Analyzing the nuclear interaction: challenges and new opportunities

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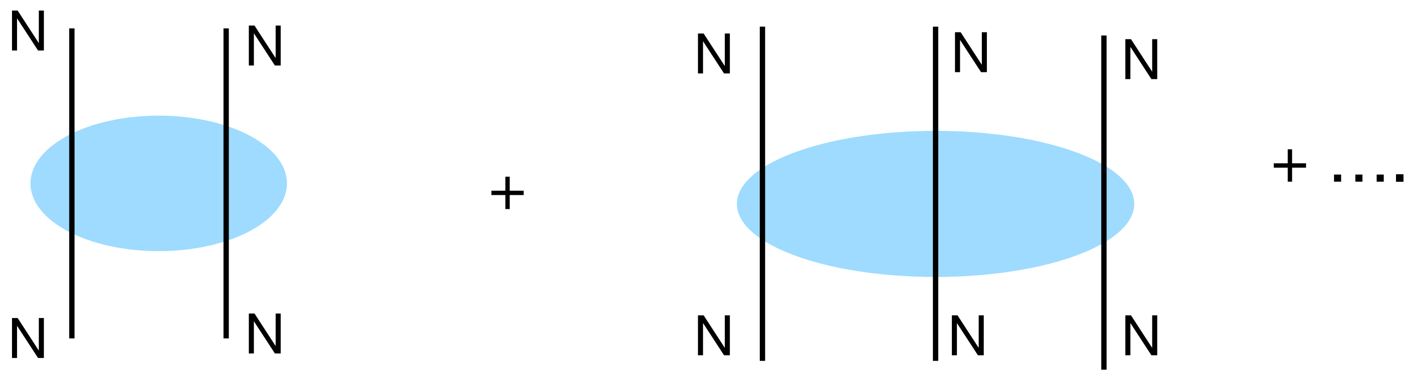
Ab initio calculations of nuclear systems

Goal: develop a predictive understanding of nuclei and nucleonic matter in terms of the interactions between individual nucleons and external probes

Two and many-body interactions:

$$H = \sum_{i=1}^{A} \frac{\mathbf{p}_i^2}{2m_i} + \sum_{i<j=1}^{A} \overbrace{v_{ij}}^{\text{th+exp}} + \sum_{i<j<k=1}^{A} \overbrace{V_{ijk}}^{\text{th+exp}} + \ldots..$$

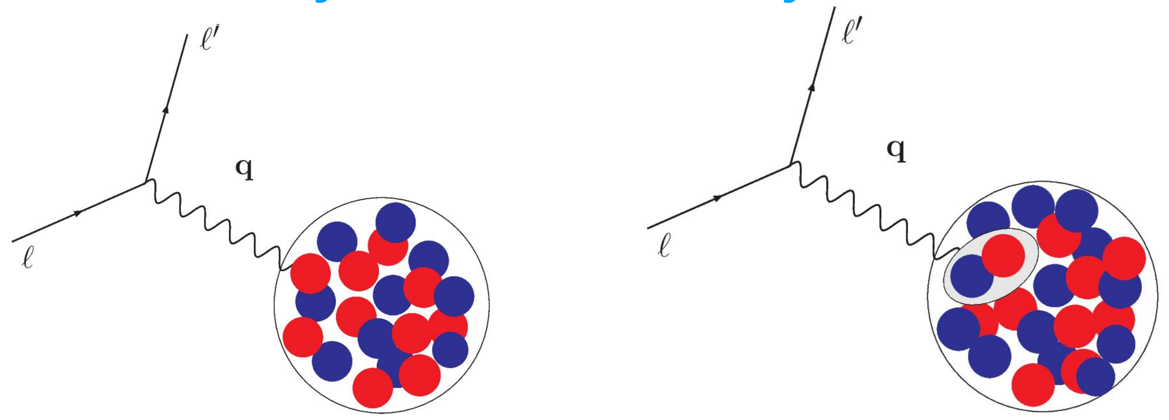
one-body   two-body (NN)   three-body (3N)



Electroweak current operators:

$$j^{\mathrm{EW}} = \sum_{i=1}^{A} j_i + \sum_{i<j=1}^{A} \overbrace{j_{ij}}^{\text{th+exp}} + \sum_{i<j<k=1}^{A} \overbrace{j_{ijk}}^{\text{th+exp}} + \ldots.$$

one-body   two-body   three-body



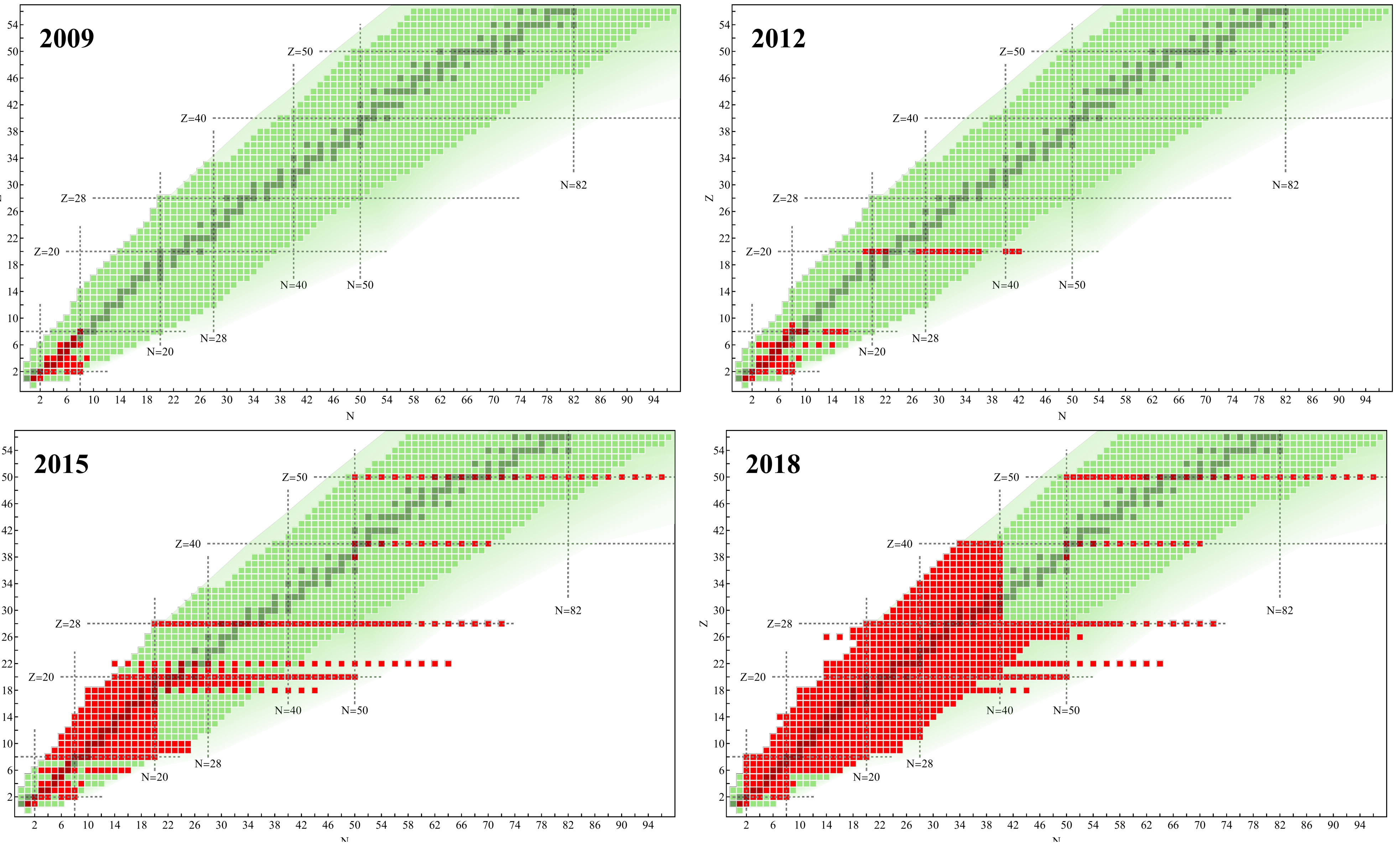
Ab-initio methods: $H\,\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_A; s_1, s_2, \ldots, s_A; t_1, t_2, \ldots, t_A)$
$= E\,\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_A; s_1, s_2, \ldots, s_A; t_1, t_2, \ldots, t_A)$

Erwin Schrödinger

Nuclear Interactions, Nuclei, and Infinite Matter

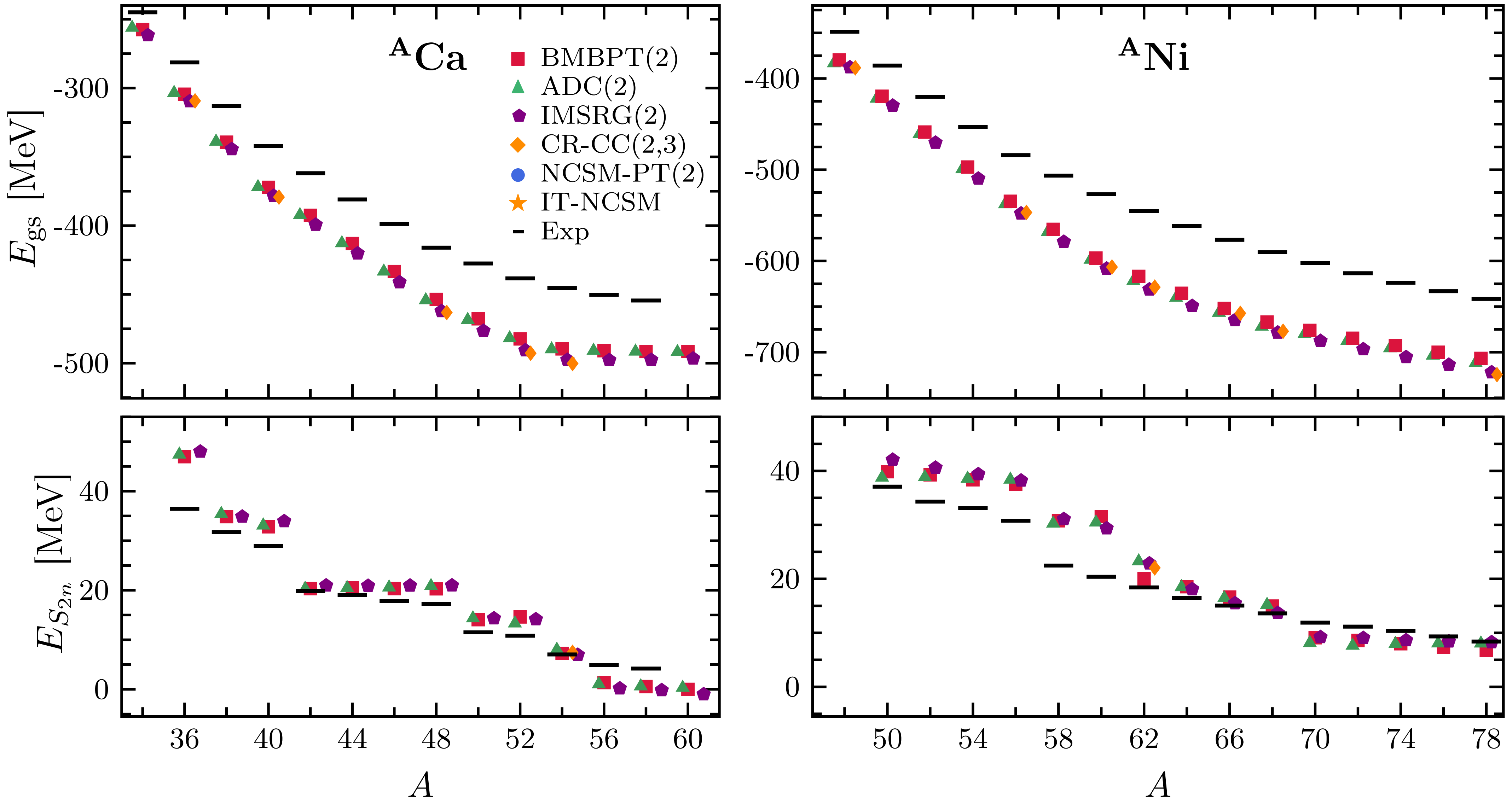
Success:

- *increased many-body capability, algorithms under control*
- *remarkable agreement between different ab intio many-body methods for the structure of nuclei (not the same for infinite matter, continuum coupling,..)*



Credit to Heiko Hergert (MSU/FRIB) for collecting the data

- Improved and novel many-body frameworks
- Increased computational resources
- Nuclear interactions and currents based on EFTs
- Theoretical uncertainty quantification



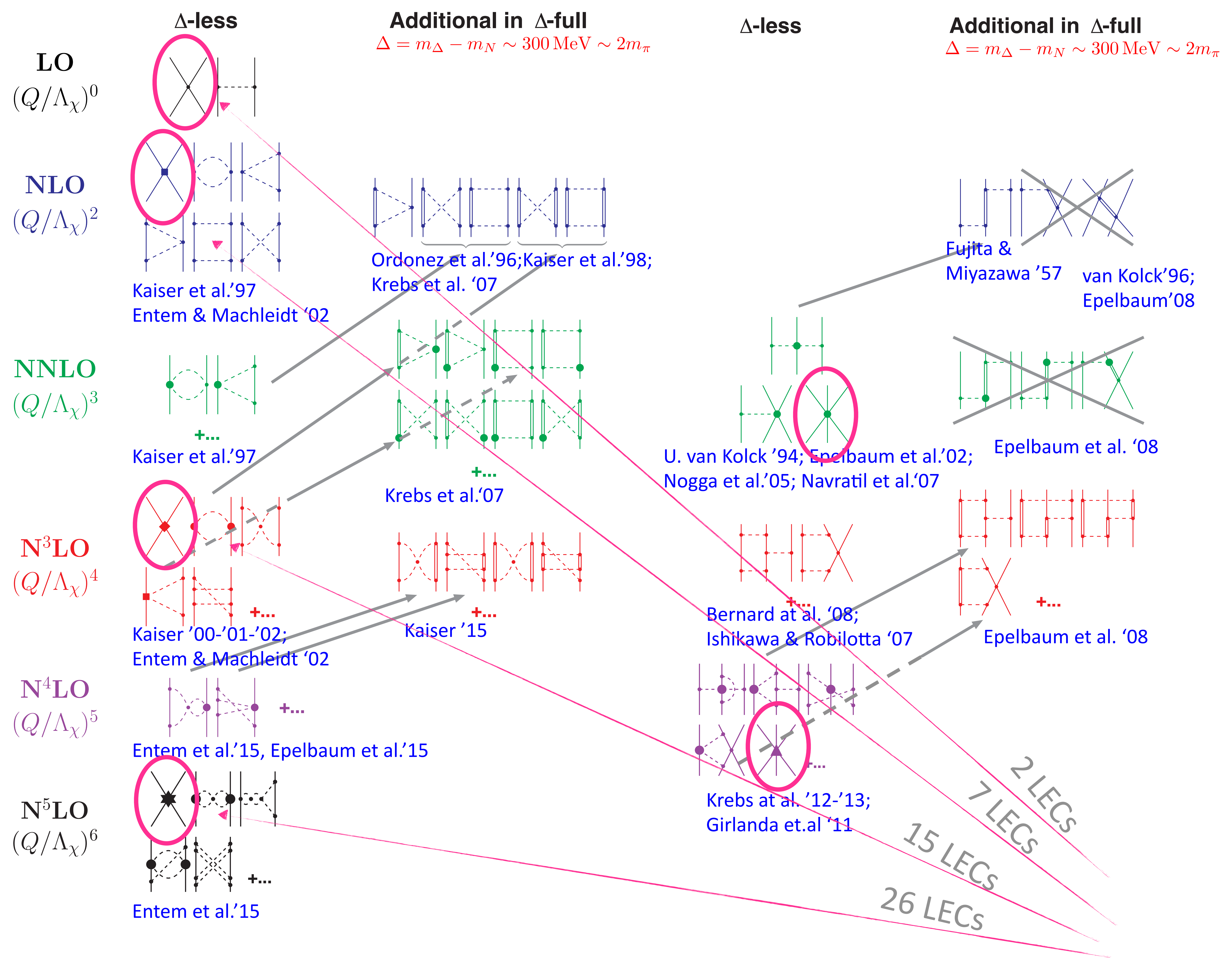
Tichai *et al.* PLB 786, 195 (2018)

Challenge: consistent description of BEs, radii, saturation properties of NM, EoS of PNM, EW properties….

Issue:

- *largest uncertainty from input Hamiltonian*
- *a deeper and more quantitative understanding of the connection between properties of matter and finite nuclei is still lacking*

State-of-the art of Chiral EFT interactions



Advantages:

- Consistent description of two- and many-body interactions and currents
- Different processes described on the same footing: piN, NN, electroweak
- UQ due to the truncation in the chiral expansion
- Scheme can be systematically improved

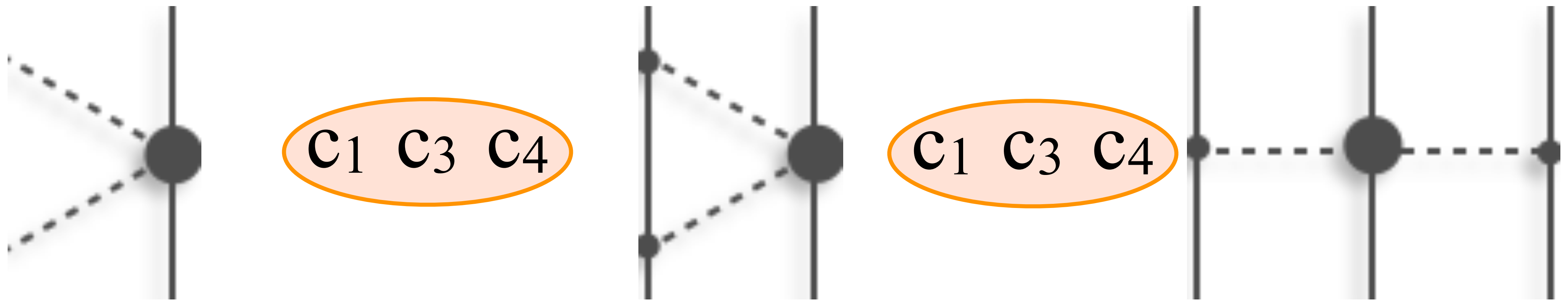
Disadvantages:

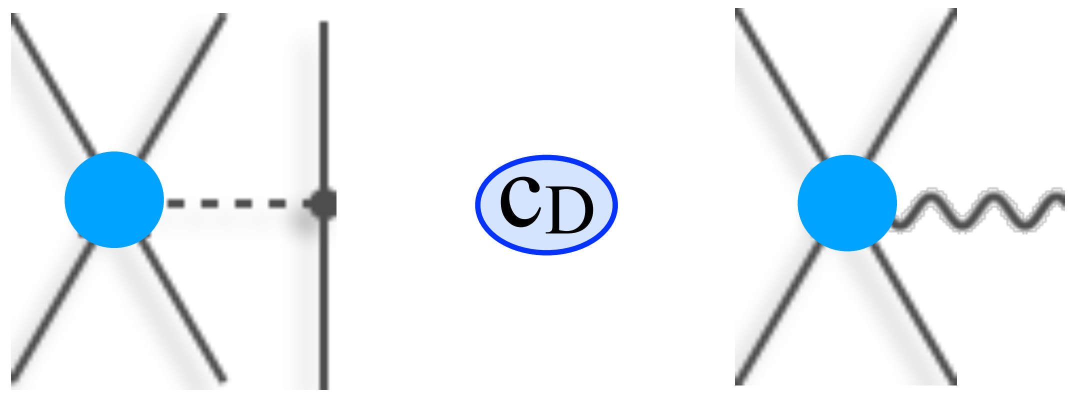
- Increase in number of diagrams at higher orders; When do we stop in the chiral expansion? Convergence, power counting, etc….
- Consistency between strong- and electroweak sector very hard to achieve
- More LECs appearing at higher orders; challenging optimization problem

How to fix the LECs?

First Challenge: *What experimental data should we use to find the LECs?*

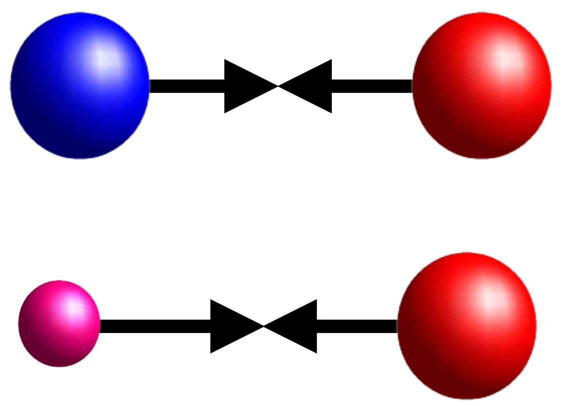
some LECs in chiral EFT appear in different low energy processes



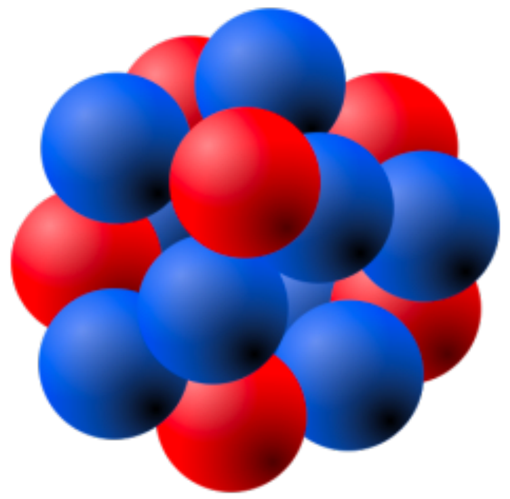


piN scattering   NN interaction   3N interaction   3N interaction   EW interaction

Remaining LECs constrained to:



Scattering observables: piN, NN, NNN..



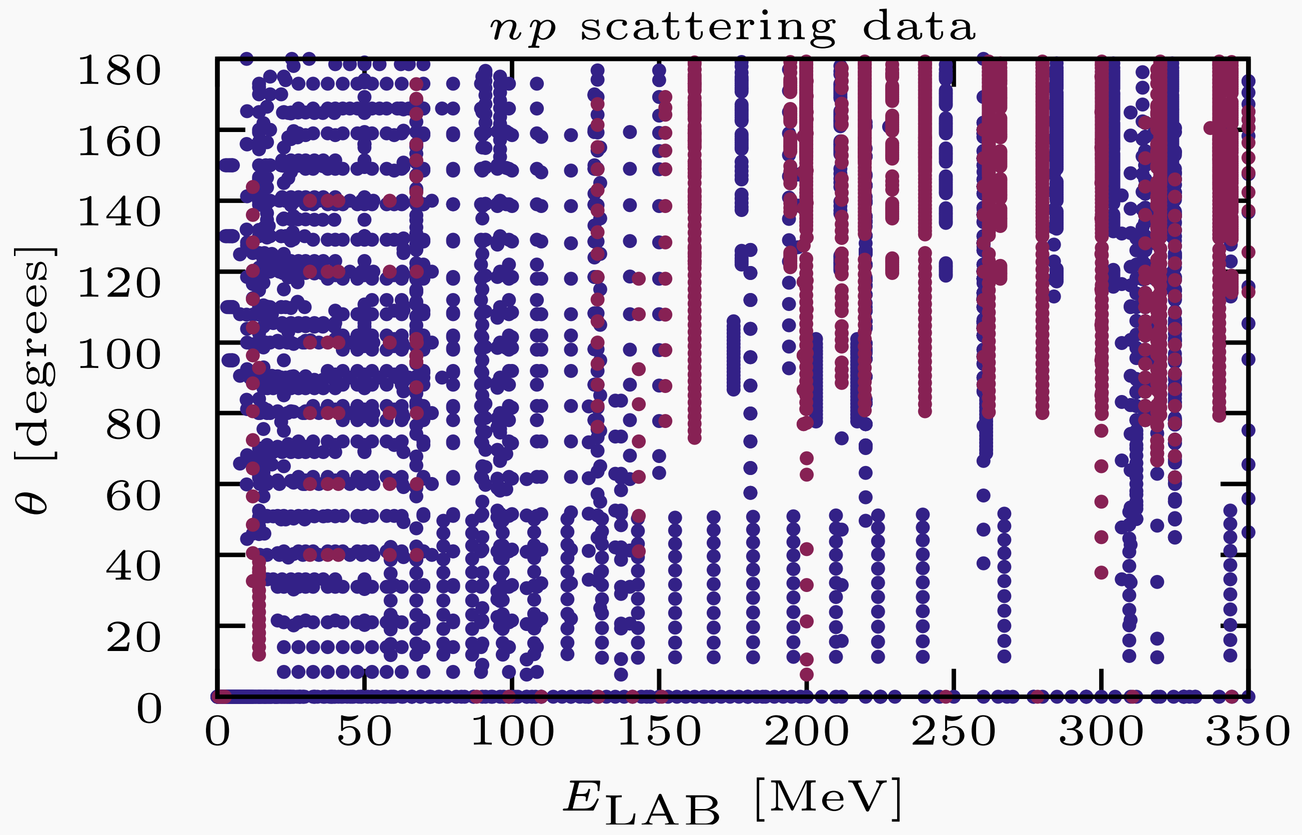
Static and dynamic properties of few- and many-body systems

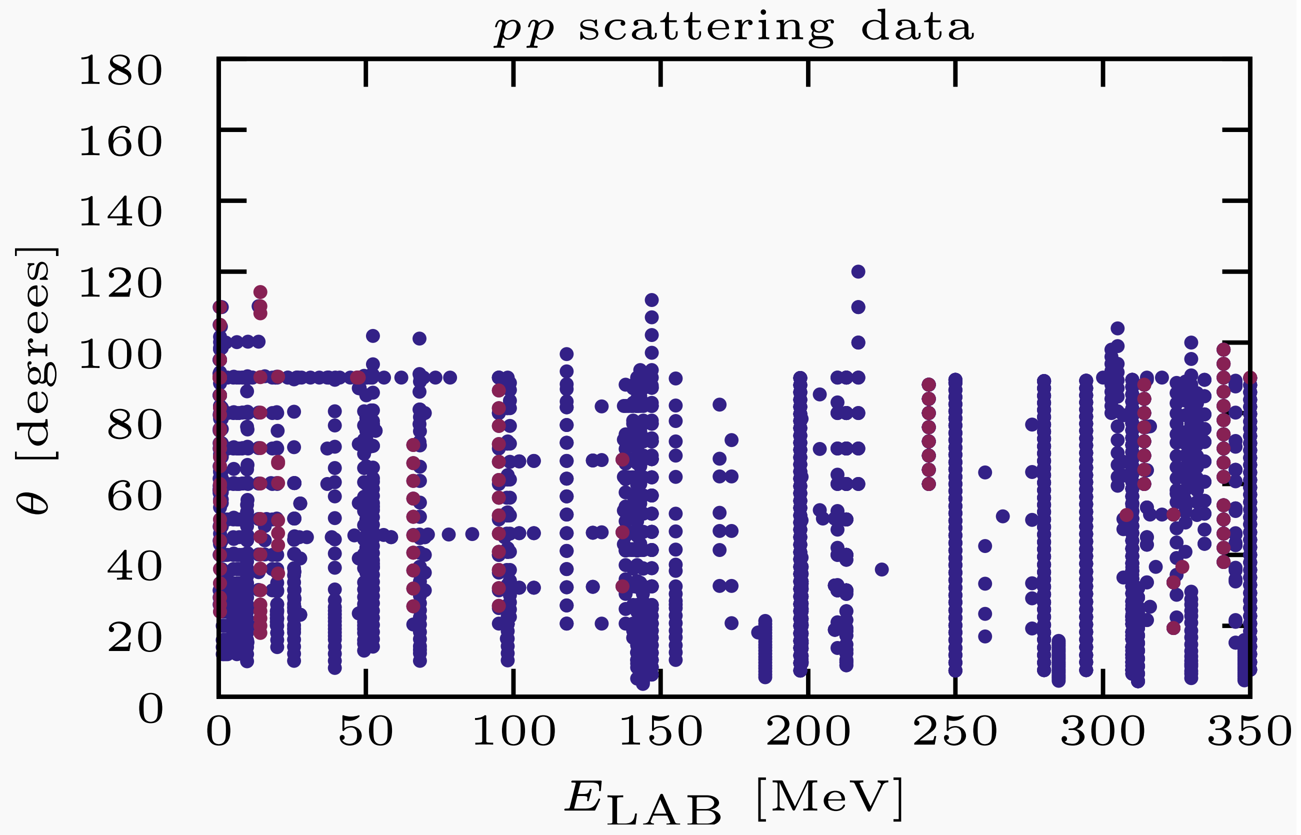
Fits of NN Interactions: nucleon-nucleon scattering data

The Granada NN database is the most up to date database. The analysis includes data within the years 1950 to 2013. http://www.ugr.es/~amaro/nndatabase/

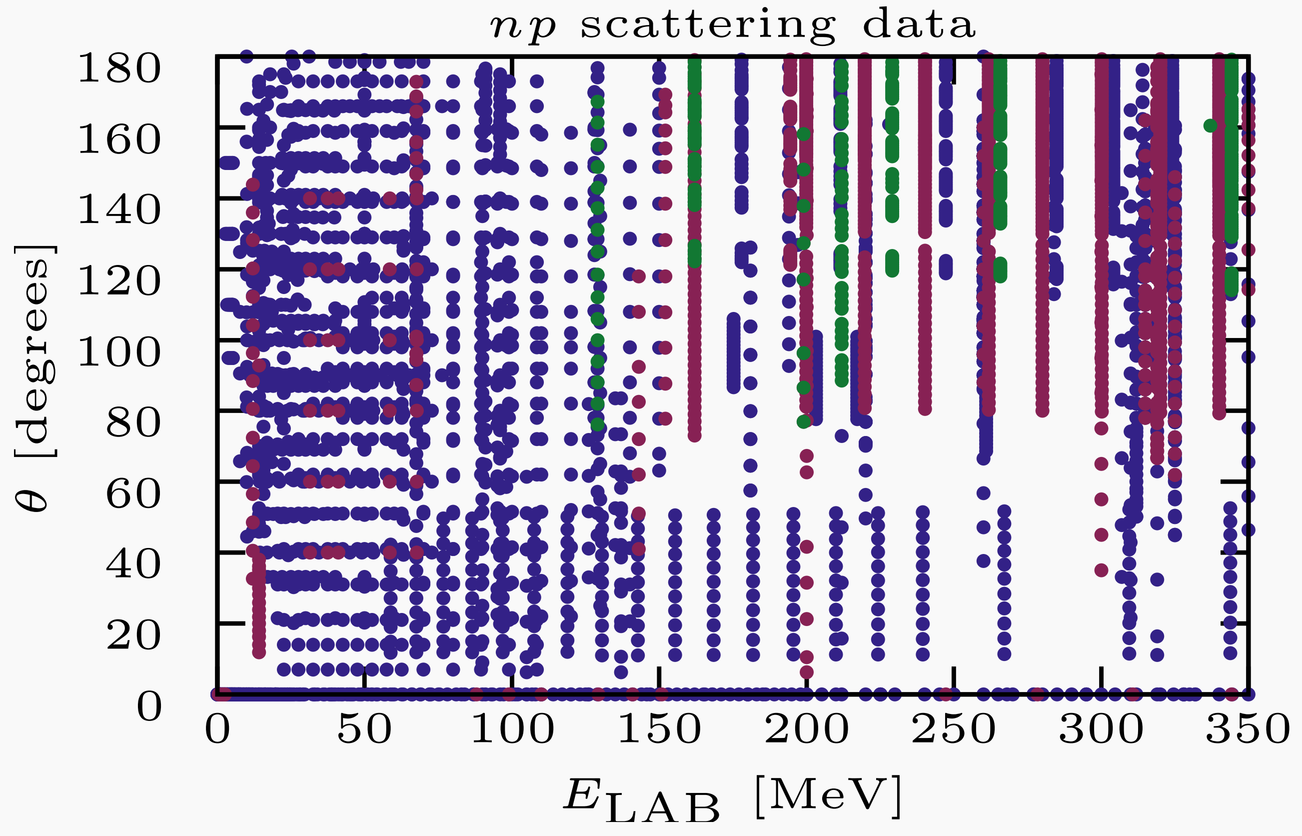
More than 7800 elastic scattering data up to E_{LAB}=350 MeV

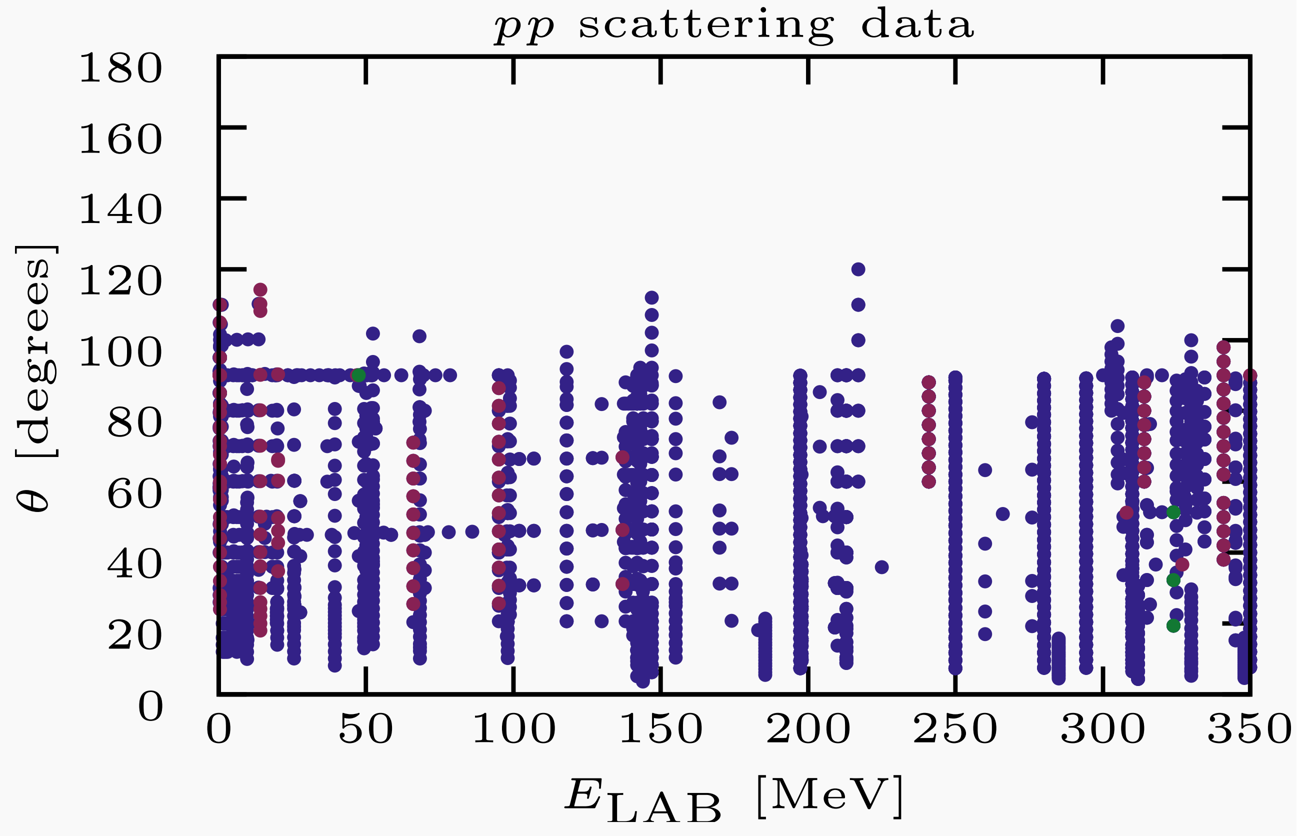
Usual Nijmegen 3σ criterion (1677 rejected data)





300 recovered data with Granada procedure





Maximization of the experimental consensus:

Fit to all data

Apply 3σ criterion

Refit parameters

Re-apply 3σ criterion to all data

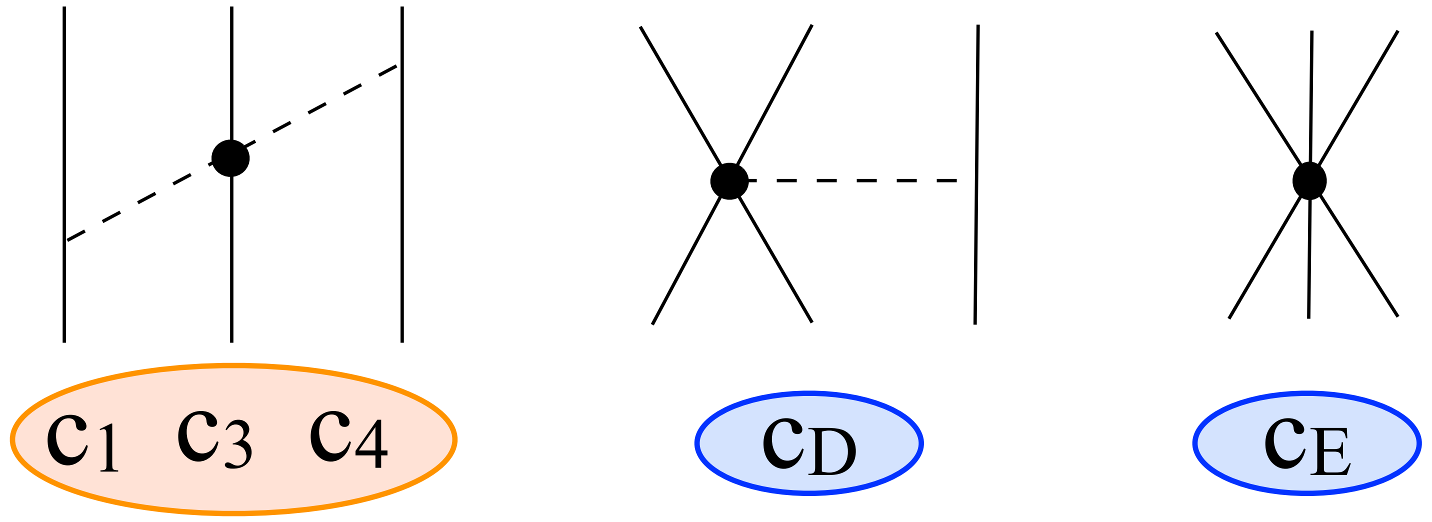
Repeat until no more data is excluded or recovered

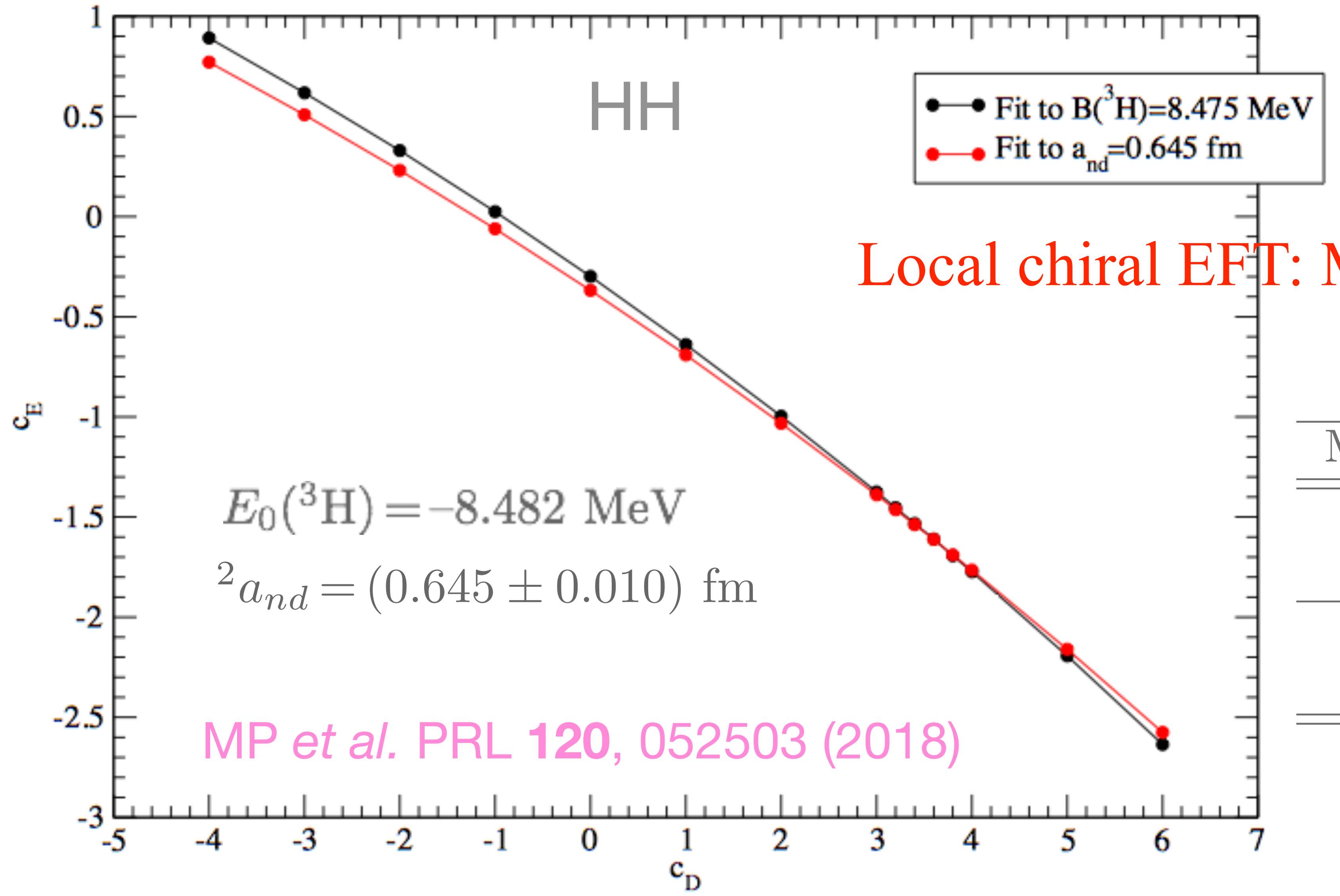
Perez, Amaro, Arriola PRC88 (2013) 064002

Fits of 3N Interactions: three-body scattering cross sections

- Inclusion of 3N forces at N2LO:

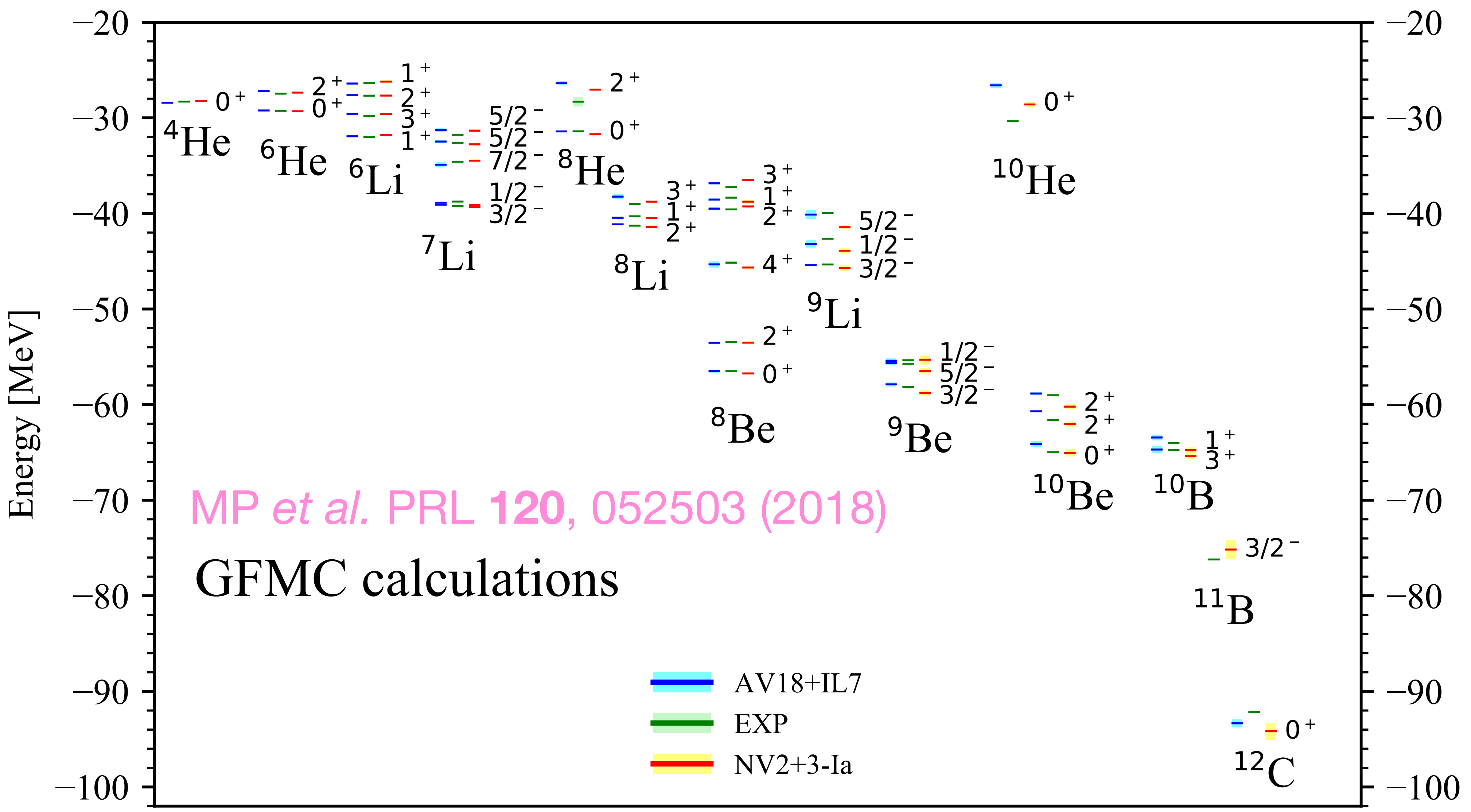
Constrained from πN scattering or NN: ex. Hoferichter et al., Phys .Rept. 625 (2016) 1



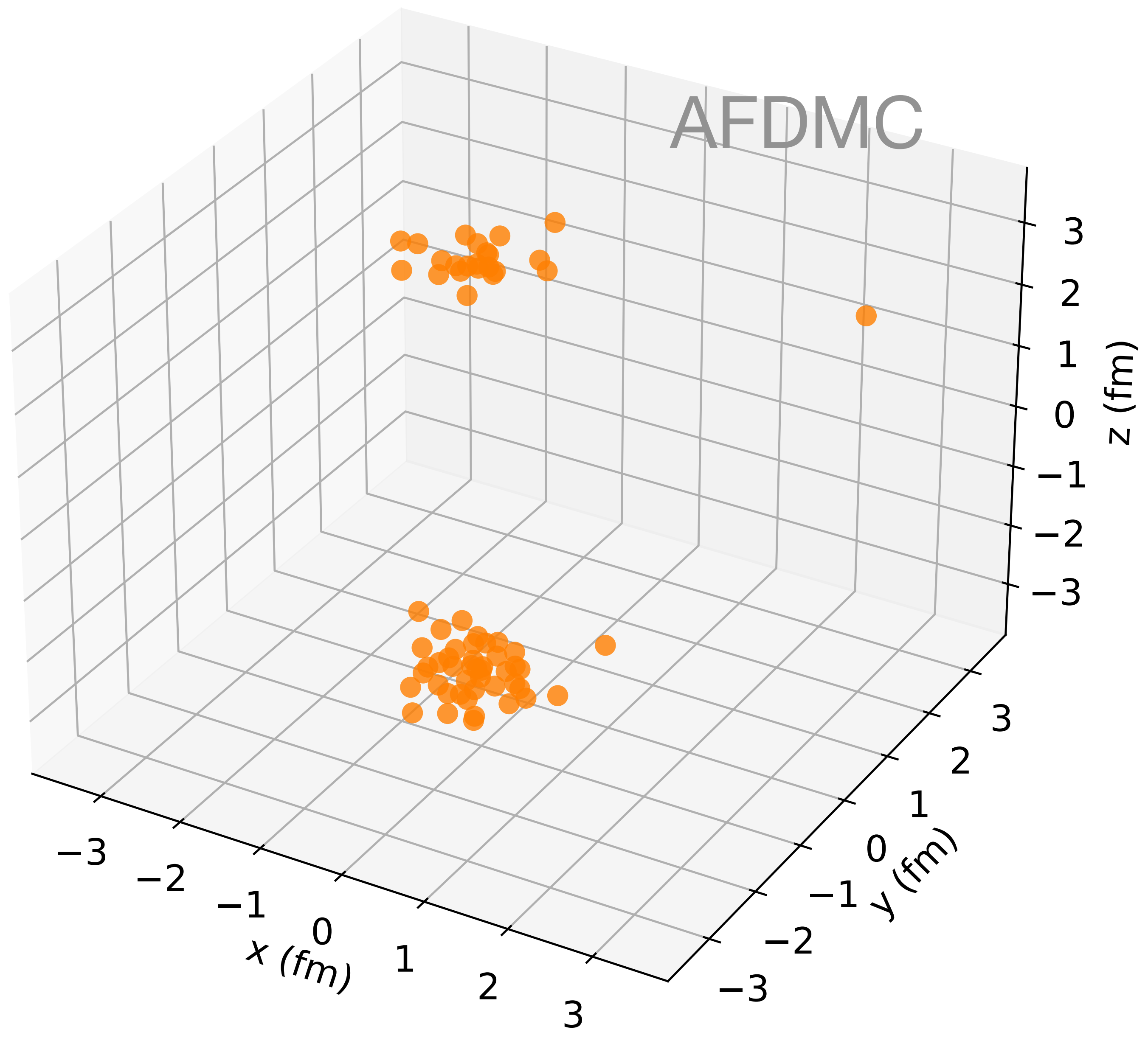


Model	c_D	c_E
Ia	3.666	−1.638
Ib	−2.061	−0.982
IIa	1.278	−1.029
IIb	−4.480	−0.412

Spectra of light nuclei and charge radii in good agreement with data but….



- ….. relatively large and negative values of c_E: "collapse" of PNM, whose energy per particles became large (~ several GeV per particle).
- The collapse is associated with the formation of "droplets" of closely packed neutrons, ultimately caused by the attractive nature of the cE term in the 3N force.



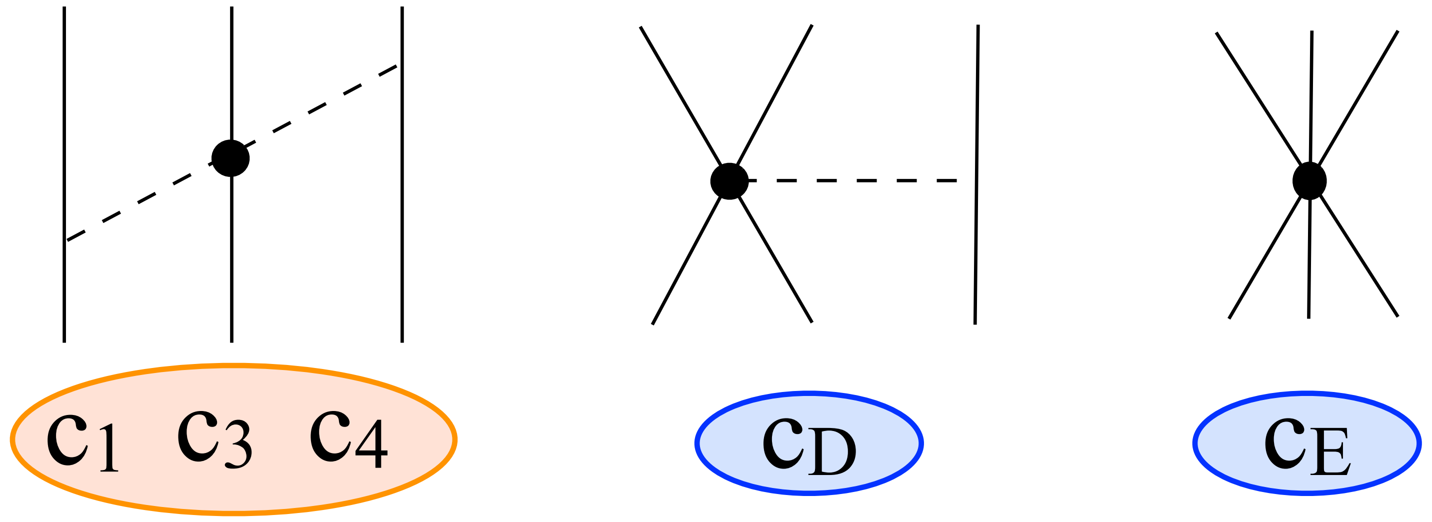
Lovato, MP *et al.* *PRC*105 (2022) 055808

a single scattering observable not too constraining (correlated with energy of ^{3}H)

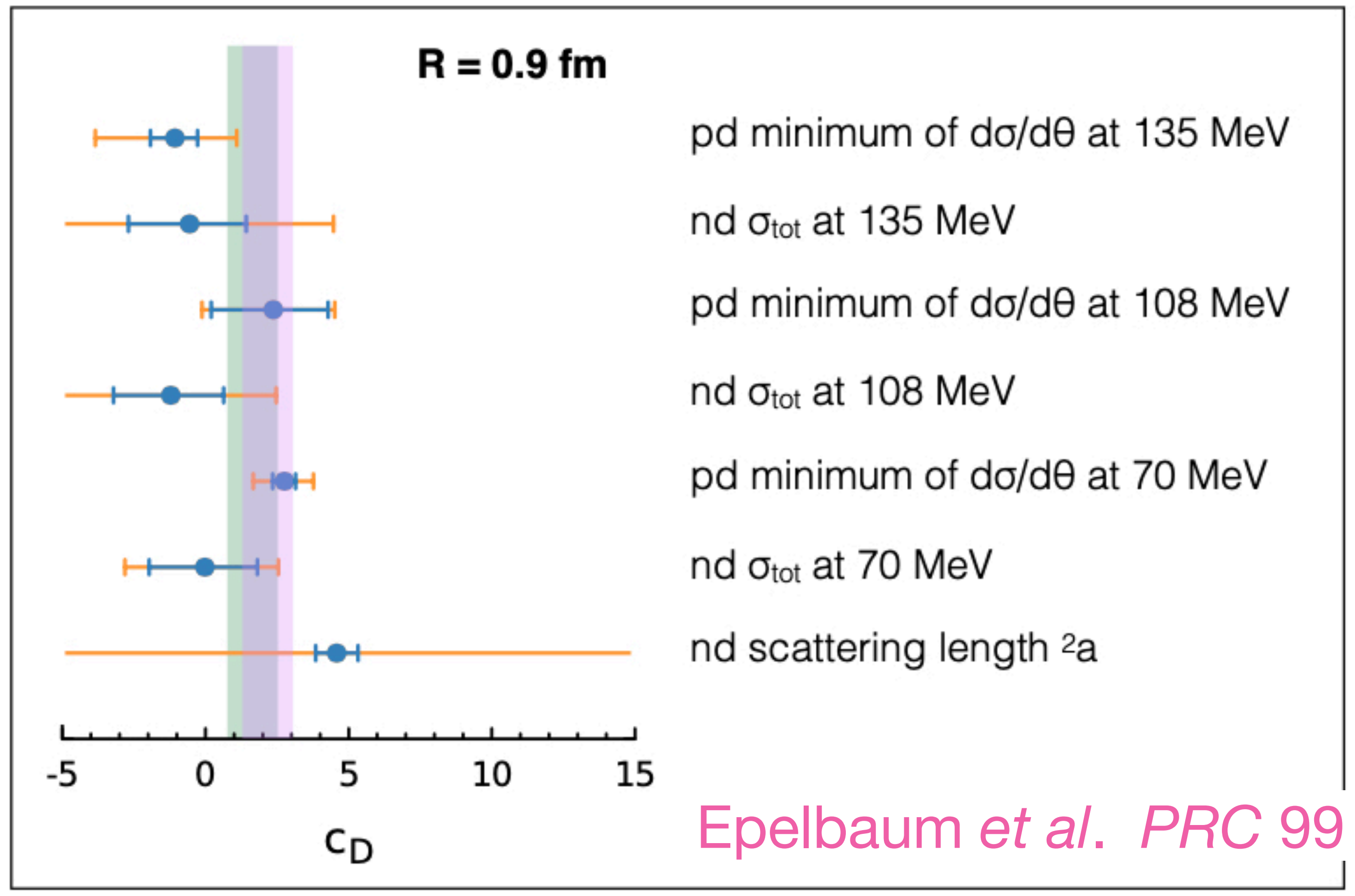
Fits of 3N Interactions: three-body scattering cross sections

- Inclusion of 3N forces at N2LO:

Constrained from πN scattering or NN: ex Hoferichter et al., Phys .Rept. 625 (2016) 1

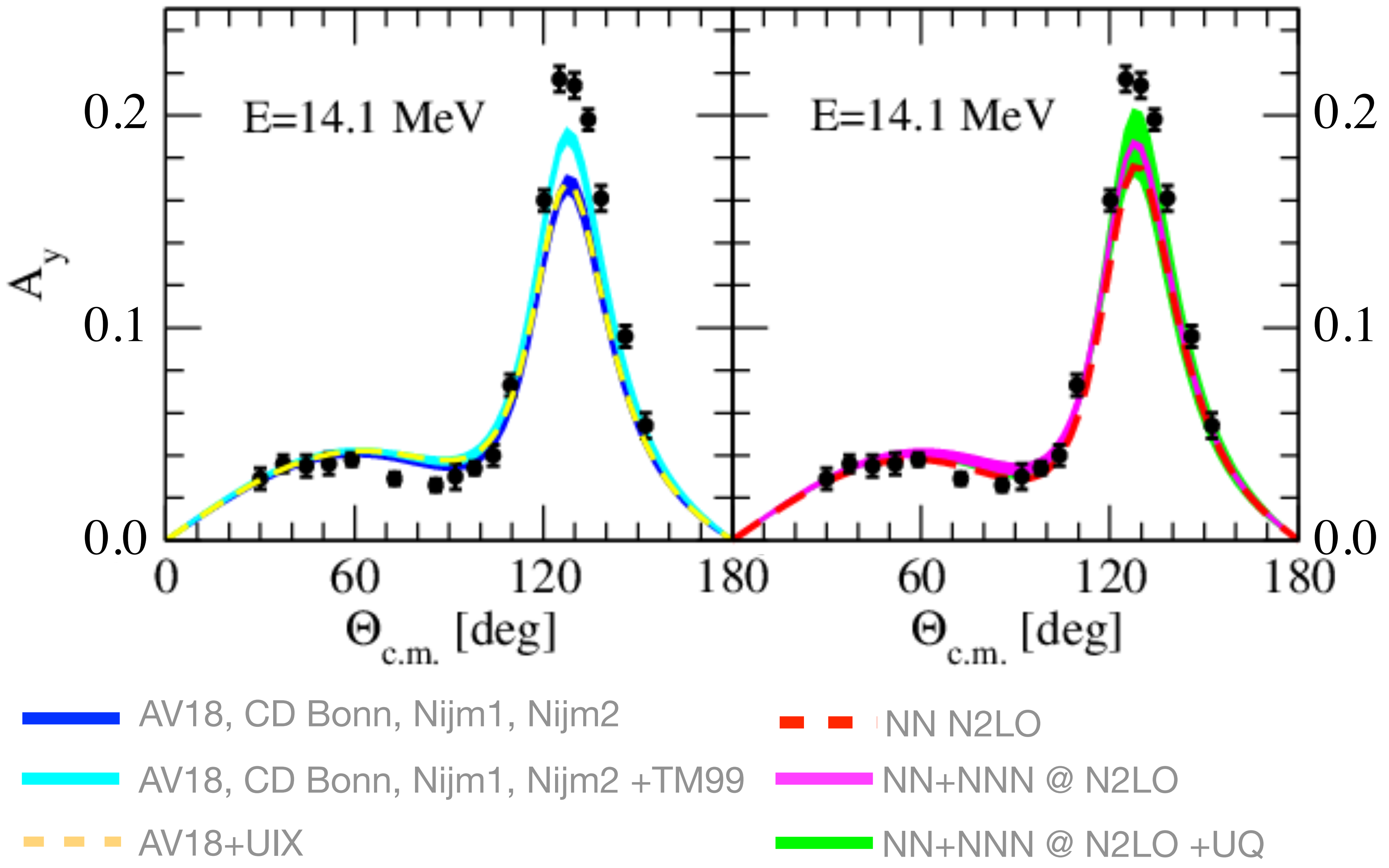


a more global fit using several observables more robust!!

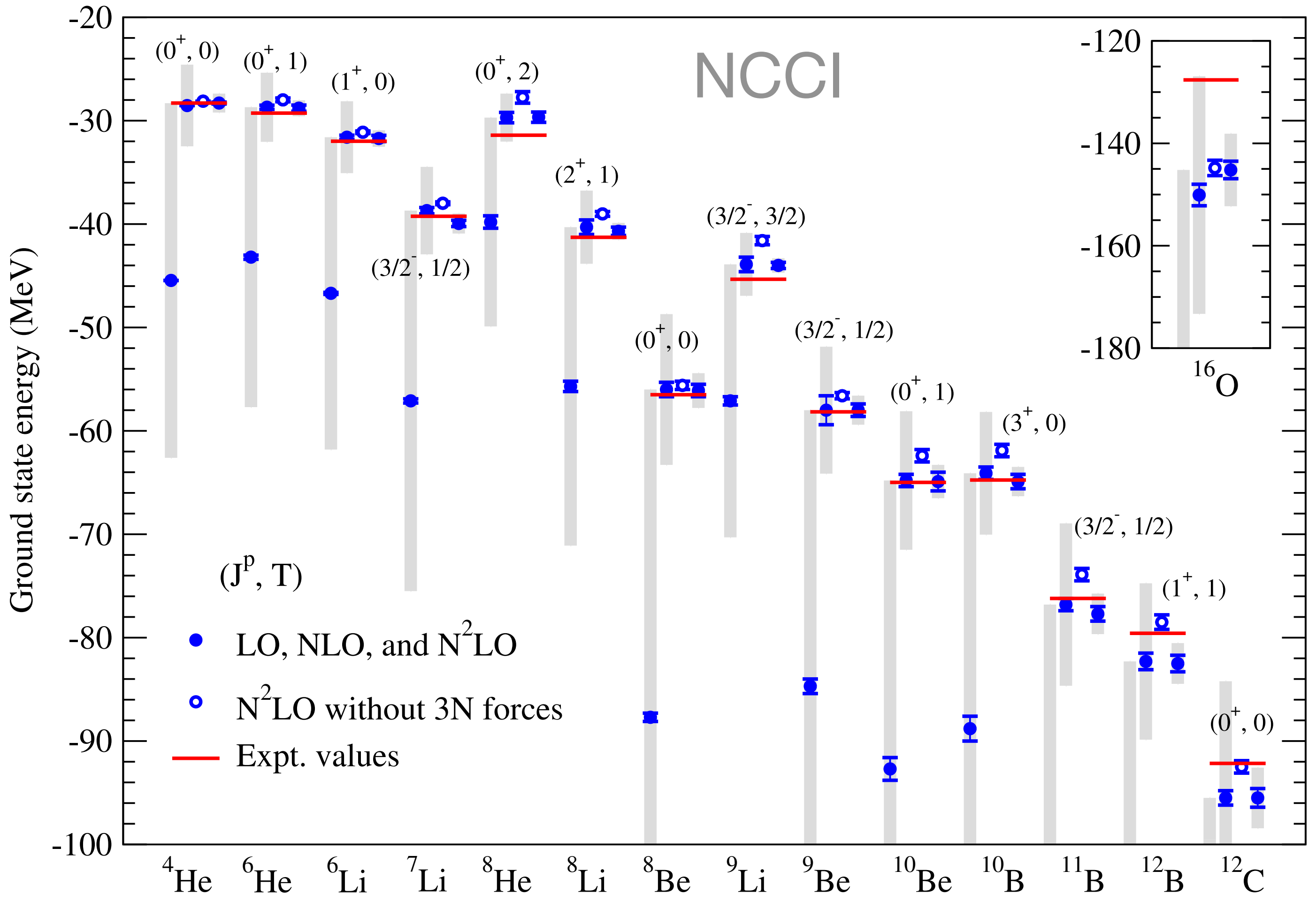


Epelbaum *et al.* *PRC* 99 (2019) 2, 024313

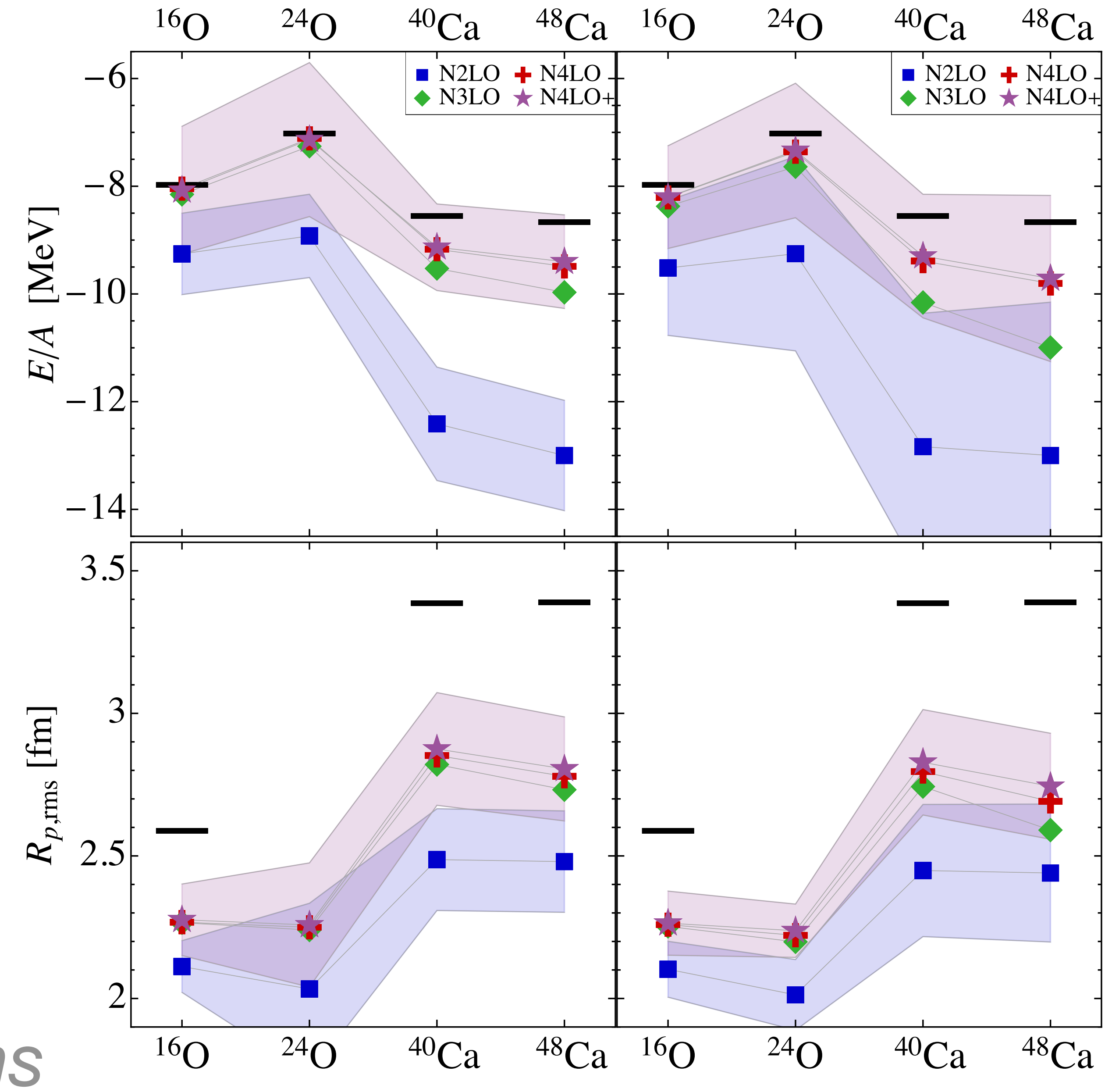
The neutron analyzing power A_y in nd elastic scattering at E_n = 14.1 MeV Epelbaum *et al.* *PRC* 99 (2019) 2, 024313



Ground-state energies in light nuclei



IM-NCSM IM-SRG



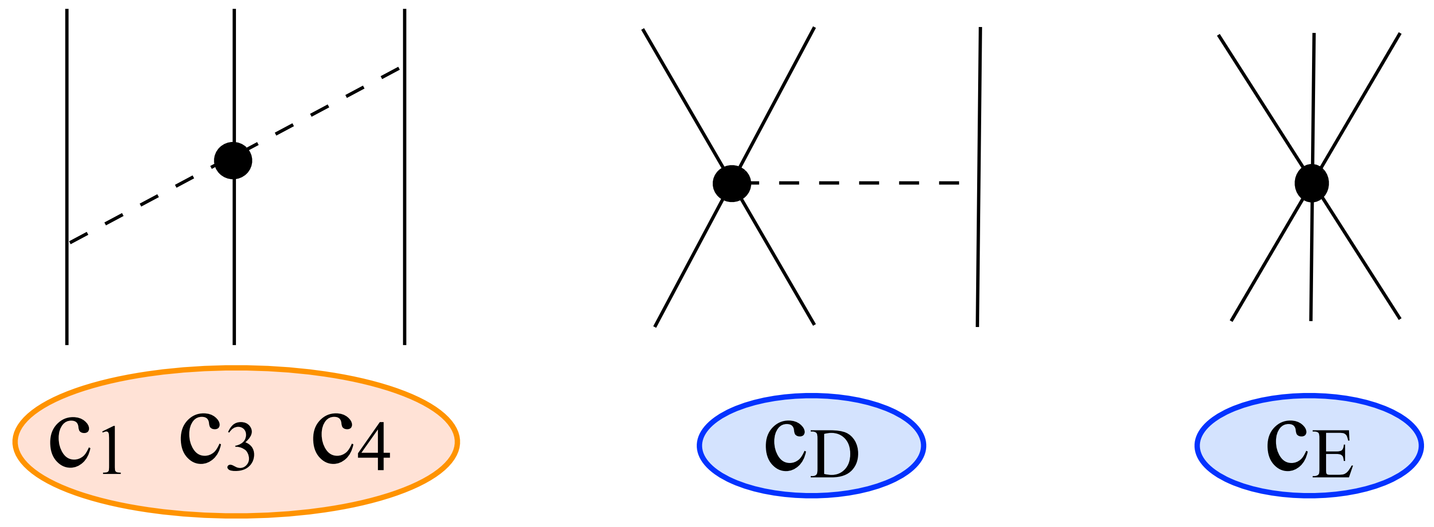
Indication that subleasing 3N contact interactions are relevant to solve the discrepancies!

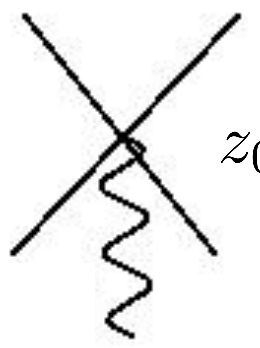
Maris *et al.* e-Print: 2206.13303 (2022)

Fits of 3N Interactions: triton beta decay half life

- Inclusion of 3N forces at N2LO:

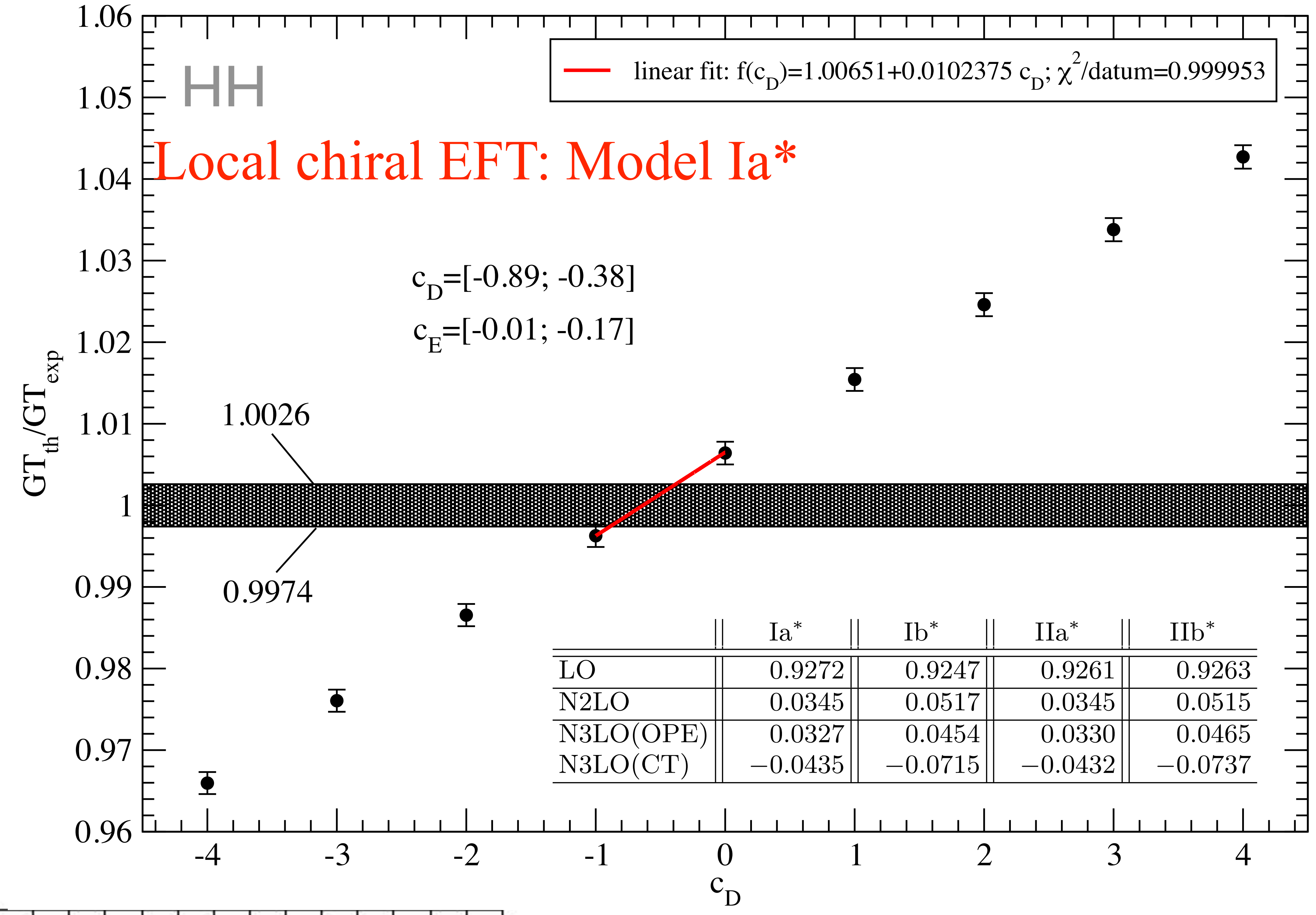
Constrained from πN scattering or NN: ex Hoferichter et al., Phys .Rept. 625 (2016) 1



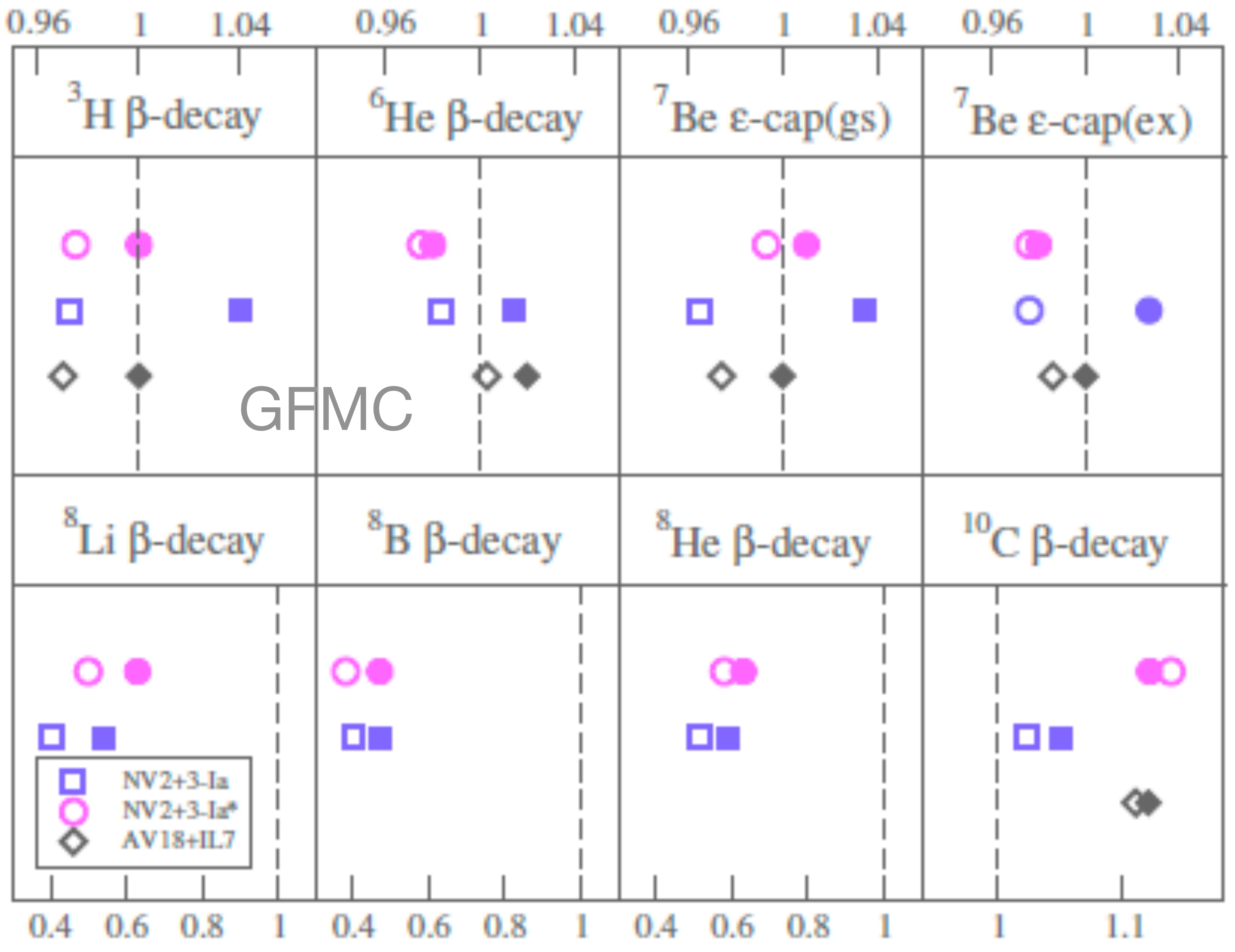


$$z_0 = \frac{g_A}{2}\frac{m_\pi^2}{f_\pi^2}\frac{1}{(m_\pi R_S)^3}\left[-\frac{m_\pi}{4\,g_A\,\Lambda_\chi}c_D + \frac{m_\pi}{3}(c_3 + 2\,c_4) + \frac{m_\pi}{6\,m}\right]$$

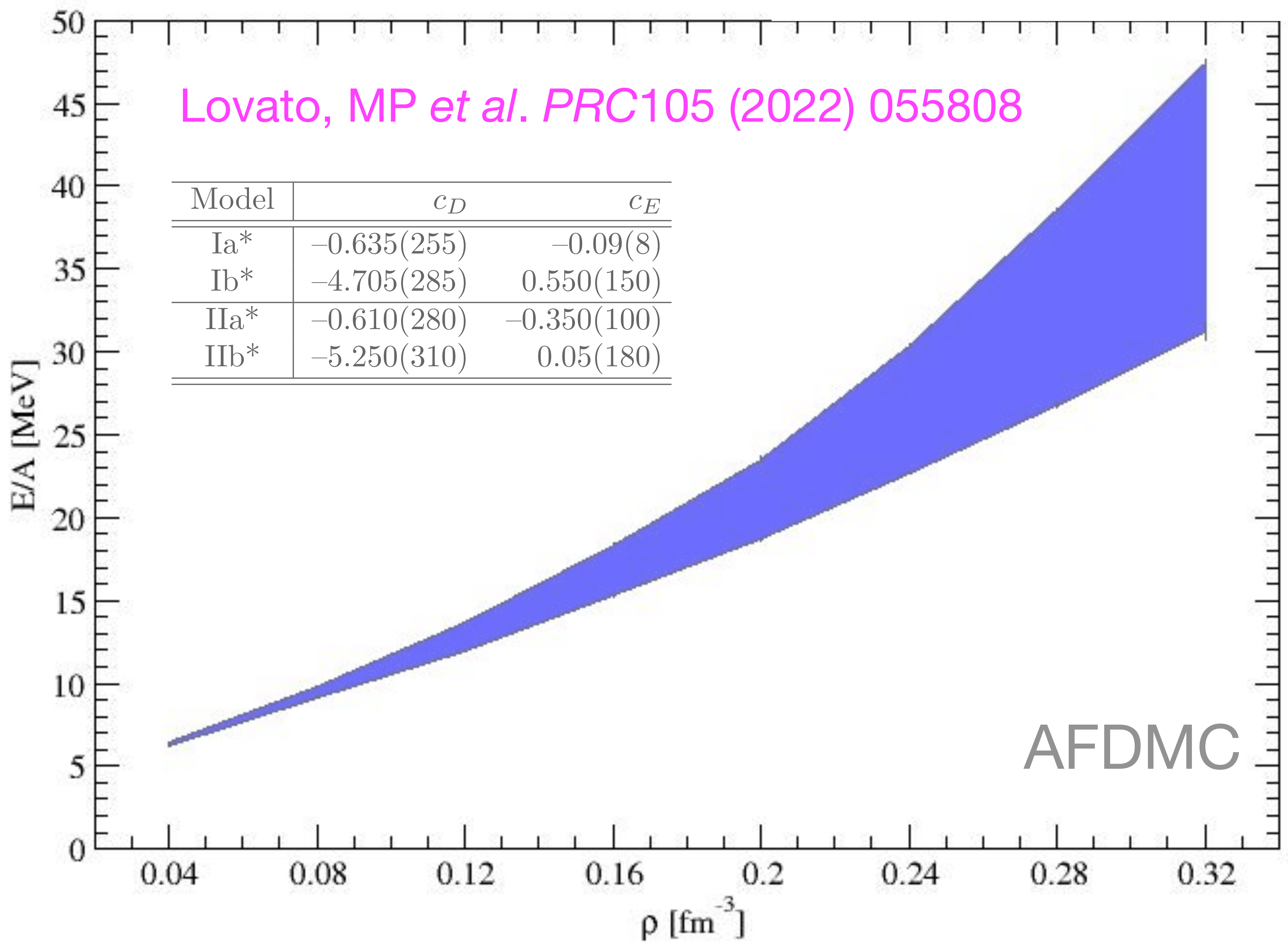
Baroni, MP *et al*. *PRC* 98 (2018) 4, 044003



	Ia*	Ib*	IIa*	IIb*
LO	0.9272	0.9247	0.9261	0.9263
N2LO	0.0345	0.0517	0.0345	0.0515
N3LO(OPE)	0.0327	0.0454	0.0330	0.0465
N3LO(CT)	−0.0435	−0.0715	−0.0432	−0.0737



G. King, MP *et al*. PRC 102, 025501 (2020)

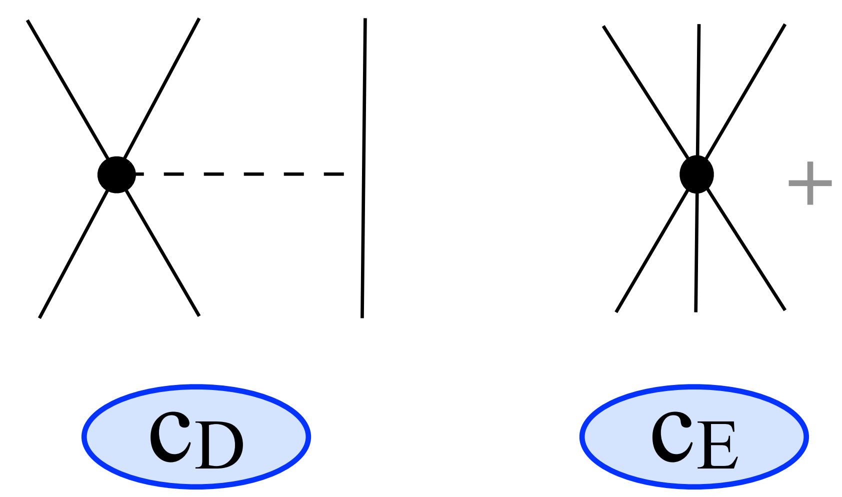


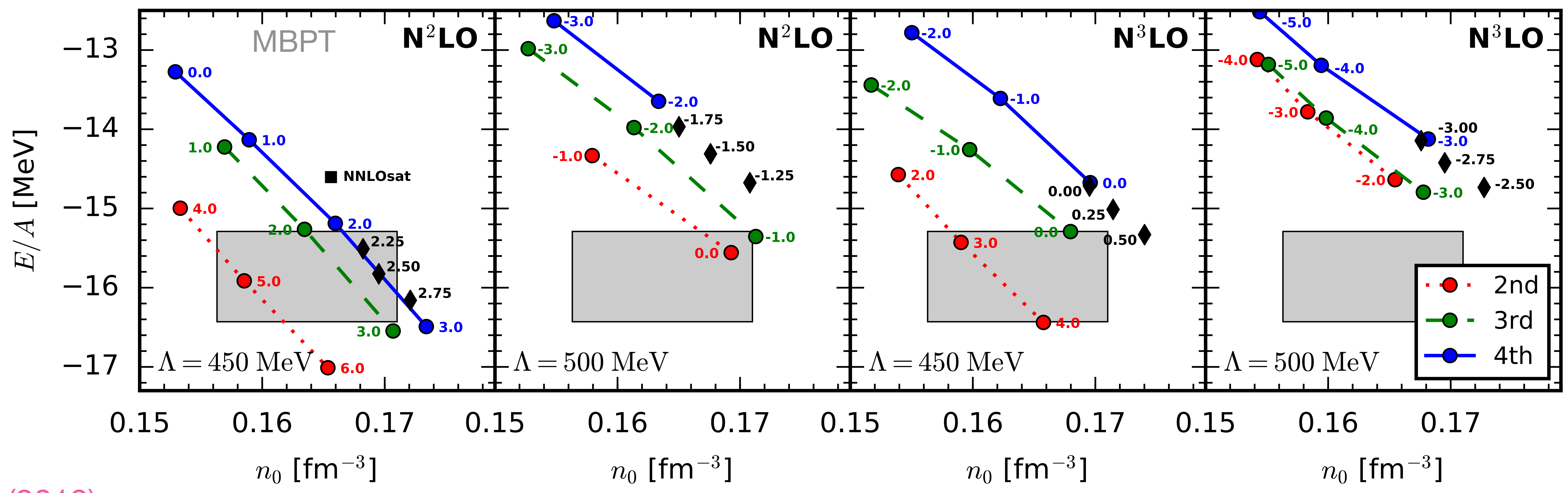
Model	c_D	c_E
Ia*	−0.635(255)	−0.09(8)
Ib*	−4.705(285)	0.550(150)
IIa*	−0.610(280)	−0.350(100)
IIb*	−5.250(310)	0.05(180)

- Model dependence of the EOS at three-body level $\rho = 2\rho_0$ (~16 MeV)
- The exp error on the 3H beta decays in the NV2+3s* (numbers in parenthesis) is not propagated yet

Fits of 3N Interactions: nuclear matter saturation point

- Inclusion of 3N forces at N2LO and N3LO:

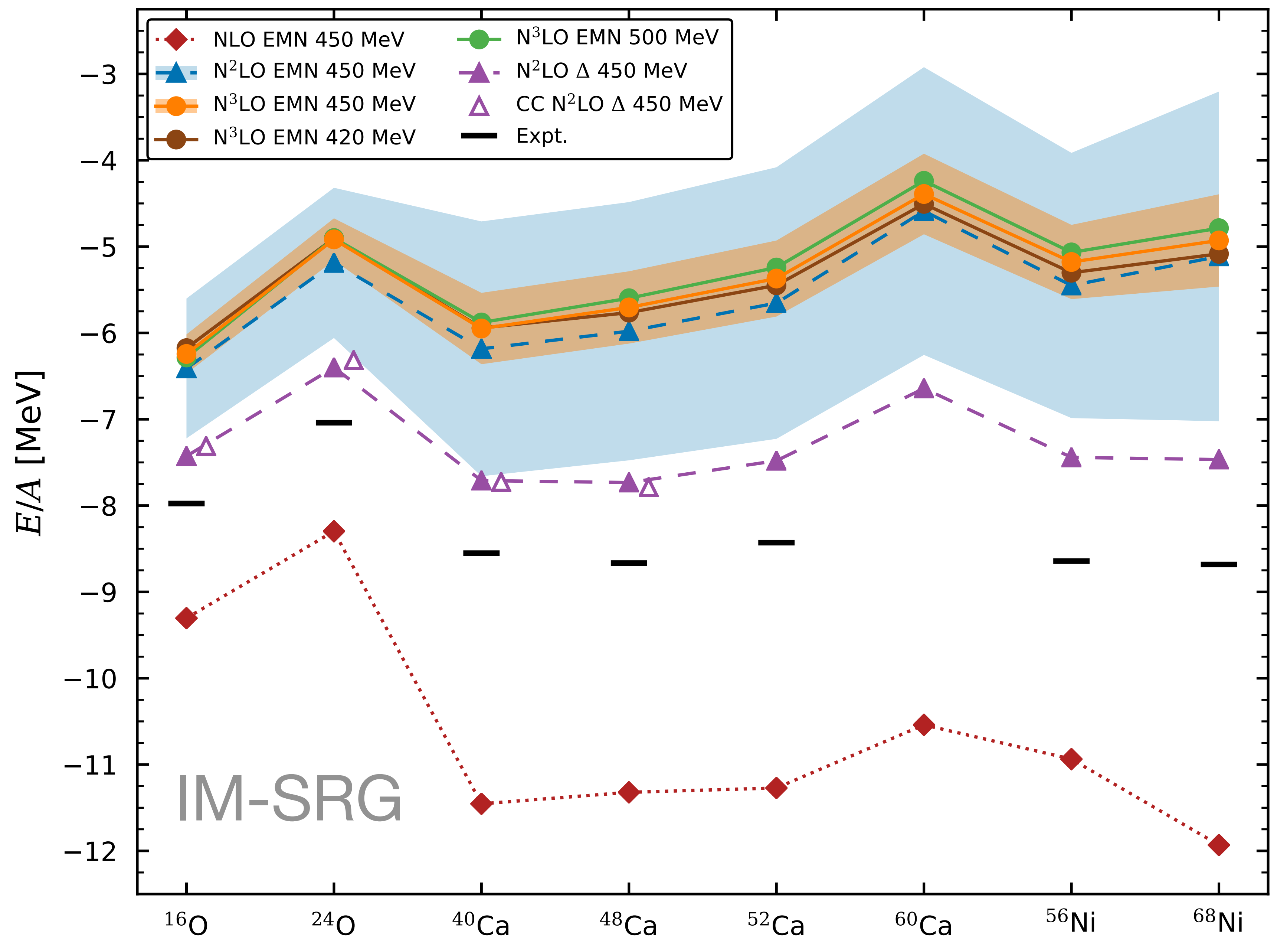


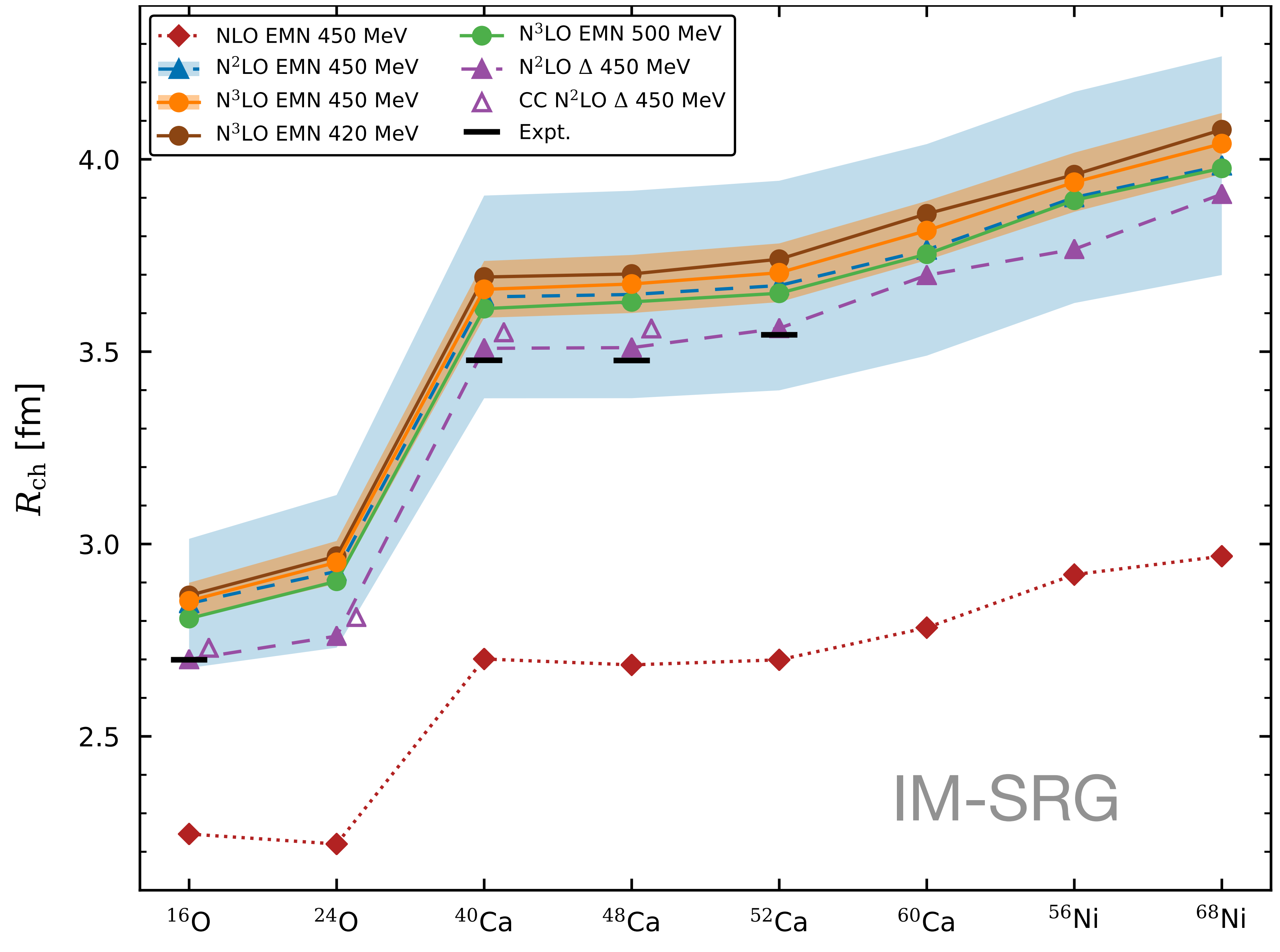


Drischler et al., PRL 122 (2019) 042501

(Thursday plenary session)

Hoppe et al. PRC 100, 024318 (2019)

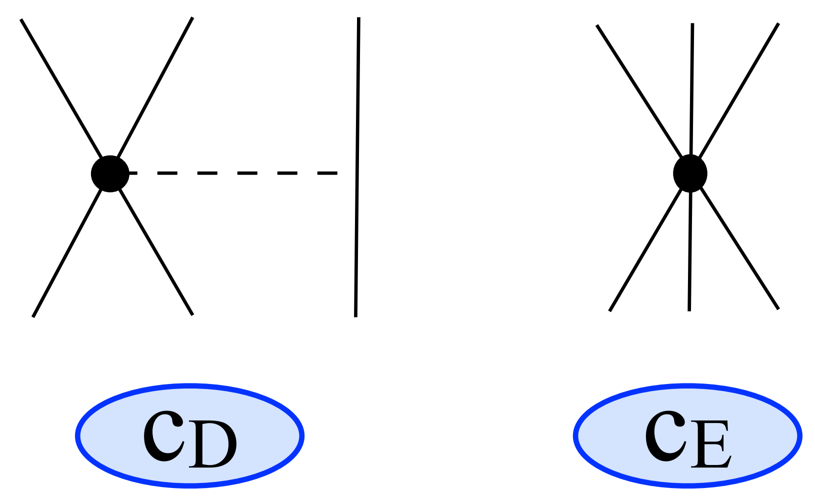




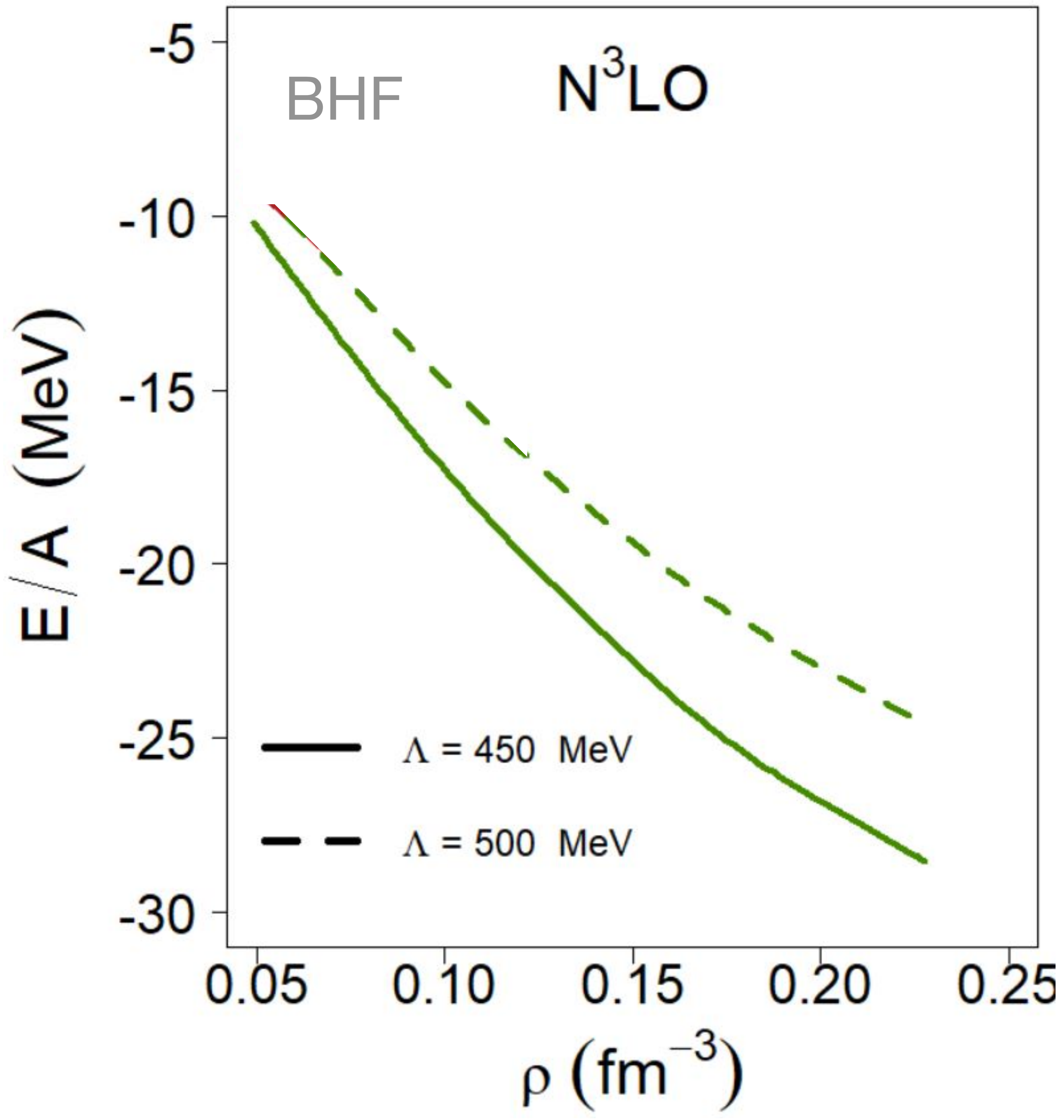
- Use nuclear matter saturation energy and density to constrain LECs
- Reasonable reproduction of both quantities possible
- Results for medium-mass nuclei still not satisfactory

Fits of 3N Interactions: g.s. energies of nuclei

- Inclusion of 3N forces at N2LO and N3LO:

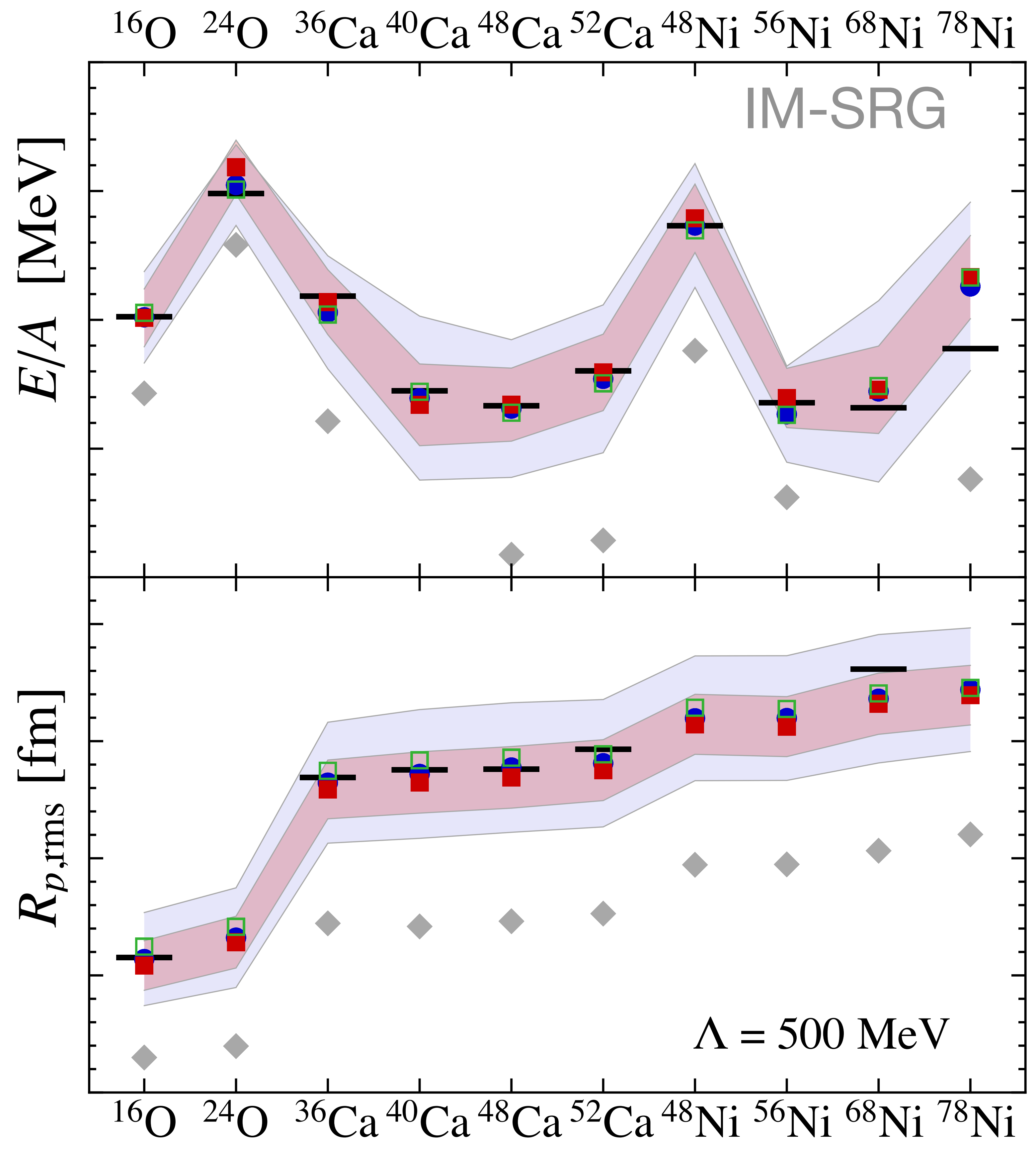


3N fitted to 3H and 16O g.s. energies



Sammarruca et al., PRC **102**, 034313 (2020)

Constraints from the few-nucleon system and a relatively light nucleus such as ^{16}O produce chiral interactions which are excessively attractive when applied in nuclear matter showing no sign of saturation.



Huther *et al.*, PLB **808**, 135651 (2020)

A good reproduction of both experimental energies and radii from p-shell nuclei up to the nickel isotopes within theoretical uncertainties

How to fix the LECs?

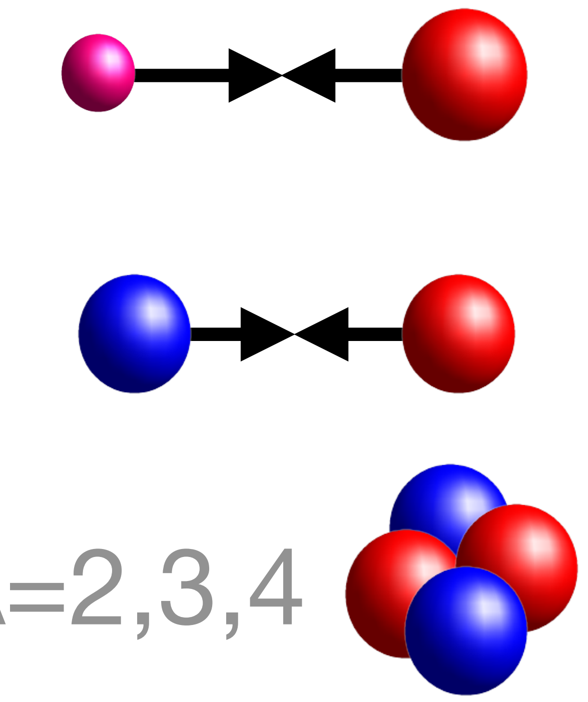
Second Challenge: *What is the best fitting procedure?*

"Traditional" approach: separate fits

piN

NN

Light nuclei, A=2,3,4



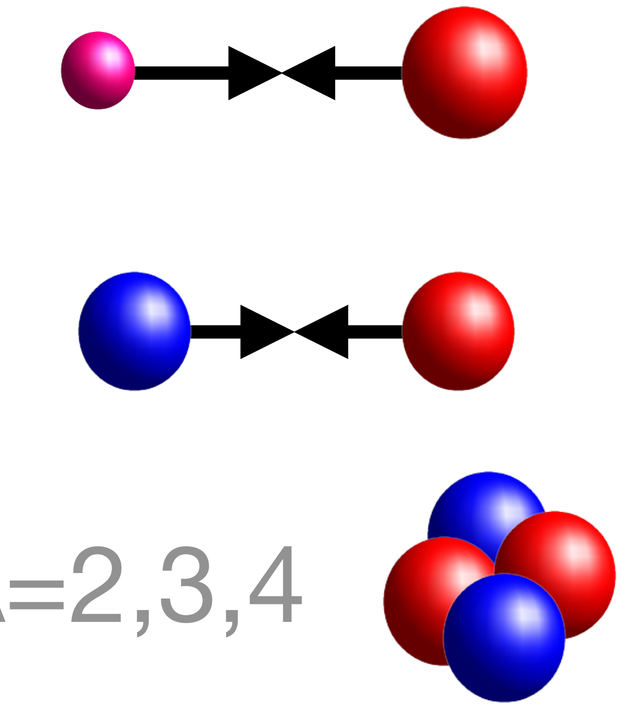
- D. R. Entem et al., Phys. Rev. C 96, 024004 2017
- A. Gezerlis et al., Phys.Rev. C 90, 054323 2014
- M. Piarulli et al., Phys. Rev. C, 024003 2015
- E. Epelbaum et al., Eur. Phys. J. A 51, 53 2015
- P. Reinert et al., Eur.Phys.J. A54 no.5, 86 2018
- Ekström et al. Phys. Rev. Lett. 110, 192502 2013 (NNLOopt)
- Ekström et al. Phys. Rev. C **97**, 024332 2018
- B. Carlsson et al., Phys. Rev. X, 011019 2015 (NNLOsep)
- .....

A "more modern" approach: simultaneous fits

piN

NN

Light nuclei, A=2,3,4

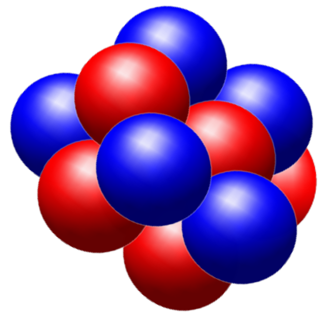


- B. Carlsson et al., Phys. Rev. X, 011019, 2015 (NNLOsim)

- Indications that simultaneous fits lead to more systematic EFT convergence
- Results for heavier systems not consistent with experimental results

Or

Heavier nuclei: A>12



- A. Ekström et al., J. Phys. G 42, 034003 2015 (NNLOsat)

- Good results for for $^{40}\mathrm{Ca}$ even though the fit included information up to oxygen.
- But NN scattering data included only up to 35 MeV E_{LAB}

Computationally a very challenging problem!

Optimization procedure for the LECs

Third Challenge: What is the best optimization scheme to find **a*** (LECs) in the parameter space?

"Conventional" least-square minimization:

Least-square objective function for a set of observables

$$\mathbf{a}^* = \min_{\mathbf{a}} \chi^2(\mathbf{a}) \quad \text{with} \quad \chi^2(\mathbf{a}) = \sum_{i=1}^{N_{\text{data}}} \left(\frac{o_i - t_i(\mathbf{a})}{\delta o_i} \right)^2$$

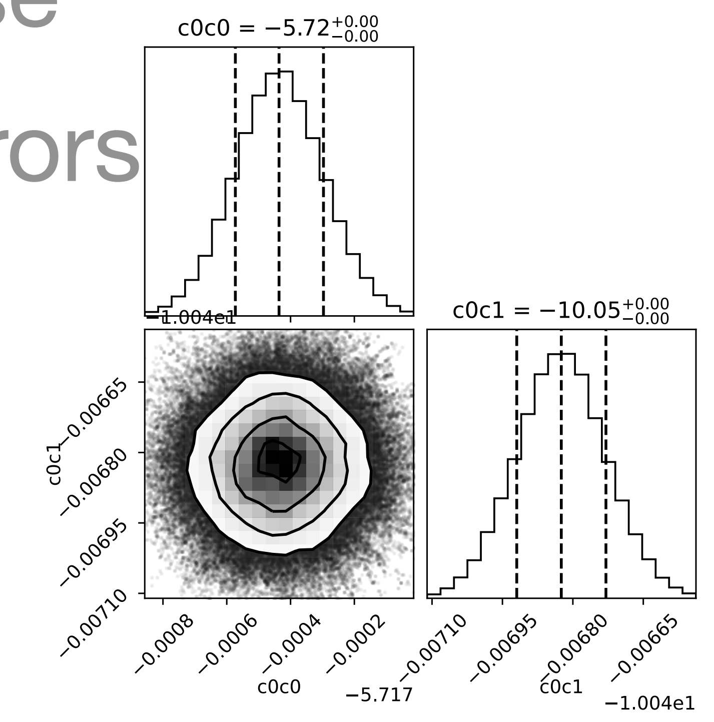
- Take δo_i to be the experimental error (or same modification to take into account theoretical errors)
- Many optimization techniques suitable for this problem such as POUNDers, Newtons Methods,….
- UQ addressed as: Covariance methods, Bootstrapping, standard protocols for chiral truncation errors, cutoff dependence
- over/under-fitting parameter ,..

Bayesian parameter estimation:

$$\underbrace{\mathrm{pr}(\mathbf{a}|\mathrm{Data}, I)}_{\text{posterior}} \propto \underbrace{\mathrm{pr}(\mathrm{Data}|\mathbf{a}, I)}_{\text{likelihood}} \times \underbrace{\mathrm{pr}(\mathbf{a}|I)}_{\text{prior}}$$

$$\propto e^{-\chi^2(\mathrm{a})/2}$$

- Particularly well suited for (any) EFT, but generally suited for theory errors
- Assumptions are made explicit (e.g. naturalness of LECs, truncation errors)
- Parameter estimation: conventional optimization recovered as special case
- Clear prescriptions for combining errors



BUQEYE collaboration

BAND collaboration

Emulation of observable calculations

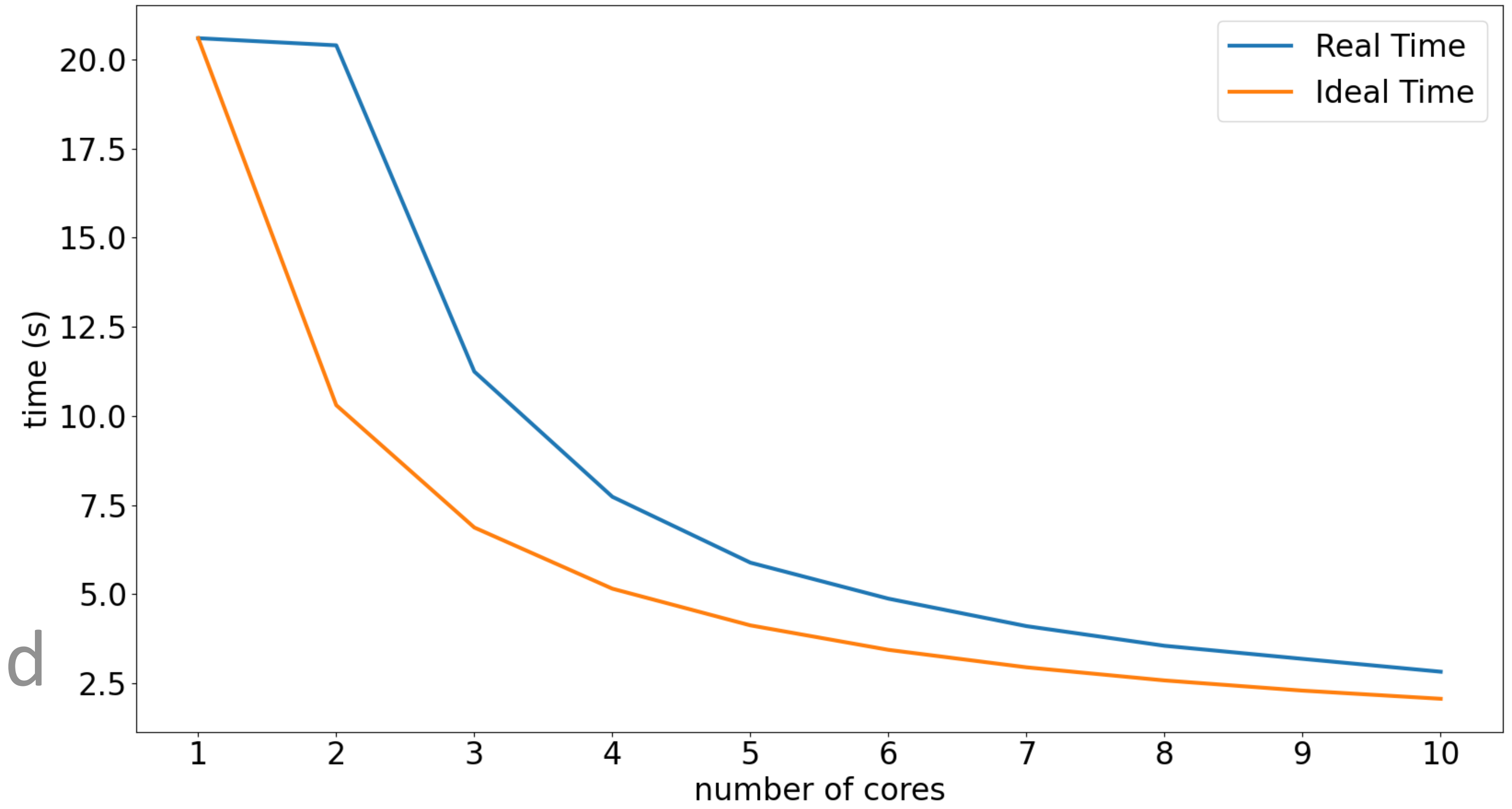
Challenge:

- A full Bayesian treatment requires millions of (MCMC) samples:
  - Likelihood calculation respect to NN data relatively expensive

    Serial likelihood calculation -> slow propagation
  - Improvement route: Parallel likelihood calculation

    Upsides: ✓ Quicker propagation
    ✓ Ability to leverage more resources

    Downsides: ✤ Inefficiencies due to MPI overhead and need for non-computing master processes



Jason Bub

Summer 2022 BAND Fellowship

Opportunity:

- Solution: Emulation
  - Use surmise from BAND Collaboration
  - Easier to emulate residuals than observables

Ozge Surer

Stefan Wild

Matt Plumlee

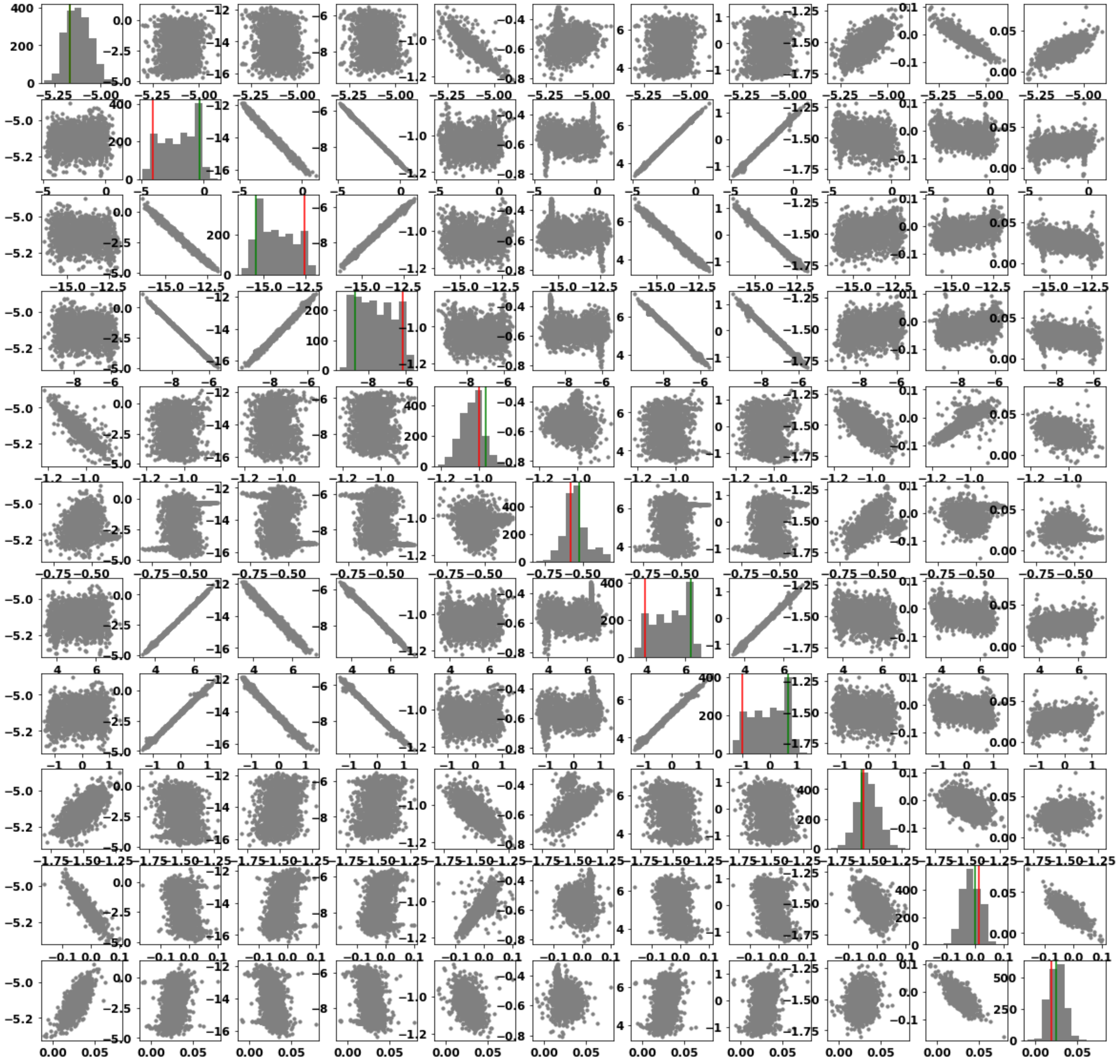
Emulator results: pionless EFT

Steps for emulation:

- Generate training dataset
  - Start with POUNDerS optimization
- Train Gaussian Process emulator
- Validate emulator

Promising steps at NLO

Preliminary!!!



Bub, MP et al in progress

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Emulation: How To

We can validate the emulator by comparing emulated value to simulated value.

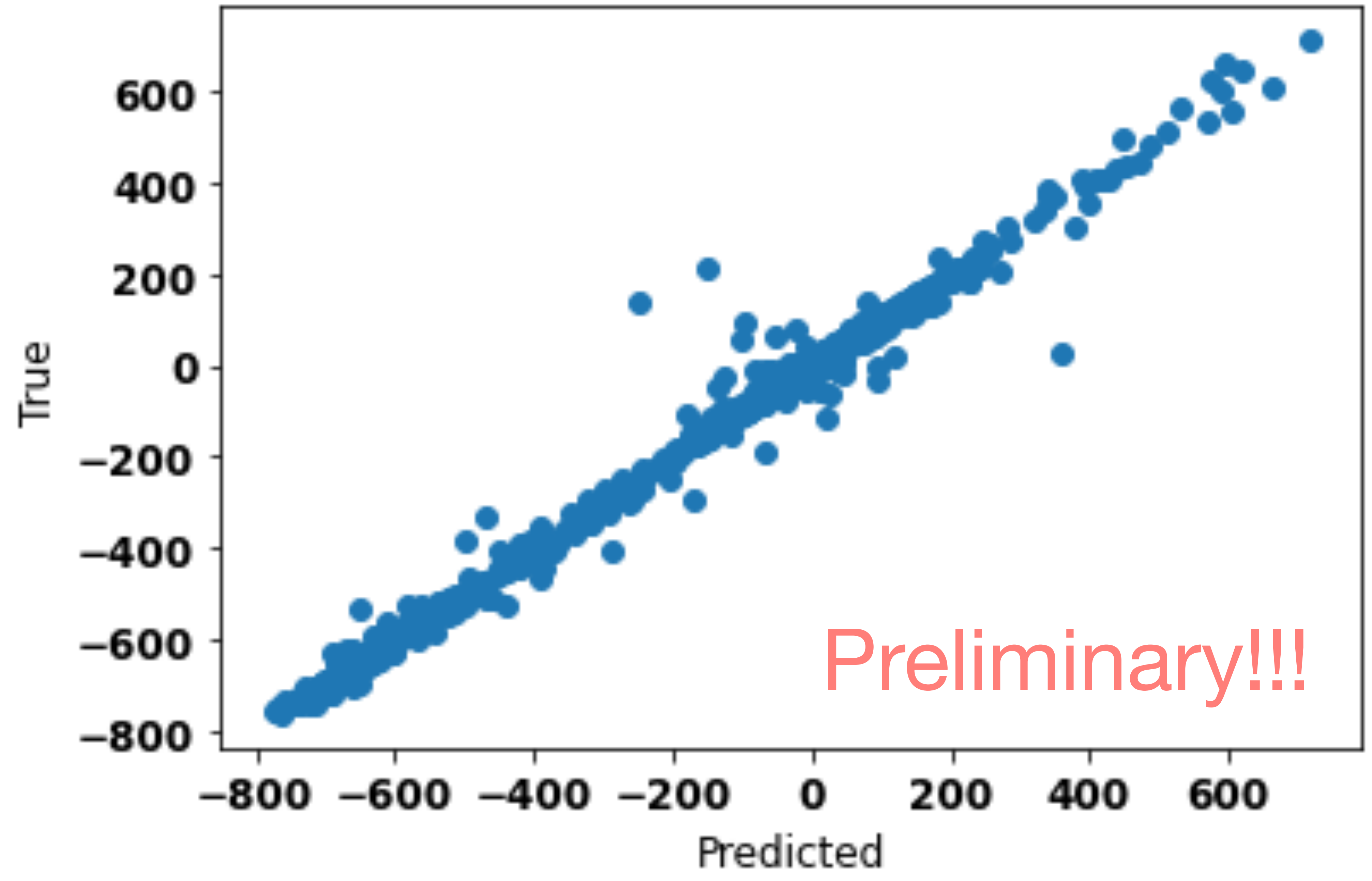
At NLO, emulator performs quite well.

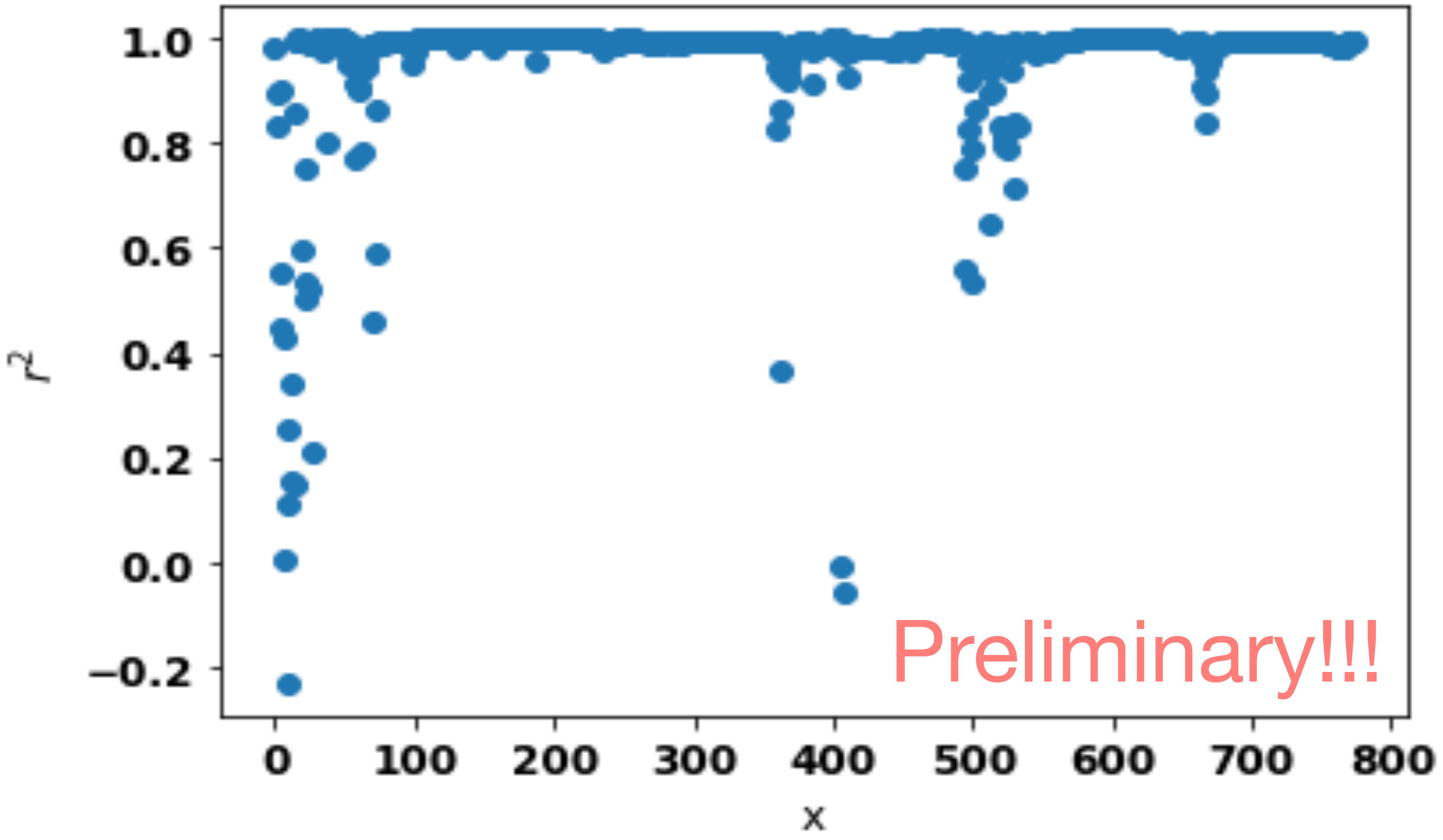
Challenge:

For N3LO, the parameter space is larger, requiring more thought in training point generation.

- Multiple POUNDerS trajectories?
- …..???

Work in progress!!!





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Full Bayesian truncation error

- To move to a full Bayesian approach, we include (uncorrelated) theoretical errors, see arXiv:2104.04441

$$\chi^2 = \sum_i \frac{(y_i - t_i)^2}{\sigma^2_{\mathrm{exp},i}} \to \chi^2 = \sum_i \frac{(y_i - t_i)^2}{\sigma^2_{\mathrm{exp},i} + \sigma^2_{\mathrm{ther},i}}$$

where

$$\sigma^2_{\mathrm{ther},i} = \frac{(y_{\mathrm{ref},i}\,\bar{c}\,Q_i^{n+1})^2}{1 - Q_i^2}, \quad Q_i = \frac{p_i}{\Lambda_b \sim m_\pi}$$

and $y_{\mathrm{ref},i}$ sets the scale of the correction for observable y_i, and $\bar{c}$ sets the magnitude of the correction.

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Dick Furnstahl

Daniel Phillips

Bub, MP et al in progress

LEC dependance on max fitting energy: pionless EFT

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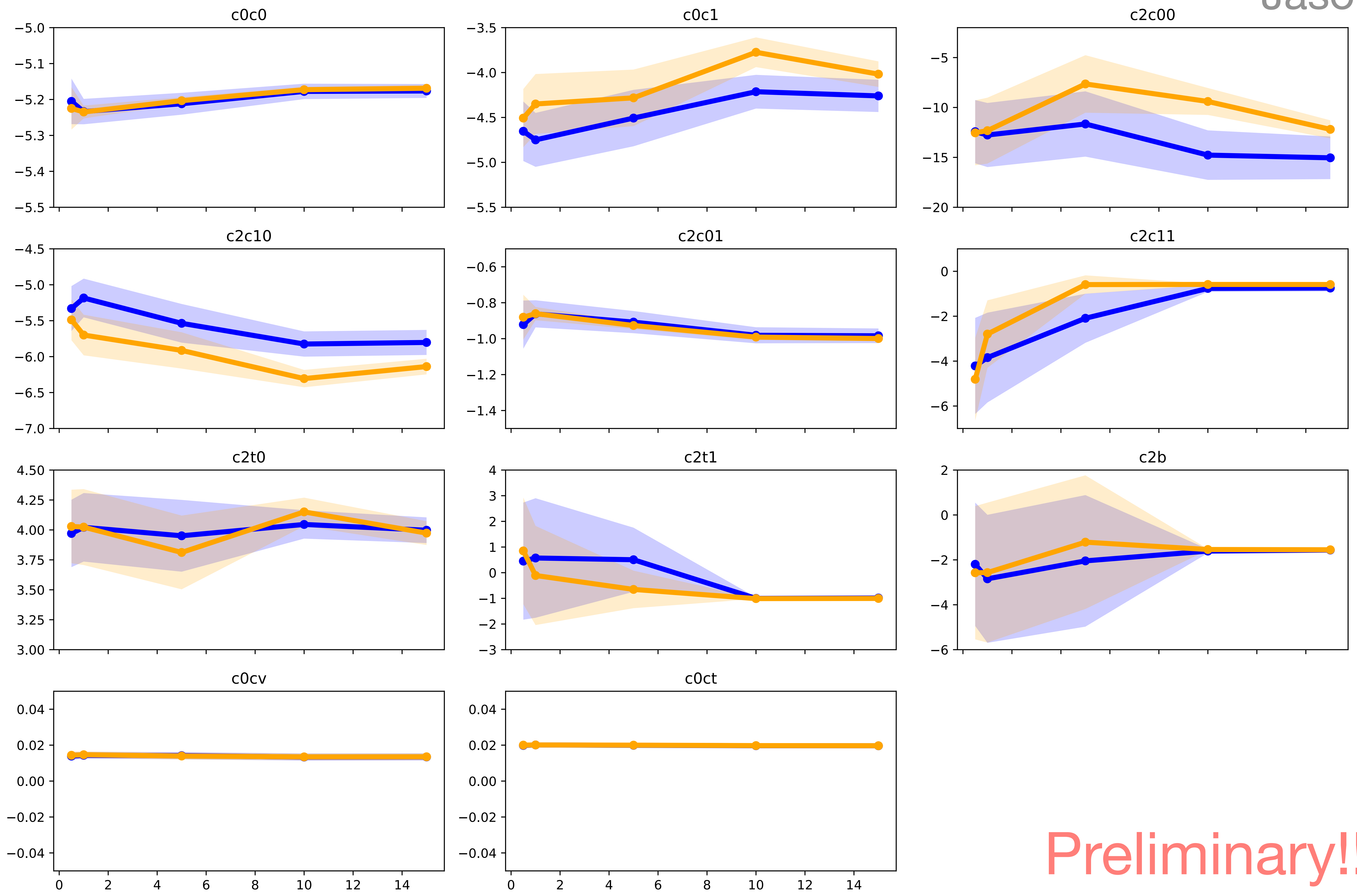
First step: Investigate how LECs change depending on max fitting energy at NLO

- No theory errors and uncorrelated theory errors have some differing dependance.
- Dependence should be resolved by correlations: correlated theory errors next!



Preliminary!!!

Summary:

- *(Progress):* Tremendous progress in ab-initio theory: algorithms and interactions
    - increased algorithm efficiency,
    - new algorithms (hybrid),
    - successful algorithm benchmarks,
    - advent of EFTs and UQ

- *(Progress):* Possibility to perform consistent calculations for nuclei and infinite matter, connecting nuclei observables to astrophysical quantities and observations

- *(Needs):* New protocols to build realistic nuclear interactions:
    which observables to use? In which mass range?
    Bayesian tools and UQ
    improvements in the formulation of the 3NFs

- *(Needs):* A deeper and more quantitative understanding of the connection between properties of matter and finite nuclei is needed

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