TALENT COURSE 11
LEARNING FROM DATA: BAYESIAN METHODS AND MACHINE LEARNING

Lecture 21: Model checking I

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TU Darmstadt
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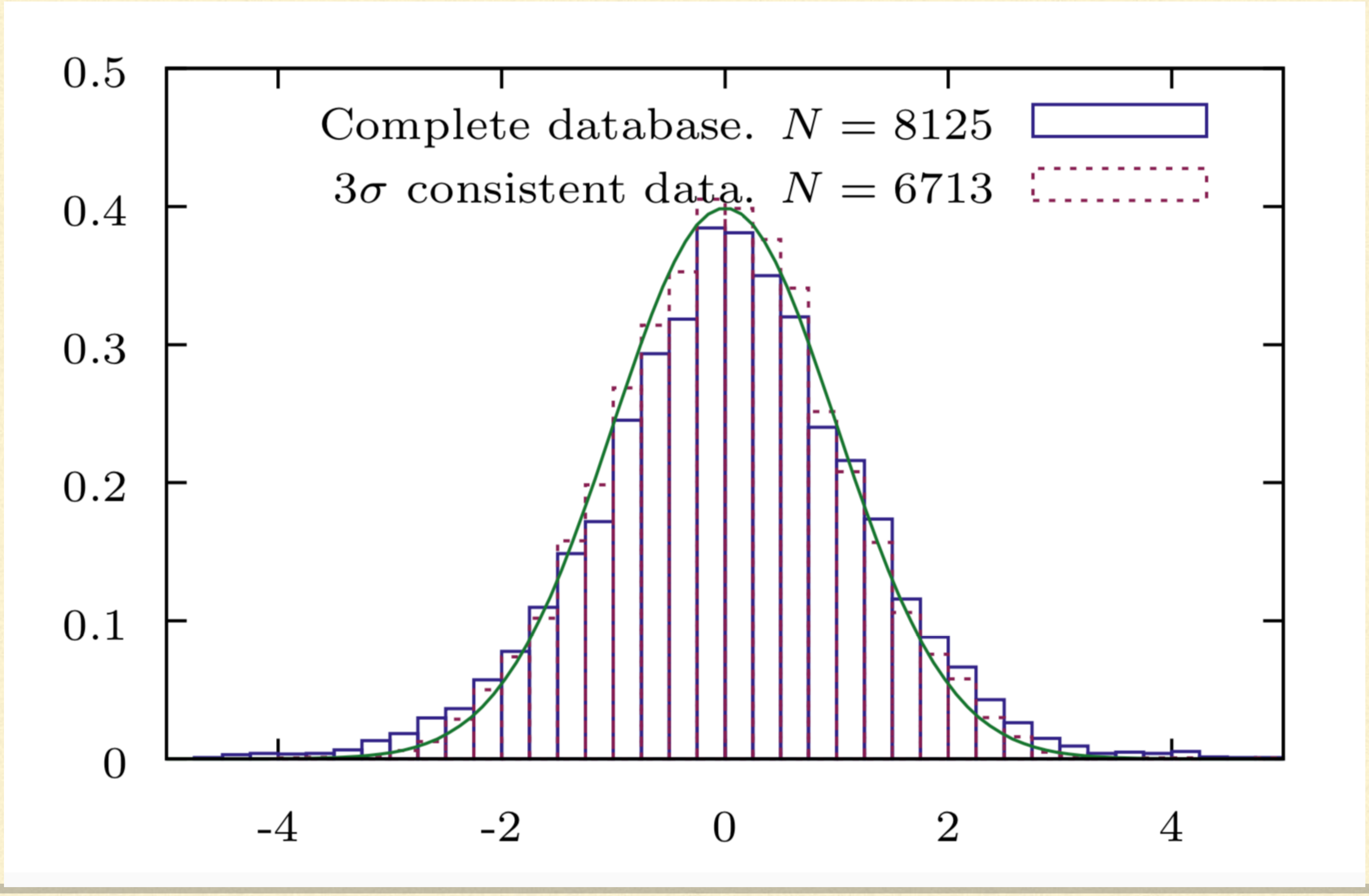
TALENT Course 11 is possible thanks to funding from the STFC

QQ plots

Navarro Perez, Ruiz Arriola, Amaro, PRC (2014)



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Arrange data residuals from most negative to most positive

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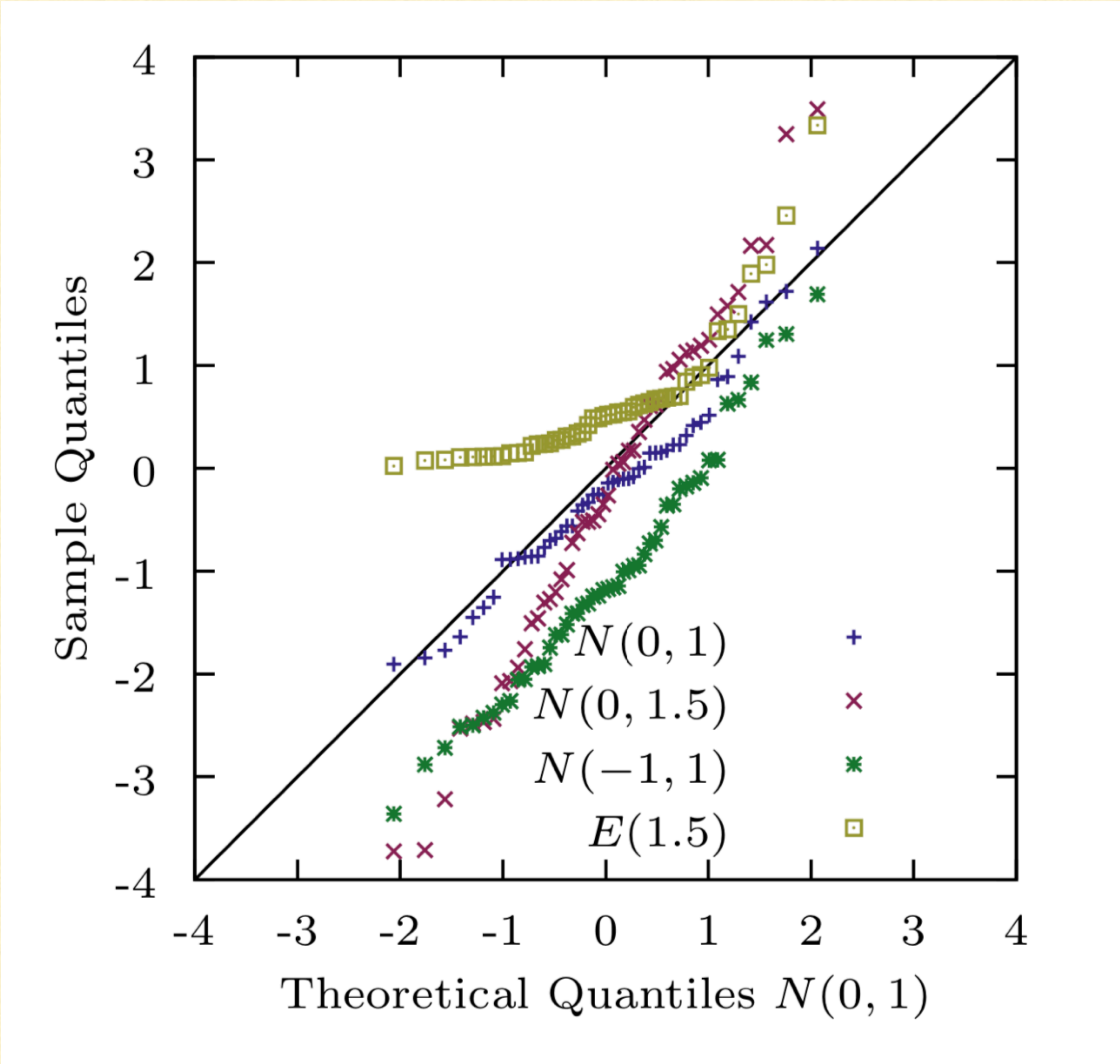

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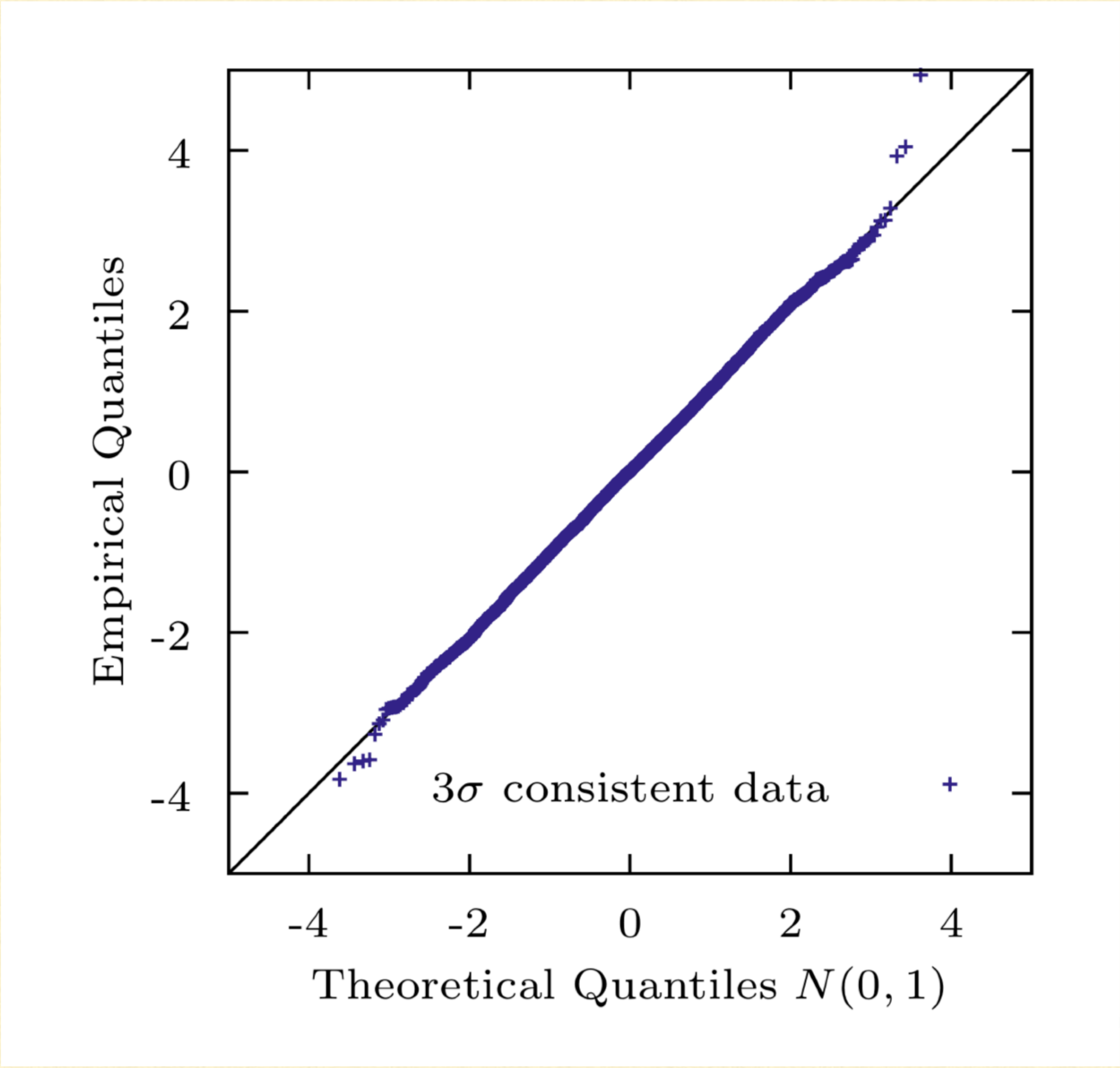

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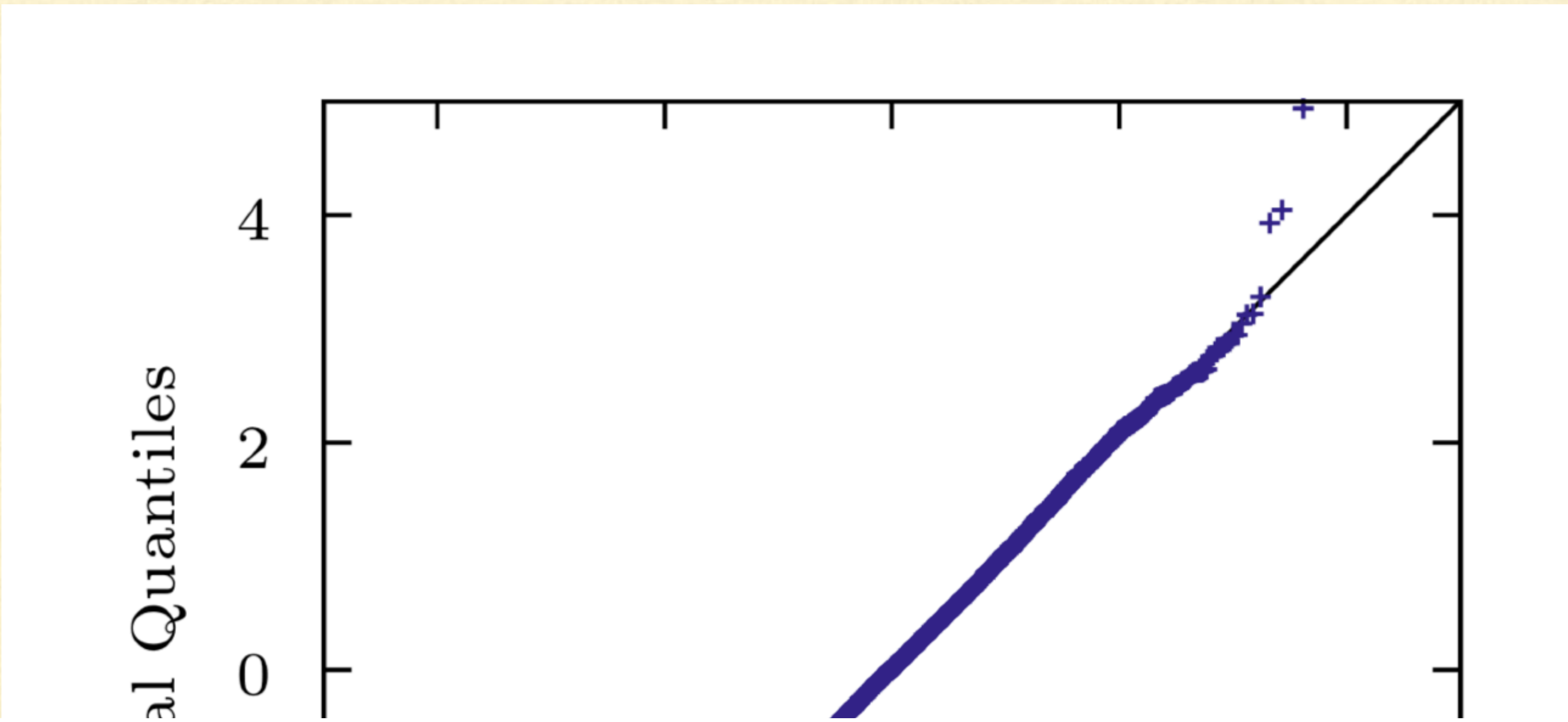

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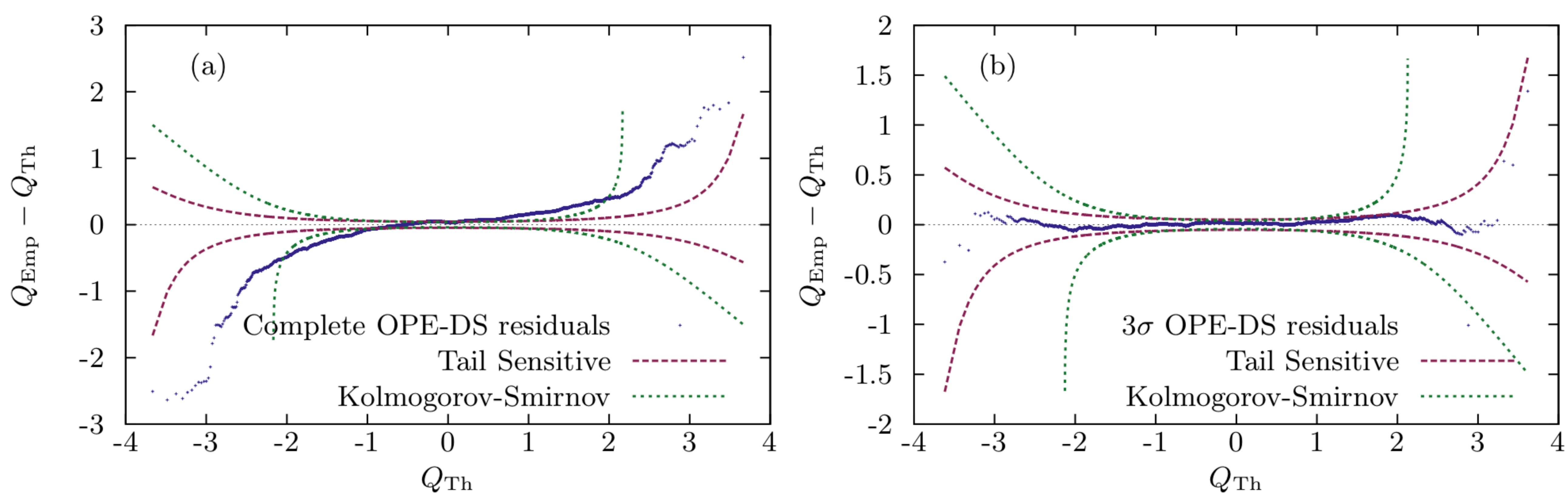

Let’s talk about the weather

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- Consider predictions for percentage probability of rain each day. Bin in 10% intervals.
- Fix a given interval: compute number of days it actually rained, compare.

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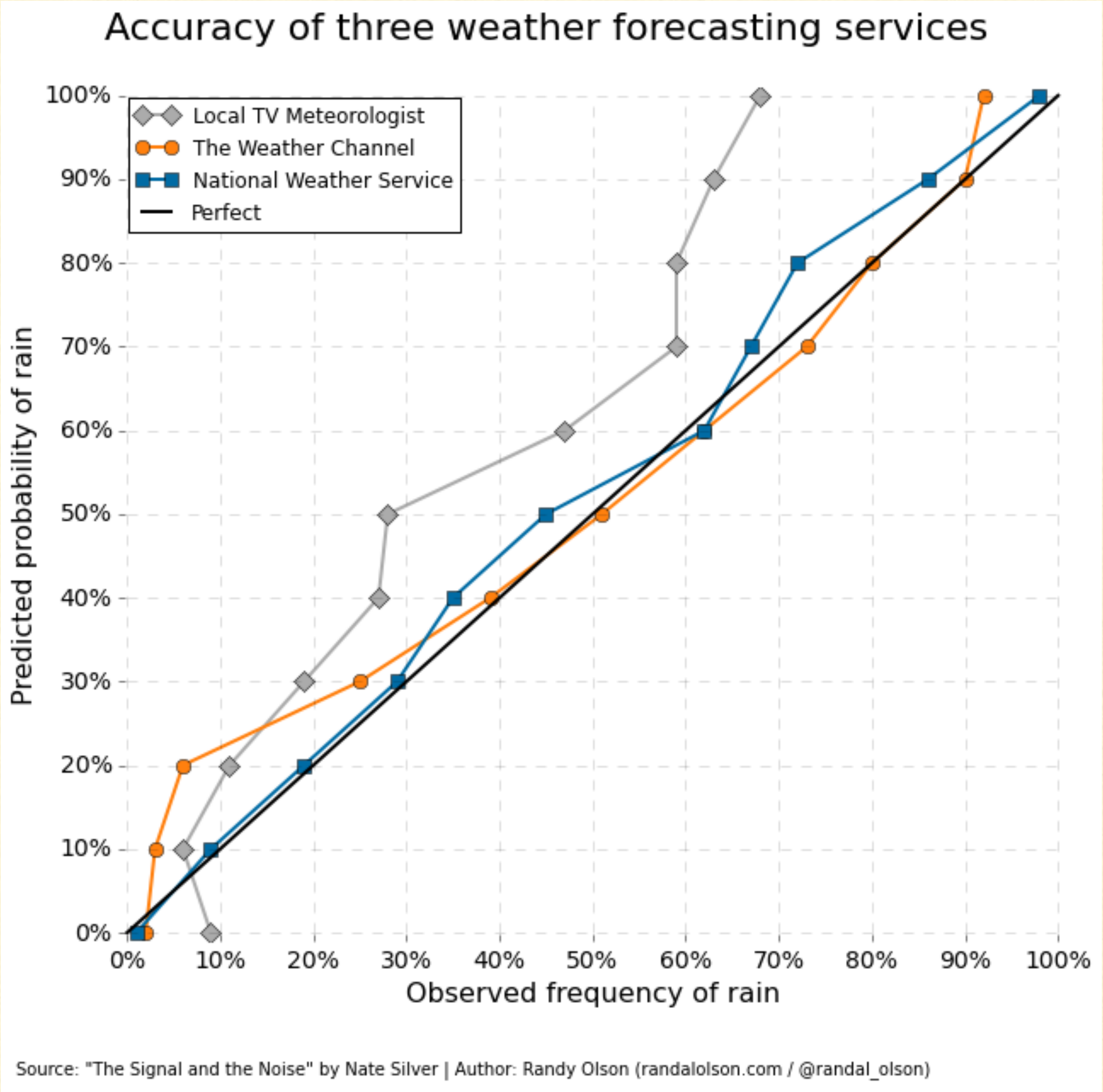

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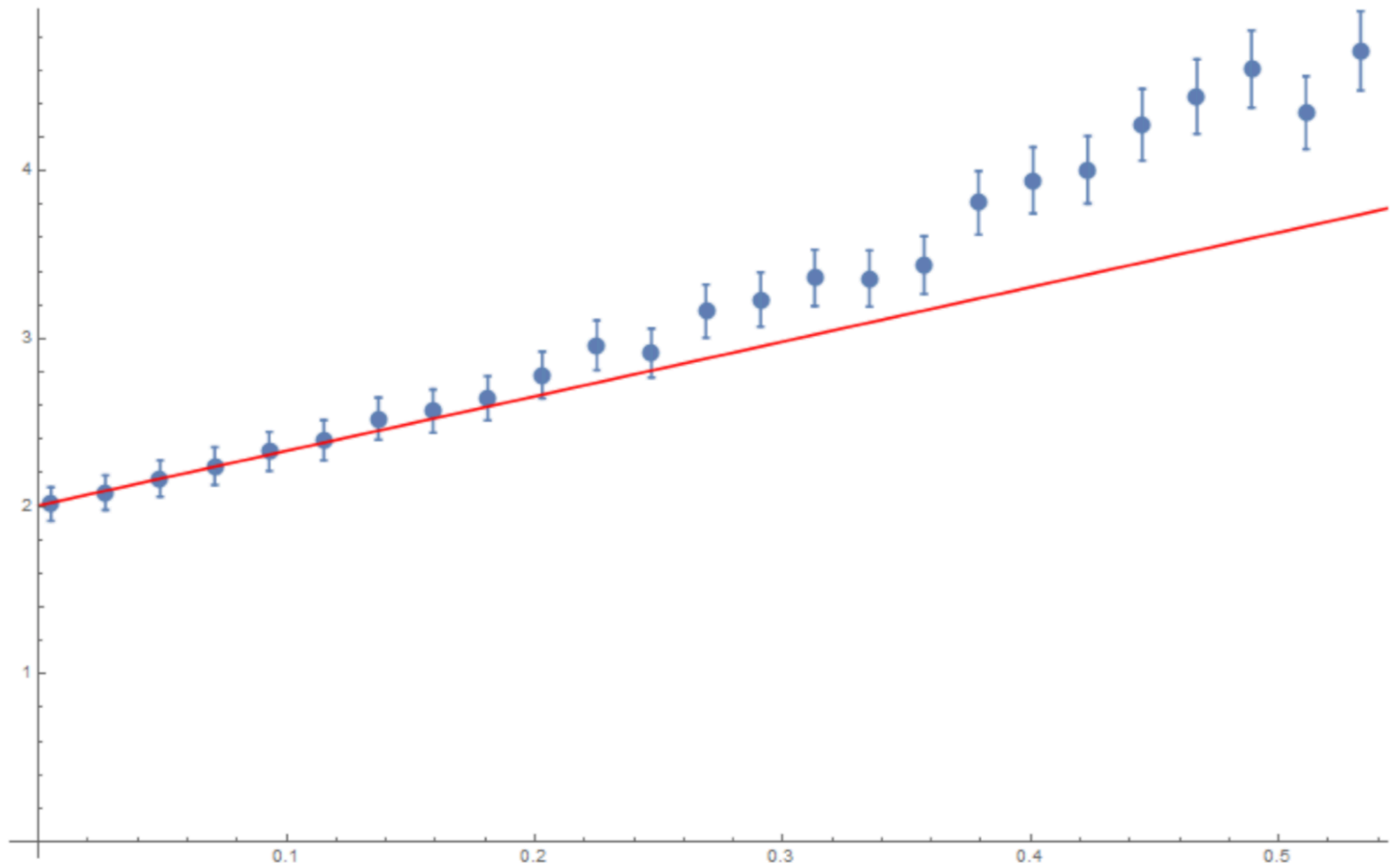
Systematic trends in residuals

Furnstahl, DP, Wesolowski, JPG (2014); Billig, HTC thesis (2019)



a0	a1
2.00473 ± 0.0834257	3.25548 ± 1.4859

Clear that a linear fit does not produce Gaussian residuals

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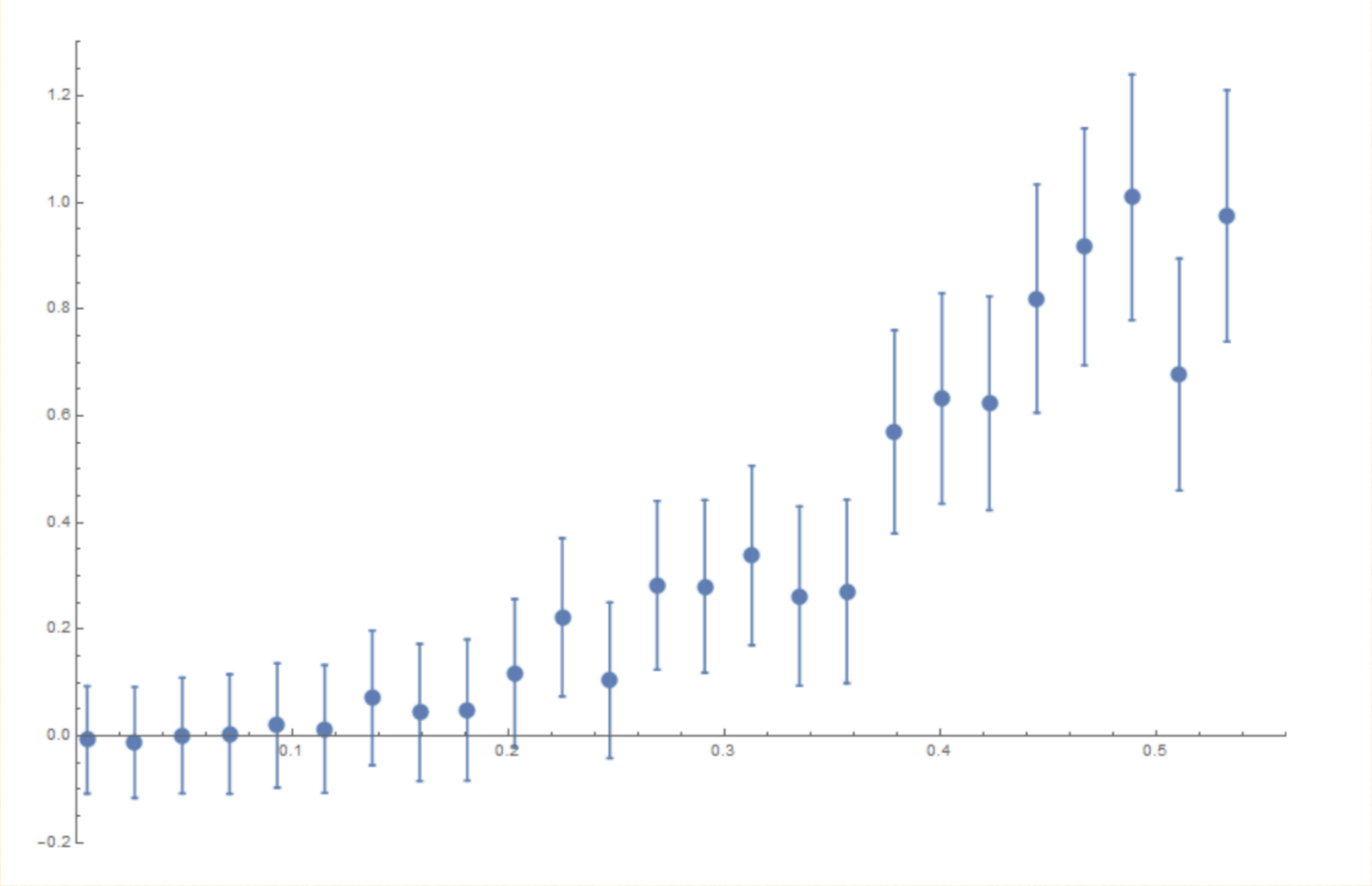
Furnstahl, DP, Wesolowski, JPG (2014); Billig, HTC thesis (2019)



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Behavior of a ChiEFT series

Behavior of a ChiEFT series

- χEFT: encodes low-energy ($p \ll \Lambda_{\chi SB} \simeq 750$ MeV) consequences of QCD's chiral symmetry and the pattern of its breaking
- Expansion in $x \equiv m_\pi/(M_\Delta - M_N) \simeq M_\Delta - M_N/\Lambda_{\chi SB} \simeq 0.4$
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- We cannot *know* the result for c_3 before we compute it, but we can use information we have to determine *what values are more or less probable*
- Two different answers, depending on what information we have:
  - What is expectation for c_3 before we know c_0, c_1, c_2?
  - In fact $\{c_n\}=\{1,-0.46,0.75\}$. What then is expectation for c_3?

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Griesshammer et al., PPNP (2012)

$c_3=1$

An EFT expansion in pictures

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

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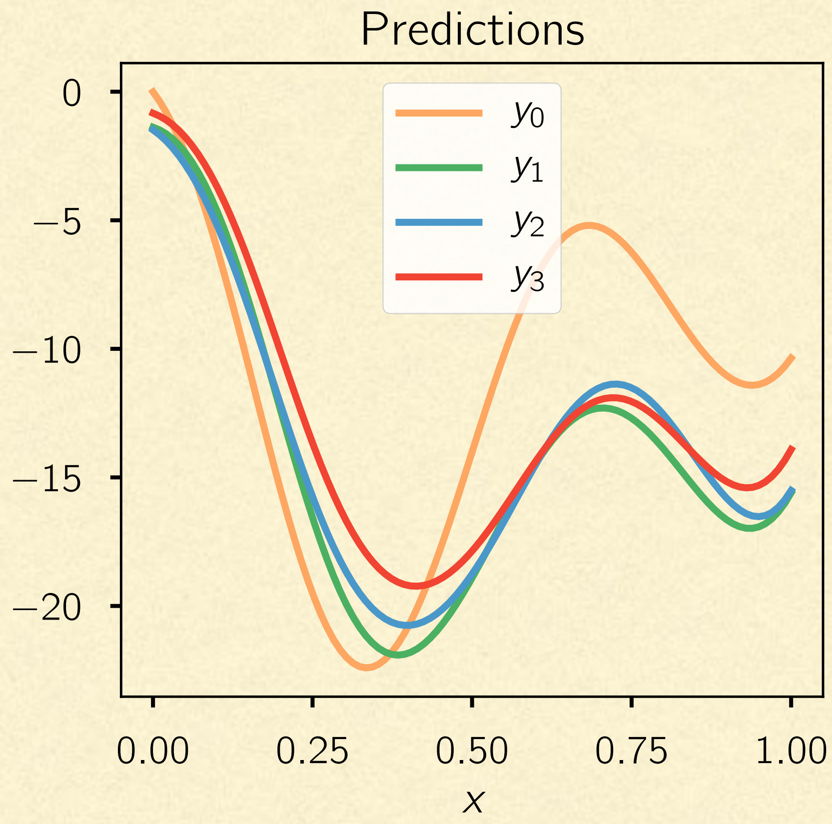

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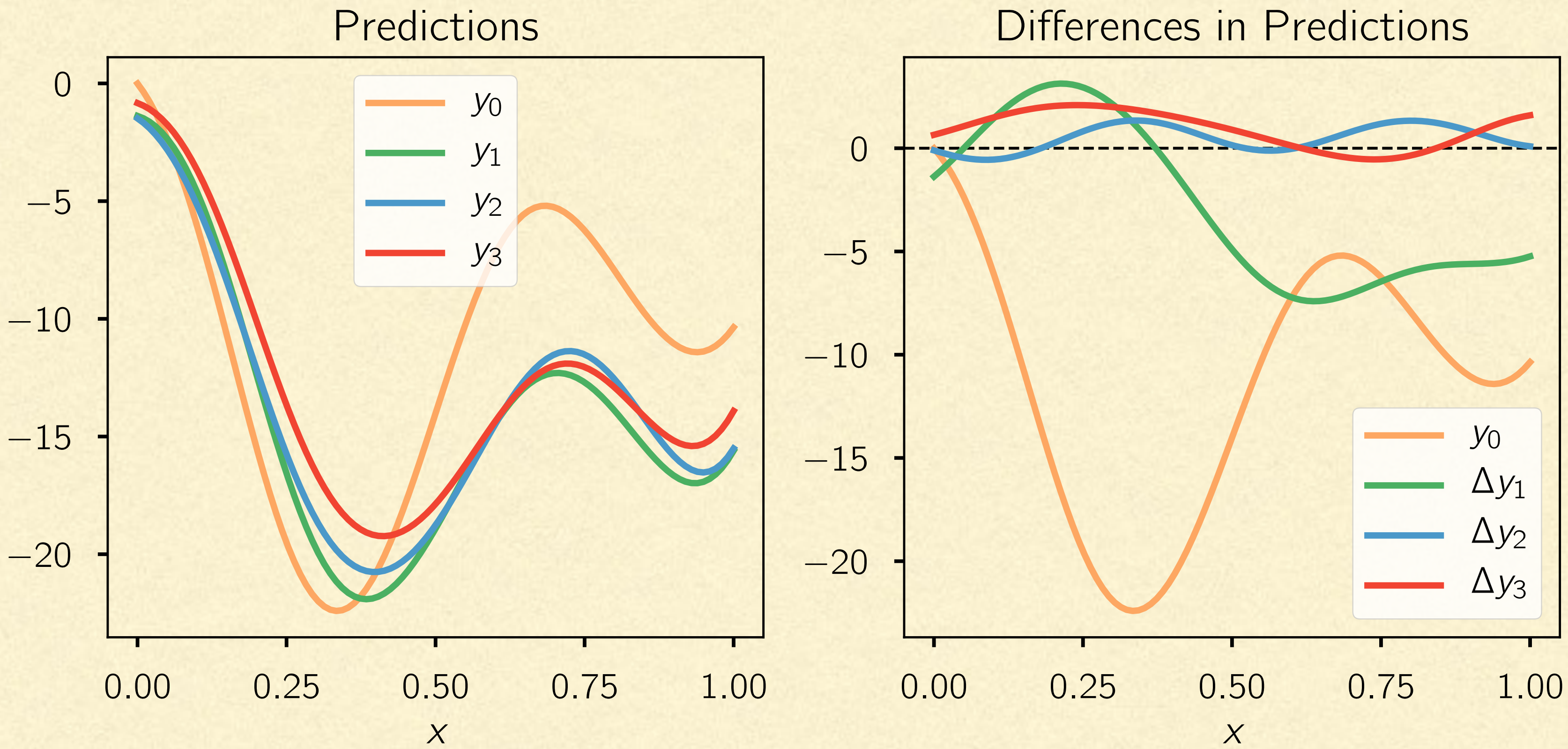

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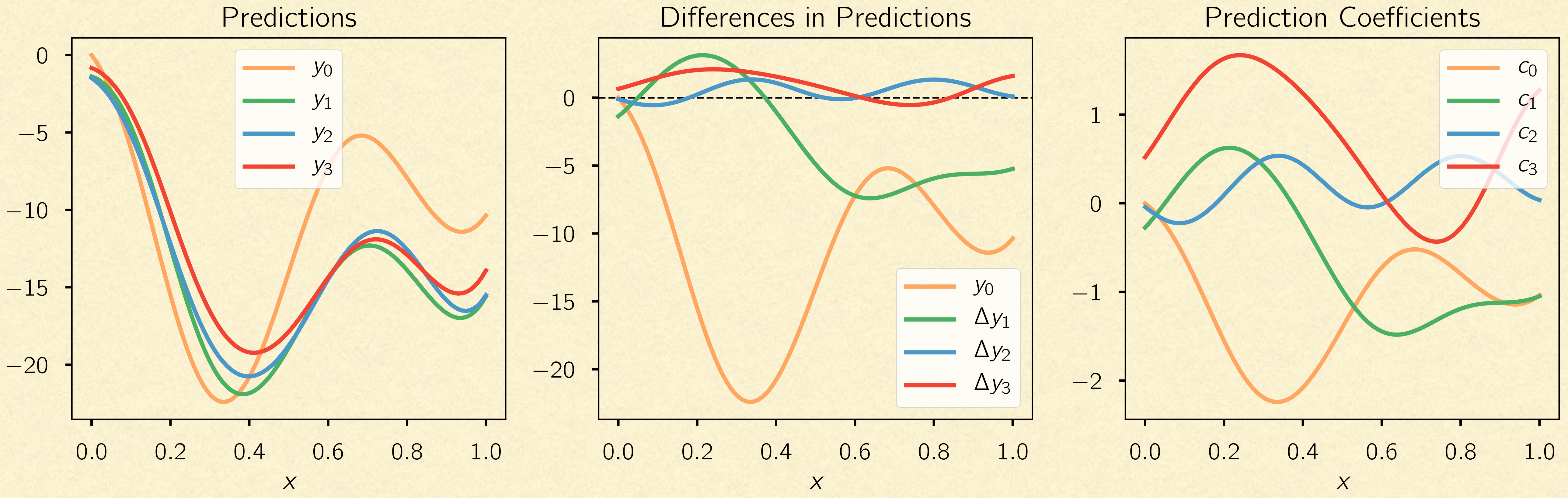

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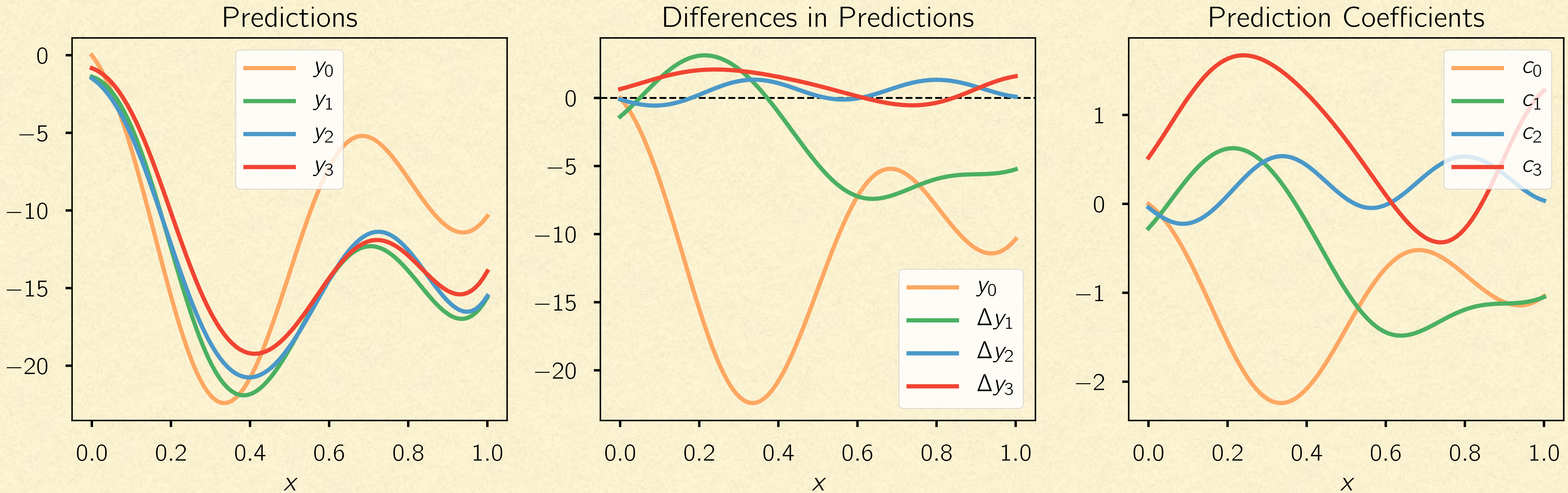

This is what a healthy observable expansion looks like: bounded coefficients, that do not grow or shrink with order.

Bayes' theorem

Thomas Bayes (1701?-1761)

$$\mathrm{pr}(A\,|\,B, I) = \frac{\mathrm{pr}(B\,|\,A, I)\,\mathrm{pr}(A\,|\,I)}{\mathrm{pr}(B\,|\,I)}$$

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Posterior

Evidence

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Posterior

Evidence

Probability as degree of belief cf. frequentist view

Probability for EFT coefficients

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

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- So can we use extracted c_0, c_1, c_2, …, c_k to estimate (in a probabilistic way) c_{k+1}? From there construct $\Delta_k = y_{ref}\, c_{k+1}\, Q^{k+1}$:truncation error

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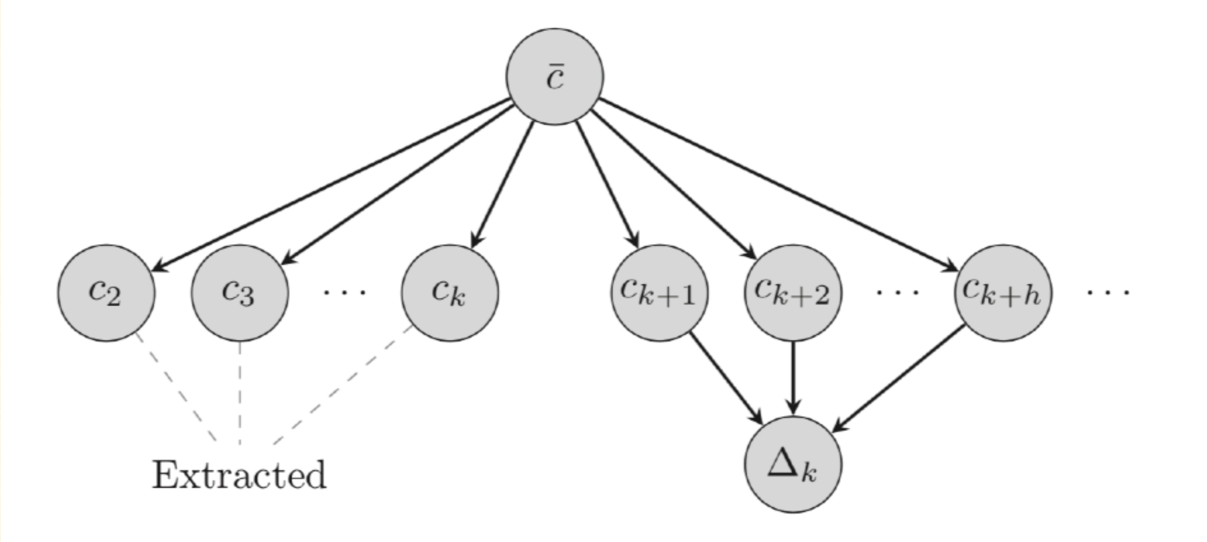
- Bayesian model:

Parameter cbar sets size of all dimensionless coefficients



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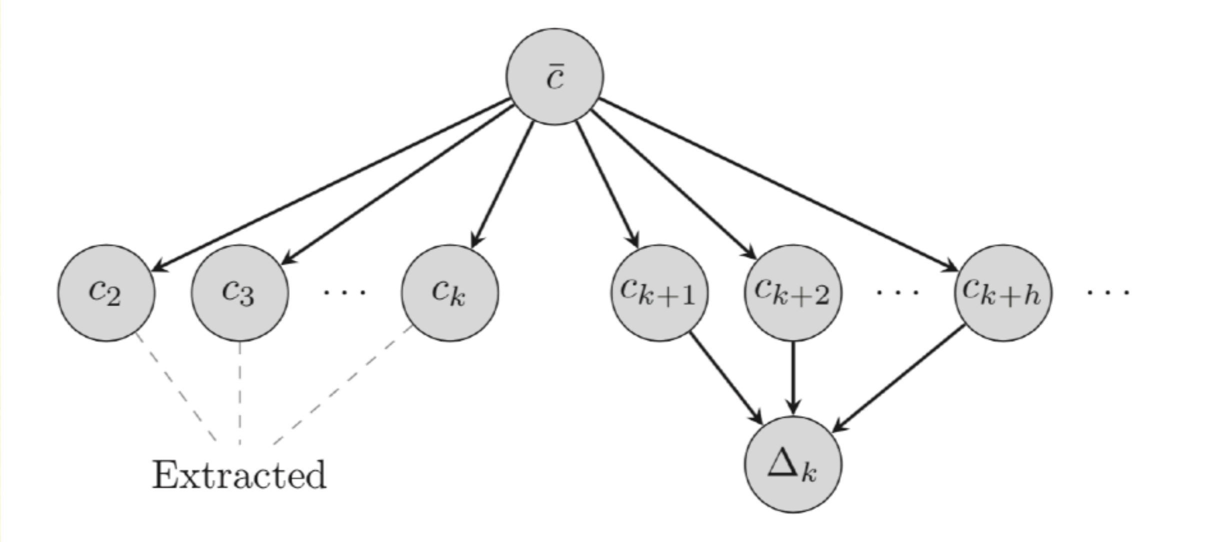

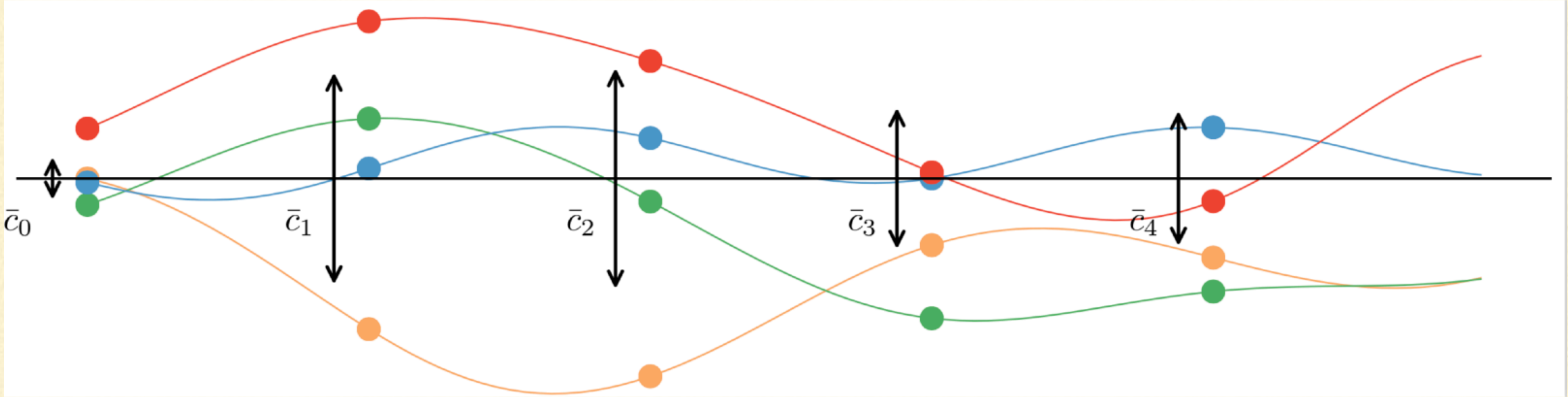

First shot: cbar can be different at different kinematic points: "uncorrelated model"

Normal naturalness

Furnstahl, Klco, DP, Wesolowski, PRC, 2015; Melendez, Furnstahl, Wesolowski, PRC, 2017

- c_n's are normally distributed, with mean 0 and standard deviation cbar. that is a) fixed or b) distributed uniformly in its logarithm

$$\mathrm{pr}(c_n|\bar{c}) = \frac{1}{\sqrt{2\pi}\bar{c}} e^{-c_n^2/2\bar{c}^2}; \ \mathrm{pr}(\bar{c}) \propto \frac{1}{\bar{c}}\theta(\bar{c} - \bar{c}_<)\theta(\bar{c}_> - \bar{c})$$

- Marginalization:

$$\mathrm{pr}(c_{k+1}|c_0, c_1, \ldots, c_k) = \int_0^\infty d\bar{c}\, \mathrm{pr}(c_{k+1}|\bar{c})\mathrm{pr}(\bar{c}|c_0, c_1, \ldots c_k)$$

$$= \int_0^\infty \frac{d\bar{c}}{\bar{c}^{k+3}} \exp\left(-\frac{c_{k+1}^2}{2\bar{c}^2}\right) \exp\left(-\frac{(k+1)\langle c^2\rangle}{2\bar{c}^2}\right)$$

- Student's t-distribution results:

$$\mathrm{pr}(c_{k+1}|c_0, c_1, \ldots, c_k) \propto \frac{\Gamma\left(\frac{k+2}{2}\right)}{\Gamma\left(\frac{k+1}{2}\right)} \left(\frac{(k+1)\langle c^2\rangle}{(k+1)\langle c^2\rangle + c_{k+1}^2}\right)^{(k+2)/2}$$

- DoB intervals computed using known results for this distribution. Size of error bar set by $<c^2>$, k, Q^{k+1}, and y_{ref}.

NN scattering

Epelbaum, Krebs, Meißner, PRC, 2015

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

χEFT: $\mathscr{L}$(N,π)→V$^{(k)}$→δ→σ_{np}

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

$$x = \frac{p_{\rm rel}}{\Lambda_b}$$

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

- 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, N^{2}LO, N^{3}LO, N^{4}LO (k=0, 2, 3, 4, 5)

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

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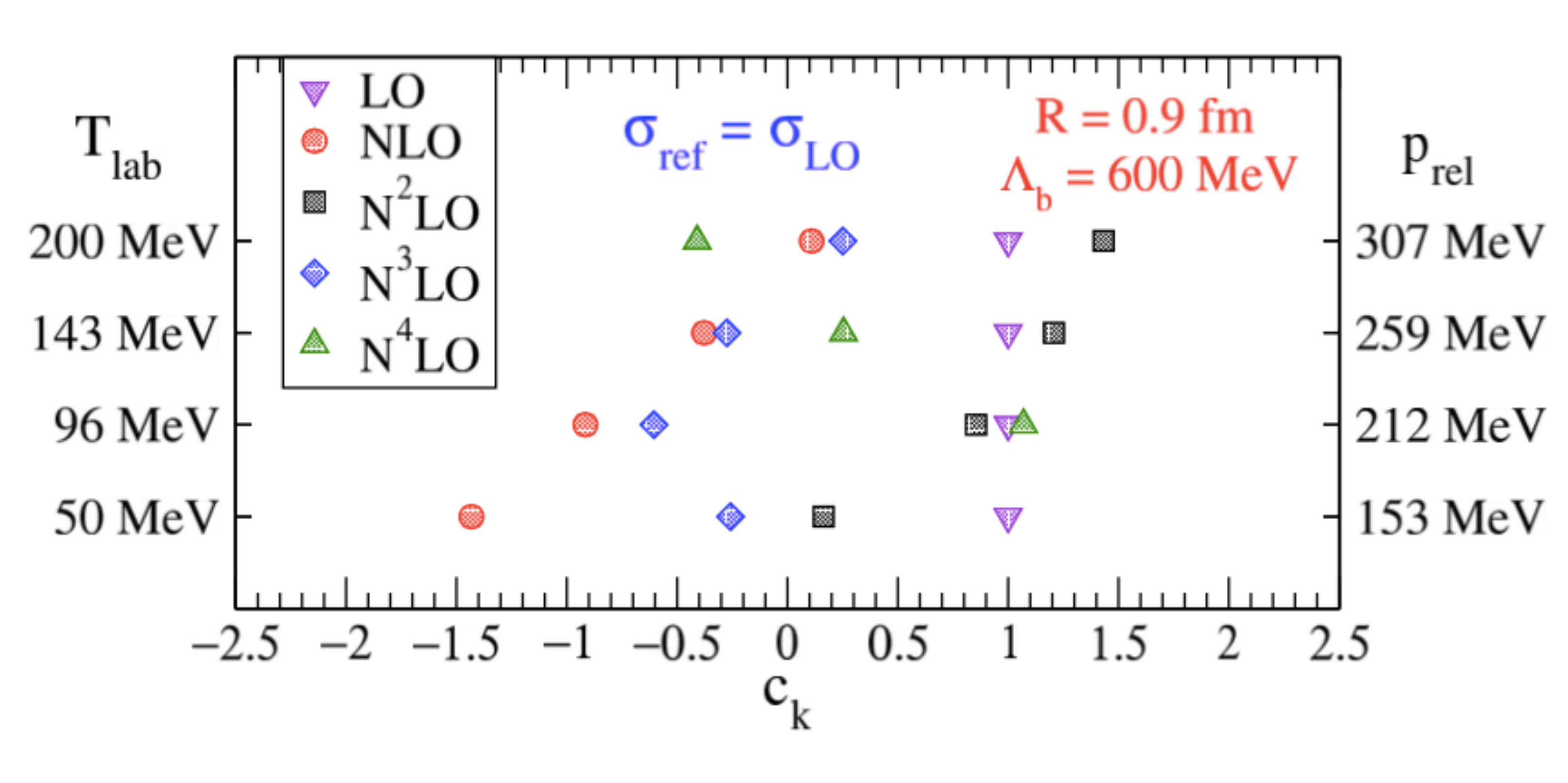
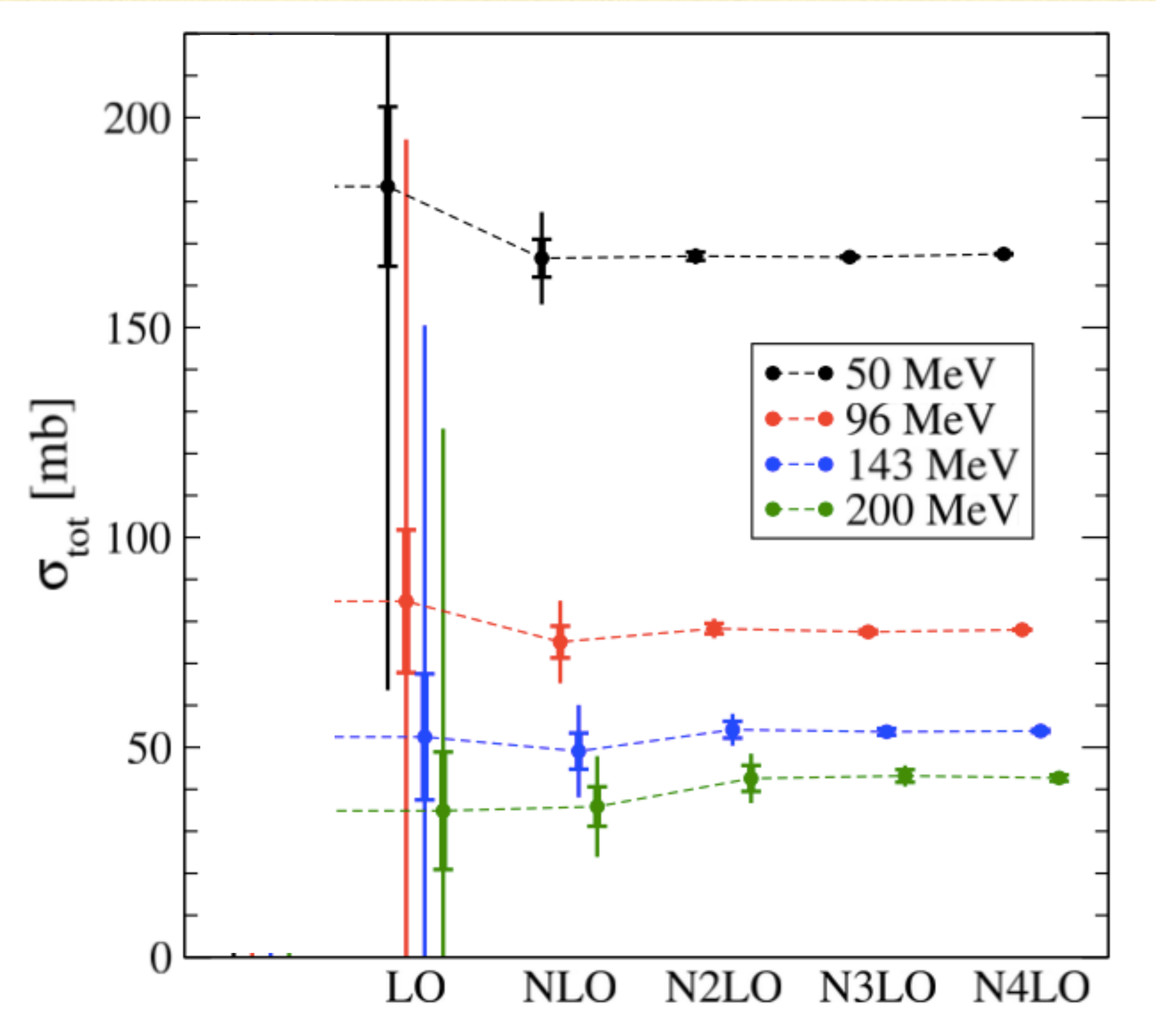
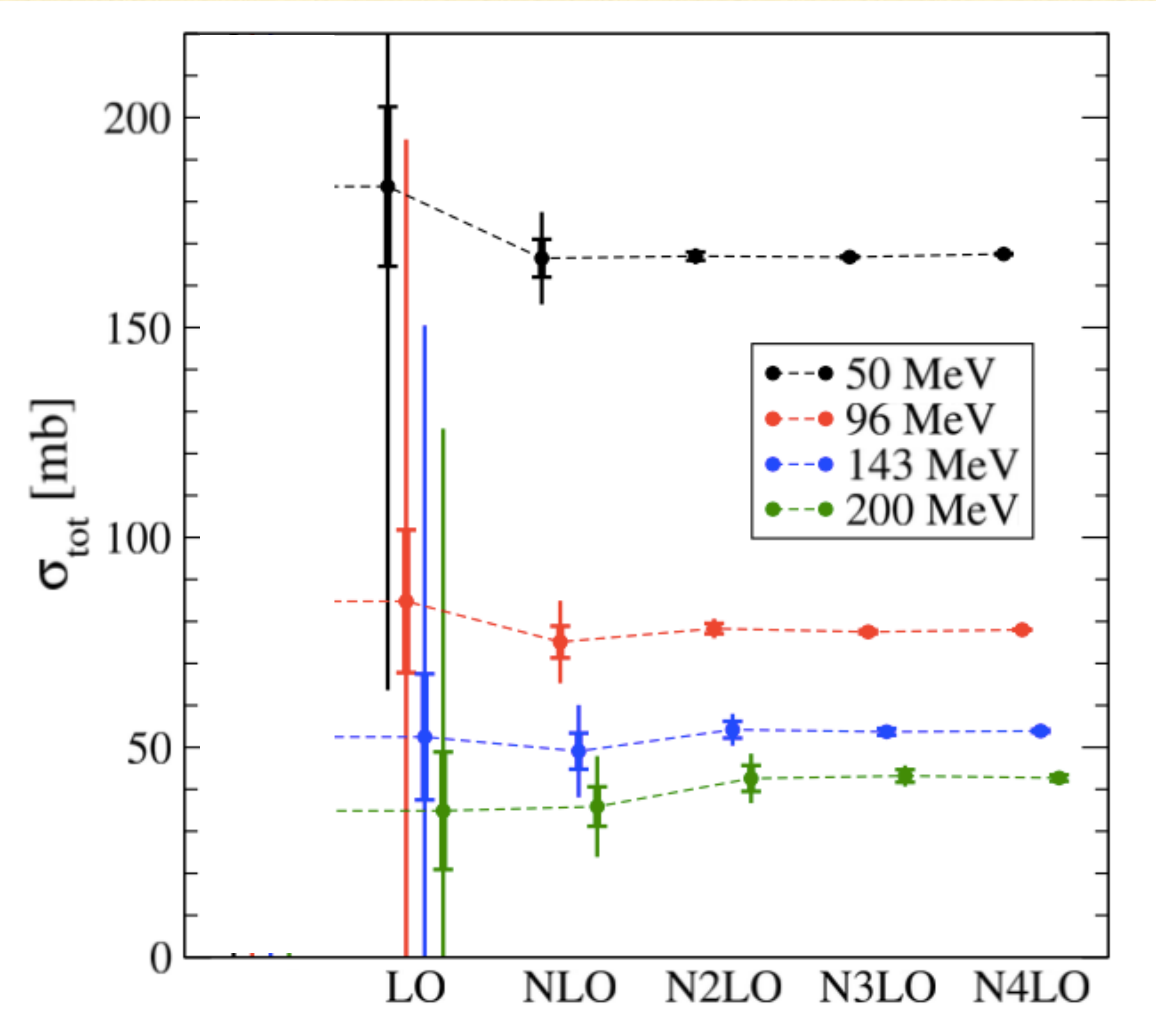


Results



200
150
100
50
0
σ_{tot} [mb]
50 MeV
96 MeV
143 MeV
200 MeV
LO
NLO
N2LO
N3LO
N4LO

Results



σ_{tot} [mb]
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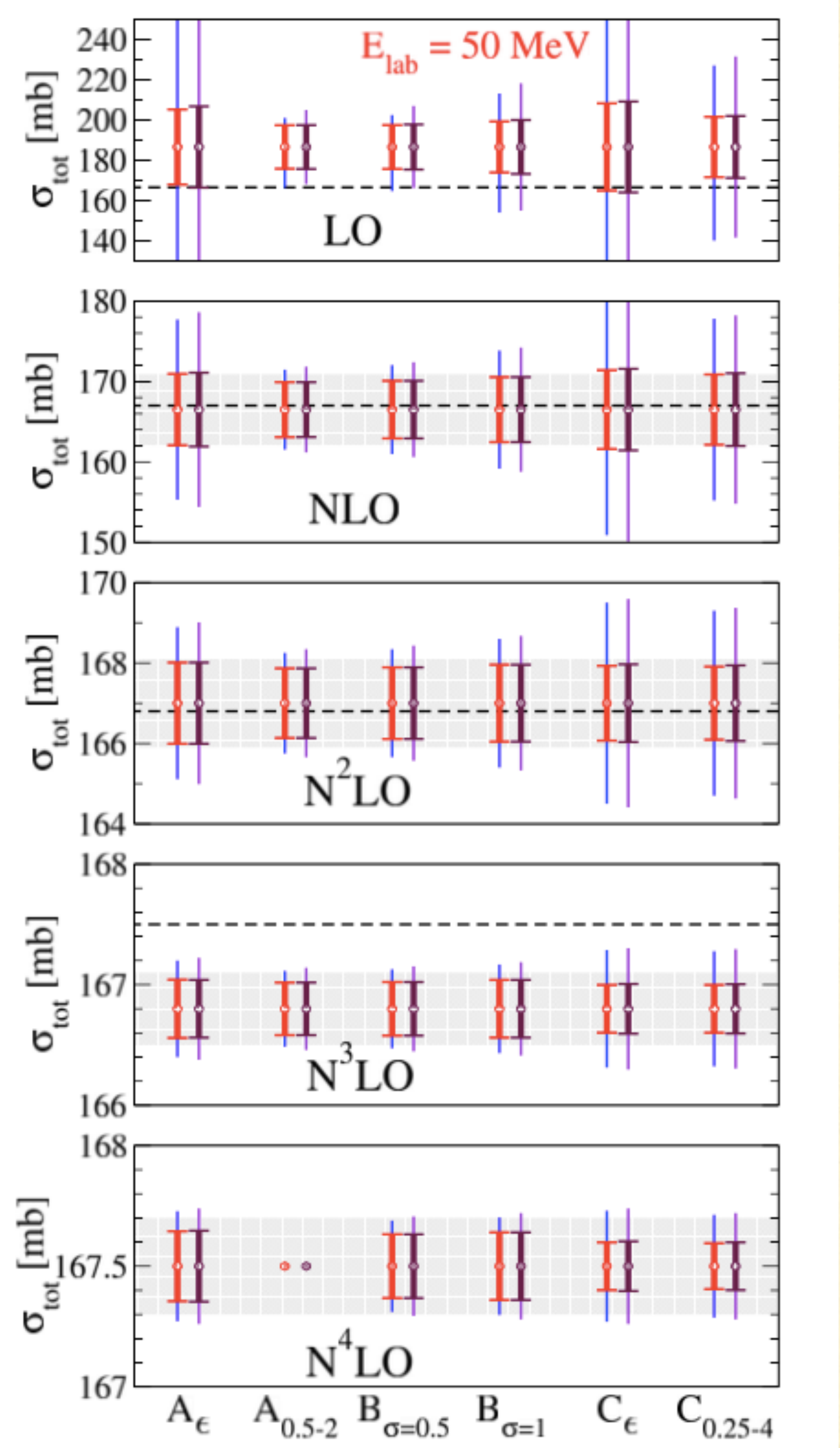
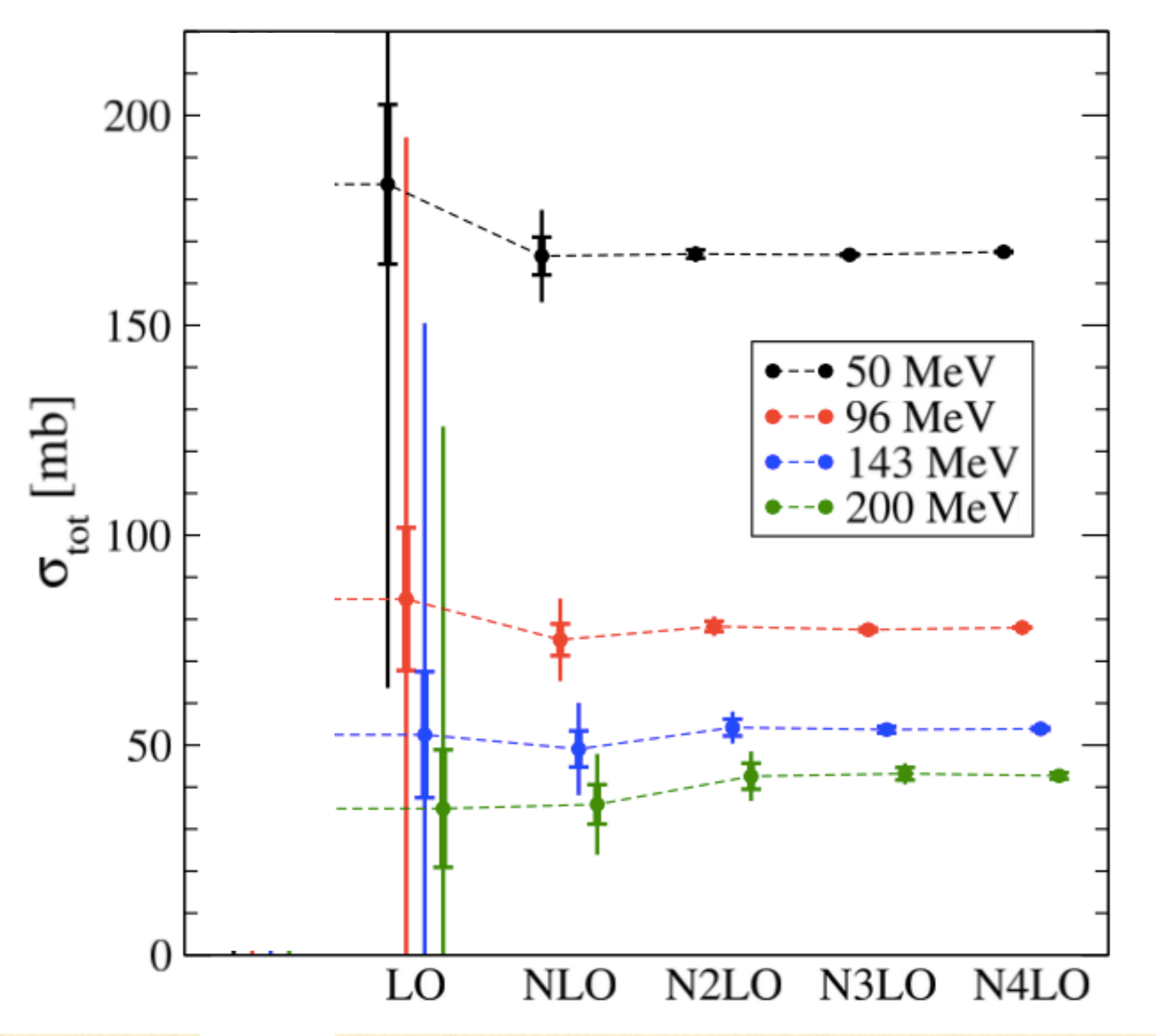


E_{lab} = 50 MeV
σ_{tot} [mb]
LO
NLO
N^2LO
N^3LO
N^4LO
A_ϵ
$A_{0.5-2}$
$B_{\sigma=0.5}$
$B_{\sigma=1}$
C_ϵ
$C_{0.25-4}$

Results



σtot [mb]
200
150
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50 MeV
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LO
NLO
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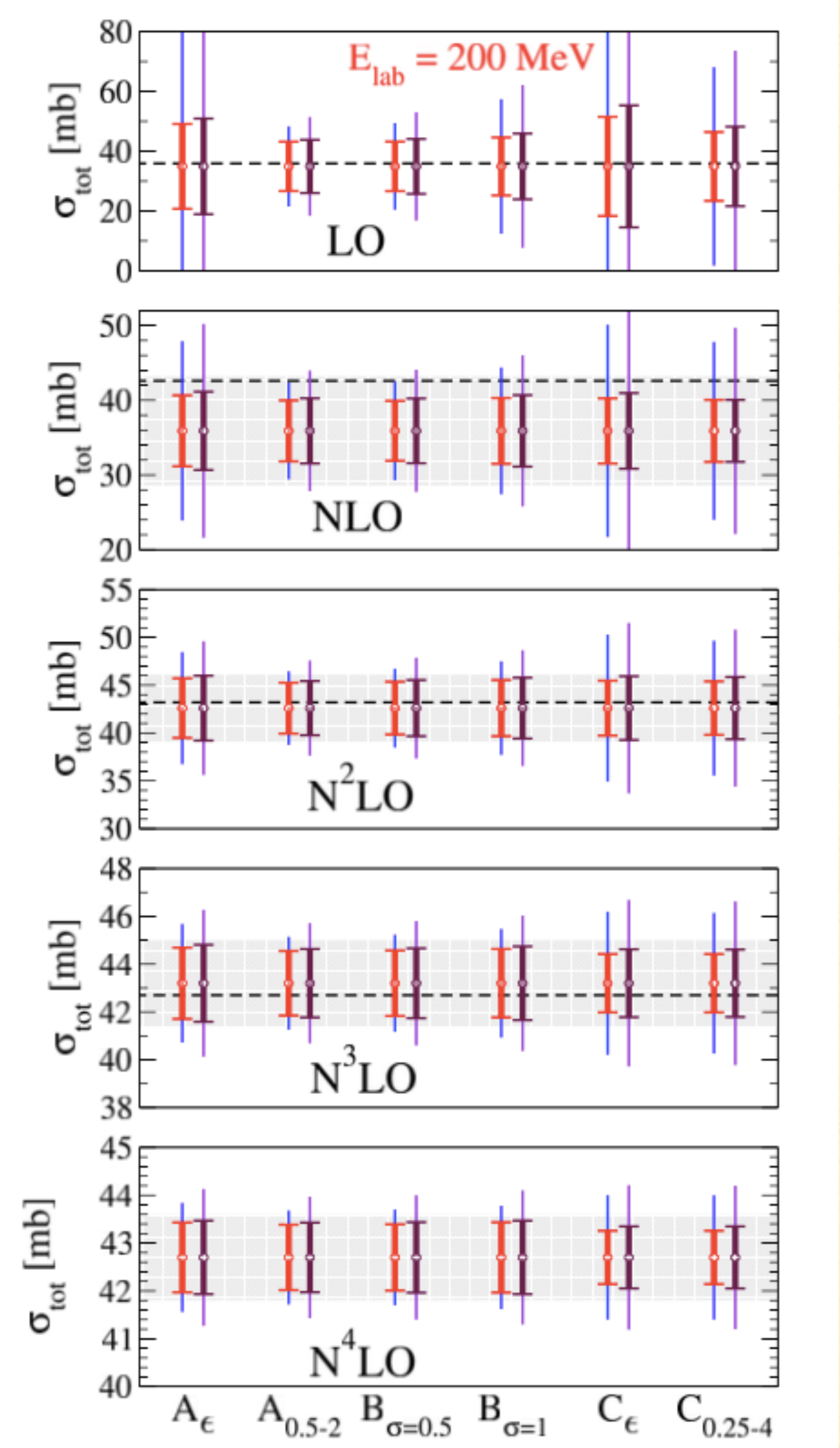

Elab = 200 MeV
σtot [mb]
LO
NLO
N2LO
N3LO
N4LO
Aϵ
A0.5-2
Bσ=0.5
Bσ=1
Cϵ
C0.25-4

Are these well calibrated?

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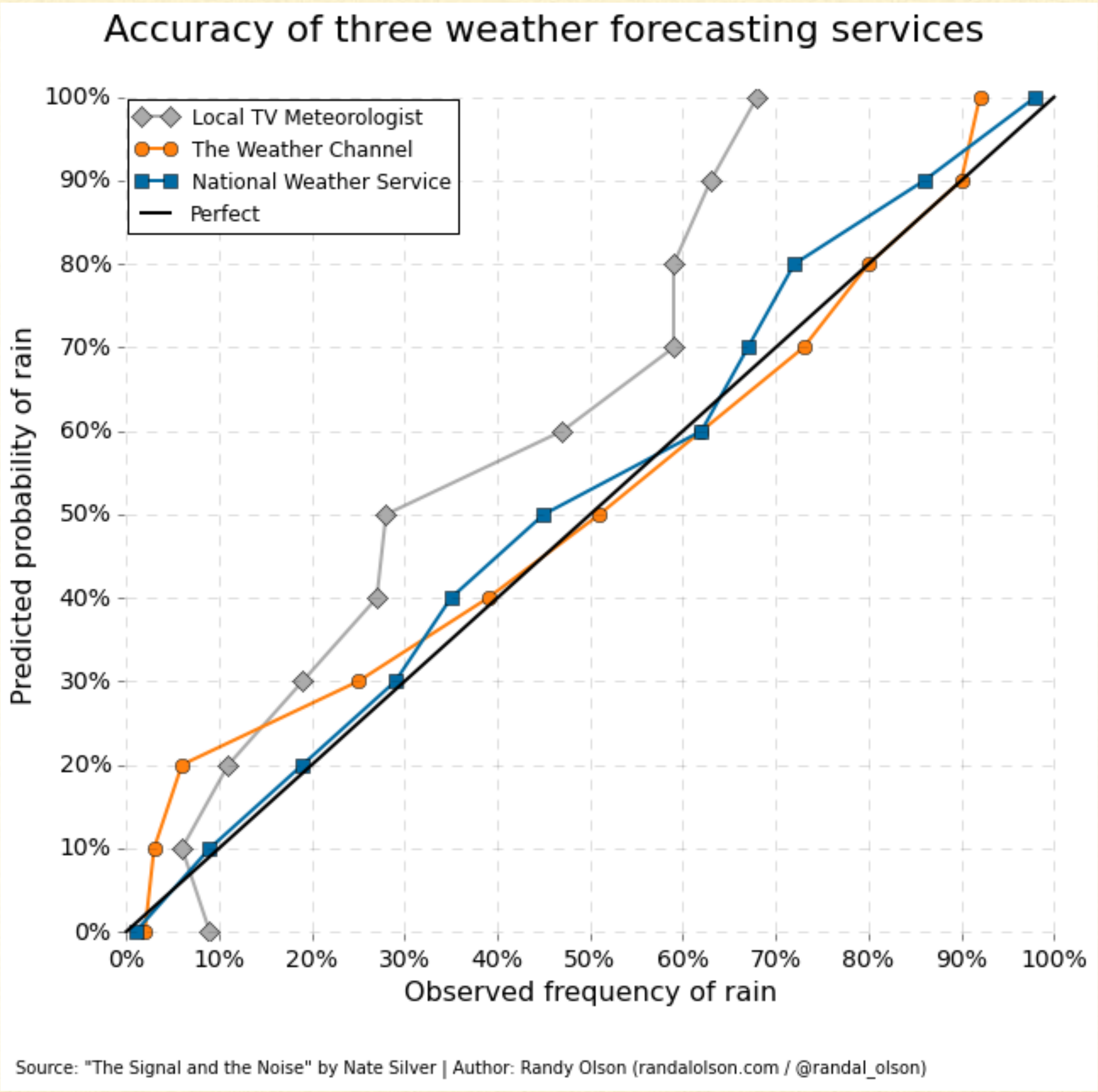

Melendez, Furnstahl, Wesolowski, PRC, 2017
after Furnstahl, Klco, DP, Wesolowski, PRC, 2015
after Bagnaschi, Cacciari, Guffanti, Jenniches, 2015

- Consider predictions at each order, with their error bars, as data and test them to see if the procedure is consistent

- Fix a given DOB interval: compute success ratio, compare

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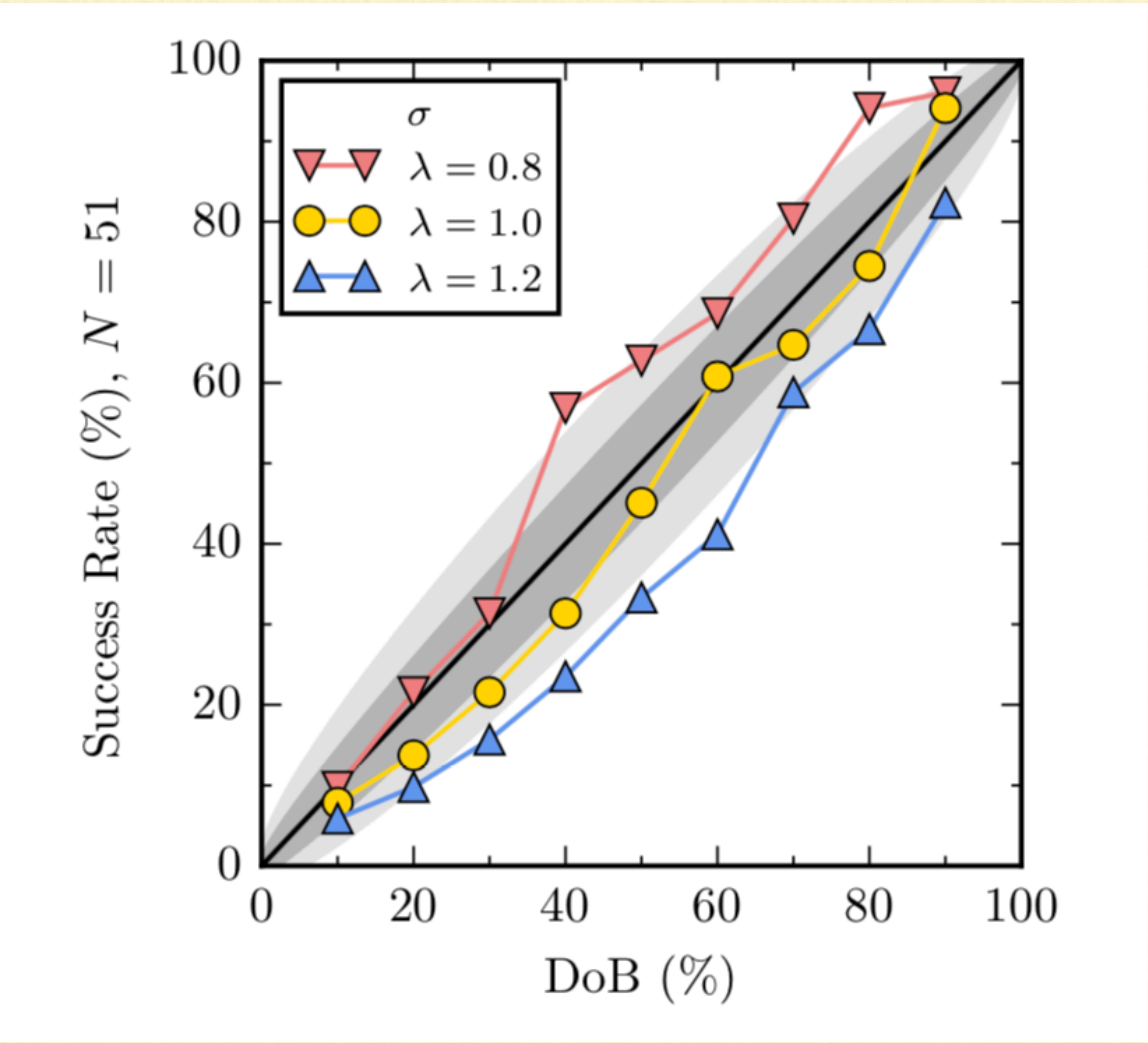

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- Fix a given DOB interval: compute success ratio, compare
- Look at this for EKM predictions at three different orders and 17 different energies
- Interpret in terms of rescaling of Λ_b by a factor λ

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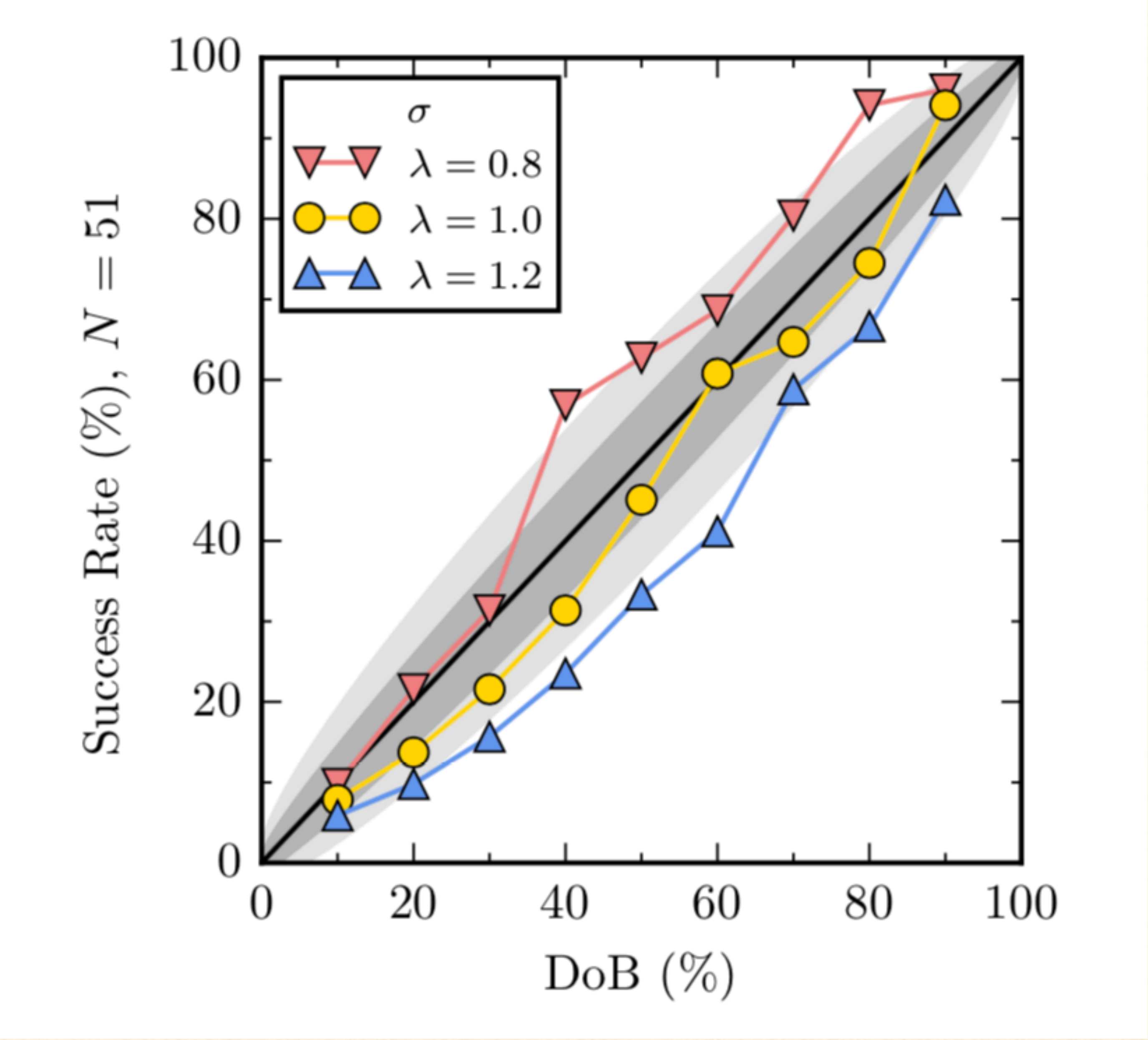

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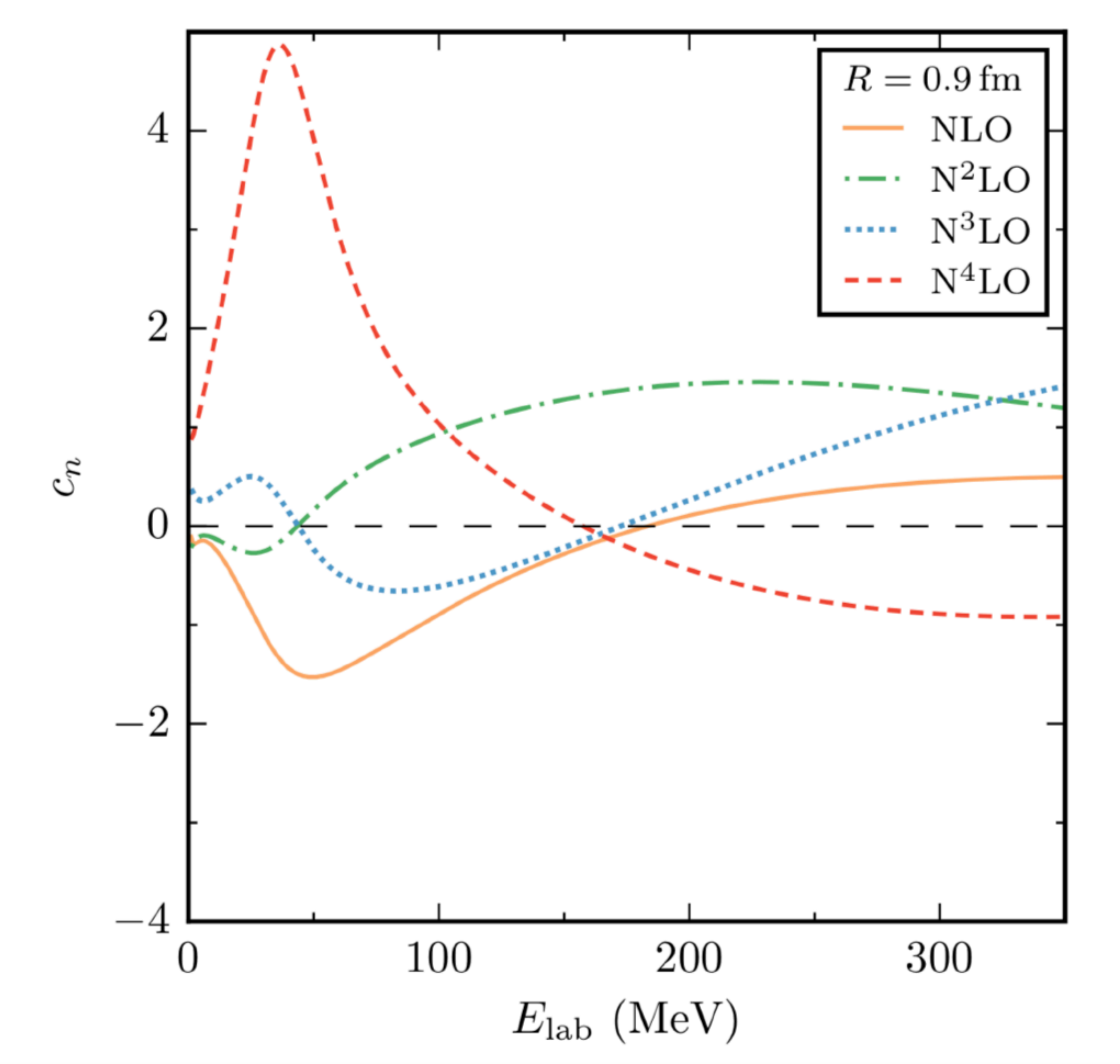
No evidence for significant rescaling of Λ_b

Error bands for NN observables

Melendez, Furnstahl, Wesolowski, PRC, 2017

EKM R=0.9 fm potential



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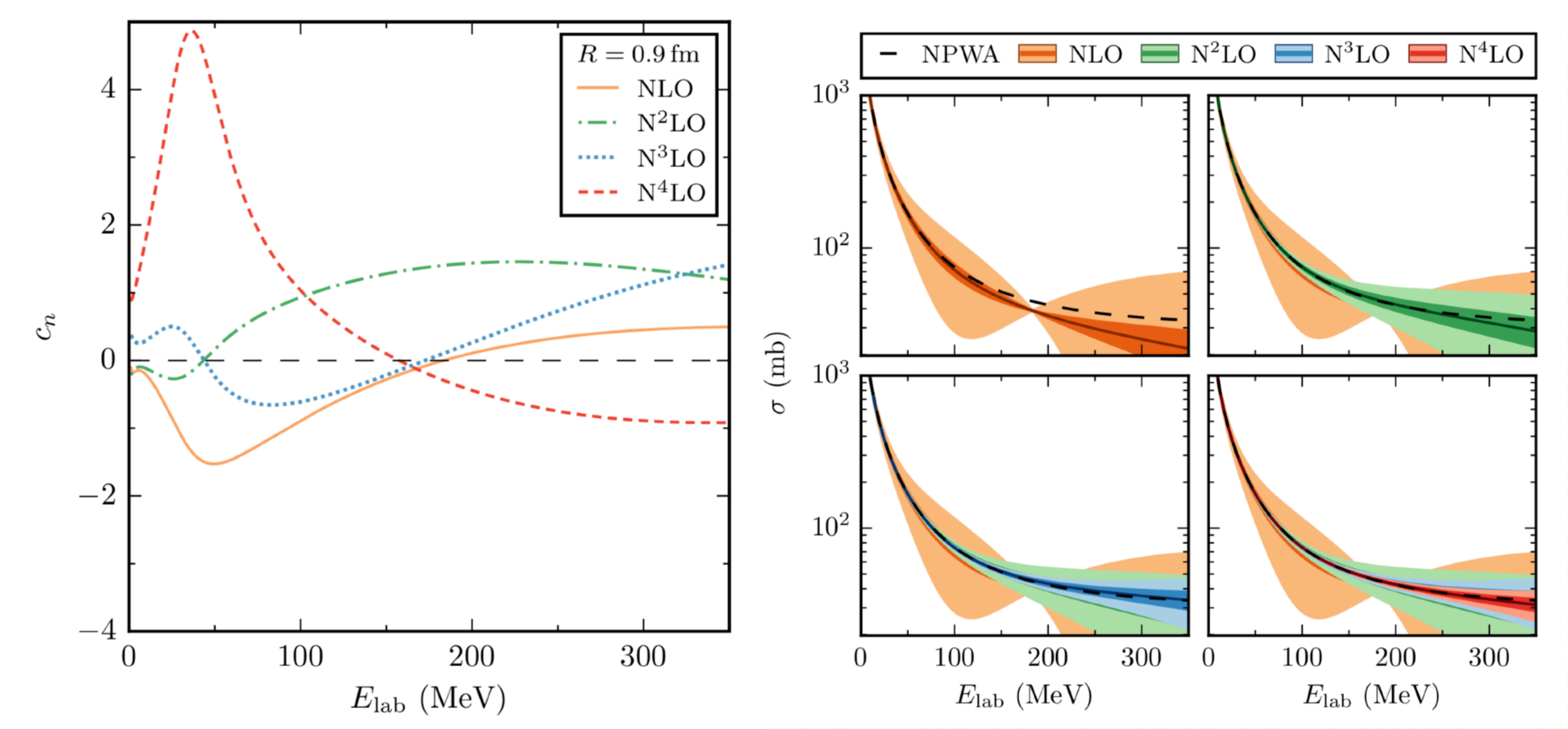

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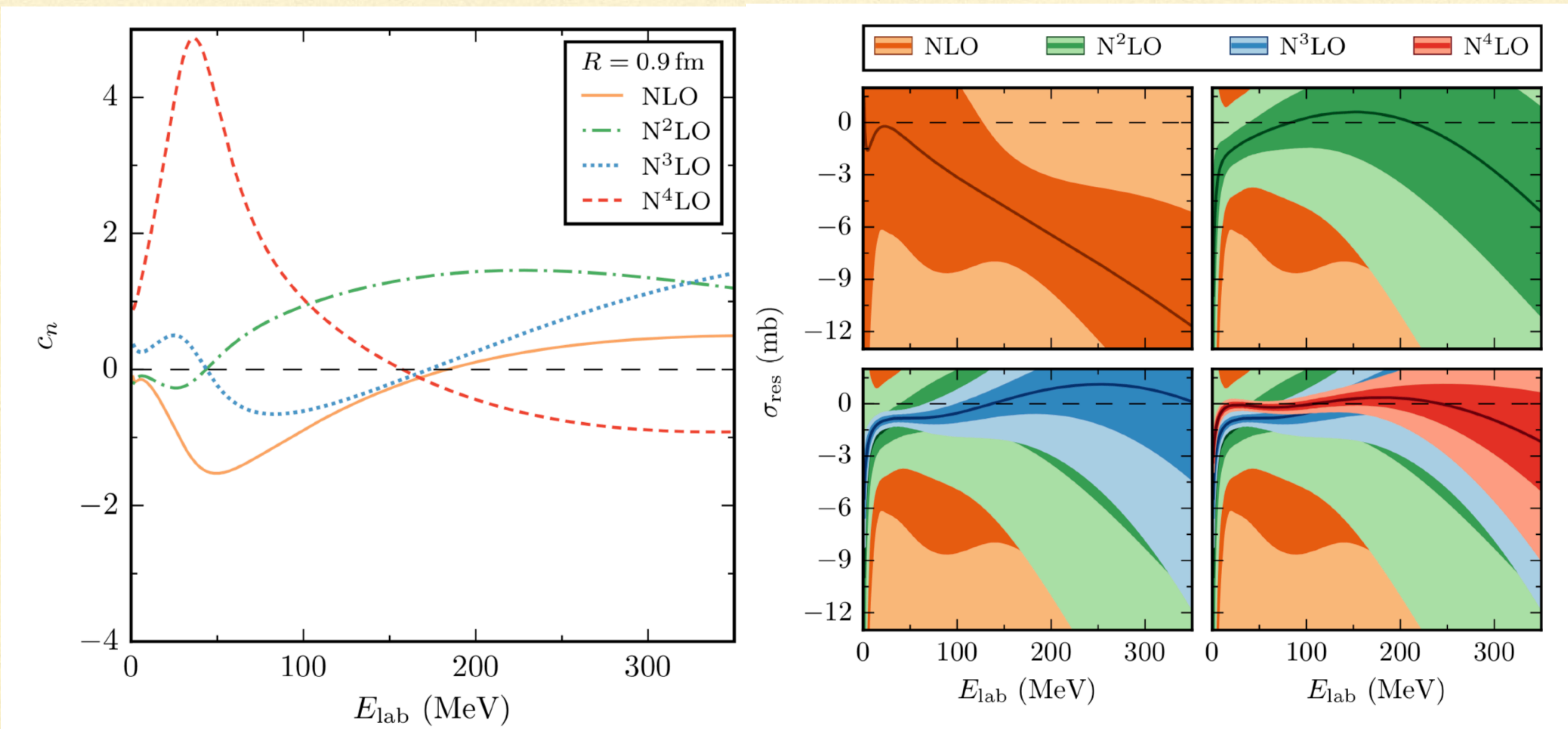

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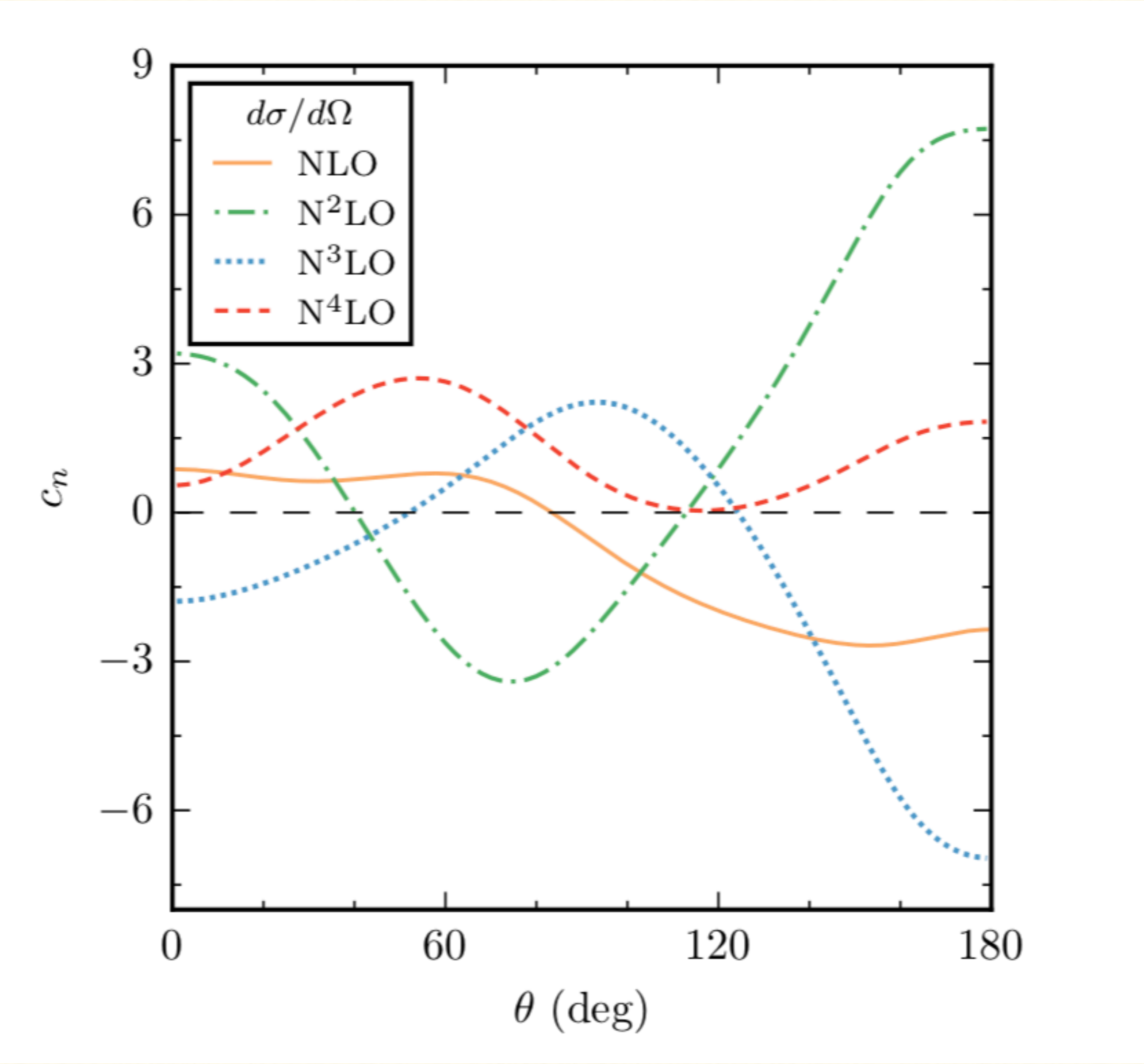

E_{lab}=96 MeV

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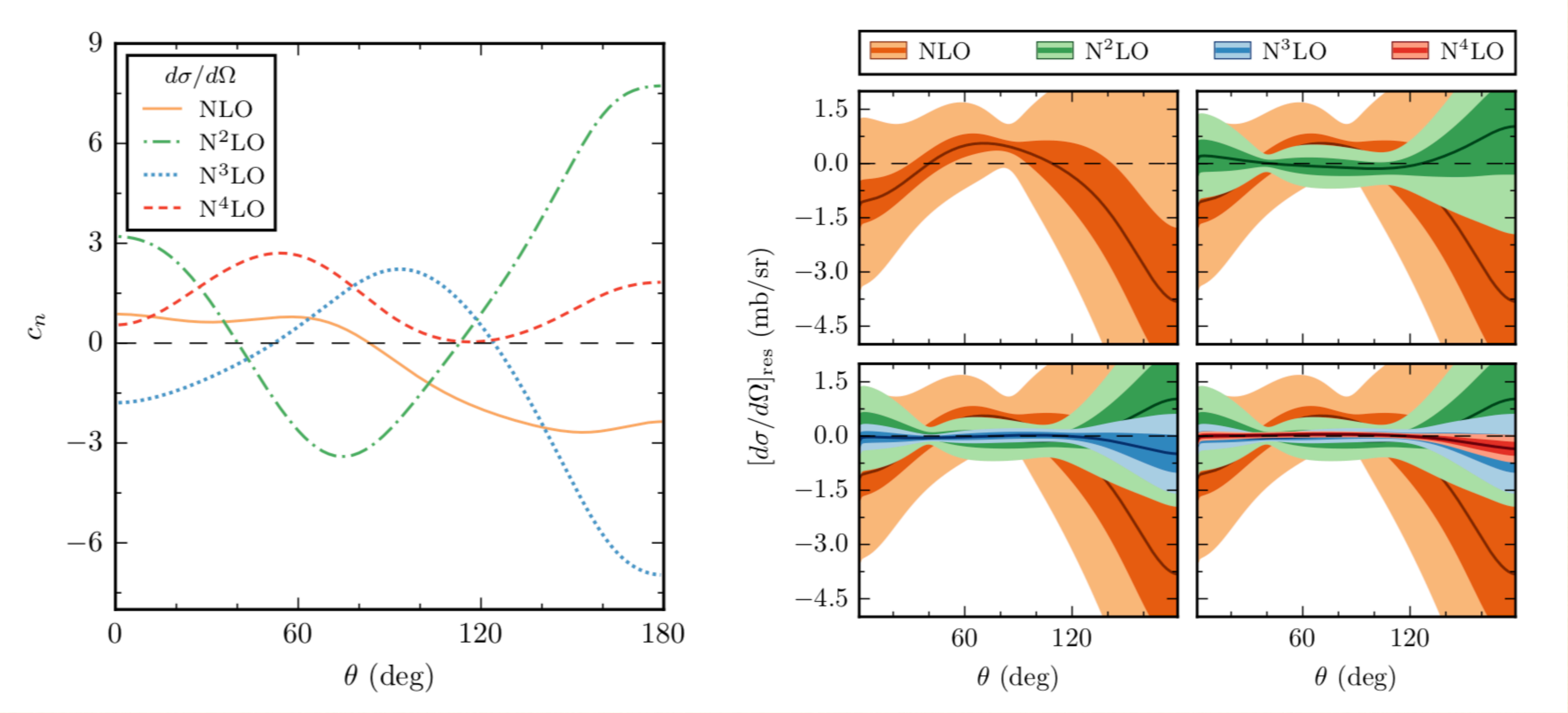
Melendez, Furnstahl, Wesolowski, PRC, 2017

EKM R=0.9 fm potential

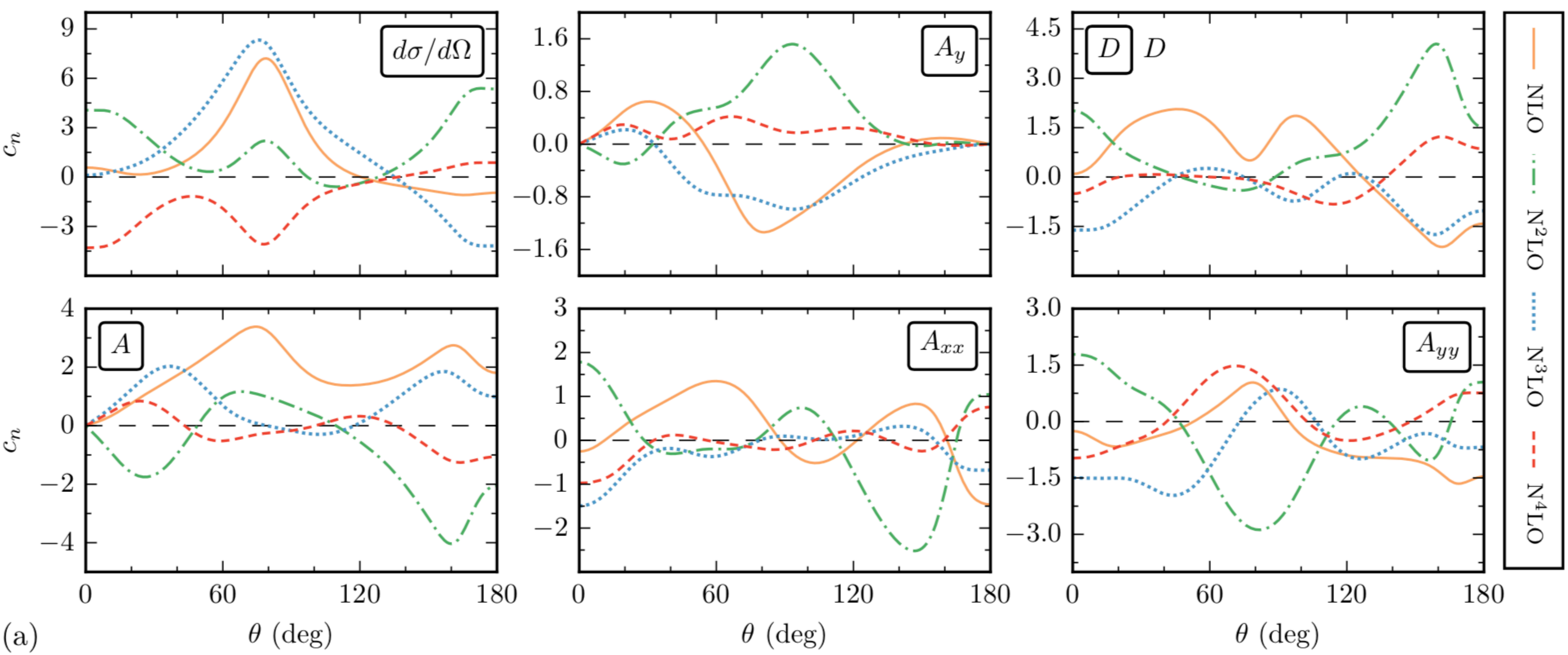


E_{lab}=96 MeV

Error bands for NN observables

Melendez, Furnstahl, Wesolowski, PRC, 2017

EKM R=0.9 fm potential

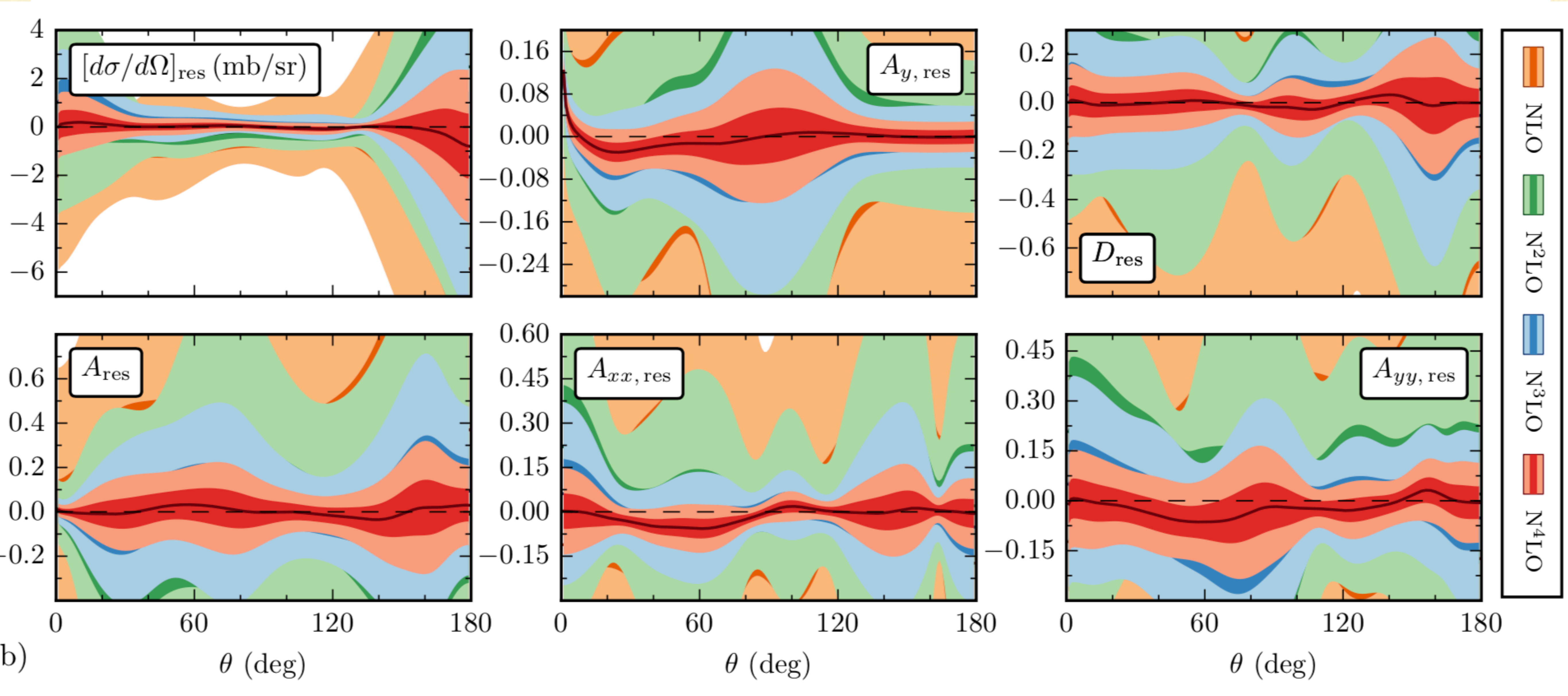


E_{lab}=250 MeV

Error bands for NN observables

Melendez, Furnstahl, Wesolowski, PRC, 2017

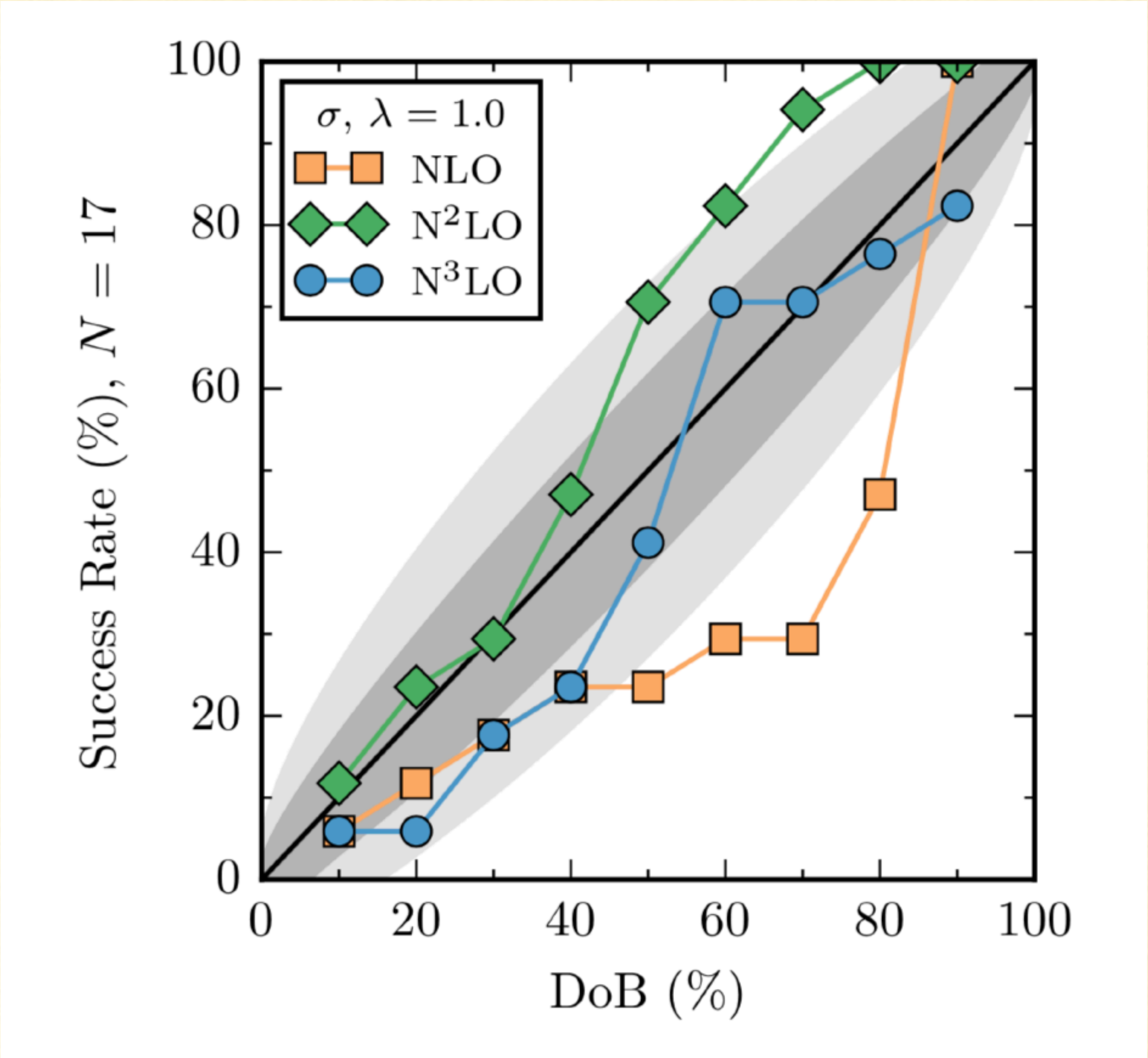
EKM R=0.9 fm potential



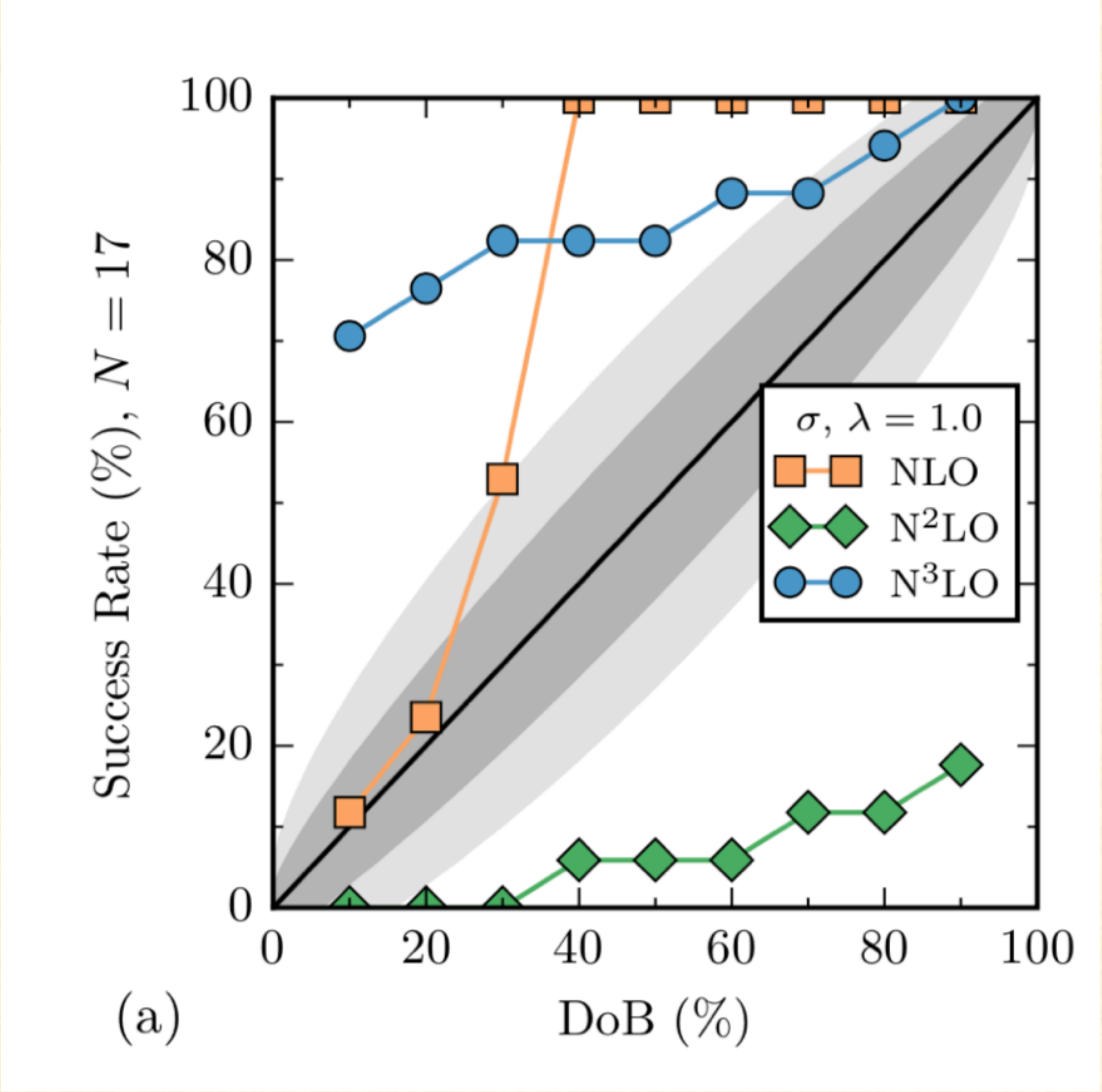
E_{lab}=250 MeV

Physics from calibration plots

R=0.9 fm



R=1.2 fm



- Allows assessment of order-by-order convergence
- Can look at differential cross section and spin observables too