



STATISTICAL ANALYSIS AND OPTIMIZATION OF CHIRAL FORCES

ANDREAS EKSTRÖM



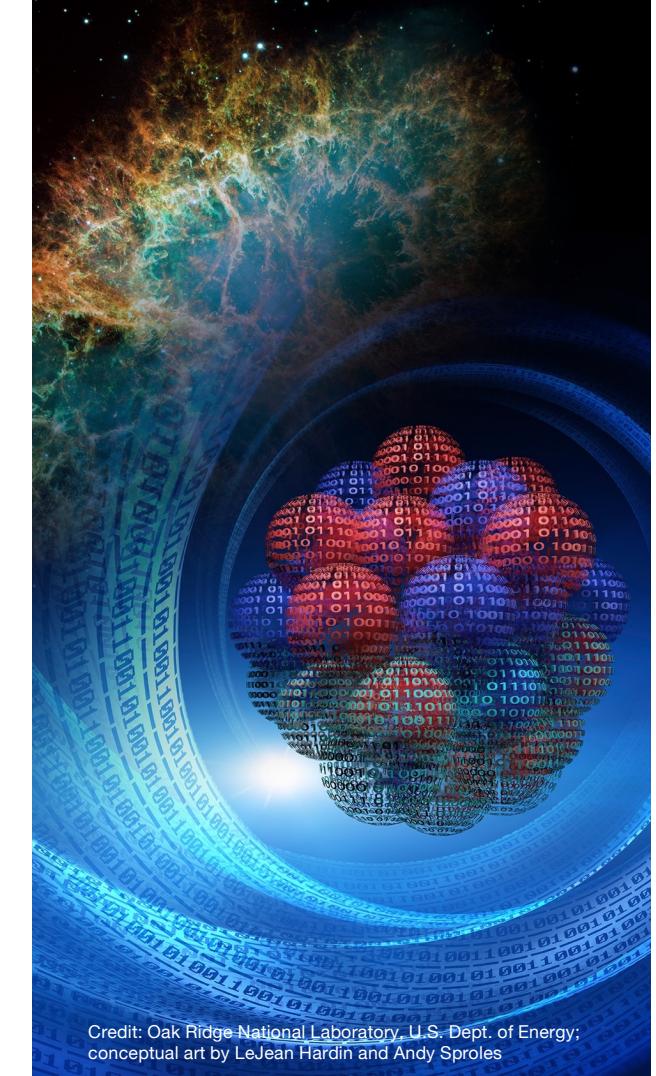
International Conference
Nuclear Theory in the Supercomputing Era – 2018 (NTSE-2018)
IBS Headquarters, Daejeon, Korea
29 October – 2 November 2018



OVERVIEW OF THIS TALK

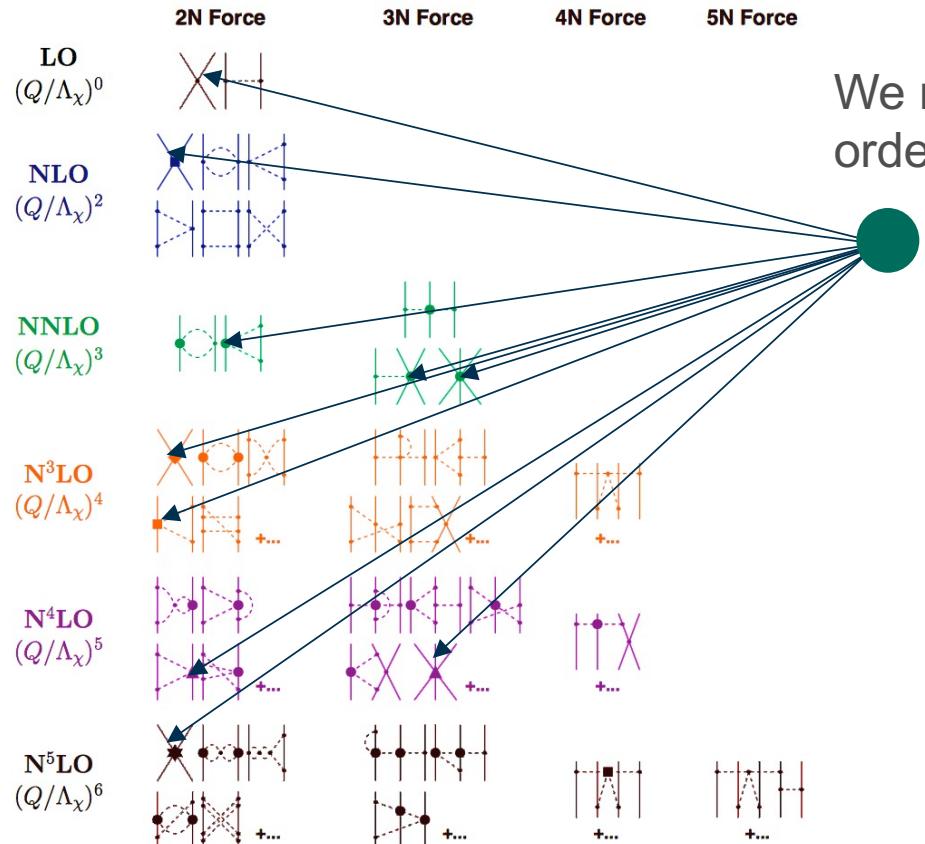
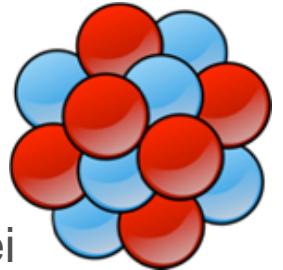
- Inferring the values of LECs from data.
B. D. Carlsson et al. Phys. Rev. X **6**, 011019 (2016)
AE, et al. Phys. Rev C **91**, 051301(R) (2015)
AE, et al. Phys. Rev. Lett. **110**, 192502 (2013)
- Uncertainty quantification.
B. Acharya, AE, and L. Platter arXiv: 1806.09481v1 [nucl-th]
B. D. Carlsson Phys. Rev. C **95**, 034002 (2017)
- **Ongoing:** Δ -full interactions and saturation.
AE, et al. Phys. Rev C **97**, 024332 (2018)
- **Ongoing:** Bayesian parameter estimation.
A. Johansson, AE, and C. Forssen, in preparation

Many thanks to all my collaborators and many colleagues in the community for enlightening and stimulating discussions!



Credit: Oak Ridge National Laboratory, U.S. Dept. of Energy;
conceptual art by LeJean Hardin and Andy Sproles

χ EFT FOR ANALYZING THE NUCLEAR INTERACTION

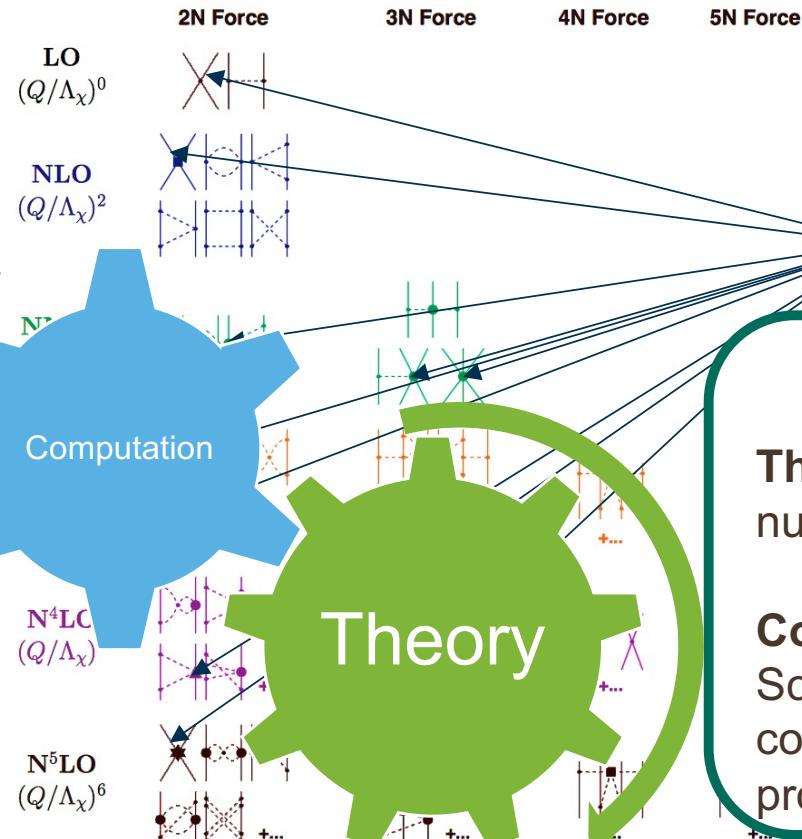
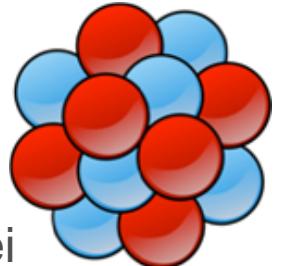


We must determine the relevant LECs in order to make predictions for atomic nuclei

Figure by R. Machleidt

Weinberg, van Kolck, Meissner, Epelbaum, Machleidt, Kaiser, Kaplan, Savage, Bernard, ...

χ EFT FOR ANALYZING THE NUCLEAR INTERACTION



We must determine the relevant LECs in order to make predictions for atomic nuclei

Nuclear Theory in the Supercomputing Era!

Theory challenge: how to formulate an EFT for atomic nuclei *and* harness its advantages (i.e. truncation errors) ?

Computing challenge: solving the many-nucleon Schrödinger equation, multi-dimensional parameter spaces, computationally expensive likelihood evaluations, error propagation to many-body systems, ...

Figure by R. Machleidt

Weinberg, van Kolck, Meissner, Epelbaum, Machleidt, Kaiser, Kaplan, Savage, Bernard, ...



EFFECTIVE FIELD THEORY IS SPECIAL

... since it promises to deliver observables in an *order-by-order* improvable fashion

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

For more on Bayes and EFT:
S. Wesolowski et al, J Phys G 43, 074001 (2016)
M. Schindler, D. Phillips, Ann. Phys. 324, 682 (2009)

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$$\mathcal{O}(p, \mathbf{a}) = \mathcal{O}^{\bar{\nu}}(p, \mathbf{a}) + \mathcal{O}_0 \sum_{\nu=\bar{\nu}+1}^{\nu_{\max}} c_\nu \left(\frac{p}{\Lambda_b} \right)^\nu$$

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Our typical setting: We want to say something about the unobserved quantities, and evaluate the fit of the parameters \mathbf{a} of the model, in the light of observed data and several sources of uncertainty.

Perhaps we also have some *a priori* belief in e.g.:

- the typical range of values for the expansion parameters ($c_\nu \sim 1$)
- the typical range of values for the LECs \mathbf{a}
- the expected breakdown scale Λ_b

How do we proceed ?

We have an idea about how observables depend on the unknowns \mathbf{a} via some data generating mechanism called the Likelihood.

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 S. Wesolowski et al, J Phys G 43, 074001 (2016)
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BAYESIAN INFERENCE

Bayes formulation of statistics offers a convenient method to guard against overfitting, to incorporating in prior knowledge (naturalness, the EFT error scaling), and to quantitatively compare models to each other!

$$P(\mathbf{a}|D, I) = \frac{P(D|\mathbf{a}, I)P(\mathbf{a}|I)}{P(D|I)}$$

Posterior **Likelihood** **Prior**
Evidence (normalization)

For more on Bayes and EFT:
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Likelihood Prior
Evidence (normalization)



If you can do Markov Chain Monte Carlo sampling “of your system”, then you can afford it. There are many pitfalls in the application of MCMC

There exists also “discounted” versions where you instead get approximate (surrogate, artificially intelligent?) descriptions of your posterior.

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Likelihood Prior

Posterior



Evidence (normalization)

Toolbox:

Marginalization

$$P(a_1|D, I) = \int da_2 \dots da_k P(\mathbf{a}|D, I)$$

$$P(D|\mathbf{a}, I) = \int dc_{\bar{\nu}+1} \dots dc_{\nu_{\max}} P(D|c_{\bar{\nu}+1} \dots c_{\nu_{\max}}, \mathbf{a}, I) \\ \times P(c_{\bar{\nu}+1} \dots c_{\nu_{\max}}|I)$$

Model comparison (Bayes factors)

$$\frac{P(M_1|D)}{P(M_2|D)} = \frac{\int P(D|\mathbf{a}, M_1)P(\mathbf{a}|M_1)d\mathbf{a}}{\int P(D|\mathbf{b}, M_2)P(\mathbf{b}|M_2)d\mathbf{b}}$$

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COMPUTATIONALLY EXPENSIVE. WORK IN PROGRESS. SEVERAL ONGOING EFFORTS.

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 M. Schindler, D. Phillips, Ann. Phys. 324, 682 (2009)

OPTIMIZATION OF THE LECS IN χ EFT

Challenge: find the point(s) \mathbf{x}^* in parameter space that minimizes some objective function, i.e:

$$\mathbf{x}^* = \underset{\mathbf{x}}{\operatorname{argmin}} f(\mathbf{x})$$

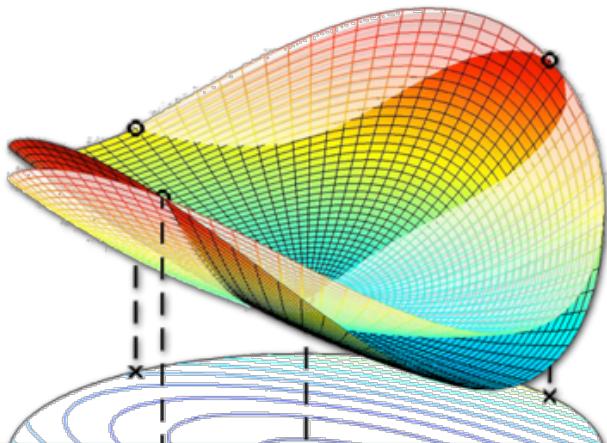
A common objective function: Reproduce thousands of nucleon-nucleon scattering data! This data can be partitioned in N_g groups where all data come from the same experiment. The systematic (norm) uncertainty within a group is lifted by including the second term.

$$f(\mathbf{x}) = \sum_{g=1}^{N_g} \min_{\nu_g} \left\{ \sum_{i=1}^{N_{d,g}} \left(\frac{\nu_g \mathcal{O}_{g,i}^{\text{model}}(\mathbf{x}) - \mathcal{O}_{g,i}^{\text{experiment}}}{\sigma_{g,i}} \right)^2 + \left(\frac{1 - \nu_g}{\sigma_{g,0}} \right)^2 \right\}$$

Finding an optimal point in a multidimensional parameter space is often very challenging, even if it is easy to evaluate the model as a function of its parameters. Any additional information is valuable.

- **Derivatives, excluded regions and/or dimensions in parameter space, ...**
- **Covariance structure of the theory and the data**

POUNDERS: MODEL-BASED OPTIMIZATION



POUNDERs exploits the known ‘squared-sum’ structure of the objective function.
POUNDERs works very well for us!

$$\min \left\{ f(x) = \frac{1}{2} \|F(x)\|_2^2 = \frac{1}{2} \sum_{i=1}^p F_i(x)^2 : x \in \mathcal{X} \subset \mathbb{R}^n \right\}$$

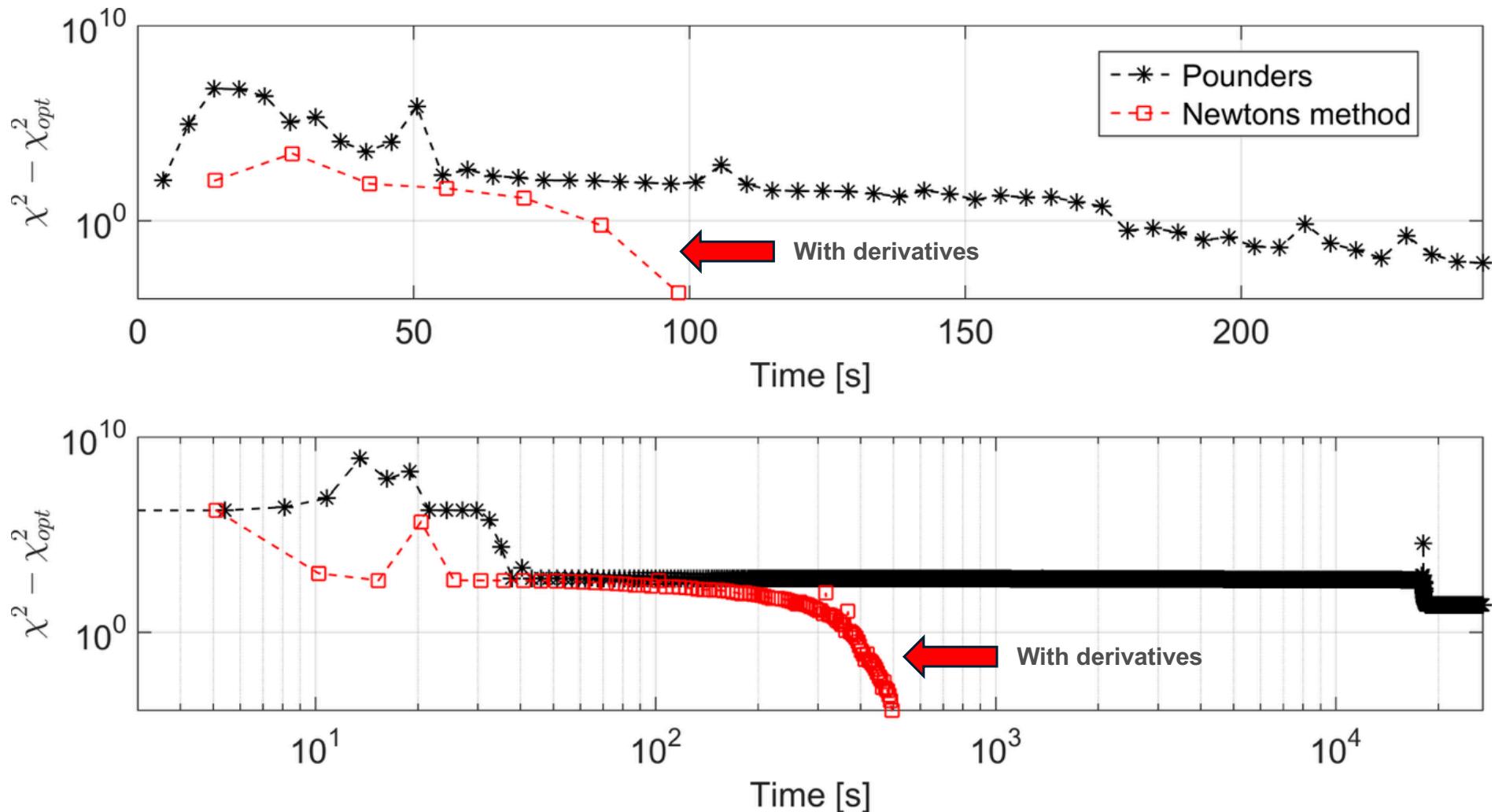
Exploit known structure (sum-of-squares) and setup interpolating quadratic model of each residual $F_i(x)$ centered around x^k .

$$q_k^{(i)} = F_i(x_k) + (x - x_k)^T g_k^{(i)} + \frac{1}{2}(x - x_k)^T H_k^{(i)}(x - x_k)$$

Solve for g_k and H_k by interpolating to subset of common function values. A master model uses second order information

$$m_k(x_k + \delta) = f(x_k) + \delta^T \sum_{i=1}^p F_i(x_k) g^{(i)} + \frac{1}{2} \delta^T \sum_{i=1}^p \left(g^{(i)} [g^{(i)}]^T + F_i(x_k) H^{(i)} \right) \delta$$

Stefan Wild, Argonne National Laboratory, Preprint ANL/MCS-P5120-0414



UQ: UNCERTAINTIES FROM ERRORS IN FIT DATA



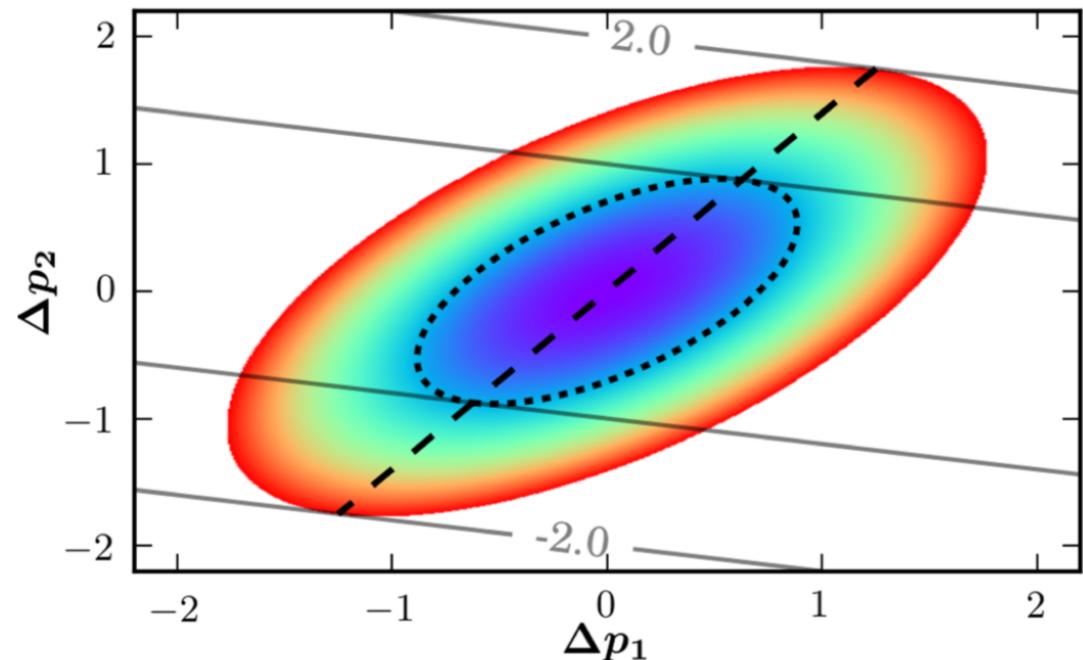
Small variations around the optimum gives

$$\chi^2(\boldsymbol{\alpha}_* + \Delta\boldsymbol{\alpha}) - \chi^2(\boldsymbol{\alpha}_*) \approx \frac{1}{2} (\Delta\boldsymbol{\alpha})^T \mathbf{H}(\Delta\boldsymbol{\alpha}),$$

where $H_{ij} = \frac{\partial^2 \chi^2(\boldsymbol{\alpha})}{\partial \alpha_i \partial \alpha_j} \Big|_{\boldsymbol{\alpha}=\boldsymbol{\alpha}_*}$

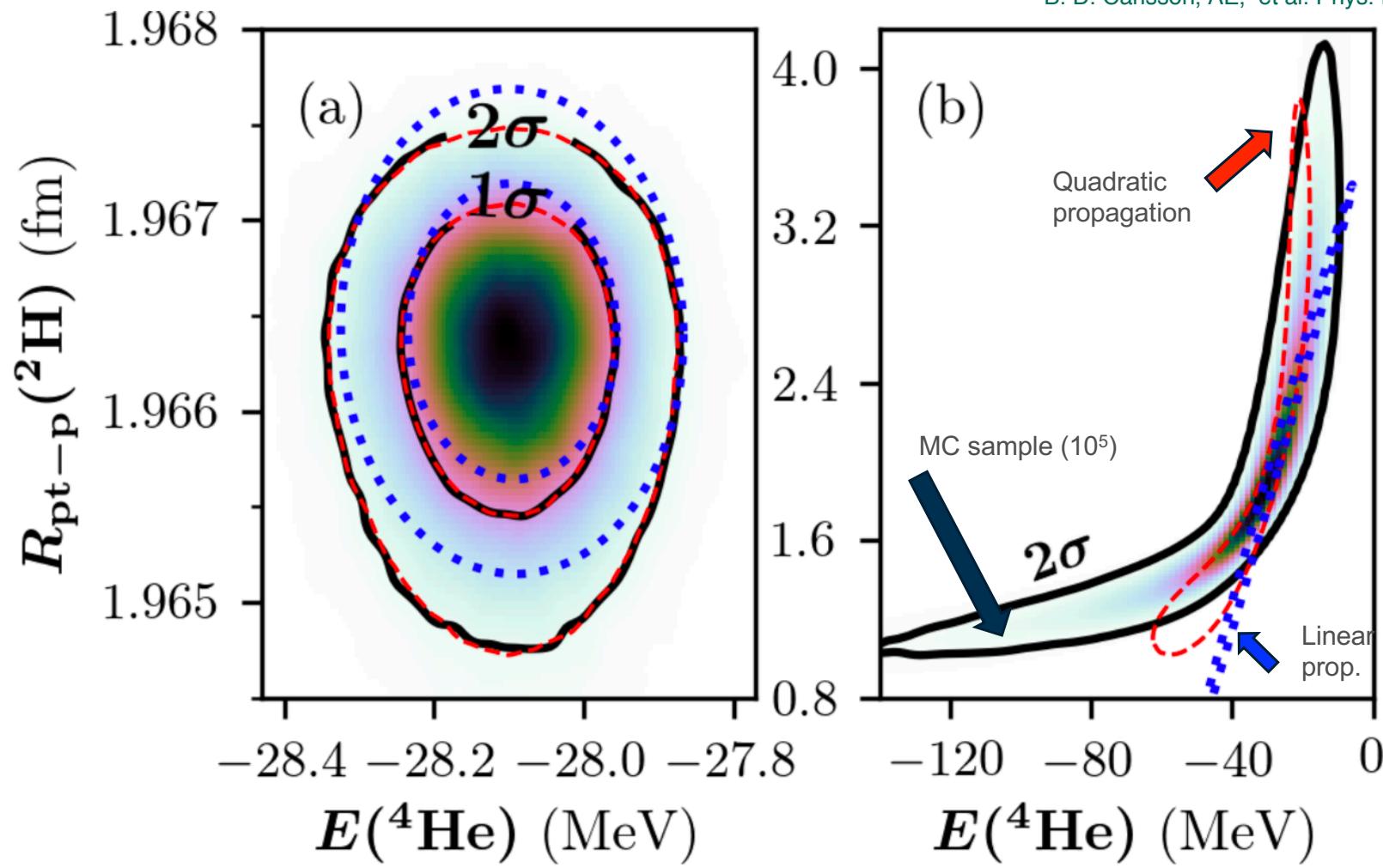
Linearized approximation to Covariance matrix of non-linear least squares objective function:

$$\text{Cov}(\boldsymbol{\alpha}_*) = 2 \frac{\chi^2(\boldsymbol{\alpha}_*)}{N_{\text{dof}}} \mathbf{H}^{-1}$$



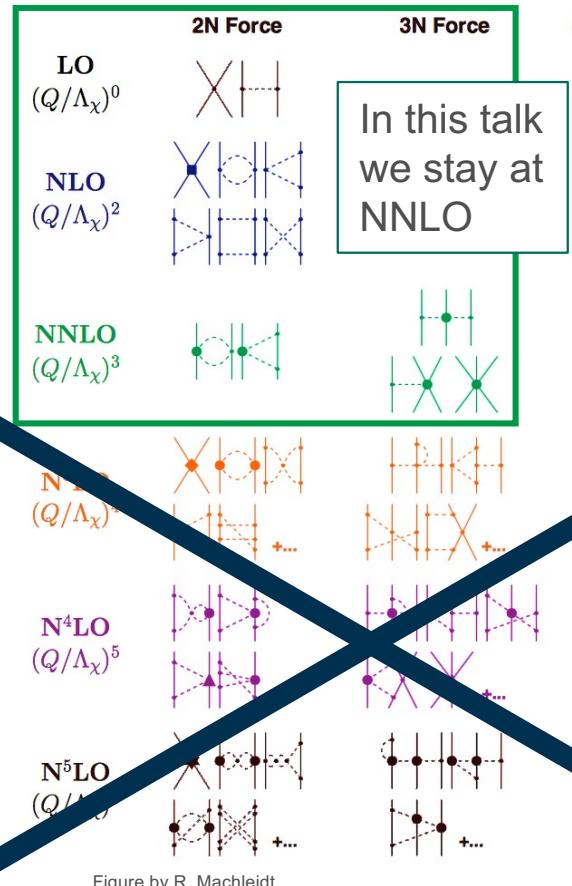
B. D. Carlsson, AE, et al. Phys. Rev. X **6**, 011019 (2016)

J Dobaczewski, W Nazarewicz, P-G Reinhard J. Phys. G: Nucl. Part. Phys. **41** (2014) 074001



Ellipses from Gaussians
“Boomerangs” traced numerically

ESTIMATING TRUNCATION ERRORS



- Effective field theories are special since they, by construction, offer a handle on the systematic uncertainty due to excluded higher-order terms (physics.)
- If we believe to have a convergent series, we can **estimate the next term**

$$\mathcal{O} = \mathcal{O}_0(c_0 Q^0 + c_1 Q^1 + c_2 Q^2 + ? Q^3 + \dots)$$

EFT expansion parameter

$$c_i = \max_{n < i} \{|c_n|\}, \quad \left(100 \times \frac{i}{i+1}\right) \% \text{ confidence}$$

For the expansion coefficients we assume iid and a boundless uniform prior distribution

E. Epelbaum et al., Eur. Phys. J. A **51**, 53 (2015)

For more on Bayes and EFT, see e.g.: M. Schindler, D. Phillips, Ann. Phys. 324, 682 (2009)

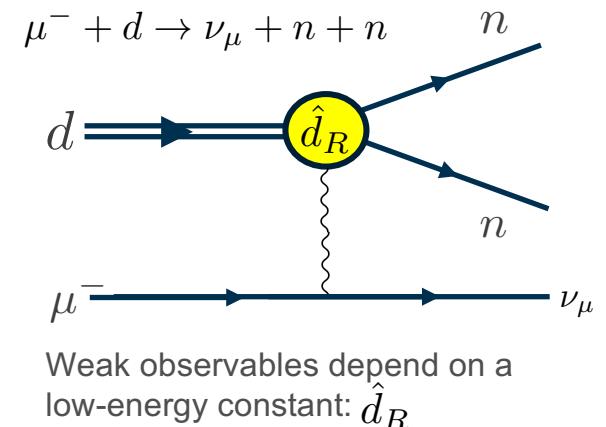
R. J. Furnstahl et al, Phys. Rev. C **92**, 024005 (2015) S. Wesolowski et al, J Phys G **43**, 074001 (2016)

PREDICTION OF THE μd CAPTURE RATE

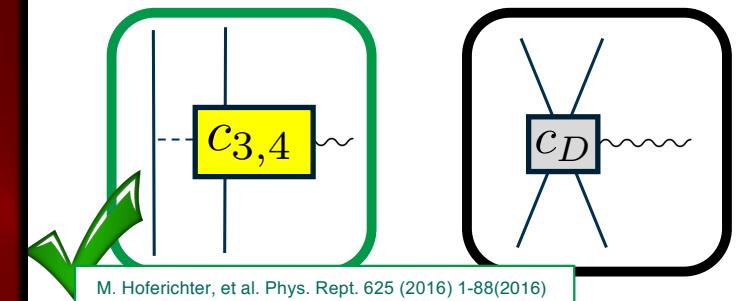
The muon-deuteron (doublet) capture rate can be measured to 1.5% precision (10x improvement), MuSun experiment: "Calibrating the Sun"

- Experimental extraction of two-body weak LEC d_R from a two-nucleon process. Previously extracted from triton β -decay
- d_R also enters in pp-fusion, the primary energy/neutrino source in the Sun and main sequence stars.
- The low-energy pp-fusion cross section cannot be measured on Earth, only inferred from theory.
- How large are the uncertainties in the theory relation between the muon-capture rate and the proton-proton fusion cross-section?
- d_R appears also in neutrino-deuteron scattering (SNO detection mechanism), and in the leading 3NF.

ppFusion: ChiEFT [Marcucci PRL 2013], Pionless EFT [Kong PRC 2001, Butler PLB 2001, PLB Ando 2008, Chen PLB 2013]
 muD capture: ChiEFT [Ando PLB 2002, Adam PLB 2012, Marcucci PRL 2013], Experiment [Cagnelli 1989]



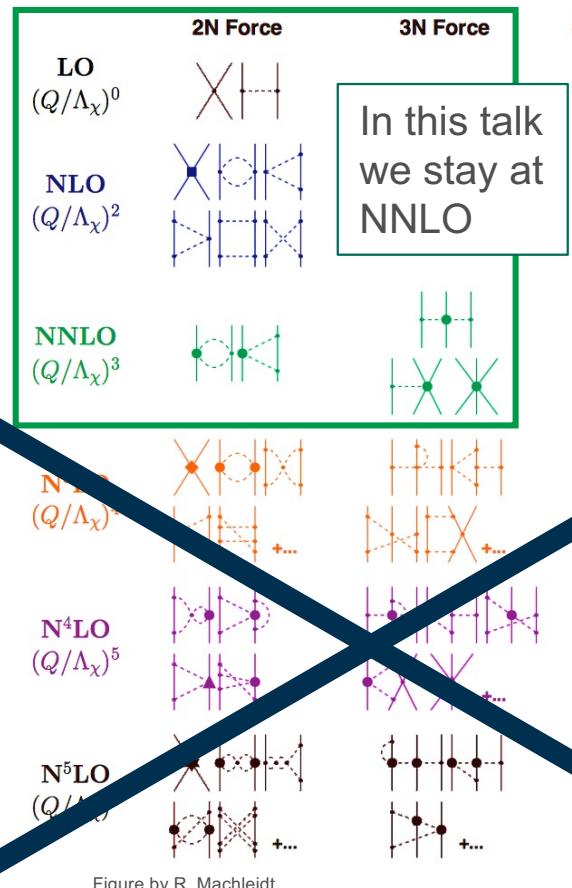
Weak observables depend on a low-energy constant: \hat{d}_R



M. Hoferichter, et al. Phys. Rept. 625 (2016) 1-88(2016)

Improved analysis (Roy-Steiner equations) determined πN couplings to 1% level. We use this in currents and potential.

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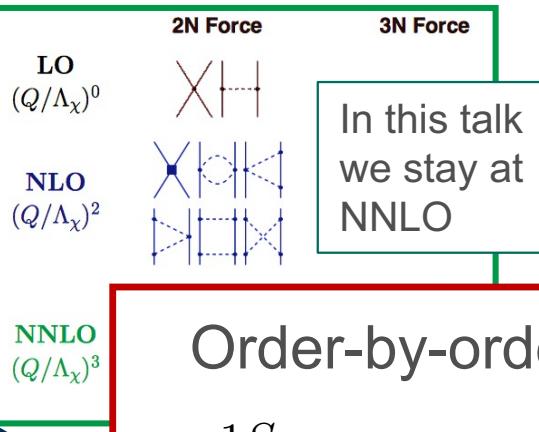
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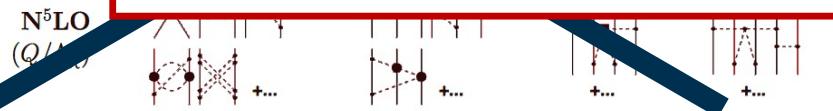
Order-by-order improvement of the capture rate:

$$\Gamma_D^{1S_0} = \underbrace{186.3}_{\text{LO}} + \underbrace{61.0}_{\text{NLO}} + \underbrace{5.5}_{\text{NNLO}} \text{ s}^{-1} \quad Q = \frac{m_\pi}{\Lambda_\chi} \sim 0.28 \text{ if } \Lambda_\chi = 500 \text{ MeV}$$

(75%-confidence) truncation error @NNLO = 4.6 s⁻¹

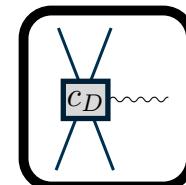
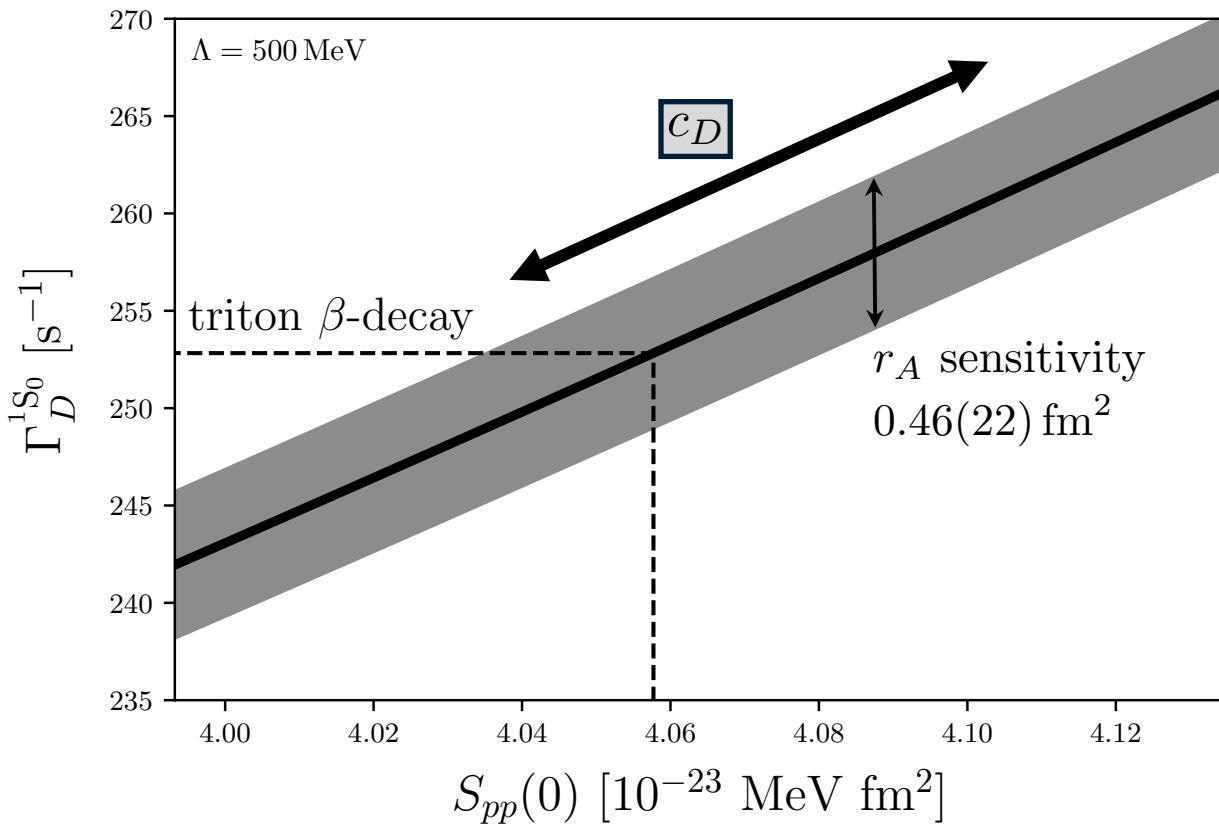
B. Acharya, AE, and L. Platter arXiv: 1806.09481v1 [nucl-th]

tribution



E. Epelbaum et al., Eur. Phys. J. A **51**, 53 (2015)
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R. J. Furnstahl et al, Phys. Rev. C **92**, 024005 (2015) S. Wesolowski et al, J Phys G **43**, 074001 (2016)

LINKING THE μd CAPTURE RATE WITH PP-FUSION



Black line correlates the capture rate with the pp-Sfactor via c_D

The axial radius error is an important error term. New analyses* of neutrino-nucleon scattering yield a larger uncertainty of the axial radius, at least $(r_A)^2=0.45(16)$ fm 2

$$\Gamma_D^{1S_0} = 252.8 \pm 4.6 \pm 3.9 \text{ s}^{-1}$$

NNLO value from triton β -decay	2% truncation error	1.5 % axial radius error
---------------------------------------	---------------------	--------------------------

Together with improved experiments (and lattice QCD ?) we can learn how the nuclear Hamiltonian correlates electroweak observables.

* Weighted ave. of z-exp of neutrino-nucleus data & MuCap exp + ChPT coupling g_P

R. J. Hill, et al. Rept. Prog. Phys. 81 (2018) no.9, 096301

C. C. Chang, et al. Nature (2018) A. S. Meyer, et al. PRD 93, 113015 (2016)

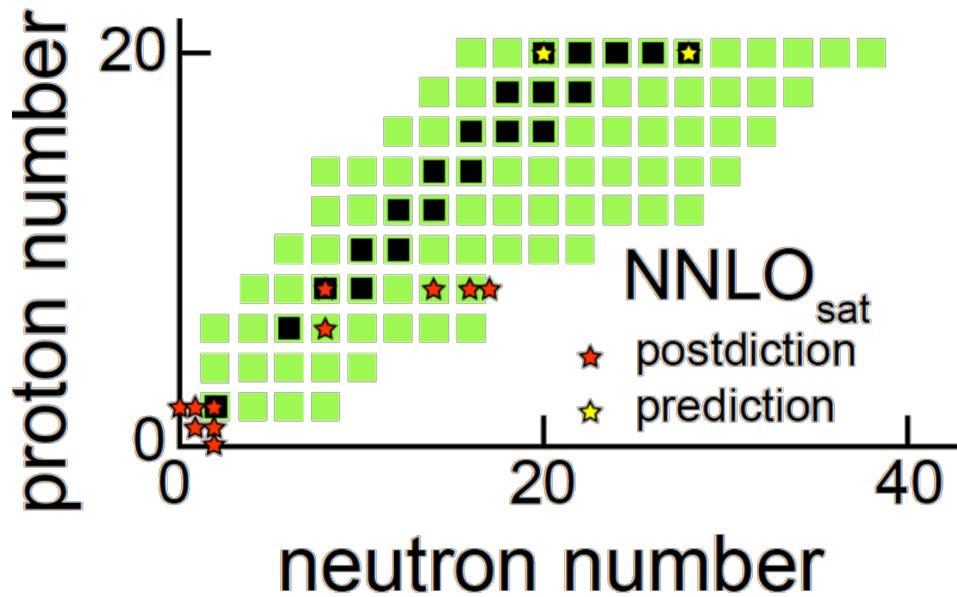
From *few-* to *many*-nucleon systems with chiral interactions

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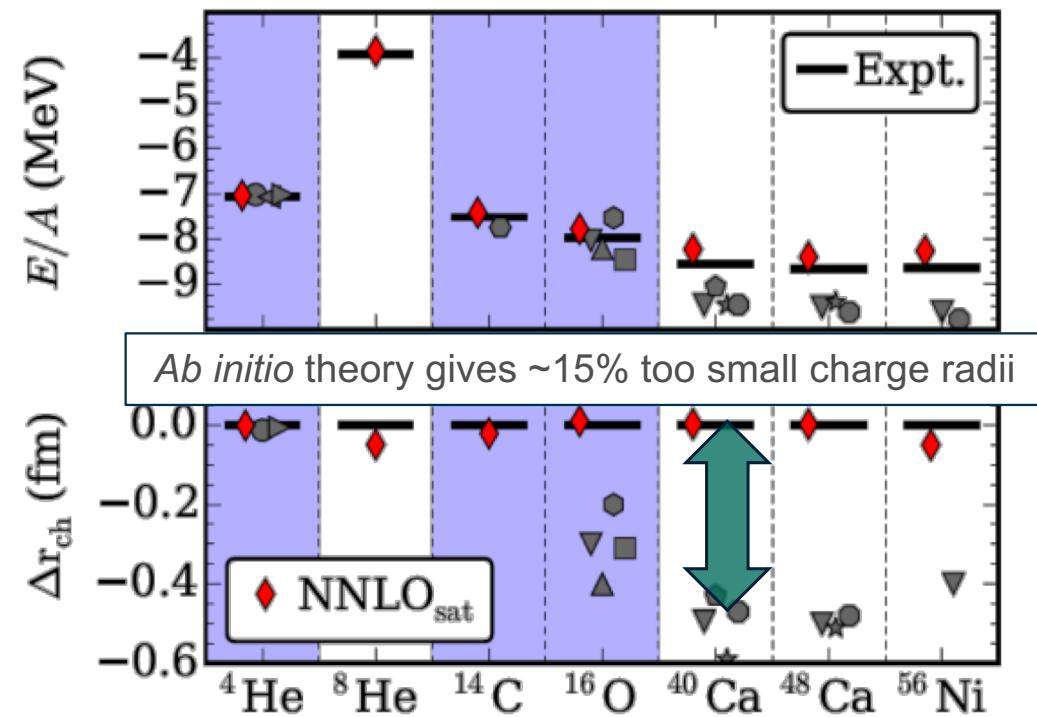
(“From a *few* challenges to *many more* challenges”)

- The likelihood/model becomes tremendously more expensive to evaluate
- We know very little about the EFT truncation error in atomic nuclei
- The theory *method* (coupled cluster, shell model, ...) error is largely unknown, although *ab initio* methods is somewhat systematic ('rules of thumb')

ACCURATE BINDING ENERGIES AND RADII FROM A CHIRAL INTERACTION



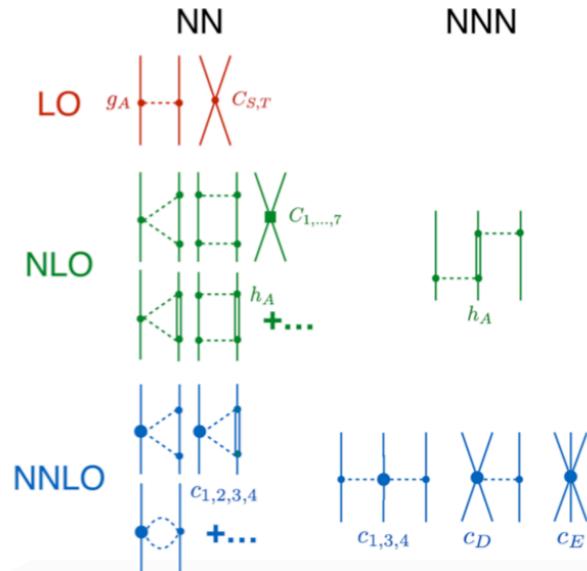
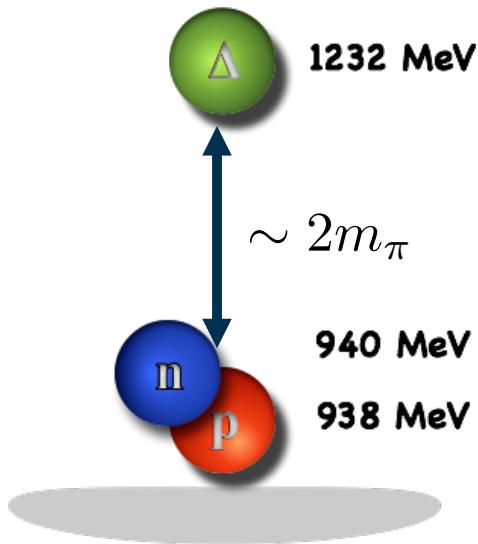
Simultaneous optimization of the chiral NN+NNN interaction at NNLO to charge radii and binding energies of ^3H , $^{3,4}\text{He}$, ^{14}C , ^{16}O and binding energies of $^{22,24,25}\text{O}$ and NN-data ($T_{\text{Lab}} < 35 \text{ MeV}$).



AE, et al. Phys. Rev C **91**, 051301(R) (2015)

^{48}Ca weak size prediction G. Hagen, et al. Nature Physics **12**, 186–190 (2016)

Δ -ISOBARS AND NUCLEAR SATURATION



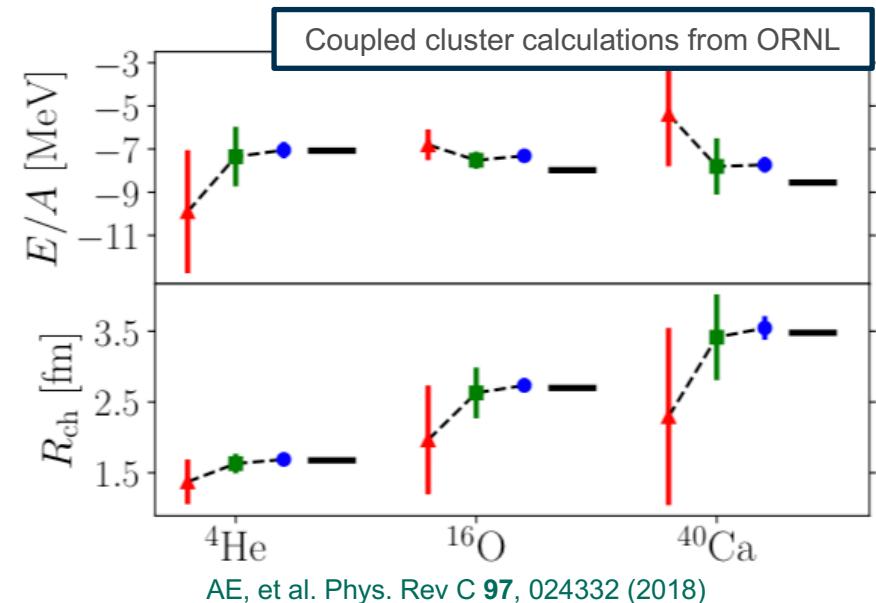
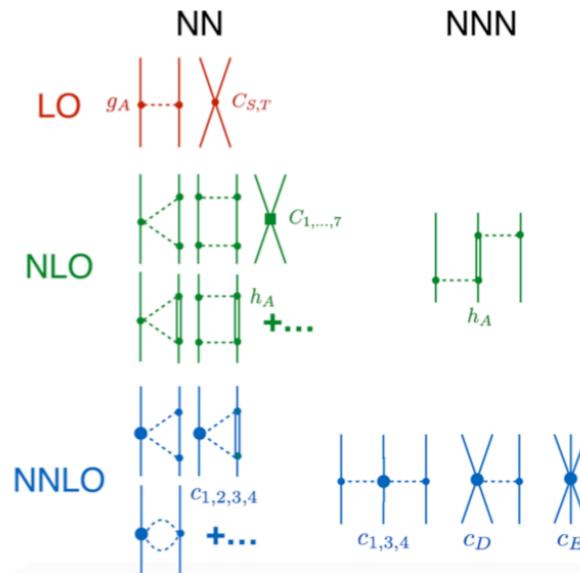
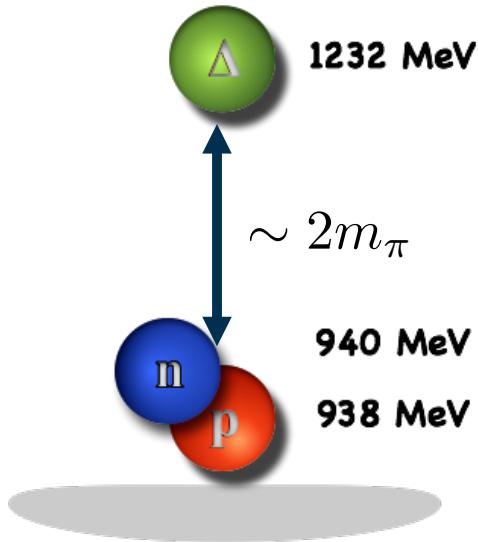
Proximity of the delta resonance motivates to explicitly including it in the effective Lagrangian.

More natural values for the LECs!
But also more LECs and diagrams (quite extensive N3LO).

(Ordoñez, Ray, van Kolck 1994) (Hemmert, Holstein, Kambor 1998)
(Kaiser, Gerstendorfer, Weise 1998) (Krebs, Epelbaum, Meissner 2007) (Krebs, Gasparyan, Epelbaum 2018)

See also: M. Piarulli et al Phys. Rev. Lett. **120**, 052503 (2018)
D. Logoteta et al. Phys. Rev. C **94**, 064001 (2016)

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LECs in δ/full interaction at LO-NLO-NNLO optimized to reproduce few-nucleon ($A \leq 4$) data (binding energies, radii, phase-shifts) yields significantly improved saturation properties.

See also: M. Piarulli et al Phys. Rev. Lett. 120, 052503 (2018)
D. Logoteta et al. Phys. Rev. C 94, 064001 (2016)

Δ -FULL/LESS OPTIMIZATION STRATEGY



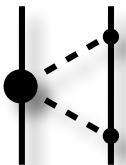
$$\mathbf{x}^* = \underset{\mathbf{x}}{\operatorname{argmin}} f(\mathbf{x})$$

With AD

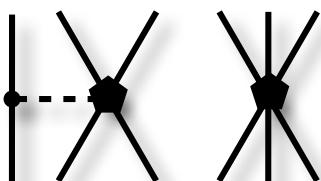
B. D. Carlsson et al. Phys. Rev. X **6**, 011019 (2016)
A. Ekström et al. Phys. Rev. Lett. **110**, 192502 (2013)

neglected EFT error the Δ -full/less optimizations

partial-wave NN scattering **phase shifts** of the Granada group up to 200 MeV scattering energy in the laboratory system. R. Navarro-Perez et al, Phys. Rev. C **88**, 064002 (2013).

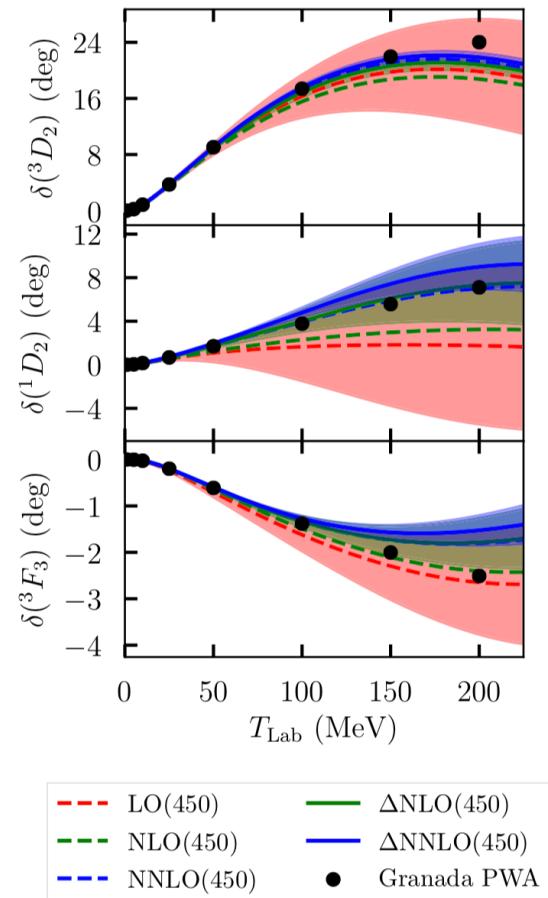
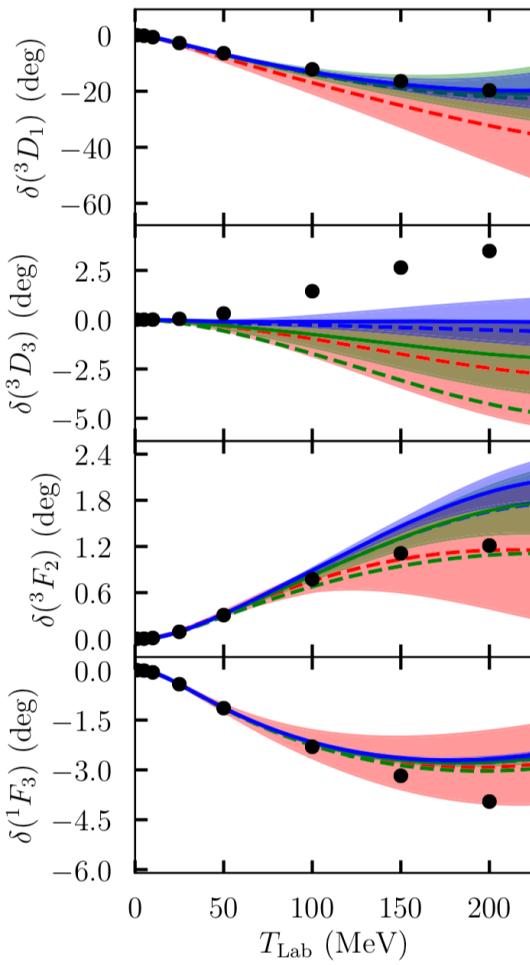


Sub-leading pi-N LECs precisely determined in recent and precise **Roy-Steiner analysis**.
D. Siemens et al. Physics Letters B **770** (2017) 27–34



Determined from **NCSM** $E_{\text{gs}}(^4\text{He})$ & $R_{\text{pt-p}}(^4\text{He})$
n.b. only relevant at NNLO.
Barrett, Navratil, Vary, Prog. Part. Nucl. Phys. **69**, 131 (2013),

Δ -full
$c_1 = -0.74(2)$
$c_2 = -0.49(17)$
$c_3 = -0.65(22)$
$c_4 = +0.96(11)$
$h_A = 1.40 \pm 0.05$
...
Δ -less
$c_1 = -0.74(2)$
$c_2 = +1.81(3)$
$c_3 = -3.61(3)$
$c_4 = +2.44(3)$

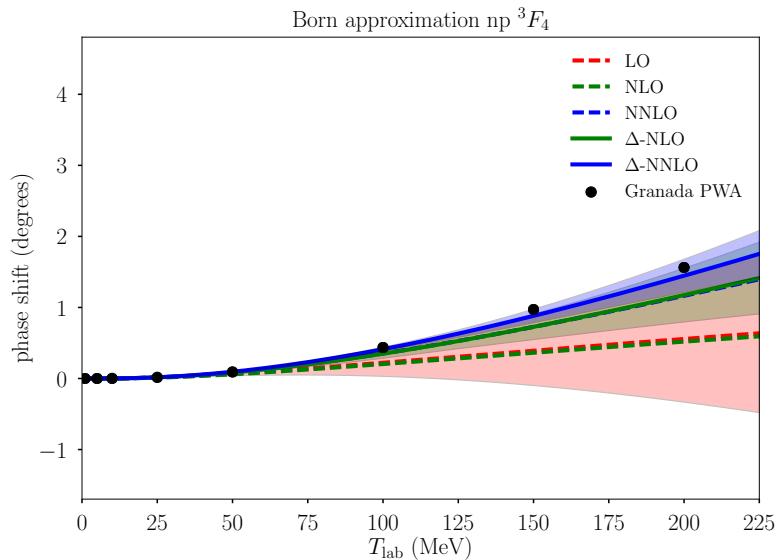


Selected proton-proton phase shifts

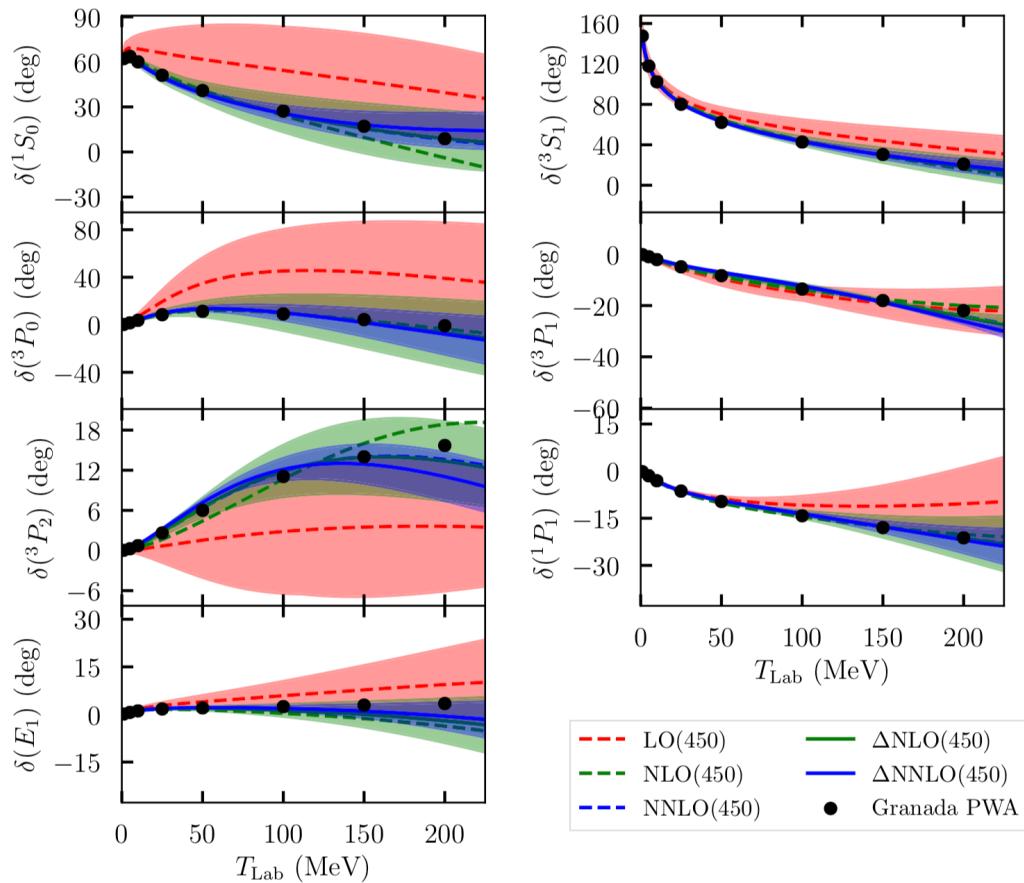
The bands indicate the estimated EFT truncation errors using a breakdown scale of 500 MeV.

As noticed already more than 10 yrs ago by H. Krebs
(H. Krebs et al, Eur. Phys. J. A 32, 127–137 (2007))

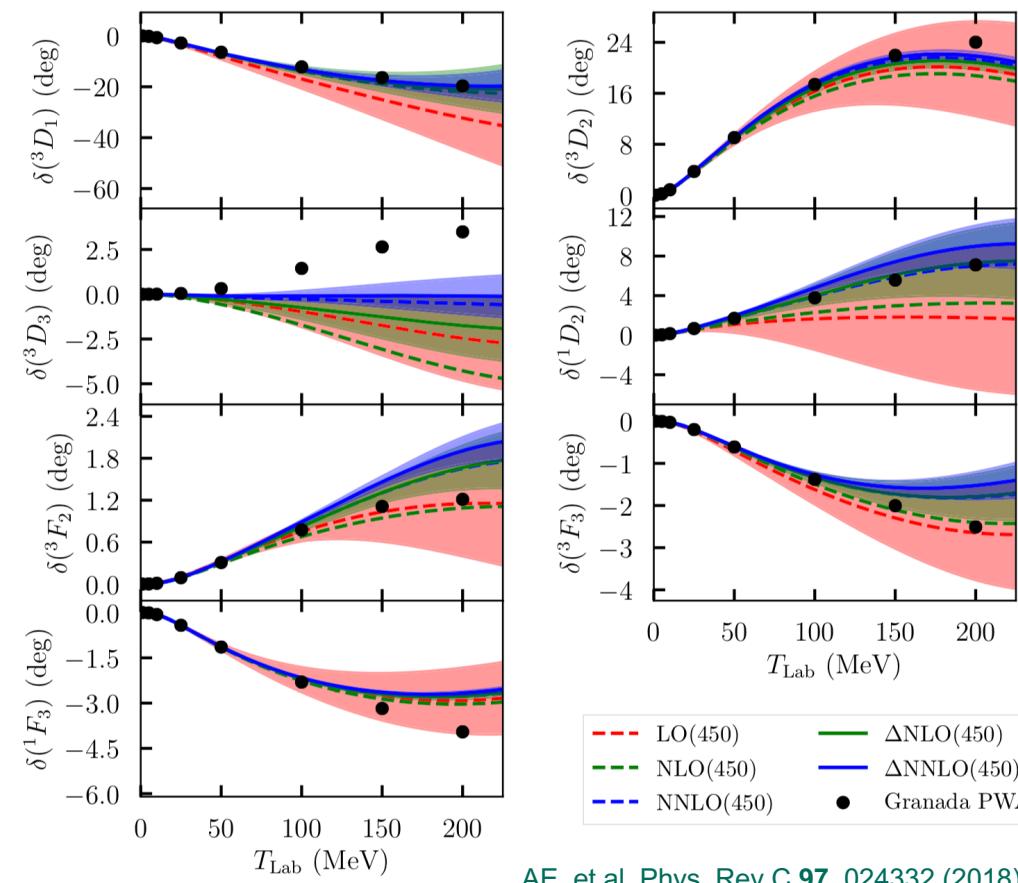
The Δ improves agreement in many peripheral waves.



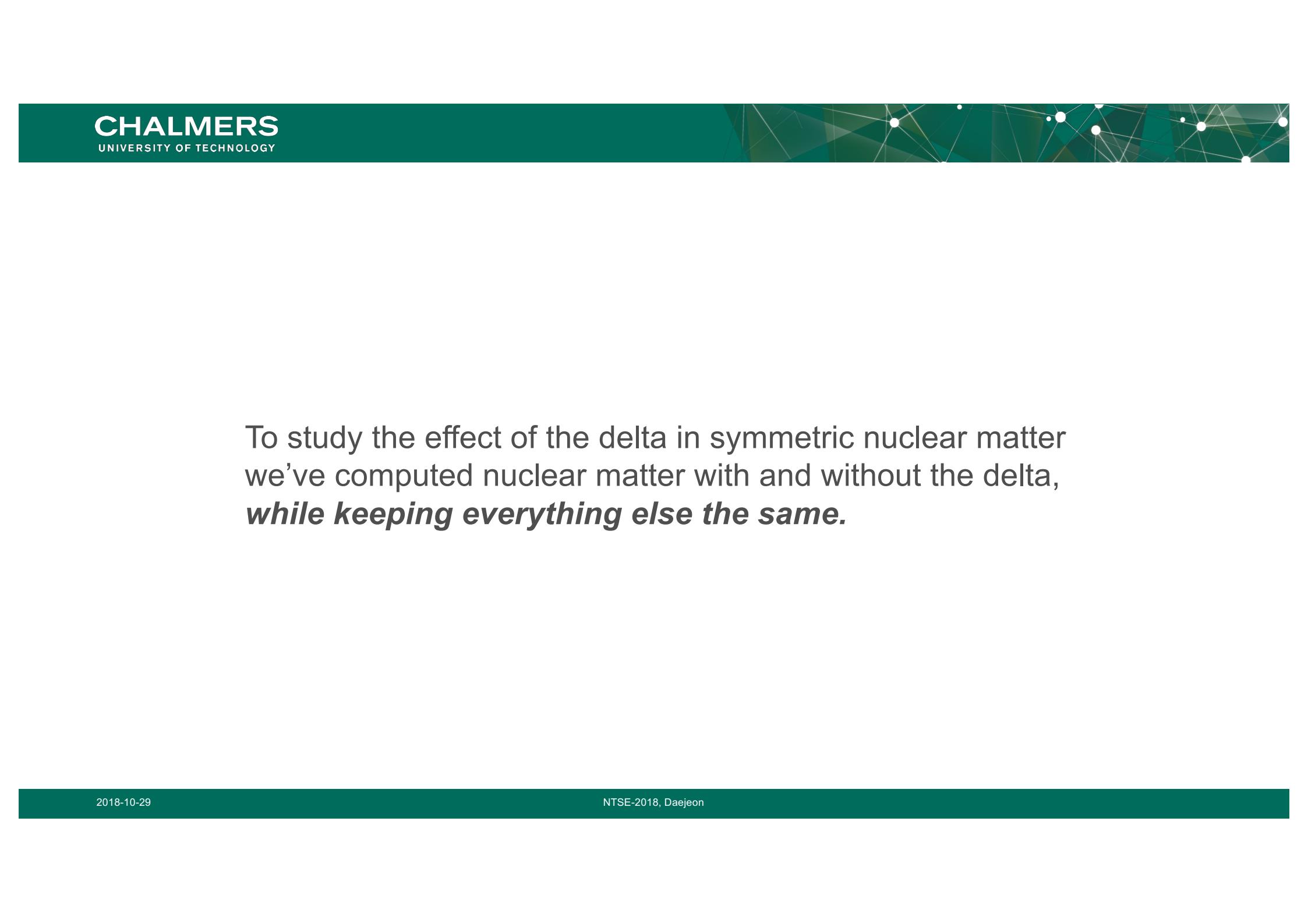
SELECTED NEUTRON-PROTON PHASES



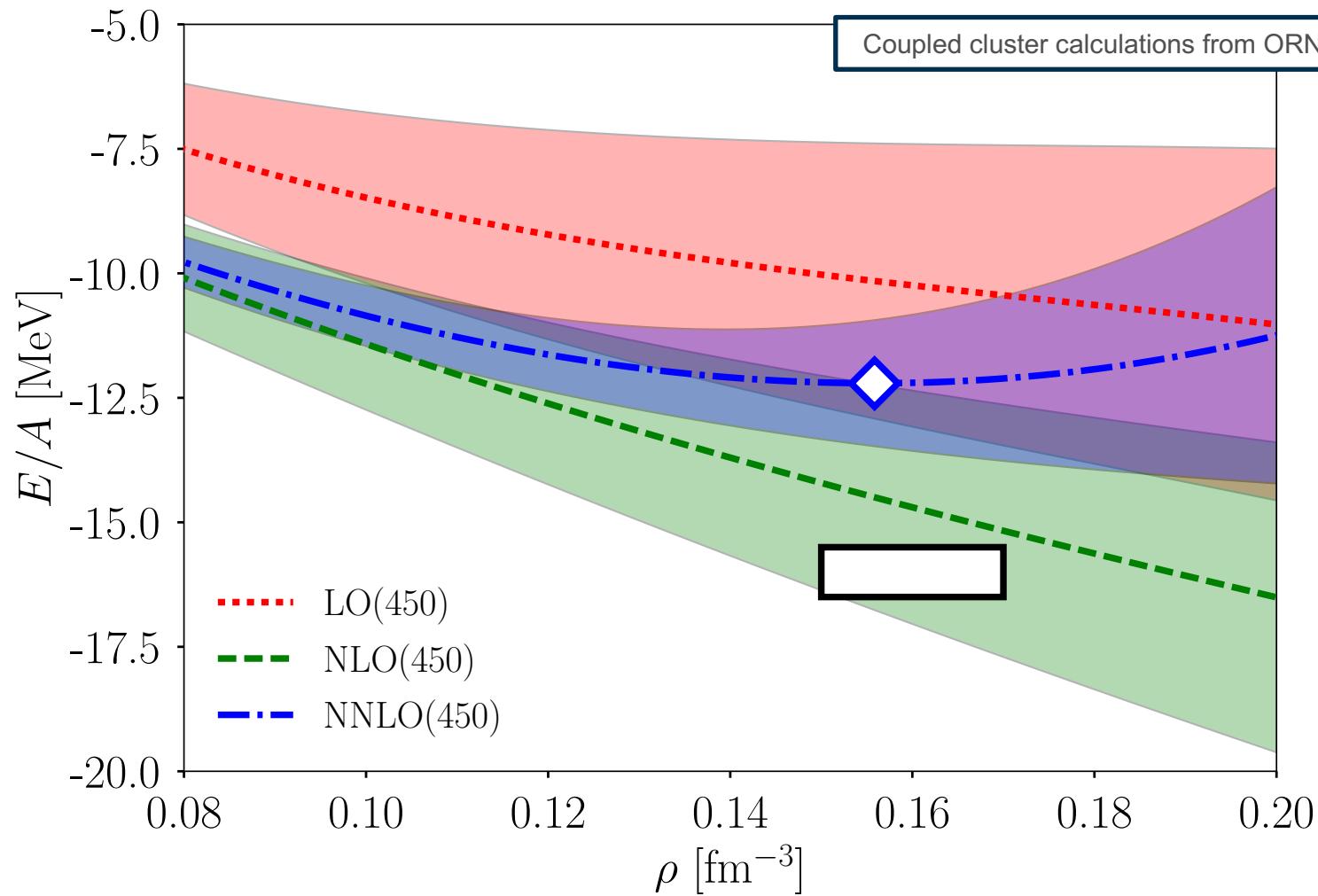
— LO(450)	— ΔNLO(450)
— NLO(450)	— ΔNNLO(450)
— NNLO(450)	● Granada PWA

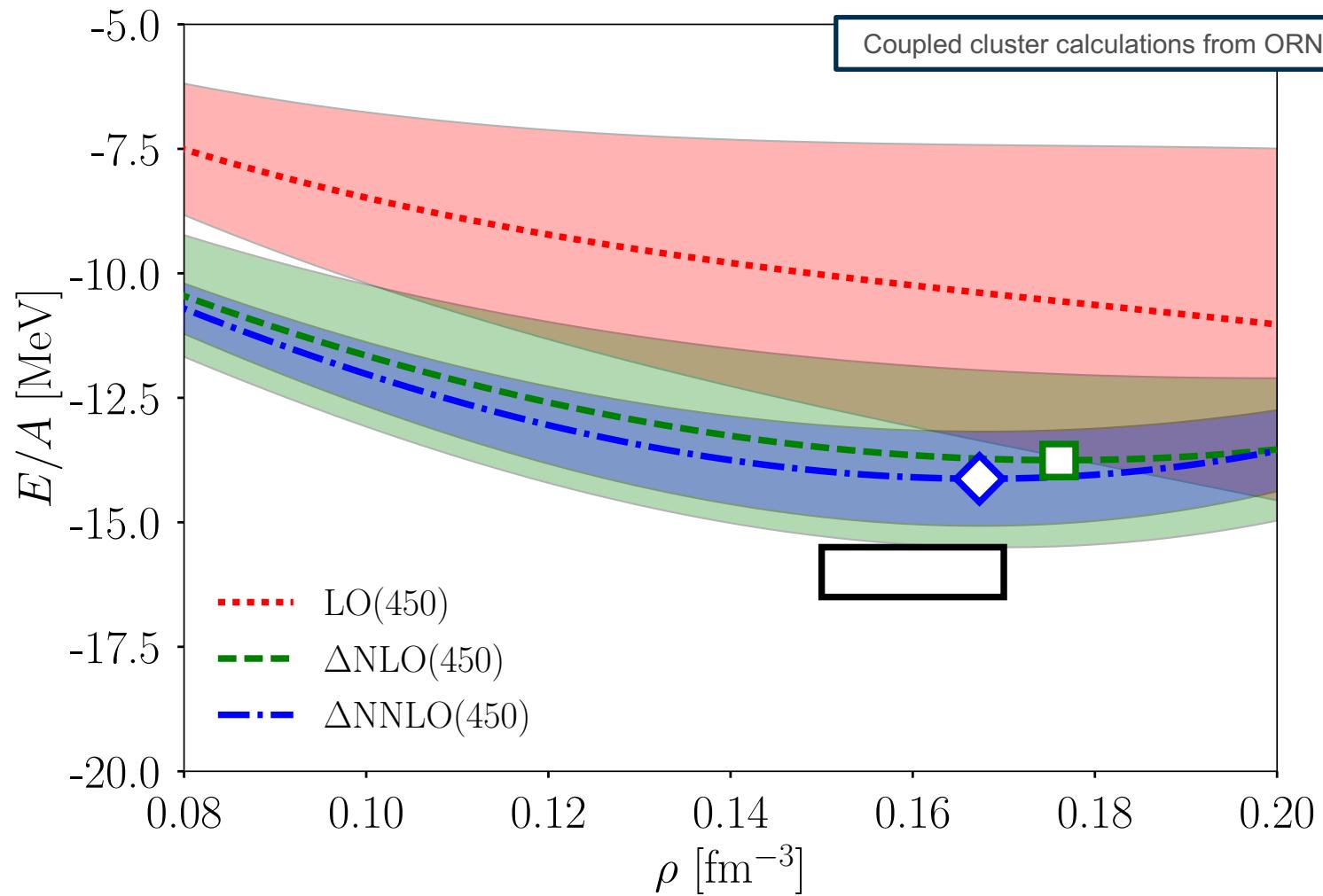


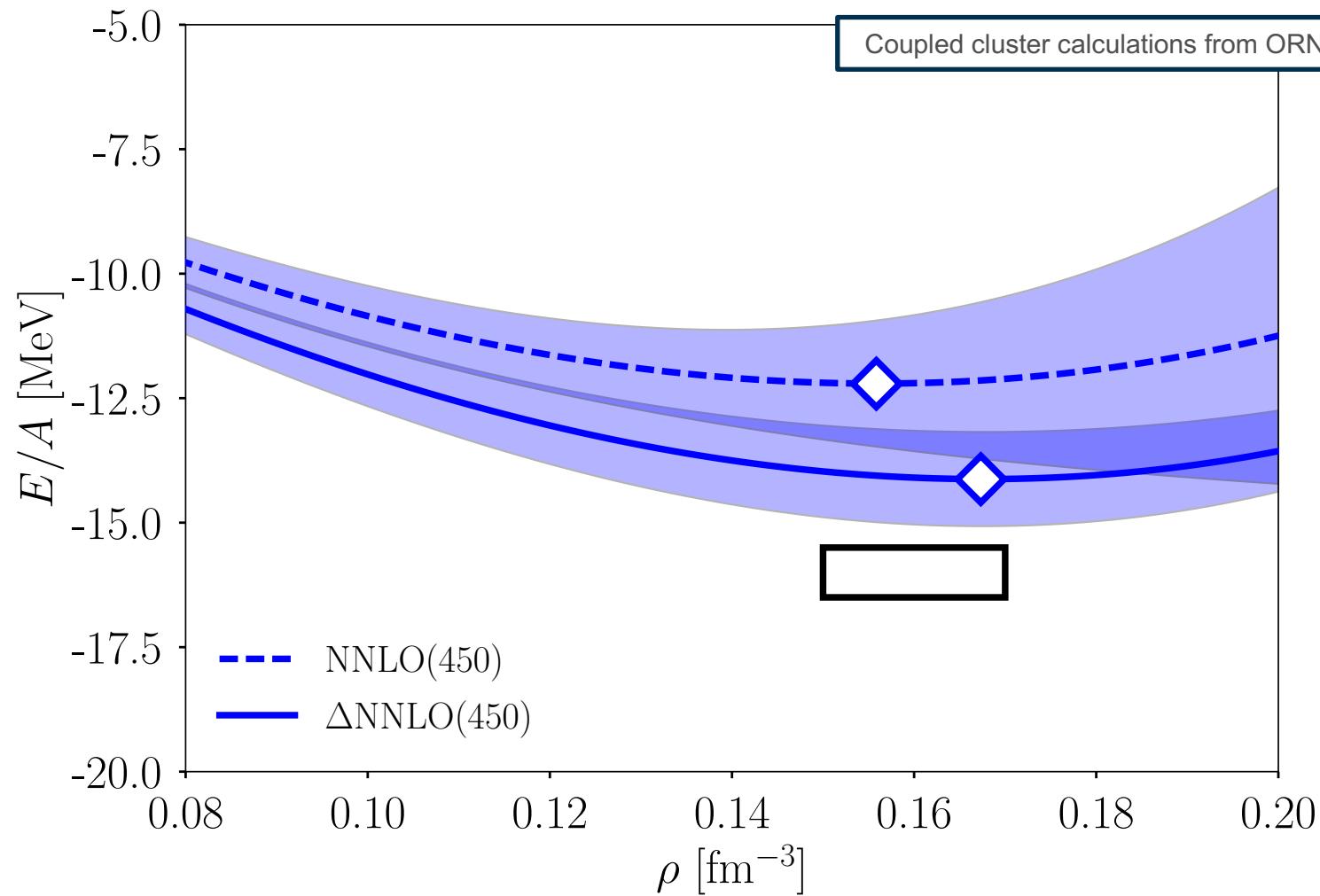
AE, et al. Phys. Rev C 97, 024332 (2018)

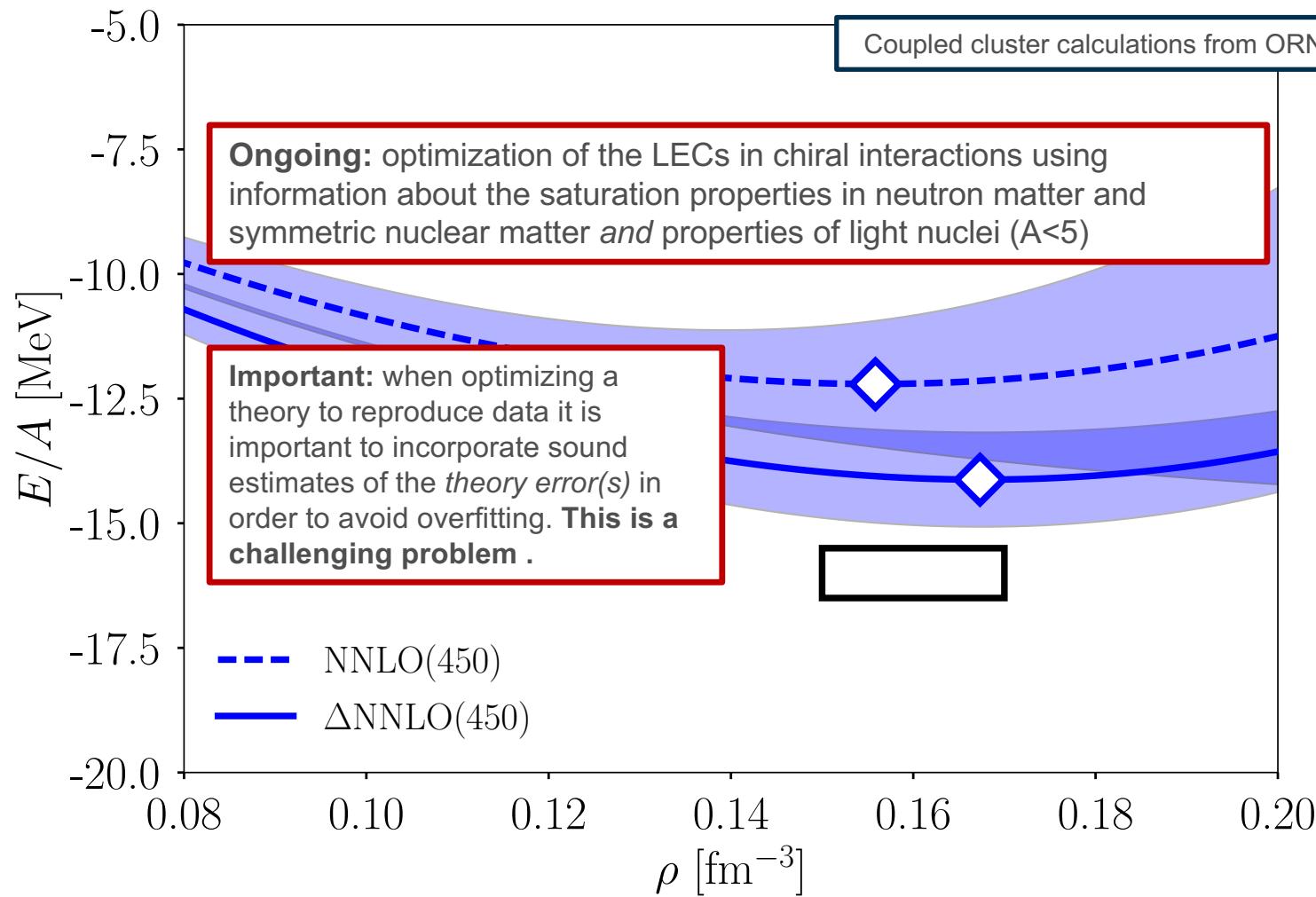


To study the effect of the delta in symmetric nuclear matter we've computed nuclear matter with and without the delta,
while keeping everything else the same.

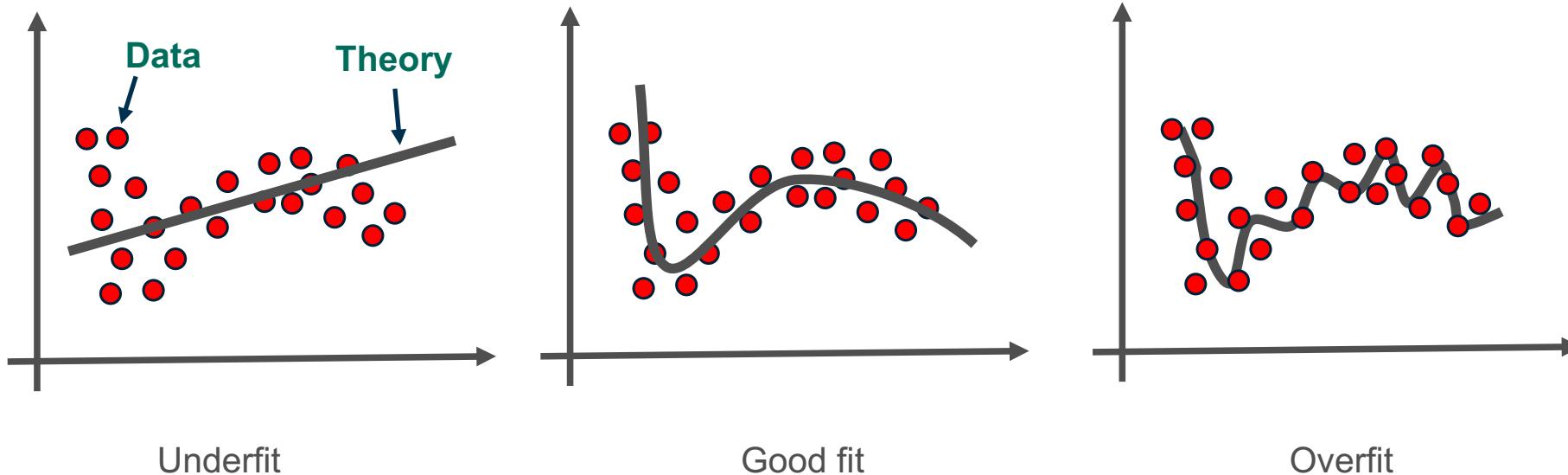








HOW WELL SHOULD THE THEORY PERFORM?



Several exciting developments and available methods in statistics, computer science, and applied mathematics that will help us answer this and many other questions about theoretical modelling of the atomic nucleus!

Talks online! ISNET-6: <https://indico.gsi.de/event/7534/timetable/#20181011>

Intro: Dick Furnstahl's "Bayes for physicists": https://github.com/furnstahl/Bayes_for_physicists

Other useful links: <http://bayesint.github.io>

BAYESIAN INFERENCE

Bayes formulation of statistics offers a convenient method to guard against overfitting, to incorporating in prior knowledge (naturalness, the EFT error scaling), and to quantitatively compare models to each other!

$$P(\mathbf{a}|D, I) \stackrel{?}{=} \frac{P(D|\mathbf{a}, I)P(\mathbf{a}|I)}{P(D|I)}$$

Likelihood Prior
Posterior **Evidence (normalization)**



Toolbox:

Marginalization

$$P(a_1|D, I) = \int da_2 \dots da_k P(\mathbf{a}|D, I)$$

$$P(D|\mathbf{a}, I) = \int dc_{\bar{\nu}+1} \dots dc_{\nu_{\max}} P(D|c_{\bar{\nu}+1} \dots c_{\nu_{\max}}, \mathbf{a}, I) \\ \times P(c_{\bar{\nu}+1} \dots c_{\nu_{\max}}|I)$$

Model comparison (Bayes factors)

$$\frac{P(M_1|D)}{P(M_2|D)} = \frac{\int P(D|\mathbf{a}, M_1)P(\mathbf{a}|M_1)d\mathbf{a}}{\int P(D|\mathbf{b}, M_2)P(\mathbf{b}|M_2)d\mathbf{b}}$$

If you can do Markov Chain Monte Carlo sampling “of your system”, then you can afford it !

There exists also “discounted” versions where you instead get approximate (surrogate, artificially intelligent?) descriptions of your posterior.

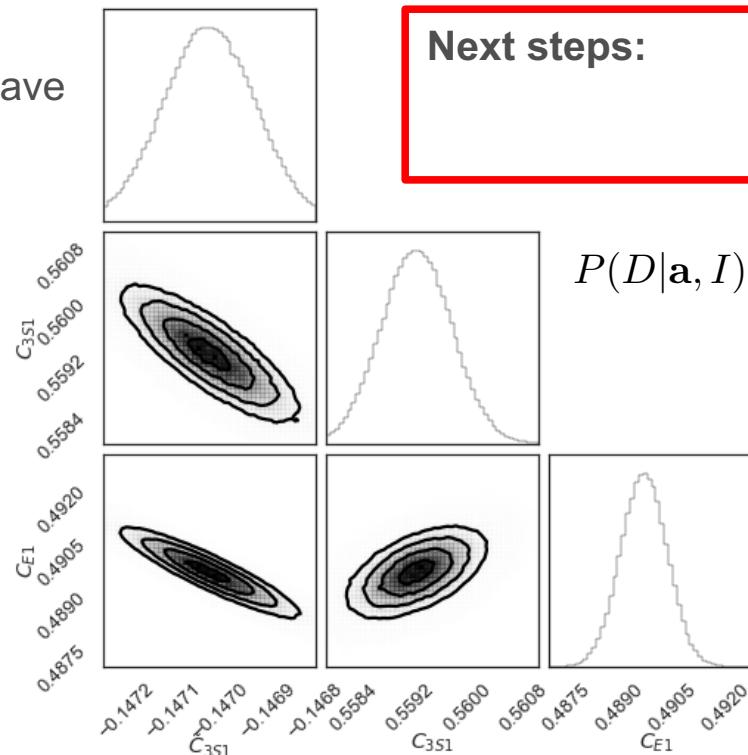
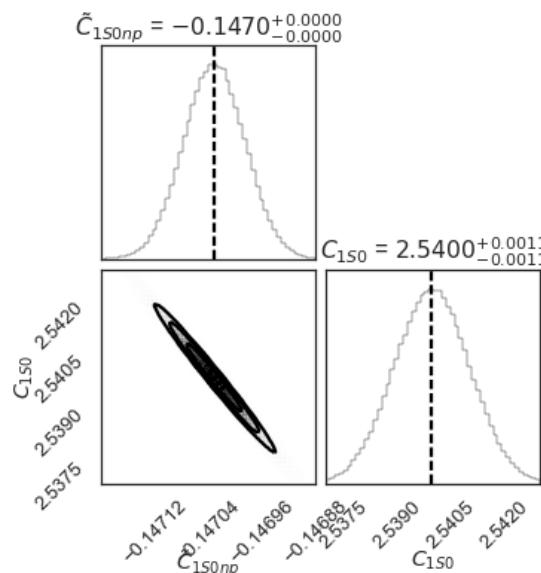
For more on Bayes and EFT:
 S. Wesolowski et al, J Phys G 43, 074001 (2016)
 M. Schindler, D. Phillips, Ann. Phys. 324, 682 (2009)

SAMPLING THE POSTERIOR DISTRIBUTION OF THE LECS

$$P(\mathbf{a}|D, I) \propto P(D|\mathbf{a}, I)P(\mathbf{a}|I)$$

↑
NNLO contact-interaction LECs

↑
NN scattering S-wave phase shifts



Next steps:

Likelihood built from NN data
Include EFT covariance
Order-by-order analysis

$$P(D|\mathbf{a}, I) = \exp \left\{ -\frac{1}{2} \mathbf{r}^T (\Sigma_{\text{exp}} + \Sigma_{\text{th}})^{-1} \mathbf{r} \right\}$$

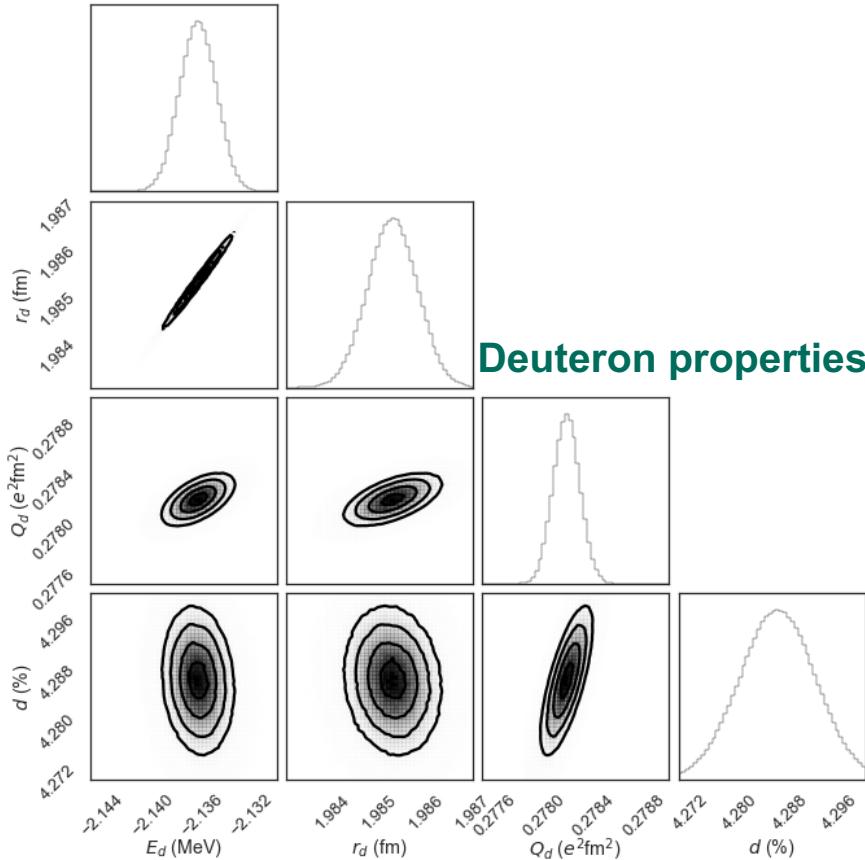
For work on EFT covariance matrices, see:
S. Wesolowski et al, arXiv 1808.08211 [nucl-th]
J. Melendez et al, ISNET-6 talk

The EFT error in BDC et al. PRX 6, 011019 (2016):
uncorrelated limit (i.e. as iid Gaussian error)

10⁷ Samples
PT-MCMC



PROPAGATING THE POSTERIOR DISTRIBUTIONS



Observables can be sampled from the posterior probability distributions for the LECs

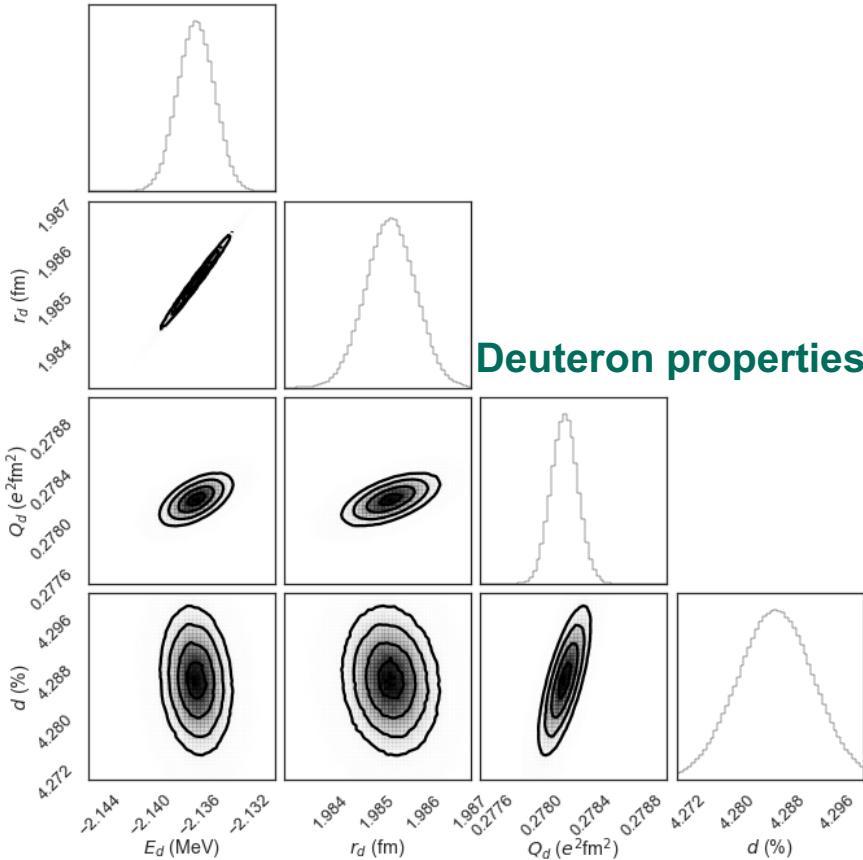
$$\langle \mathcal{O}(\mathbf{a}) \rangle = \int d\mathbf{a} P(\mathbf{a}|D, I) \mathcal{O}(\mathbf{a}) \approx \frac{1}{N} \sum_{j=1}^N \mathcal{O}(\mathbf{a}_j)$$

MCMC samples $\{\mathbf{a}_j\}$ according to the posterior pdf

**10⁷ Samples
PT-MCMC**



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MCMC samples $\{\mathbf{a}_j\}$ according to the posterior pdf

Challenges: to take this kind of analysis to larger parameter spaces in a computationally efficient fashion, and try to assess the convergence behavior of the sampled posterior.

Try to answer questions like:

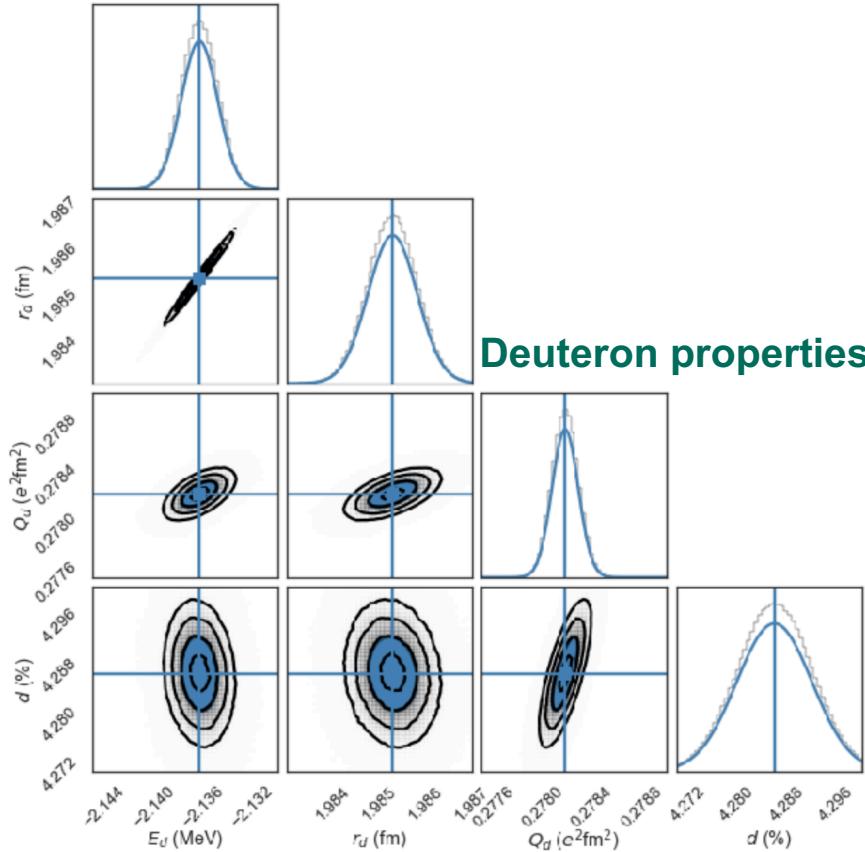
How large is the EFT error in my observable ?
To which order should I go to describe data D ?

...

**10⁷ Samples
PT-MCMC**



PROPAGATING THE POSTERIOR DISTRIBUTIONS



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**10⁷ Samples
PT-MCMC**



- The computational capabilities in *ab initio* nuclear physics exceed the accuracy of available interactions
- Chiral interactions are advantageous for analyzing low-energy nuclear physics with quantified uncertainties. But do we have an EFT of low-energy QCD yet ?
- The inclusion of the Δ -isobar in the nuclear interaction addresses some long-standing problems regarding nuclear saturation
- Our ongoing efforts to obtain "precision nuclear physics":
 - ❑ **Quantify** systematic uncertainties in theoretical predictions using Bayesian statistics
 - ❑ **Incorporate** EFT truncation errors, and possible prior knowledge, when fitting nuclear interactions. How do we represent the EFT truncation error in bound state observables of atomic nuclei ?
 - ❑ **Exploit** information from 3N scattering, and saturation properties of infinite matter when optimizing the LECs of chiral nuclear interactions. (opportunities with lattice QCD for EFT & EFT for lattice QCD)
 - ❑ **Demonstrate** a connection between EFT(s) applied to nuclei and low-energy QCD (e.g. test power counting for RG invariance and predict finite nuclei)
 - ❑ **Explore** the usefulness of emulators for leveraging expensive calculations

Thank you for your attention !