Ab initio nuclear physics with chiral EFT

optimization and uncertainty estimates

Andreas Ekström
Department of Physics
Chalmers University of Technology
Gothenburg, Sweden
andreas.ekstrom@chalmers.se

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Vetenskapsrådet

MARIE CURIE ACTIONS

Many Thanks to all my collaborators

@Chalmers: B. D. Carlsson, C. Forssén

@UT/ORNL: S. Binder, G. Hagen,
G. R. Jansen, T. Papenbrock, L. Platter,
B. Acharya

@MSU: W. Nazarewicz

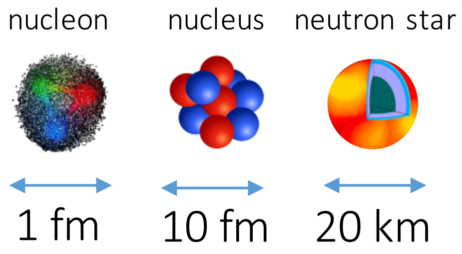
@MSU/UiO: M. Hjorth-Jensen

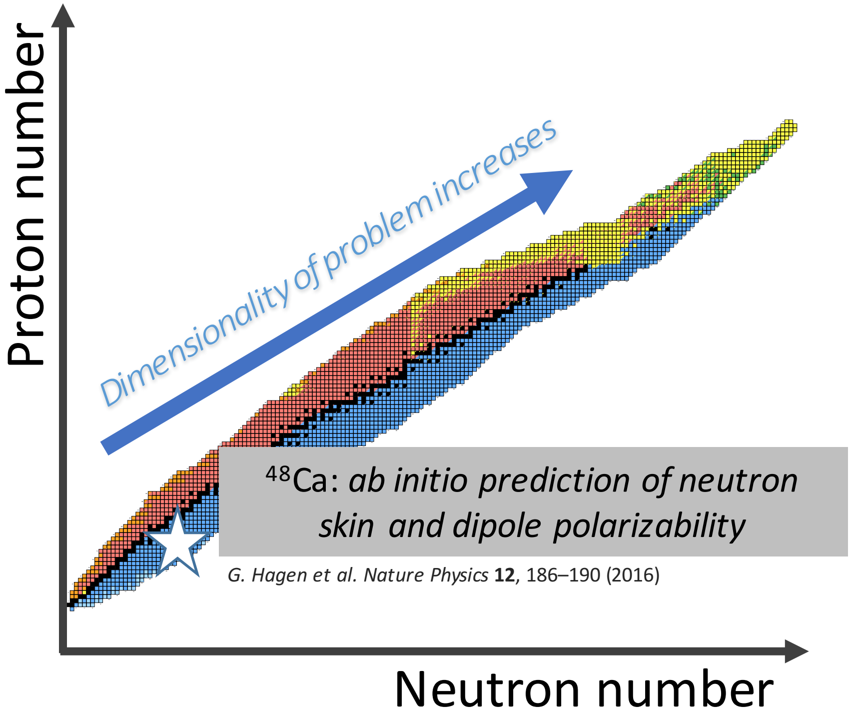
@U. Idaho: R. Machleidt

@TU Darmstadt: K. Hebeler,
A. Schwenk, K. Wendt

Overview

Nuclear physics spans a broad scientific scope. We would like to understand the origin, stability, and evolution of subatomic matter; how it organizes itself and what phenomena emerge.





G. Hagen et al. Nature Physics **12**, 186–190 (2016)

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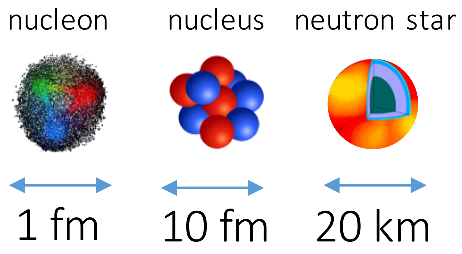

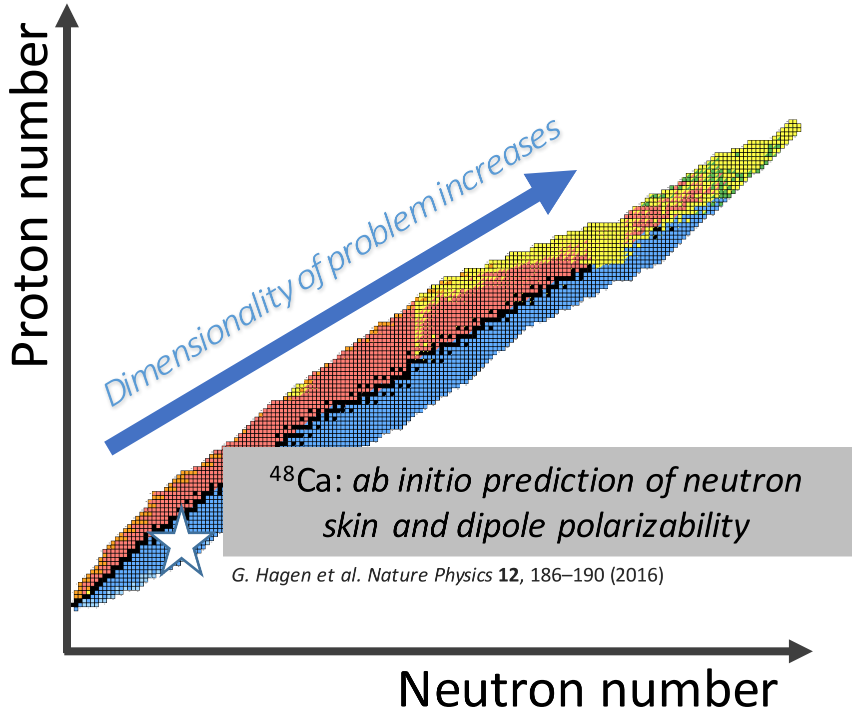

Many-body methods that scale polynomially with A

- e.g. Coupled-Cluster, In-Medium SRG, SC Green's function theory,…

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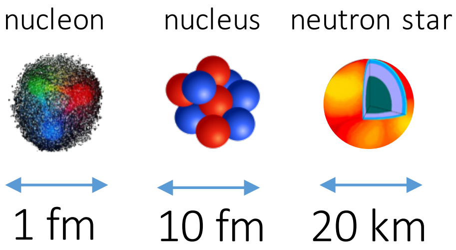

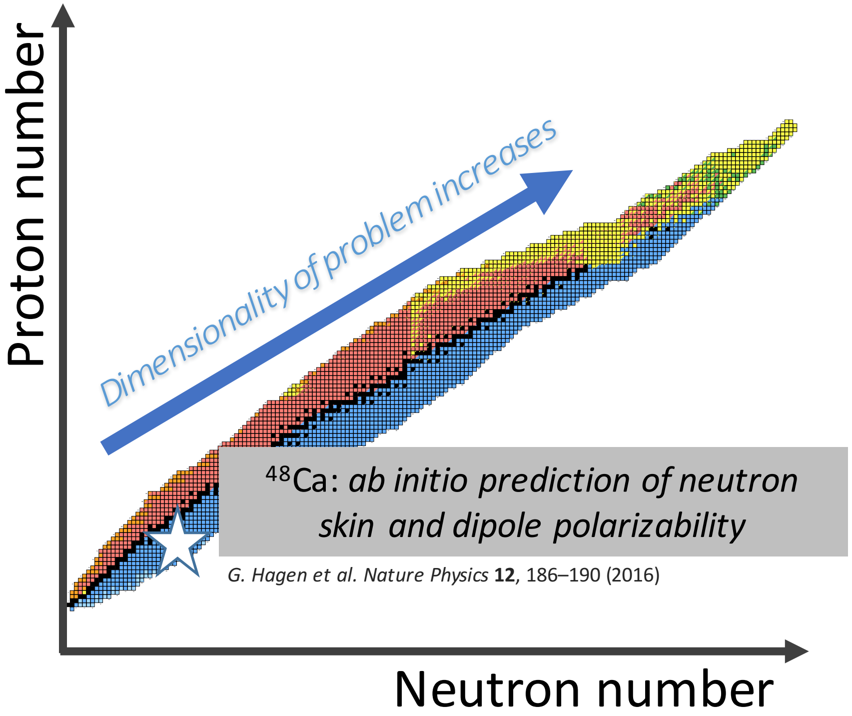

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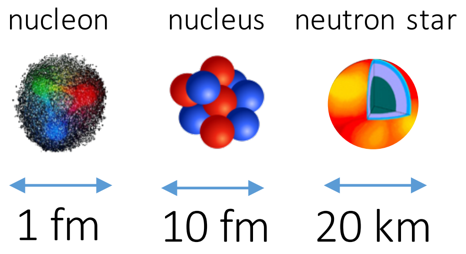

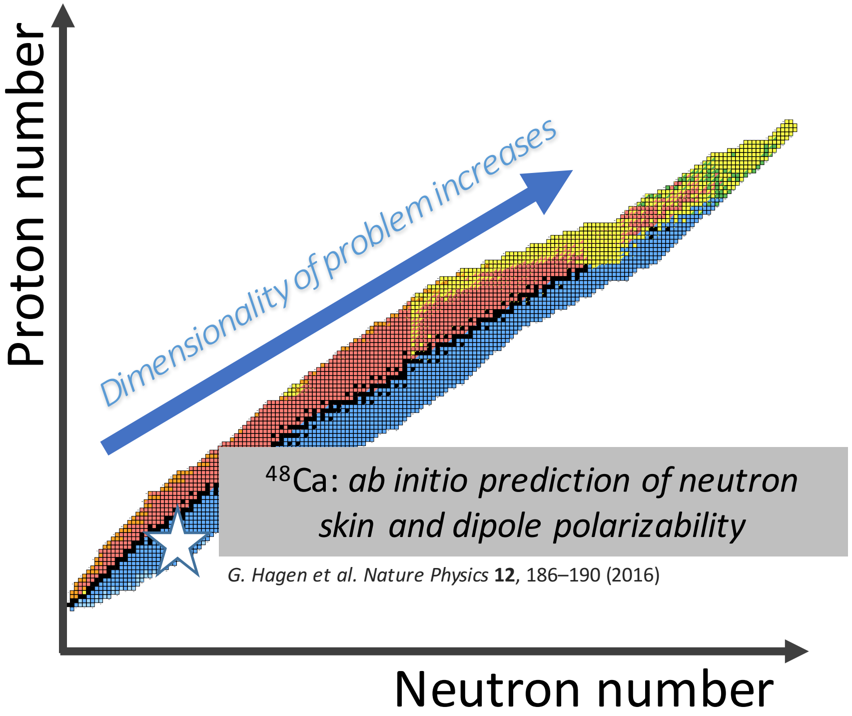

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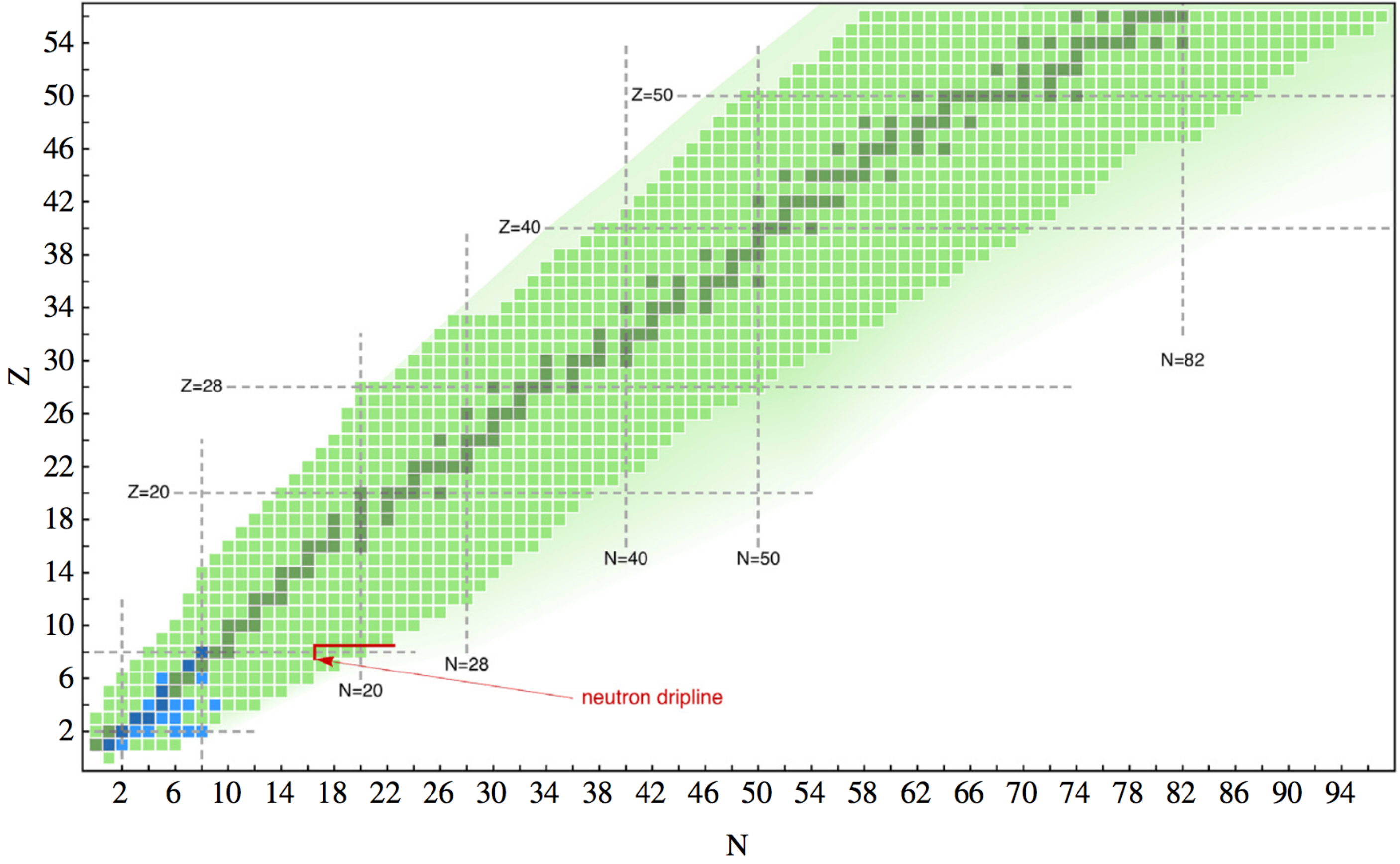
Emergence of uncertainty estimates in ab initio theory

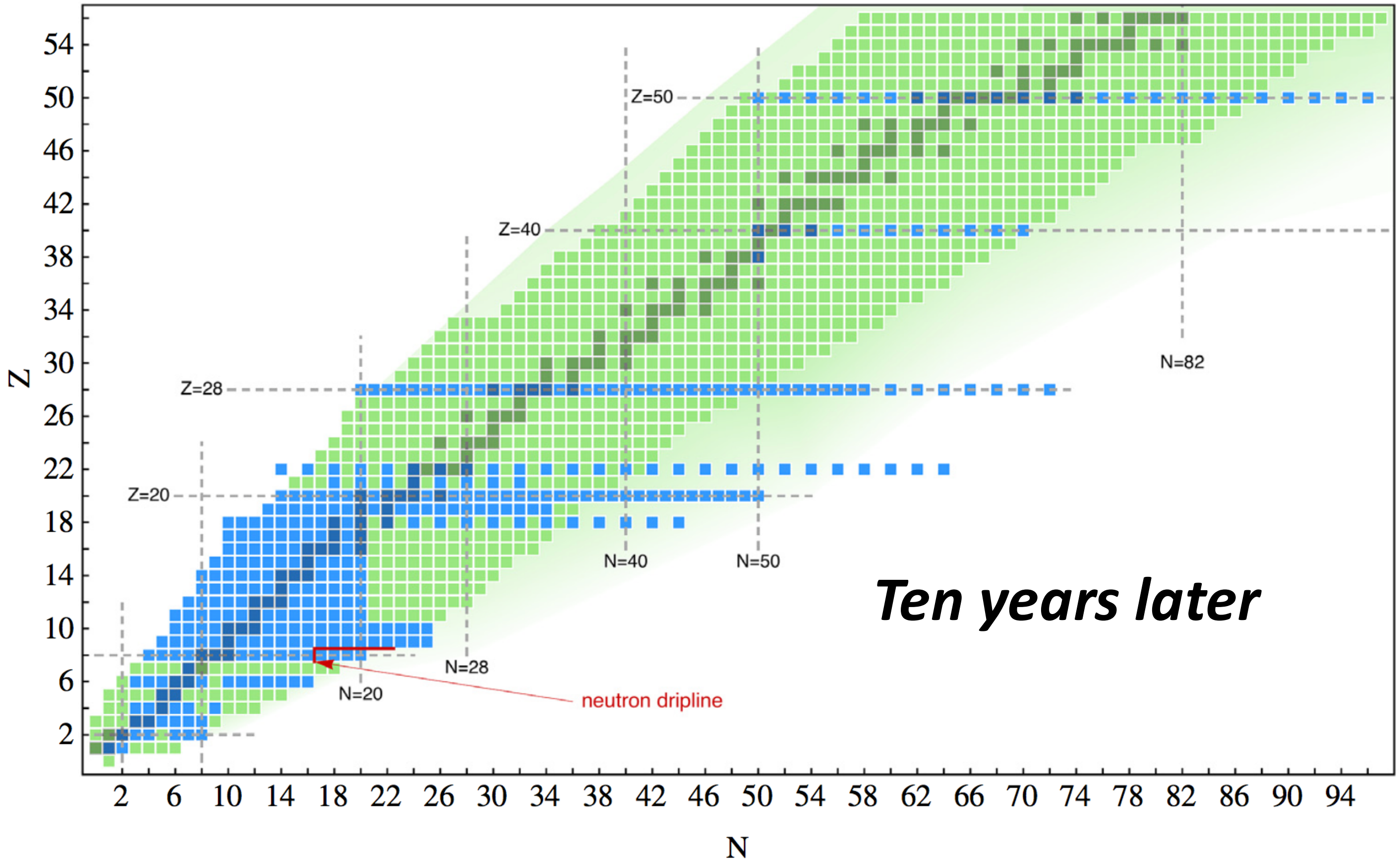
- Tools: Frequentist and Bayesian analyses of predictions

Ab initio reach in **2005**



H. Hergert et al. Phys. Rep. **621**, 165-222 (2016)

Ab initio reach in **2015**

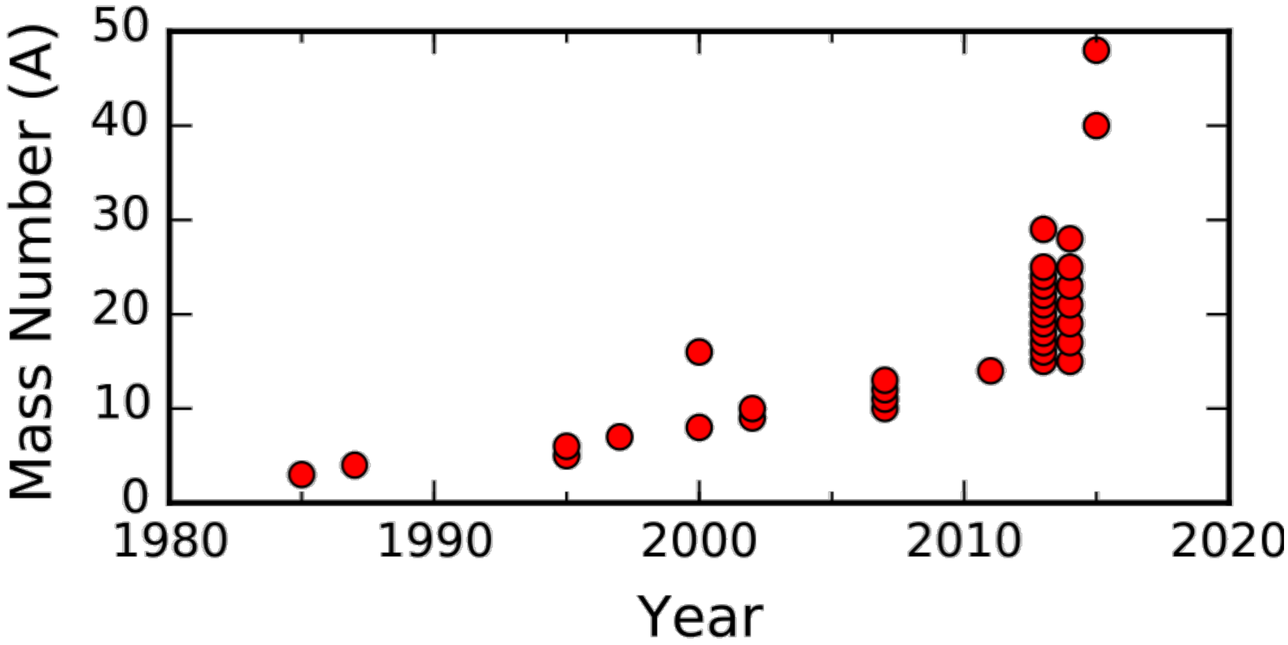


Ten years later

H. Hergert et al. Phys. Rep. **621**, 165-222 (2016)

Trend of accurate *ab initio* capabilities

Extended computational capabilities and polynomial A-scaling.
However, limited by accuracy of available interactions



G. Hagen, AE, et al. Nature Physics **12**, 186–190 (2016)
S. Binder et al, Phys. Lett. ***B*** *736 (2014) 119*

$$\left(\frac{Q}{\Lambda}\right)^{\nu}$$

Our tool to analyze forces: χEFT

(Weinberg, van Kolck, Epelbaum, Meissner, Machleidt, ...)

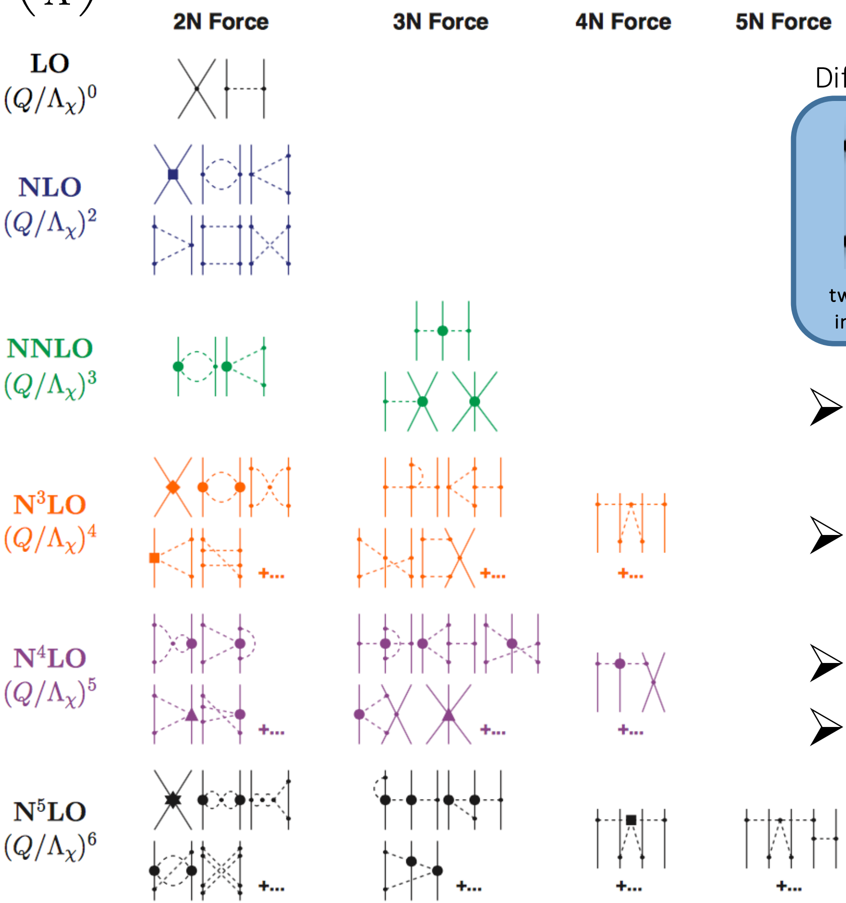
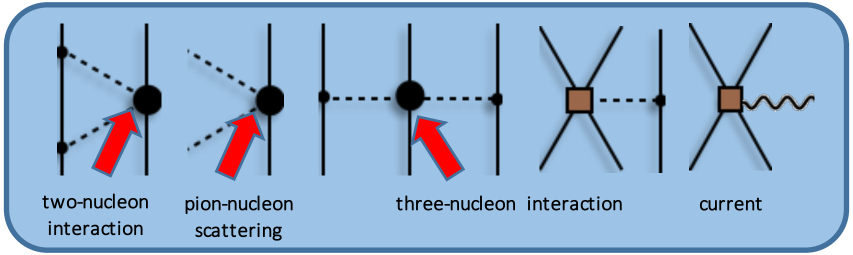


Figure from: R. Machleidt and F. Sammarruca, Phys. Scr. **91** (2016) 083007

Different low-energy processes share coupling constants (LECs).



- Chiral symmetry and pion dynamics constrain long-range physics.
- Systematic low-q expansion consistent with QCD symmetries.
- 2N, 3N, 4N, 5N, … forces.
- Local, non-local, semi-local formulations.

R. Machleidt and D. R. Entem Phys. Rep. ***503*** *(2011) 1-75*
E. Epelbaum et al., Rev. Mod. Phys. ***81*** *(2009) 1773-1825*

Optimizing interactions from χEFT

Short range physics included as contact interactions.
*With LECs **p** to be extracted/optimized from data.*

$$\chi^2(\mathbf{p}) = \sum_i \left(\frac{\mathcal{O}_{i,\mathrm{theo}}(\mathbf{p}) - \mathcal{O}_{i,\mathrm{exp}}}{\sigma_{i,\mathrm{tot}}} \right)^2$$

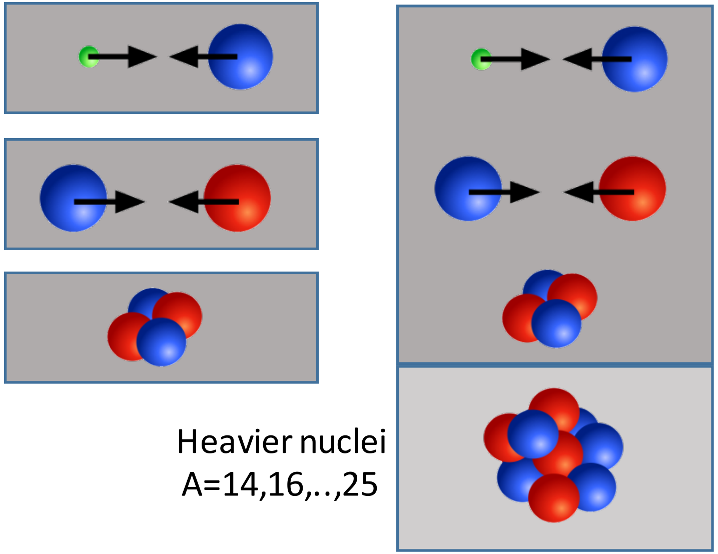
Optimization strategy matters

Separate ('historic') Fit | Simultaneous Fit

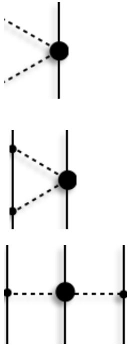
piN

NN

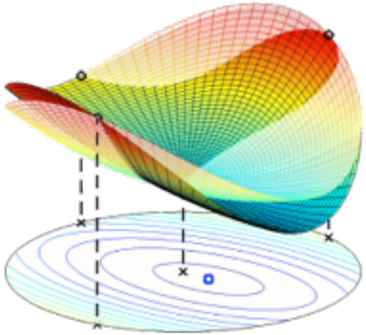
Light nuclei
A=2,3,(4)



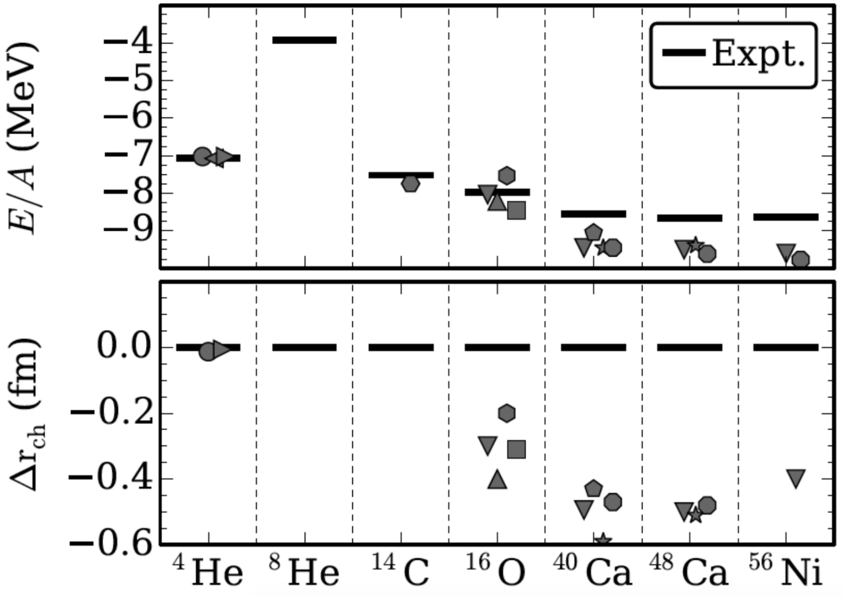
Heavier nuclei
A=14,16,..,25

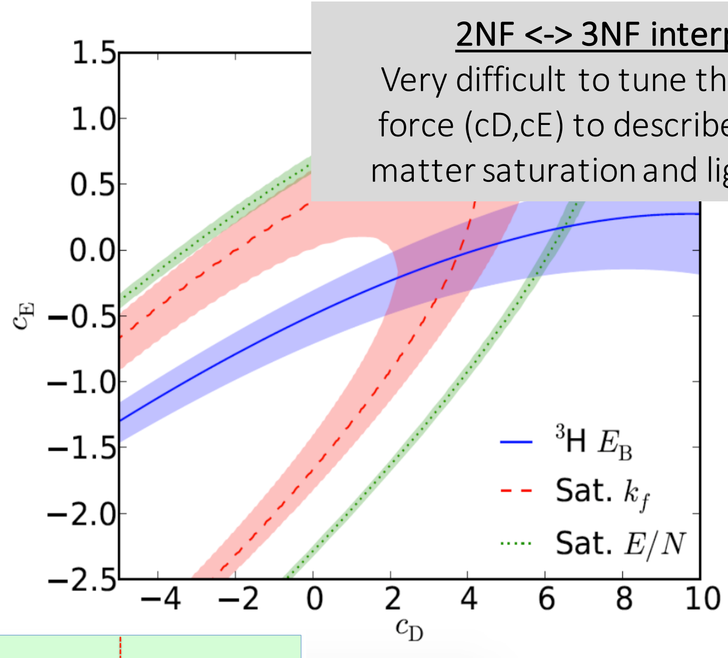


NNLO$_{\mathrm{sat}}$



AE et al. Phys. Rev. C. ***91****, 051301(R) (2015)*
AE et al. Phys. Rev. Lett. ***110****, 192502 (2013)*



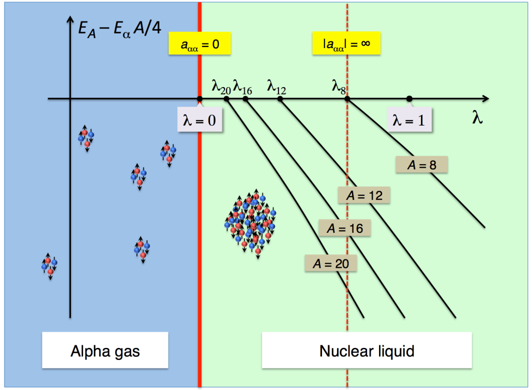


2NF <-> 3NF interplay

Very difficult to tune three-body force (cD,cE) to describe nuclear matter saturation and light nuclei

Predictive Power

Fitting 2NF and 3NF separately to NN / πN / A=2,3,4 energies and radii is not enough

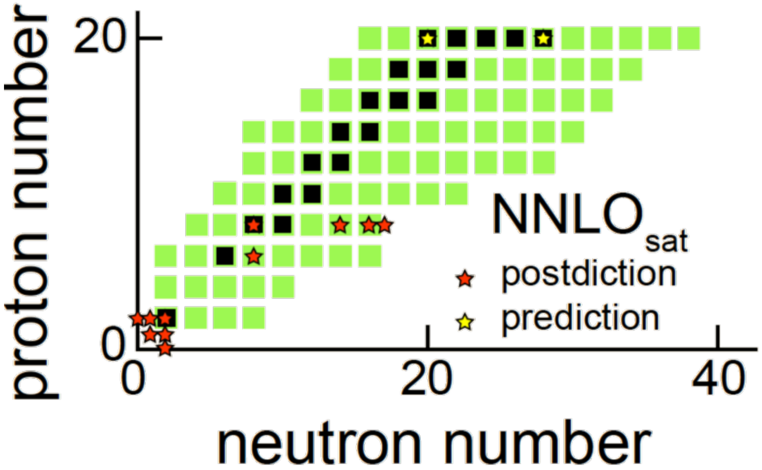


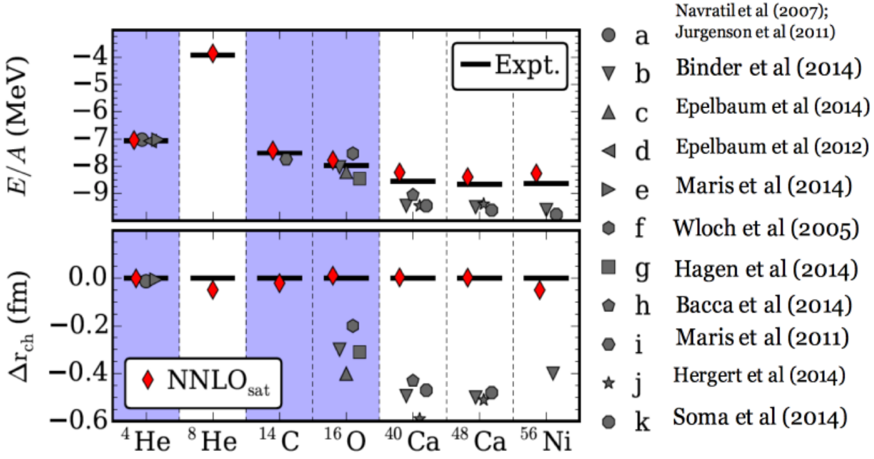
Local, non-local, or semi-local ?

Lattice EFT investigations at LO suggest that nuclei are close to a quantum phase transition, and that it is key to probe the degree of locality of interactions.

S. Elhatisari et al, Phys. Rev. Lett (2016)
G. Hagen, AE, et al. Phys. Rev. C ***89****, 014319 (2014)*
AE et al. Phys. Rev. C. ***91****, 051301(R) (2015)*
A. Dyhaldo et al, Phys. Rev. C ***94,*** *034001 (2016)*

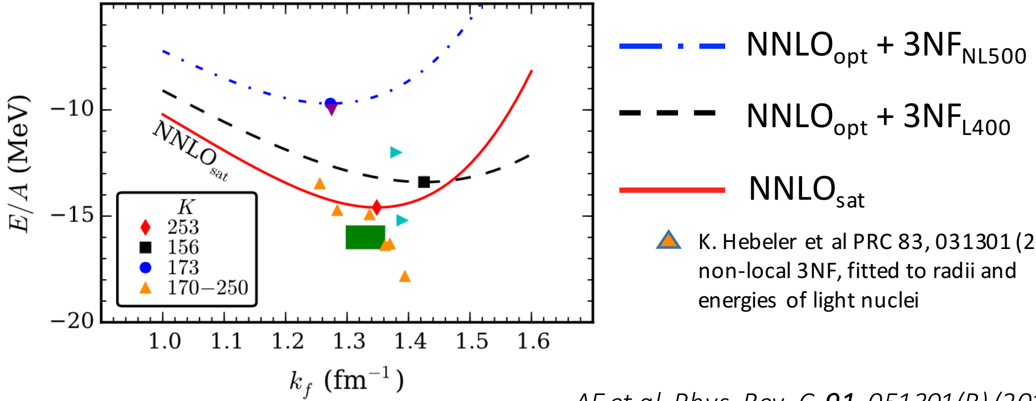
$NNLO_{sat}$ – designed for radii and binding energies





Stabilize extrapolations by simultaneously optimizing the chiral 2NF+3NF to charge radii and binding energies of ^{3}H, $^{3,4}He$, ^{14}C, ^{16}O and binding energies of $^{22,24,25}O$ and NN-data (T_{Lab} <35 MeV).

Three-nucleon force with non-local regulator.

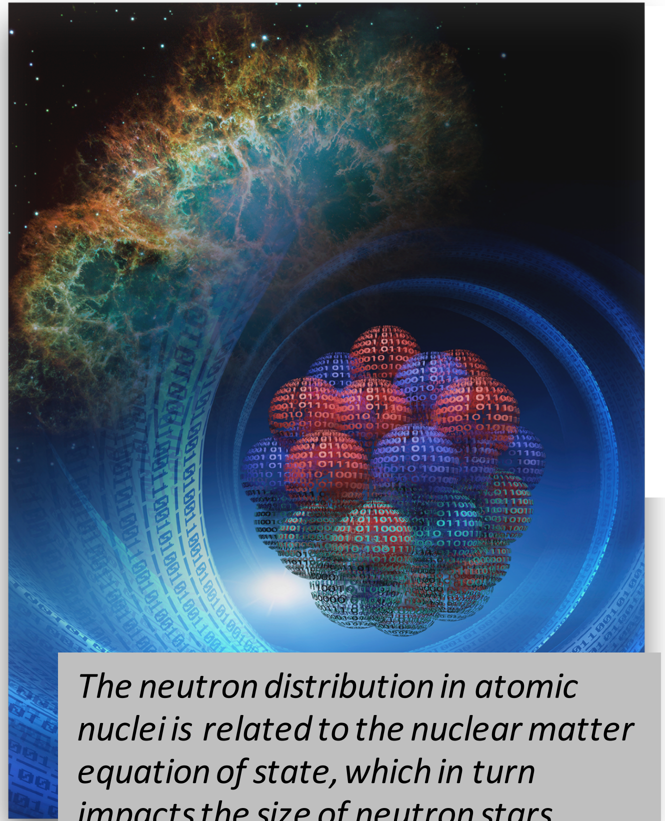


K. Hebeler et al PRC 83, 031301 (2011) non-local 3NF, fitted to radii and energies of light nuclei

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

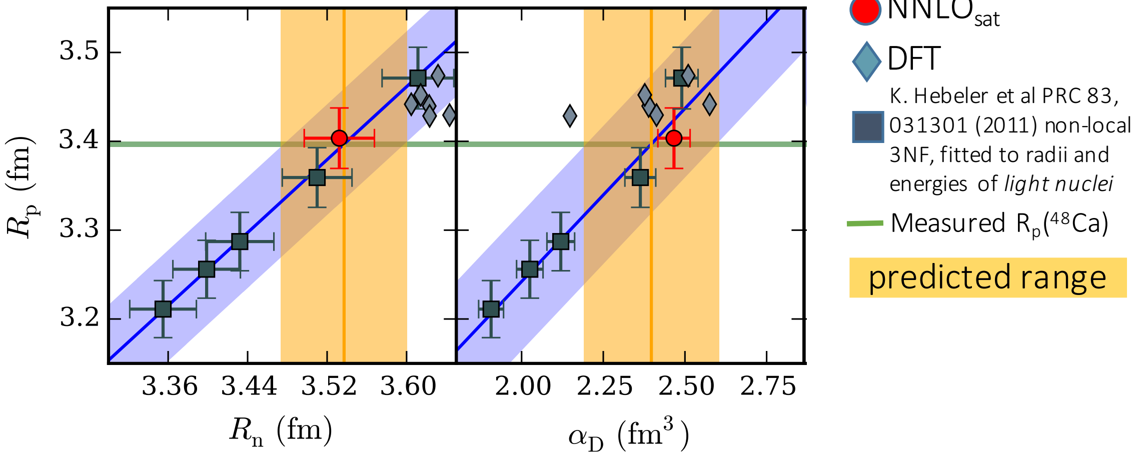
Predicting the skin thickness in ^{48}Ca

(skin = difference between the radii of the neutron and proton distributions)



The neutron distribution in atomic nuclei is related to the nuclear matter equation of state, which in turn impacts the size of neutron stars.

G. Hagen, AE, et al. Nature Physics **12**, 186–190 (2016)



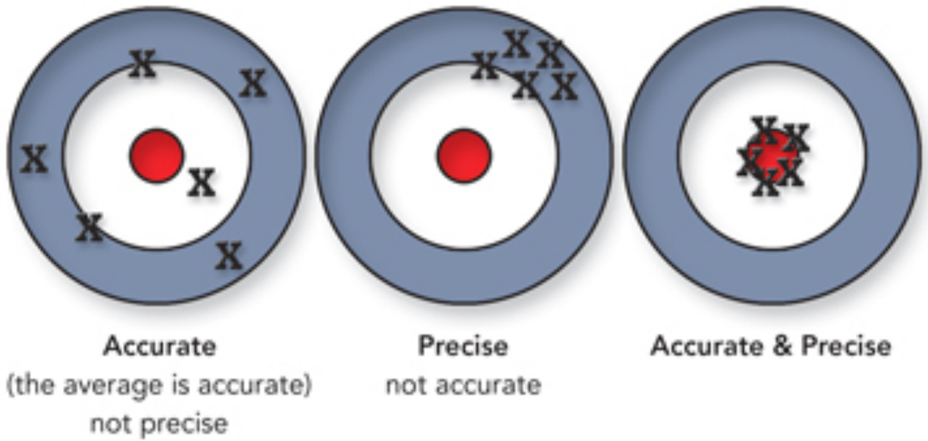
- Bridging EFT and DFT
- Skin nearly independent of Hamiltonian.

  measurement possible via parity-violating electron scattering (P-REX/C-REX at JLab)
- Correlated with dipole polarizability (α_D).

Large charge radius of ^{52}Ca challenge for ab initio.

R. F. Garcia Ruiz et al. Nature Physics **12**, 594–598 (2016)

Key scientific questions

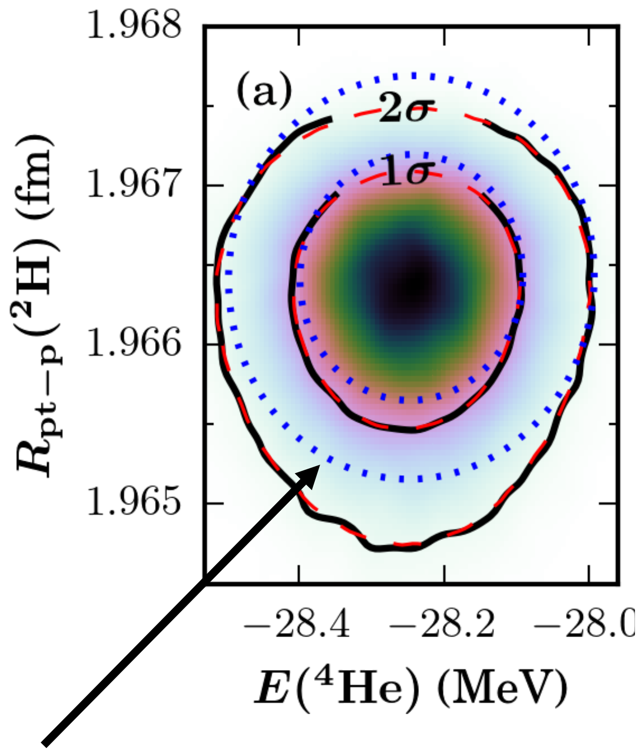


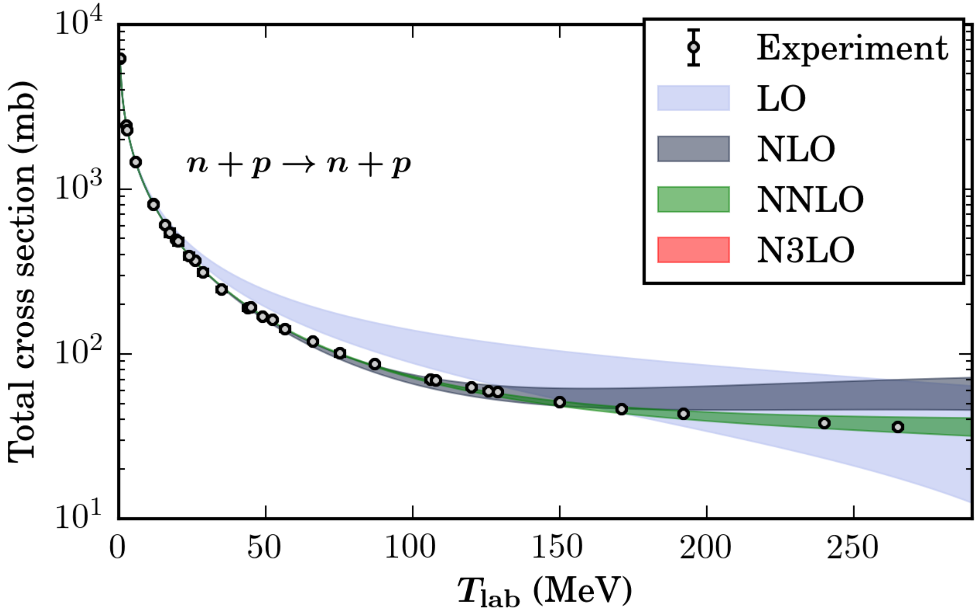
What is the **accuracy** of ab initio nuclear structure calculations with χEFT ?

What is the **precision** of ab initio nuclear structure calculations with χEFT ?

Useful guide: J. Dobaczewski, et al. J. Phys. G **41**, 074001, (2014).
M .R. Schindler et al. Ann. Of. Phys **324**, 682, (2009).
AE et al, J. Phys. G **42**, 034002, (2015).
R. N. Perez et al. Phys. Rev. C **91**, 064002, (2015).
E. Epelbaum et al. Phys. Rev. Lett. **115**, 122301 (2015).
B. D. Carlsson, AE, et al. Phys. Rev. X **6,** 011019, (2016).
S. Wesolowski et al. J. Phys. G.**43**, 074001, (2016).

Monte Carlo sampled joint statistical probability distributions





Simultaneously optimized non-local chiral NNLO interactions (NN+NNN). Λ=450-600 MeV.

Covariance matrix for all LECs available.
Enables statistical regression analysis of any ab initio calculation. (blue dashed)

All 2N, 3N, πN - coupling constants calibrated to reproduce pion-nucleon and nucleon-nucleon scattering data, as well as binding energies and charge radii of ^2H ^3H ^3He ^4He.

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

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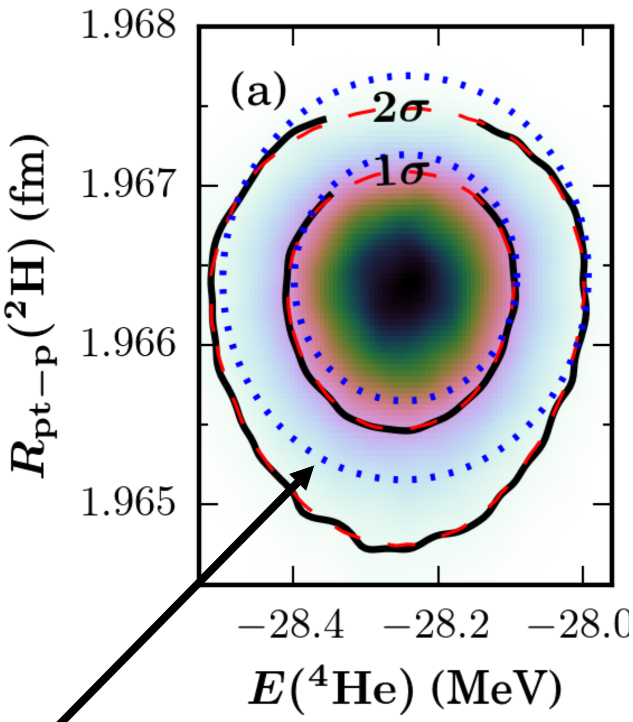

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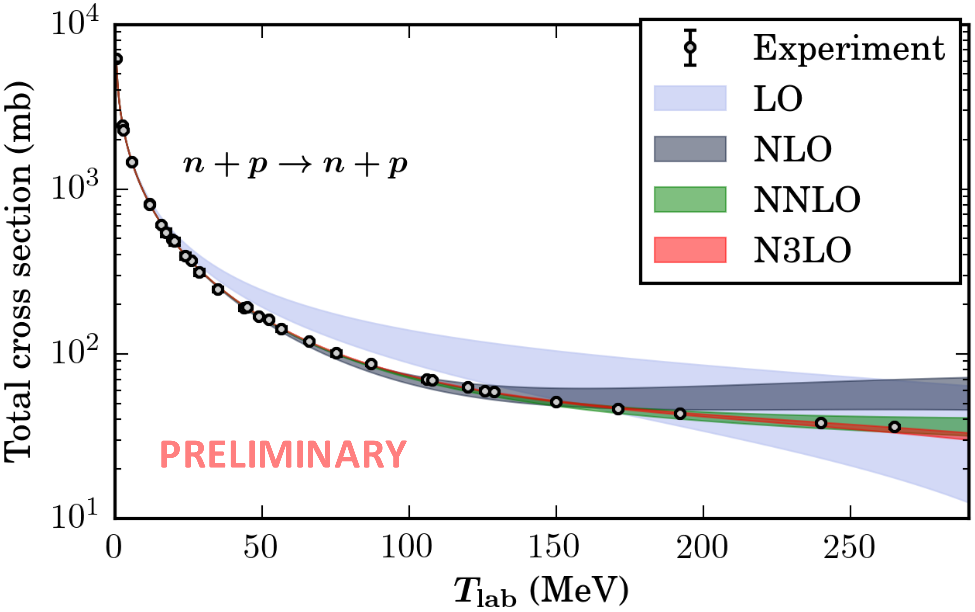

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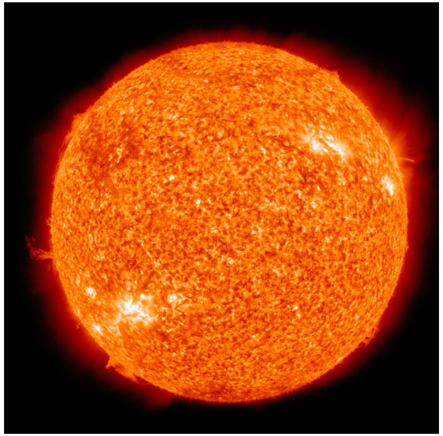
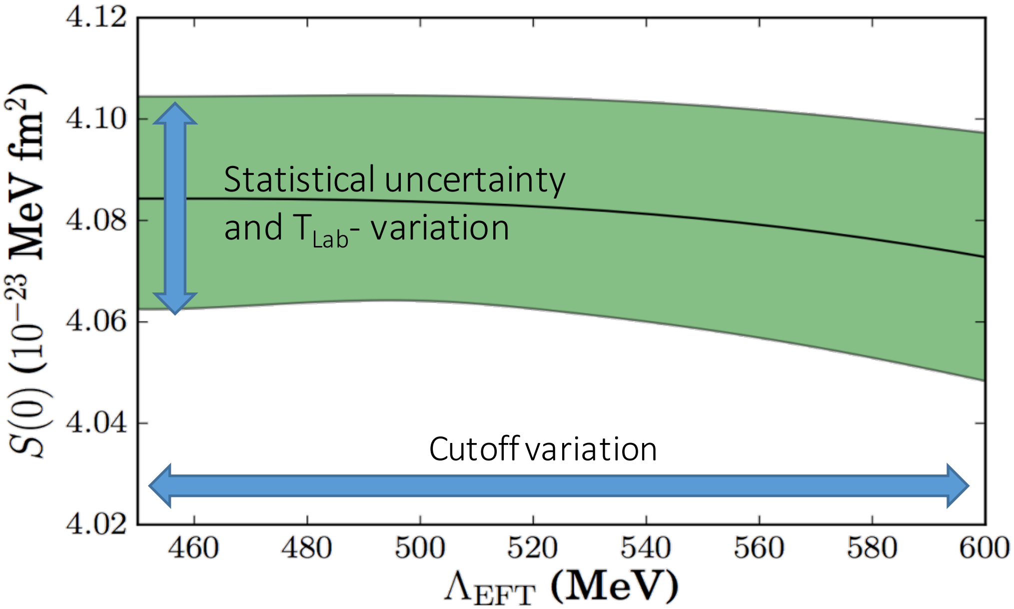
UQ of proton-proton fusion at NNLO in χEFT

$p + p \rightarrow d + e^{+} + \nu_e$



In the core of the Sun, energy is released through sequences of nuclear reactions that convert hydrogen into helium. The primary reaction is thought to be the fusion of two protons with the emission of a low-energy neutrino and a positron.



$$S(0) = \left(4.047^{+0.024}_{-0.032}\right) \times 10^{-23}\ \mathrm{MeVfm}^2$$

If we also correct for higher order e.m. effects

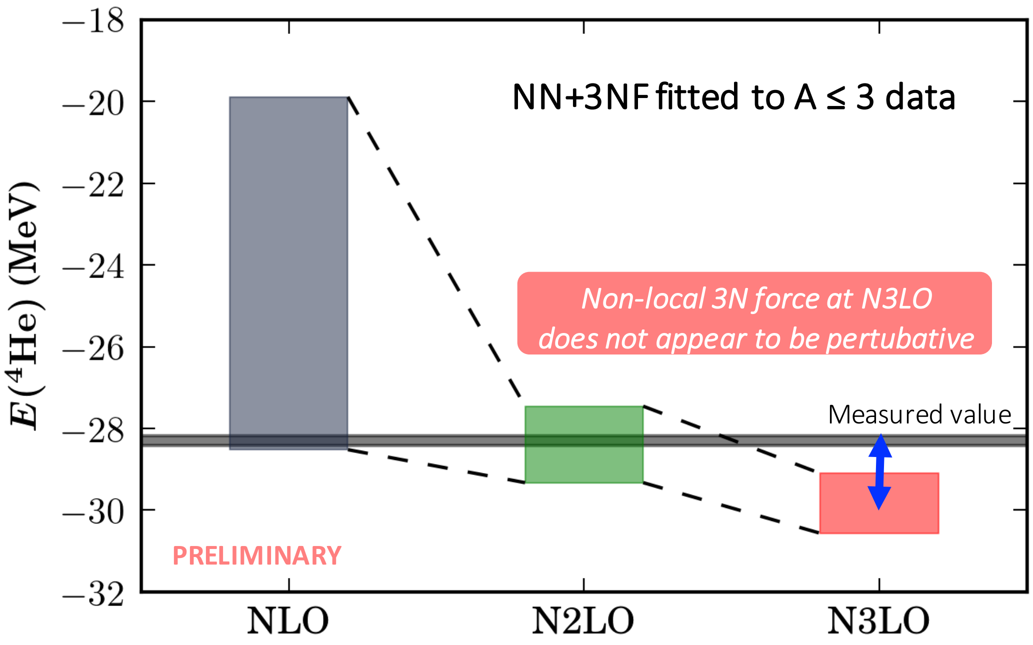
Marcucci et al. PRL 2013 $S = (4.030 \pm 0.006) \times 10^{-23}$ MeV fm^2

Adelberger et al. RMP 2011 $S = (4.01 \pm 0.04) \times 10^{-23}$ MeV fm^2

B. Acharya, AE, et al. Phys. Lett. ***B*** *760 (2016) 584-589*

^{4}He with 3N force at N3LO

(No new parameters in the 3NF at this order)



Bands indicate effect of cutoff variation and different truncations in the NN scattering database

@N3LO: at least over 100 minima, all with a good description of A = 2,3 & πN data

- More data (heavy nuclei, 3N scattering) !
- πN sector from Roy-Steiner analysis ?
- Other regulators ?

Fitting to heavy nuclei and/or 3N-scattering cross sections is more expensive.

- Requires efficient code
- Use surrogate model from machine learning
- Sensitivity analysis to select/suggest data

V. Bernard et al, Phys. Rev. C 77, 064004 (2007), V. Bernard et al, Phys. Rev. C 84, 054001 (2011)
K. Hebeler et al, Phys. Rev. C 91, 044001 (2015), M. Hoferichter et al, Phys. Rev. Lett 115, 192301 (2015)
T. Krüger et al, Phys. Rev. C ***88*** *025802 (2013),*

Summary

- ***Ab initio* nuclear theory is developing very rapidly:**
  - *Several highly capable many-body methods.*
  - *Interactions (and currents) from* χEFT *are continuously improved.*
  - *First link between ab initio/EFT and DFT .*
  - *Well-founded estimates of theory errors are emerging.*

- **Chiral interaction $NNLO_{sat}$ for *ab initio* description of radii and binding energies:**
  - *Weak charge form factor, neutron radius, and dipole polarizability in ^{48}Ca.*
  - *Advantageous to fit chiral interactions to selected heavier nuclei.*
  - *Strong arguments for optimizing coupling constants simultaneously.*

- **Statistical errors are small (≤ 1%) for the simultaneously optimized potentials. The total error budget is dominated by systematic errors (‘theory’ errors).**
  - *Few-body systems accessible for detailed regression analyses.*
  - *Detailed uncertainty analysis of proton-proton fusion in* χEFT
  - *Codes for potentials and covariance matrices available for download.*

- **Exciting future:**
  - *Bayesian parameter estimation and model selection.*
  - *Machine Learning approaches (Gaussian Process Modeling).*
  - *Model mixing for assessing systematic uncertainties.*
  - *Continued efforts on modified power-counting and effects due to regulators.*

Thank You