

AB INITIO NUCLEAR THEORY WITH UNCERTAINTY QUANTIFICATION

CHRISTIAN FORSSÉN

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MANY THANKS TO MY COLLABORATORS

- ❖ **Boris Carlsson, Andreas Ekström, Tor Djärv, Daniel Gazda, Andreas Johansson, Håkan Johansson, Sean Miller, Isak Svensson, Chieh-Yen Yang (Chalmers)**
- ❖ **Gustav Jansen, Gaute Hagen, Thomas Papenbrock, Weiguang Jiang (ORNL/UT)**
- ❖ **And many people in the *ab initio nuclear theory* community for enlightening discussions**

Research funded by:

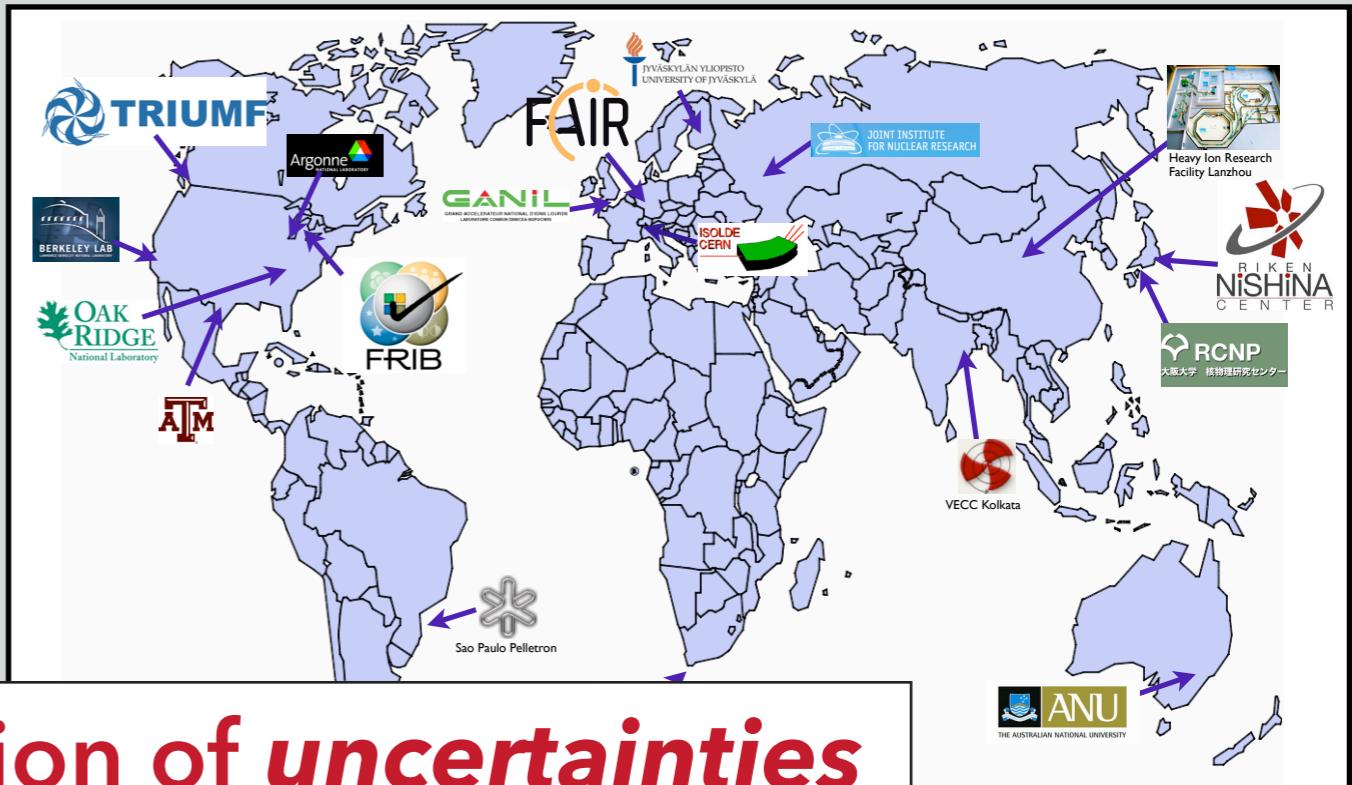
- STINT
- Vetenskapsrådet
- European Research Council



PROGRESS IN NUCLEAR EXPERIMENT AND THEORY

Experimental facilities and technology

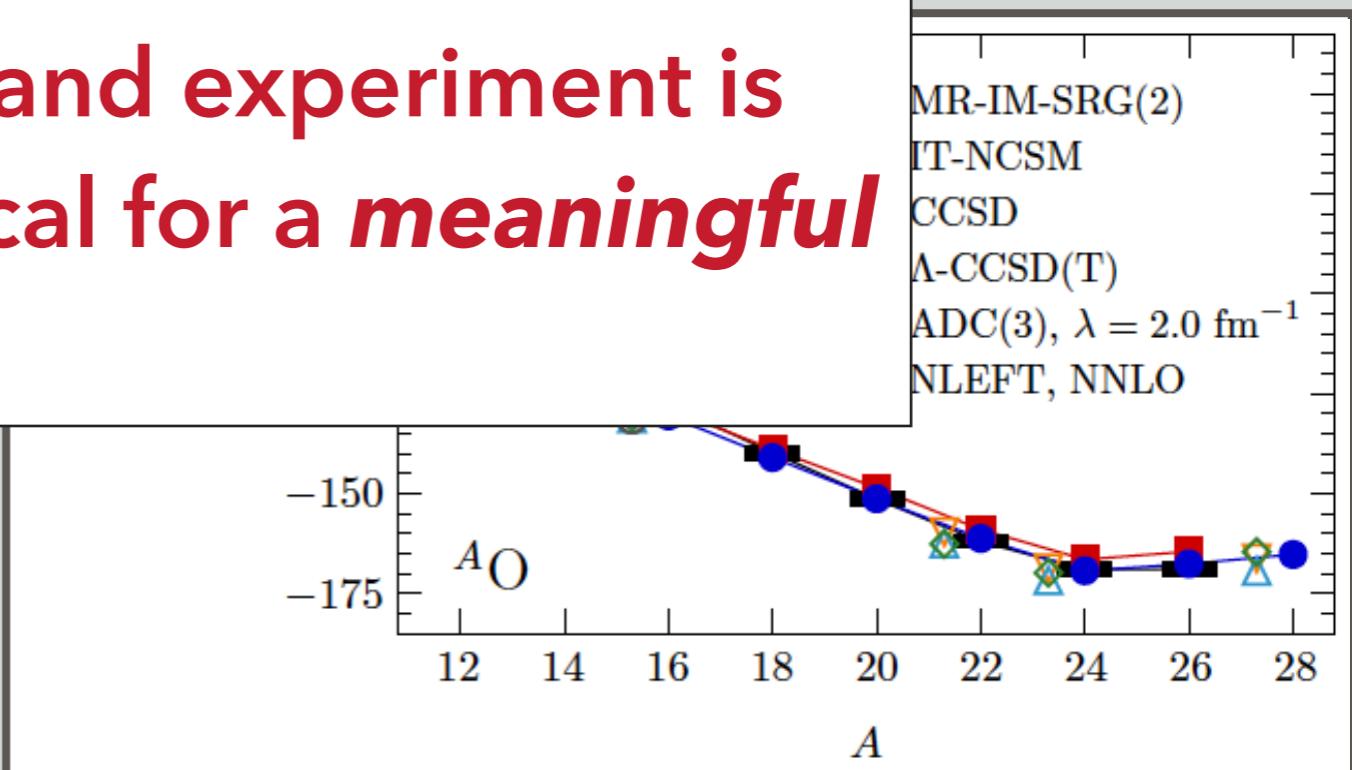
- ▶ Precise + accurate mass measurements (e.g., Penning traps)
- ▶ Access to exotic nuclei (isotope chains, halos, etc.)
- ▶ Knock-out reactions (of many varieties)
- ▶ ...



The quantification of *uncertainties* in both **theory** and experiment is absolutely critical for a **meaningful comparison**.

Theory advances (catalyzed by large datasets)

- ▶ Explosion of coupled-body methods
- ▶ Inputs: effective field theory (EFT) and renormalization group (RG)
- ▶ Computational power and advanced algorithms
- ▶ ...



Hergert et al., PRL110 (2013) 242501, Phys. Rep. 621, 165 (2016); Phys. Scripta 92, 023002 (2017). Cipollone et al. (2013)

FRONTIERS IN LOW-ENERGY NUCLEAR PHYSICS (AB INITIO THEORY)

New territory frontier

- ▶ Heavier systems
- ▶ Away from closed shells
- ▶ Hypernuclei

Continuum frontier

- ▶ Approaching the drip lines
- ▶ Unified theory of structure and reactions

Technology frontier

- ▶ New computational hardware
- ▶ Algorithms, applied math.

Service frontier

- ▶ Deliver reliable input to other communities
- ▶ Cross sections, masses, etc ($0\nu\beta\beta$, dark matter, astrophysics processes, ...)

Precision and accuracy frontiers

- ▶ Accurate results
- ▶ Precise results:
 - Uncertainty quantification, Error propagation

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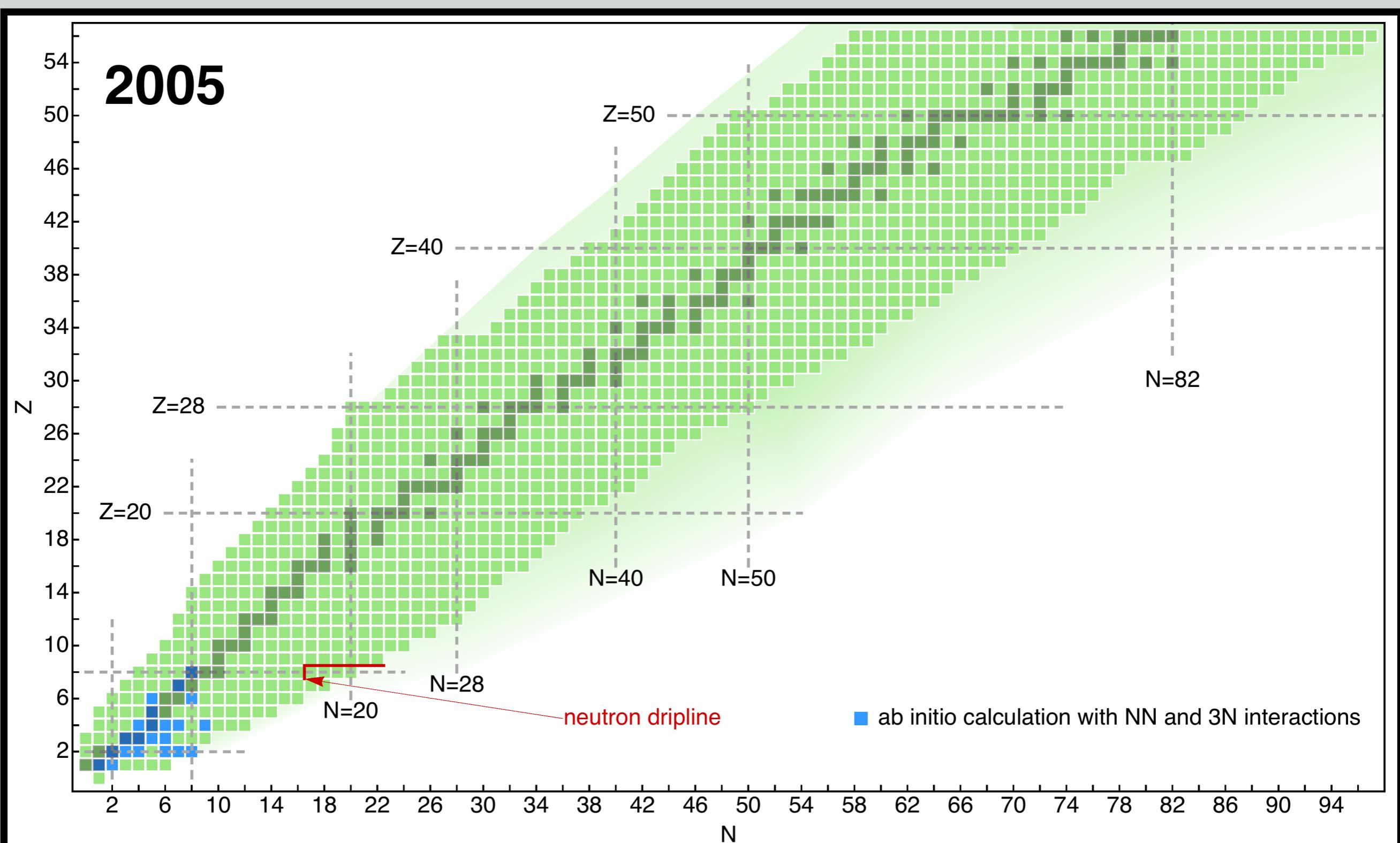
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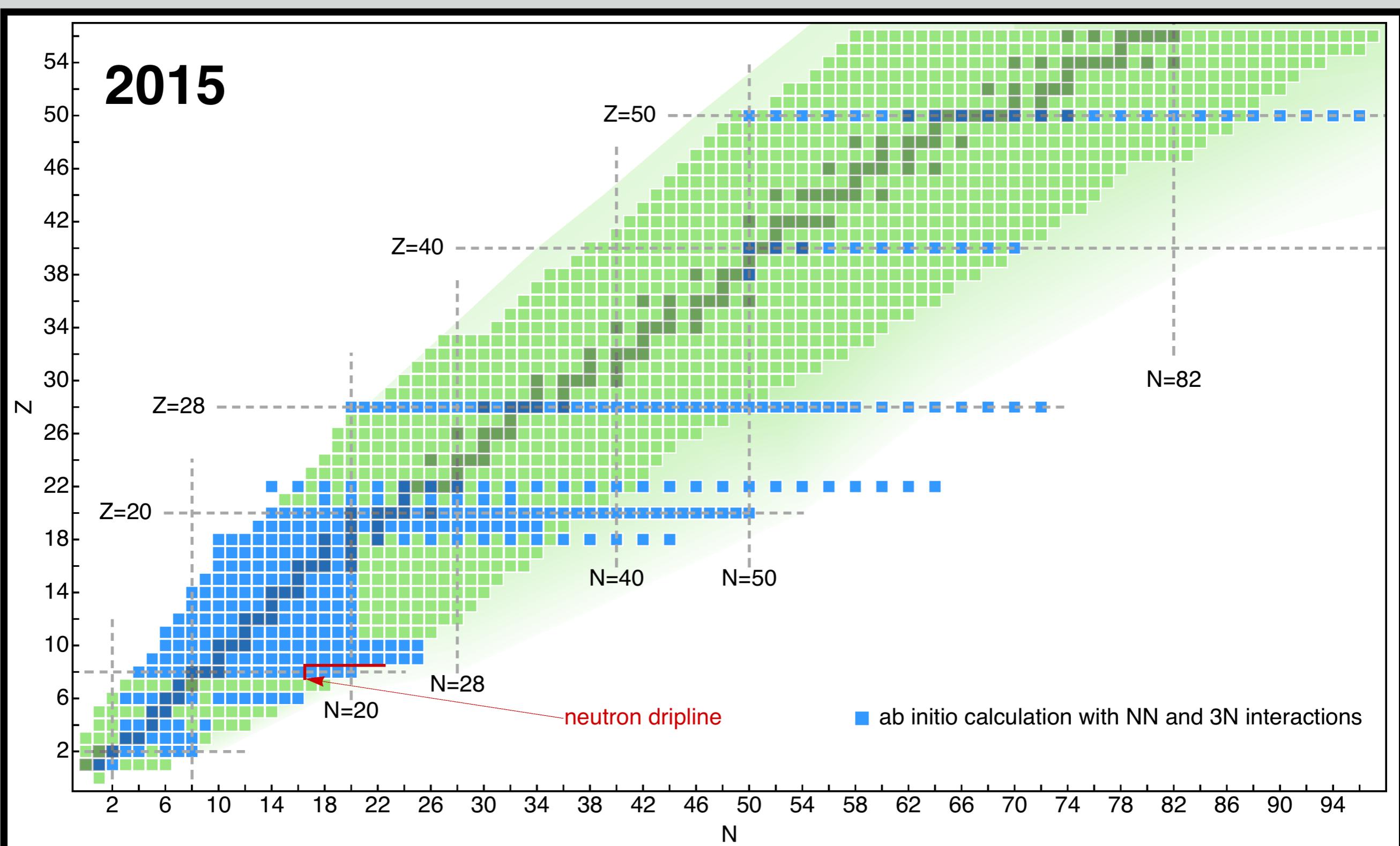
PART 1

New territory frontier for ab initio calculations

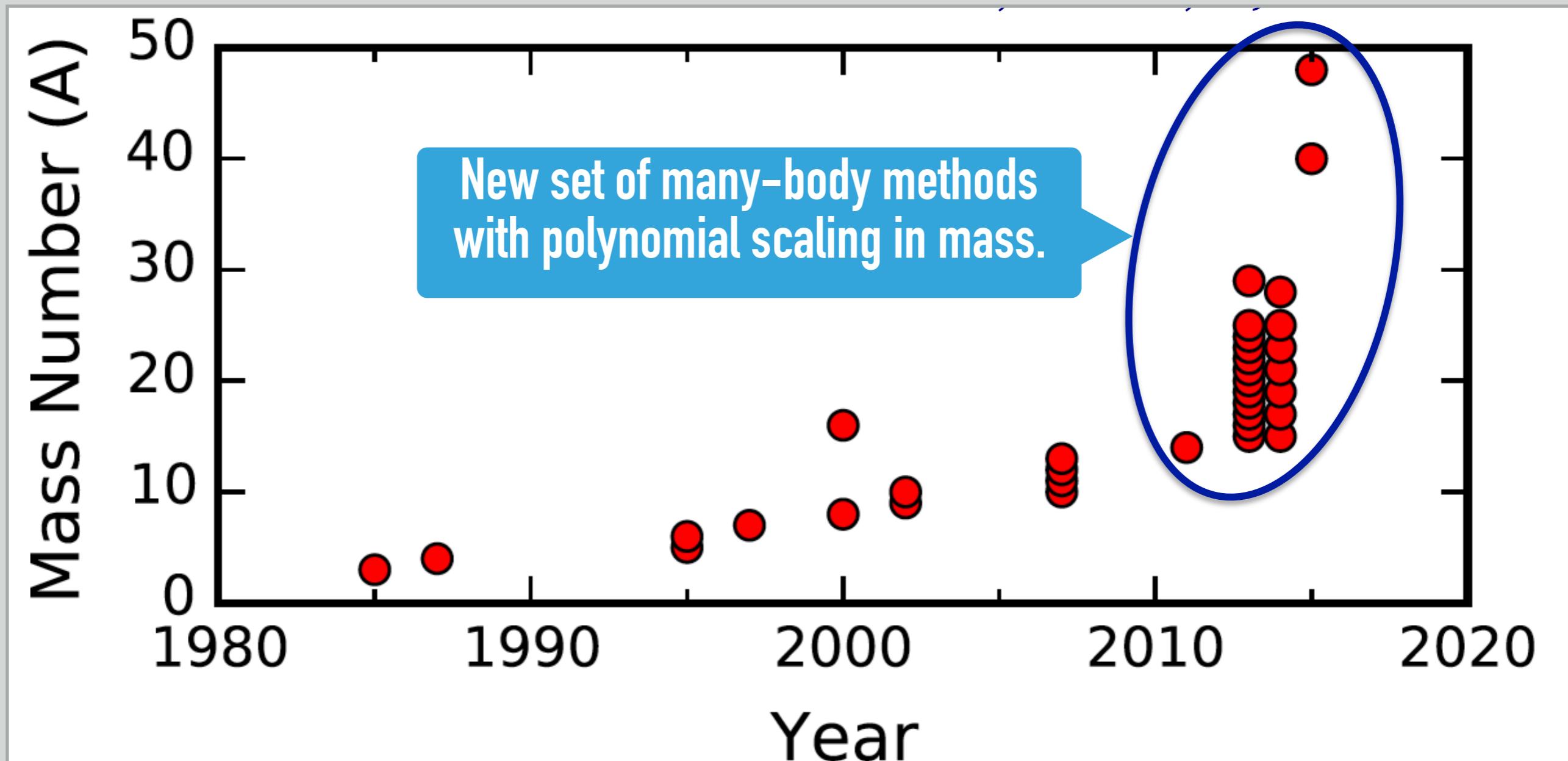
REACH OF AB INITIO CALCULATIONS



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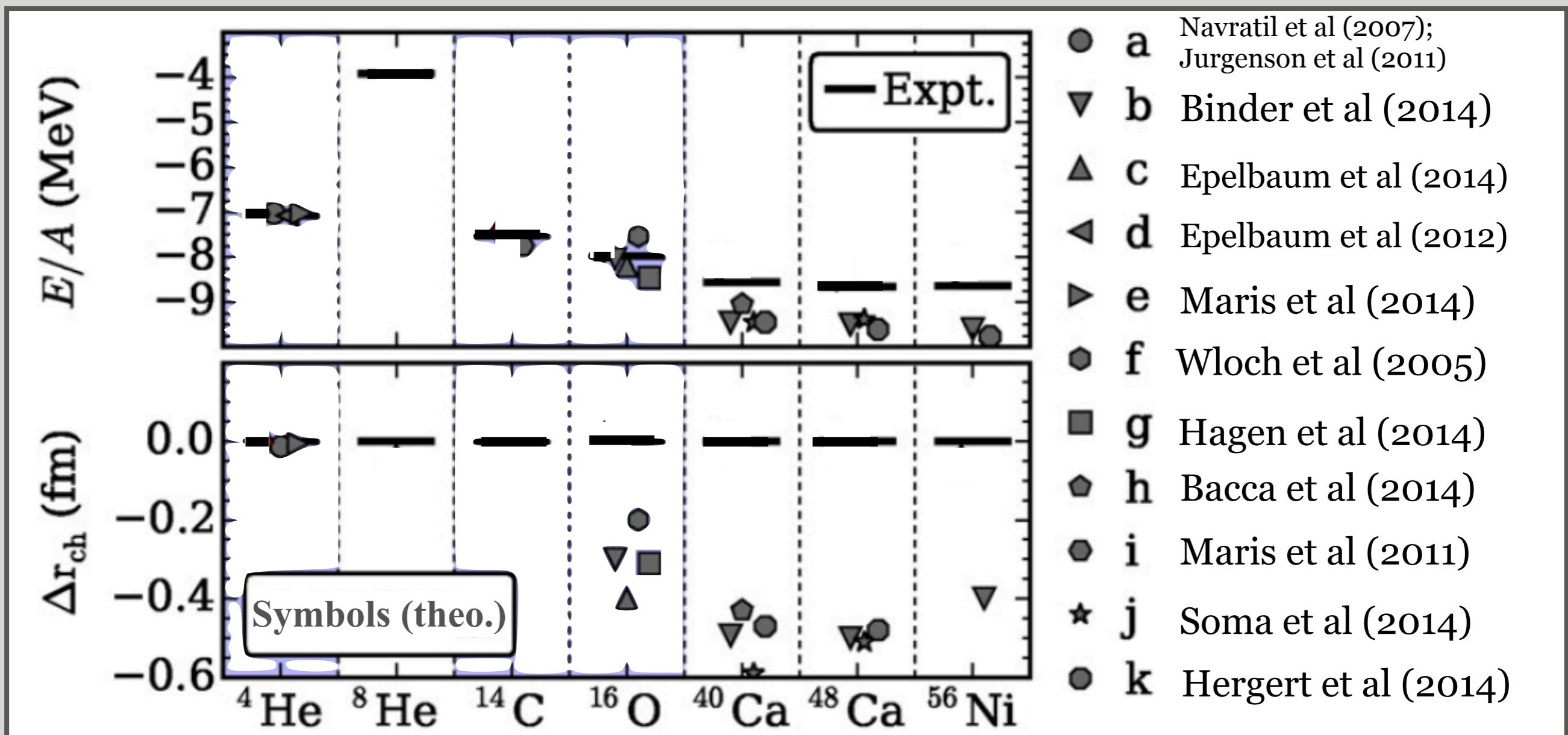


TREND IN REALISTIC AB INITIO CALCULATIONS

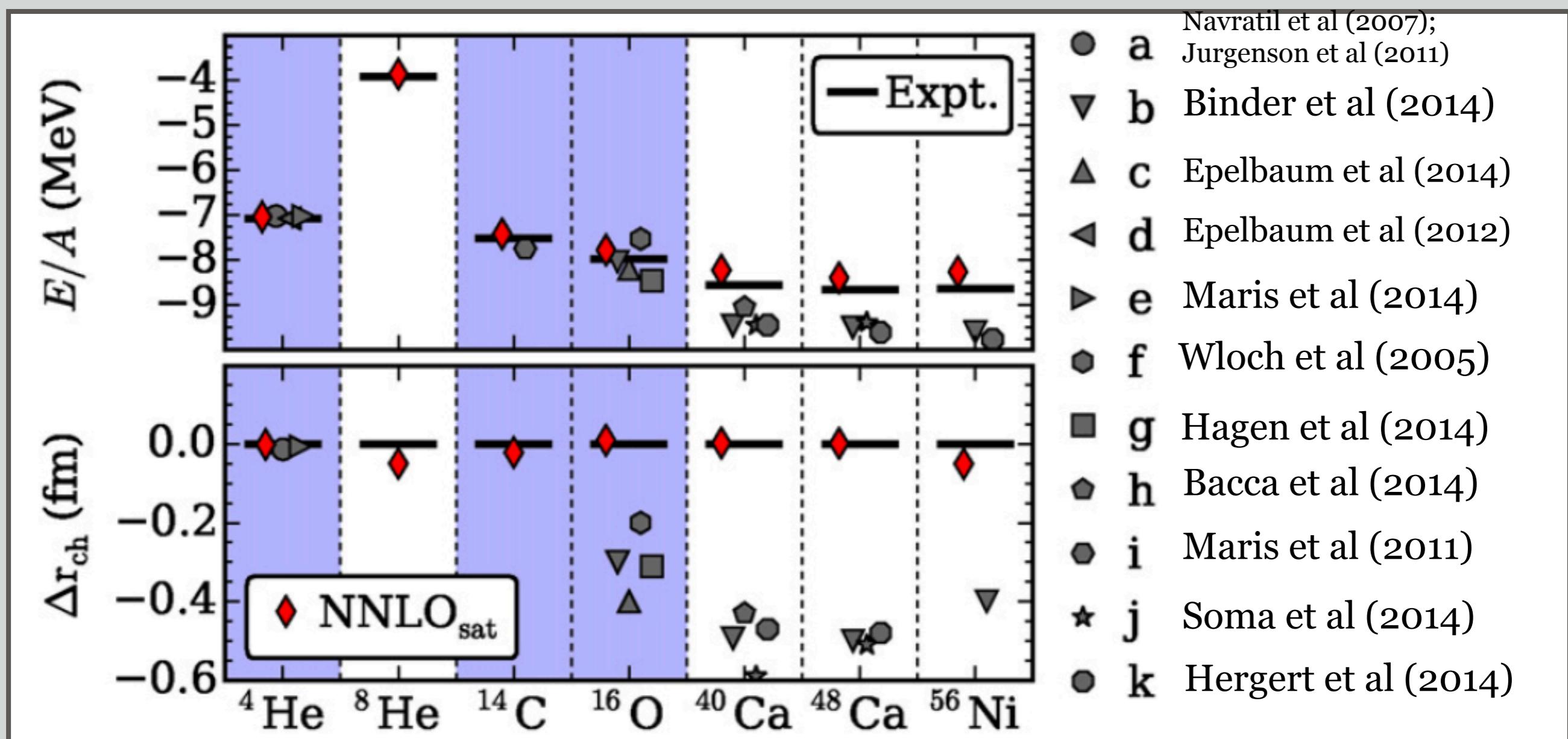


Ab initio calculations with existing chiral interactions

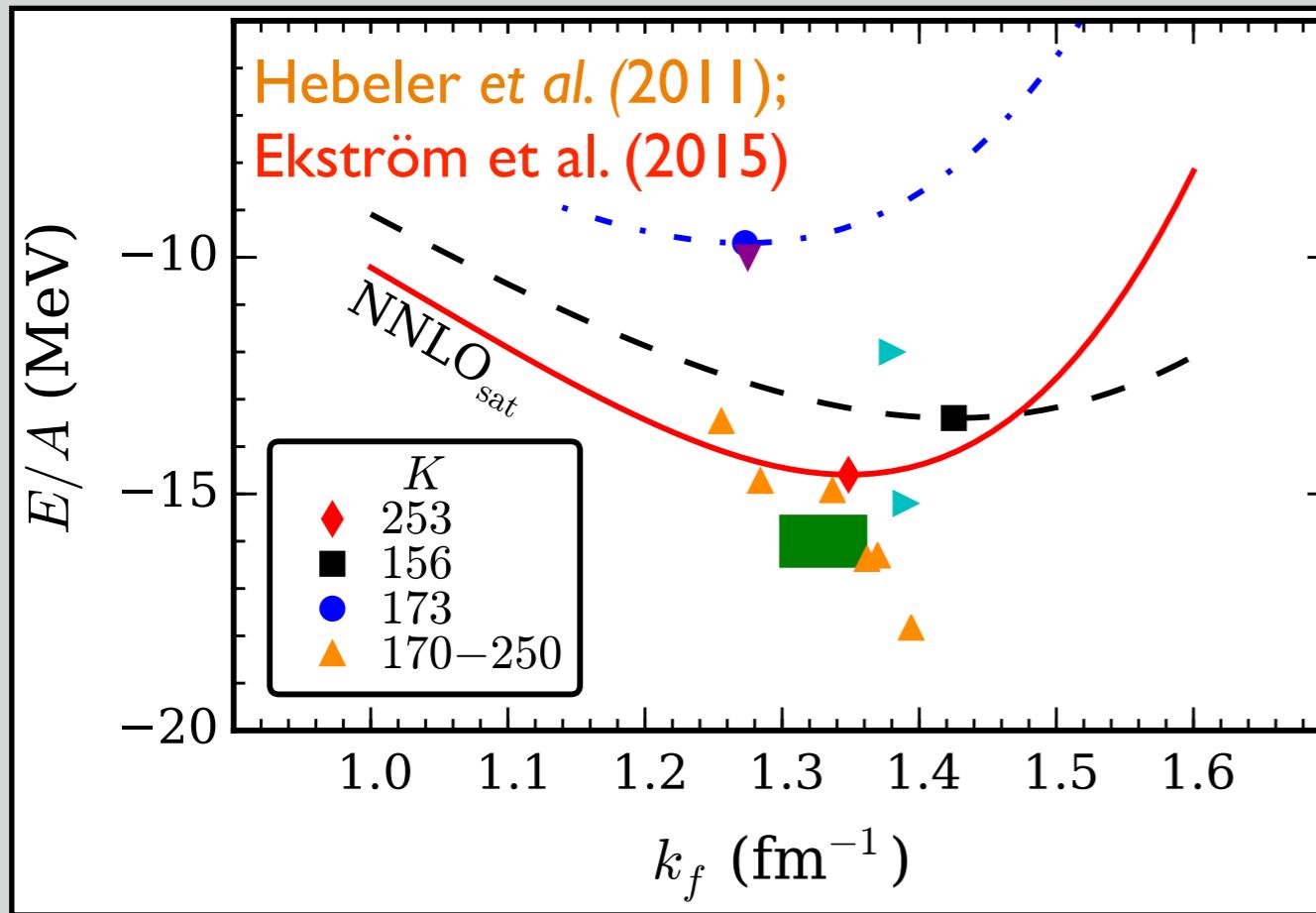
- **overbind** medium-mass and heavy nuclei, and
- **underestimate charge radii.**



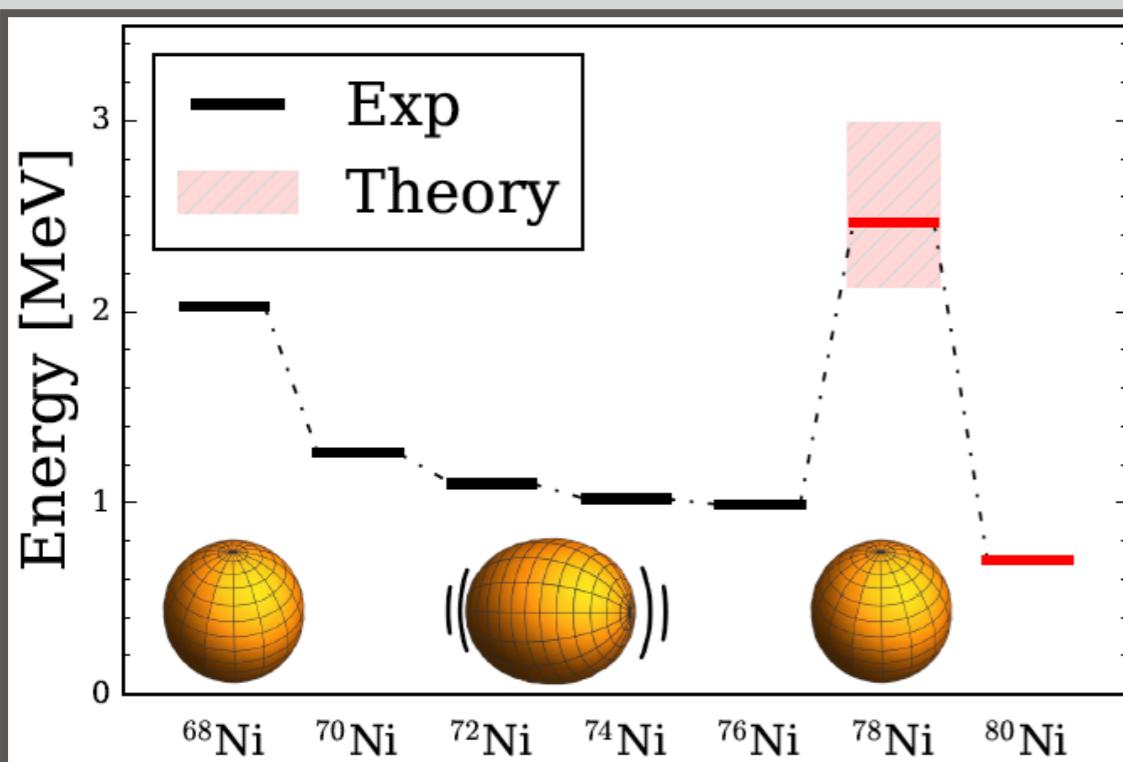
- **Simultaneous optimization** of NN and NNN LECs at NNLO.
- NCSM and CC calculations performed within the optimization.
- Adjusted to **NN scattering data** ($T_{\text{lab}} < 35$ MeV) ... and to $A=2,3,4$ nuclei, ... and to **BEs of ^{14}C , $^{16,22,24,25}\text{O}$** , and to **radii of ^{14}C and ^{16}O**



ACCURATE PREDICTIONS FOR FINITE NUCLEI AND NUCLEAR MATTER



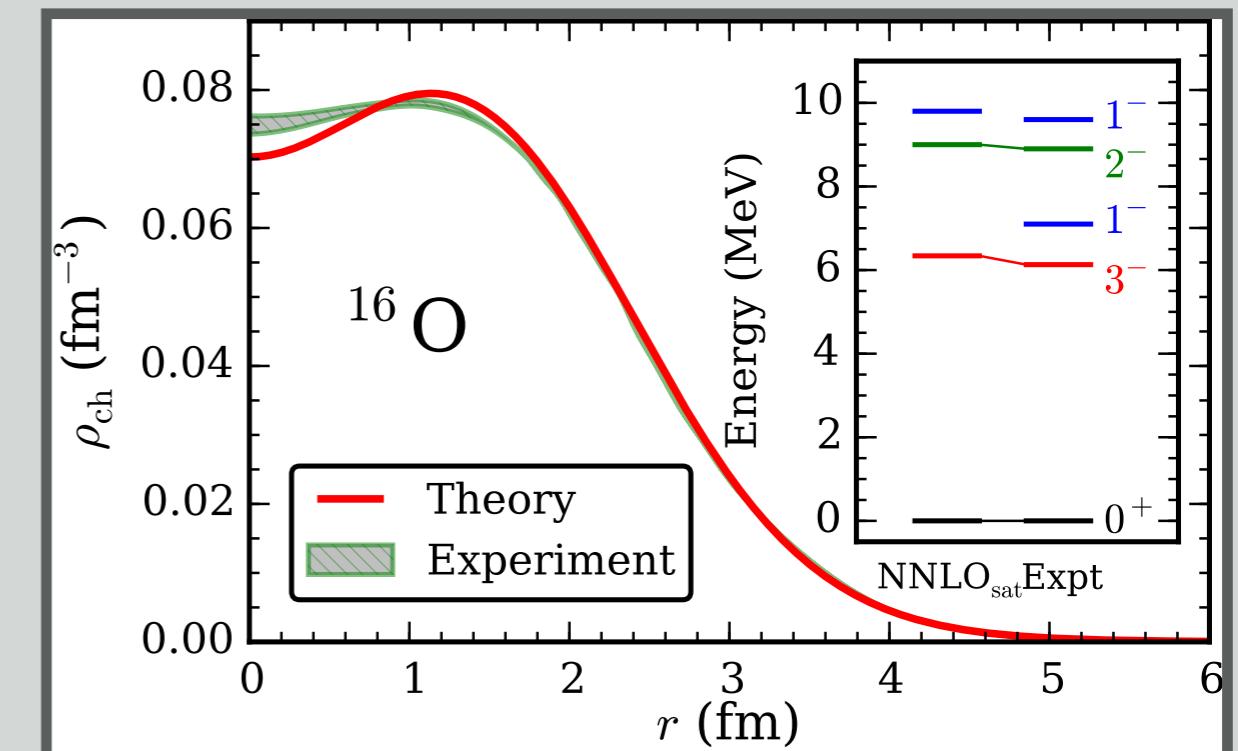
Accurate saturation



G. Hagen et al, Nat. Phys. 12 (2016) 186

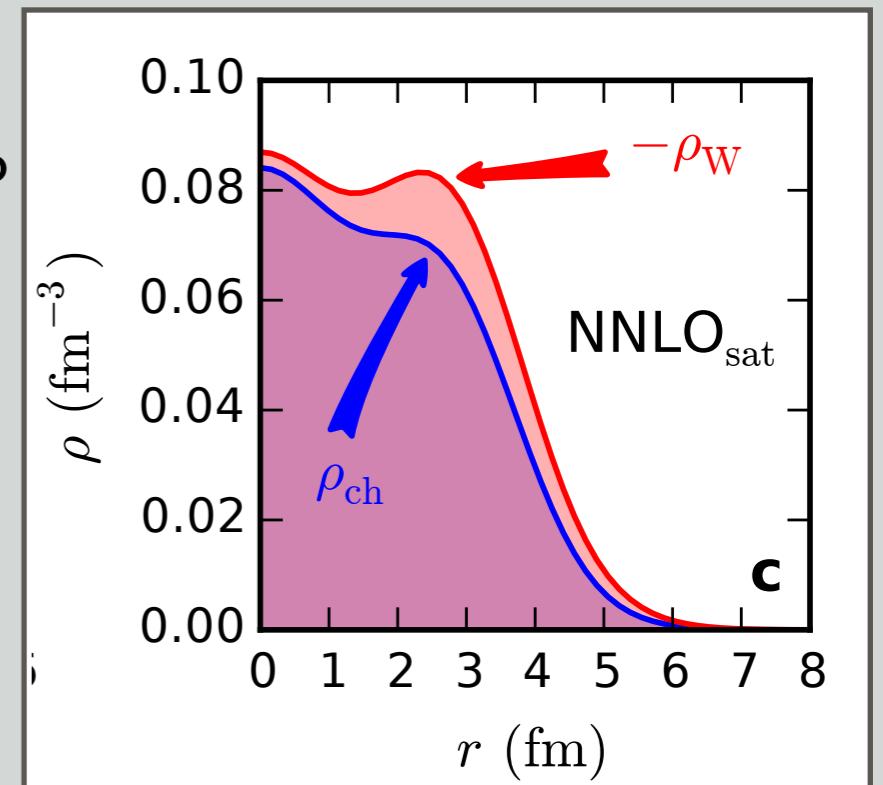
Structure of ^{78}Ni

G. Hagen, et al., Phys. Rev. Lett. 117, 172501 (2016).



^{16}O charge radius

Neutron skin of ^{48}Ca



OUTLOOK — PART 1

- ▶ Many-body methods with polynomial scaling (CC, IMSRG, SCGF) reach calcium and nickel regions, and even beyond...
- ▶ Development of effective interactions for valence-space shell model from ab initio interactions (IMSRG, CC)
- ▶ Computational capabilities exceed accuracy of available interactions.
- ▶ New generation of nuclear interactions:
 - different fitting strategies (saturation point), including intermediate delta particle.

Precision and accuracy frontiers

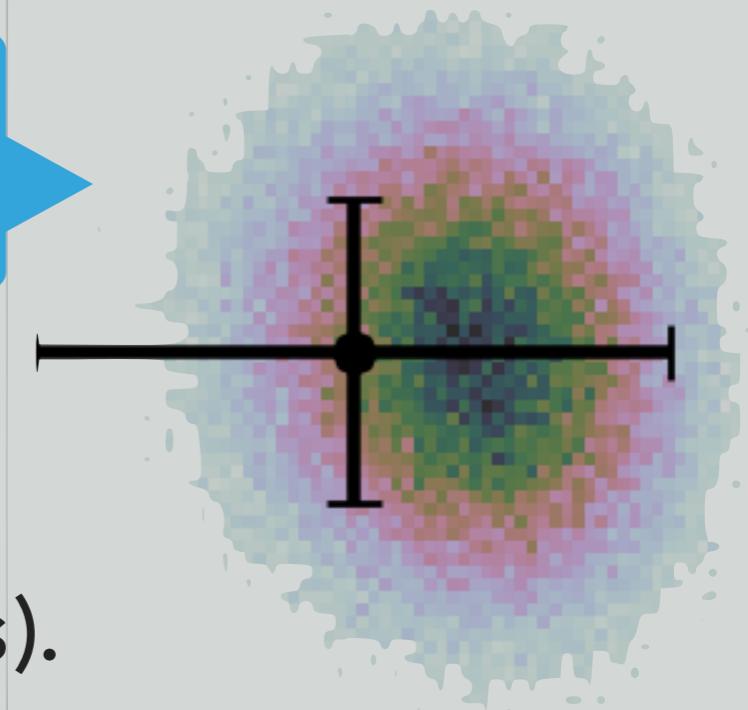
- ▶ Accurate results
- ▶ Precise results:
 - Uncertainty quantification,
 - Error propagation

PART 2

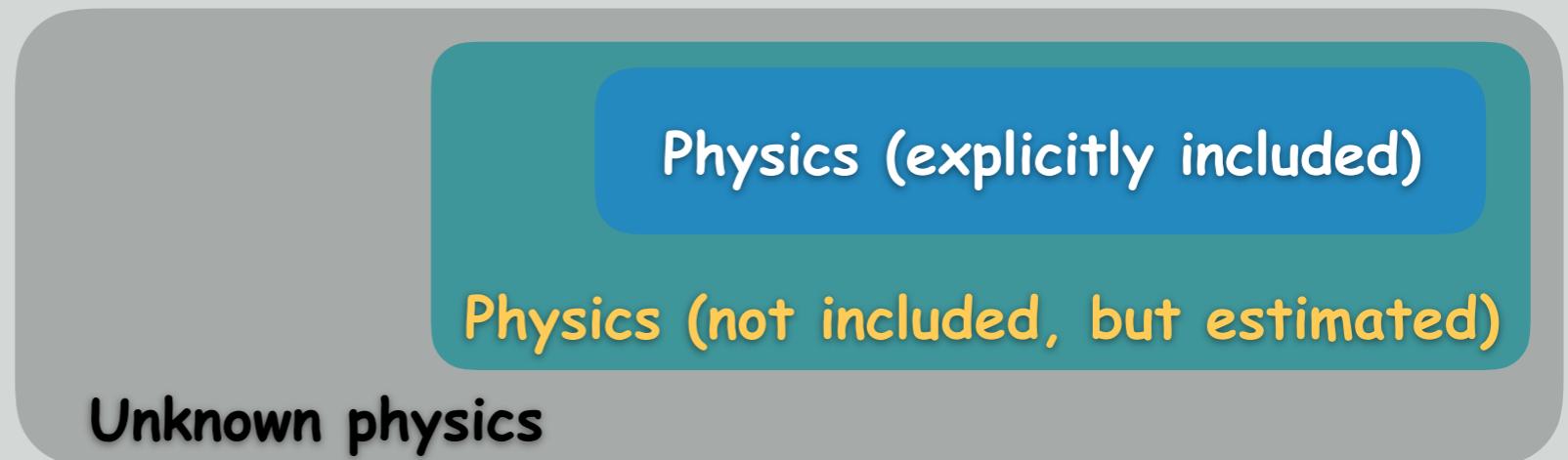
The precision and accuracy frontiers of nuclear theory

QUANTIFIED THEORETICAL UNCERTAINTIES

*“Does my model agree
with the data?”*



- ▶ **Statistical:** parametric uncertainties (should be done also for phenomenological models).
- ▶ **Systematic:** method (many-body solver) and numerical uncertainty.
- ▶ **Systematic:** physics model uncertainty.



ADVERTISEMENTS

- ▶ Annual series of workshops: ***ISNET*** = Information and Statistics in Nuclear Experiment and Theory
 - with topical issue in J. Phys. G;
 - **ISNET-8 at Chalmers** next fall;
- ▶ New ***TALENT*** course:
 - **Learning from data** – Bayesian Methods and Machine Learning” in **York, UK, June, 2019**;
 - email me at christian.forssen@chalmers.se to get on mailing list, or visit nucleartalent.org;

PARAMETRIC MODELS

- ▶ Assume that hypothesis H_i is a model M_i with parameters θ_i .
- ▶ In **Bayesian statistics** we assess an hypothesis by calculating its probability $p(H_i | \dots)$ conditional on known and/or presumed information using the rules of probability theory.
 - **Parameter estimation:**
Assume that the model M_i is true;
Compute: $p(\theta_i | D_{\text{obs}}, M_i, I)$
- ▶ In **Frequentist statistics** we would often use a statistical model in combination with a **maximum-likelihood estimator**.

BAYESIAN PARAMETER ESTIMATION

Bayes' theorem (follows from probability product rule):

posterior	likelihood	prior
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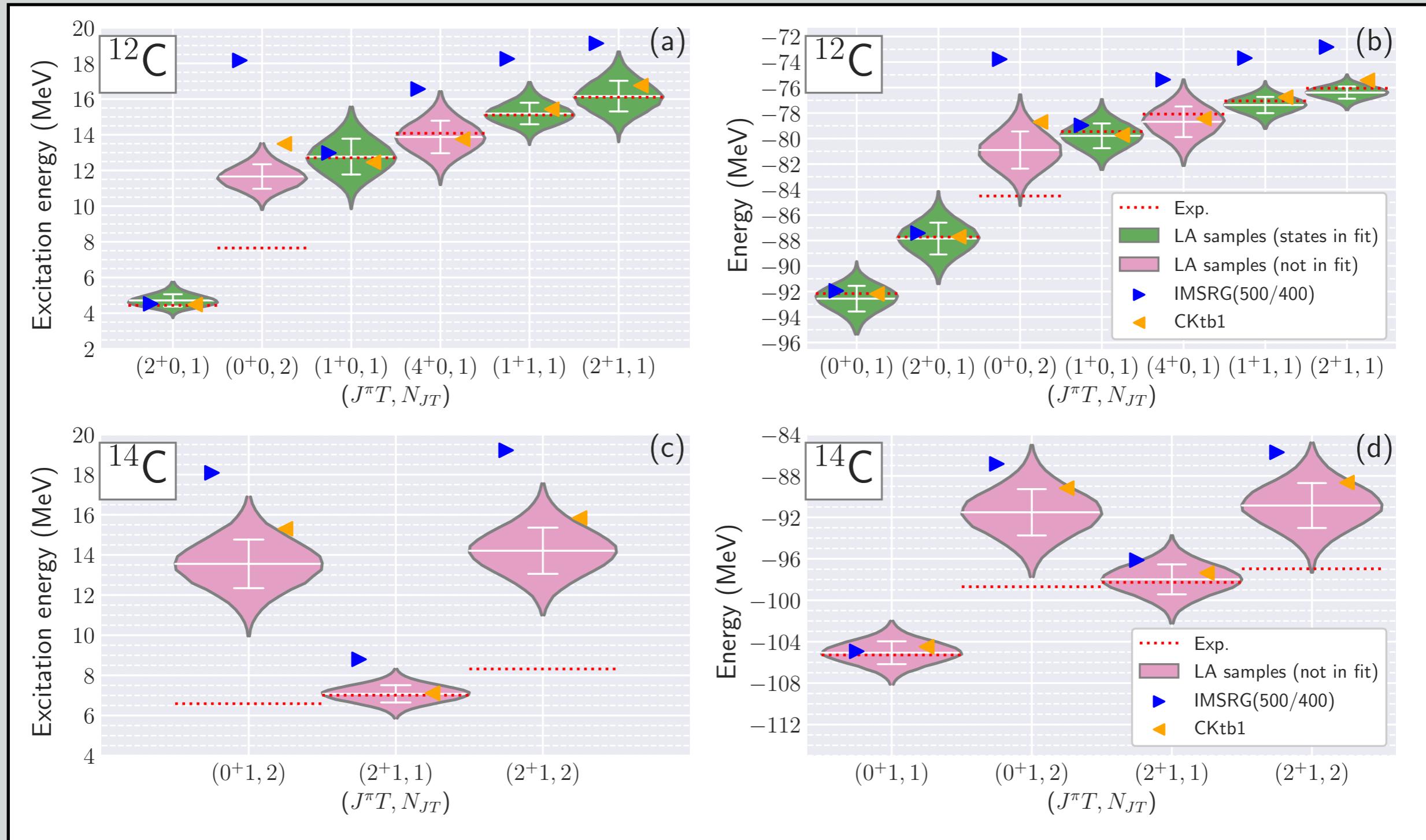
$$p(\theta | D, I) = \frac{p(D | \theta, I)p(\theta | I)}{p(D | I)}$$

Bayesian evidence

Marginalization:

$$p(\theta_1 | D, I) = \int d\theta_2 \dots d\theta_k p(\theta | D, I)$$

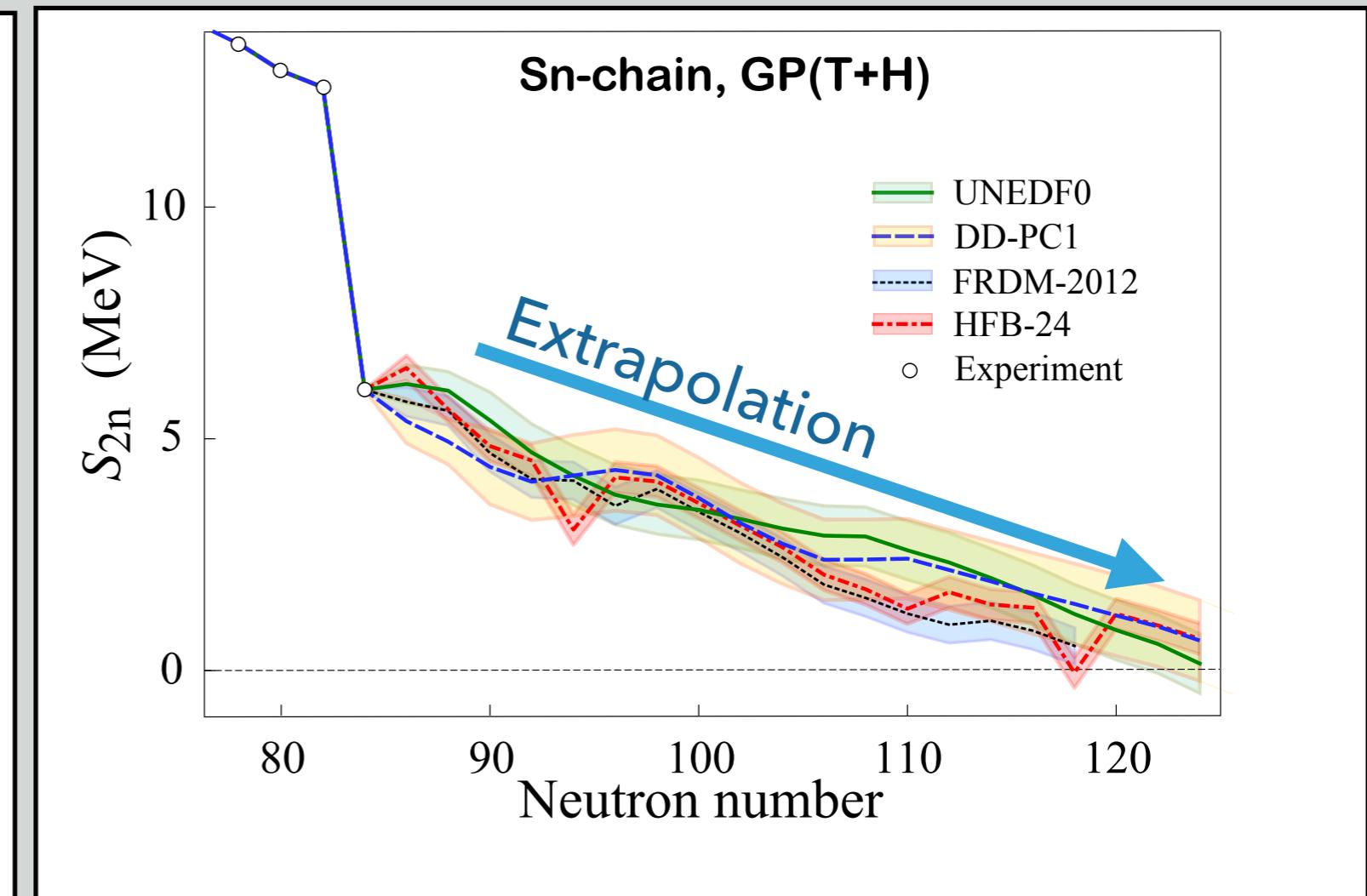
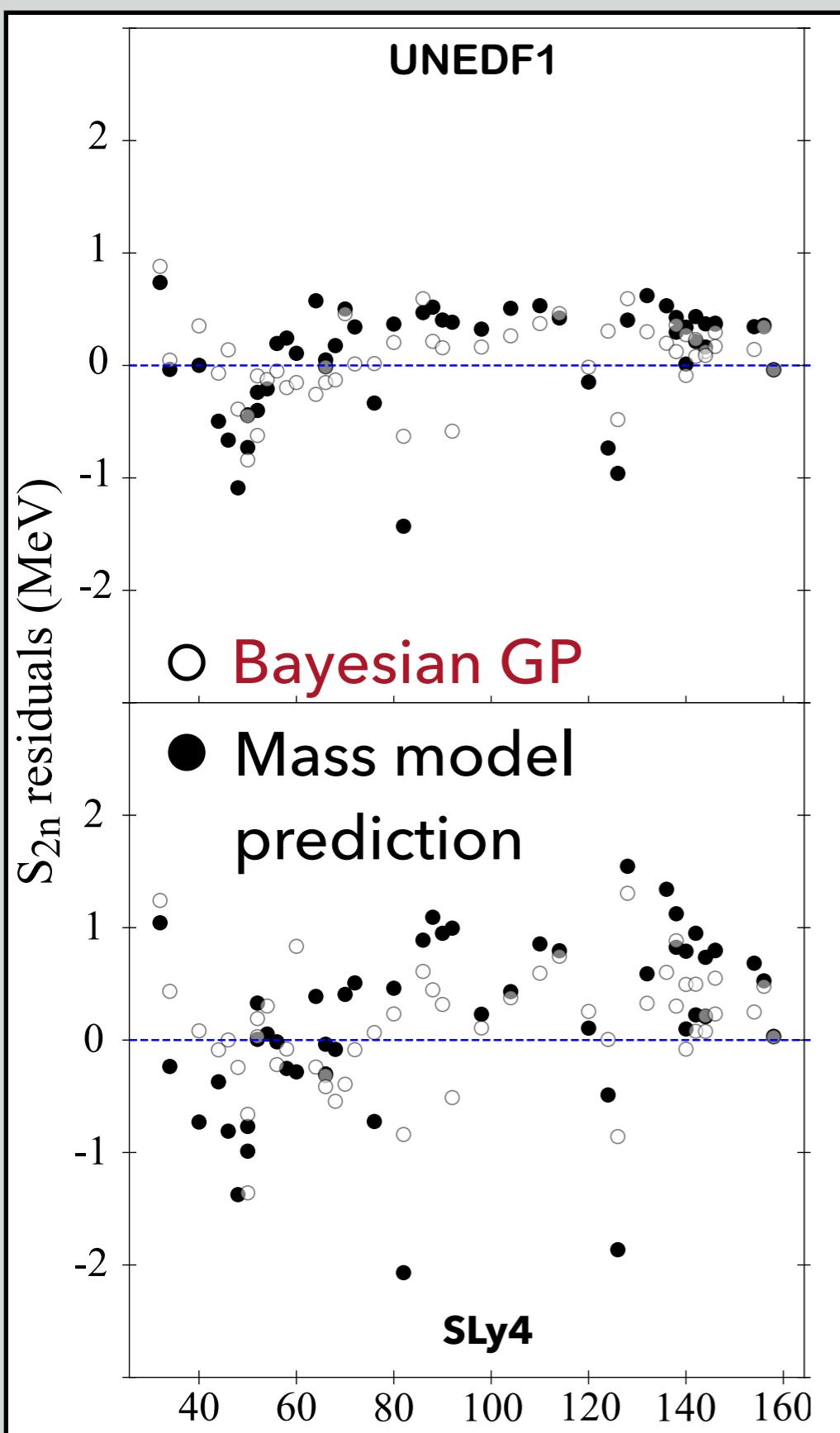
TOWARDS UNCERTAINTY QUANTIFICATION IN NUCLEAR SHELL MODEL



S. Yoshida et al., arXiv:1810.03263

Bayesian-inspired analysis of p-shell interaction (17 parameters, 33 fit data)

BAYESIAN APPROACH TO MASS MODEL EXTRAPOLATIONS



Emulators of S_{2n} residuals (and Bayesian confidence intervals) are constructed using Bayesian Gaussian processes for several different mass models.

Training set of masses (<2003 database) and testing set (>2003).

Ab initio approaches



Uncertainty quantification

AB INITIO NUCLEAR PHYSICS – NUCLEONIC DEGREES OF FREEDOM

OUR AIM: A credible program for uncertainty quantification in *ab initio* nuclear theory

- ▶ Start from nucleonic degrees of freedom and construct an effective inter-nucleon force based on effective field theory. σ_{model}
- ▶ The parameters (LECs) of this force will have to be constrained by data. σ_{data}
- ▶ Solve the few- or many-nucleon problem and compute observables. $\sigma_{\text{num+method}}$

LIKELIHOOD CHI-SQUARED FUNCTION

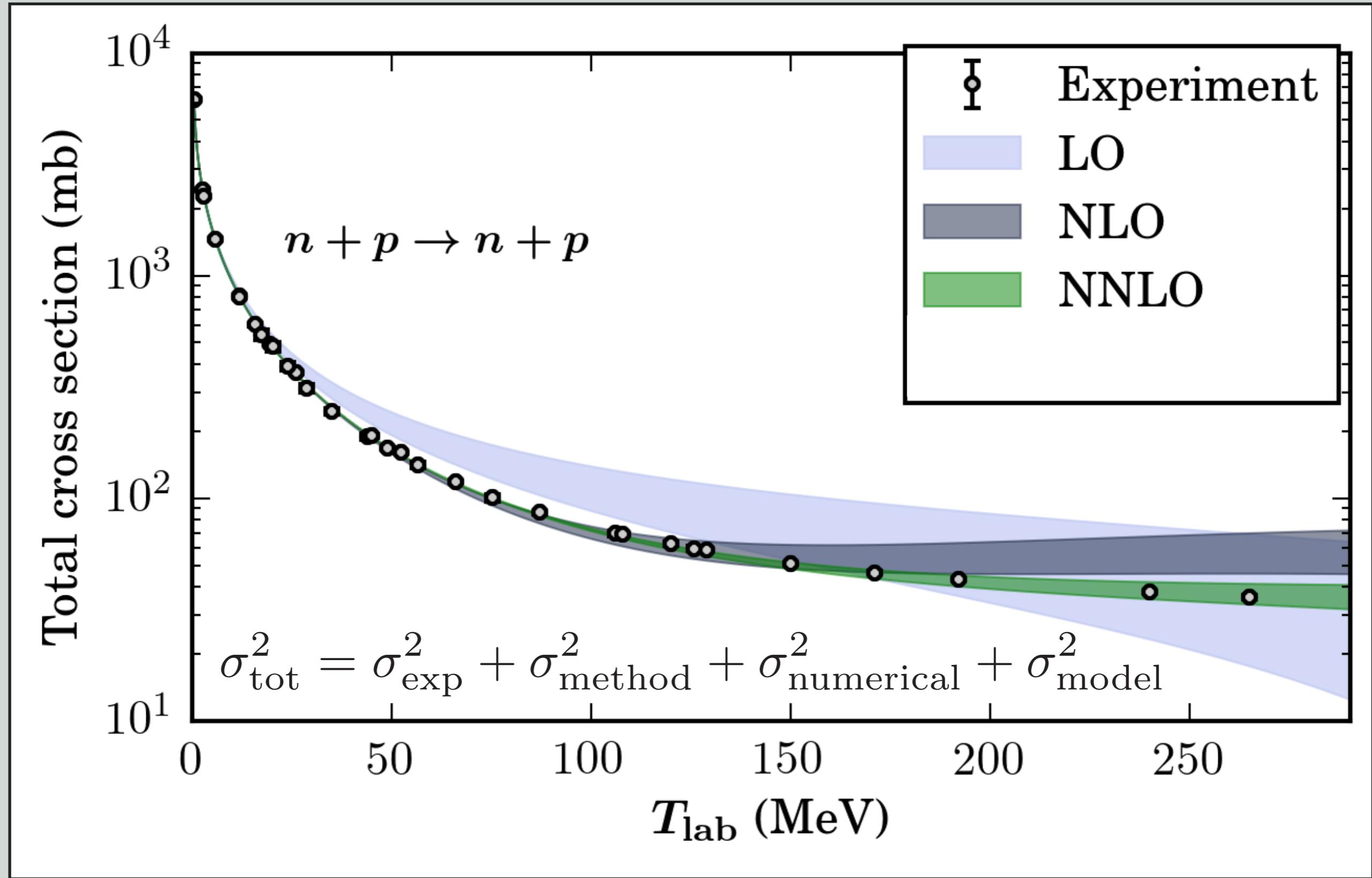
Low-energy constants (LECs) enter through contact interactions and need to be fitted to experimental data.

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

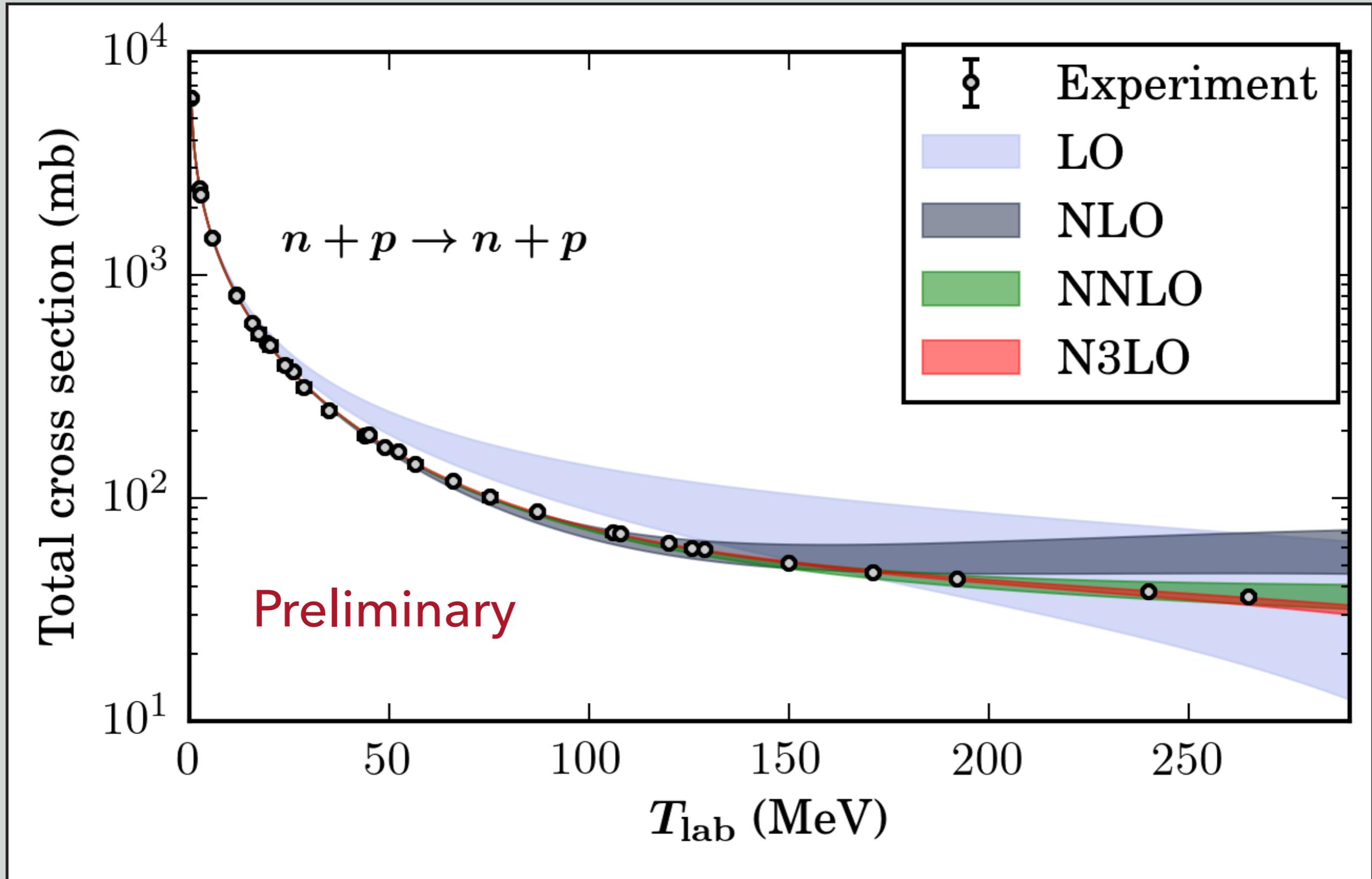
Maximum-Likelihood optimization

- ❖ **Standard approach:** sequential, chi-by-eye optimization; fits to phase shifts; N³LO needed for high-accuracy fit up to T_{lab}=290 MeV.
- ❖ From 2013: **Optimization technology** significantly improved.
- ❖ From 2015: Fits to **experimental data including uncertainties**.
- ❖ From 2016: **Algorithmic Differentiation (AD)** to get precise derivatives.

TOTAL np CROSS SECTION



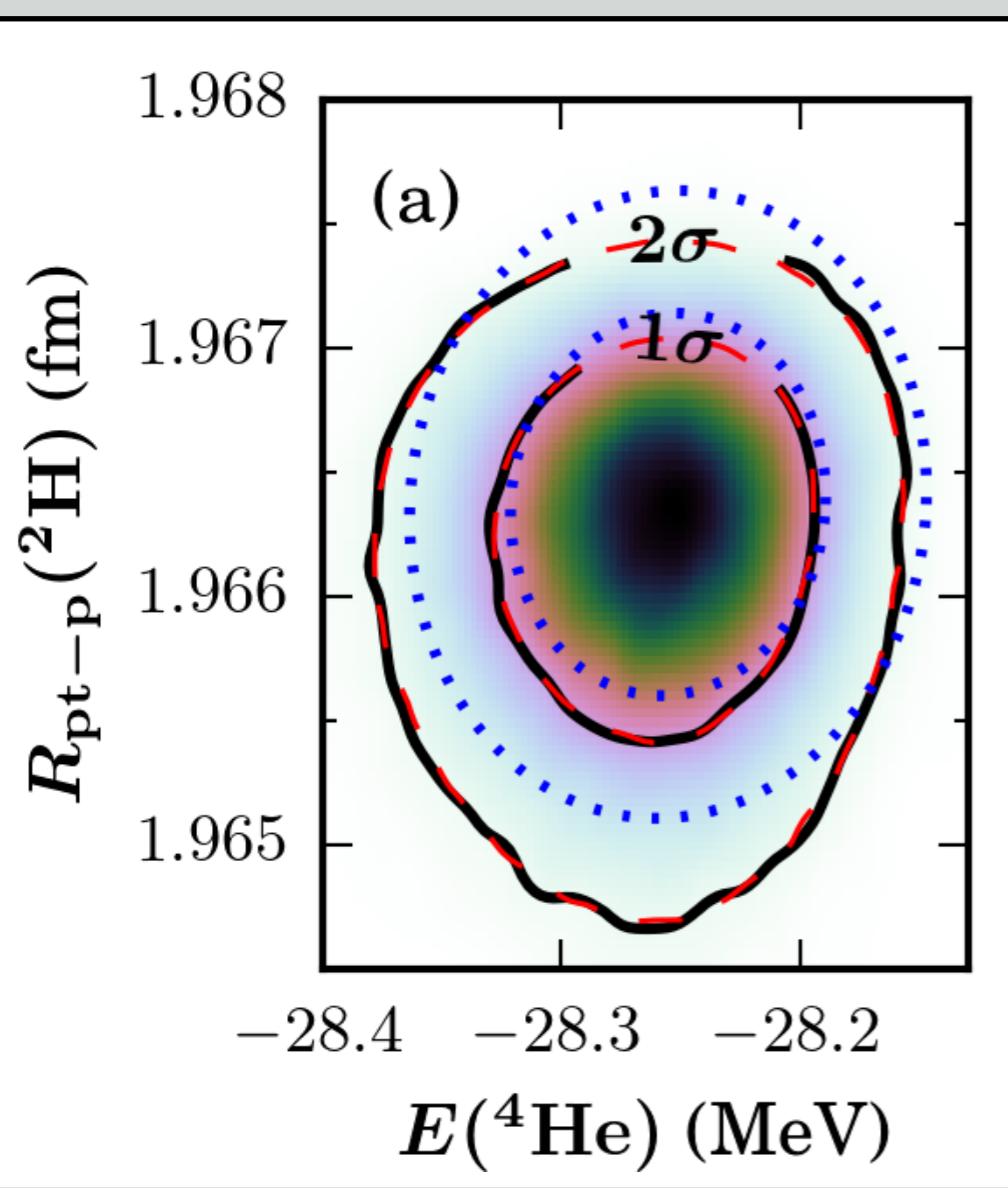
TOTAL np CROSS SECTION



UNCERTAINTY QUANTIFICATION IN THE FEW-BODY SECTOR

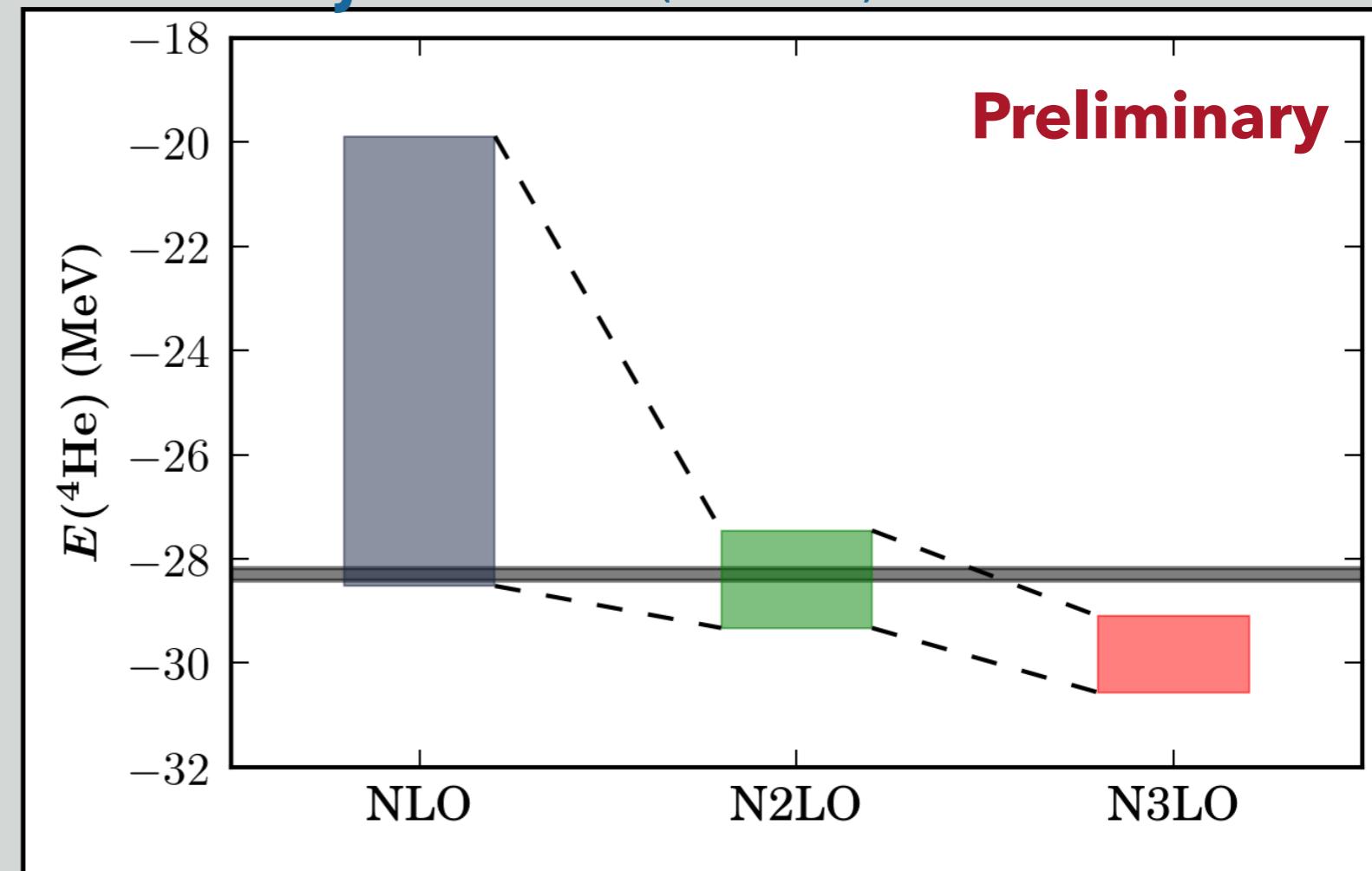
Statistical error propagation

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



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

Systematic (model) error estimate

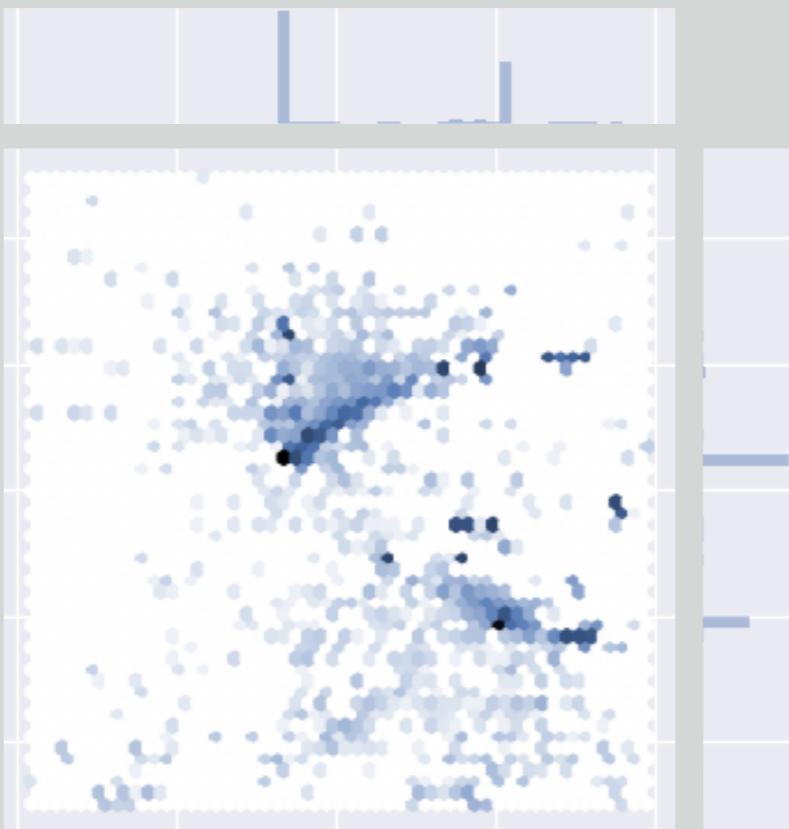


Bands indicate effects of cutoff variation and different truncations in the NN database.

BAYESIAN PARAMETER ESTIMATION

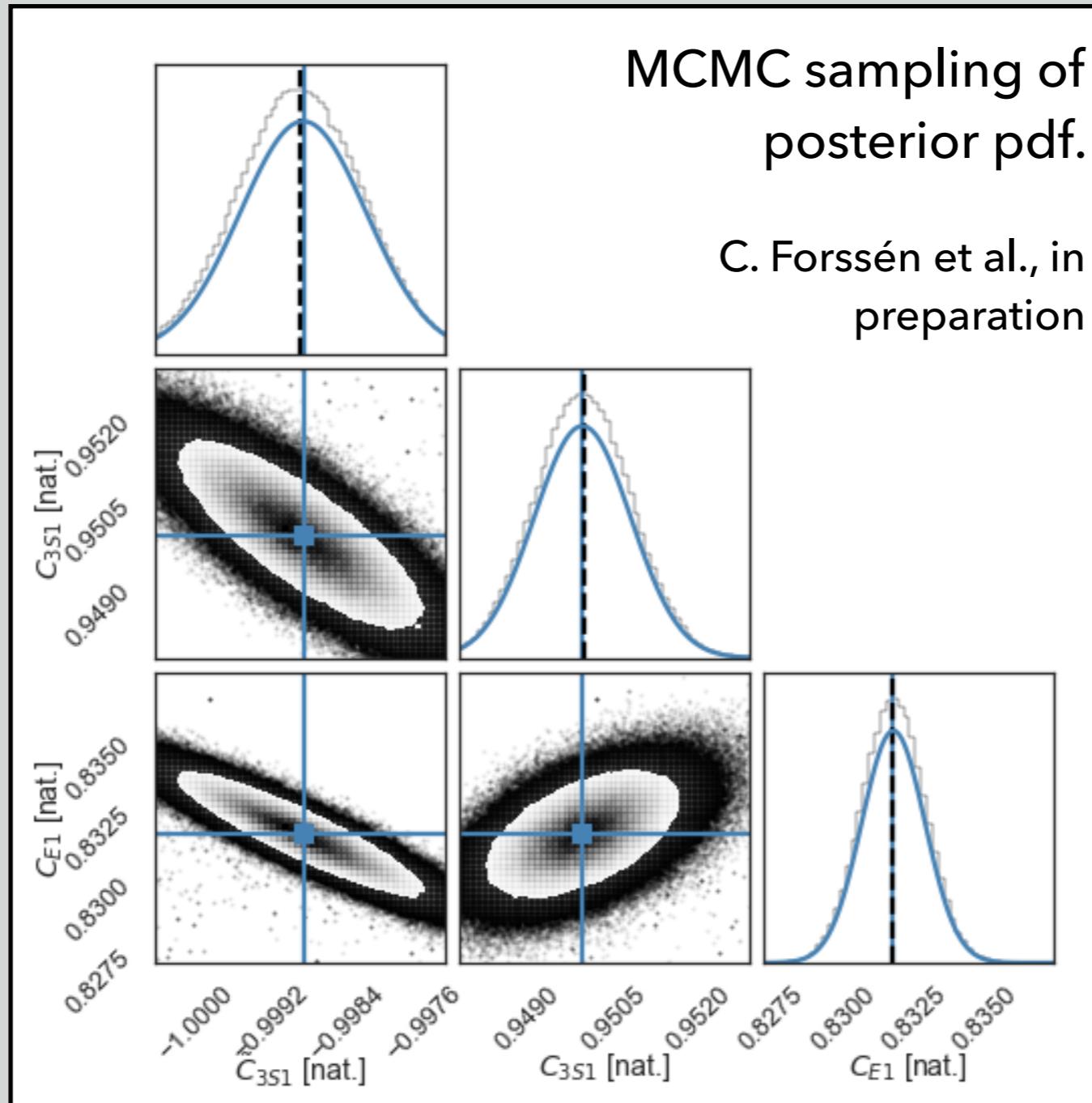
Bayes' theorem:

$$p(\theta | D, I) = \frac{p(D | \theta, I)p(\theta | I)}{p(D | I)}$$



- ▶ Bayes → consistent analysis of error in *ab initio* calculations
- ▶ Prior input information: naturalness of LEC:s
- ▶ Framework outputs (LEC) parameter posteriors with uncertainties consistently included:
- ▶ Can also add EFT truncation error

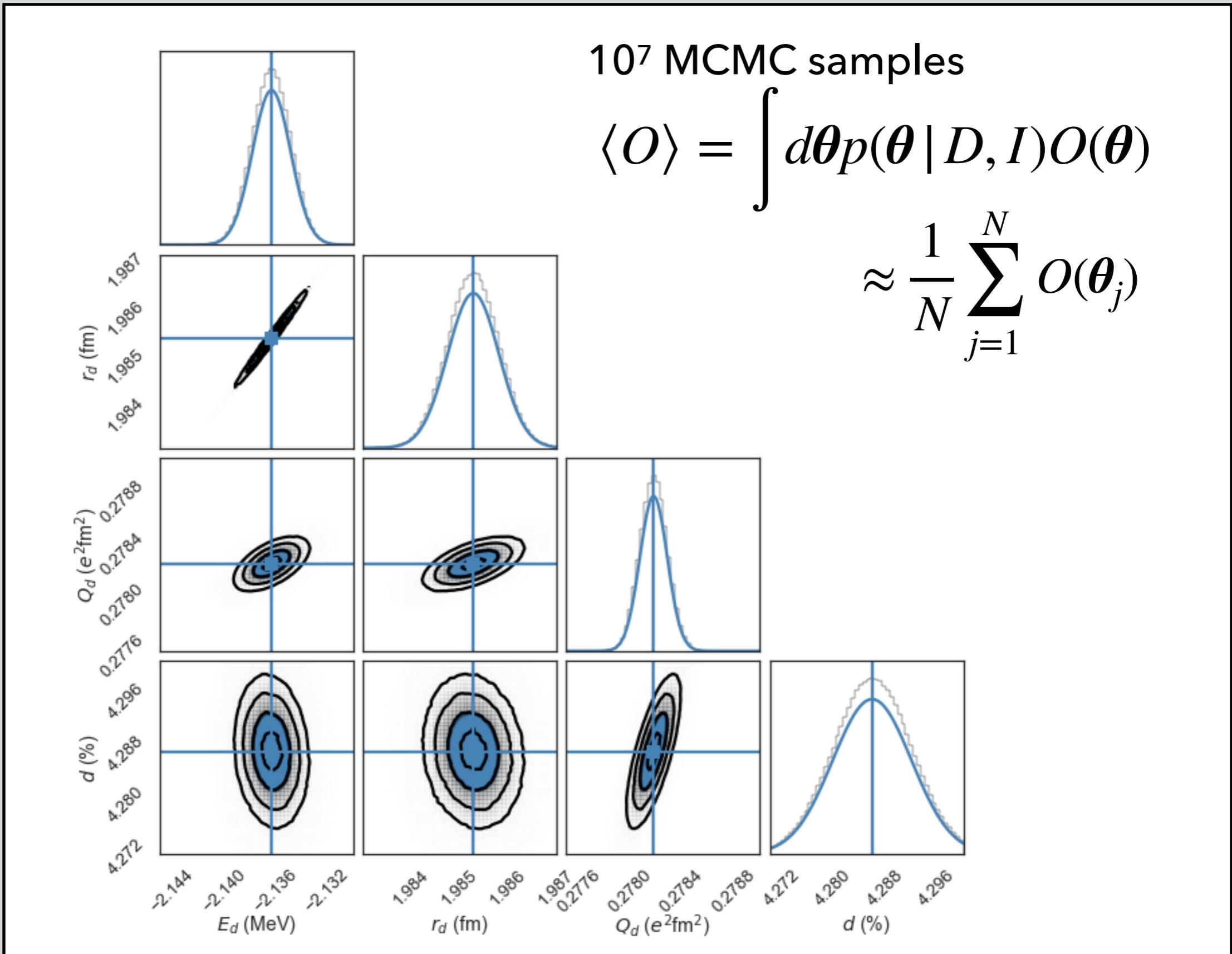
BAYESIAN PARAMETER ESTIMATION: DEUTERON CHANNEL



$$p(\tilde{C}_{1S0}, C_{1S0} | D, I) \propto p(D | \tilde{C}_{1S0}, C_{1S0}, I) p(\tilde{C}_{1S0}, C_{1S0} | I)$$

posterior likelihood prior

BAYESIAN ERROR PROPAGATION: DEUTERON OBSERVABLES



OUTLOOK

We're in a golden age for low-energy nuclear physics theory

- ▶ EFT and RG have become important tools for precision when combined with mathematical optimization algorithms and *ab initio* many-body methods.
- ▶ New generation of many-body methods that scale polynomially with A .
- ▶ Next generation of nuclear interactions will probe new aspects of the EFT approach
- ▶ Emergence of uncertainty estimates in *ab initio* theory.
- ▶ The use of advanced computational methods and new technologies are key for progress.

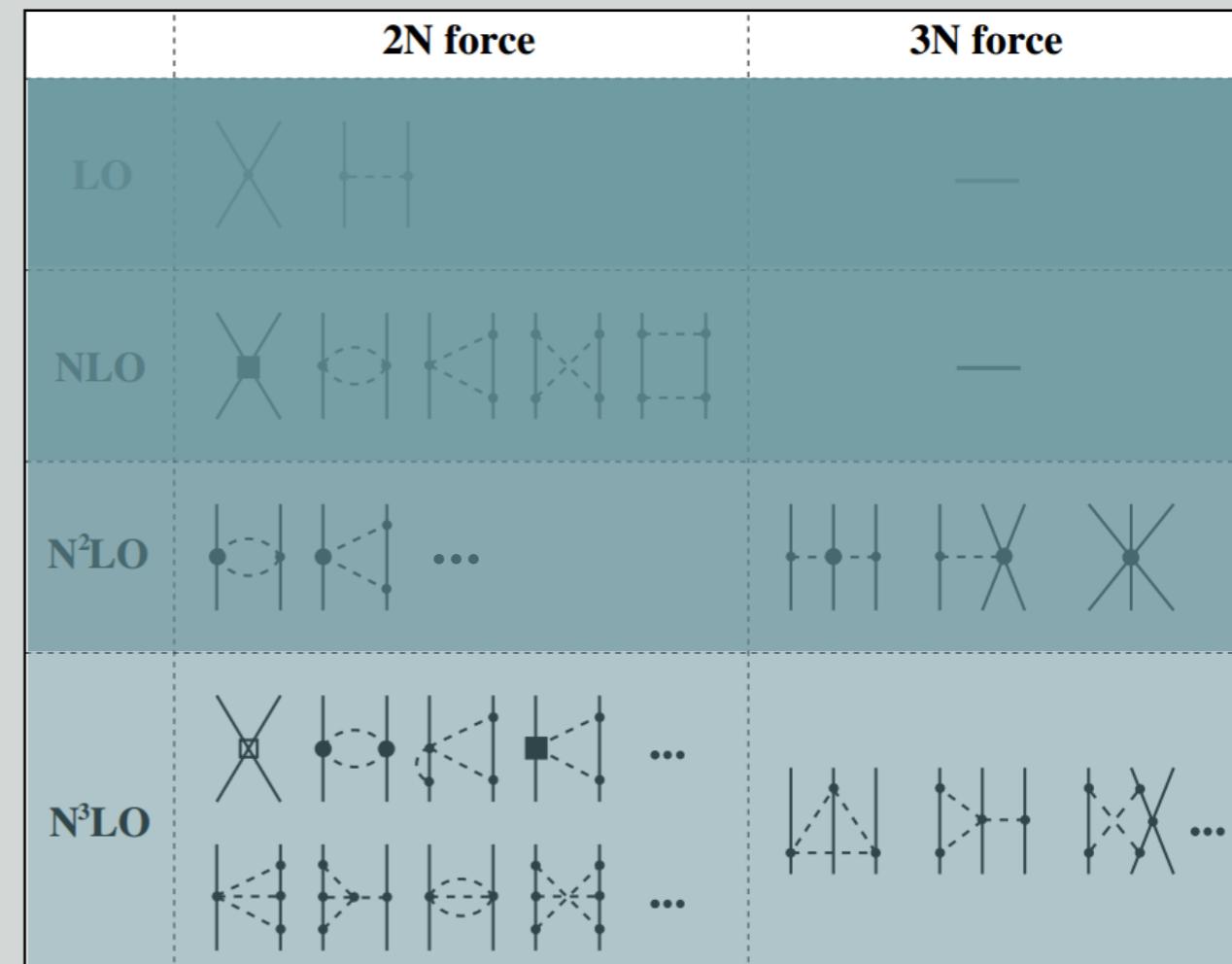
Stay tuned!

We're entering the era of *precision nuclear physics*!

CHIRAL EFFECTIVE FIELD THEORY

Chiral EFT

- Utilize a separation of scales.
- Chiral symmetry and pion dynamics constrain long-range physics;
- Short-distance unresolved – capture in LECs. Need to be fitted to data.
- Systematic low-energy expansion: $(Q/\Lambda_X)^\nu$
- Connects several sectors:
 πN , NN , NNN , j_N



Chiral EFT

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

INPUT AND TECHNOLOGY

πN scattering

- WI08 database
- T_{lab} between 10-70 MeV
- $N_{\text{data}} = 1347$
- $\chi^2 \text{EFT}(Q^4)$ to avoid underfitting

NN scattering

- SM99 database
- T_{lab} between 0-290 MeV
- $N_{\text{data}} = 2400(\text{np}) + 2045(\text{pp})$
- $\chi^2 \text{EFT}(Q^0, Q^2, Q^3)$

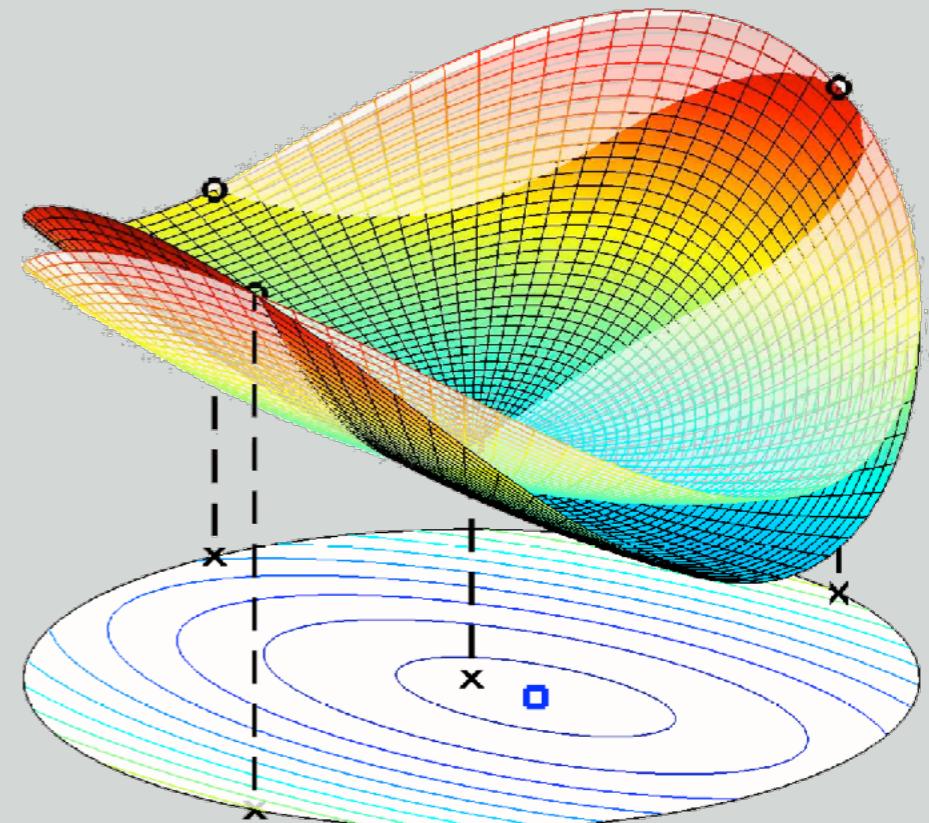
All 6000 residuals computed on 1 node in ~90 sec.

$A=3$ bound states

- ${}^3\text{H}, {}^3\text{He}$ (binding energy, radius, ${}^3\text{H}$ half life)

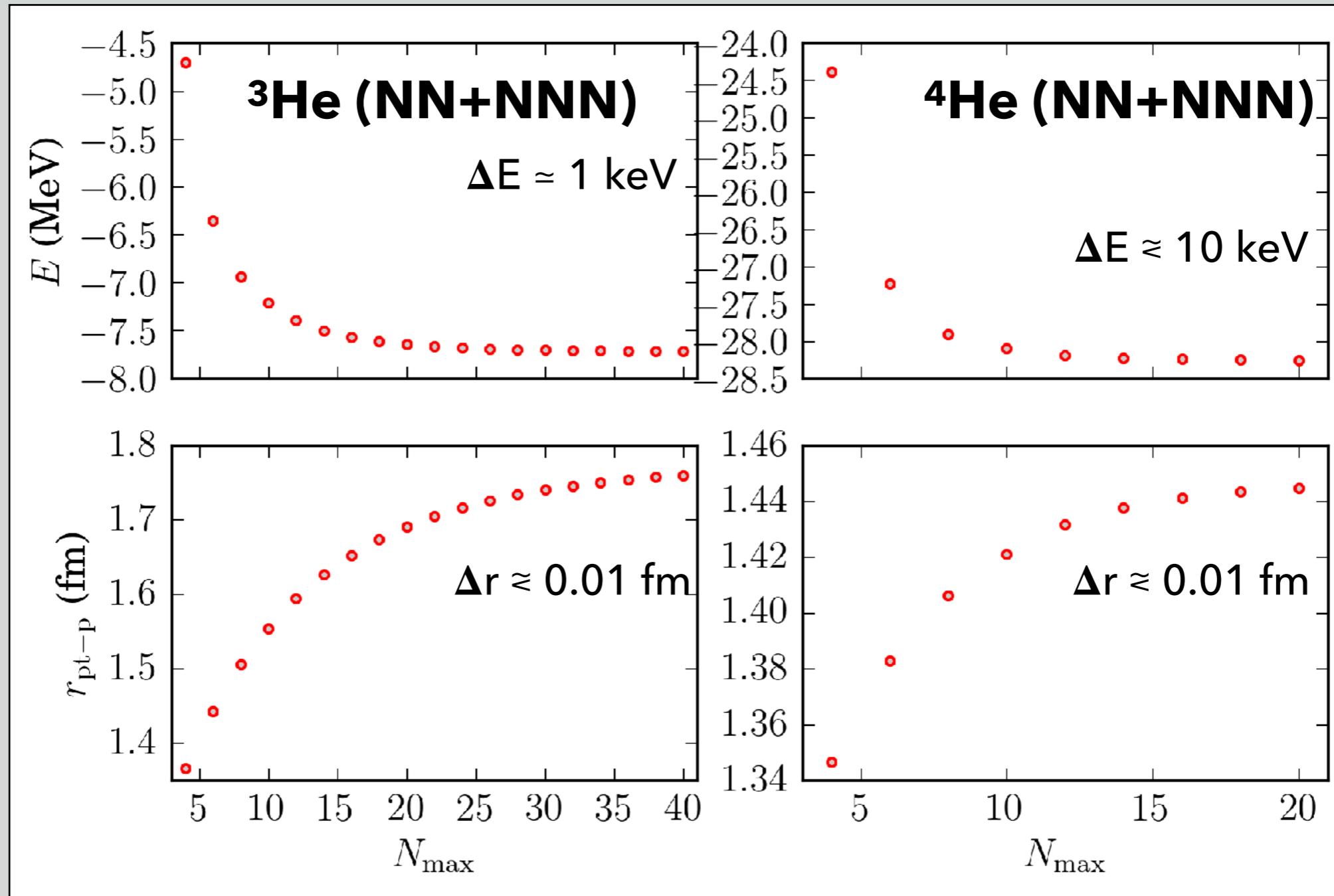
On 1 node in ~10 sec

+ derivatives! ($\times 2-20$ cost)



FEW-BODY CALCULATIONS

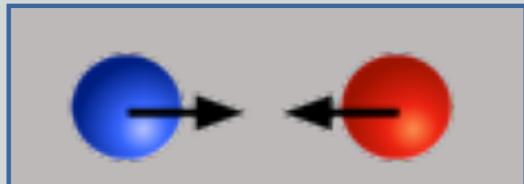
NCSM (rel. coord.)



~ 10 sec.

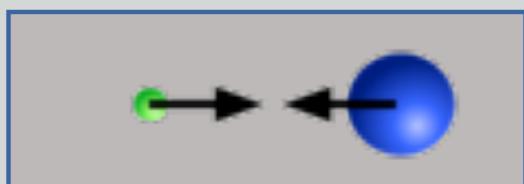
~ 45 sec.

EXPERIMENTAL DATA



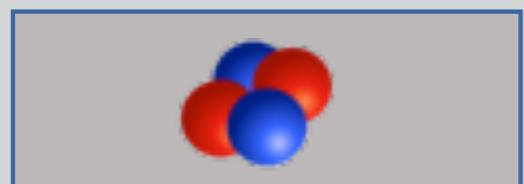
Granada NN database (0-290 MeV)

R. Navarro Pérez et al. PRC 88, 064002 (2013)



Washington Institute WI08 πN database (0-70 MeV)

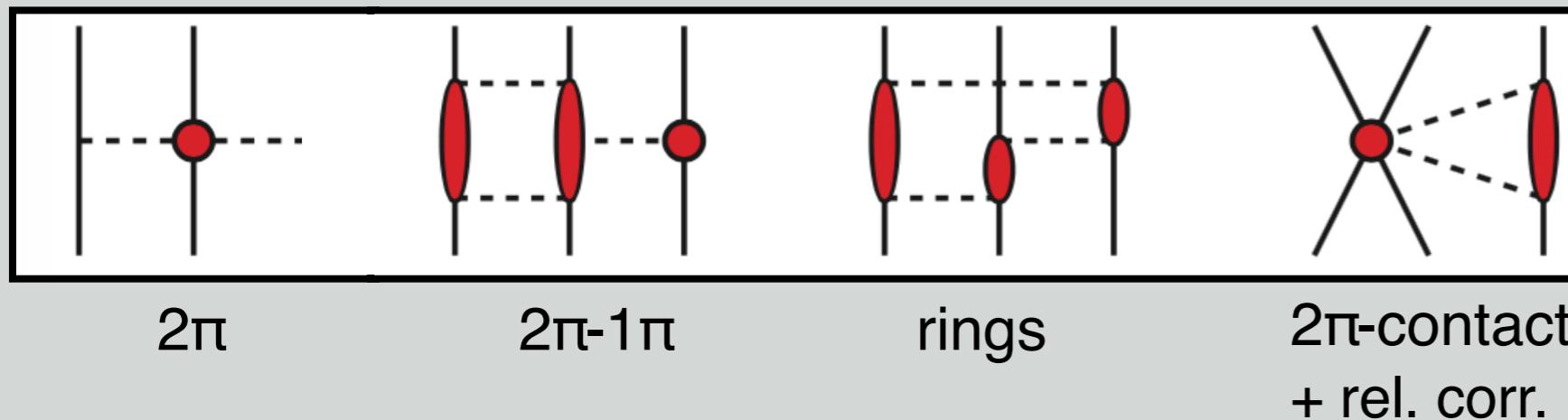
R. Workman et al. PRC 86, 035202 (2012)



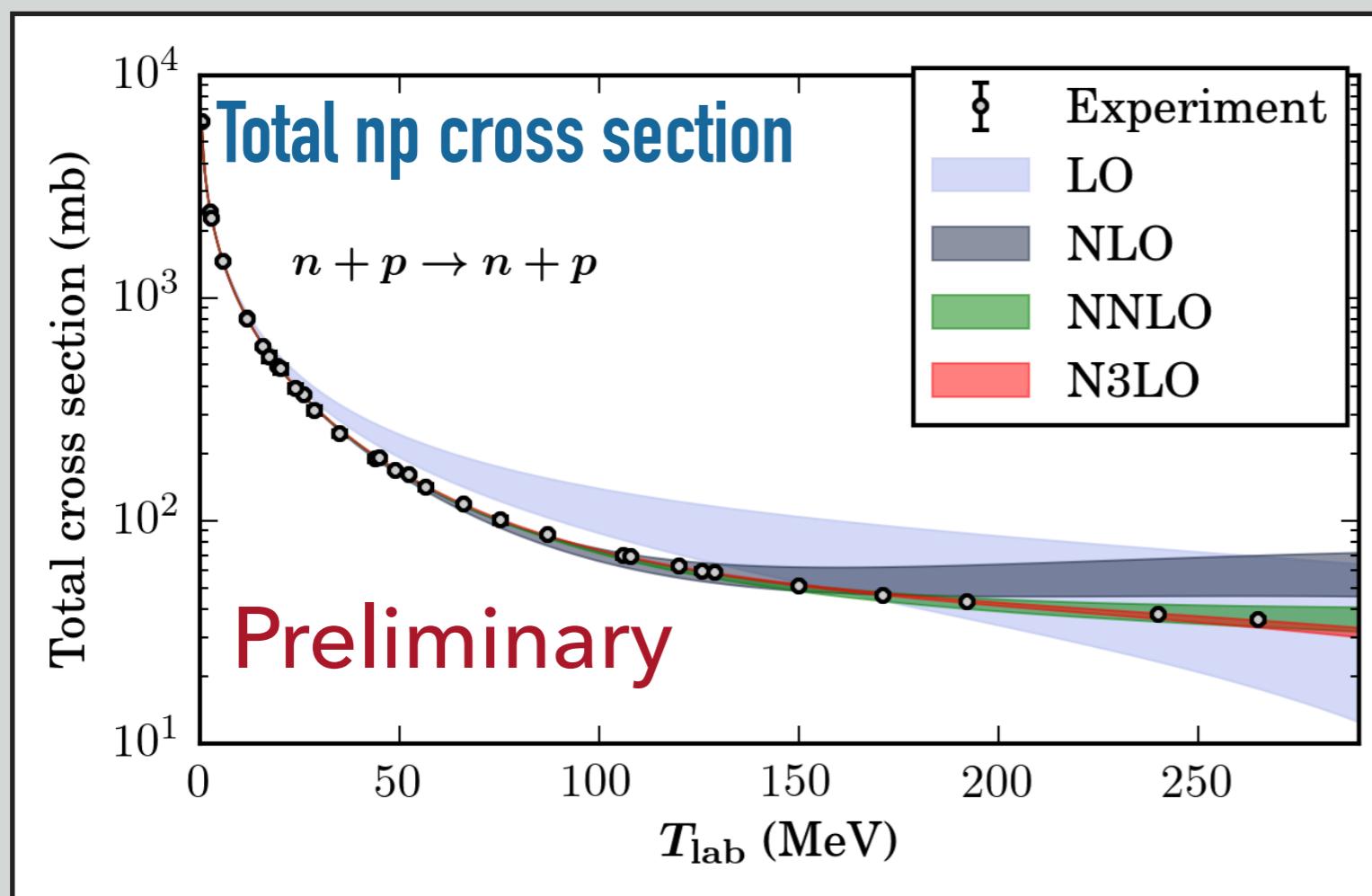
	Experimental value	$\sigma_{\text{exp+method}}$
$E(^2\text{H})$	-2.22456627(46)	0.22×10^{-3}
$E(^3\text{H})$	-8.4817987(25)	0.028
$E(^3\text{He})$	-7.7179898(24)	0.019
$E(^4\text{He})$	-28.2956099(11)	0.11
$r_{\text{pt-p}}(^2\text{H})$	1.97559(78) ^a	0.79×10^{-3}
$r_{\text{pt-p}}(^3\text{H})$	1.587(41)	0.041
$r_{\text{pt-p}}(^3\text{He})$	1.7659(54)	0.013
$r_{\text{pt-p}}(^4\text{He})$	1.4552(62)	0.0071
$Q(^2\text{H})$	0.27(1) ^b	0.01
$E_A^1(^3\text{H})$	0.6848(11)	0.0011

ORDER-BY-ORDER CONVERGENCE

N3LO optimizations are challenging



2π 2π-1π rings 2π-contact
+ rel. corr.



41 parameters to optimize,
No new parameters in the
three-nucleon force.

3NF matrix elements recently
made available (K. Hebeler)

@N3LO:

- at least 100 minima
- all with a good description
of πN , NN, NNN data
- perform differently for $A > 3$

Possible solutions:

- Additional data... NNN
scattering, heavier systems,...
- Bayesian statistics...

are all **computationally very
costly**