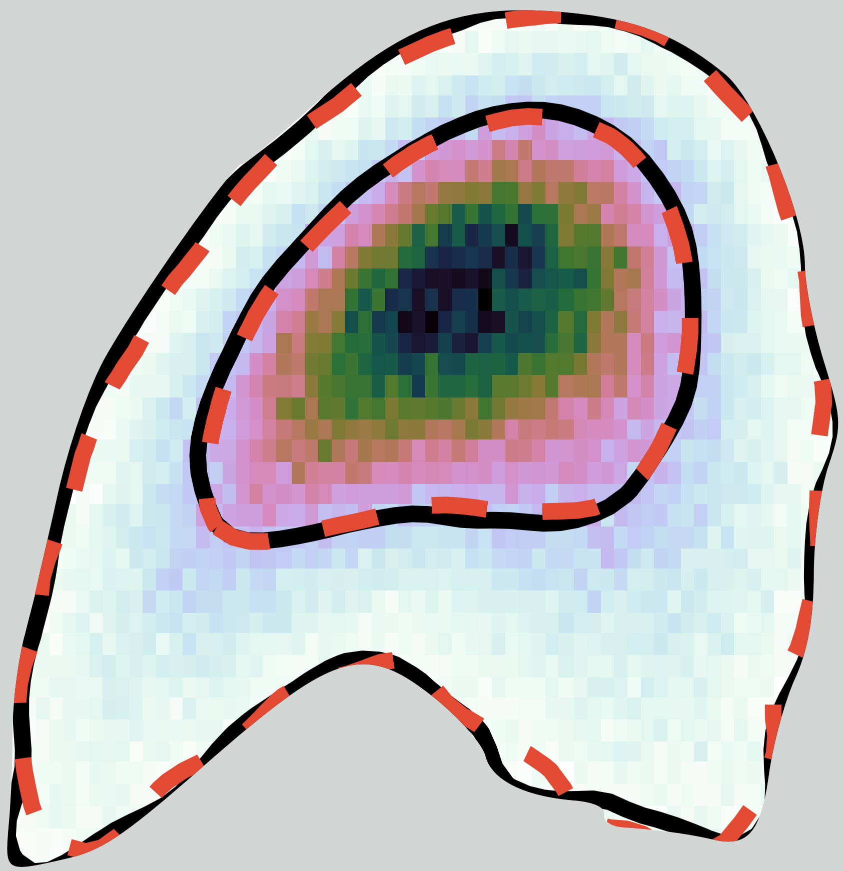

THE DATA PERSPECTIVE ON CHIRAL EFFECTIVE FIELD THEORY

CHRISTIAN FORSSÉN

Department of Physics, Chalmers, Sweden

ISNET-5 workshop, York,
Nov. 6-9, 2017

MANY THANKS TO MY COLLABORATORS

- **Boris Carlsson**, **Andreas Ekström** (Chalmers)
- Kai Hebeler (Darmstadt), Gustav Jansen (ORNL), Kyle Wendt (ORNL/UT now LLNL)

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INTRODUCTION

ONE-BULLET OVERVIEW

- What information does available nuclear scattering data[1,2] impose[3] on a state–of-the-art “model”[4] of the strong force between nucleons?

[1] only πN and NN
[2] plus A=2-3 bound-state data
[3] using a frequentist approach.
[4] chiral effective field theory => systematically improvable

FIVE-BULLET OVERVIEW (FOR PHYSICISTS)

- Optimize LECs at N3LO of chiral EFT (Weinberg PC) with respect to πN, NN scattering data and A=2-3 bound states.
- There are many LECs – making this a very difficult optimization problem.
- We attempt uncertainty quantification and error propagation to few-body observables.
- The analysis is repeated using information from a Roy-Steiner analysis of πN data with resulting constraints on ci:s, di:s, ei:s.
- Summary and Outlook

FIVE-BULLET OVERVIEW (TRANSLATED)

- Optimize LECs at N3LO of chiral EFT (Weinberg PC) with respect to πN, NN scattering data and A=2-3 bound states.
  Translation: 41 model parameters. 6000 experimental data points with small-to-large error bars. There is some prior knowledge of the model error.

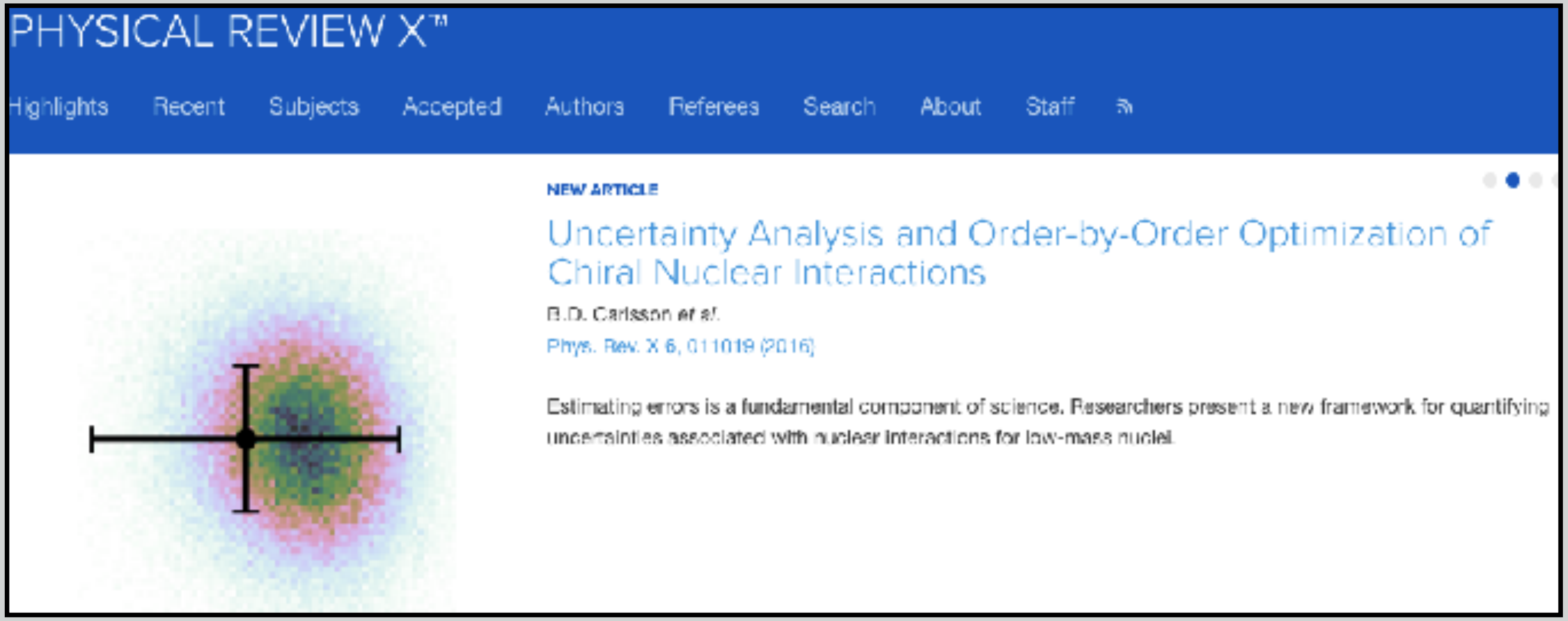
- There are many LECs – making this a very difficult optimization problem.
  Translation: We encounter a very flat chi2-surface with many local minima (sometimes non-quadratic).
  Question: How could this optimization problem be handled? (see also Andreas' talk)

FIVE-BULLET OVERVIEW (TRANSLATED)

- We attempt uncertainty quantification and error propagation to few-body observables.
  Question: How to best perform uncertainty quantification and error propagation in this situation?

- The analysis is repeated using information from a Roy-Steiner analysis of πN data with resulting constraints on ci:s, di:s, ei:s.
  Question: How to handle the errors when combining experimental data with information from a theory analysis?

- Summary and Outlook
  Translation: Summary and Outlook



Based on work presented in:

- B. Carlsson, A. Ekström, **CF** et al., Phys. Rev. X 6 (2016) 011019

- B. Carlsson, PhD thesis, manuscript in preparation

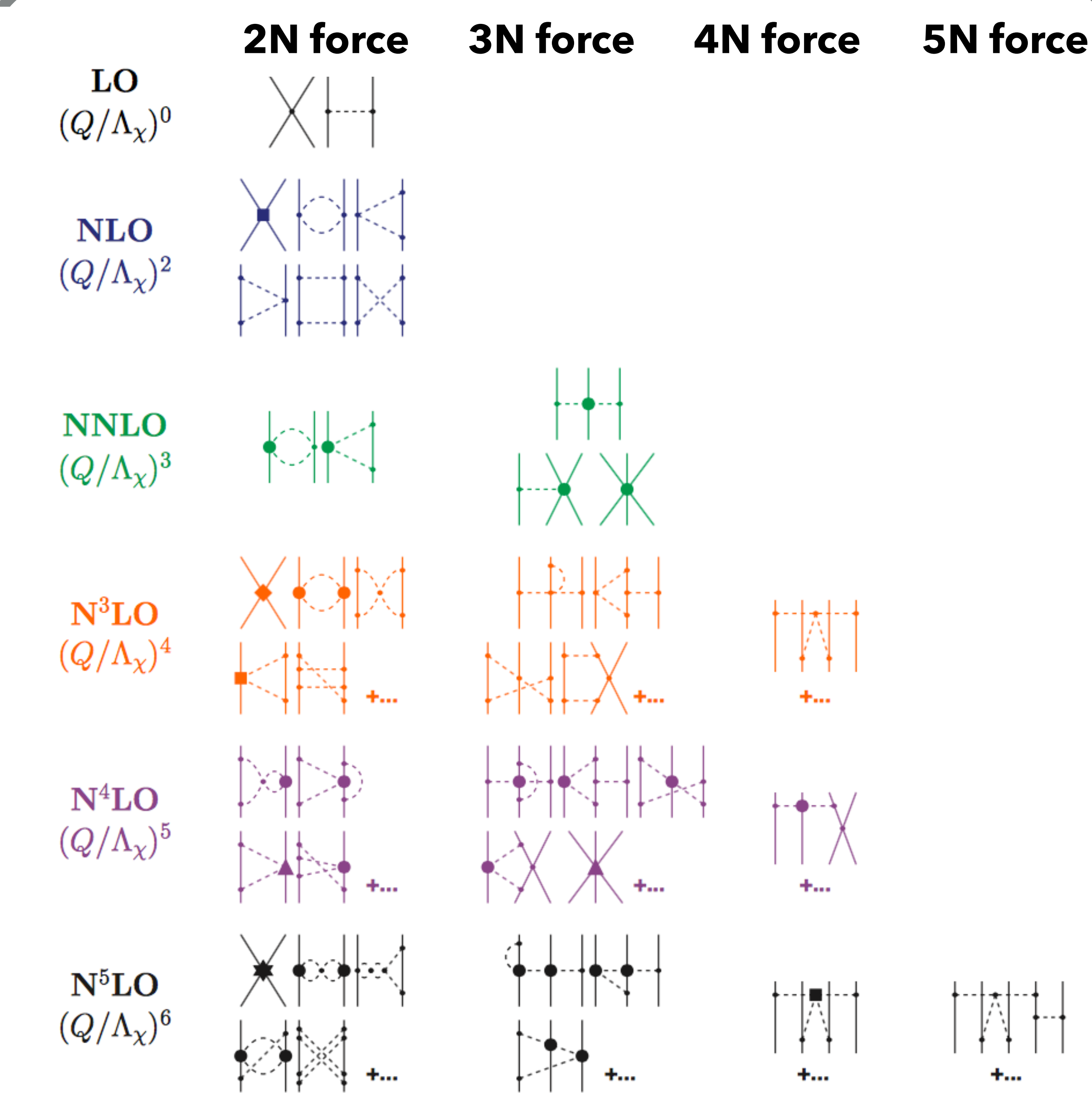
FROM πN AND NN TO A=4 WITH CHIRAL EFT AND ERROR ANALYSIS

CHIRAL EFT FOR NUCLEAR INTERACTIONS

Chiral EFT

- Systematic low-energy expansion: $(q/\Lambda_\chi)^\nu$
- Connects several sectors: πN, NN, NNN, j_N
- (Unknown) short-range physics included as contact interactions.
- LECs need to be fitted to data.

$$\chi^2(\vec{p}) = \sum_i \left(\frac{O_i^{\text{theo}}(\vec{p}) - O_i^{\text{exp}}}{\sigma_{\text{tot},i}} \right)^2$$

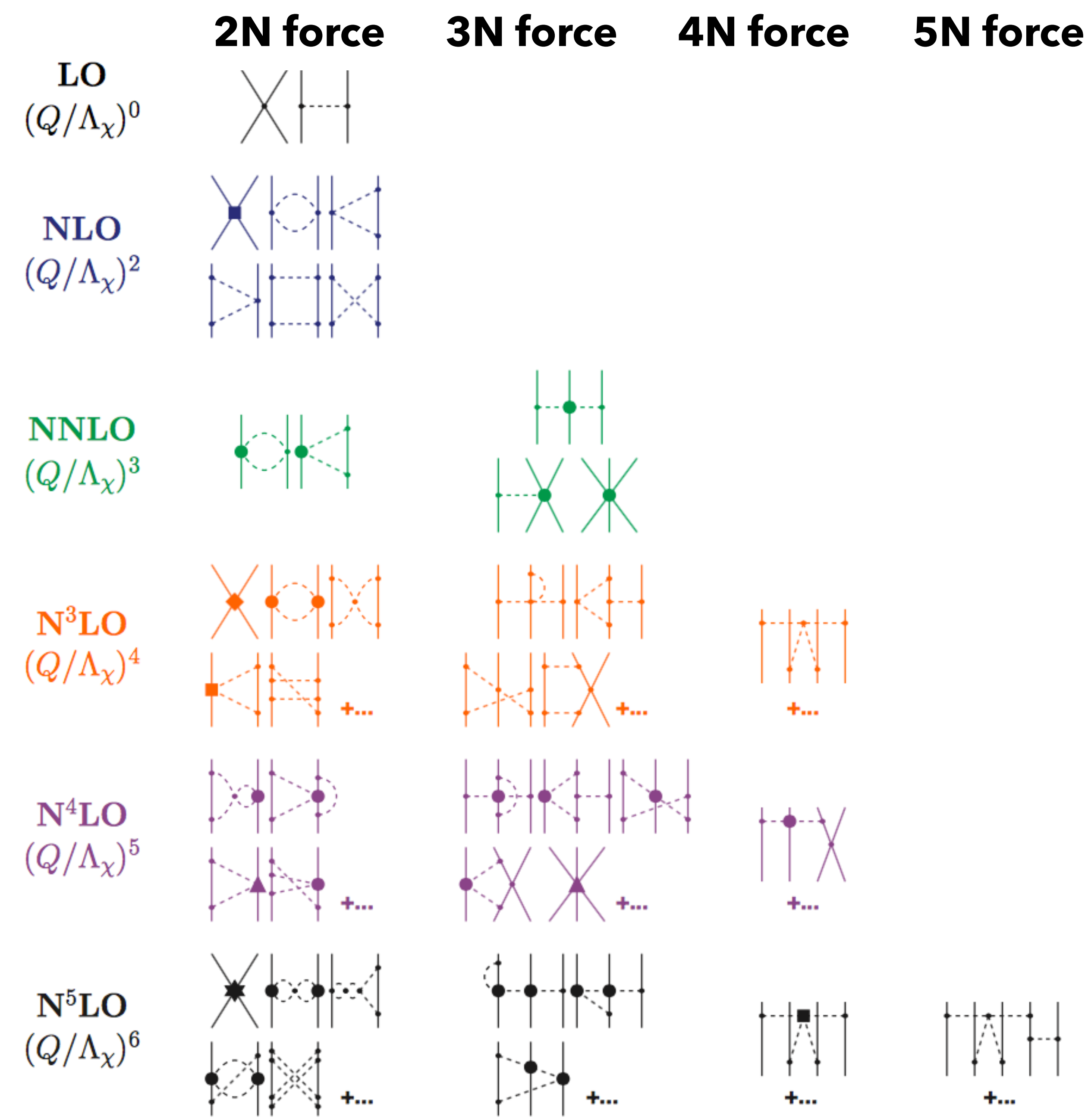


See Evgeny's presentation

CHIRAL EFT FOR NUCLEAR INTERACTIONS

Selected key results

- Non-local, 2NF up to N5LO
  - D. R. Entem et al. PRC 91, 014002 (2015)
  - R. Machleidt et al. Phys. Rep. 503 (2011)
- Non-local, leading 3NF
  - E. Epelbaum et al. PRC 66, 064001 (2002)
  - K. Hebeler et al. PRC 91, 044001 (2015)
- Non-local, sub-leading 3NF
  - V. Bernard et al. PRC 77, 064004 (2008)
  - V. Bernard et al. PRC 84, 054001 (2011)
  - K. Hebeler et al. PRC 91, 044001 (2015)
- 4th-order πN scattering
  - H. Krebs et al. PRC 85, 054006 (2015)



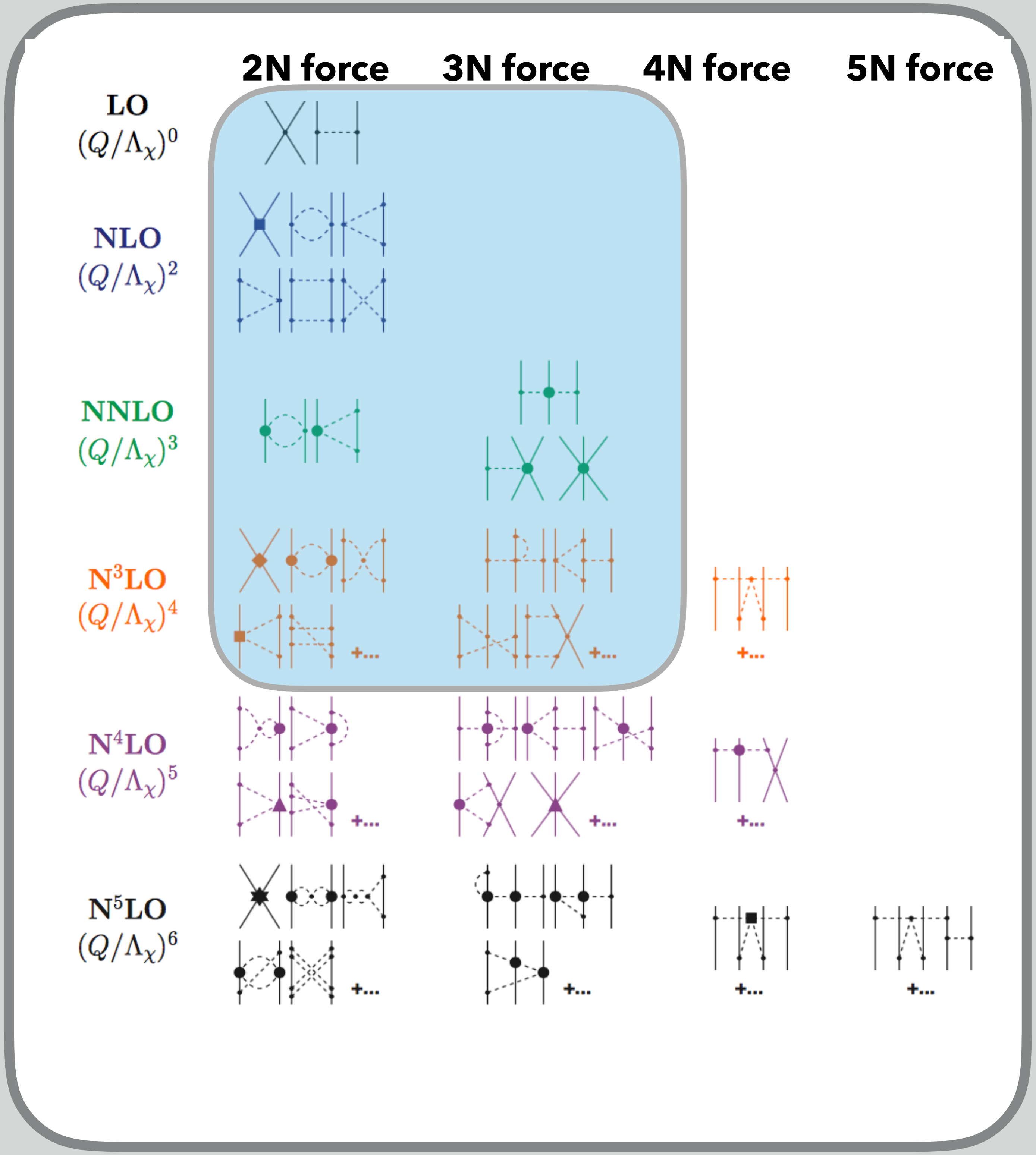
See Evgeny's presentation

CHIRAL NUCLEAR INTERACTIONS

Number of LECs

- Non-local, 2NF up to N3LO
  26 contacts
  4 c_i:s + 4 d_i:s
- Non-local, leading 3NF
  c_D, c_E
  3 c_i:s
- Non-local, subleading 3NF
  c_S, c_T
- 4th-order πN scattering
  c_i:s + d_i:s
  5 e_i:s

TOTAL:
41 parameters



INPUT AND TECHNOLOGY

πN scattering

- WI08 database
- T_{lab} between 10-70 MeV
- N_{data} = 1347
- R. Workman et al. (2012)

NN scattering

- Granada '13 database
- T_{lab} between 0-290 MeV
- N_{data} = 4753 (np + pp)
- R. Navarro Pérez et al. (2013)

All 6000 residuals computed on 1 node in ~90 sec.

A=2,3 bound states

- ^{2}H,^{3}H,^{3}He [binding energy, radius, Q(^{2}H), ^{3}H half life]

On 1 node in ~10 sec

+ derivatives! (×2-20 cost)

Alternatively… theoretical analysis of data

πN scattering

- Roy-Steiner analysis
  M. Hoferichter et al. (2015)

NN scattering

- Phase shifts from partial wave analysis

OPTIMIZATION STRATEGY

Low-energy constants (LECs) need to be fitted to experimental data.

$$\chi^2(\vec{p}) \equiv \sum_i \left(\frac{O_i^{\text{theo}}(\vec{p}) - O_i^{\text{expr}}}{\sigma_{\text{tot},i}} \right)^2 \equiv \sum_i r_i^2(\vec{p})$$

- Derivative-free optimization using POUNDerS was used in our earliest works
- More efficient minimization algorithms (Levenberg-Marquardt, Newton), and statistical error analysis require **derivatives**

$$\frac{\partial r_i}{\partial p_j} \quad \text{and} \quad \frac{\partial^2 r_i}{\partial p_j \partial p_k}$$

- Numerical derivation using **finite differences** is plagued by **low numerical precision** and is **computationally costly.**
- Instead, we use **Automatic Differentiation** (AD)

TOTAL ERROR BUDGET

- The total error budget is

E.g. , NCSM   Neglected

$$\sigma^2_{\text{tot}} = \sigma^2_{\text{exp}} + \sigma^2_{\text{method}} + \sigma^2_{\text{numerical}} + \sigma^2_{\text{model}}$$

- At a given chiral order v, the omitted diagrams should be of order

$$\mathcal{O}\left((Q/\Lambda_\chi)^{\nu+1}\right)$$

- Still needs to be converted to actual numbers σ_{model}

- We translate this EFT knowledge into an error in the scattering amplitudes

$$\sigma^{(\text{amp})}_{\text{model,x}} = C_x \left(\frac{Q}{\Lambda_\chi}\right)^{\nu+1}, \quad x \in \{NN, \pi N\}$$

- which is then propagated to an error in the observable.

OPTIMIZATION STRATEGY

Low-energy constants (LECs) need to be fitted to experimental data.

$$\chi^2(\vec{p}) \equiv \sum_i r_i^2(\vec{p}) = \boxed{\boxed{\sum_{j\in NN} r_j^2(\vec{p})} + \boxed{\sum_{k\in \pi N} r_k^2(\vec{p})} + \boxed{\sum_{l\in 3N} r_l^2(\vec{p})}}$$

 # parameters that are allowed to vary:

13	1-8 per channel	25	2+1=3	41
FIT πN-SECTOR TO πN DATA	FIT NN CONTACTS TO NN PHASE SHIFTS	FIT NN CONTACTS TO NN DATA	FIT C_D,C_E (+ Ct^{nn}_{1S0}) TO A=3 DATA	SIMULTANEOUS OPTIMIZATION
1	2^5x5=160	2^5x4=128	160	104

 # minima at each stage
(used as starting points for the next stage); (Λ=500 MeV)

c_1	$-0.69(50)$
c_2	$+3.0(14)$
c_3	$-4.12(32)$
c_4	$+5.35(81)$
d_1+d_2	$+6.22(44)$
d_3	$-5.31(30)$
d_5	$-0.46(18)$
$d_{14}-d_{15}$	$-11.00(42)$
e_{14}	$-0.63(95)$
e_{15}	$-7.7(26)$
e_{16}	$+5.9(49)$
e_{17}	$+2.1(18)$
e_{18}	$-8.1(42)$

2 per channel: 2 per channel: Some cases with 2 c_D, c_E optima

$^1S_0$, $^1P_1$, $^3P_0$, $^3P_1$, $^3P_2$–$^3F_2$

5 in the deuteron channel: 4 in the deuteron channel:

$^3S_1$, $^3D_1$, $^3S_1$–$^3D_1$

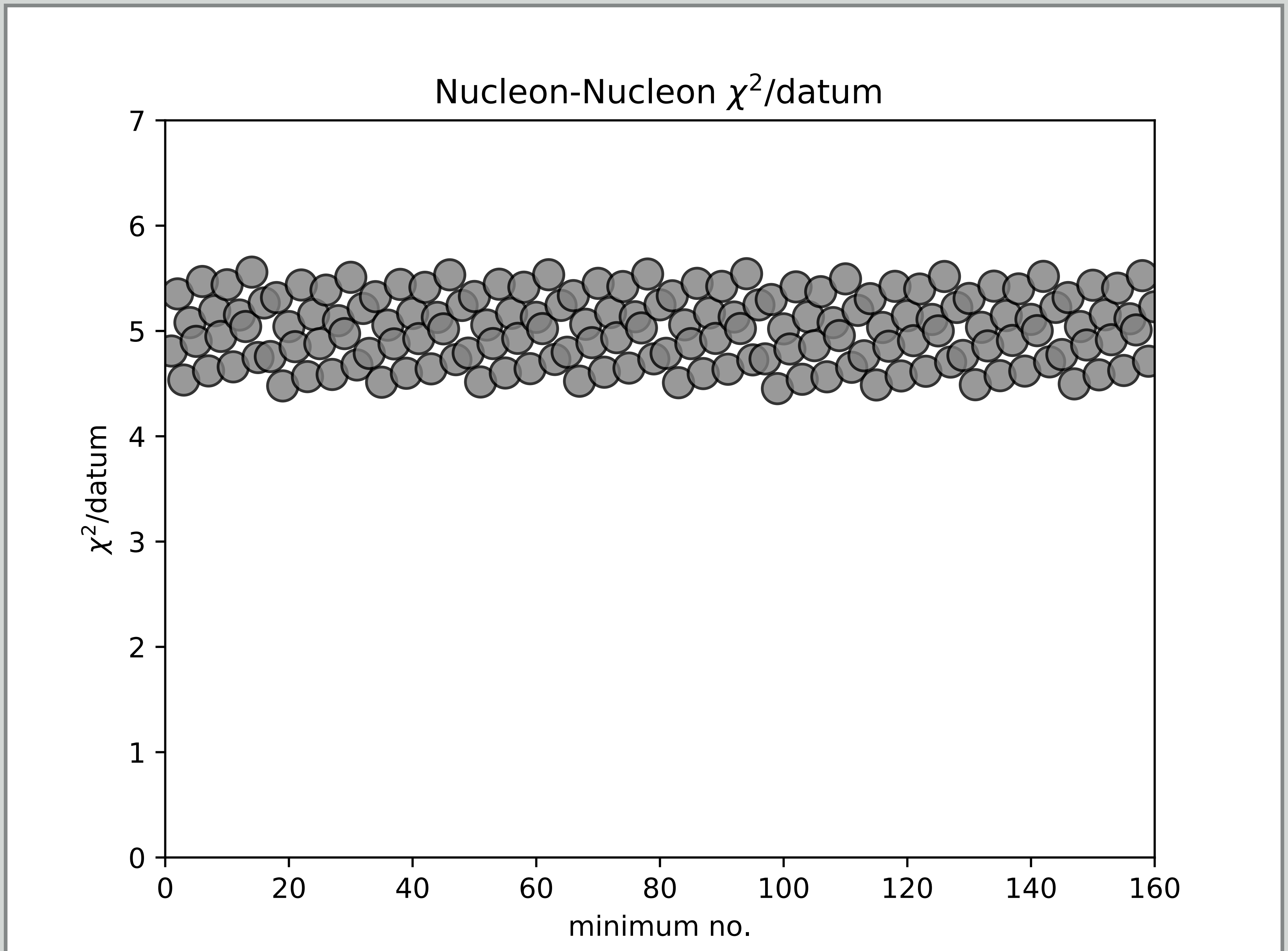
FIT πN-SECTOR TO πN DATA

FIT NN CONTACTS TO NN PHASE SHIFTS

FIT NN CONTACTS TO NN DATA

FIT C_D, C_E TO A=3 DATA

SIMULTANEOUS OPTIMIZATION



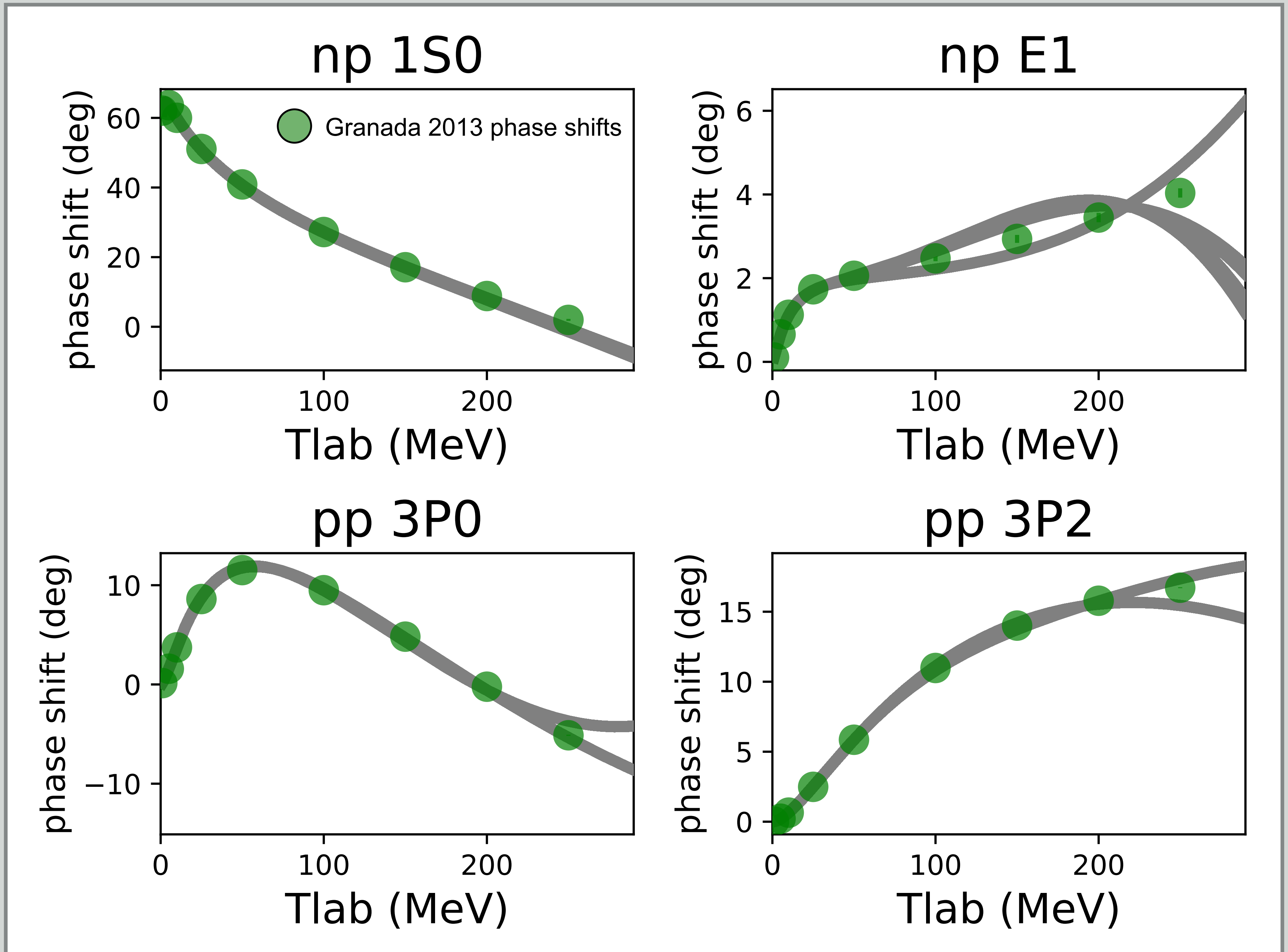
FIT πN-SECTOR TO πN DATA

FIT NN CONTACTS TO NN PHASE SHIFTS

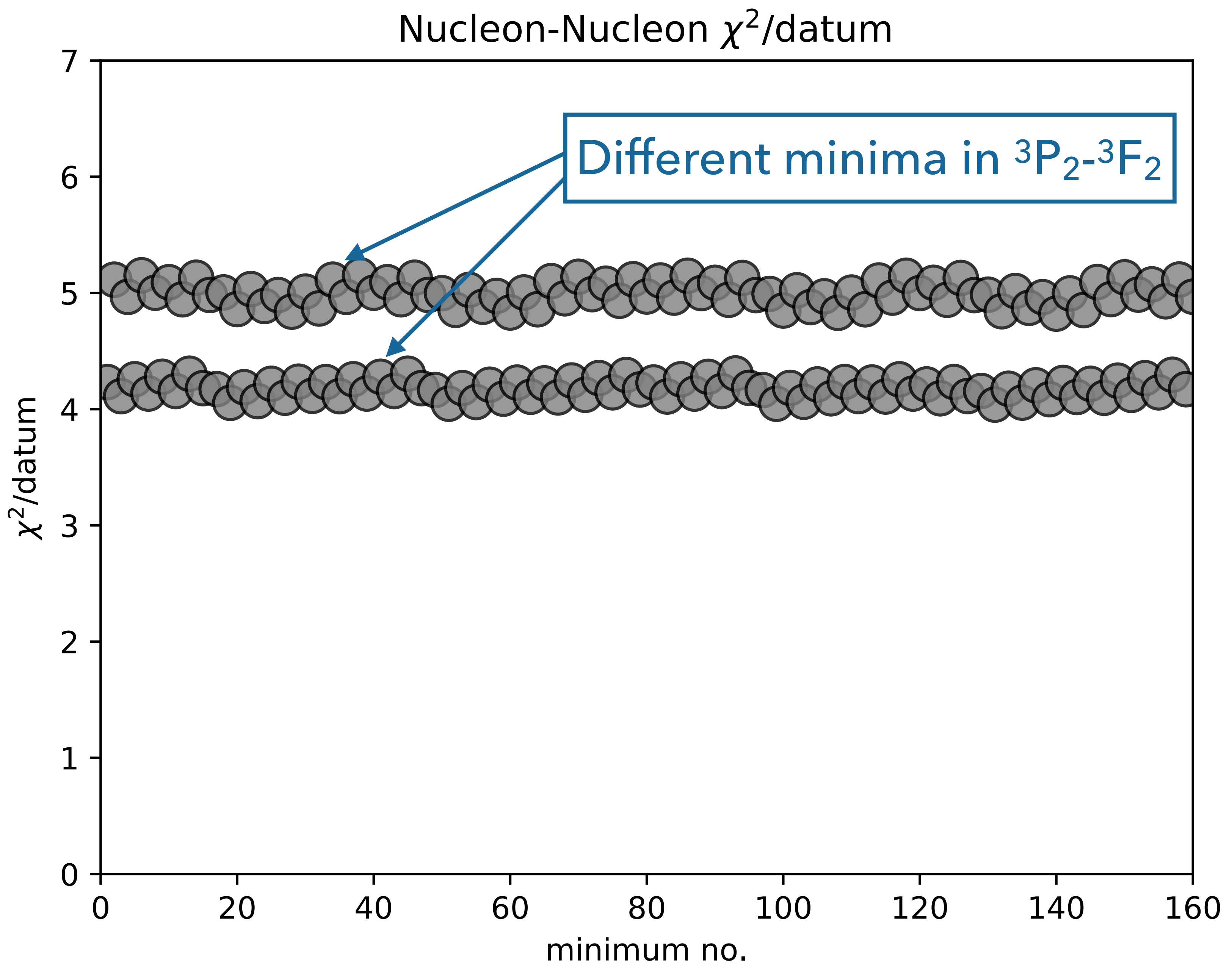
FIT NN CONTACTS TO NN DATA

FIT C_D,C_E TO A=3 DATA

SIMULTANEOUS OPTIMIZATION



FIT πN-SECTOR TO πN DATA → FIT NN CONTACTS TO NN PHASE SHIFTS → **FIT NN CONTACTS TO NN DATA** → FIT C_D, C_E TO A=3 DATA → SIMULTANEOUS OPTIMIZATION



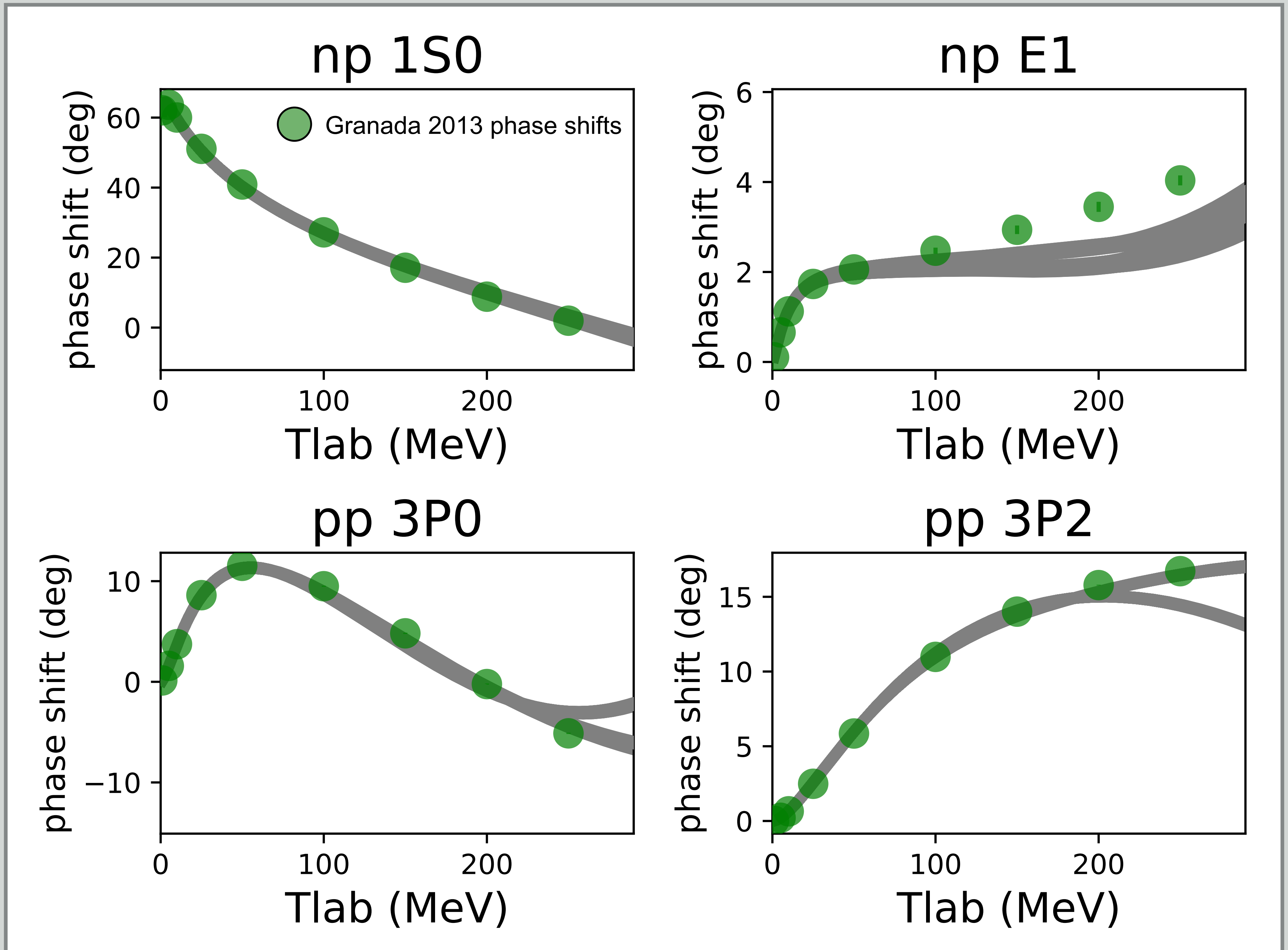
FIT πN-SECTOR TO πN DATA

FIT NN CONTACTS TO NN PHASE SHIFTS

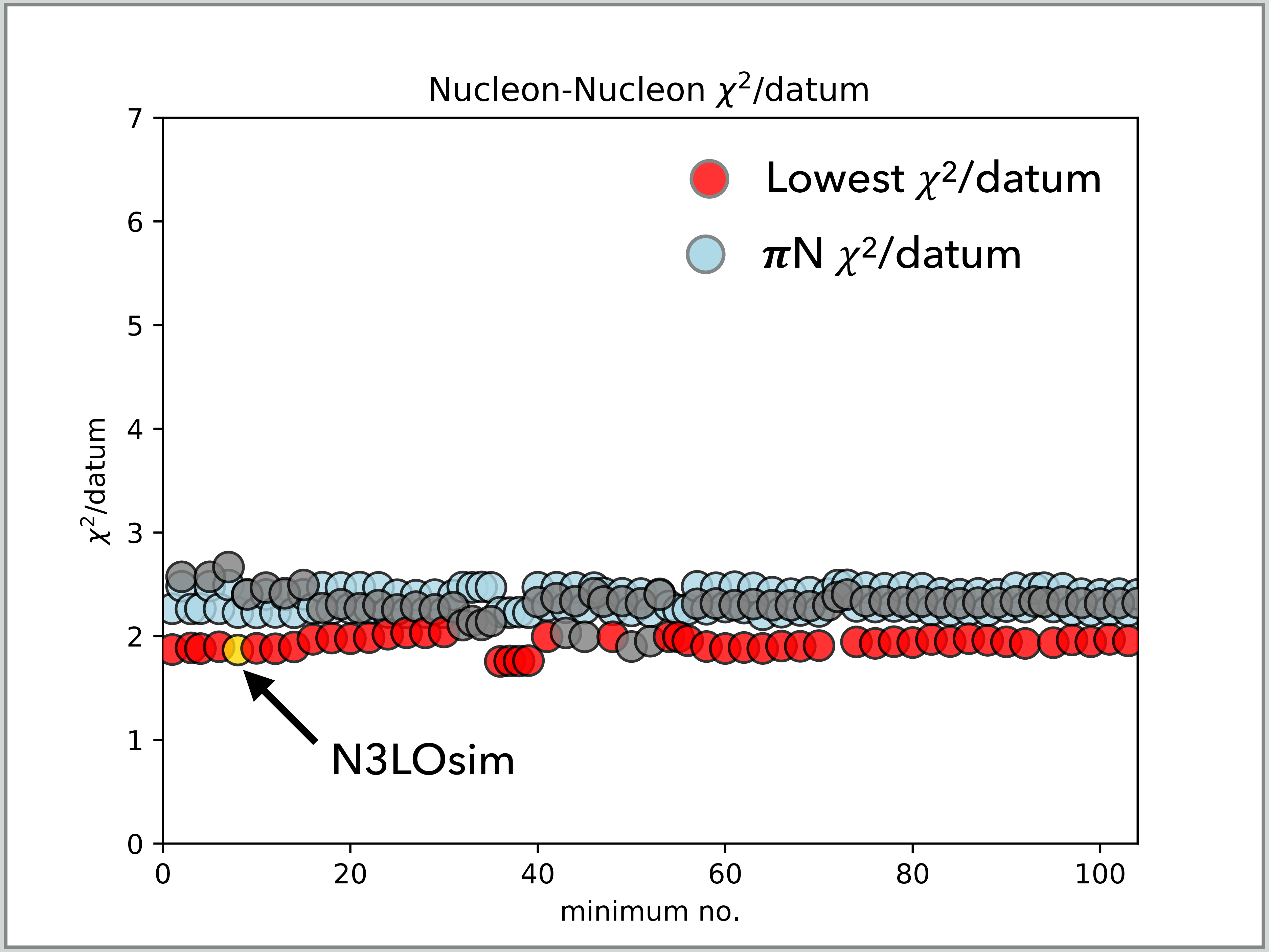
FIT NN CONTACTS TO NN DATA

FIT C_D, C_E TO A=3 DATA

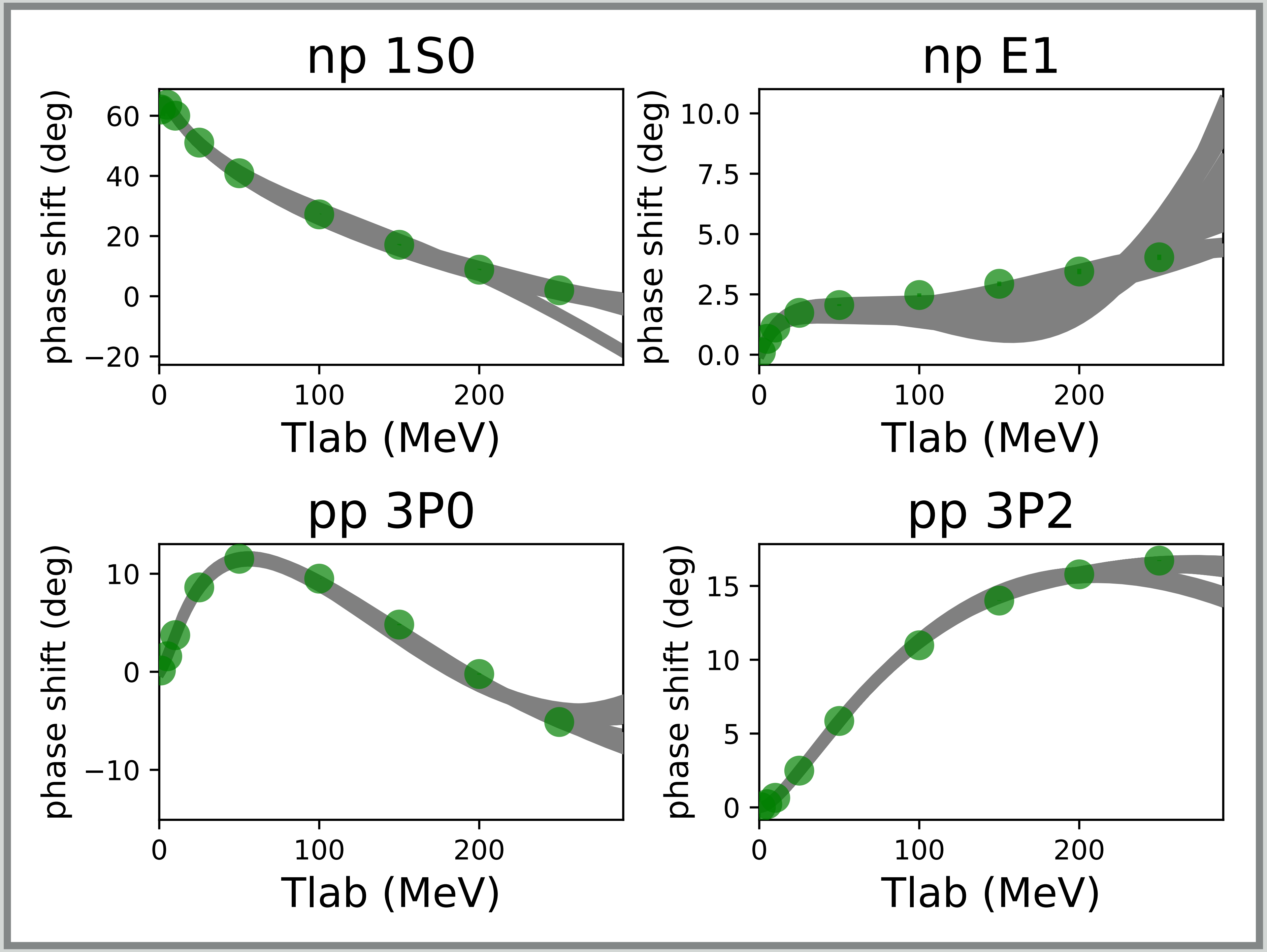
SIMULTANEOUS OPTIMIZATION



FIT πN-SECTOR TO πN DATA → FIT NN CONTACTS TO NN PHASE SHIFTS → FIT NN CONTACTS TO NN DATA → FIT C_D,C_E TO A=3 DATA → **SIMULTANEOUS OPTIMIZATION**

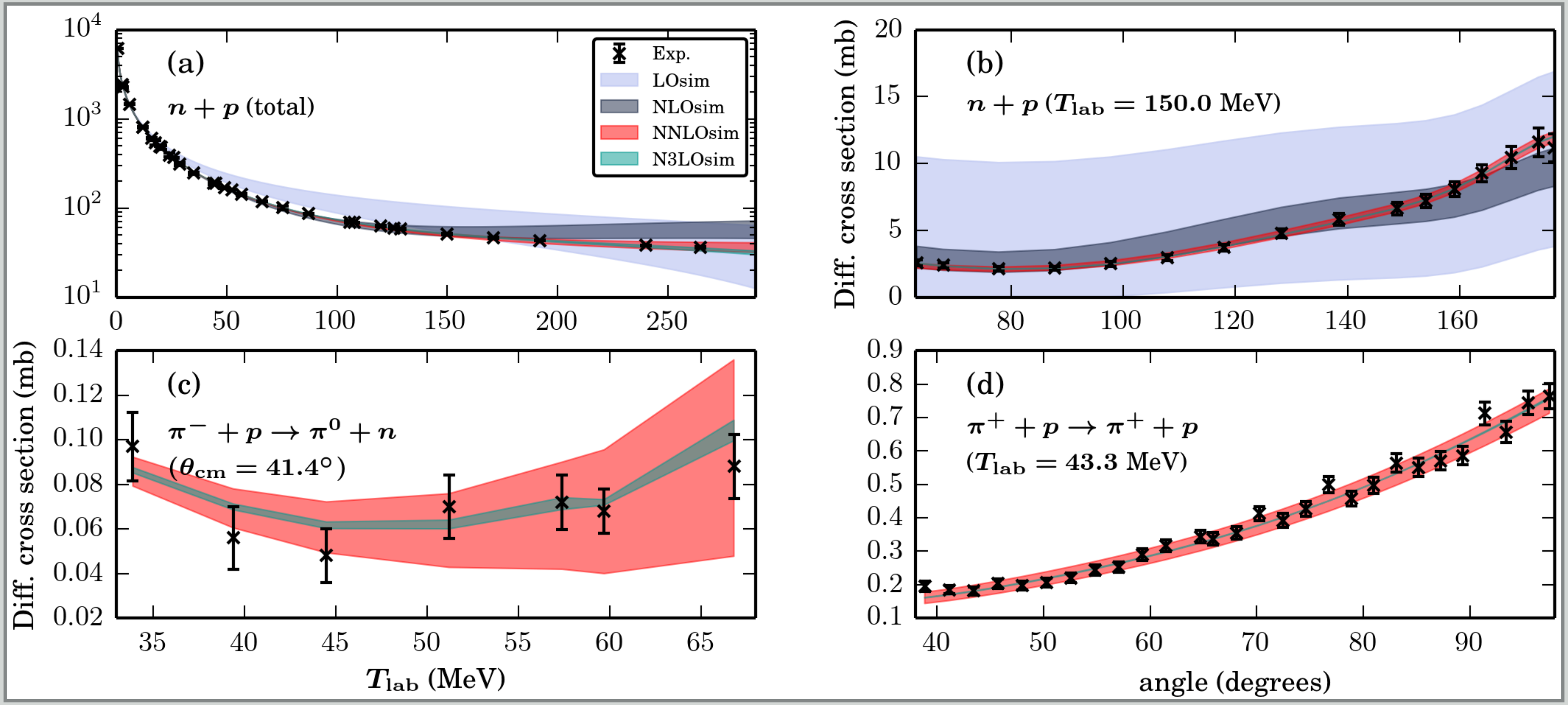


FIT πN-SECTOR TO πN DATA → FIT NN CONTACTS TO NN PHASE SHIFTS → FIT NN CONTACTS TO NN DATA → FIT C_D,C_E TO A=3 DATA → **SIMULTANEOUS OPTIMIZATION**



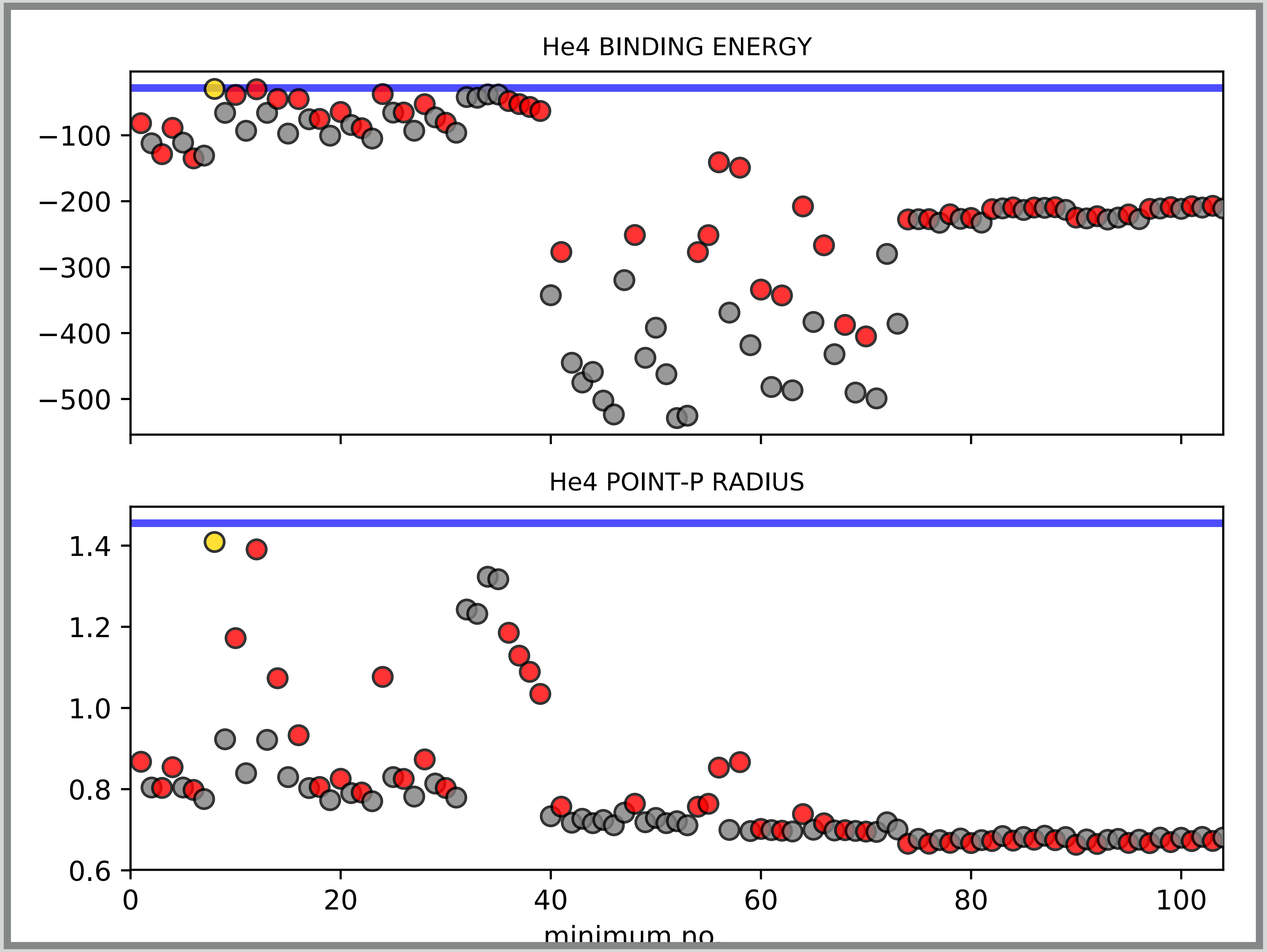
SCATTERING OBSERVABLES, ORDER-BY-ORDER (SIM)

FIT πN-SECTOR TO πN DATA → FIT NN CONTACTS TO NN PHASE SHIFTS → FIT NN CONTACTS TO NN DATA → FIT C_D, C_E TO A=3 DATA → **SIMULTANEOUS OPTIMIZATION**

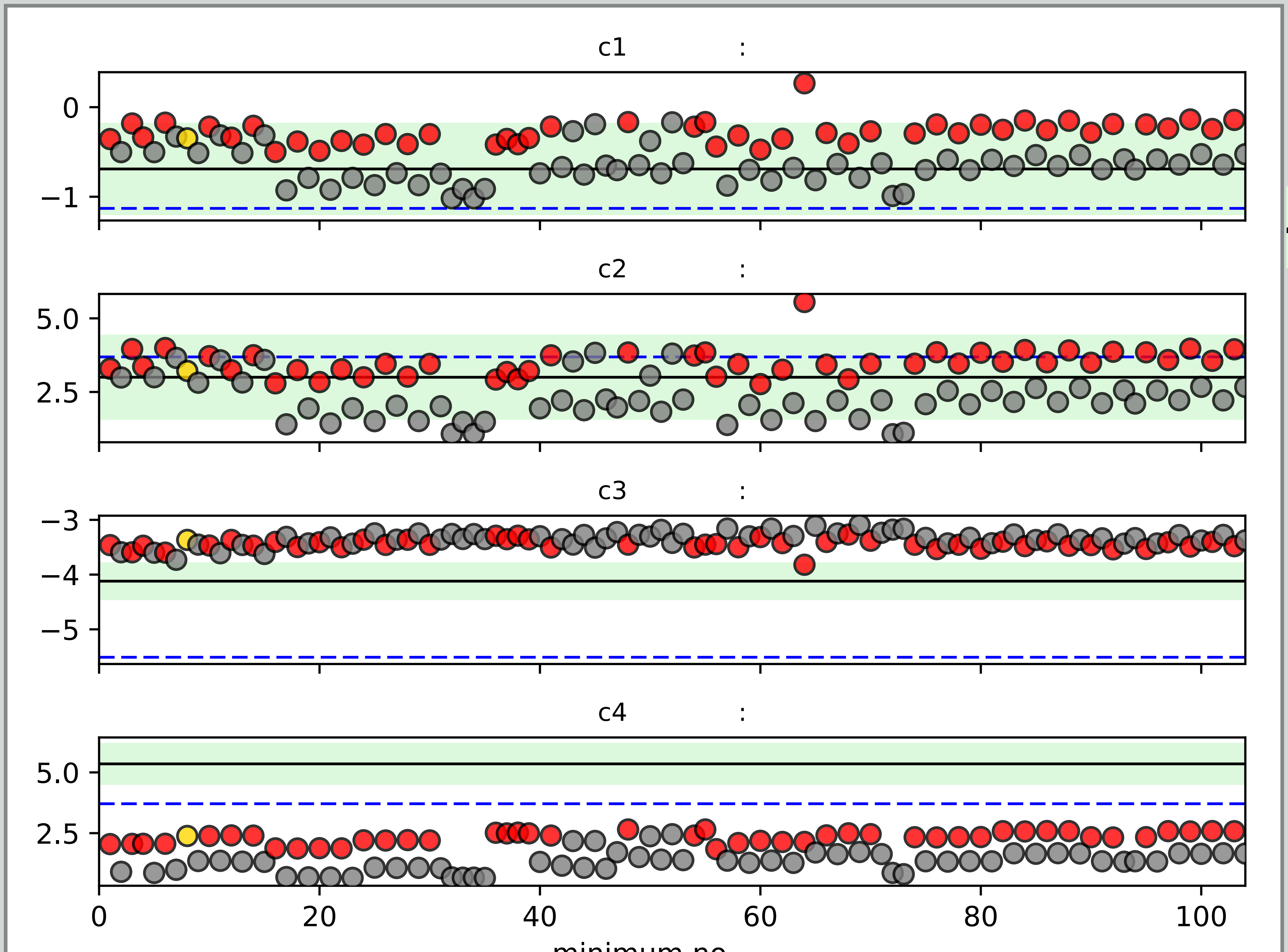


FIRST PREDICTIONS (A=4)

FIT πN-SECTOR TO πN DATA → FIT NN CONTACTS TO NN PHASE SHIFTS → FIT NN CONTACTS TO NN DATA → FIT C_D,C_E TO A=3 DATA → **SIMULTANEOUS OPTIMIZATION**



- FIT πN-SECTOR TO πN DATA
- FIT NN CONTACTS TO NN PHASE SHIFTS
- FIT NN CONTACTS TO NN DATA
- FIT C_D, C_E TO A=3 DATA
- **SIMULTANEOUS OPTIMIZATION**



stage 1:
πN only fit

Krebs et al
PRC85, 054006

ROY-STEINER ANALYSIS OF πN SCATTERING

FIT πN-SECTOR TO SUBTHRESHOLD PARAMETERS → FIT NN CONTACTS TO NN PHASE SHIFTS → FIT NN CONTACTS TO NN DATA → FIT C_D, C_E TO A=3 DATA → SIMULTANEOUS OPTIMIZATION

Preliminary

- Physical values of the momentum transfer in *NN* scattering is much closer to subthreshold kinematics in πN scattering than to the physical region.
- Hoferichter et al. recently matched subthreshold parameters of πN scattering from a solution of Roy-Steiner equations to χPT.
- We allow these results to determine the long-range dynamics of the nuclear force within our optimization framework [πN LECs and covariance matrix from PRL 115, 192301 (2015)].

ROY-STEINER ANALYSIS OF πN SCATTERING

FIT πN-SECTOR TO SUBTHRESHOLD PARAMETERS → FIT NN CONTACTS TO NN PHASE SHIFTS → FIT NN CONTACTS TO NN DATA → FIT C_D, C_E TO A=3 DATA → SIMULTANEOUS OPTIMIZATION

Preliminary

- We still find multiple minima in the *NN* optimization.
- Keeping only the most promising one we perform the simultaneous optimization of the final stage replacing the optimization w.r.t. πN data with

$$2f(\vec{p}_{\pi N} - \vec{p}_{RS})^T C_{RS}^{-1} (\vec{p}_{\pi N} - \vec{p}_{RS})$$

- We use f=1000 to stay close to the RS values for the ci:s.

Question: How to best combine experimental data with information from a theory analysis?

ROY-STEINER ANALYSIS OF πN SCATTERING

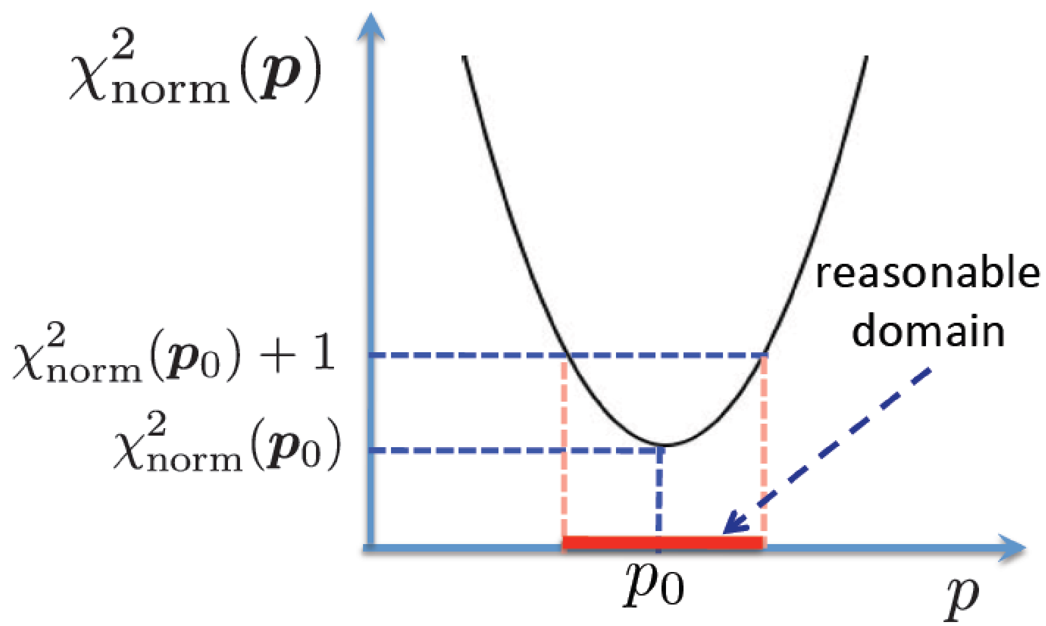
FIT πN-SECTOR TO SUBTHRESHOLD PARAMETERS → FIT NN CONTACTS TO NN PHASE SHIFTS → FIT NN CONTACTS TO NN DATA → FIT C_D, C_E TO A=3 DATA → SIMULTANEOUS OPTIMIZATION

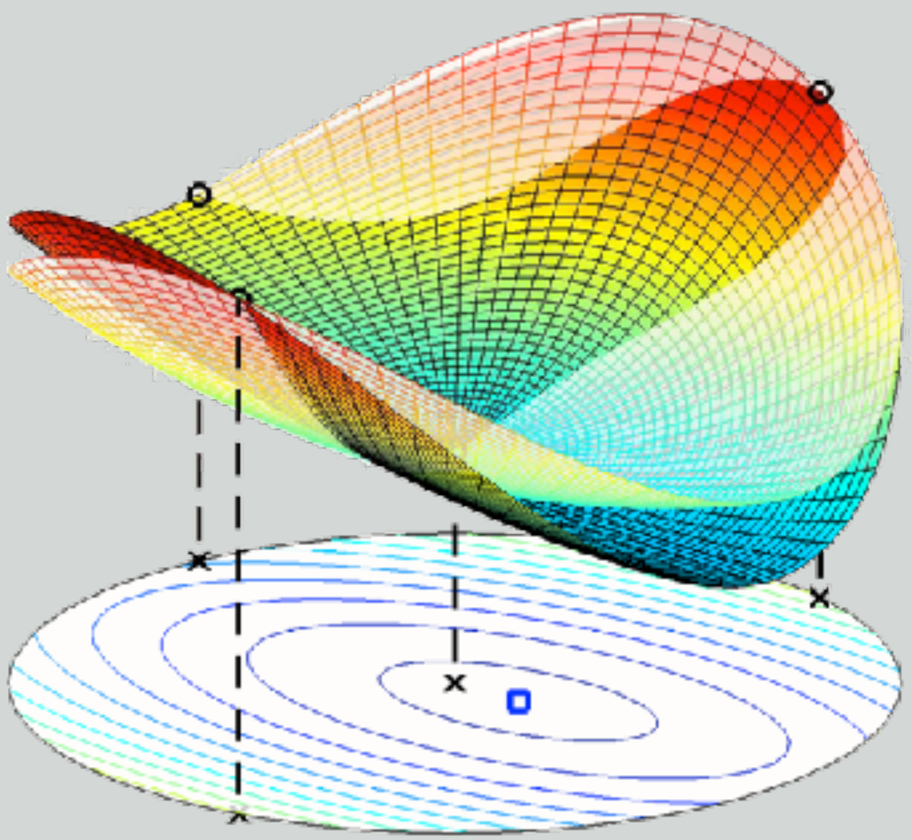
Preliminary

- A simultaneous optimization of this objective function leads to a good description on all *NN* and *NNN* data.
  - For instance *np* χ^2/datum = 3.5.
- The LECs remain in the Roy-Steiner region (to ~1σ)
- Predictions for 4He still disagree with experiments
  - E(4He) = -29.4 MeV
  - R(4He) = 1.38 fm

STATISTICAL ERROR ANALYSIS

- In a minimum there will be an **uncertainty in the optimal parameter values $\mathbf{p}_0$** given by the χ^2 surface.[1]





- Approximate the objective function with a quadratic form in the vicinity of the optimum. Compute the hessian matrix.

- Expand observables similarly, to second order

$$\mathcal{O}(\mathbf{p_0}+\Delta\mathbf{p})-\mathcal{O}(\mathbf{p_0})\approx\left(\Delta\mathbf{p}^T\right)\mathbf{J}_{\mathcal{O}}+\frac{1}{2}\left(\Delta\mathbf{p}^T\right)\mathbf{H}_{\mathcal{O}}\left(\Delta\mathbf{p}\right)$$

- The covariance between two observables is then

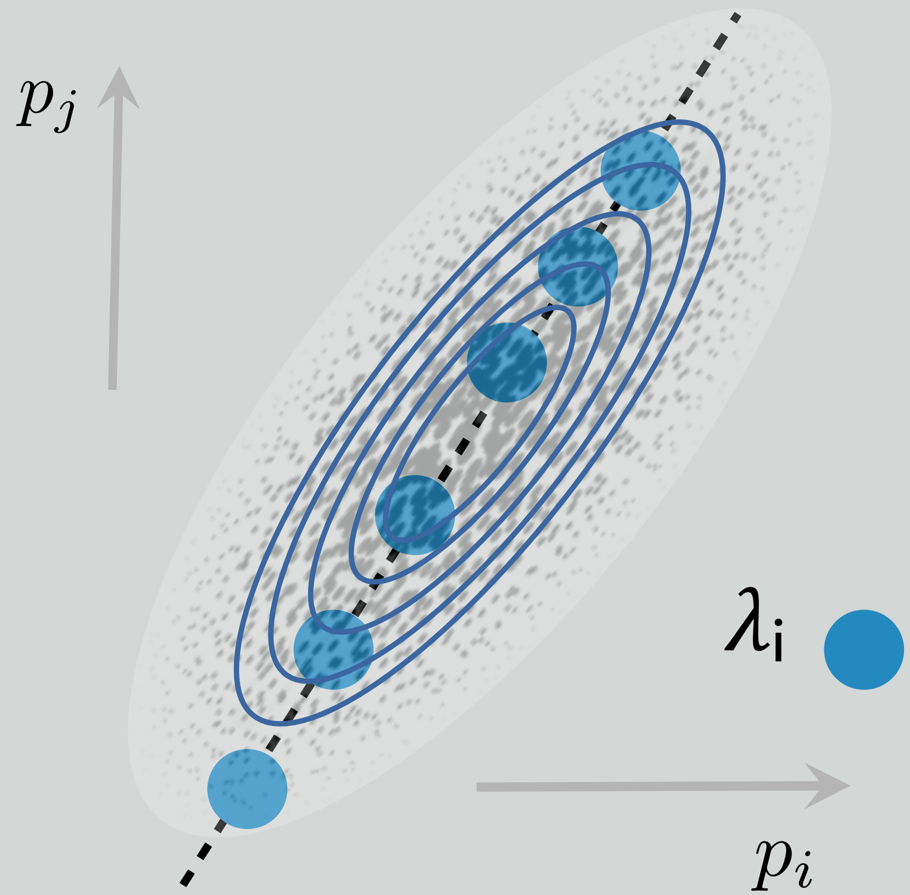
$$\mathrm{Cov}(\mathcal{O}_A,\mathcal{O}_B)\approx\mathbf{J}^T_{\mathcal{O}_A}\mathrm{Cov}(\mathbf{p_0})\mathbf{J}_{\mathcal{O}_B}+\text{second order}$$

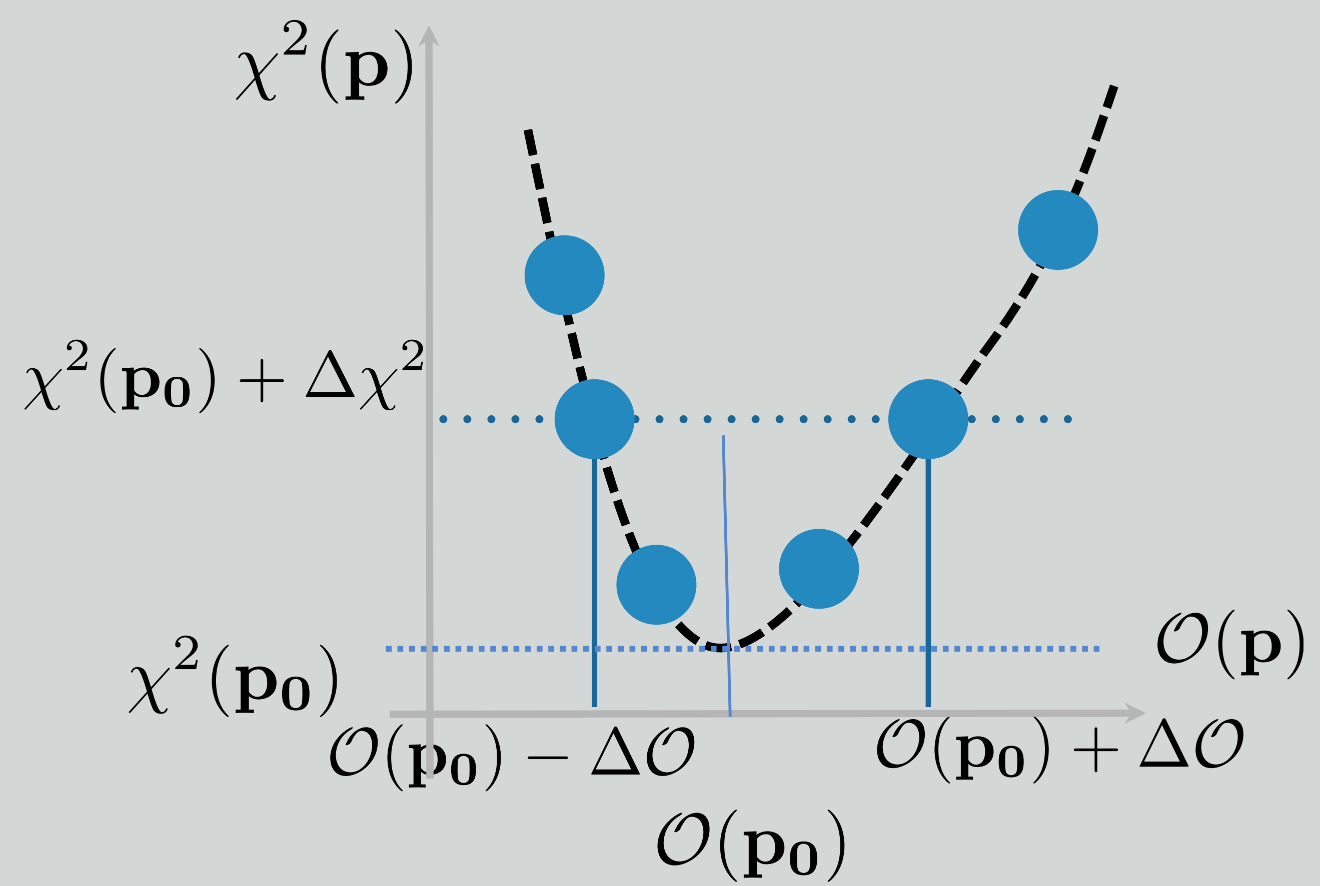
HESSIAN UNCERTAINTY QUANTIFICATION

	LOsim	NLOsim	NNLOsim	N3LOsim	Exp.
$E(^2\mathrm{H})$	-2.223	$-2.224^{(+1)}_{(-6)}$	$-2.224^{(+0)}_{(-1)}$	$-2.225^{(+1)}_{(-2)}$	-2.225
$E(^3\mathrm{H})$	-11.43	$-8.268^{(+26)}_{(-38)}$	$-8.482^{(+26)}_{(-30)}$	$-8.482(28)$	$-8.482(28)$
$E(^3\mathrm{He})$	-10.43	$-7.528^{(+20)}_{(-31)}$	$-7.717^{(+17)}_{(-21)}$	$-7.717(19)$	$-7.718(19)$
$E(^4\mathrm{He})$	$-40.38(1)$	$-27.44^{(+13)}_{(-15)}$	$-28.24^{(+9)}_{(-11)}$	$-29.75(18)$	$-28.30(11)$
$r_{\text{pt-p}}(^2\mathrm{H})$	$+1.912$	$+1.972^{(+0)}_{(-2)}$	$+1.966^{(+0)}_{(-1)}$	$+1.977(1)$	$+1.976(1)$
$r_{\text{pt-p}}(^3\mathrm{H})$	$+1.292$	$+1.614^{(+2)}_{(-3)}$	$+1.581(2)$	$+1.590(2)$	$+1.587(41)$
$r_{\text{pt-p}}(^3\mathrm{He})$	$+1.368$	$+1.791(3)$	$+1.761(2)$	$+1.760(2)$	$+1.766(13)$
$r_{\text{pt-p}}(^4\mathrm{He})$	$+1.080$	$+1.482(3)$	$+1.445(3)$	$+1.407(5)$	$+1.455(7)$
$E^1_A(^3\mathrm{H})$	–	–	$+0.6848(11)$	$+0.6848(11)$	$+0.6848(11)$
$D(^2\mathrm{H})$	$+7.807$	$+2.876^{(+85)}_{(-82)}$	$+3.381^{(+46)}_{(-45)}$	$+8.682^{(+96)}_{(-99)}$	–
$Q(^2\mathrm{H})$	$+0.3030$	$+0.2589^{(+17)}_{(-19)}$	$+0.2623(8)$	$+0.2897(7)$	$+0.270(11)$
a^{N}_{nn}	$-26.04(8)$	$-18.95^{(+38)}_{(-41)}$	$-19.28^{(+74)}_{(-80)}$	$-19.50^{(+79)}_{(-89)}$	$-18.95(40)$
a^{N}_{np}	$-25.58(8)$	$-23.60^{(+10)}_{(-13)}$	$-23.83(11)$	$-23.75^{(+3)}_{(-6)}$	-23.71
a^{C}_{pp}	$-7.579(6)$	$-7.799^{(+1)}_{(-3)}$	$-7.811(1)$	$-7.812^{(+2)}_{(-6)}$	$-7.820(3)$
r^{N}_{nn}	$+1.697(1)$	$+2.752^{(+7)}_{(-8)}$	$+2.793(14)$	$+2.785(15)$	$+2.75(11)$
r^{N}_{np}	$+1.700(1)$	$+2.648(3)$	$+2.686(2)$	$+2.683(2)$	$+2.750(62)$
r^{C}_{pp}	$+1.812(1)$	$+2.704(3)$	$+2.758(2)$	$+2.755(2)$	$+2.790(14)$

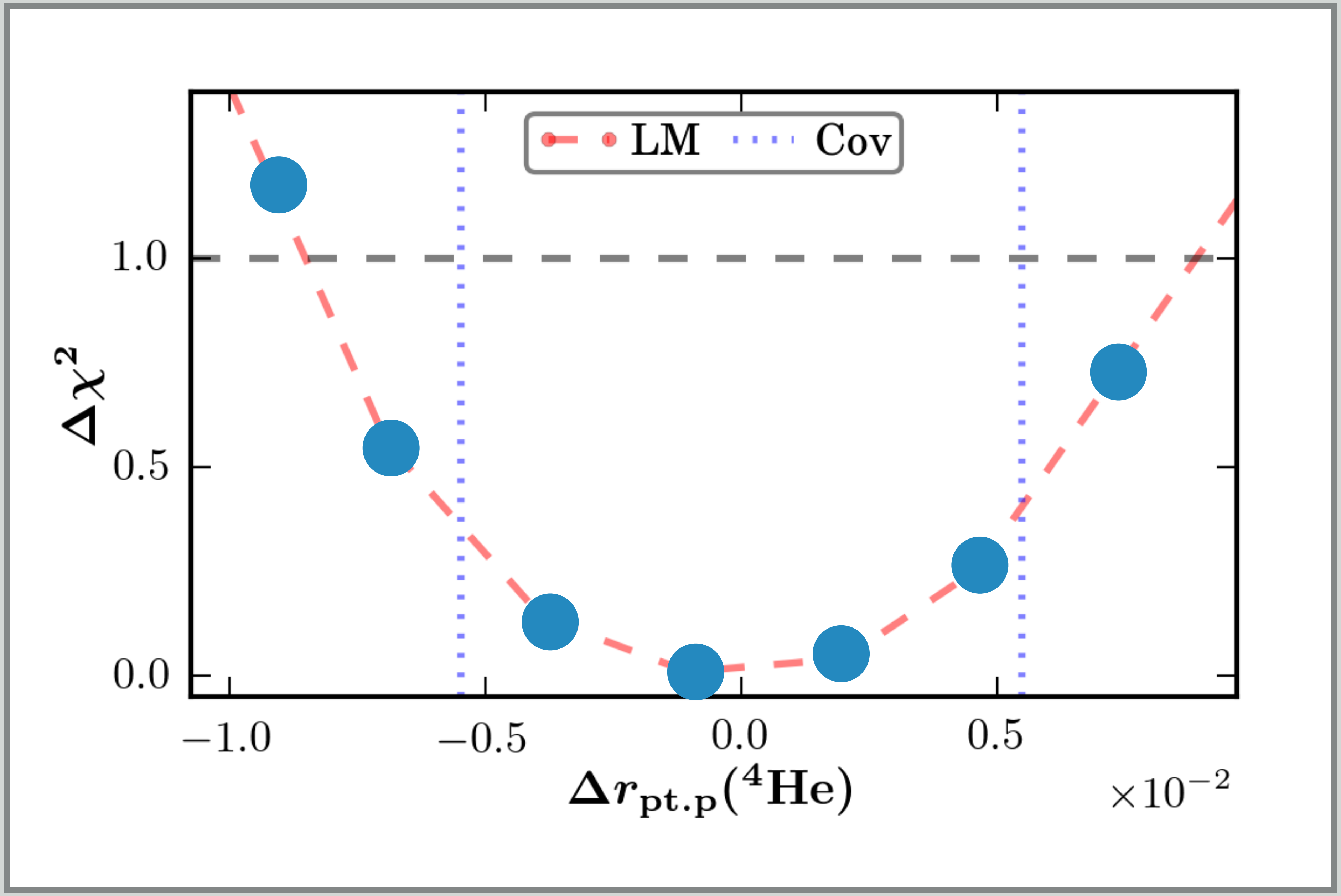
LAGRANGE MULTIPLIER

- The hessian UQ relies on a quadratic shape of the χ^2-surface.
- The local minima of our χ^2-surface are often very flat in some directions. Curvature is dominated by fourth-order terms.
- A possible solution: Lagrange multiplier optimization:
  - Minimize $$F(\mathbf{p}, \lambda) = \chi^2(\mathbf{p}) + \lambda \cdot \mathcal{O}(\mathbf{p})$$





COMPARISON: HESSIAN UQ VS LAGRANGE-MULTIPLIER UQ

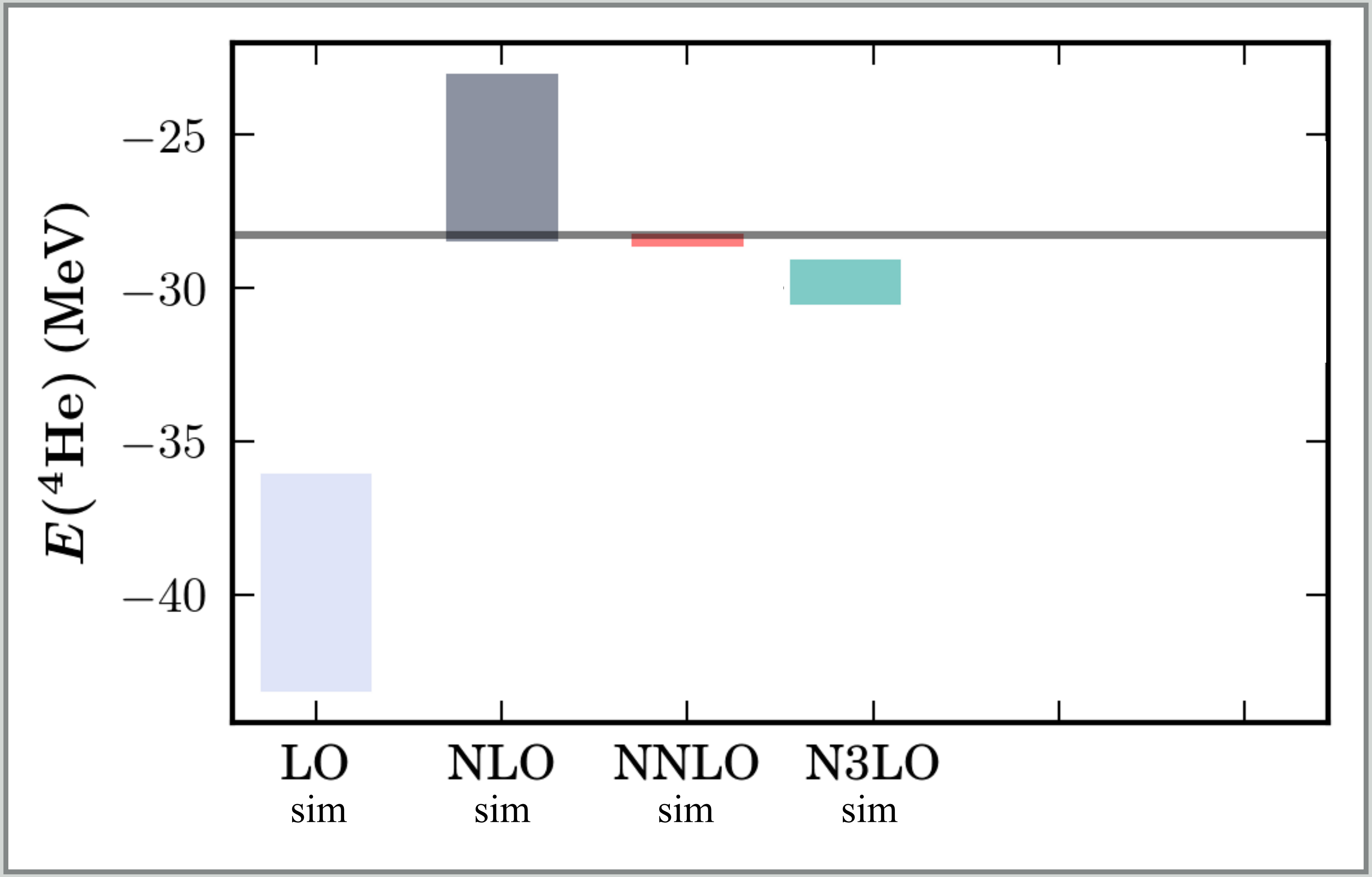


see also B. Carlsson et al., Phys. Rev. C 95 (2017) 034002

EXPLORING FURTHER SYSTEMATIC UNCERTAINTIES

- So far, all results have been obtained with a non-local regulator with cutoff Λ=500 MeV.
  - A subset of systematic uncertainties can be probed by varying Λ.
- Reoptimizing with different Λ (450-575 MeV) will give us a **family** of models.
- **All of them will reproduce the same few-body physics.**

SYSTEMATIC UNCERTAINTIES



CONCLUSION

SUMMARY (MAINLY FOR PHYSICISTS)

- There are roughly 100 local minima when the non-local N3LO *NN*+*NNN* interaction is optimized w.r.t. A=2,3 data.
  - Typically, the *NN* and πN chi2/datum is 2 across the board.
  - The best few (2-4) candidate(s) predict the E(4He) within 2 MeV, however the radii are too small.
- In few-nucleon calculations, the non-local 3N-interaction is not a small perturbation, compared to N2LO,
- πN coupling constants are of expected size.
  - However, they are very poorly constrained from πN data alone.
  - When fitted simultaneously, c3 c4 deviate significantly from the values obtained when fitted w.r.t. πN scattering data.
- Lagrangian multiplier optimization and UQ for non-quadratic cases. No need for derivatives.

OUTLOOK

- The inclusion of more data in the objective function requires other approaches to the optimization problem needed. (See also Andreas' presentation.)
- The frequentist approach does not offer an easy and transparent method for handling systematic uncertainties or imposing prior knowledge.
- Bayesian parameter estimation is advantageous, but costly.
  - avoiding the need to 'judge', a priori, what data can be included in order to safely avoid overfitting.
  - not obvious whether local minima will vanish.
  - offers a viable approach to include prior knowledge of certain parameters from Roy-Steiner analysis.
- Investigate other chiral EFT power-counting schemes. (See also Andreas' presentation.)