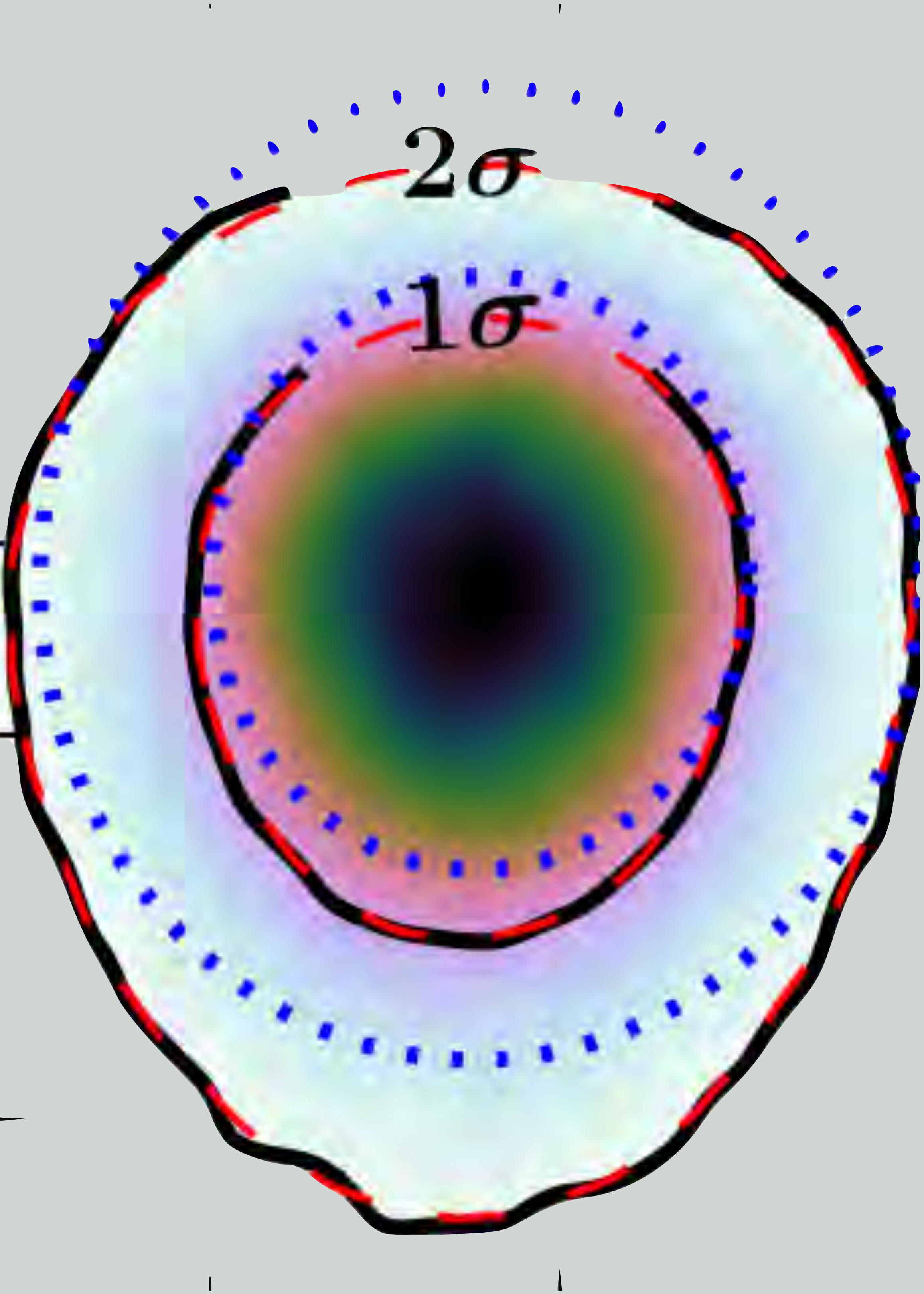

PRAGMATIC VS RIGOROUS VIEW ON CHIRAL EFT(–BASED) INTER-NUCLEON INTERACTIONS

CHRISTIAN FORSSÉN

Department of Physics, Chalmers, Sweden

ESNT workshop, CEA Saclay, France, Jan. 16-20, 2017

MANY THANKS TO MY COLLABORATORS

❖ **Boris Carlsson**, **Andreas Ekström**, Dag Strömberg, Oskar Lilja, Mattias Lindby, Björn Mattsson (Chalmers)

❖ Kai Hebeler (TU Darmstadt), Kyle Wendt (ORNL, LLNL)

and

❖ Gaute Hagen, Gustav Jansen, Thomas Papenbrock (ORNL/UT), Morten Hjorth Jensen (UiO, MSU), Petr Navrátil (TRIUMF), Witek Nazarewicz (ORNL, MSU)

STINT
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erc

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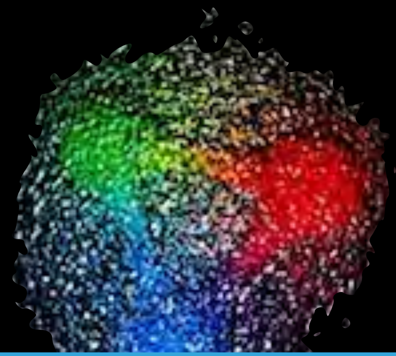
MODERN NUCLEAR PHYSICS

INTRODUCTION

PROFOUND INTERSECTIONS

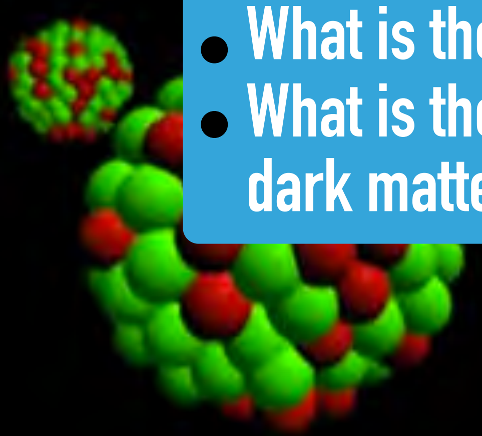
- Can we solve QCD to describe hadronic structures and interactions?
- Can we employ the separation of scales to build successful effective field theories?
- What is the new standard model of particle physics?

subfemto…



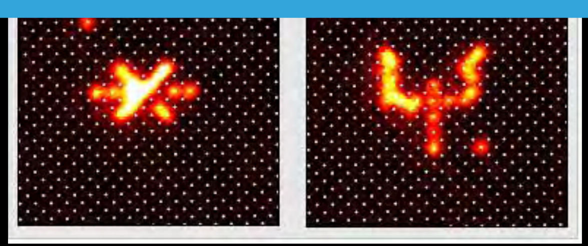
- What controls nuclear saturation?
- What are the properties of nuclei with extreme neutron/proton ratios?
- Can we predict useful cross sections that cannot be measured?
- Can nuclei provide precision tests of fundamental symmetries?

femtophysics



- How do nuclei shape the physical universe?
- What is the origin of the elements?
- What is the interaction between baryonic and dark matter?

ARTICLES



PHYSICS OF NUCLEI

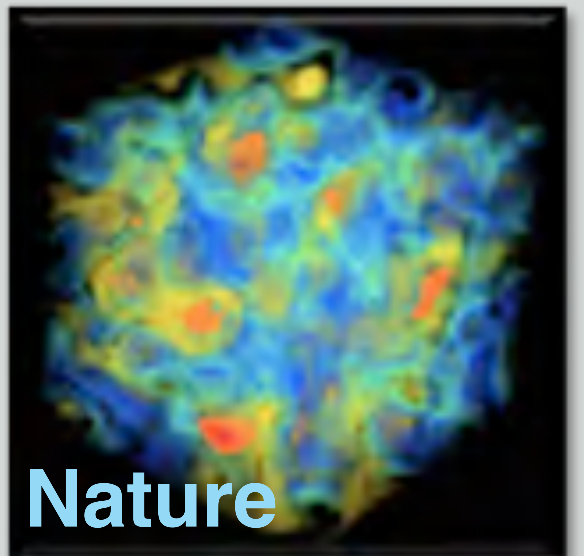
QUANTUM MANY-BODY PHYSICS

giga…

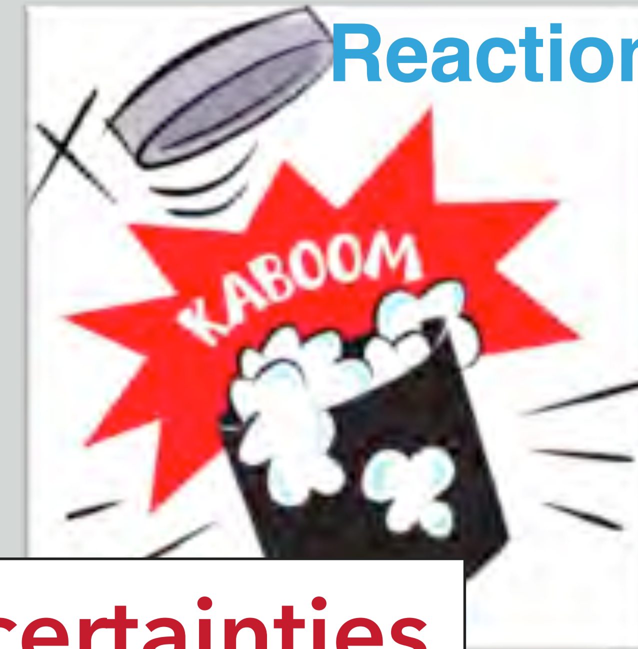
- How do collective phenomena emerge from simple constituents?
- How can complex systems display astonishing simplicities?
- What are unique properties of open quantum systems?

HYSICS AND COSMOLOGY

THE SCIENTIFIC METHOD



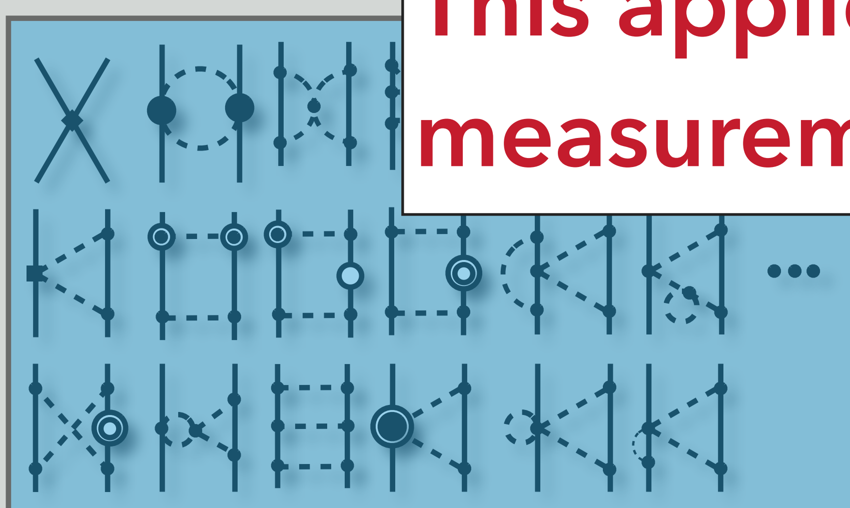
Manifests itself in



e accessible to

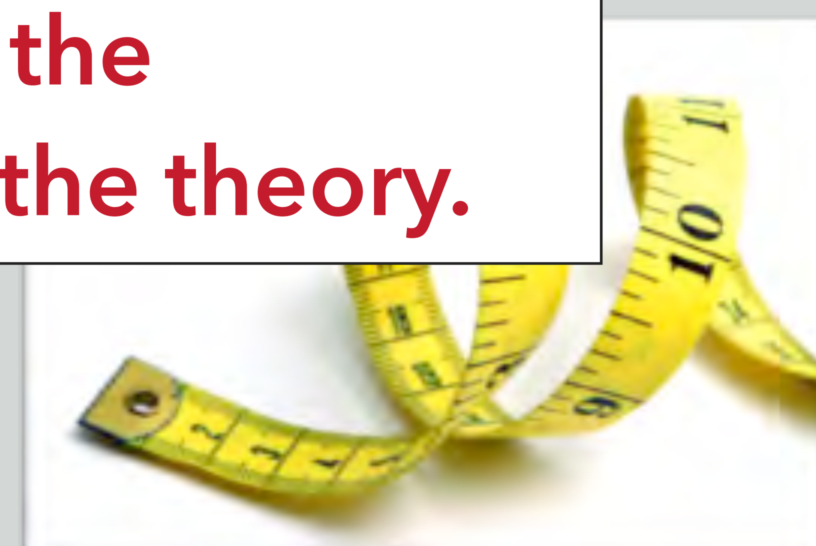
h

The quantification of uncertainties is absolutely critical for progress. This applies BOTH to the measurement and to the theory.

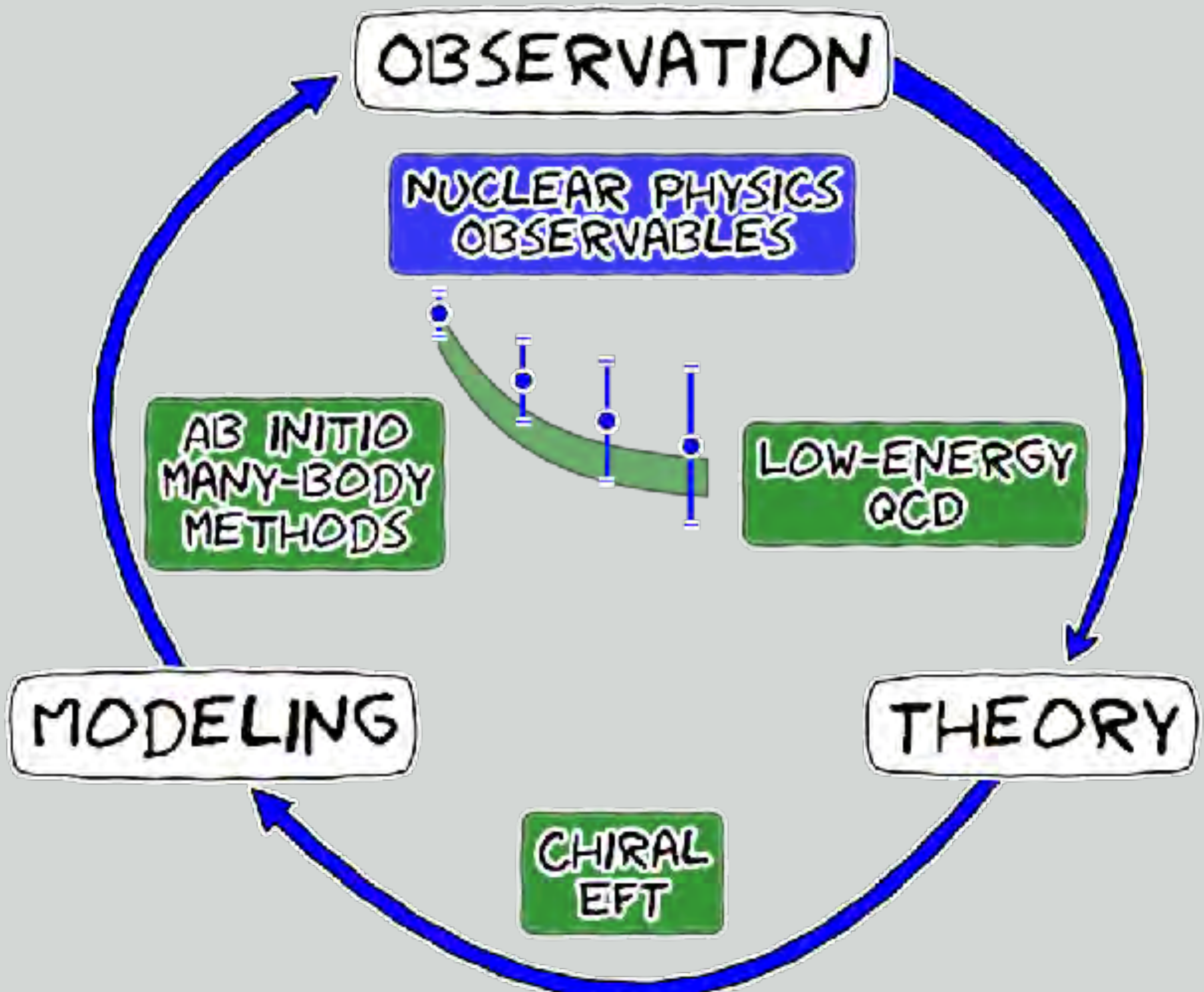


Theories

inspire



THE SCIENTIFIC METHOD: NUCLEAR PHYSICS



An EFT approach offers many nice features;
No free lunch: there are a number of parameters;
How do we determine those? Does this EFT deliver?

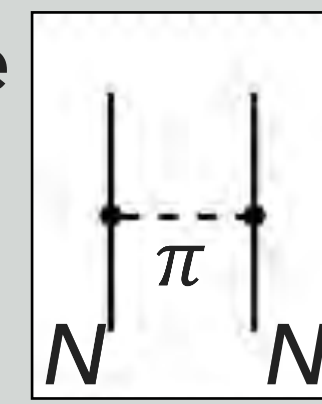
CHIRAL EFT BASED NUCLEON-NUCLEON INTERACTIONS

"BLACK BOX" =
CHIRAL EFT FOR THE
MANY-NUCLEON SECTOR

See work by: Weinberg, van Kolck, Epelbaum, Meissner, Krebs, Entem, Machleidt…

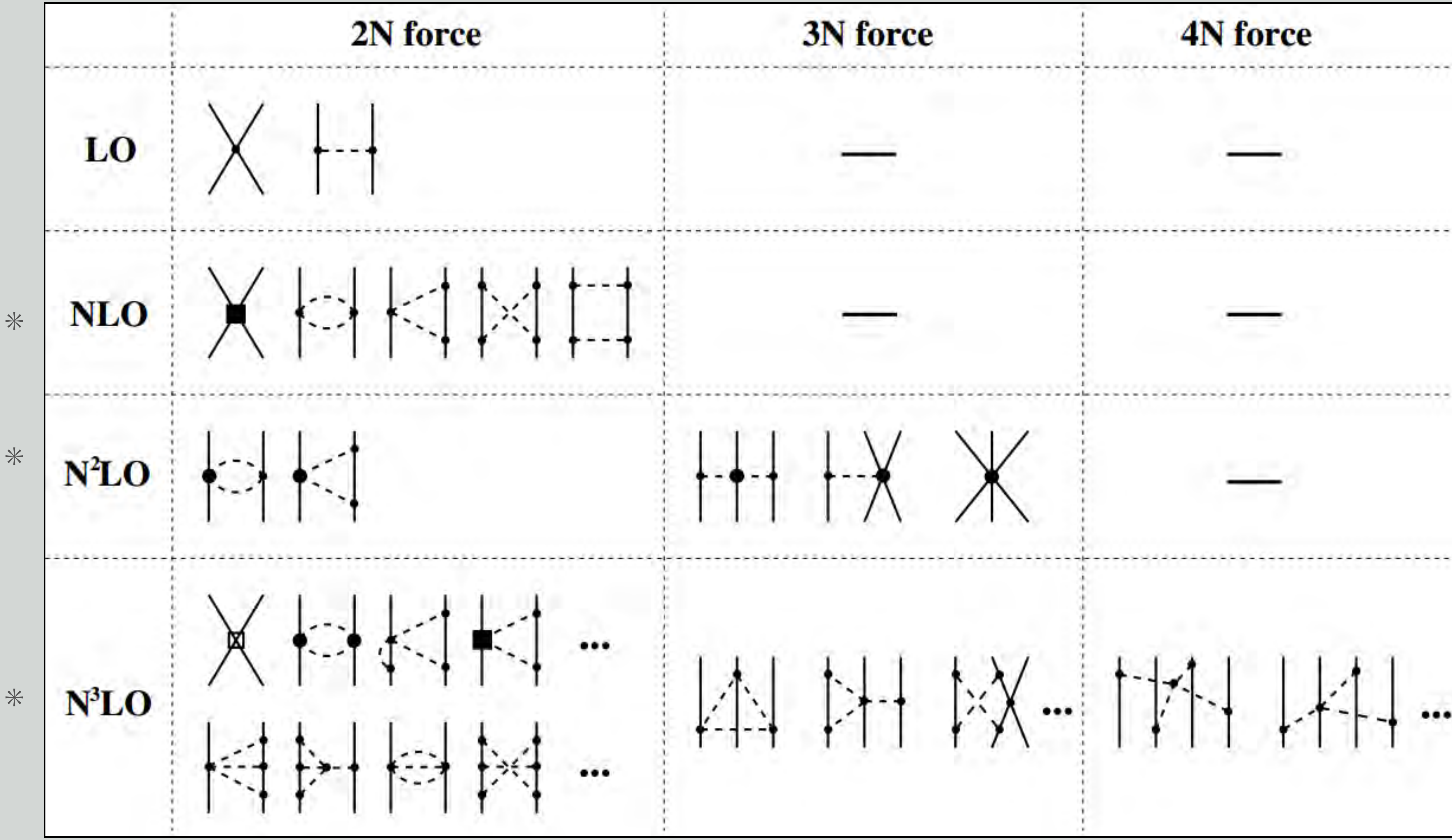
… however, with different instructions

- Separation of scales in nuclear physics.
- Pions (π) and nucleons (N) as relevant degrees of freedom.
- One-pion exchange = long-range physics



- Contact interactions capture physics at very short distances

CHIRAL EFT BASED NUCLEON-NUCLEON INTERACTIONS



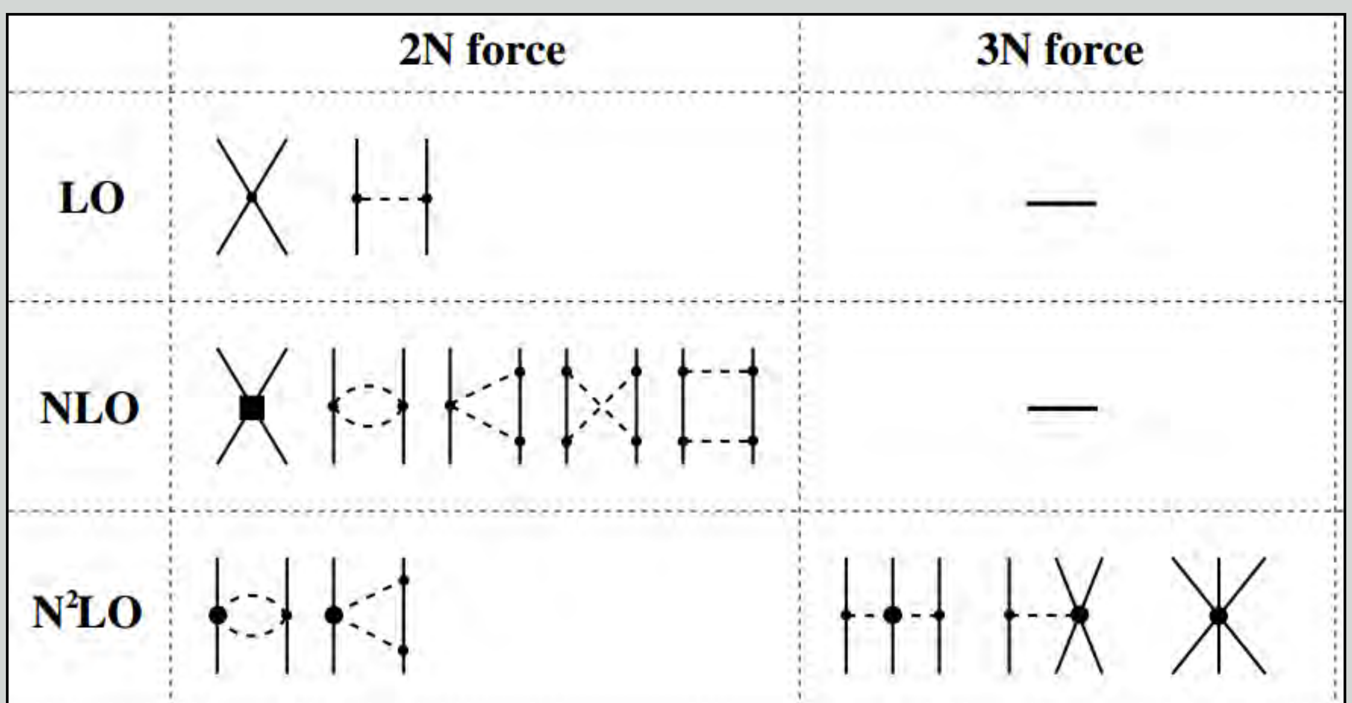
Chiral EFT

- E. Epelbaum, H. Hammer, U. Meissner Rev. Mod. Phys. **81** (2009) 1773
- R. Machleidt, D. Entem, Phys. Rep. **503** (2011) 1

* For non-germans: add an extra 'N'

EXPECTATIONS

- Should simultaneously give a good description of πN, NN, and many-nucleon observables.
- LECs should be fitted to low-energy data (uncertainties will propagate)
- Fits and predictions should improve with increasing order in the expansion.
- We should be able to estimate the systematic model error.



higher-order corrections:

$$+\mathcal{O}(q/\Lambda)$$

$$+\mathcal{O}((q/\Lambda)^3)$$

$$+\mathcal{O}((q/\Lambda)^4)$$

THE NUCLEAR MANY-BODY PROBLEM

"BLACK BOX" =
SOLVING THE MANY-NUCLEON PROBLEM

- Strongly-interacting $\Longrightarrow$ Strongly correlated
- Fermionic $\Longrightarrow$ Exchange (a)symmetry
- Quantum mechanical many-body $\Longrightarrow$ Many-dimensional coupled differential equations
- The solution of this many-body problem used to be the bottleneck

AB INITIO METHODS

- Consider an A-body system described by a well- defined microscopic Hamiltonian (A = # of particles)
- Ab initio methods solve the relevant QM many-body equations without uncontrolled approximations
- Controlled approximations are allowed as they can be systematically improved.
- Converged results are considered precise ab initio results.
- Ab initio methods: No-Core Shell Model, Coupled clusters, Green's function Monte Carlo, In-Medium SRG, Lattice EFT

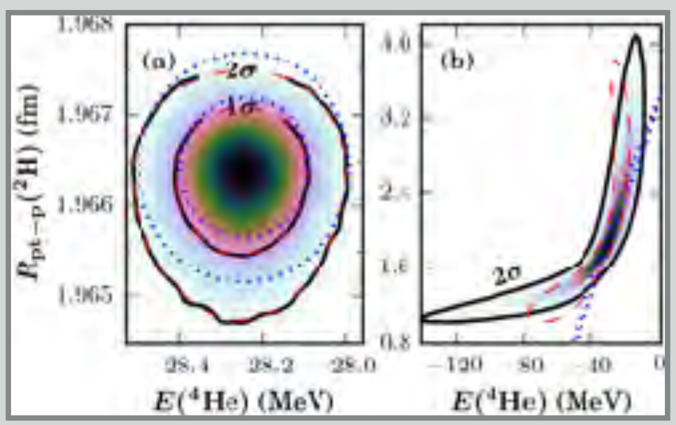
“PRAGMATIC” VS “RIGOROUS” VIEW

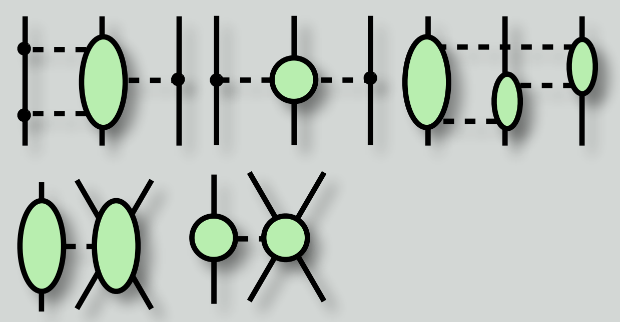
FROM EFT-BASED NUCLEAR INTERACTIONS TO EMERGENT PHENOMENA

Overview of our research efforts

We aim to develop the technology and ability to:

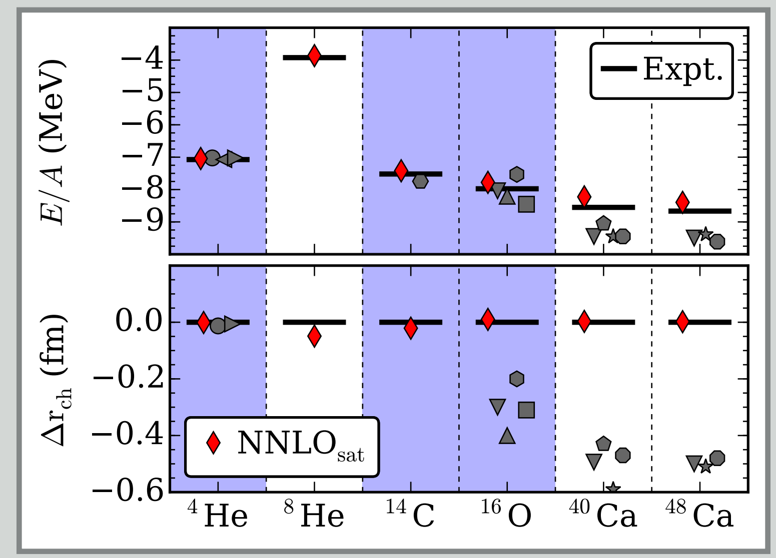
Diversify and extend the **statistical analysis** of chiral-EFT based nuclear interactions in a **data-driven** approach.





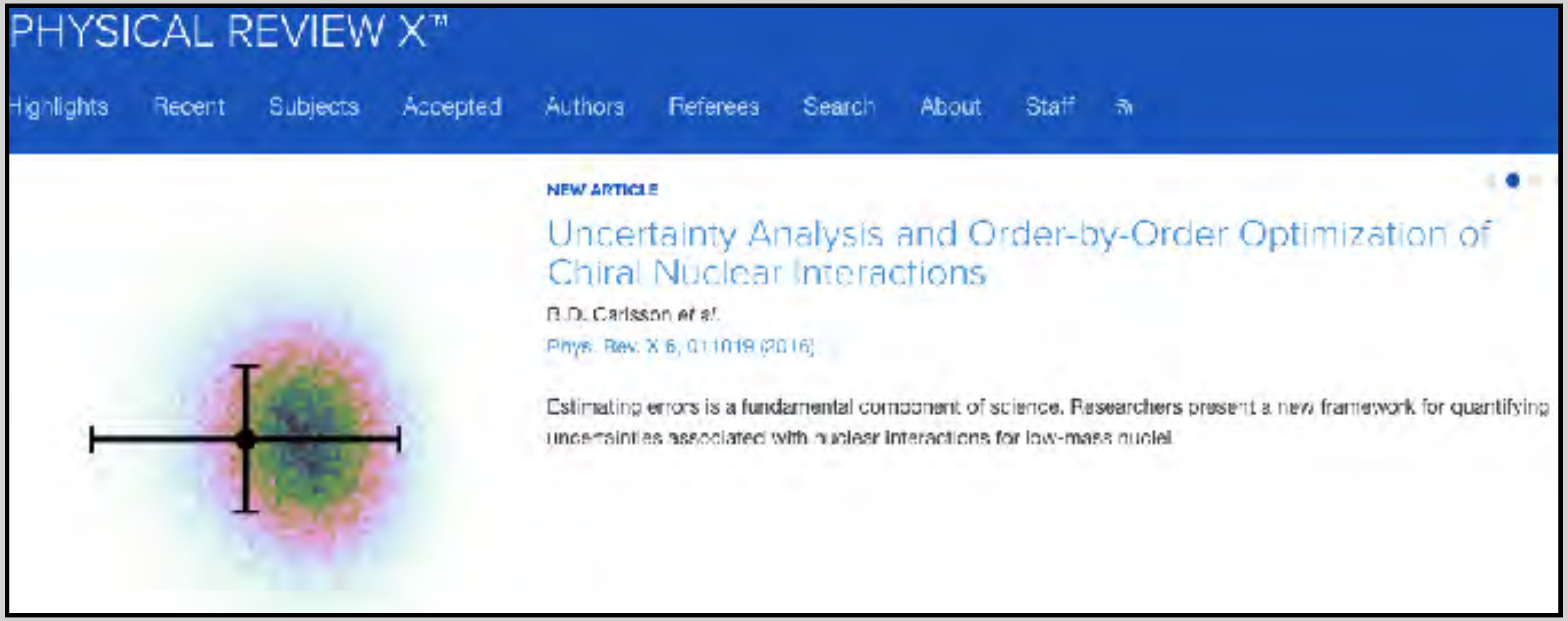
- **Does nuclear-physics phenomena emerge in a “from few to many” ab initio approach?**
- **Is available few-body data sufficient to constrain this model? Does the model become fine-tuned?**

Explore **alternative strategies of informing** the model about low-energy many-body observables.



- **Can/should emergent phenomena be used to constrain the model?**
- **How to quantify model uncertainties in such an approach?**

Based on: B.D. Carlsson, A. Ekström, C. Forssén et al, Phys. Rev. X **6** (2016) 011019
B. D. Carlsson et al., In preparation



THEORETICAL UNCERTAINTY QUANTIFICATION

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

OPTIMIZATION STRATEGY

Low-energy constants (LECs) are the parameters of the EFT.
In practice they need to be fitted to experimental data.

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

Historic approach:

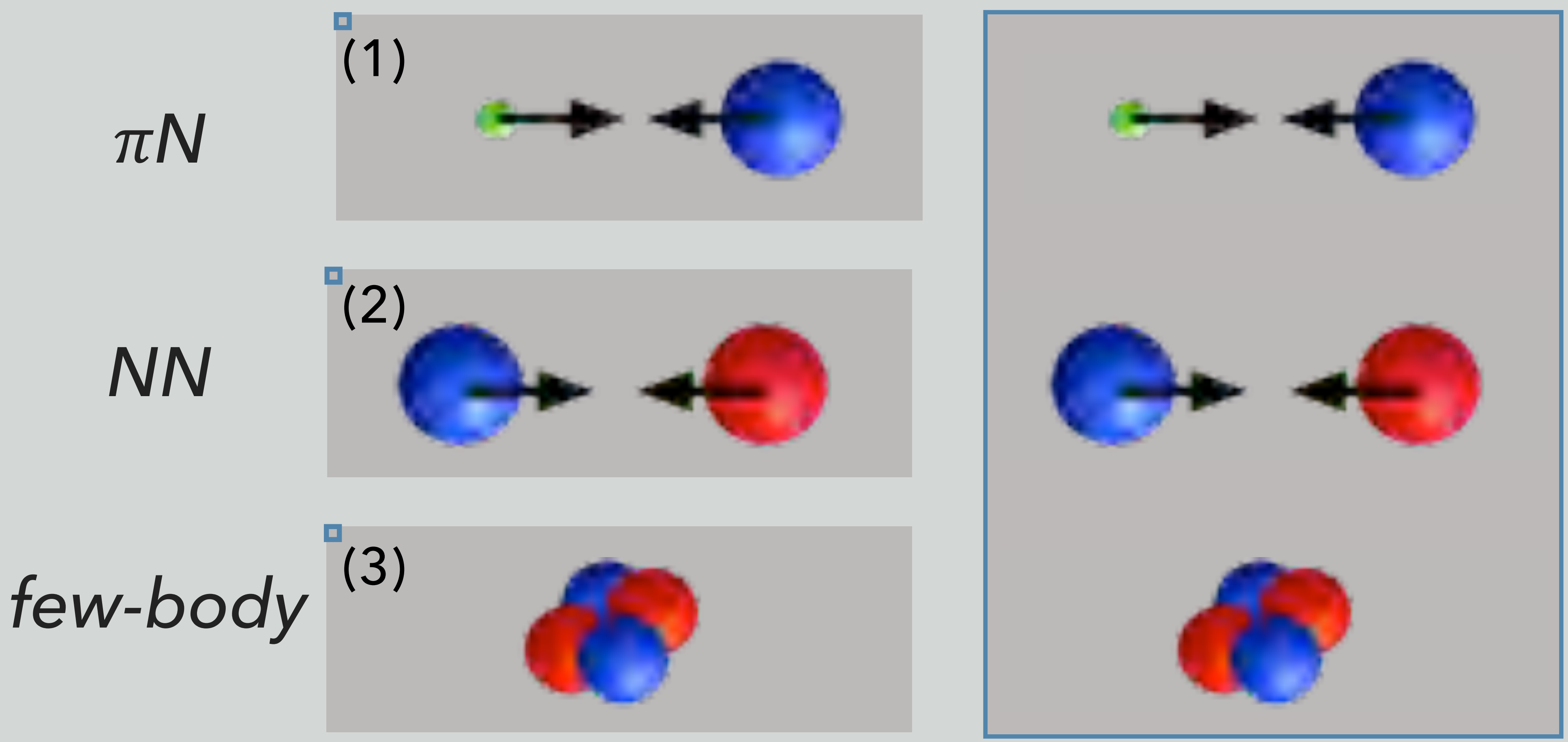
1. **πN LECs determined first;** either from Pion-Nucleon scattering phase shifts or from NN phase shifts in peripheral waves
2. **(NN-only) objective function based on Nijmegen phase shift analysis**
   - Chi-by-eye optimization; "it's an art" (Machleidt)
   - N^3LO needed for high-accuracy fit up to T_{lab}=290 MeV
3. **NNN LECs determined at the end** given the NN part. Usually at NNLO. First results at N^3LO are coming.

OPTIMIZATION STRATEGY

Low-energy constants (LECs) are the parameters of the EFT.
In practice they need to be fitted to experimental data.

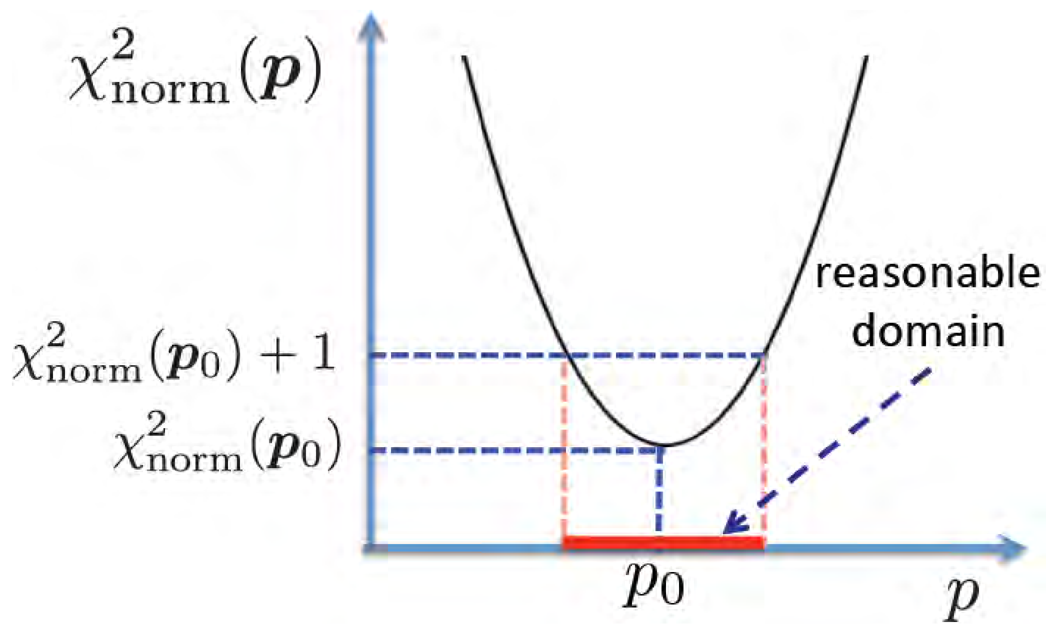
$$\chi^2(\vec{p}) \equiv \sum_i \left(\frac{O_i^{\rm theo}(\vec{p}) - O_i^{\rm expr}}{\sigma_{{\rm tot},i}} \right)^2 \equiv \sum_i r_i^2(\vec{p})$$

Sequential (historic) approach: **Simultaneous** approach:



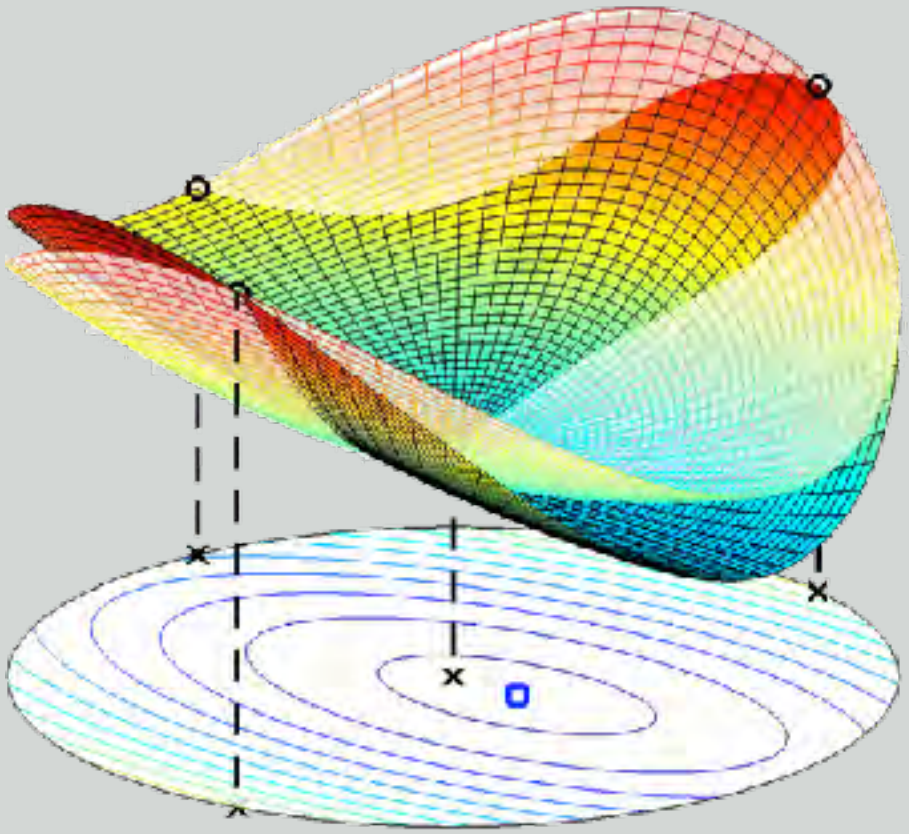
Statistical error analysis

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



- From the hessian at $\mathbf{p}_0$ we can calculate a **covariance matrix** and from that a **correlation matrix**.

[1] J Dobaczewski et al 2014 J. Phys. G: Nucl. Part. Phys. 41 074001



HESSIAN

$$H_{ij} = \frac{1}{2}\left.\frac{\partial^2\chi^2}{\partial x_i \partial x_j}\right|_{\mathbf{x}=\mathbf{x}_\mu}$$

COVARIANCE MATRIX

$$\boldsymbol{\Sigma} = \frac{\chi^2}{N_{df}}\mathbf{H}^{-1}$$

CORRELATION MATRIX

$$R_{ij} = \frac{\Sigma_{ij}}{\sqrt{\Sigma_{ii}\Sigma_{jj}}}$$

Input and technology

πN scattering
- WI08 database
- T_{lab} between 10-70 MeV
- N_{data} = 1347
- χEFT(Q^4) to avoid underfitting

NN scattering
- SM99 database (+Granada)
- T_{lab} between 0-290 MeV
- N_{data} = 2400(np) + 2045(pp)
- χEFT(Q^0,Q^2,Q^3,Q^4)

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

A=3 bound states
- ^3H,^3He (binding energy, radius, ^3H half life)

On 1 node in ~10 sec

+ derivatives! (×2-20 cost)

Total error budget

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

- The total error budget is

E.g. , NCSM　　Neglected

$$\sigma_{\rm tot}^2 = \sigma_{\rm exp}^2 + \sigma_{\rm method}^2 + \sigma_{\rm numerical}^2 + \sigma_{\rm model}^2$$

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

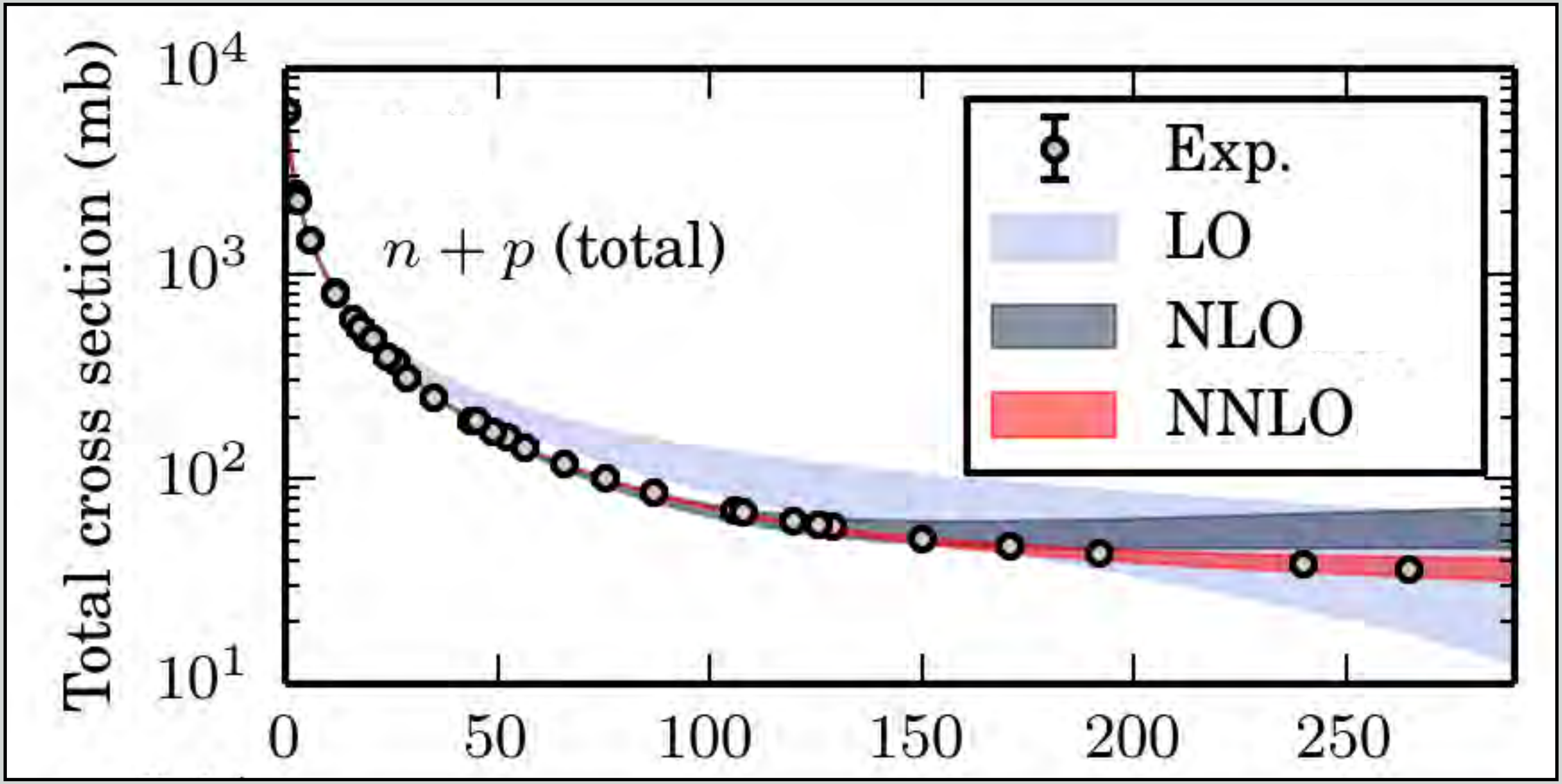
$$\mathcal{O}\left((Q/\Lambda_\chi)^{\nu+1}\right)$$

- Still needs to be converted to actual numbers $\sigma_{\rm model}$
- We translate this EFT knowledge into an error in the scattering amplitudes

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

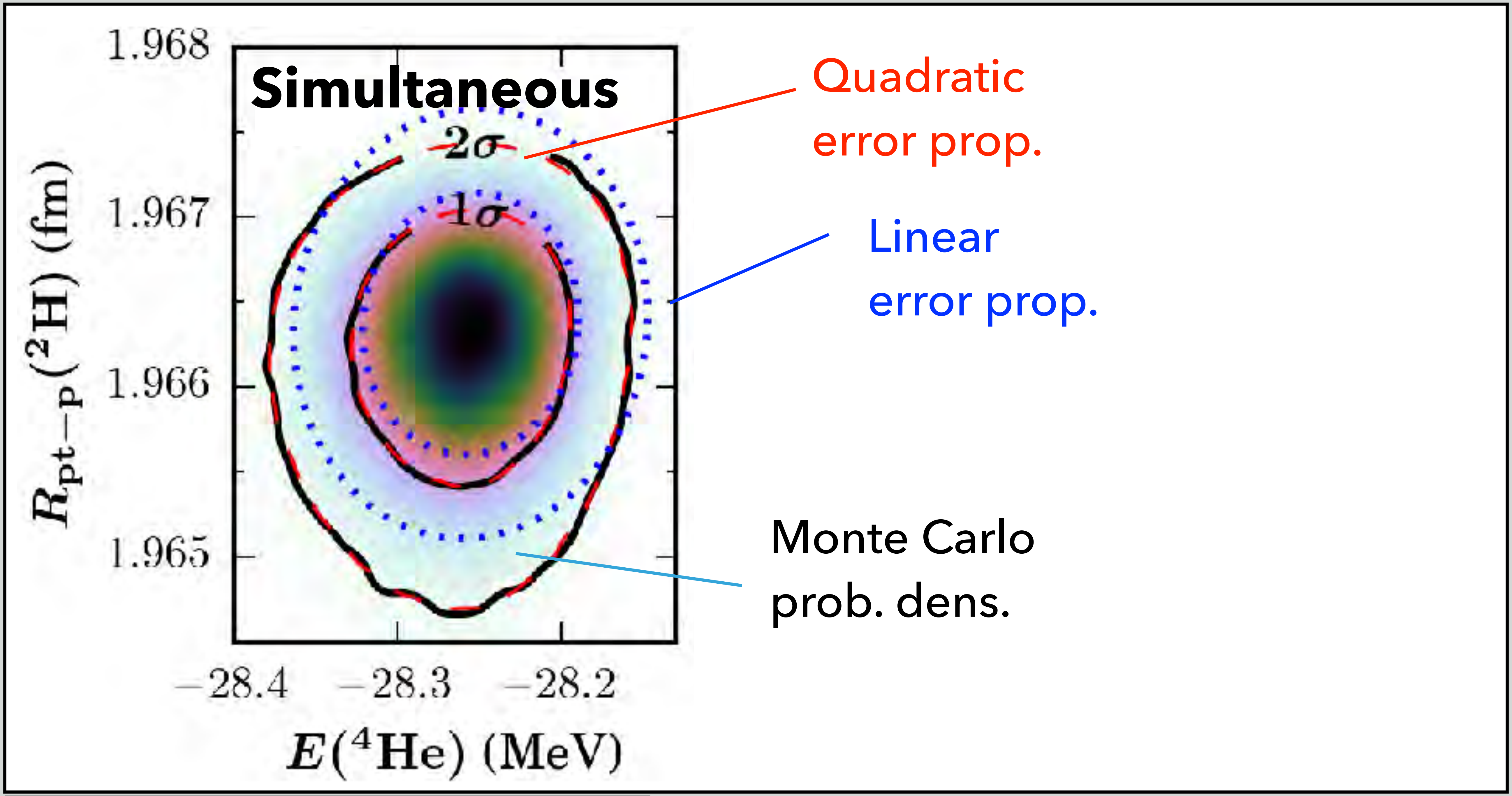
- which is then propagated to an error in the observable.

TOTAL NP CROSS SECTION



Quadratic error propagation vs Brute force sampling

$$O(\mathbf{p}) \approx O(\mathbf{p}_0) + J_O \Delta\mathbf{p} + \frac{1}{2}\Delta\mathbf{p}^T H_O \Delta\mathbf{p}$$

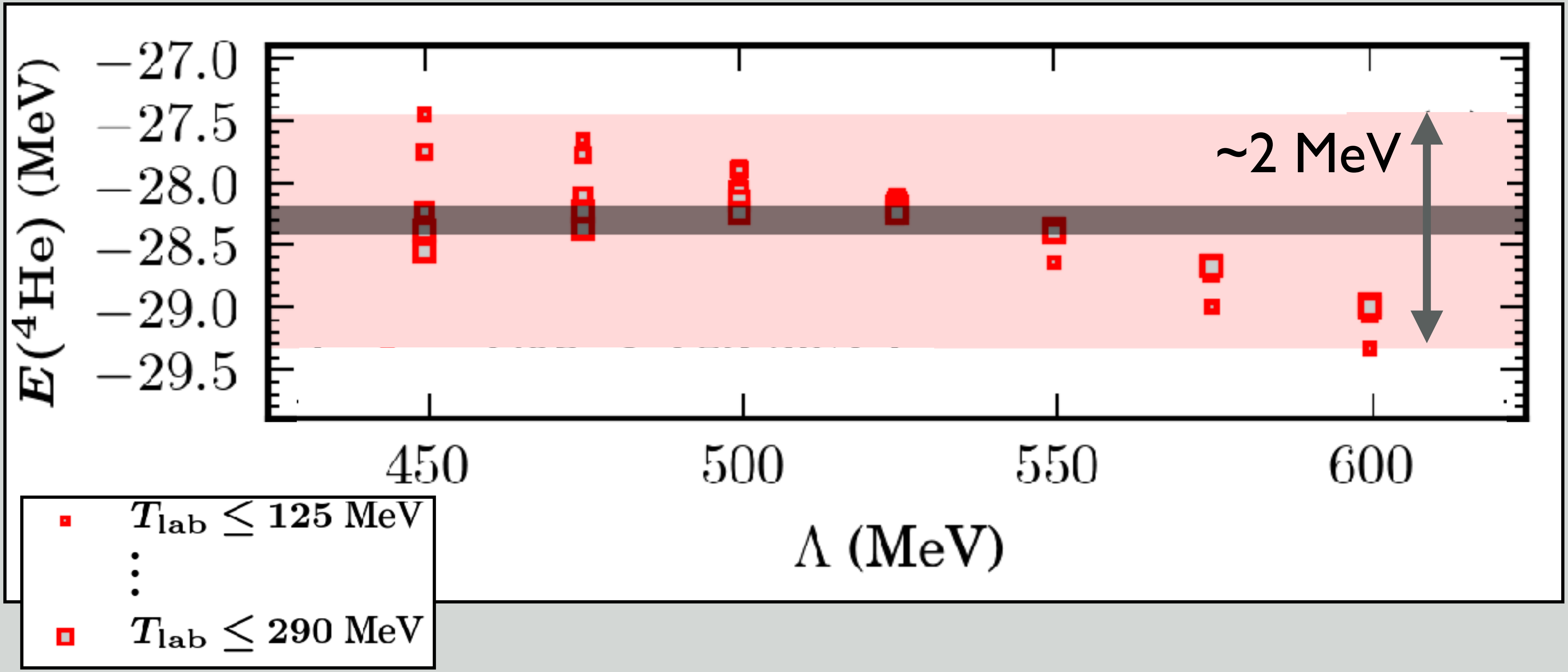


$E(^4He) = -28.24^{+9}_{-11}$ (MeV) Statistical uncertainty

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.
- The bulk of input data comes from *NN* scattering. We have truncated the data base at T_{lab}=290 MeV
  - Always with model error that gives more weight to low E.
  - A subset of systematic uncertainties can be probed by varying the truncation max(T_{lab})
- Reoptimizing with different Λ and T_{lab} and will give us a **family** of models.
- **All of them will reproduce the same few-body physics.**

Systematic uncertainties: input data, regulator cutoff



- 7 different regulator cutoffs: Λ=450, 475, ..., 575, 600 MeV
- 6 different *NN*-scattering datasets $T_{lab} \in [0, T_{lab,max}]$, with $T_{lab,max}$=125, ..., 290 MeV

Do-it-yourself

$$\begin{aligned}\mathrm{Cov}(\mathrm{A},\mathrm{B}) &\equiv \mathbb{E}[(\mathcal{O}_{\mathrm{A}}(\mathbf{p})-\mathbb{E}[\mathcal{O}_{\mathrm{A}}(\mathbf{p})])(\mathcal{O}_{\mathrm{B}}(\mathbf{p})-\mathbb{E}[\mathcal{O}_{\mathrm{B}}(\mathbf{p})])] \\ &\approx \mathbb{E}[(\tilde{J}_{A,i}x_i + \frac{1}{2}\tilde{H}_{A,ij}x_ix_j - \frac{1}{2}\tilde{H}_{A,ii}\sigma_i^2) \\ &\times (\tilde{J}_{B,k}x_k + \frac{1}{2}\tilde{H}_{B,kl}x_kx_l - \frac{1}{2}\tilde{H}_{B,kk}\sigma_k^2)] \\ &= \tilde{\mathbf{J}}_A^T\mathbf{\Sigma}\tilde{\mathbf{J}}_B + \frac{1}{2}(\boldsymbol{\sigma}^2)^T(\tilde{\mathbf{H}}_A \circ \tilde{\mathbf{H}}_B)\boldsymbol{\sigma}^2,\end{aligned}$$

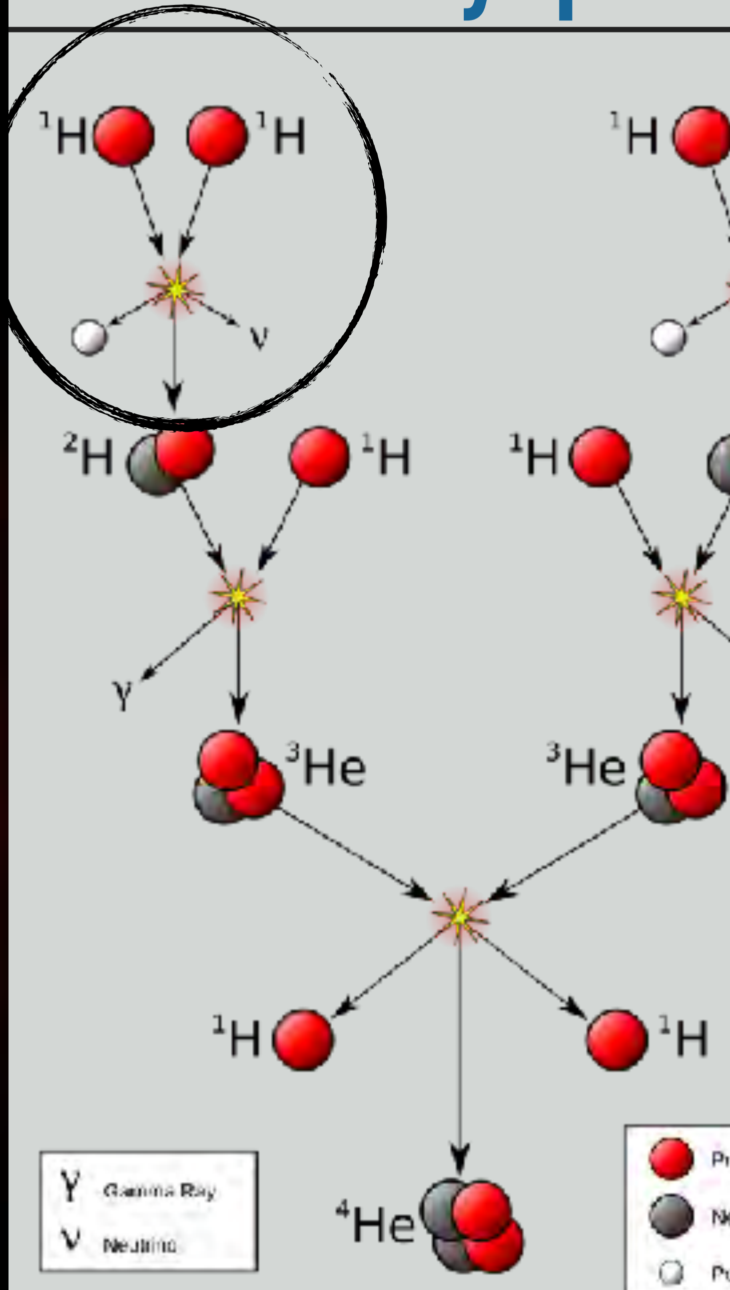
All 42 different sim/sep potentials, as well as the respective covariance matrices are available as supplemental material.

- LO-NLO-NNLO
- with 7 different cutoffs: 450,475,..,600 MeV
- from 6 different NN-scattering datasets

compute the derivatives of your own observables wrt LECs, then explore:

- cutoff variations
- order-by-order evolution
- LEC UQ/correlations

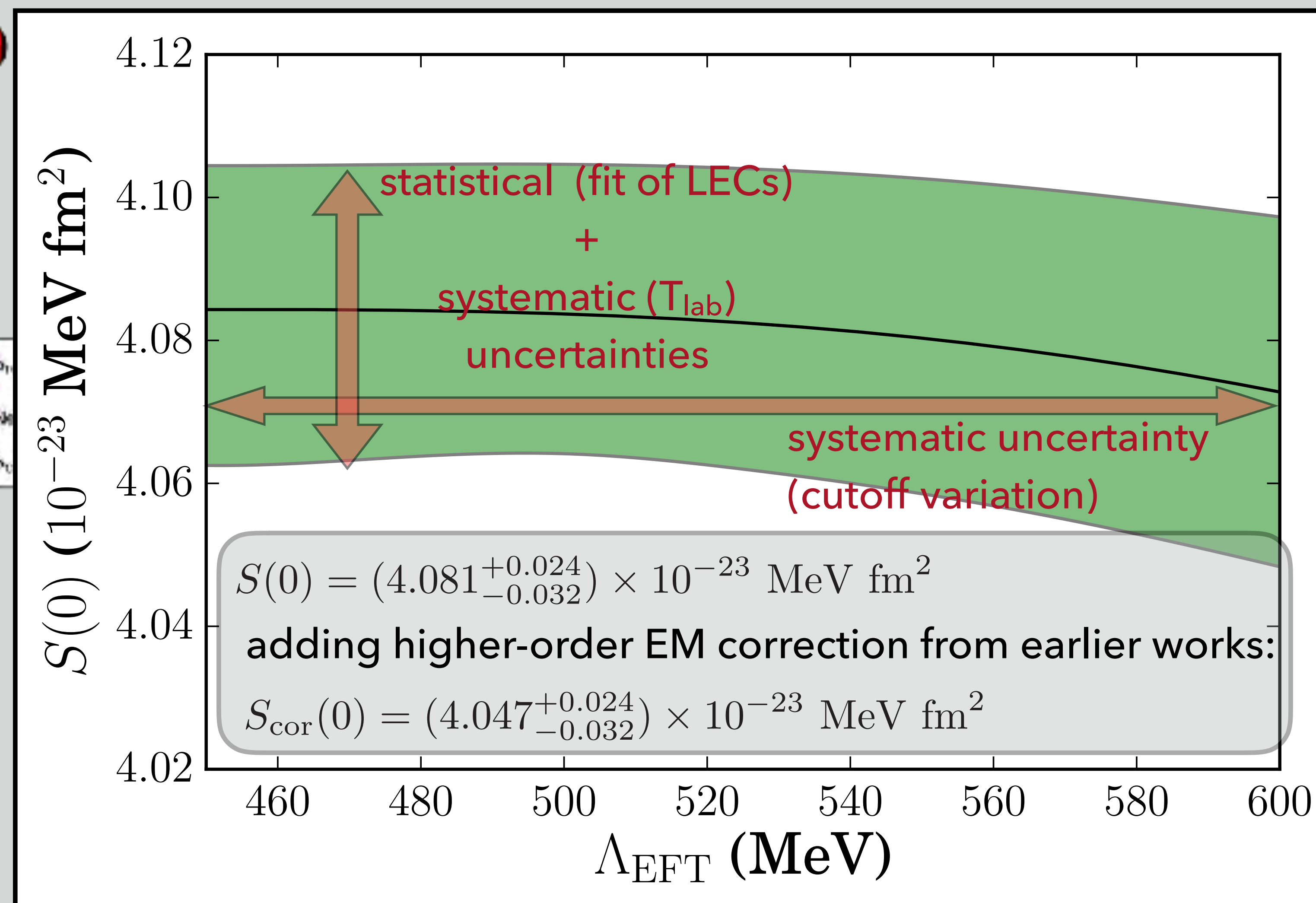
Uncertainty quantification applied to pp fusion



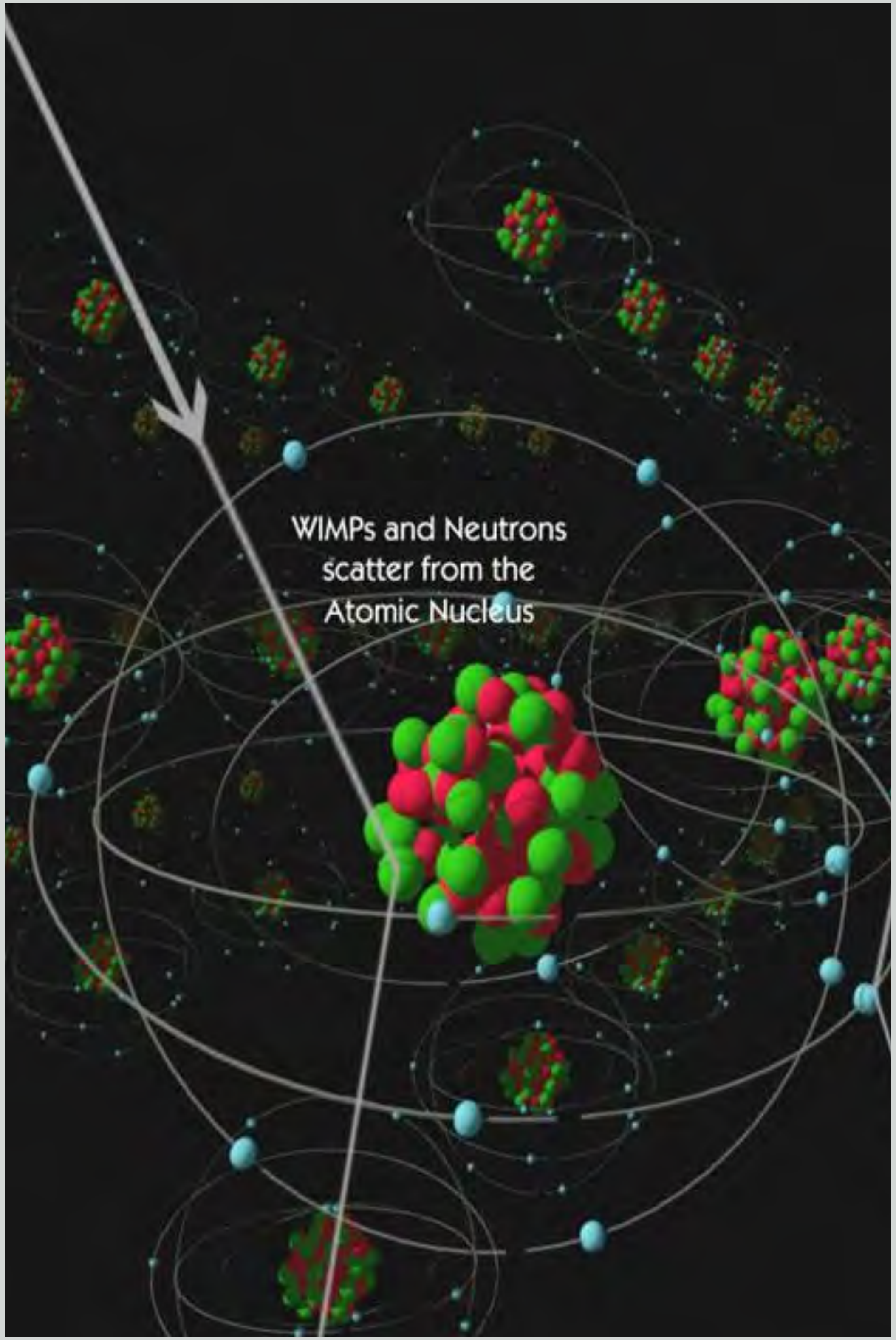
$$p + p \rightarrow d + e^+ + \nu_e$$
$$S(E) = \sigma(E) E e^{2\pi\eta}$$

L. E. Marcucci et al PRL 110, 192503 (2013)
R. Schiavilla et al PRC 58, 1263 (1998)
J-W. Chen et al. PLB 720, 385 (2013)

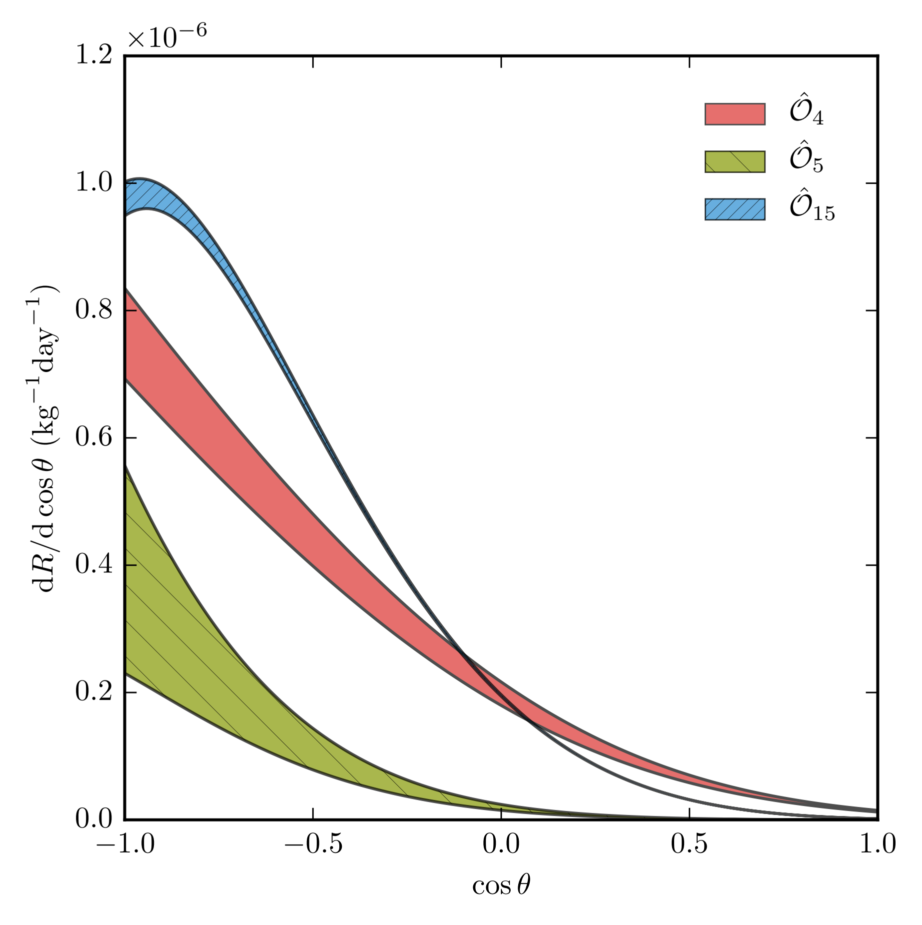
B. Acharya et al, Phys. Lett. B 760 (2016) 584



Uncertainty quantification applied to dark-matter nucleus scattering



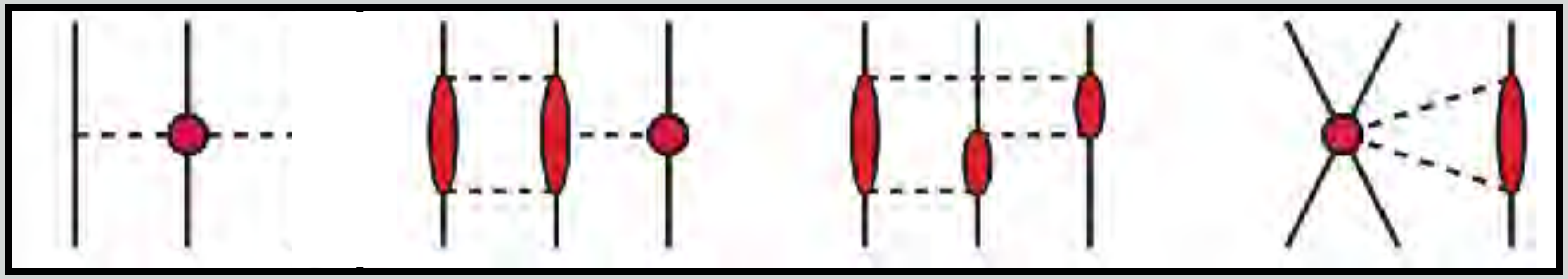
- WIMP scattering off ^{3,4}He described in NR-EFT
- Nuclear response functions from NCSM wave functions
- Studied rates of dark matter–nucleus scattering events



D. Gazda et al, arXiv:1612.09165

Work in progress: N3LO

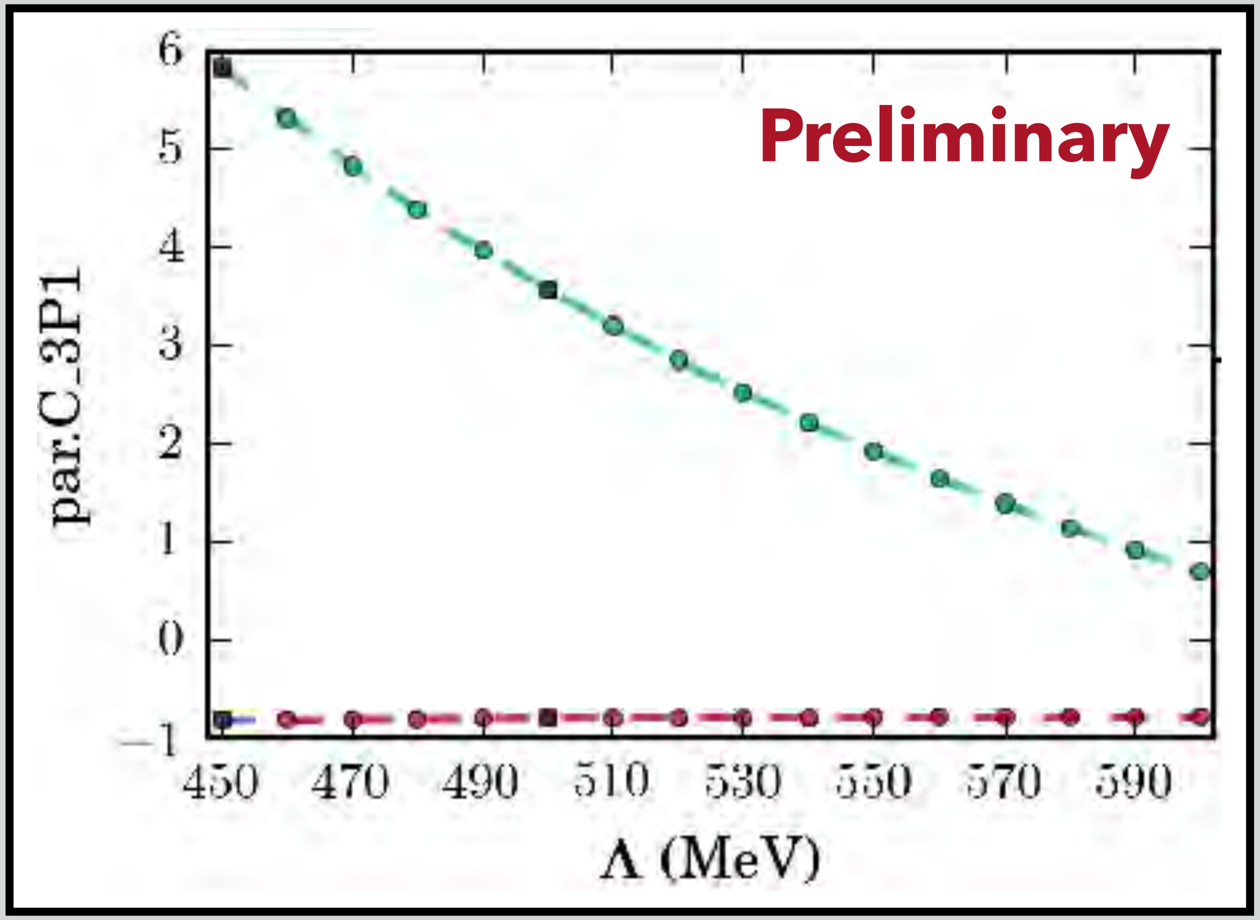
N3LO optimizations are challenging



+ rel. corr.

41 parameters to optimize,
3NF matrix elements recently made available (K. Hebeler)

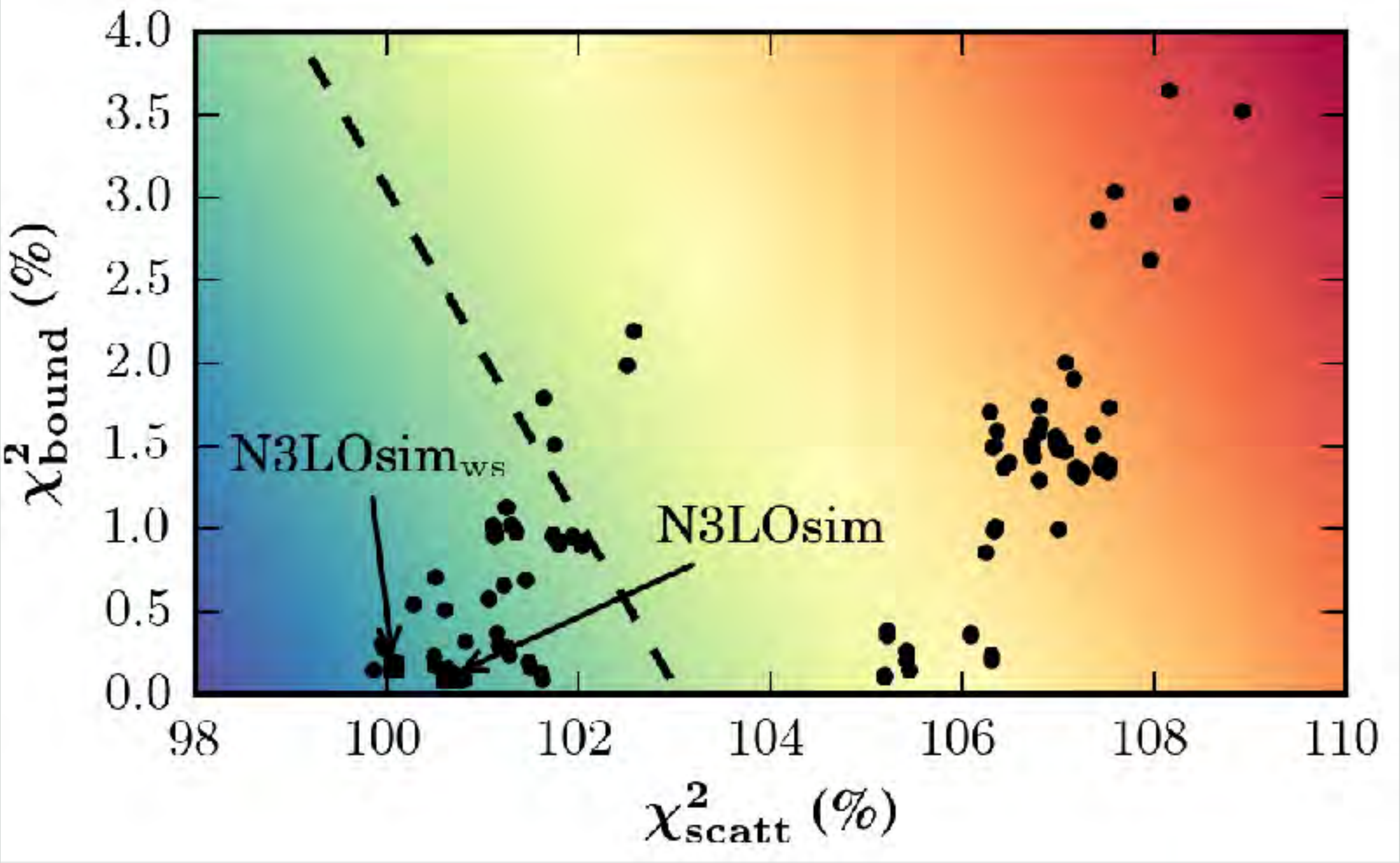
Initialize by computing phase shifts for 10^5 random contact LEC values for each partial wave and select the ~1000 best values and optimize. This leads to [5x2x2x2x2x2=160] different optima (for cutoff 500 MeV) with respect to phase shifts. (pi-N LECs from sep-optimization).



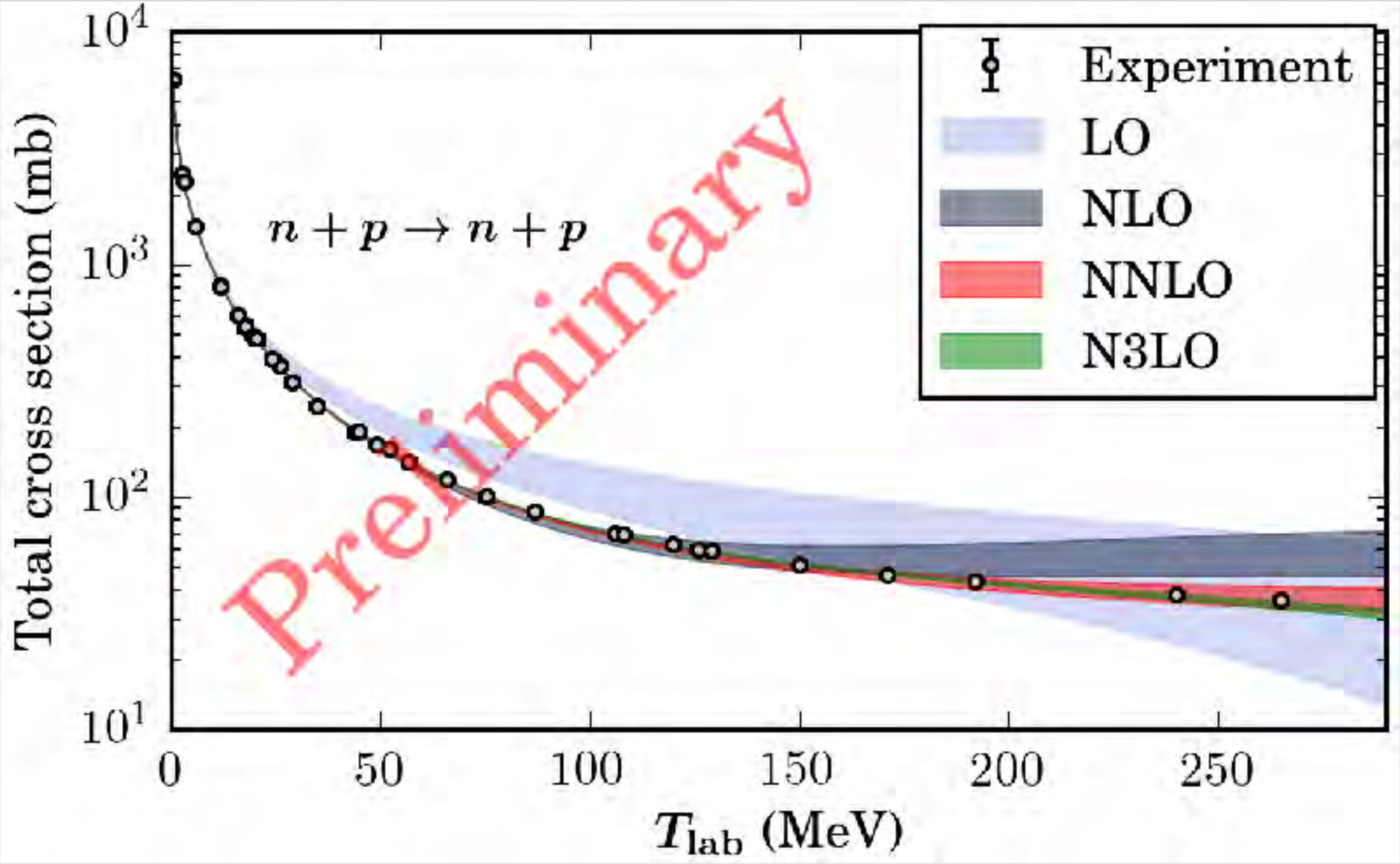
These minima perform equally well in the NN sector. But the LECs display rather different Λ-dependence.

N3LO MINIMA

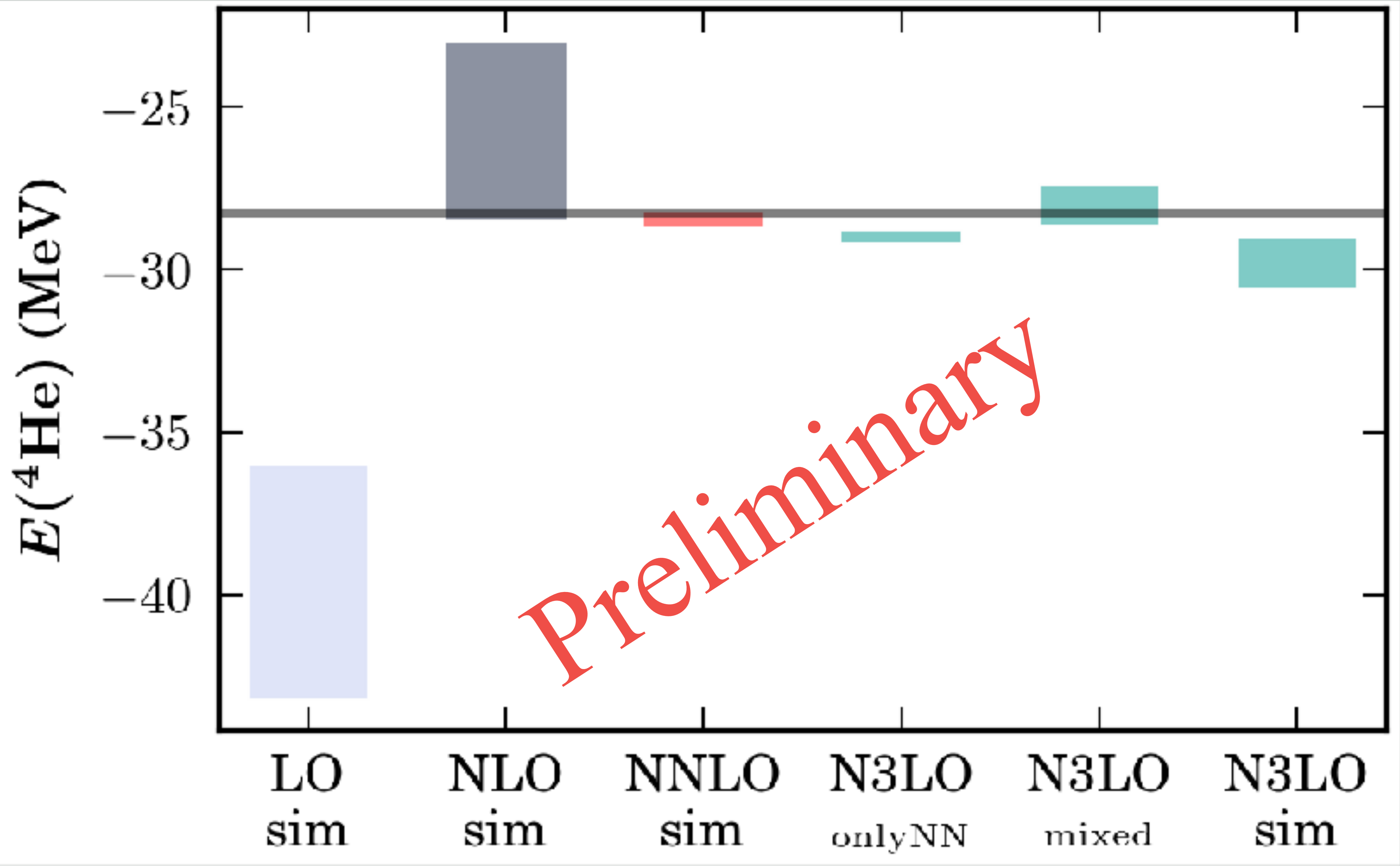
≳100 optima remain after performing simultaneous optimizations from these starting points



N3LO SCATTERING



SYSTEMATIC UNCERTAINTIES: INPUT DATA, REGULATOR CUTOFF



Based on: A. Ekström et al, Phys. Rev. C **91** (2015) 051301(R)

Rapid Communication

Accurate nuclear radii and binding energies from a chiral interaction

A. Ekström, G. R. Jansen, K. A. Wendt, G. Hagen, T. Papenbrock, B. D. Carlsson, C. Forssén, M. Hjorth-Jensen, P. Navrátil, and W. Nazarewicz

Phys. Rev. C **91**, 051301(R) – Published 1 May 2015

See also: G. Hagen et al, Nat. Phys. **12** (2015) 186

nature physics

NATURE PHYSICS | ARTICLE

Neutron and weak-charge distributions of the ^{48}Ca nucleus

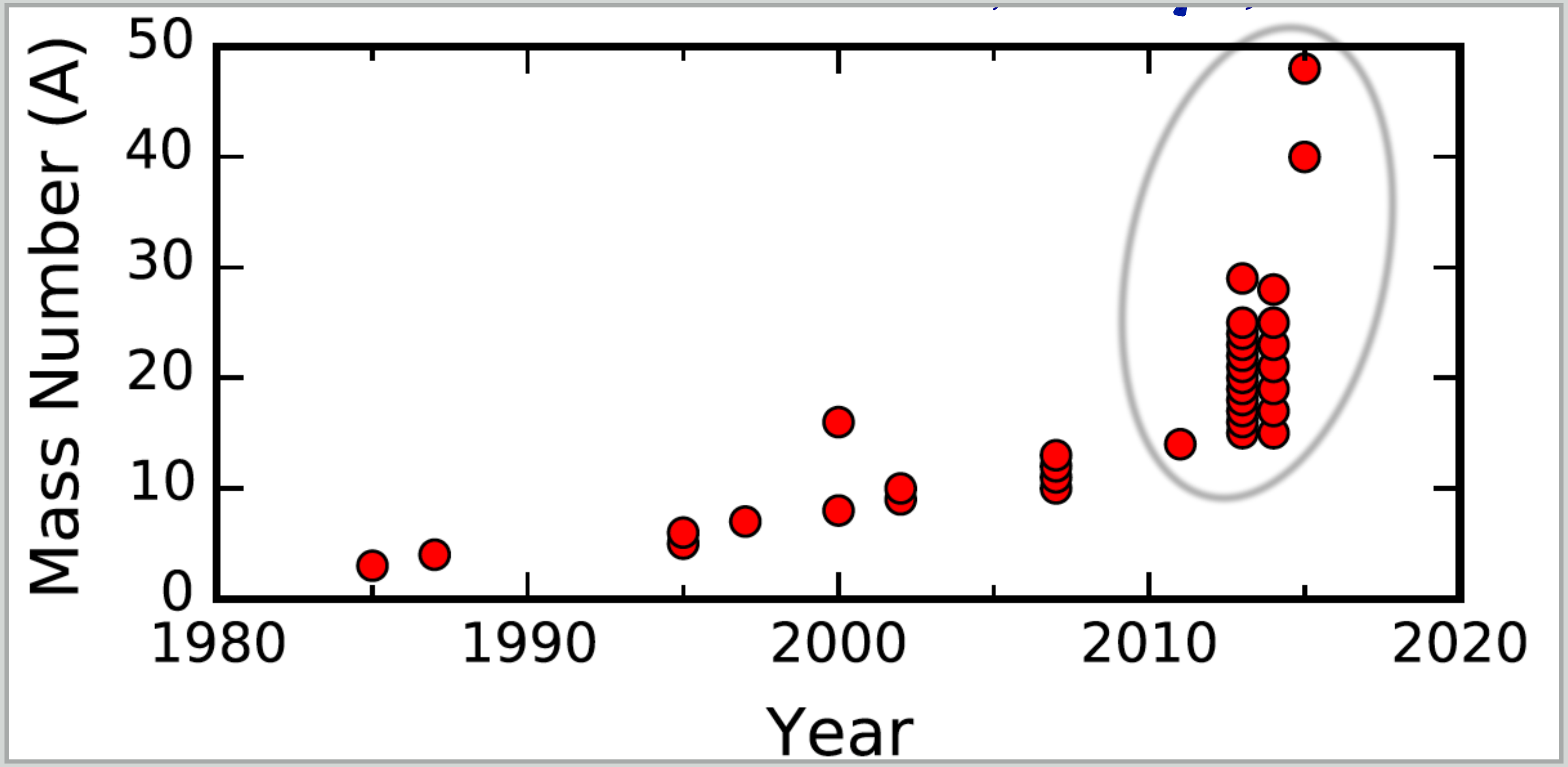
G. Hagen, A. Ekström, C. Forssén, G. R. Jansen, W. Nazarewicz, T. Papenbrock, K. A. Wendt, S. Bacca, N. Barnea, B. Carlsson, C. Drischler, K. Hebeler, M. Hjorth-Jensen, M. Miorelli, G. Orlandini, A. Schwenk & J. Simonis

FROM FEW TO MANY

IS NUCLEAR SATURATION AN EMERGENT PHENOMENON?

TREND IN REALISTIC AB INITIO CALCULATIONS

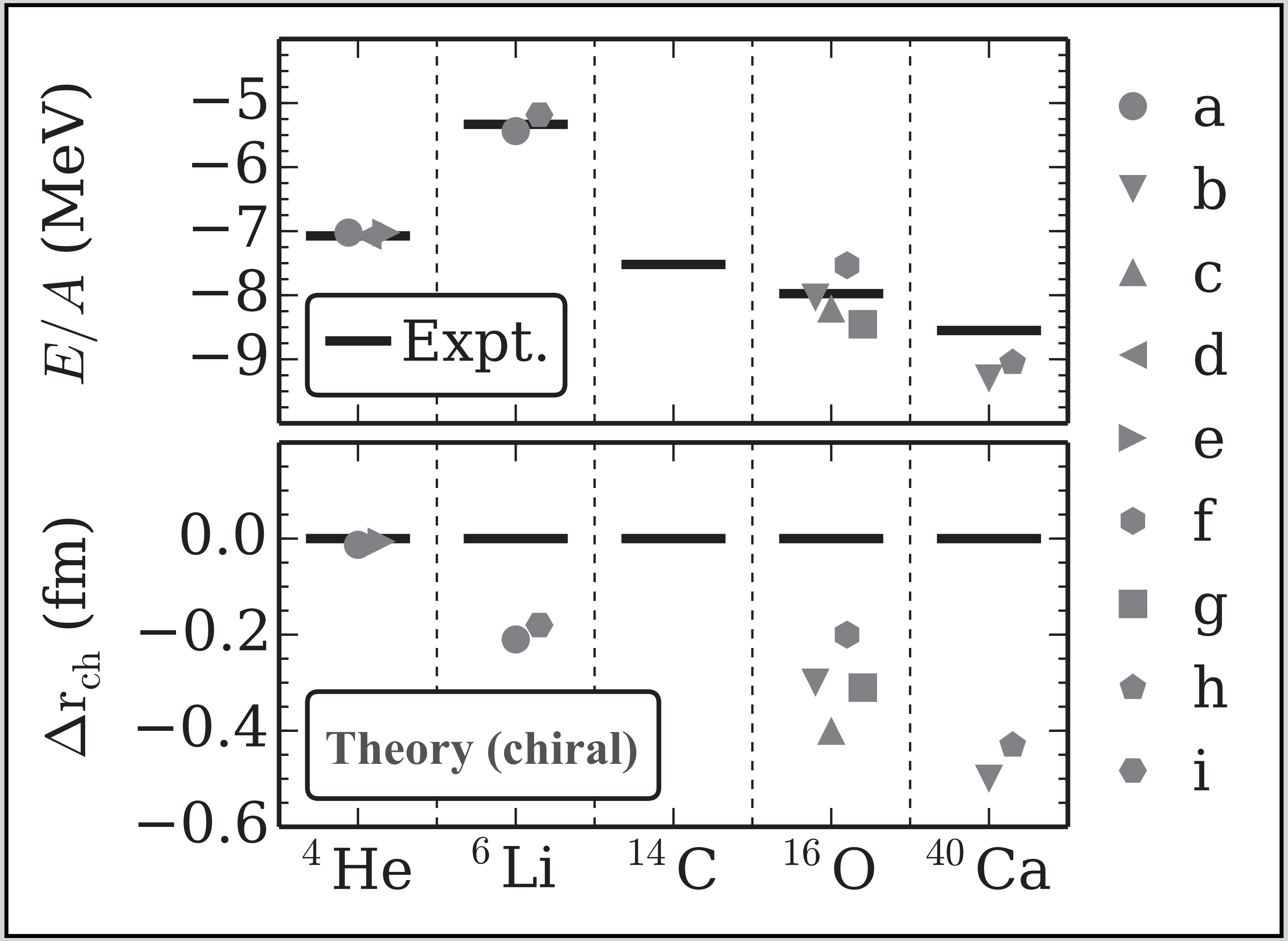
Explosion of many-body methods
(Coupled clusters, Green's function Monte Carlo, In- Medium SRG, Lattice EFT, No-Core Shell Model, Self-Consistent Green's Function, UMOA, ...)



"Computational capabilities exceed accuracy of available interactions "

[Binder et al, Phys. Lett. B 736 (2014) 119]

STATUS OF CHIRAL-FORCE PREDICTIONS

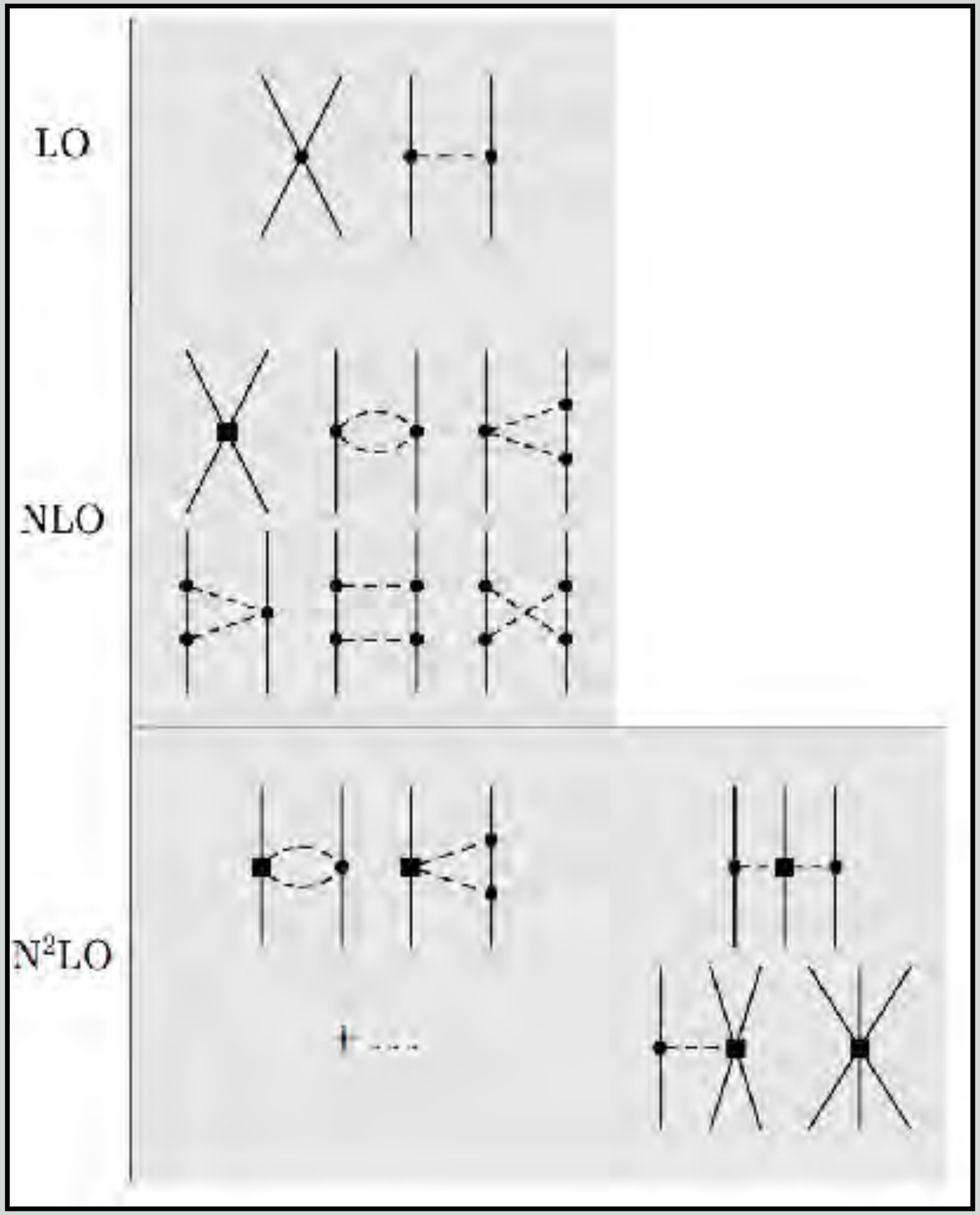


Ab initio calculations with existing chiral interactions

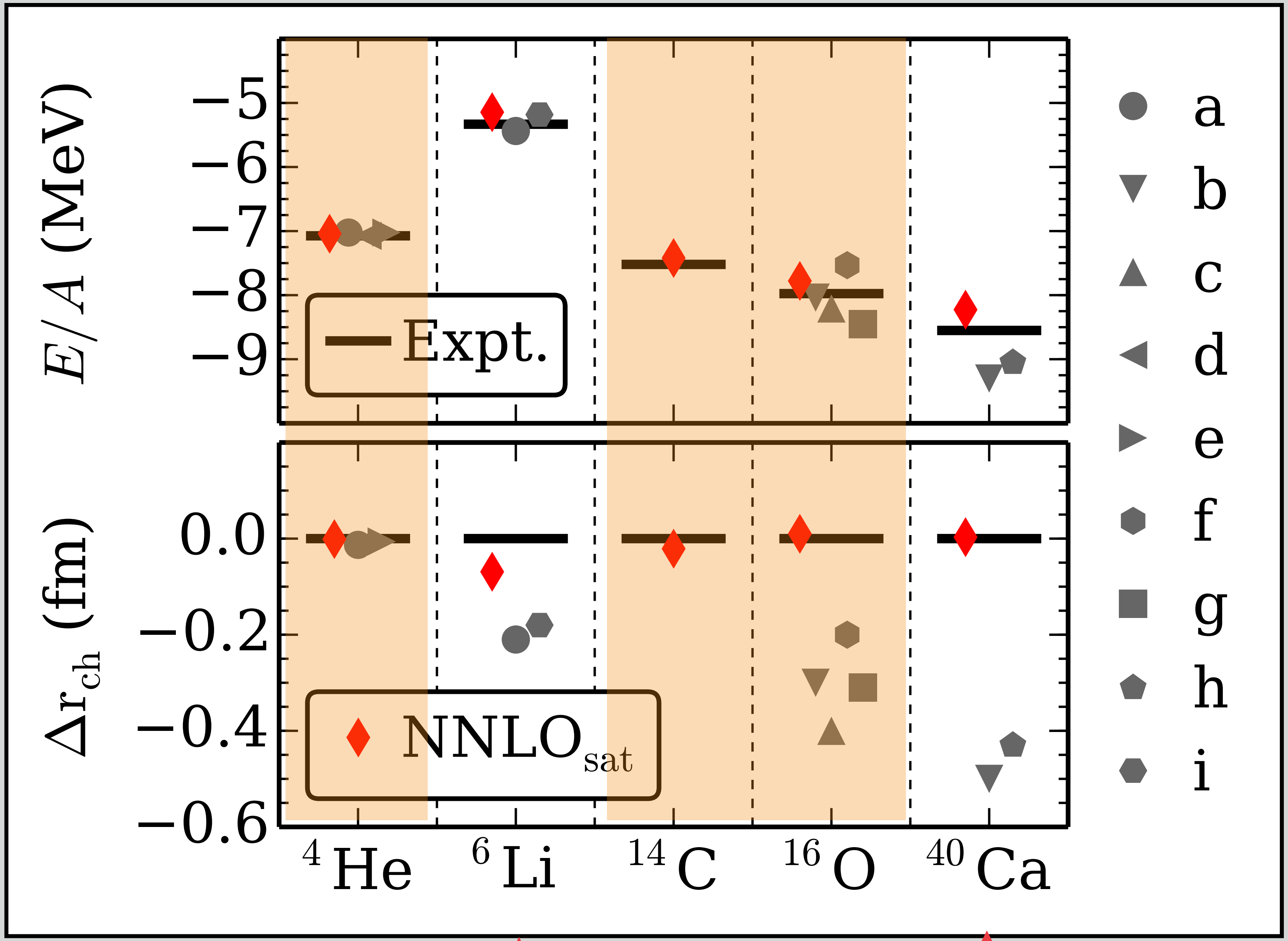
- **overbind** medium-mass and heavy nuclei, and
- **underestimate charge radii**.

PRAGMATIC OPTIMIZATION STRATEGY

- Simultaneous optimization of NN and NNN LECs at NNLO.
- NCSM and CC calculations are performed within the optimization
- Objective function contains:
  - deuteron properties and *NN* scattering data (T_{lab}< 35 MeV)
  - A=3,4 binding energies, radii
  - ^{14}C,^{16}O binding energies, radii
  - ^{22,24,25}O binding energies



CHIRAL INTERACTION WITH ACCURATE SATURATION: N2LO$_{SAT}$

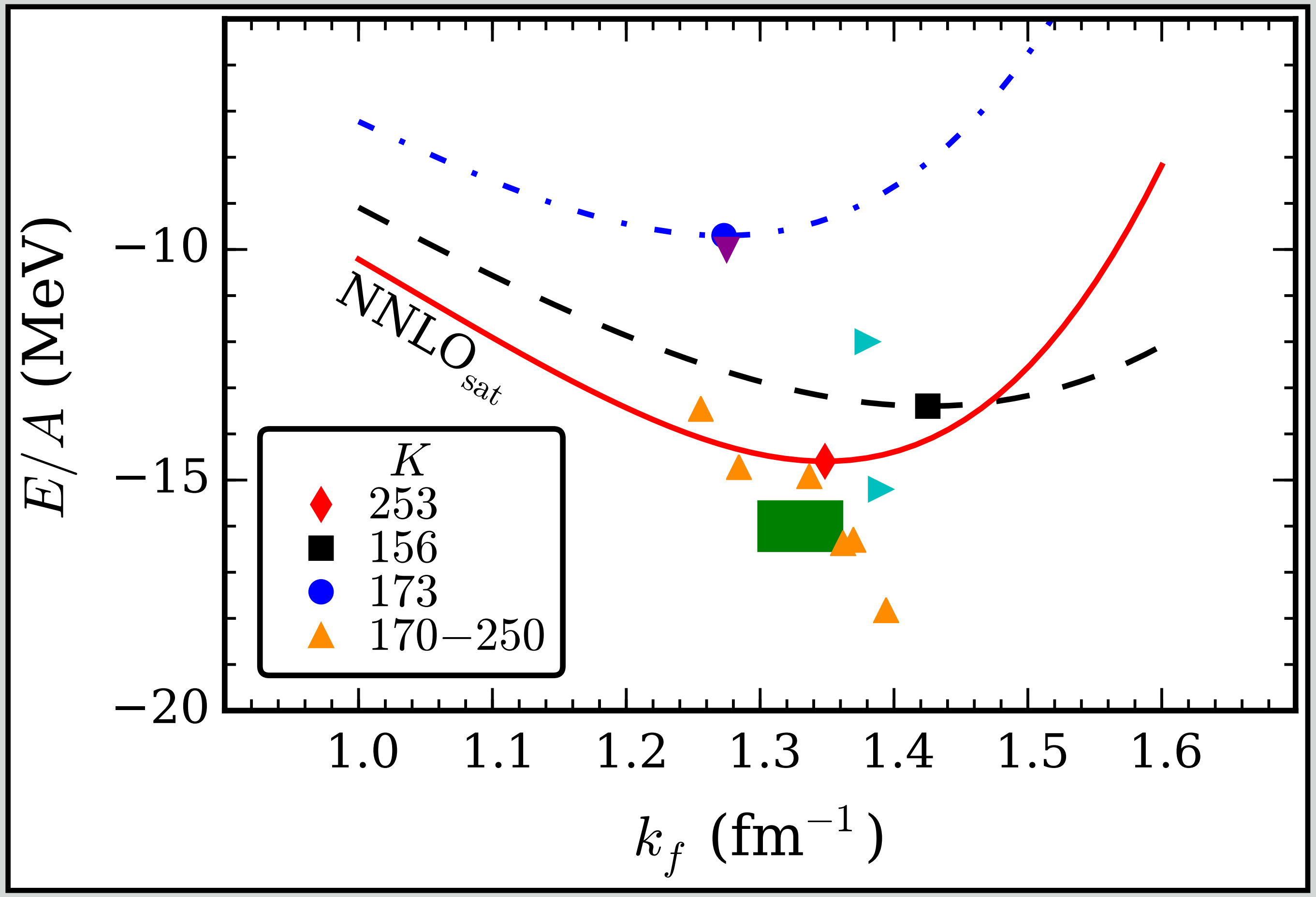


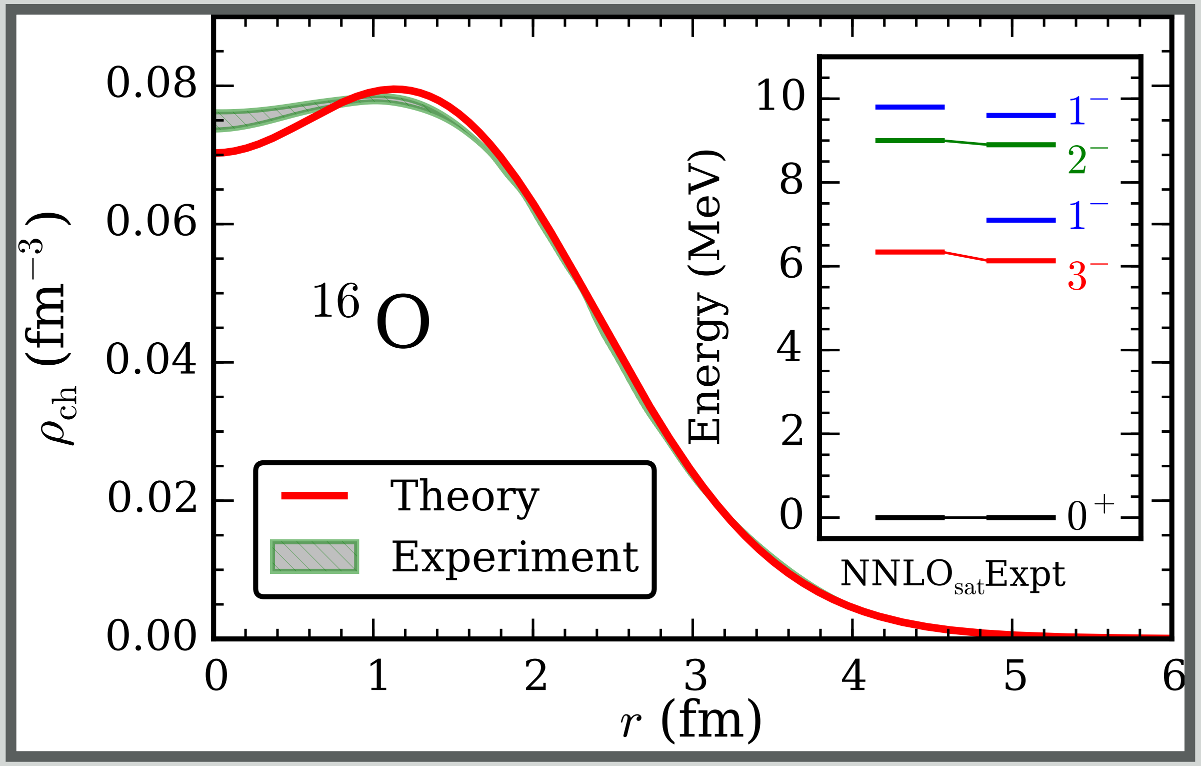
Interpolation

Extrapolation

CHARGE, NEUTRON DISTRIBUTION, AND WEAK SIZE OF THE ATOMIC NUCLEUS

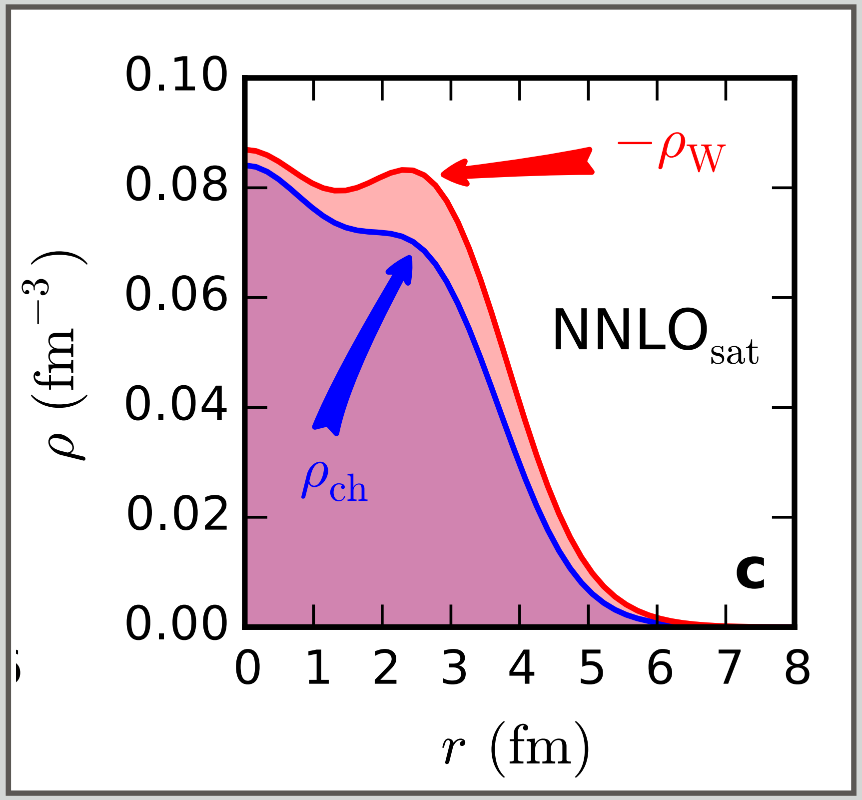
Accurate saturation





^{16}O charge radius

Neutron skin of ^{48}Ca



CONCLUSION

SUMMARY

Chiral EFT with error analysis

- **Uncertainty quantification** is a **unique opportunity** when employing **systematic approaches (EFT + ab initio).**
- First results for correlations, parameter uncertainties and **error propagation in the few and many-body sectors.**
- **Simultaneous optimization of all LECs** at LO, NLO, NNLO, N3LO using NN, NNN and piN data is critical in order to:
  - capture all correlations between the parameters, and
  - reduce the statistical errors.
- We find that **statistical errors** are small ($\lesssim$1%), and the total error budget is dominated by **systematic model errors.** Statistical errors increase dramatically for sequentially optimized potentials.