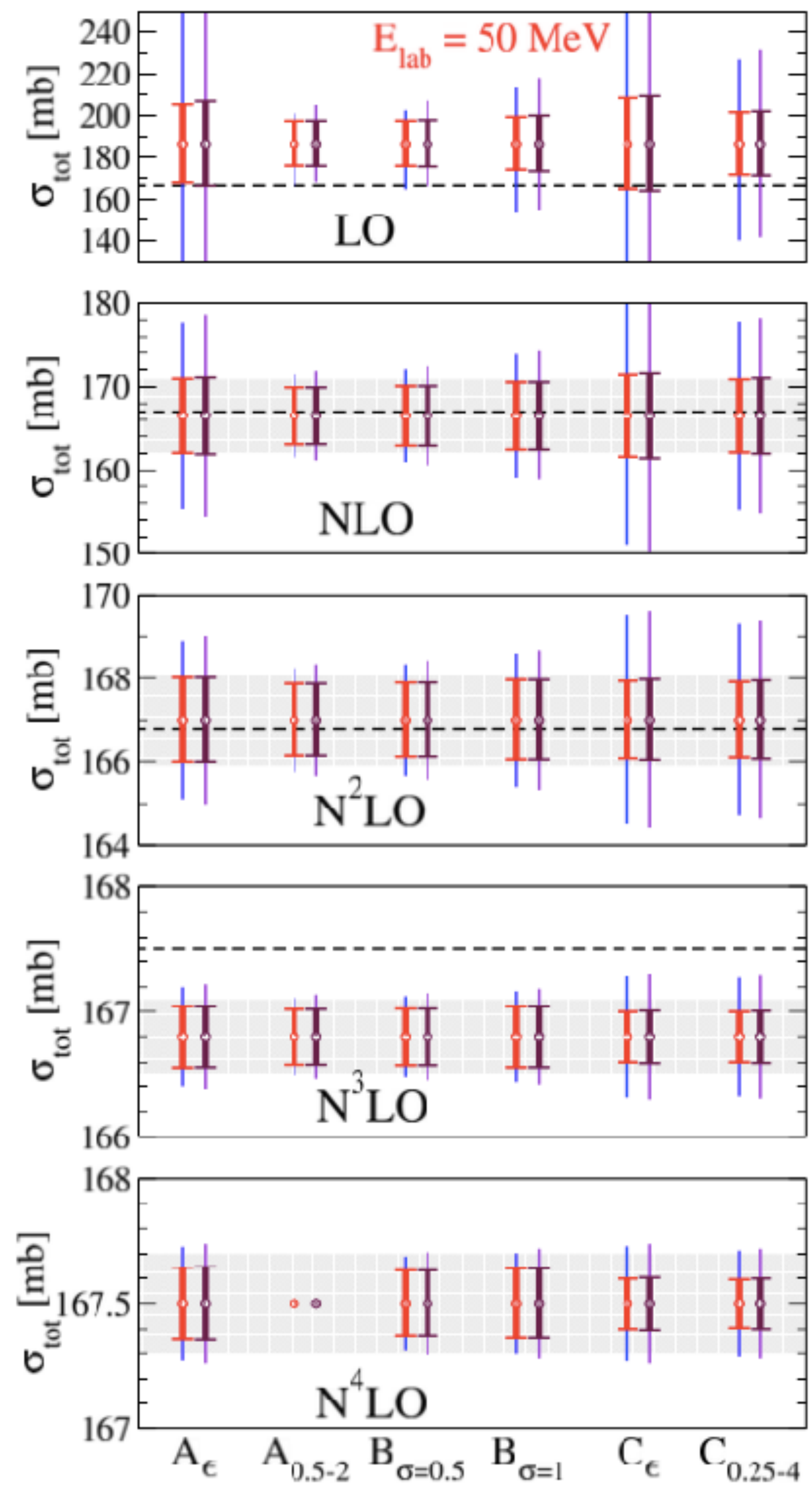
- NN cross section at T_{lab}=50, 96, 143, 200 MeV
- Potential regulated by local function, parameterized by R
- EKM identify Λ_b=600 MeV for smaller R values
- Here: R=0.9 fm data
- Results at LO, NLO, N²LO, N³LO, N⁴LO (k=0, 2, 3, 4, 5)

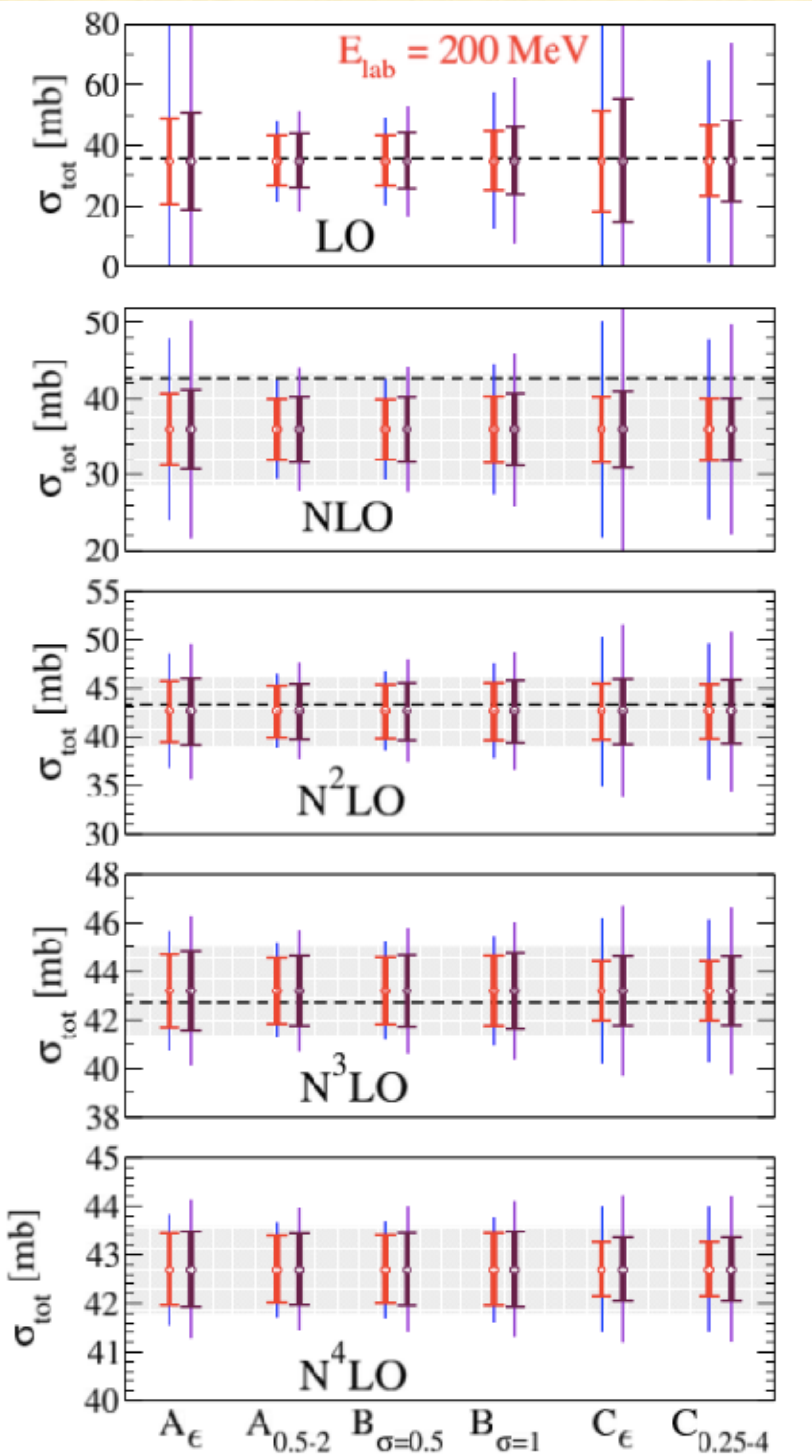


Results



E_{lab} = 50 MeV
σ_{tot} [mb]
LO
NLO
N^{2}LO
N^{3}LO
N^{4}LO
A_ϵ
$A_{0.5\text{-}2}$
$B_{\sigma=0.5}$
$B_{\sigma=1}$
C_ϵ
$C_{0.25\text{-}4}$

Res


E_{lab} = 200 MeV
σ_{tot} [mb]
LO
NLO
N^2LO
N^3LO
N^4LO
A_ϵ
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$B_{\sigma=0.5}$
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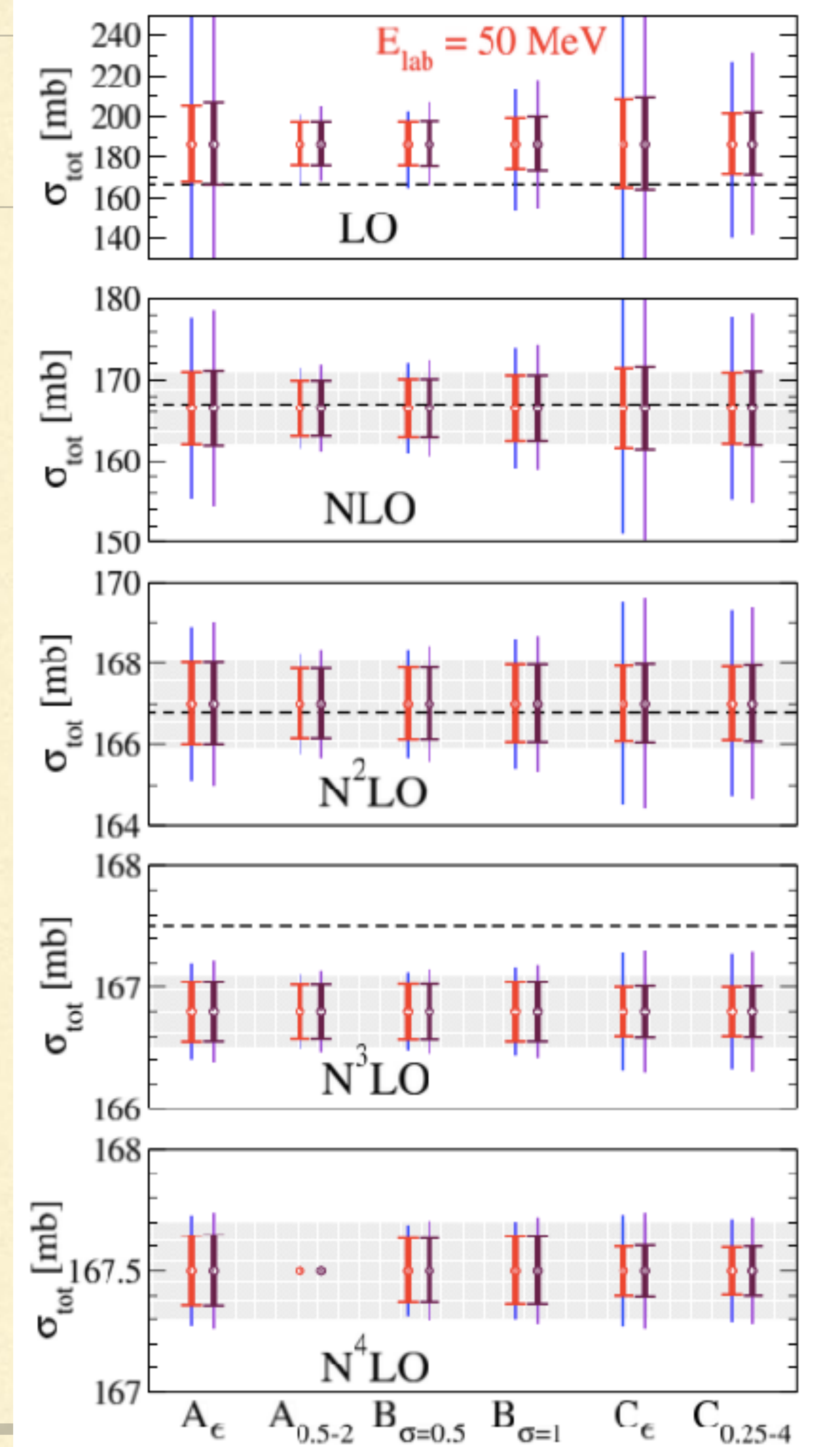
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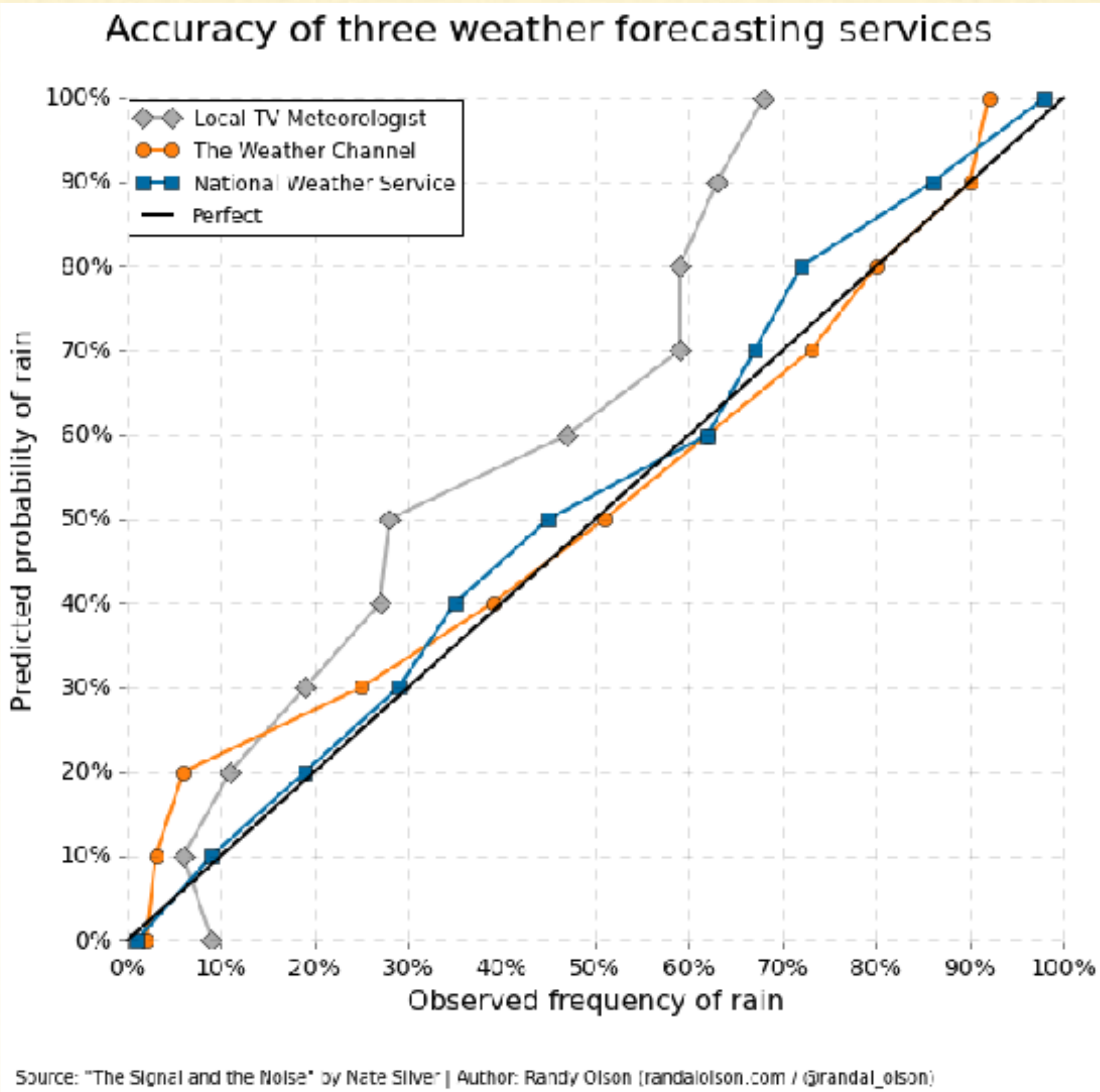

Melendez, Furnstahl, Wesolowski, PRC, 2017
after Furnstahl, Klco, DP, Wesolowski, PRC, 2015
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- Fix a given DOB interval: compute success ratio, compare

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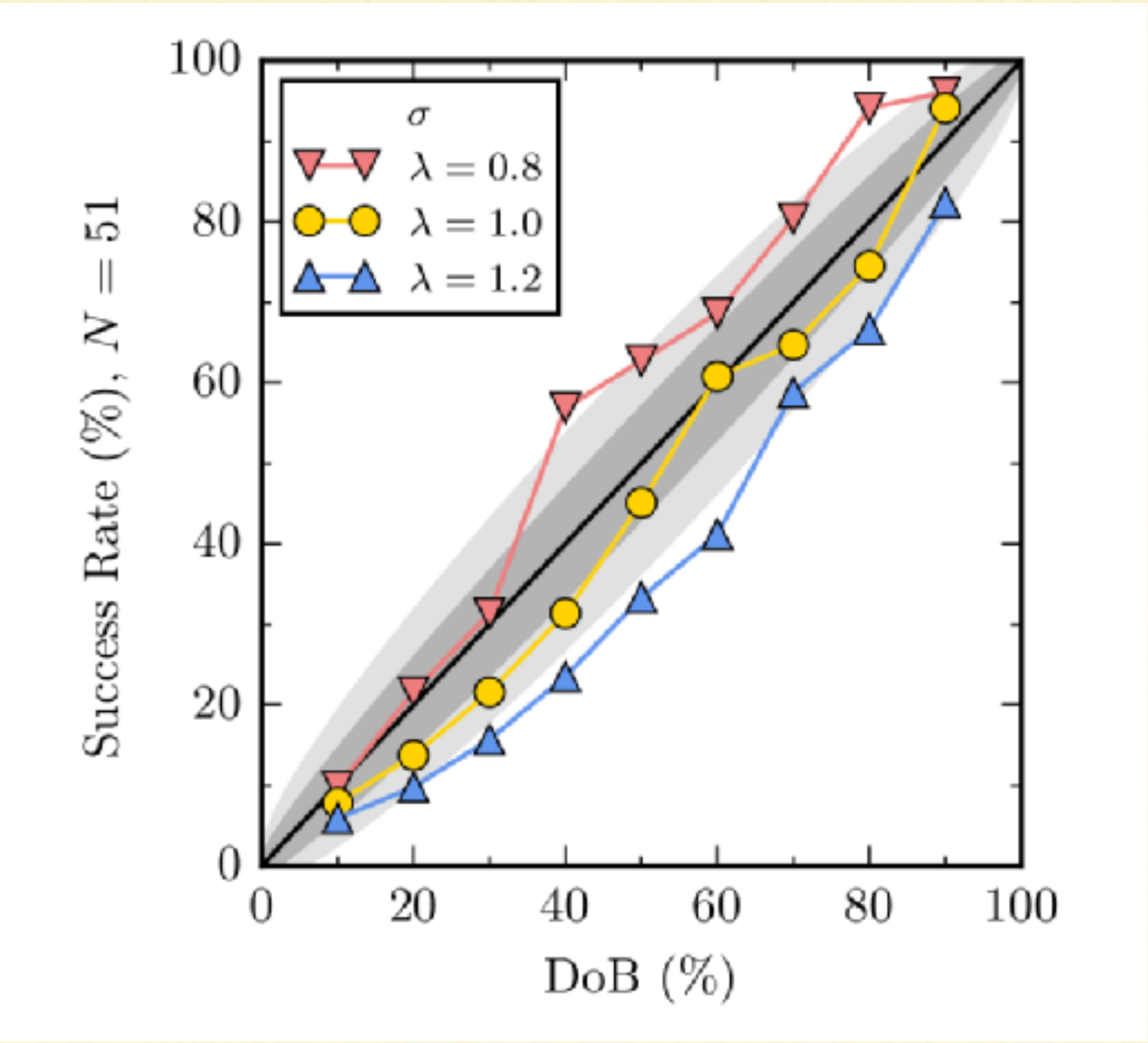

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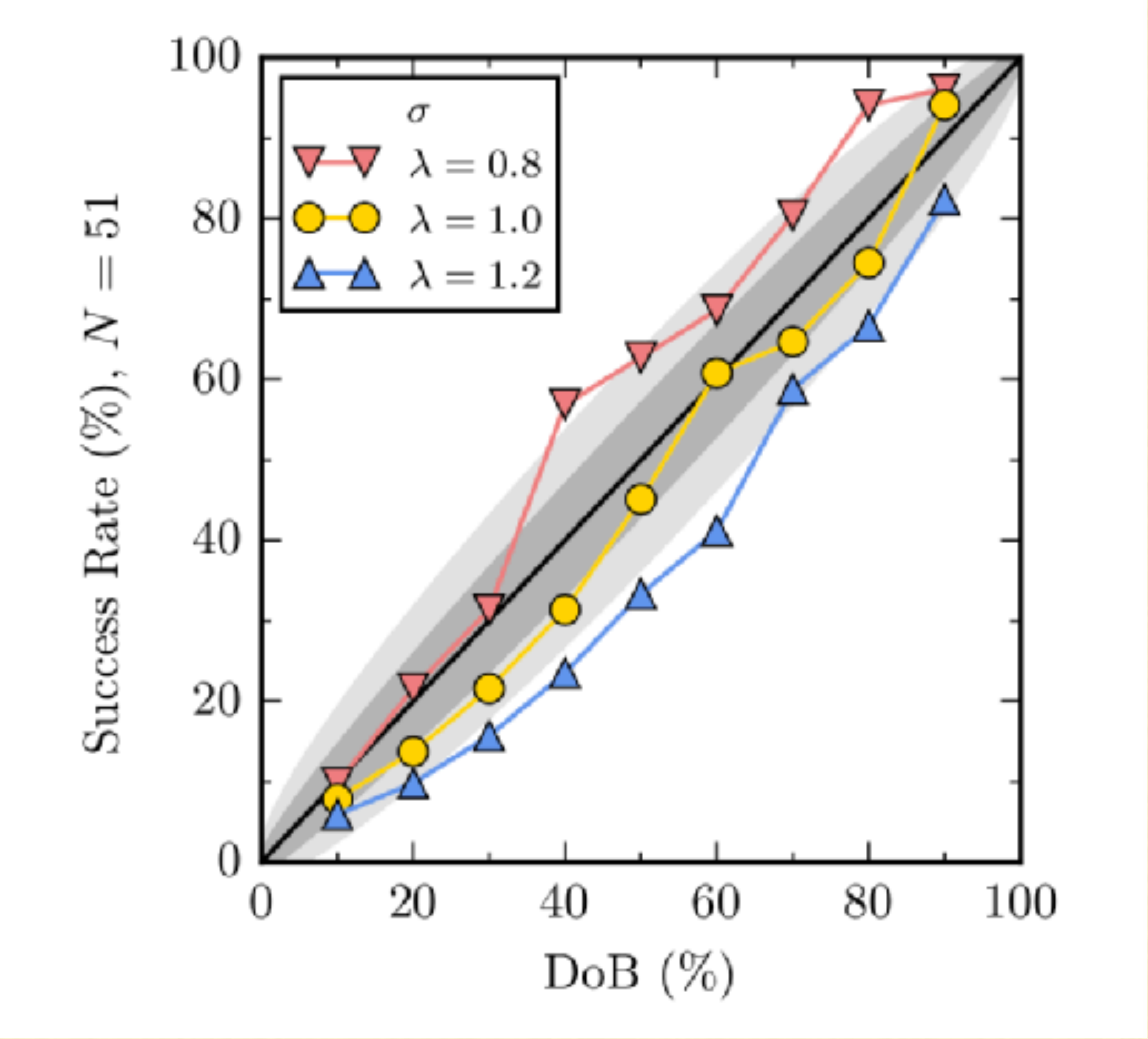

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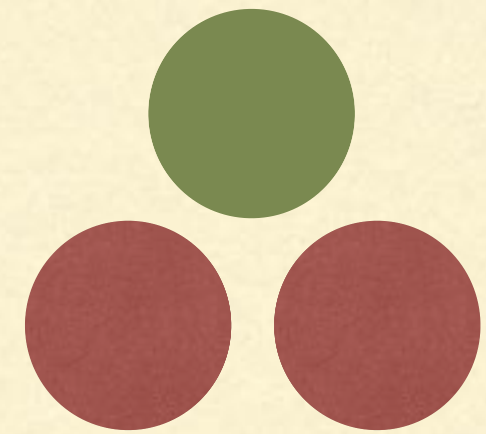
No evidence for significant rescaling of Λ_b

Parameter estimation from few-body data

Wesolowski, Svennson, Ekström, Forssén, Furnstahl, Melendez, DP, PRC 2021

Let's try and estimate the parameters of the three-nucleon force; for the moment we stick to bound-state observables

- Binding energy of three-nucleon nuclei: ^{3}H
- Binding energy of ^{4}He
- Charge radius of ^{4}He
- Beta-decay half-life of ^{3}H, aka "GT matrix element"



Solve Schrödinger equation for ^{3}He and ^{4}He and compute radii, GT matrix element

Done at $O(Q^0)$, $O(Q^2)$, $O(Q^3)$

Emulation via a Reduced-Basis Method (EC) makes fast evaluation possible

3N error model

$$y_{\rm exp} = y_{\rm th} + \delta y_{\rm exp} + \delta y_{\rm th}$$

$$y_{\rm th} = y_{\rm ref} \sum_{i=0}^{k} c_i(\{a_j\}) Q^i \qquad Q = \frac{p_{\rm typ}}{\Lambda_b} \qquad y_{\rm ref} = y_{\rm LO} \text{ here}$$

- Assume c_i's Gaussian random variables with mean zero $\Rightarrow \delta y_{\rm th} = y_{\rm ref} \bar{c} \dfrac{Q^{k+1}}{\sqrt{1 - Q^2}}$
- Q is not obvious: we will actually make it a parameter and sample it.
- We will also sample $\bar{c}^2$, the mean-square value of the higher-order coefficients
- $\bar{c}^2$ and Q are also constrained by information from the lower-order calculations
- As a first go we take the covariance matrix $\delta y_{\rm th}$ to be diagonal, although we will assume that all observables share a common $\bar{c}$

Posterior and priors

$$\mathrm{pr}(c_D, c_E, \bar{c}^2, Q \,|\, D, I) \propto \exp\left(-\frac{1}{2}\mathbf{r}^T(\boldsymbol{\Sigma}_{\mathrm{exp}} + \boldsymbol{\Sigma}_{\mathrm{th}})^{-1}\mathbf{r}\right) \exp\left(-\frac{c_D^2 + c_E^2}{2\bar{a}^2}\right) \mathrm{pr}(\bar{c}^2 \,|\, Q, \bar{a}, I)\mathrm{pr}(Q \,|\, c_D, c_E, I)$$

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- Can include NN in "fit" by expanding meaning of $\vec{a}$ to include NN parameters. Incorporate NN information by using posterior from that analysis as a prior on $\vec{a}_{NN}$, the NN piece of $\vec{a}$, here
- $\mathrm{pr}(\bar{c}^2 \,|\, Q, \vec{a}, I)$ is taken to be an inverse-χ^2 distribution. Information on the order-to-order shift NNLO-NLO included there
- $\mathrm{pr}(Q \,|\, \mathbf{a}, I)$ then also affected by that information. Starts as weakly informative Beta distribution.

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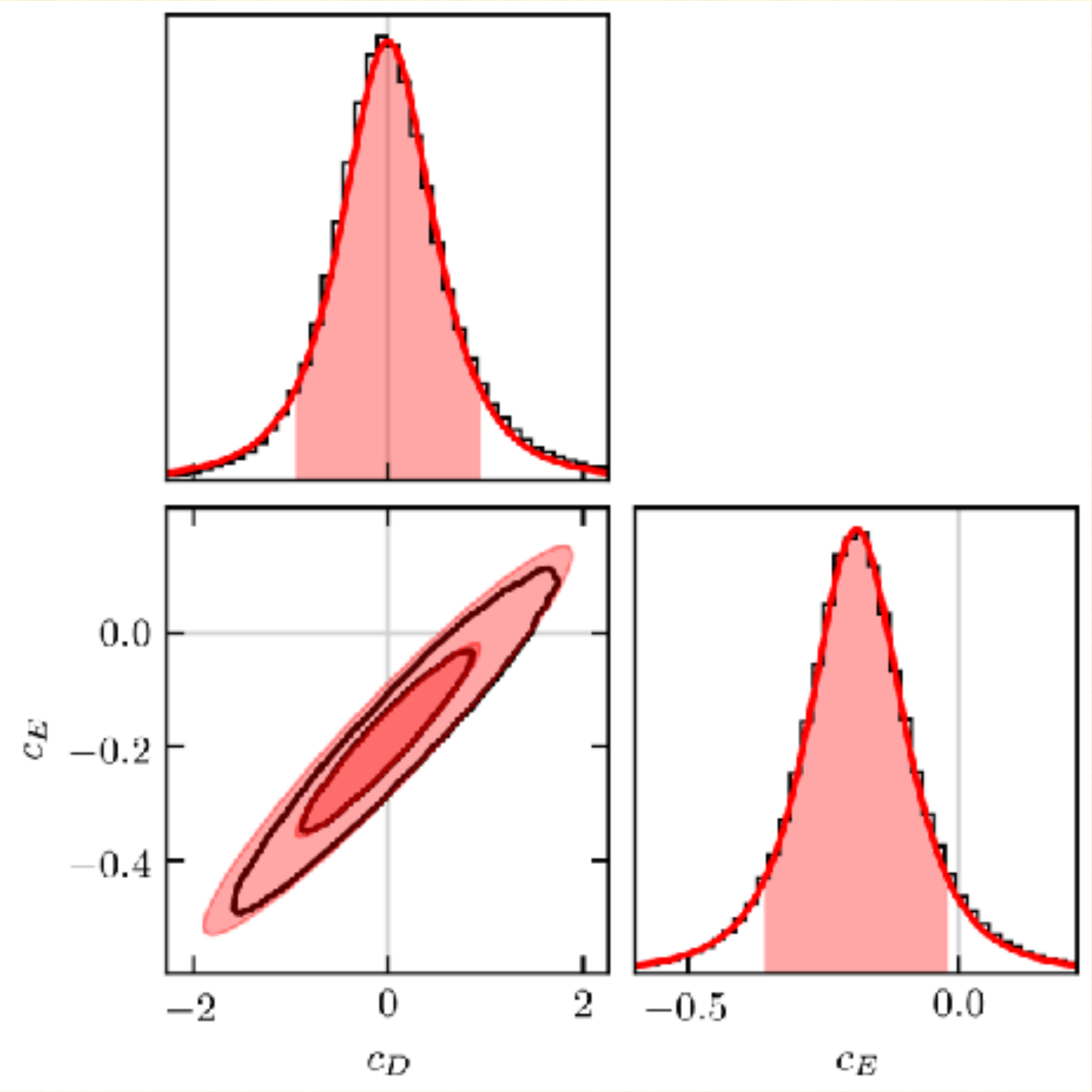

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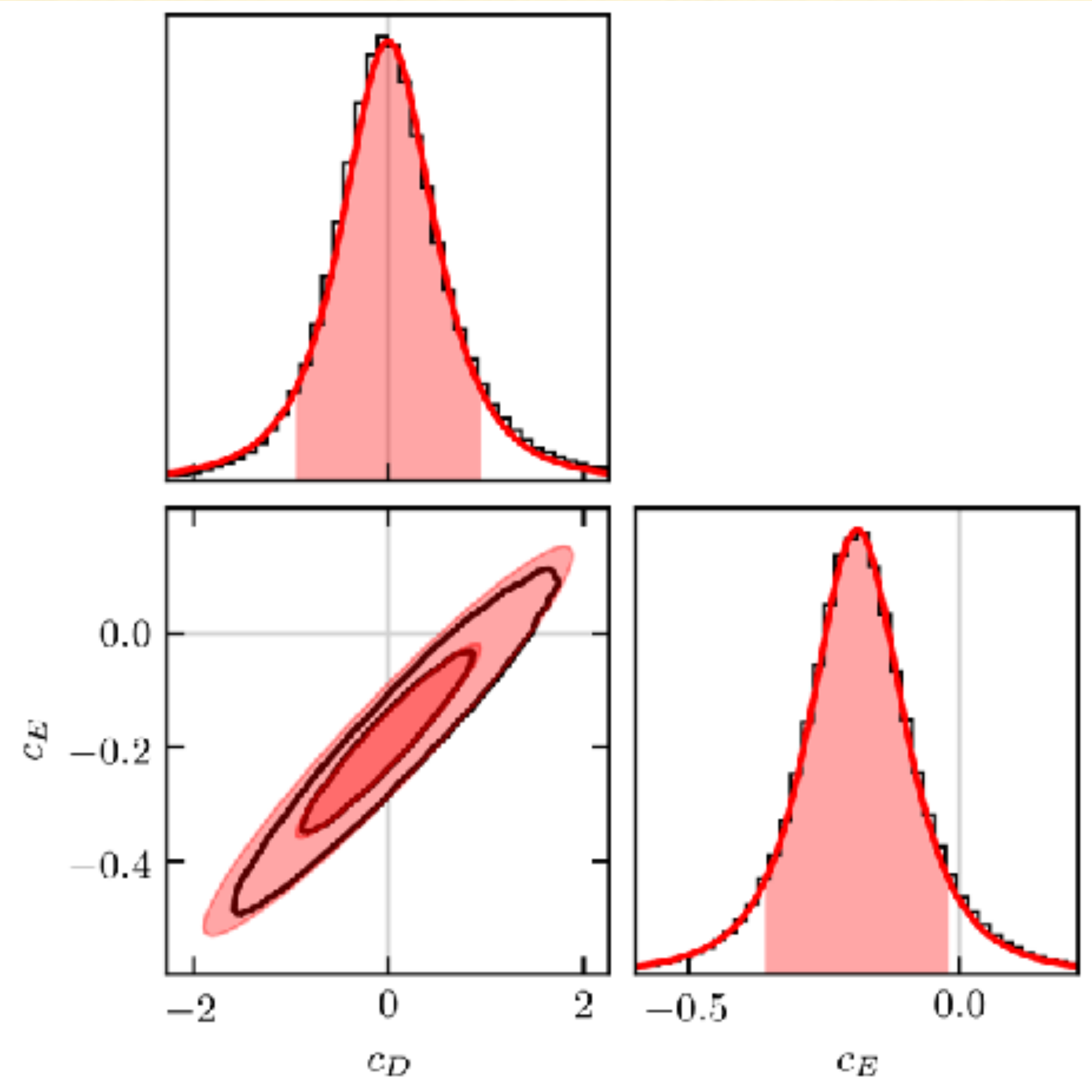

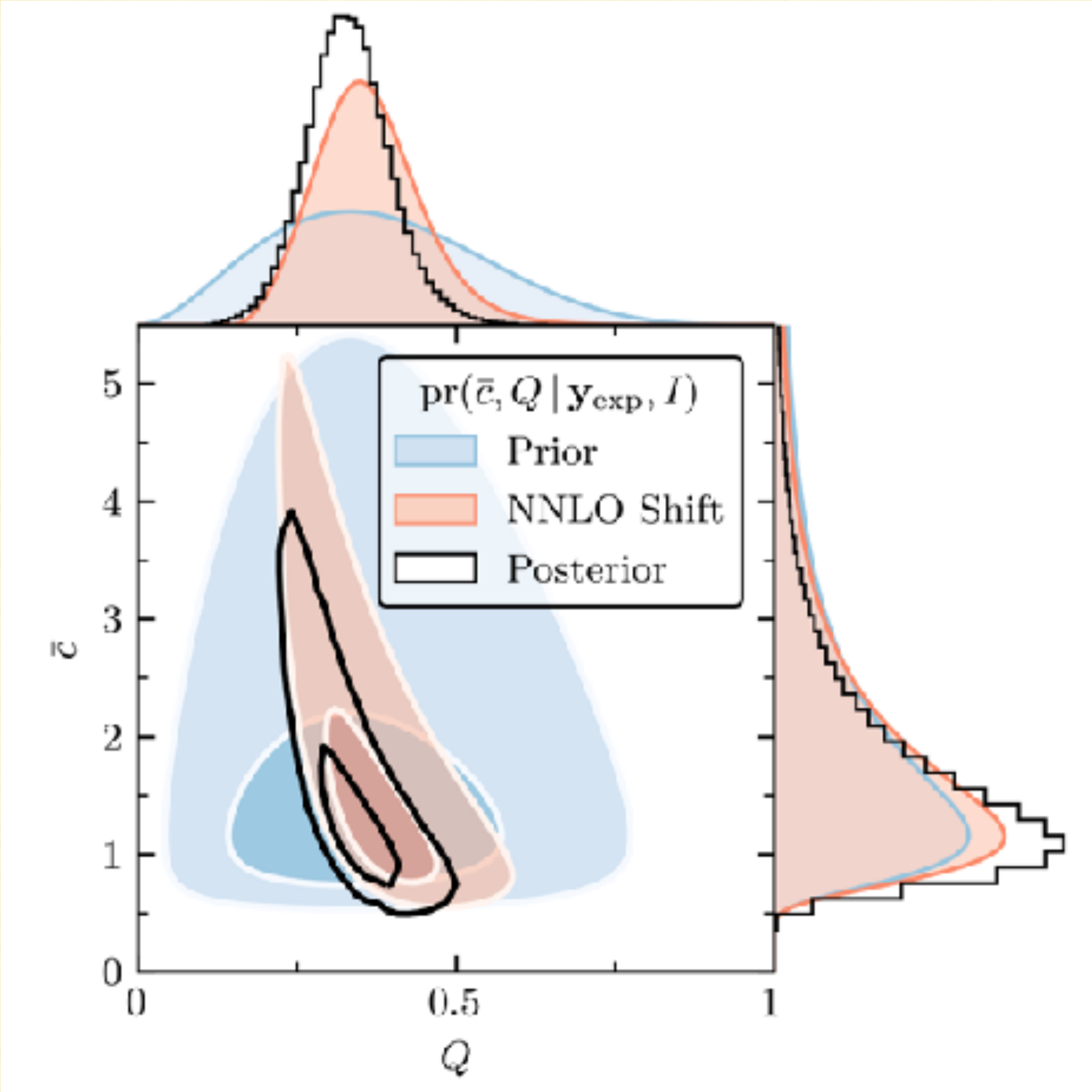

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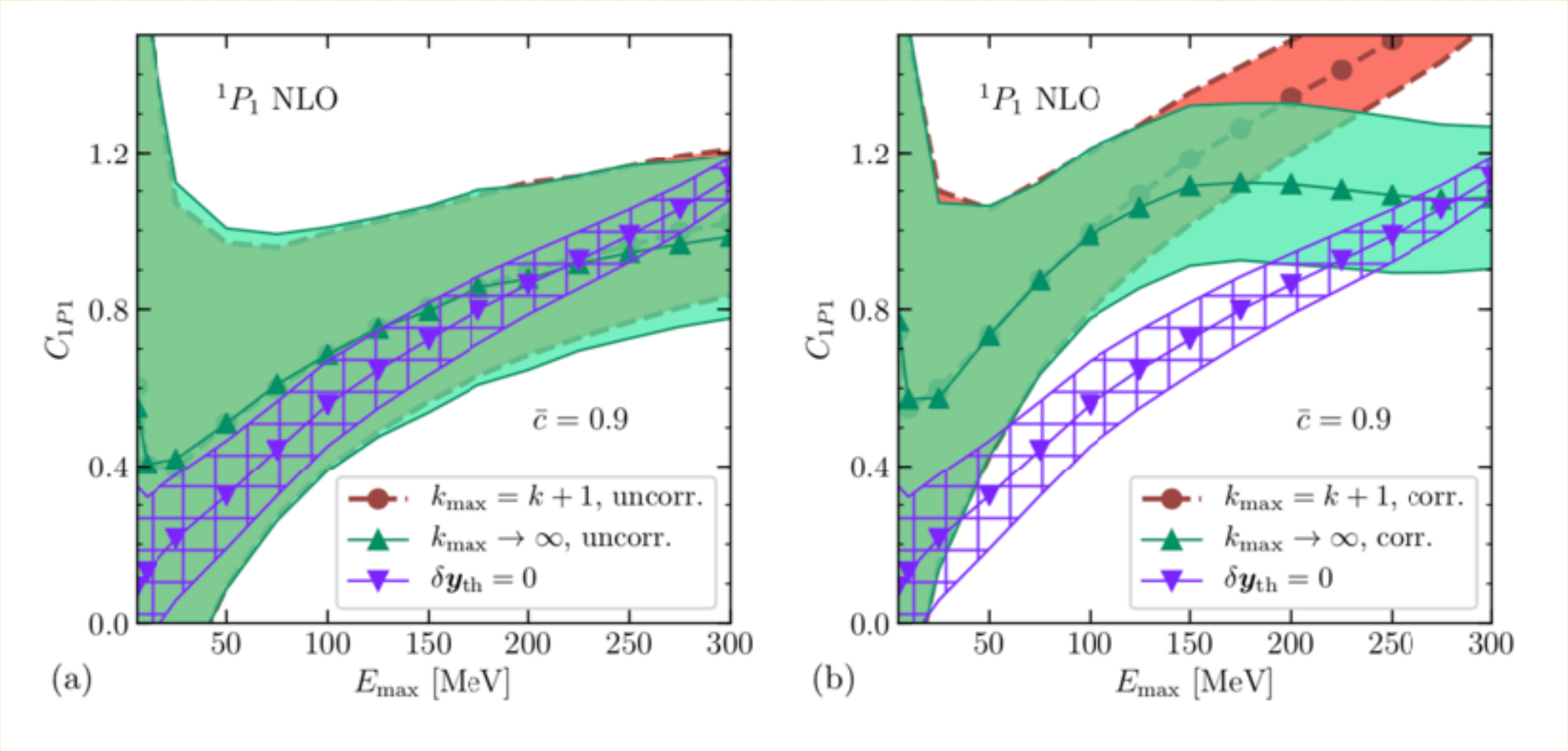
Q inferred from data, convergence pattern

E_{max} plots in the $^1P_1$

Wesolowski, Furnstahl, Melendez, DP, JPG 2018



$$(\Sigma_{\mathrm{th,diag}})_{ij} = (\mathbf{y}_{\mathrm{ref}})^2 \bar{c}^2 \delta_{ij} \sum_{n=k+1}^{k_{\max}} Q_i^{2n} \qquad (\Sigma_{\mathrm{th,corr}})_{ij} = (\mathbf{y}_{\mathrm{ref}})_i (\mathbf{y}_{\mathrm{ref}})_j \bar{c}^2 \sum_{n=k+1}^{k_{\max}} Q_i^n Q_j^n$$

- Can resum truncation error to all orders (under assumptions about its correlation across orders): tests validity of first-omitted term approximation

A Gaussian Process hypothesis

Melendez, Wesolowski, Furnstahl, DP, Pratola, PRC (2019)

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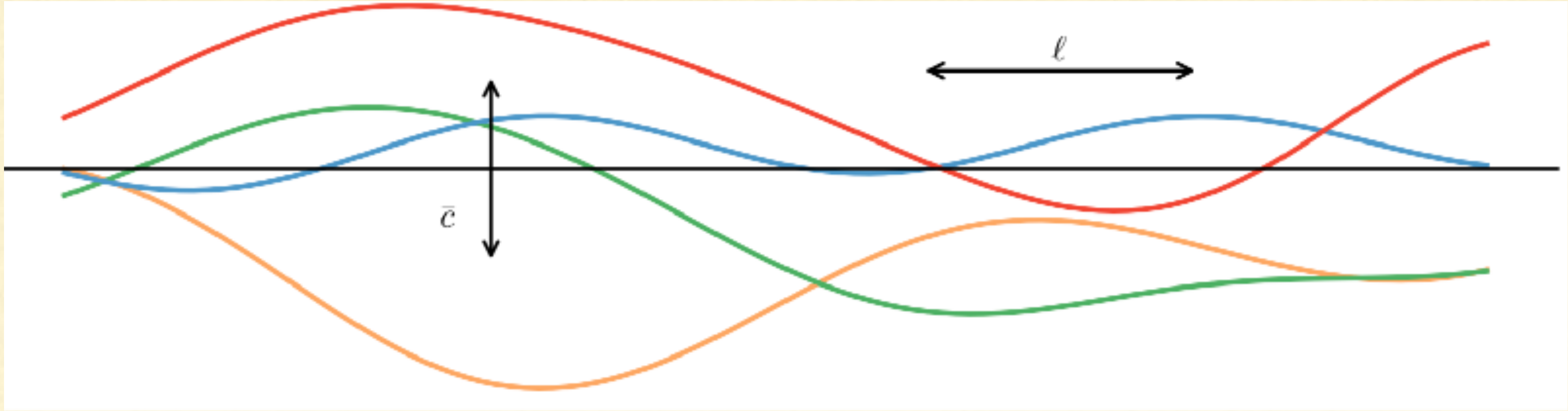
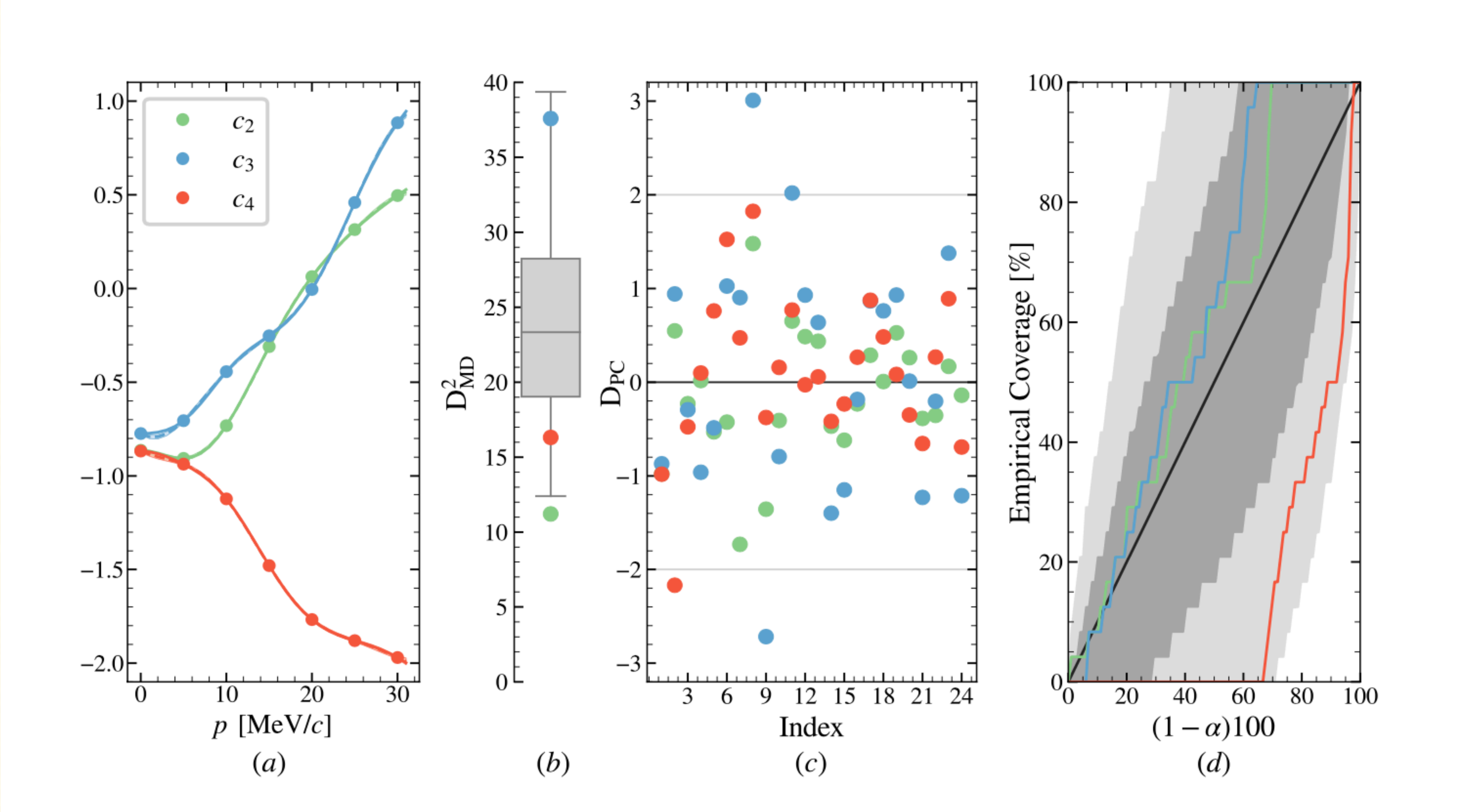
EFT coefficients at different orders can be modeled as independent draws from a *Gaussian Process* with a stationary kernel



- Gaussian distribution at each point
- With correlation structure parameterized by a single $\bar{c}^2$ and ℓ at all orders

Application to np→dγ

Acharya, Bacca, PLB 2022



Publicly available package gsum

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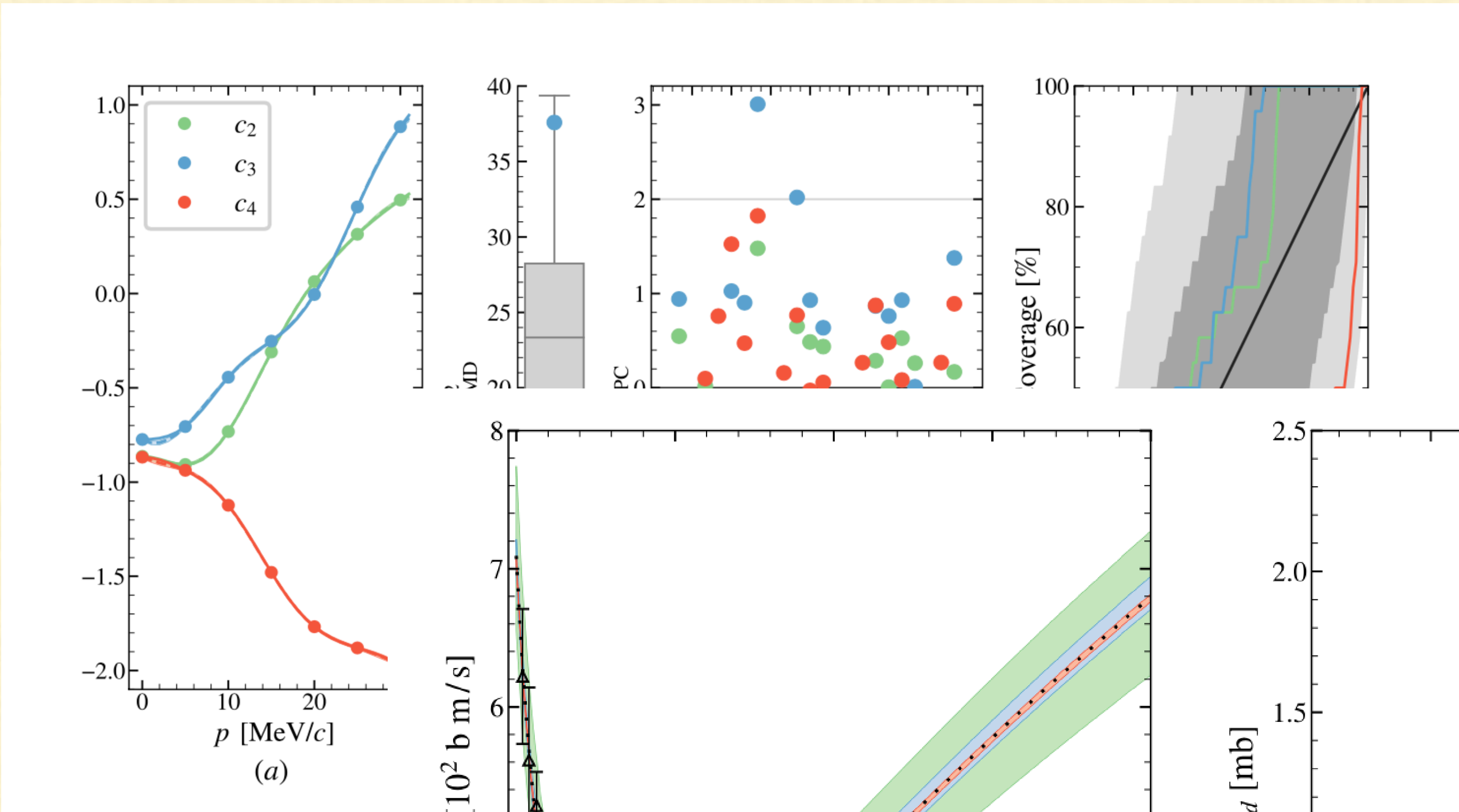
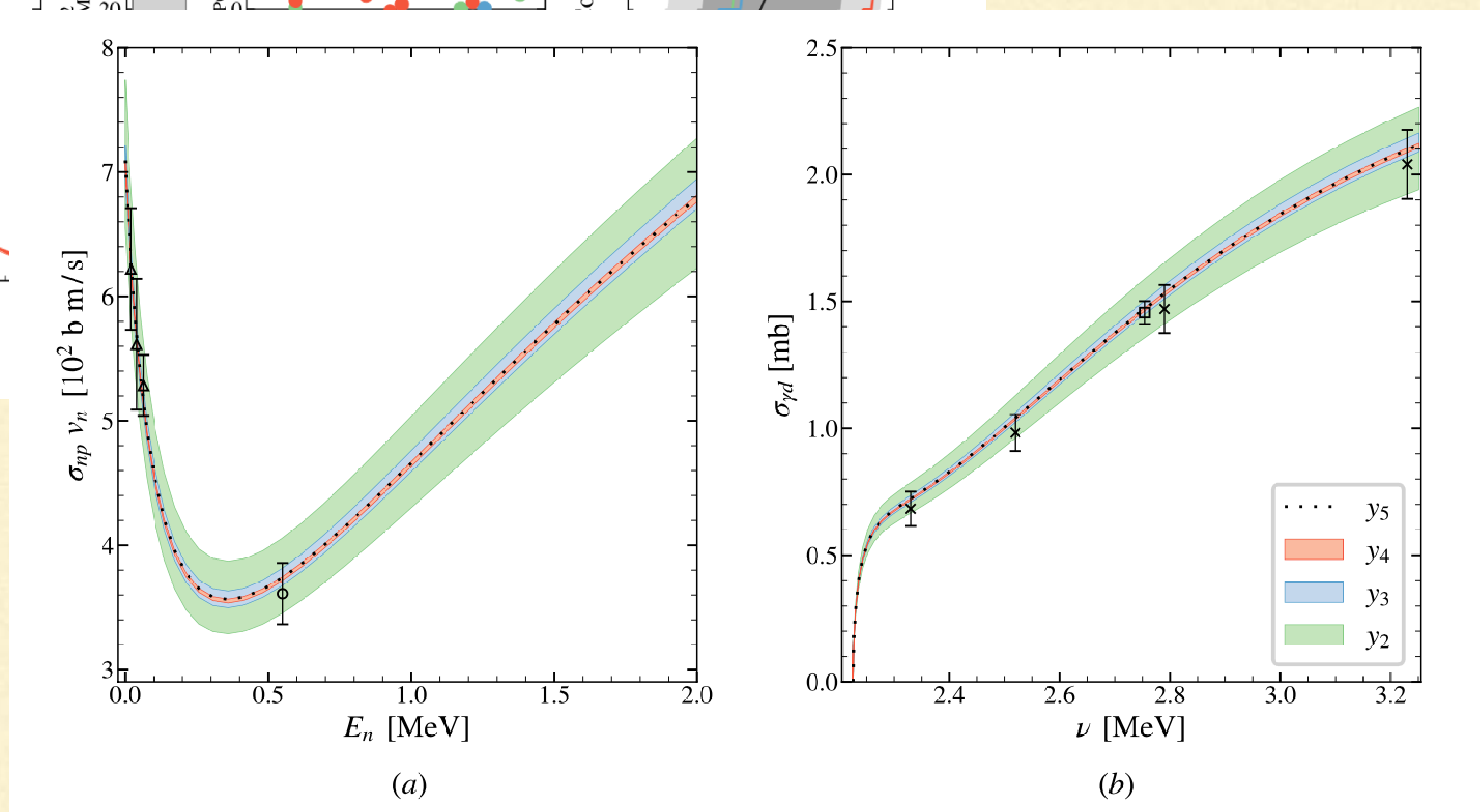
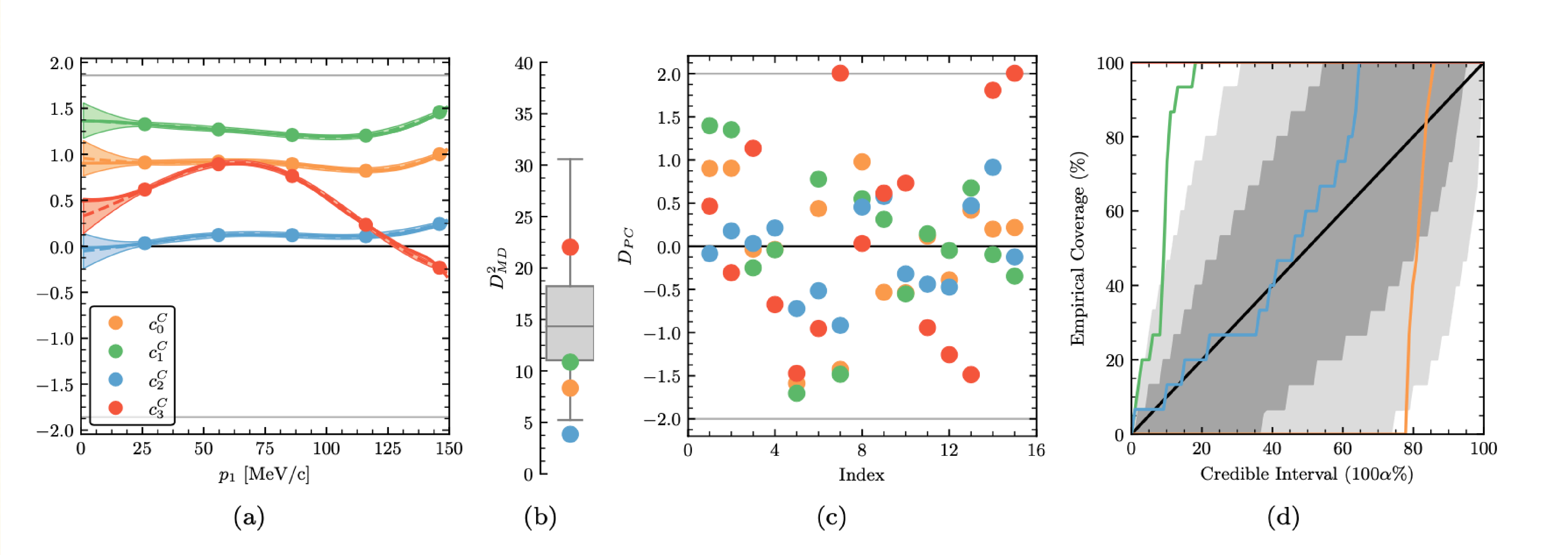




Publicly available package gsum

Application to $\mu^- d \rightarrow nn\nu_\mu$

Gnech, Marcucci, Viviani, arXiv 2023

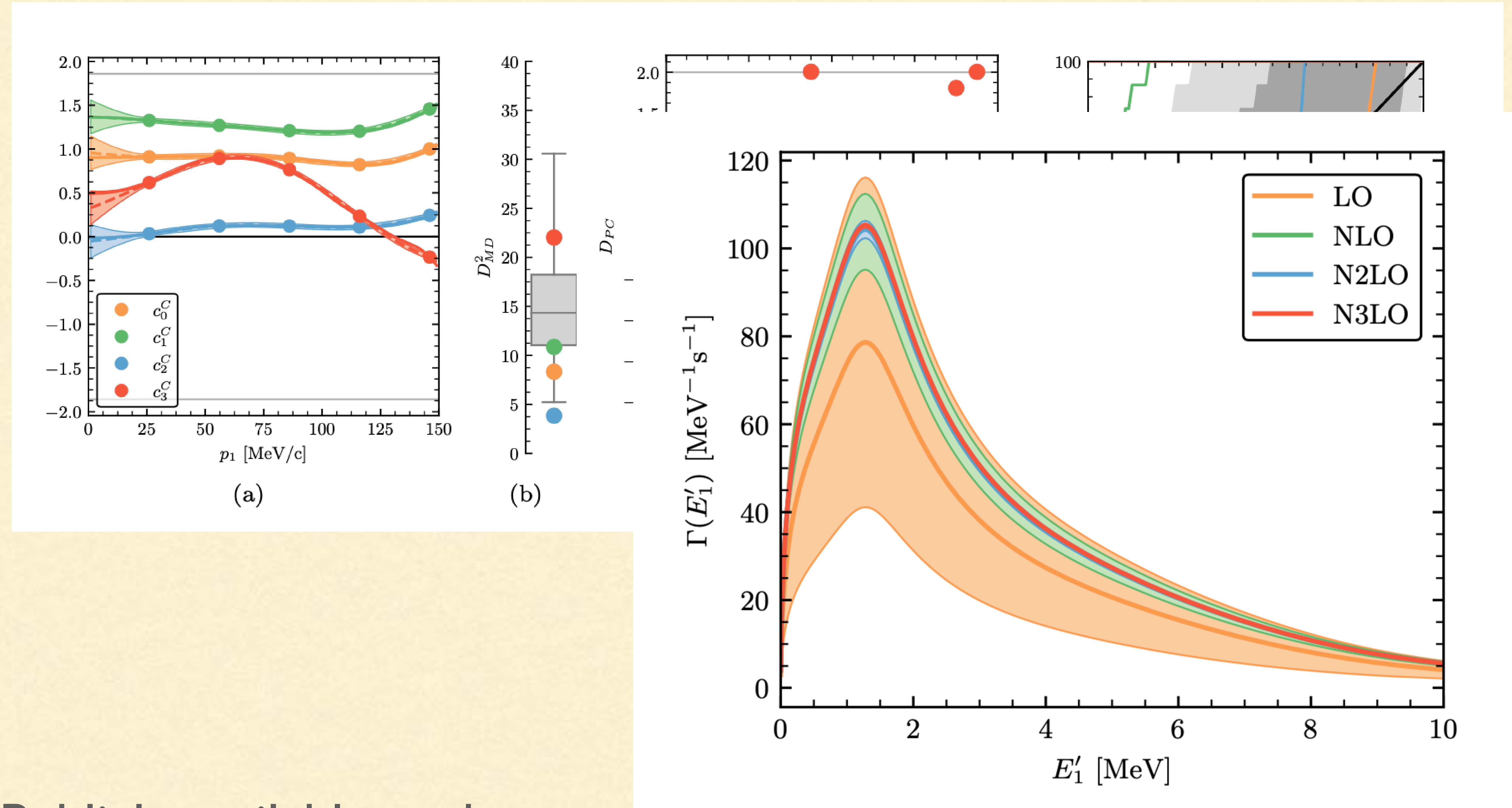


Publicly available package:

https://github.com/buqeye/gsum

Application to $\mu^- d \to nn\nu_\mu$

Gnech, Marcucci, Viviani, arXiv 2023



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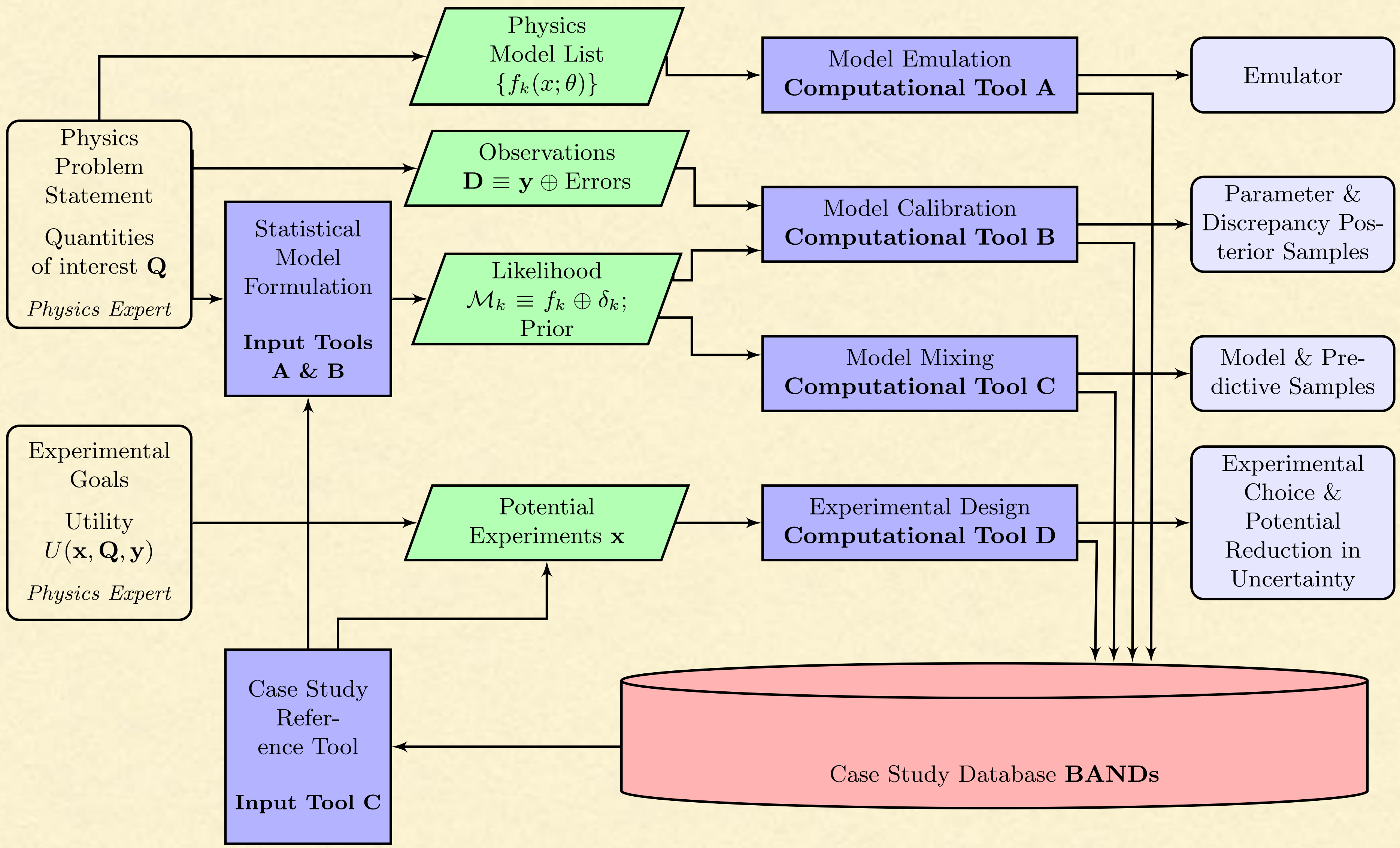
BAND Software Framework

Goal: *Facilitate principled Uncertainty Quantification in Nuclear Physics*



DP et al., "BAND manifesto", JPG 2021 https://bandframework.github.io/

Research scientists and grad students


Pablo Giuliani


Kyle Godbey


Sunil Jaiswal


Moses Chan


Manuel Catacora-Rios


Dan Liyanage


Alexandra Semposki


Mookyong Son


John Yannotty

BAND Framework v0.3

Bayesian Analysis of Nuclear Dynamics

Now available at https://github.com/bandframework/bandframework

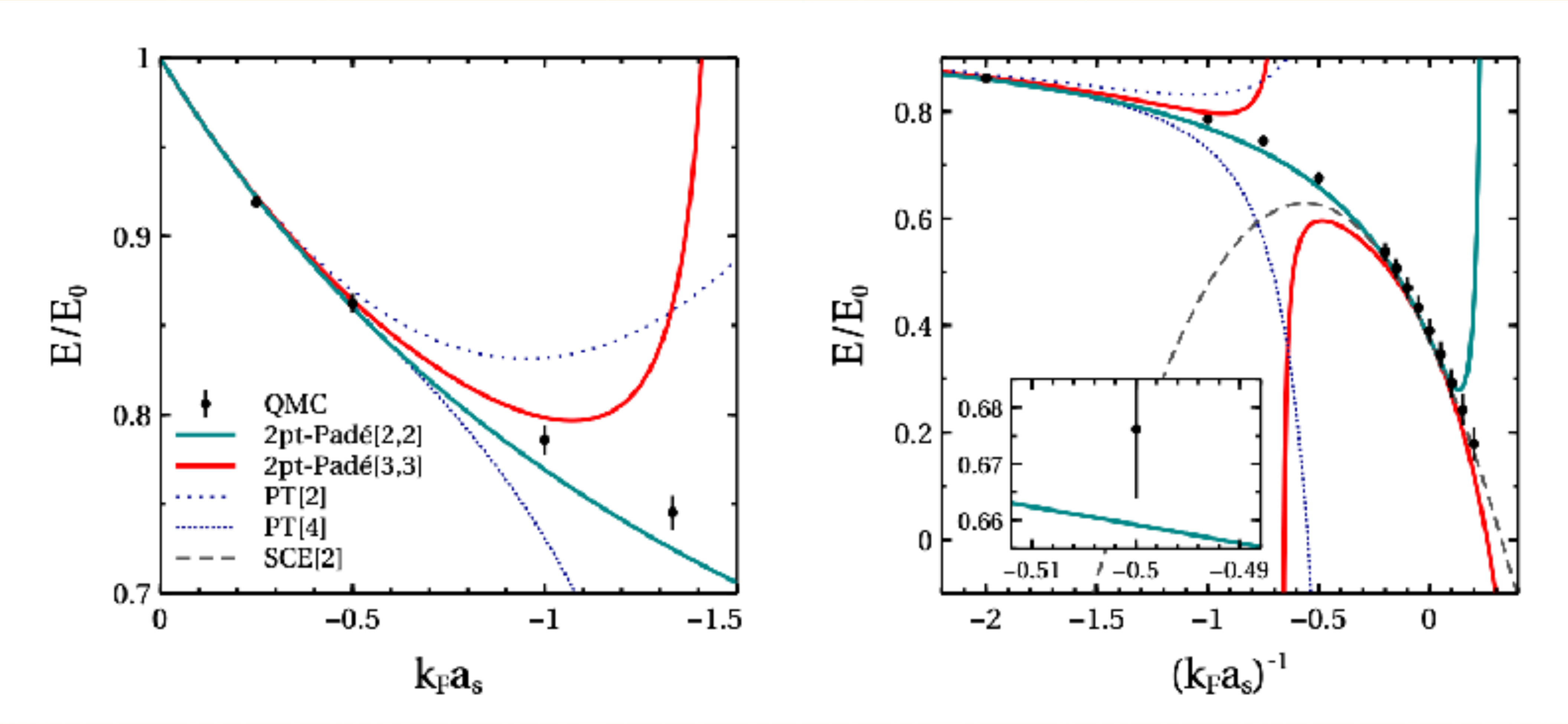
- Tools:
  - surmise: for model emulation via Gaussian Processes and calibration
  - SaMBA: Sandbox for Mixing via Bayesian Analysis
  - Taweret: Model Mixing software
  - BMEX: Bayesian Mass Explorer
  - par moo: parallel multiobjective simulation optimization.
  - rose: a reduced-order scattering emulator
- Examples:
  - QGP_Bayes: tutorial on Bayesian analysis of QGP simulations
  - BRICK: Bayesian R-matrix Inference Code Kit
  - BFRESCOX: Emulation and model calibration of coupled-channels treatment of nuclear reactions

We welcome contributions (tools, examples, and suggestions) from the community

Bayesian Model Mixing

What if we have two (or more) nuclear-physics models, each of which works well in its own region of validity. How do we make reliable predictions across the entire space?

Example: gas of fermions with short-range interactions

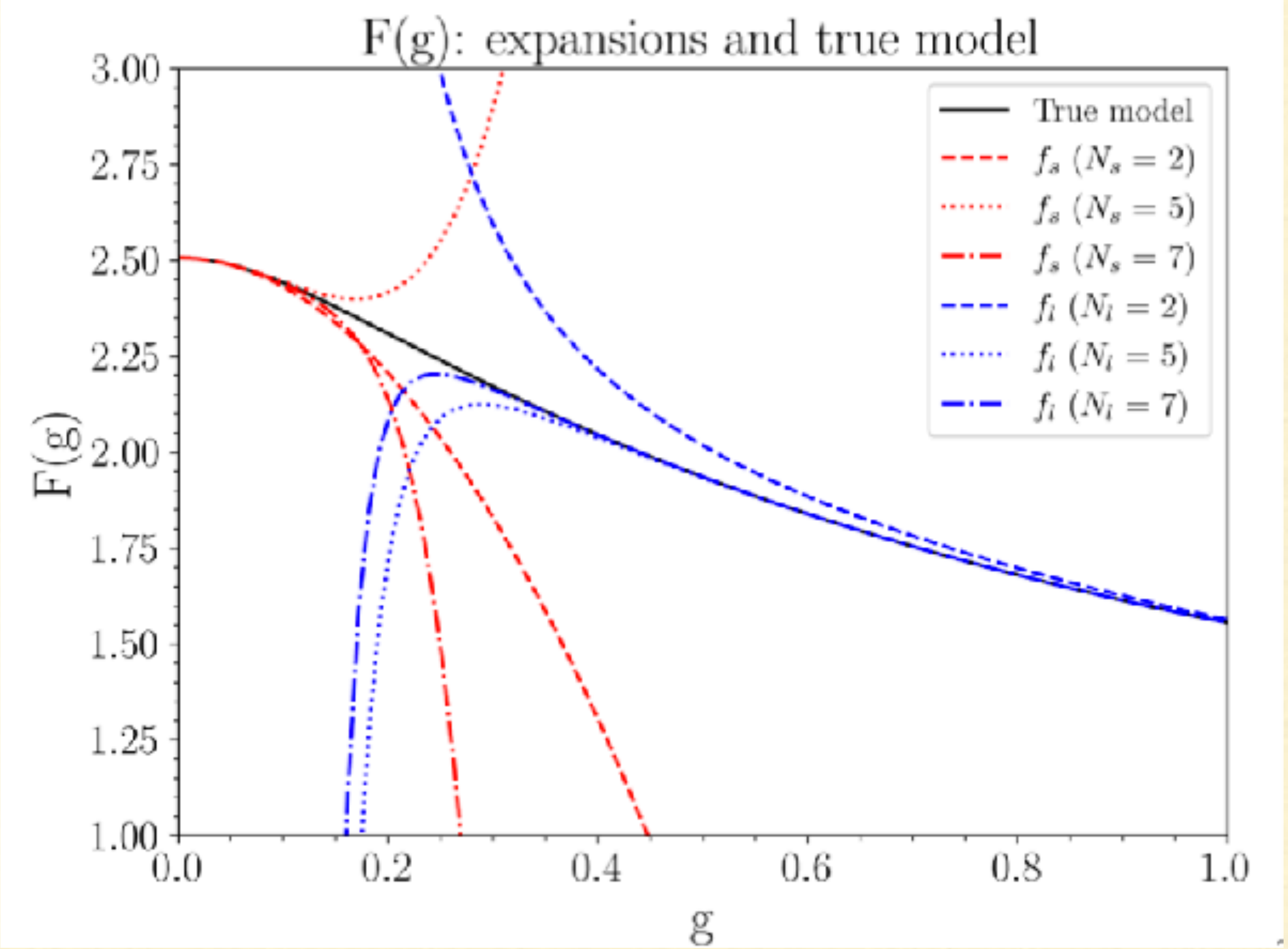


Wellenhofer, DP, Schwenk, PSS B (2021)

A toy problem

Semposki, Furnstahl, DP Phys. Rev. C (2022)

- Consider weak-coupling expansion: $f_s(g) = \sum_{k=0}^{N_s} s_k g^k$
- And strong-coupling expansion for same thing: $f_l(g) = \frac{1}{\sqrt{g}} \sum_{k=0}^{N_l} l_k g^{-k}$



- E.g., 0d partition function of ϕ^4 theory:

$$f(g) = \int d\phi \exp\left(-\phi^2/2 - g^2\phi^4\right)$$

Honda, JHEP 2014, 19 (2014)

Step 1: "error model" for each physics model

- BUQEYE™ approach to truncation errors
- Rewrite perturbation-theory expansion as $\sum_{n=0}^{k} c_n Q^n$
- Put a prior on behavior of c_n (e.g. naturalness prior in EFT)
- Update prior based on known values $\{c_0, \ldots, c_k\}$: $\mathrm{pr}(c_{k+1} | \{c_n\}, I)$
- Estimate error due to next term as $\sqrt{\langle c_n^2 \rangle} Q^{k+1} \equiv \bar{c} Q^{k+1}$
- Here we take the values of $f_{s,l}(g)$ to be normally distributed around the result of order $N_{s,l}$ with a standard deviation given by
  - Uninformative: $\sigma_{N_s} = \bar{c} g^{N_s+2} (N_s + 2)!$; $\sigma_{N_l} = \bar{d} \dfrac{1}{(N_l + 1)!} \dfrac{1}{g^{N_l+1}}$
  - Informative: standard deviation includes additional factors of 4^{N_s} and $1/4^{N_l}$ to more closely match behavior of low-order coefficients

Step 2: Combine the Gaussians

- Combine K models by weighting them by their precision

$$f_\dagger = \frac{1}{Z_P}\sum_{k=1}^{K}\frac{1}{v_k}f_k; \quad Z_P = \sum_{k=1}^{K}\frac{1}{v_k}$$

- Then, e.g. if f_1 and f_2 are both normally distributed, so is the combination:

$$f_\dagger \sim \mathcal{N}\left(\frac{v_2 f_1 + v_1 f_2}{v_1 + v_2}, \frac{v_1 v_2}{v_1 + v_2}\right)$$

Phillips et al., "Get on the BAND Wagon: a Bayesian framework for quantifying model uncertainties..."

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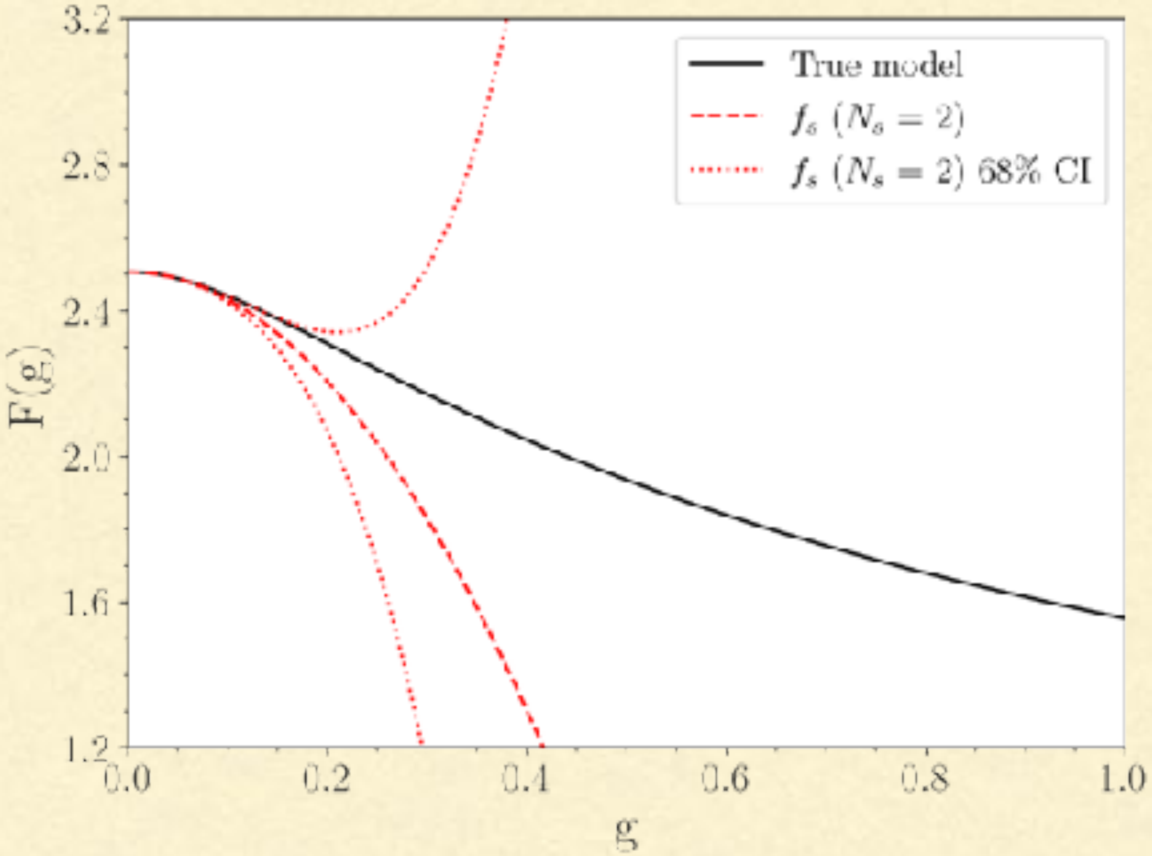

$N_s=N_l=2$

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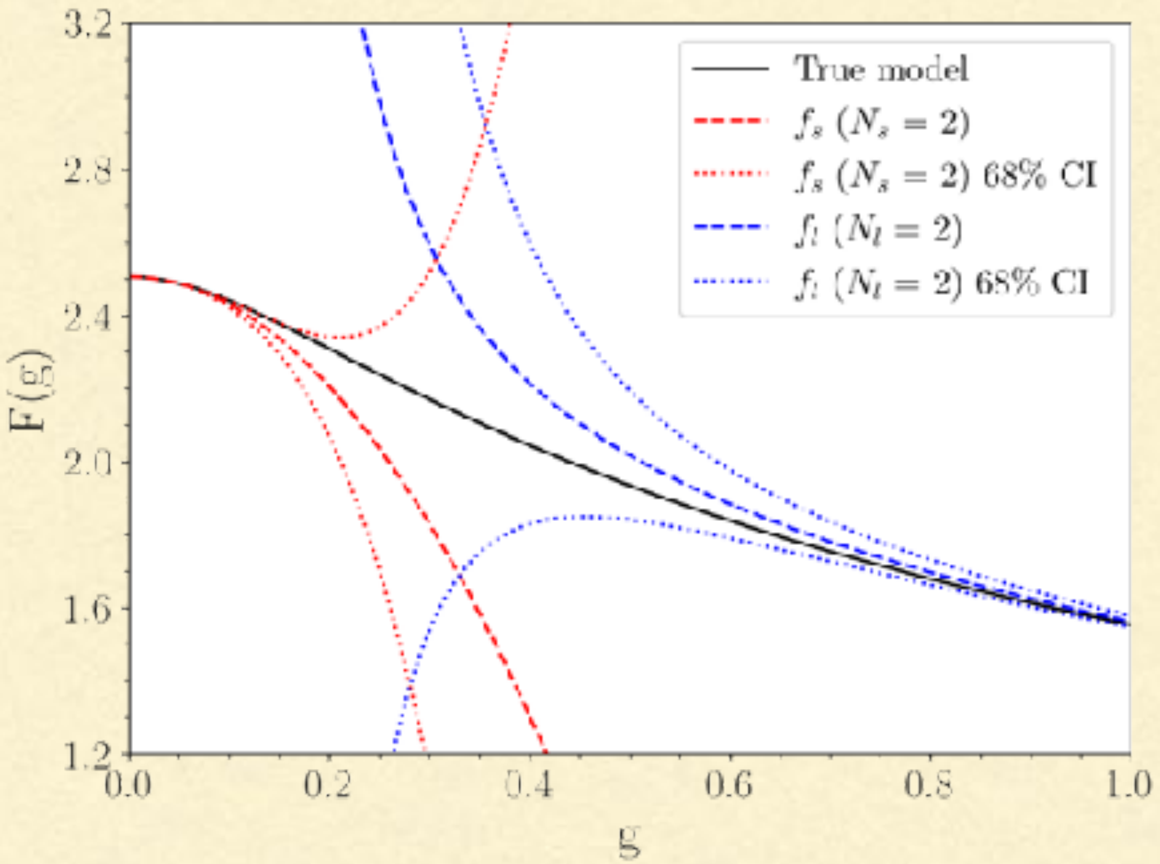

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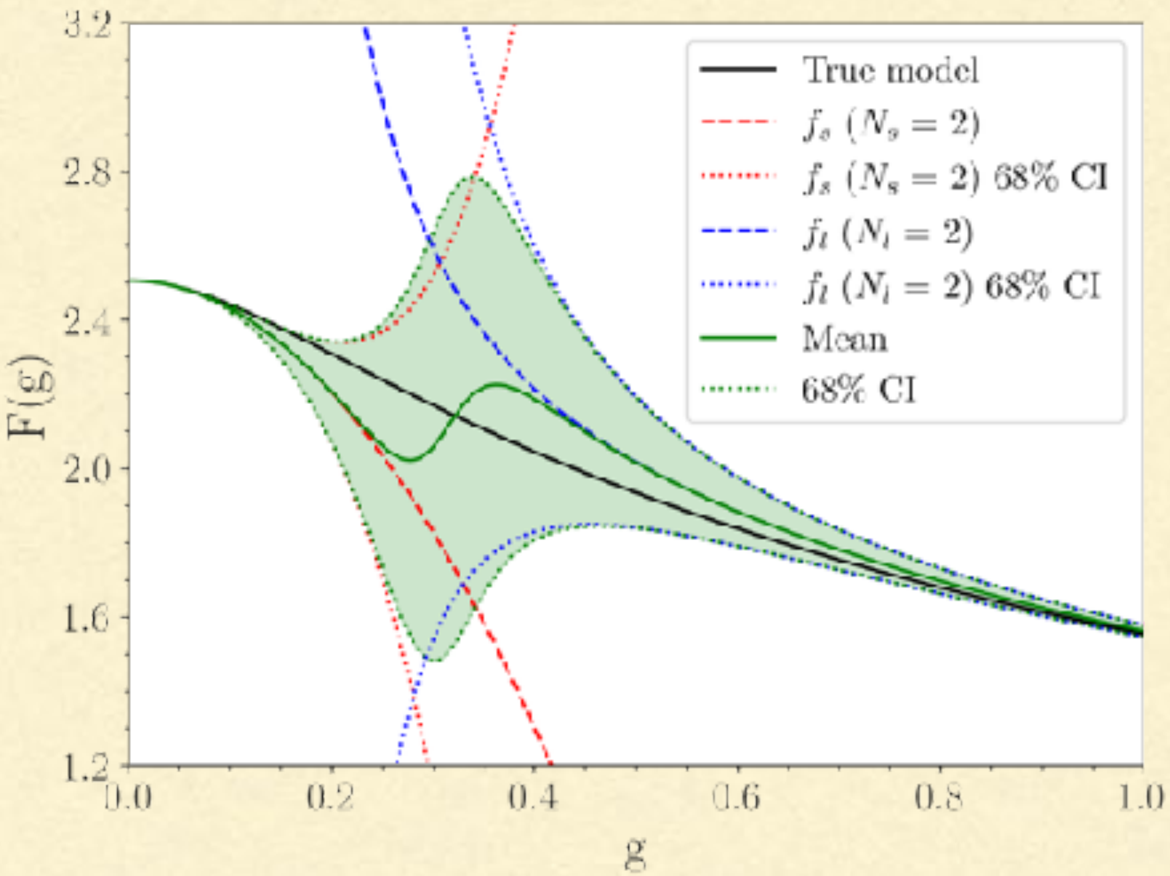

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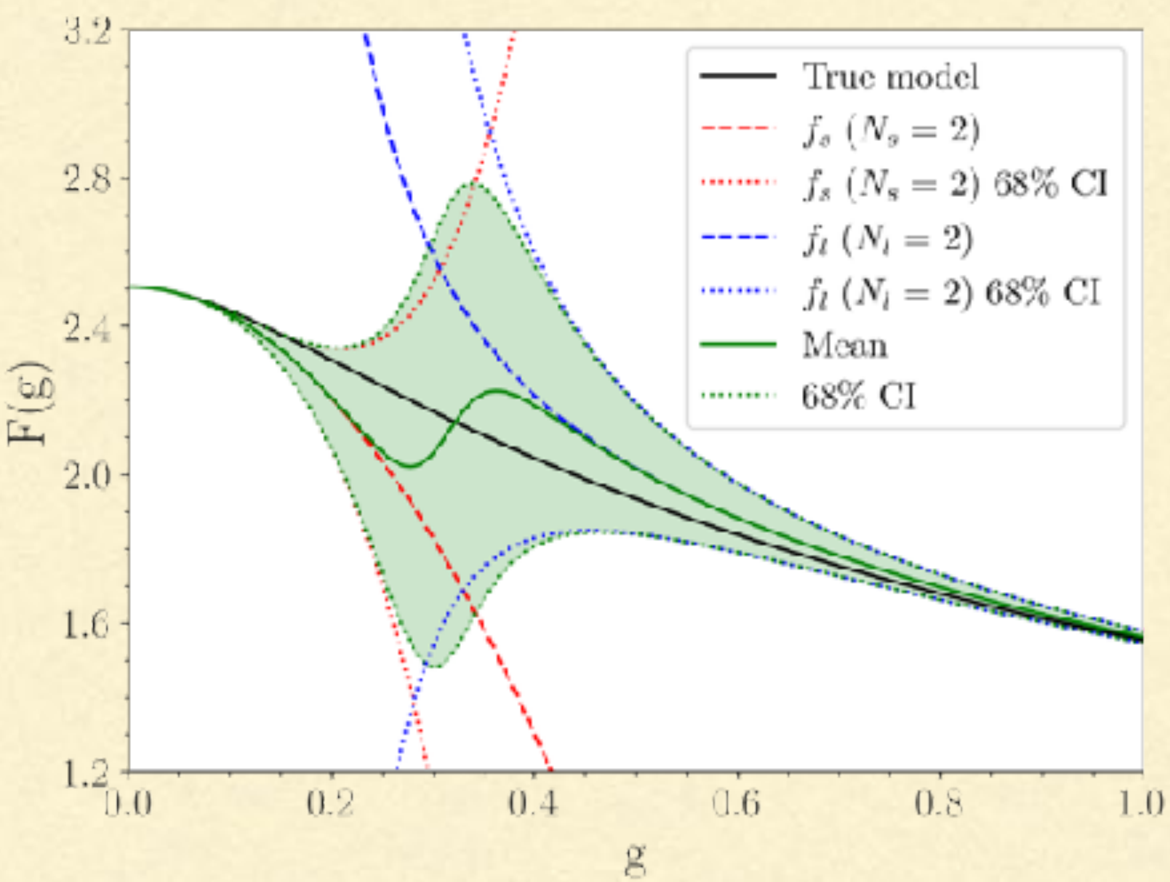
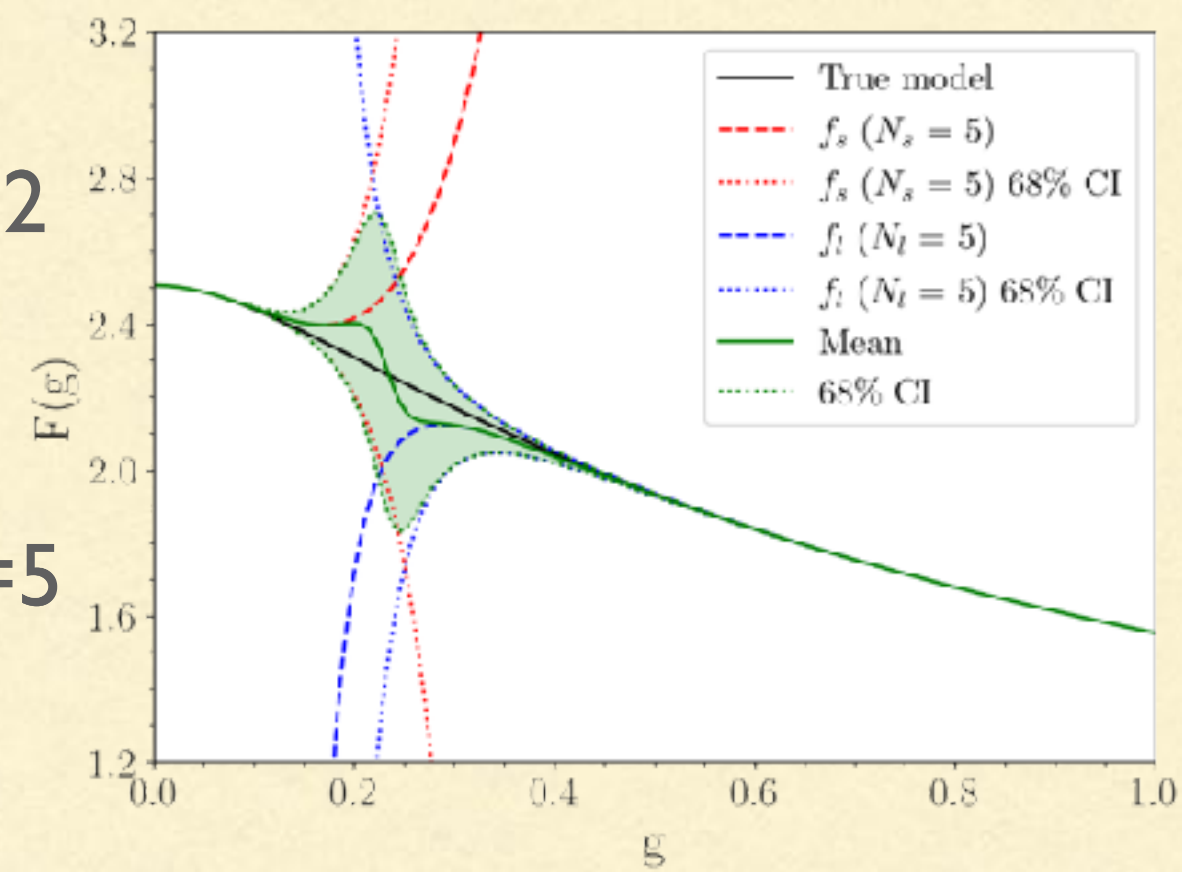
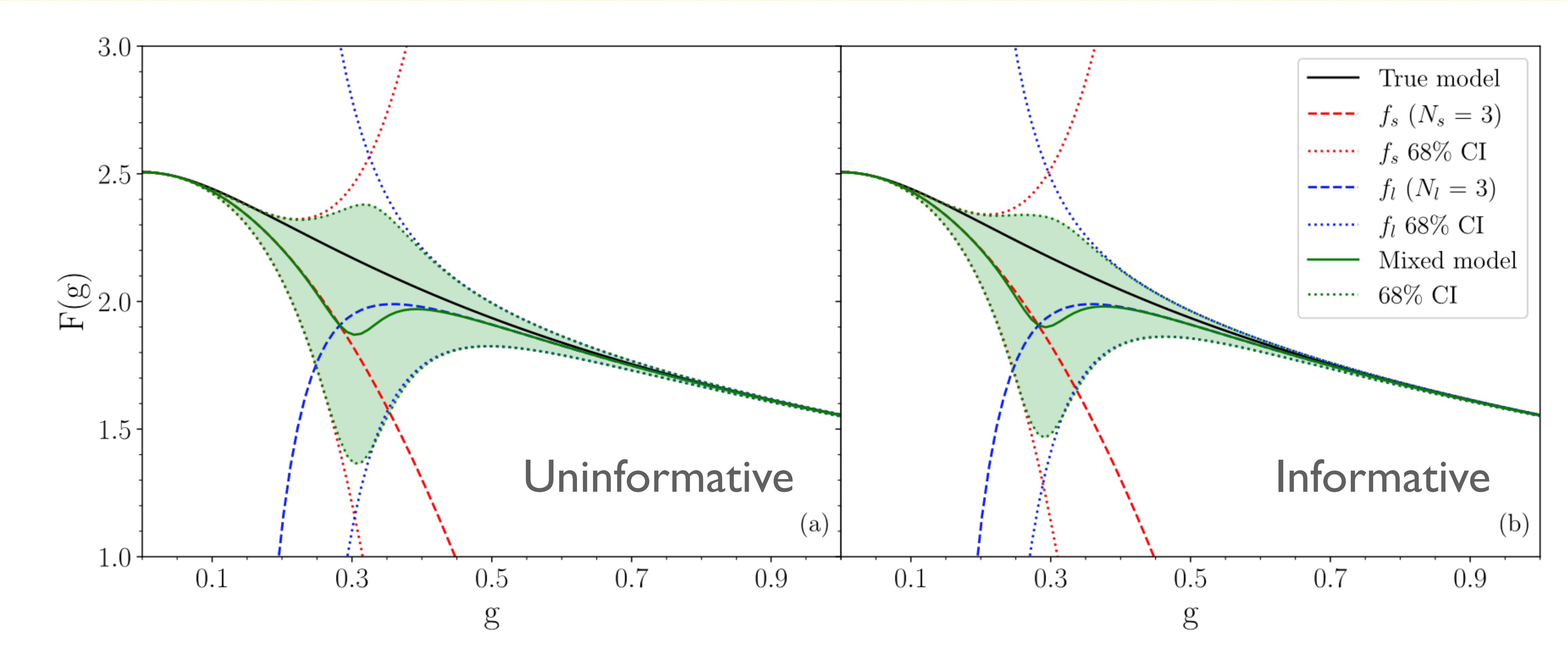


N_s=N_l=2

N_s=N_l=5



Bugs—or features?



- Result is sensitive to choice of error model
- Median has unexpected sinusoidal structure
- Error bands are wide compared to variation of function

Step 3: add a GP as third model

Step 3: add a GP as third model

- **IF** you think the connection is smooth
- Want to impose a prior on ways small-g and large-g expansion can connect
- Gaussian Process (GP): non-parametric interpolant that comes with uncertainty
- Take two training data in small-g and two in large-g region and formulate a GP; include estimated truncation uncertainties in these training data
- Pick three testing points, compute Mahalanobis distance to check validity of GP
- Include GP as third model

Results

Semposki, Furnstahl, DP Phys. Rev. C (2022)

Uncertainty now much smaller in the gap

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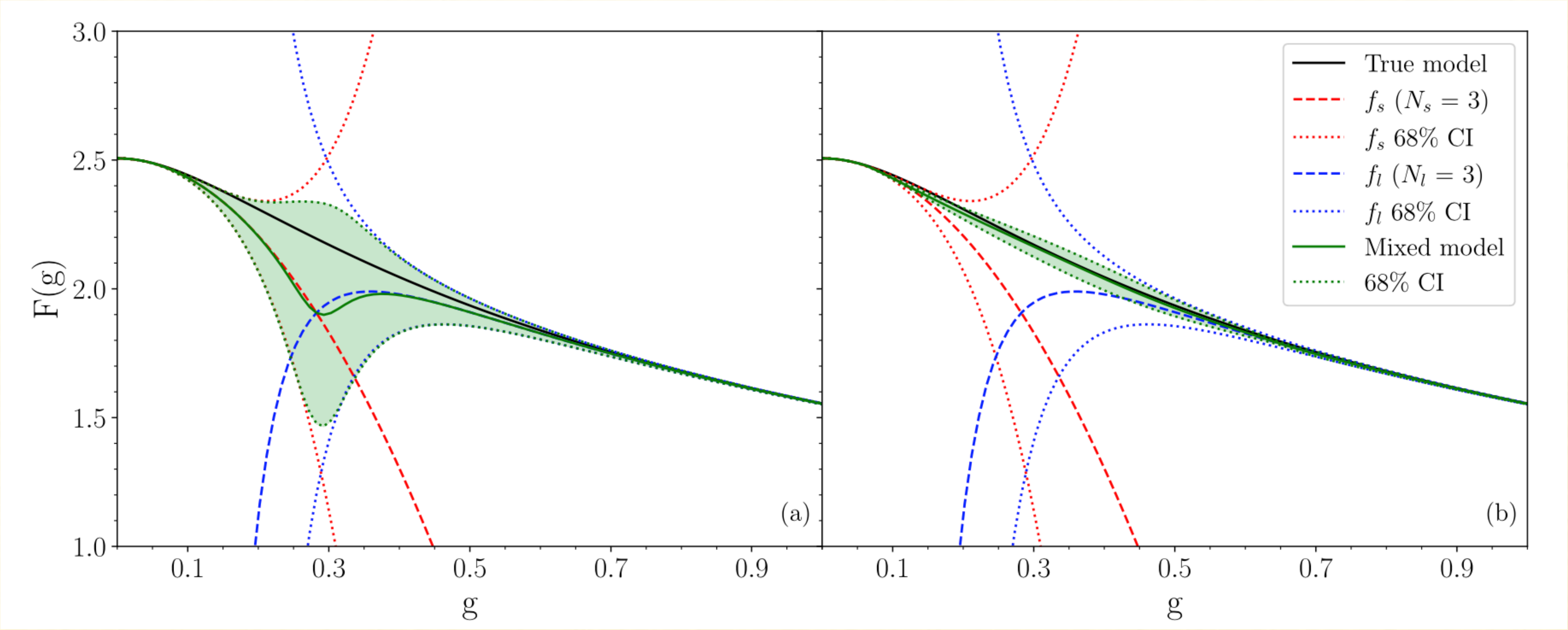

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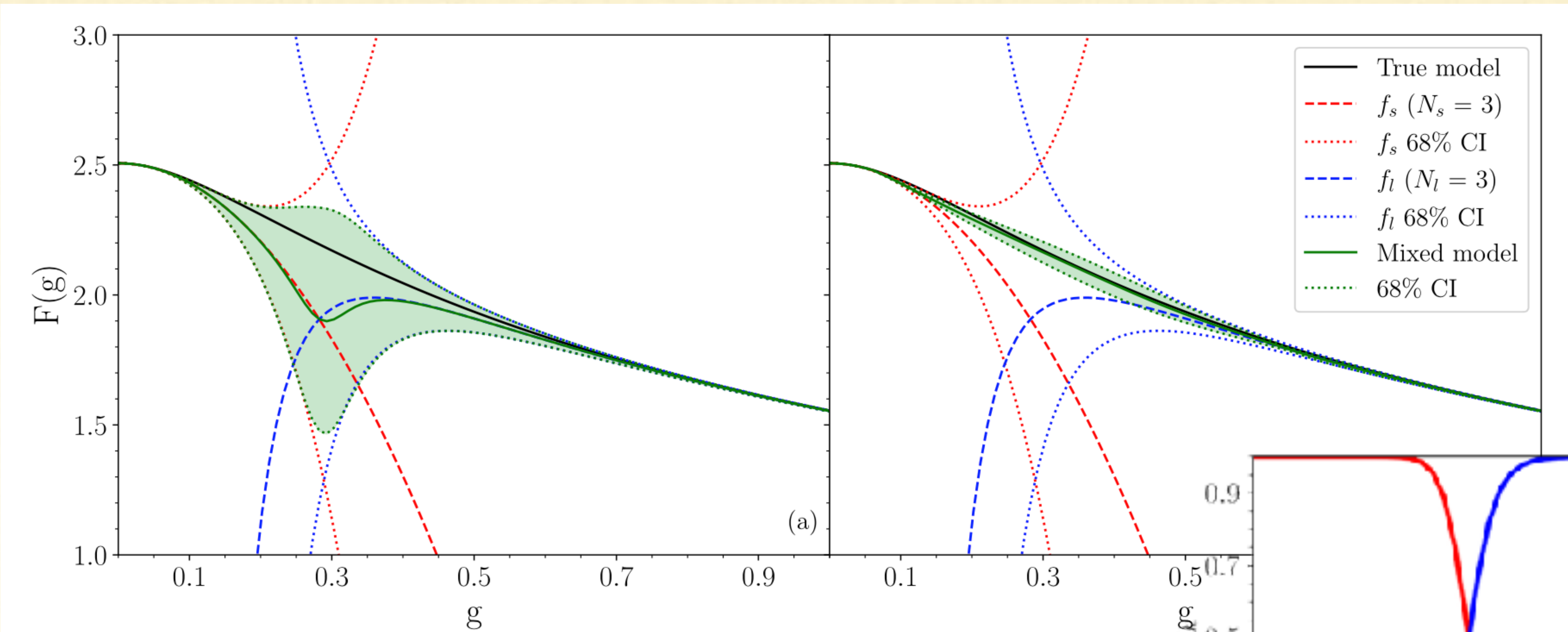
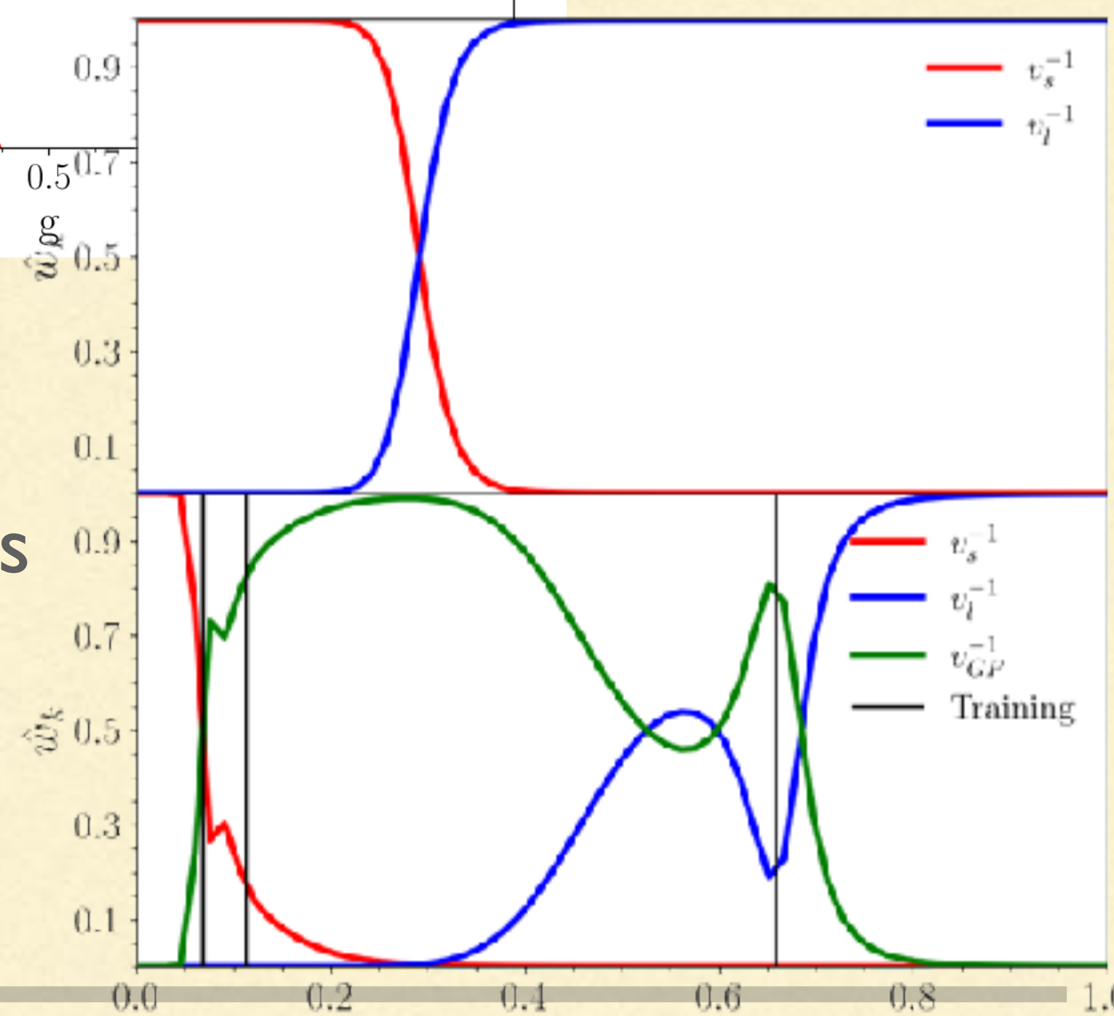


Model weights



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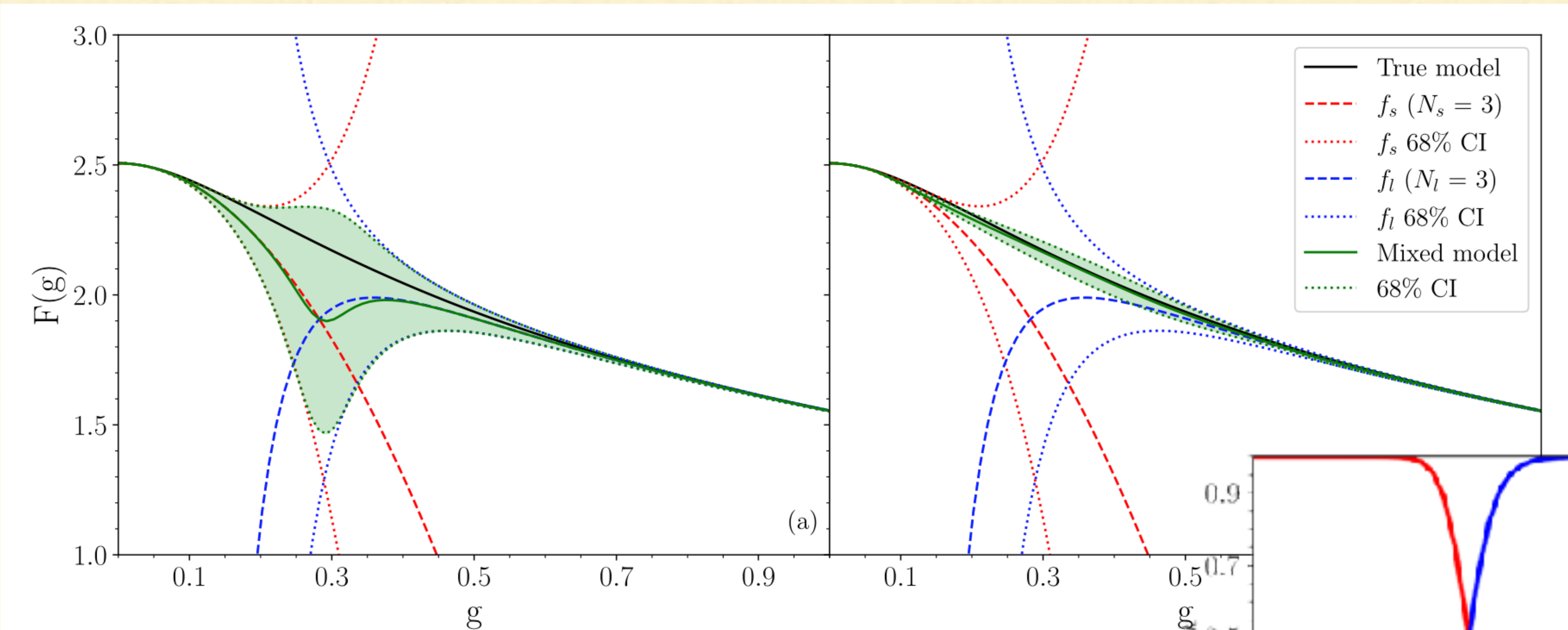
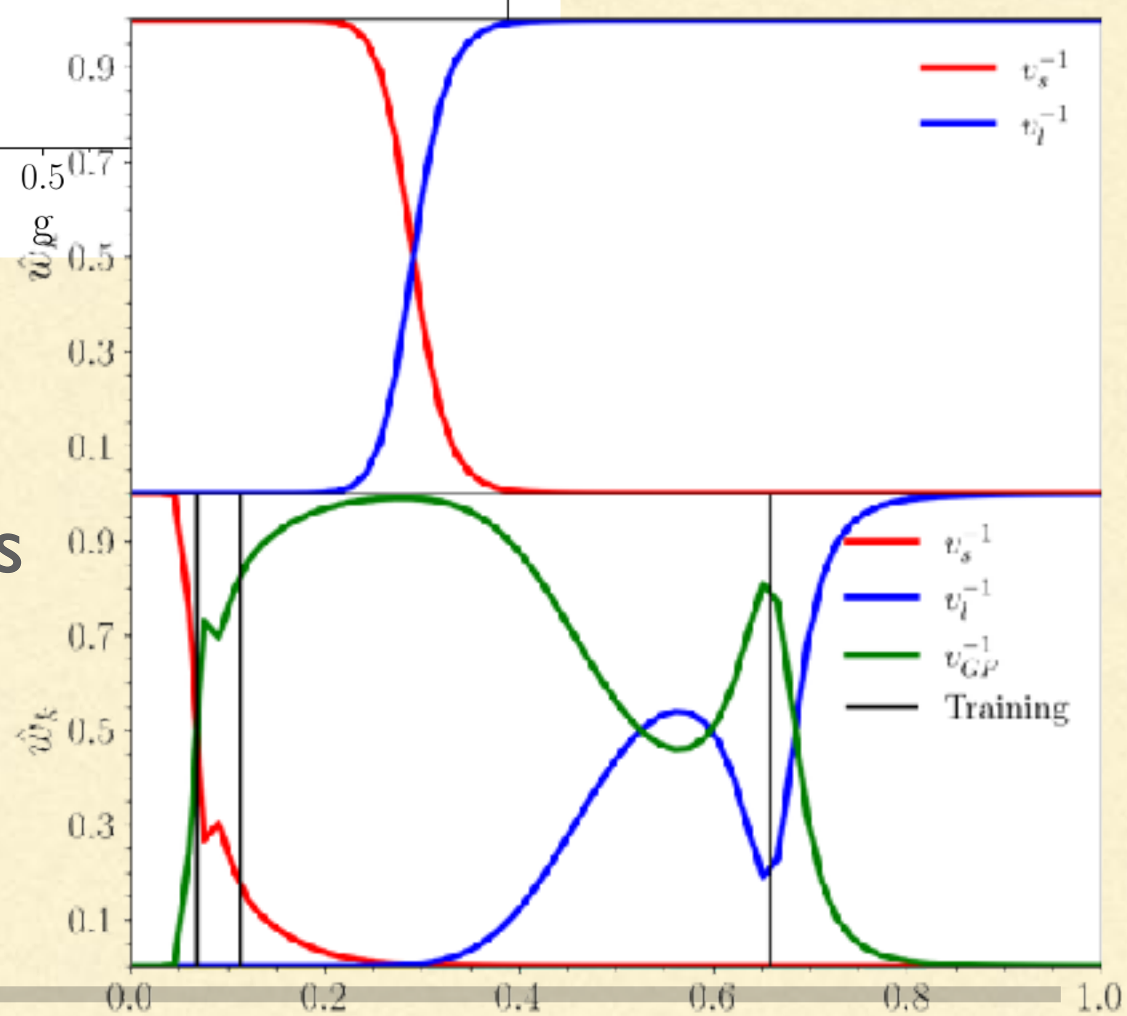


Performance improves as N_s and N_l increase

TABLE II. Calculated areas of each uncertainty band per truncation order in N_s and N_l. As expected, as both N_s and N_l increase, the uncertainty reduces.

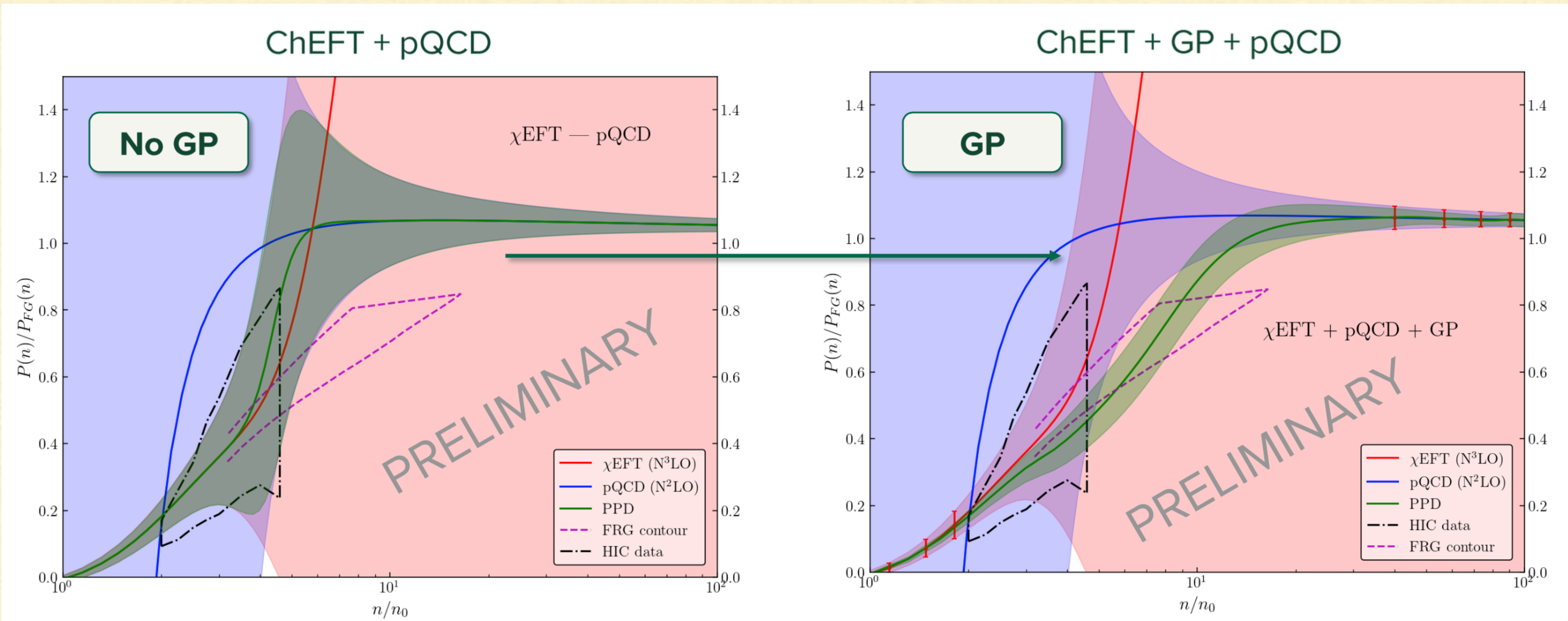
N_s	N_l	Gap length (g)	Gap area
2	2	0.92	0.05
2	4	0.60	0.02
3	3	0.92	0.04
4	4	0.26	0.03
5	5	0.21	0.02
8	7	0.13	0.01
5	10	0.11	0.003

Model weights



Results for symmetric nuclear matter

Semposki, Drischler, Furnstahl, DP, in preparation



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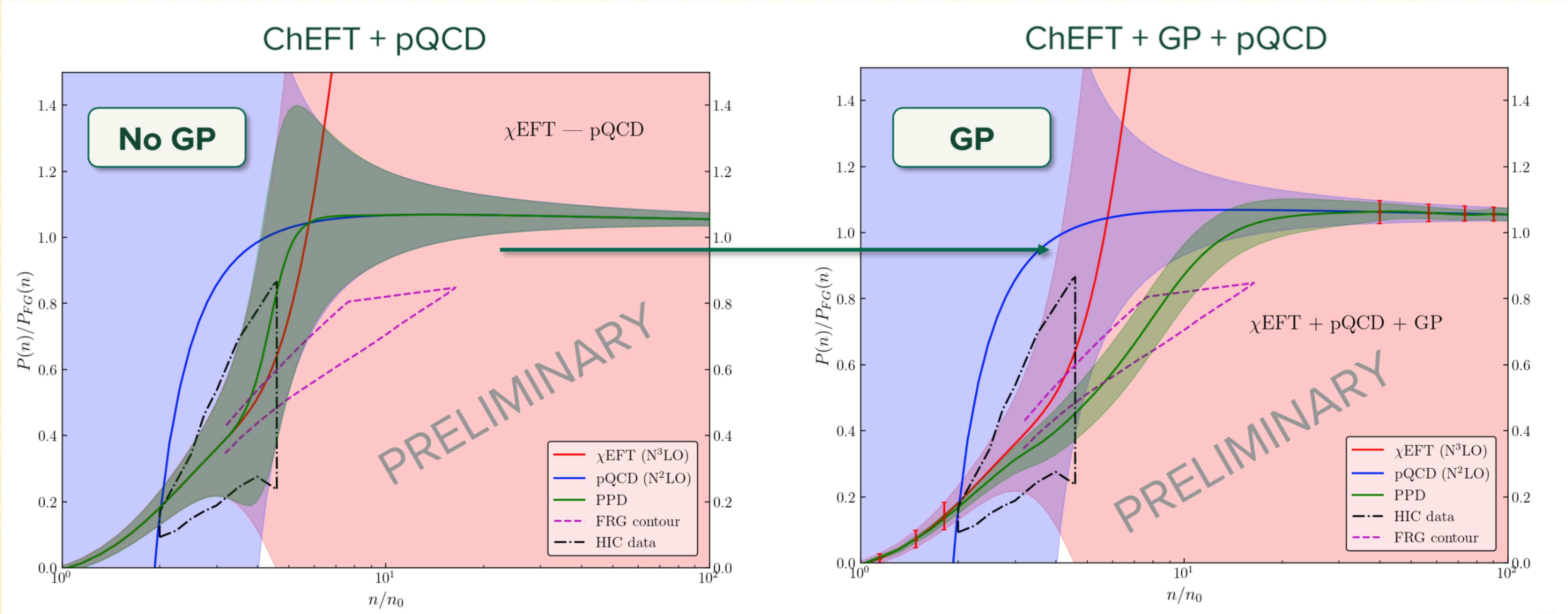

- pQCD uncertainties estimated from p(n) using BUQEYE™ technology
- Technical issues with GP training still under investigation for r.h. figure

Future work along these lines

- Gaussian Process model for order-by-order coefficients in χEFT for NN scattering observables

  Millican, Melendez, Furnstahl, Wesolowski, DP

- Extraction of NN parameters using model for correlated uncertainties

  Thim, Ekström, Forssén; Svennson, Ekstrom, Forssén

- Use BUQEYE™ technology to simultaneously extract scattering parameters and breakdown scale in other EFTs

  Bub, Piarulli, Pastore, Furnstahl, DP

- And for other reactions

  Burnelis, DP; Capel, Svennson, DP

- Use these ideas to do UQ for electroweak reactions

  Acharya, Bacca; Gnech, Marcucci, Viviani, ...?

- Treatment of symmetric nuclear matter, neutron star matter via Bayesian Model Mixing

  Semposki, Drischler, Furnstahl, DP

- Applications of model mixing in nuclear structure and heavy-ion physics

  Liyanage, Ingles, Jaiswal, Heinz, et al.; Kejzlar, Neufcourt, Nazarewicz; Giuliani, Godbey, Kejzlar, Nazarewicz

Backup slides

Bayesian EFT parameter estimation

$$y_{\text{exp}} = y_{\text{th}} + \delta y_{\text{exp}} + \delta y_{\text{th}}$$

Bayesian EFT parameter estimation

- $\delta y_{\rm th} = y_{\rm ref}(p)[c_{k+1}Q^{k+1} + \ldots]$ $\qquad$ $y_{\rm exp} = y_{\rm th} + \delta y_{\rm exp} + \delta y_{\rm th}$

- Posterior for parameters **a**={$a_0,\ldots,a_k$} by marginalizing:

$$\mathrm{pr}(\mathbf{a}|D,k,k_{\rm max}) = \int dc_{k+1}\ldots dc_{k_{\rm max}}\mathrm{pr}(\mathbf{a},c_{k+1},\ldots,c_{k_{\rm max}}|D,k,k_{\rm max})$$

and Bayesing $$= \int dc_{k+1}\ldots dc_{k_{\rm max}} \frac{\mathrm{pr}(D|\mathbf{a},c_{k+1},\ldots,c_{k_{\rm max}},k,k_{\rm max})\mathrm{pr}(\mathbf{a}|\bar{a}_{\rm fix})\prod_{j=k+1}^{k_{\rm max}}\mathrm{pr}(c_j|\bar{c}_{\rm fix})}{\mathrm{pr}(D|k,k_{\rm max})}$$

Bayesian EFT parameter estimation

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- Marginalization over c's produces revised correlation matrix in standard likelihood, accounts for uncertainties (and correlation structure) induced by omitted terms

$$\mathrm{pr}(\mathbf{a}\,|\,D,k,k_{\rm max}) \propto \exp\left(-\frac{1}{2}\mathbf{r}^T(\boldsymbol{\Sigma}_{\rm exp}+\boldsymbol{\Sigma}_{\rm th})^{-1}\mathbf{r}\right)\exp\left(-\frac{\mathbf{a}^2}{2\bar{a}^2}\right) \qquad \mathbf{r} \equiv \mathbf{y}_{\rm exp} - \mathbf{y}_{\rm th}$$

$$(\boldsymbol{\Sigma}_{\rm th,corr})_{ij} = (\mathbf{y}_{\rm ref})_i(\mathbf{y}_{\rm ref})_j\bar{c}^2\sum_{n=k+1}^{k_{\rm max}} Q_i^nQ_j^n \qquad (\boldsymbol{\Sigma}_{\rm th,uncorr})_{ij} = (\mathbf{y}_{\rm ref})^2\bar{c}^2\delta_{ij}\sum_{n=k+1}^{k_{\rm max}} Q_i^{2n}$$

Bayesian EFT parameter estimation

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- Normal naturalness (i.e. Gaussian) prior for LECs. Here we take a fixed $\bar{a}$, could also marginalize over it.

A bit more on Gaussian Processes

- Non-parametric, probabilistic model for a function
- Suppose we already know f at $x_1, x_2, x_3, \ldots, x_n$.
- Specify how f(y) is correlated with $f(x_1)$, $f(x_2)$, …..; don't specify underlying functional form.
- But value of f(y) is not deterministic: it's given by a (Gaussian) probability distribution.
- Correlation decreases as points get further away from each other.
- Specify correlation matrix of f at x and y, e.g.:

$$k(f(x), f(y)) = \bar{c}^2 \exp\left(-\frac{(x-y)^2}{2\ell^2}\right)$$

- Two parameters cbar and ℓ

BAND timeline

- July 2020: beginning of grant from NSF OAC
- December 2020: virtual BAND camp
- December 2021: hybrid BAND camp
- Summer 2022: Release of v0.2
- Summer 2023: Release of v0.3, including additional model-mixing methods, emulators (ROSE), and additional physics examples, e.g., BMEX
- Summer 2024: Release of v0.4, including experimental-design capability and additional physics examples
- Summer 2025: Release of v1.0: full functionality