Uncertainty quantification in ab initio nuclear theory

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Bayesian Methods in Nuclear Physics
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Vetenskapsrådet

Outline

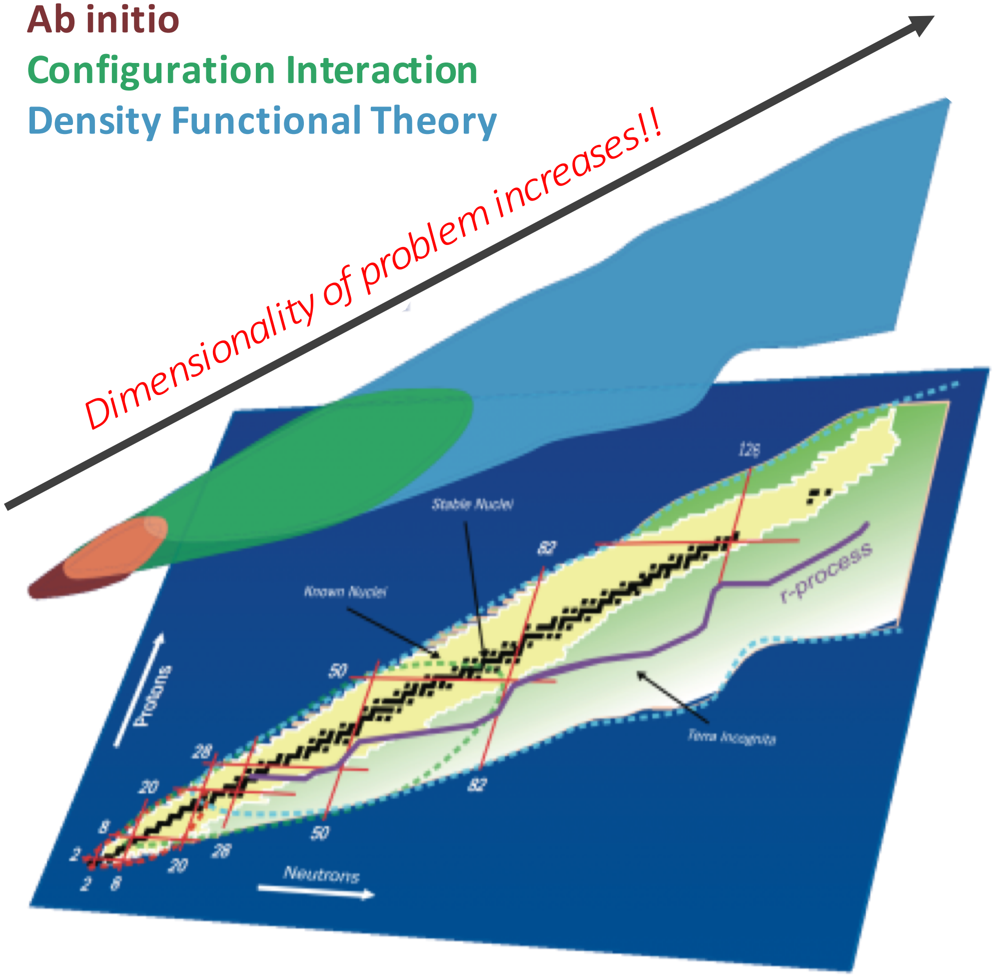
- Chiral EFT: Optimization and UQ (frequentist so far…)
- Our technology (codes, stat. methods)
- Examples: Solar pp-Fusion
  Few-body systems
- First steps with Gaussian process modeling

This talk is based on:

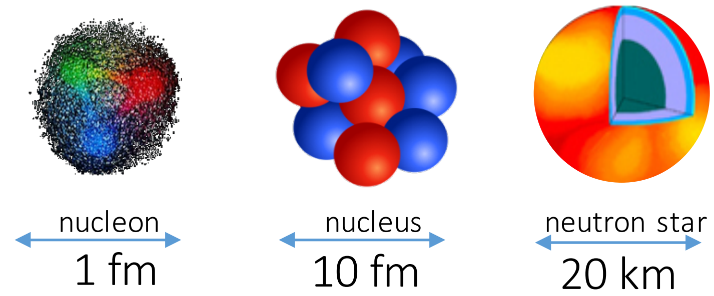
A. Ekström et al. Phys. Rev. C. 91, 051301(R) (2015)
G. Hagen et al. *Nature Physics* 12, 186–190 (2016)
B. Carlsson et al. Phys. Rev. X 6 011019 (2016)
B. Acharya et al. arXiv 1603.01593 (2016)
J. Aspman et al. Bachelor's thesis TIFX04-16-04, Chalmers (2016)

Overview: physics

Ab initio
Configuration Interaction
Density Functional Theory



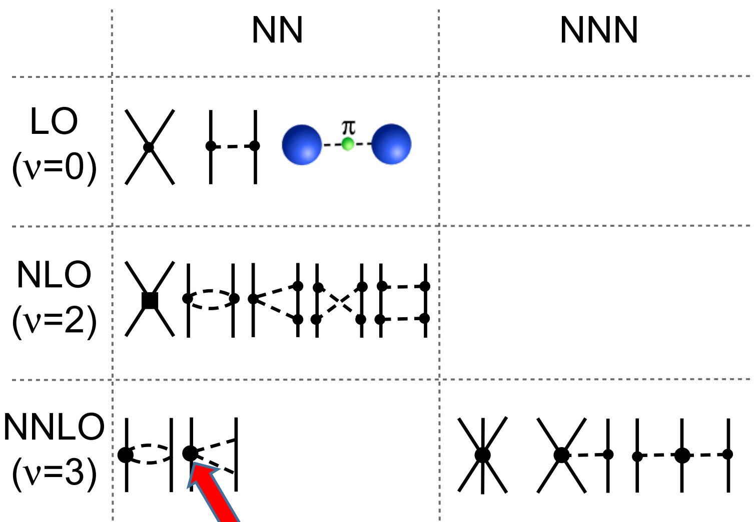
A multi-scale problem



We are after:

- *Common theory for nuclear phenomena*
- *Well-founded formulation that is linked to (Lattice) QCD*
- *Determine e.g. the limits for the existence of nuclei*
- *Credible error estimates of predictions*
- *....*

Ab initio approach with chiral EFT

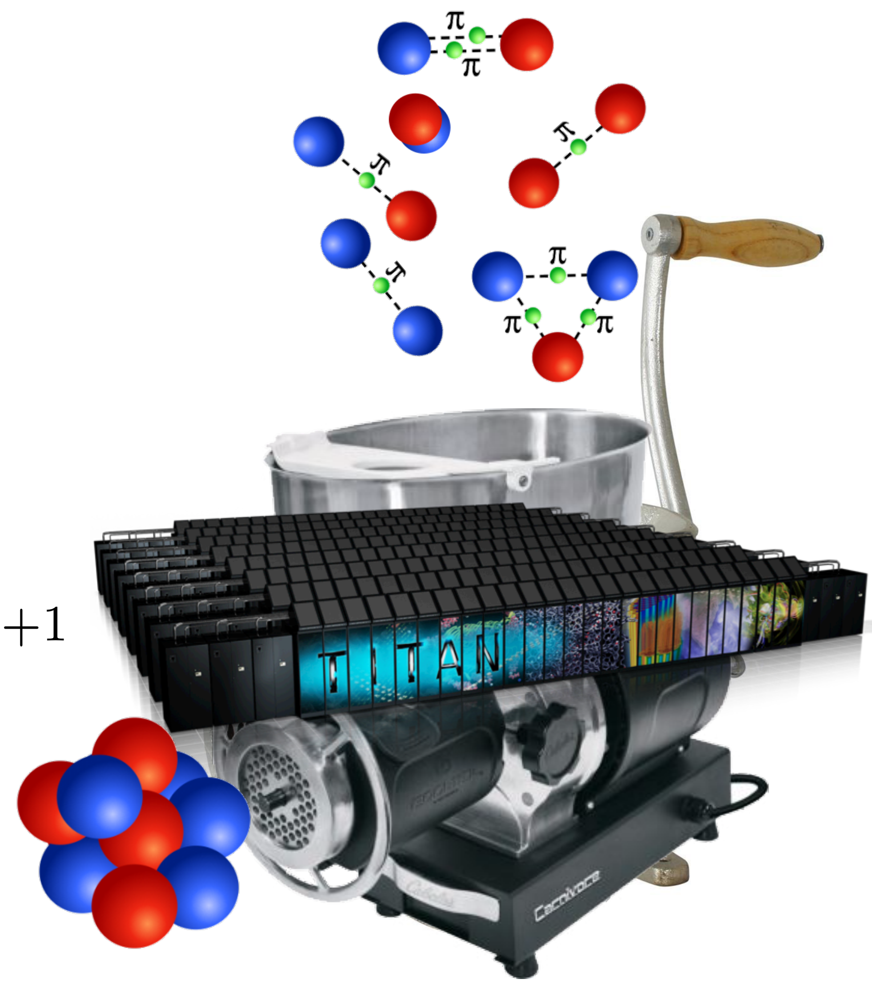


16 parameters in NN+NNN sector up to Q^3
Additional 10 from inclusion of piN up to Q^4

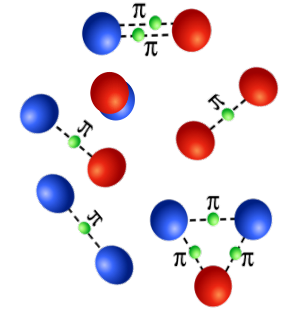
$$\left(\frac{Q}{\Lambda}\right)^{\nu+1}$$

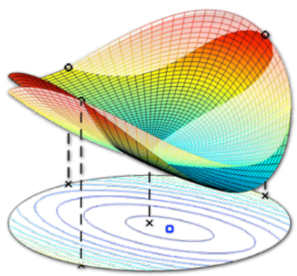
What data to include? …
(in practice governed by)

Physics arguments.
Reliable predictions.
Systematic uncertainties.
Local minima.
Computationally expensive model.
….. and more



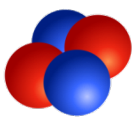
Optimization strategy



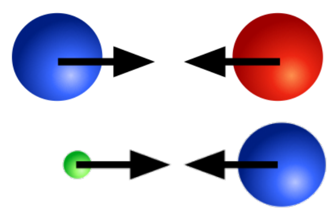


We wish to explore the physics capabilities and limitations of chiral EFT by forming different objective functions

$$\theta_\star = \operatorname{argmin} \chi^2(\theta)\,, \;\; \chi^2 = \sum_{\mathrm{i}}^{\mathrm{N_{data}}} \left(\frac{\mathrm{y_i}(\theta) - \mathrm{d_i}}{\sigma_\mathrm{i}} \right)^2$$

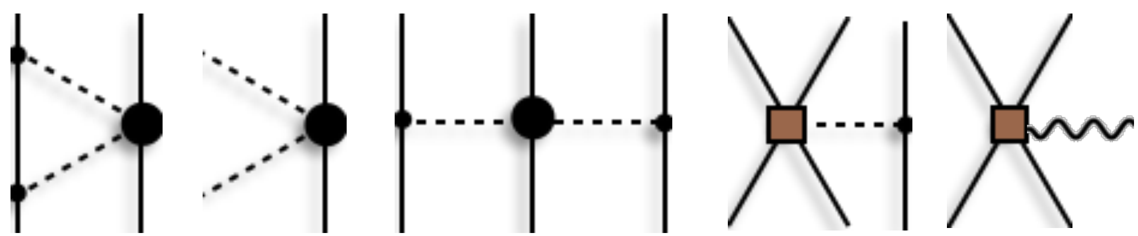


Bound state properties (so far, mainly masses and radii)



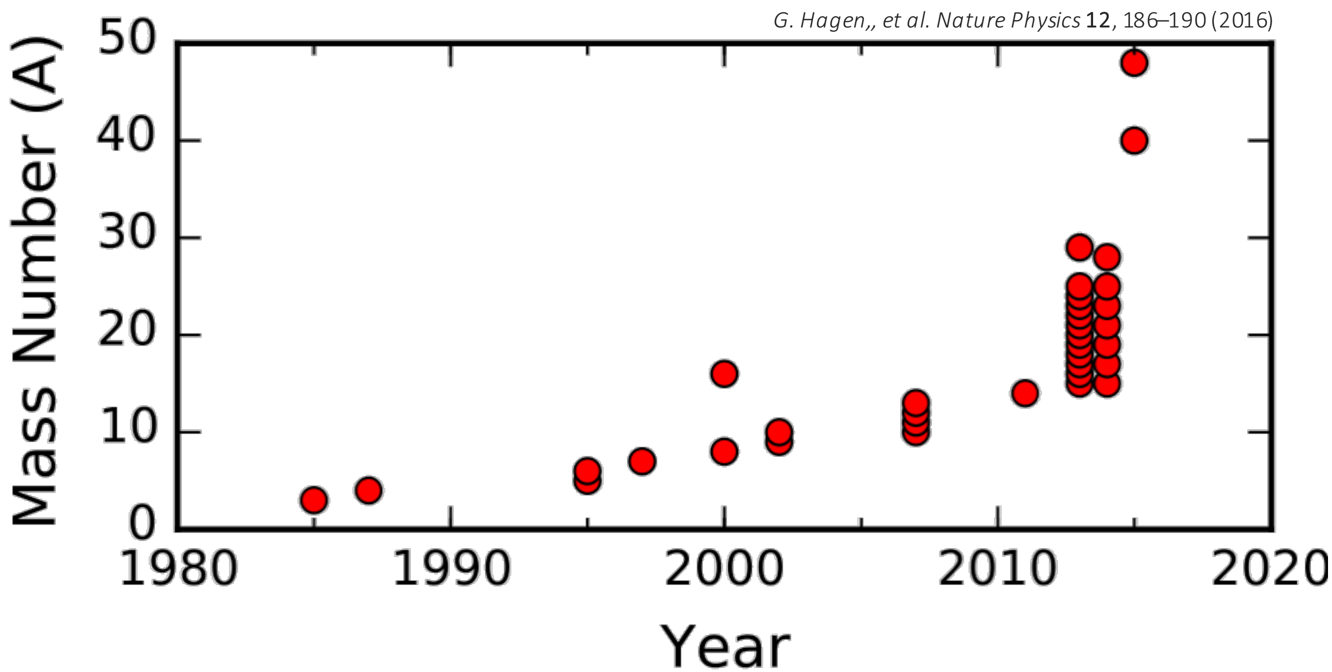
Scattering cross sections (so far, only NN, piN)

Same LECs appear in various low-energy processes



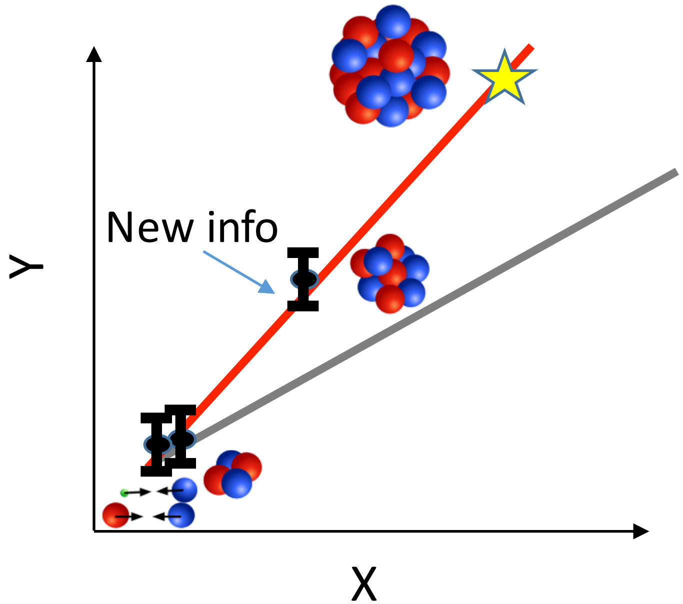
two-nucleon interaction | pion-nucleon scattering | three-nucleon interaction | current

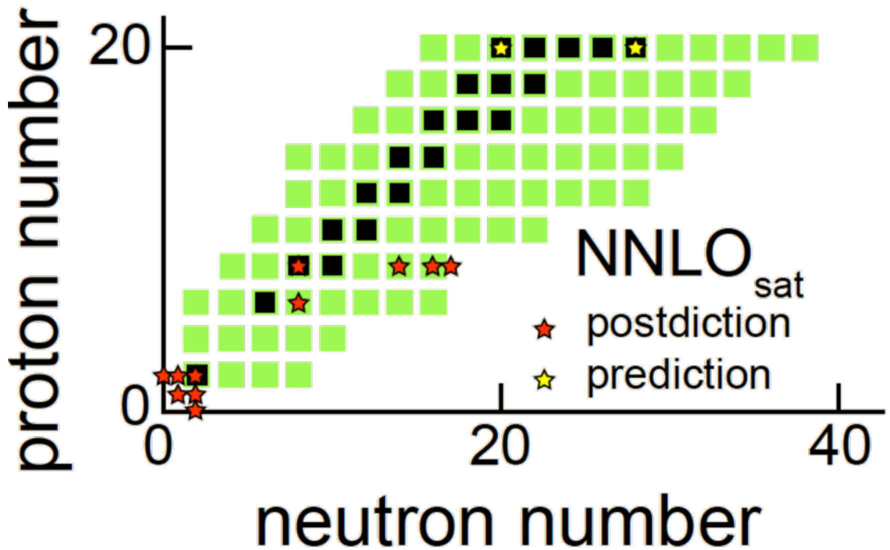
We are making progress



Rather expensive calculations
(use surrogate for UQ instead?)

… and here's why (in part)





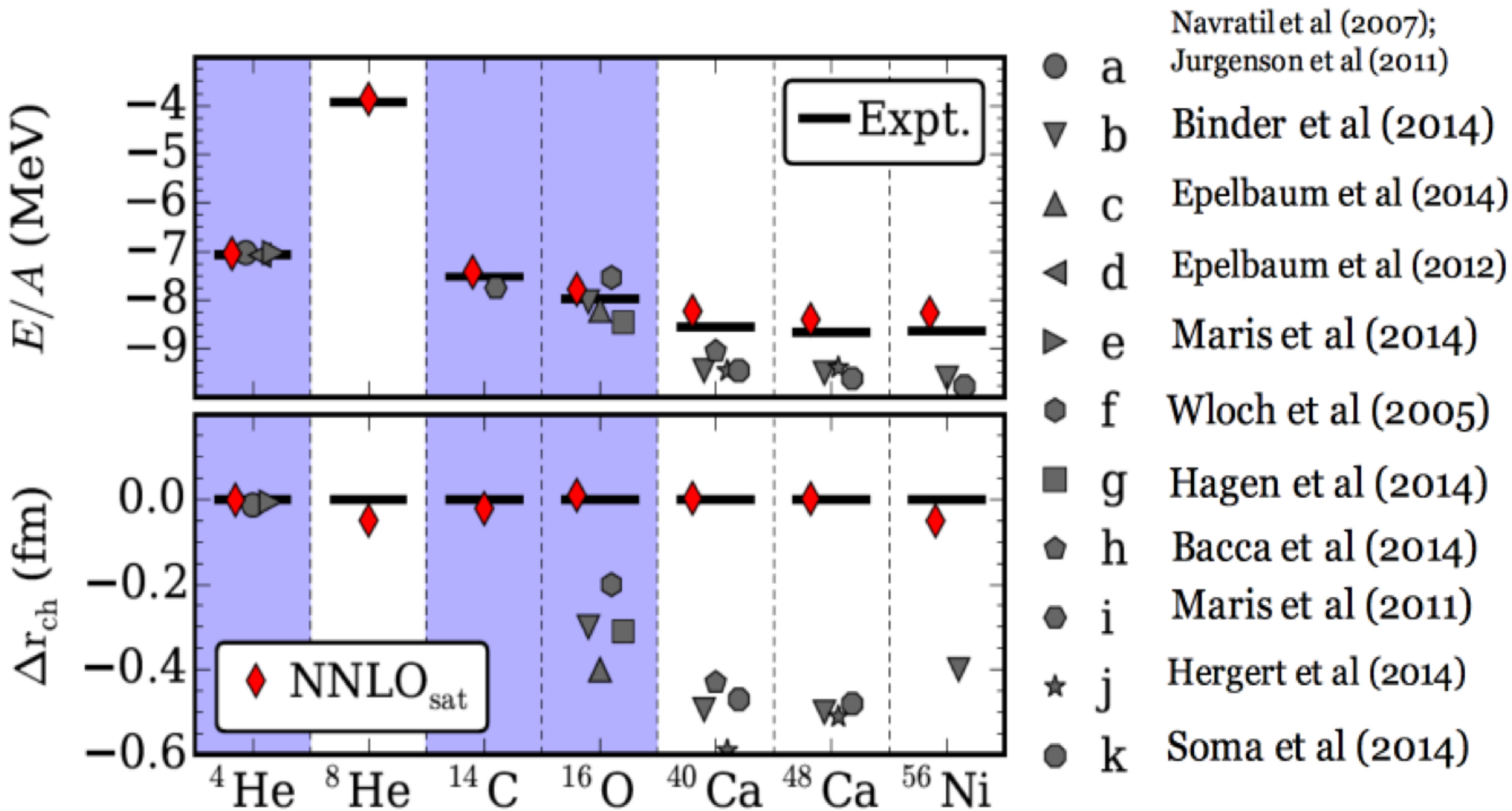
Calibration data "incomplete"
(e.g. T=3/2 insensitivity small-A,
Multiple minima, …)

The inclusion of some observables, like e.g. heavy nuclei (or 3N-scattering cross sections) **make the model evaluations expensive.**

Stabilize extrapolations by simultaneously optimizing the NN+NNN chiral interaction with respect to charge Radii and binding energie of ^{3}H, $^{3,4}He$, ^{14}C, ^{16}O As well as binding energies of $^{22,24,25}O$ and two-nucleon scattering data (T_{Lab} <35 MeV).

Three-nucleon force with **non-local regulator.**

Ab initio predictions



See K. Wendt's talk from last week

UQ challenges

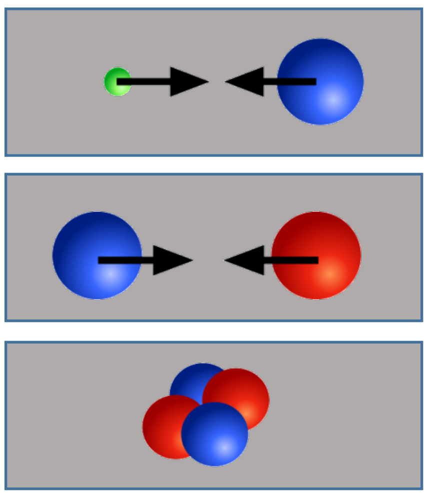
One reason for the observed progress is an improved understanding and appreciation of using optimization algorithms and statistical methods as well as a critical assessment of what data that we should included in the pool of fit data.

Separate ('historic') approach

piN

NN

Light nuclei
A=2,3,(4)



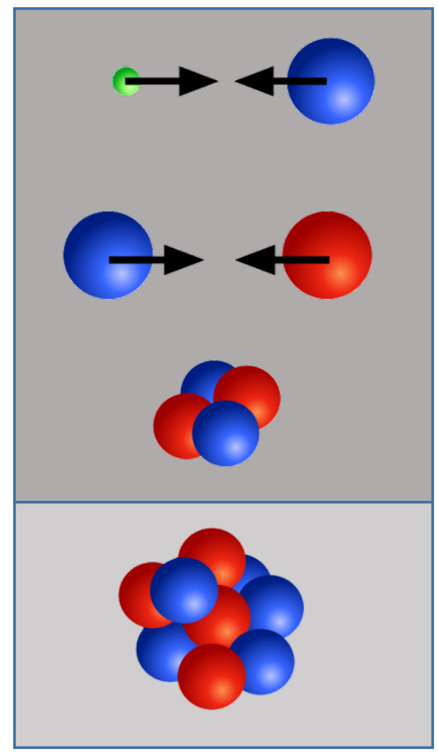
Simultaneous approach

piN

NN

Light nuclei
A=2,3,(4)

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

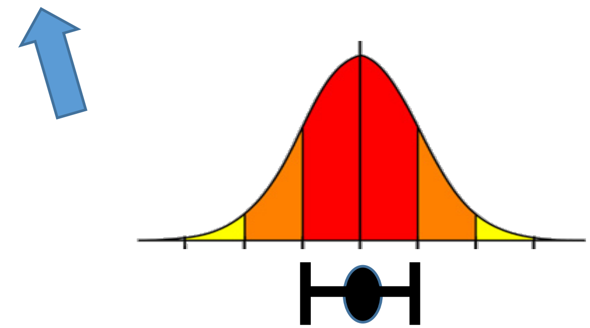


$NNLO_{sat}$

We have carried out a statistical analysis of chiral forces (up to NNLO) in **light** nuclei

$$\chi^2 = \sum_{\mathrm{i}}^{\mathrm{N_{data}}} \left(\frac{\mathrm{y_i}(\theta) - \mathrm{d_i}}{\sigma_{\mathrm{i}}} \right)^2$$

Error budget



$$\sigma^2_{\mathrm{tot}} = \sigma^2_{\mathrm{exp}}$$

Quoted (syst. and/or stat.) error in published analysis of measurement

$$+\sigma^2_{\mathrm{numerical}}$$

Algorithmic origin and intrinsic limitations. E.g. Machine epsilon of float 10^{-16}.

$$+\sigma^2_{\mathrm{method}}$$

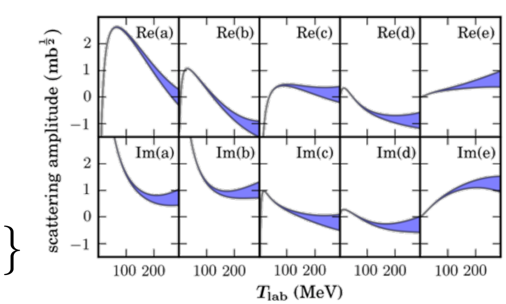
Due to method-approximations in the solution of the Schrodinger equation.

$$H|\Psi_A\rangle = E|\Psi_A\rangle,$$

$$+\sigma^2_{\mathrm{model}}$$

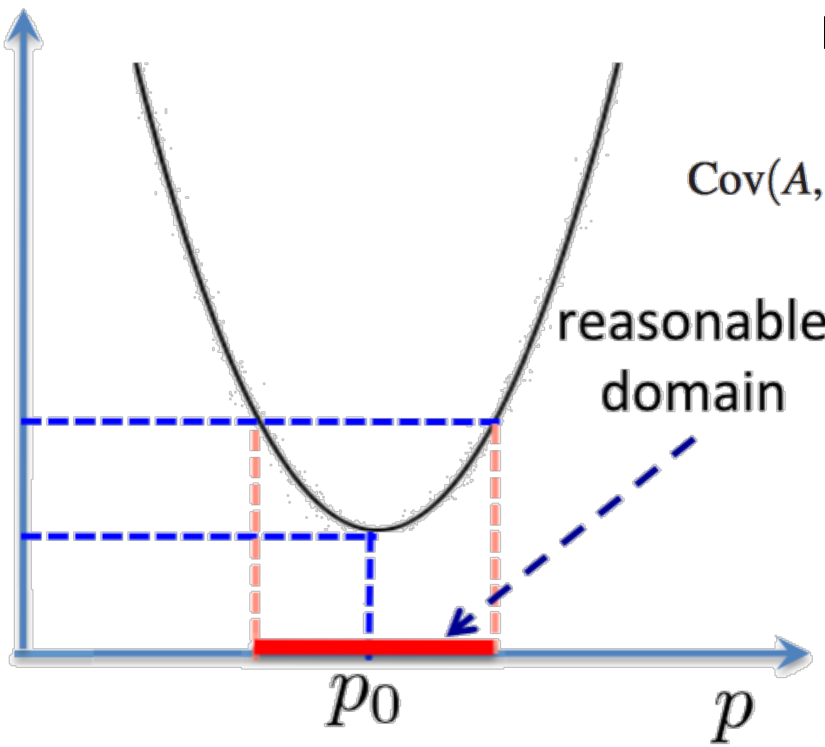
Imperfect modeling and missing physics. In χEFT we can *estimate* this from:

$$\sigma^{(\mathrm{amplitude})}_{\mathrm{model,x}} = \mathcal{C}_x \left(\frac{Q}{\Lambda} \right)^{\nu+1}, \; x \in \{\mathrm{NN}, \pi\mathrm{N}\}$$



Error propagation

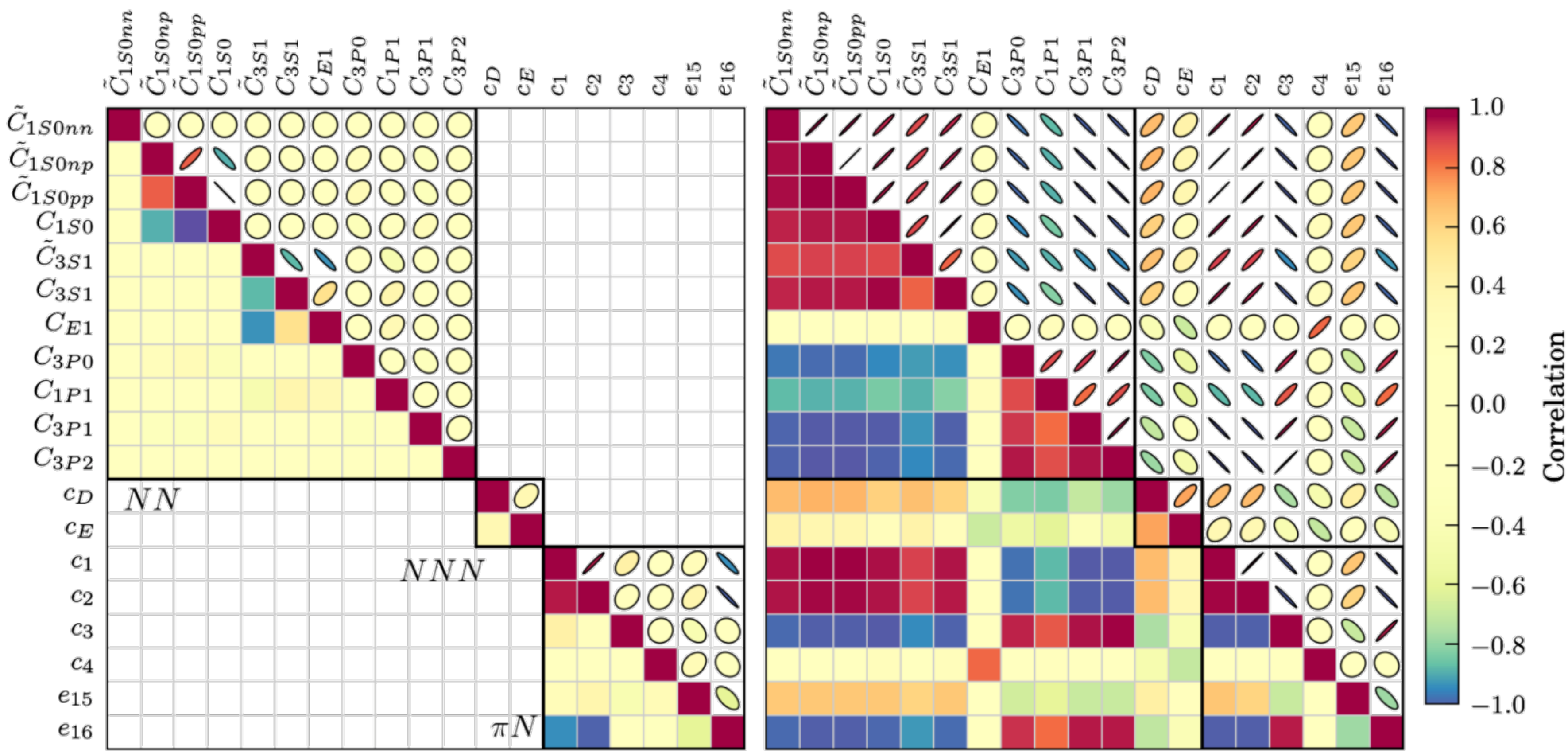
We can write a quadratic approximation to the covariance between two observables. Keeping only the first term gives the well-known first-order estimate.



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

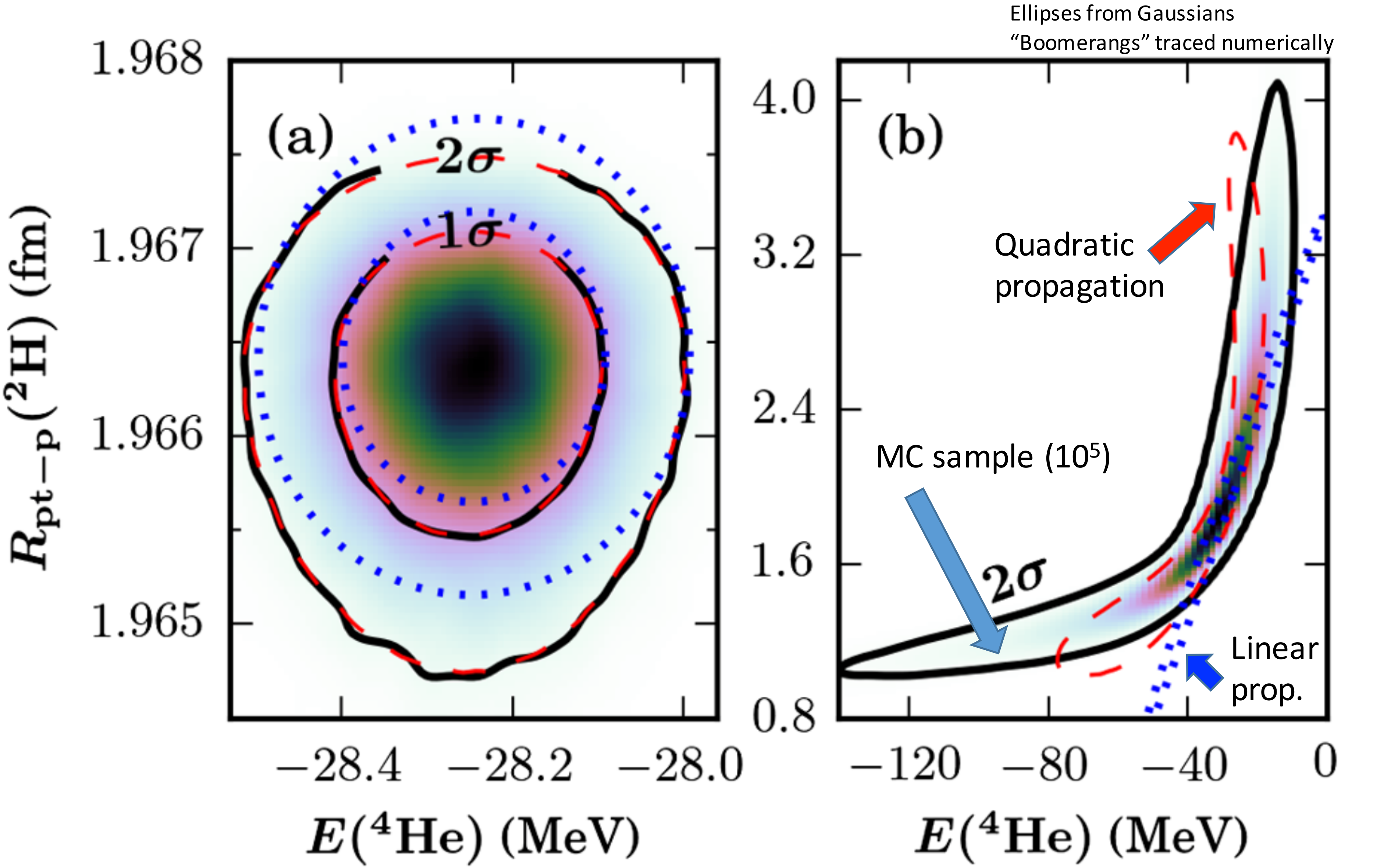
Figure from J. Dobaczewski et al J. Phys. G 41 (2014) 074001

Linear Correlations at NNLO



SEPARATE **SIMULTANEOUS**

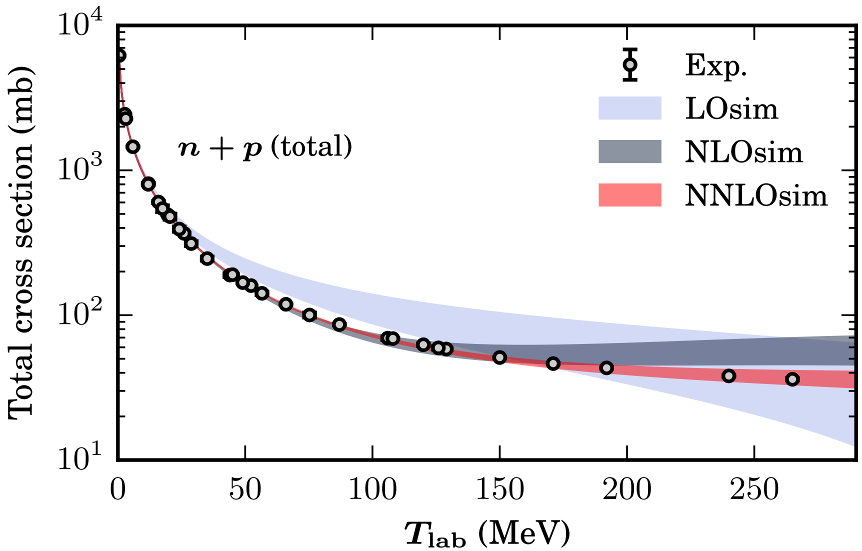
Joint probability distributions



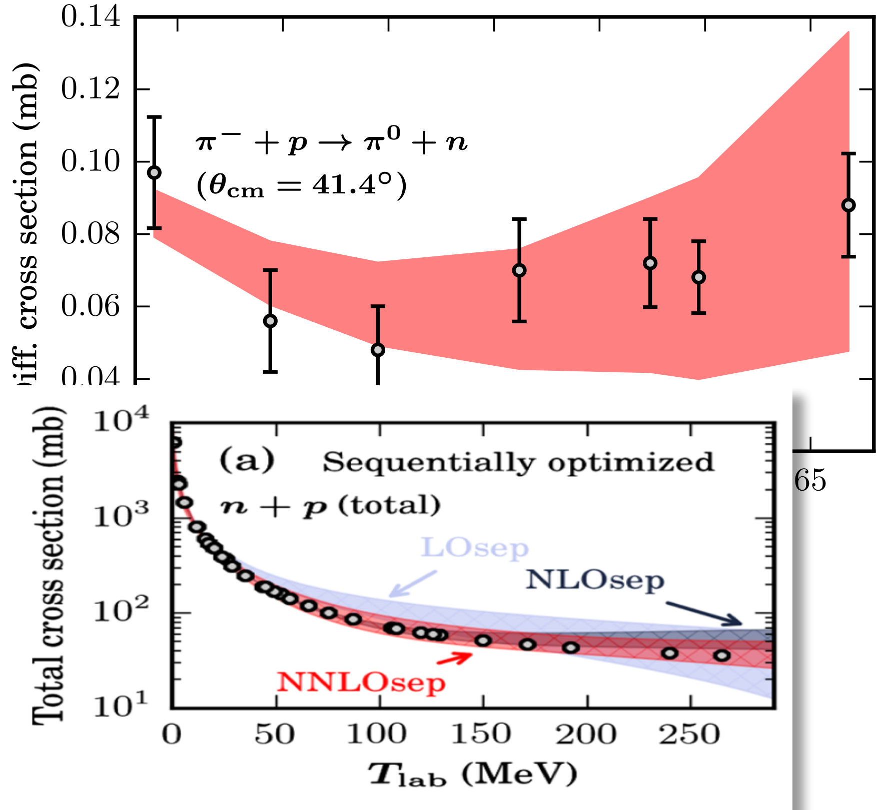
SIMULTANEOUS OPTIMIZATION **SEPARATE OPTIMIZATION**

Predicting cross sections and UQ

neutron – proton integrated cross sections



πN charge-exchange differential cross section

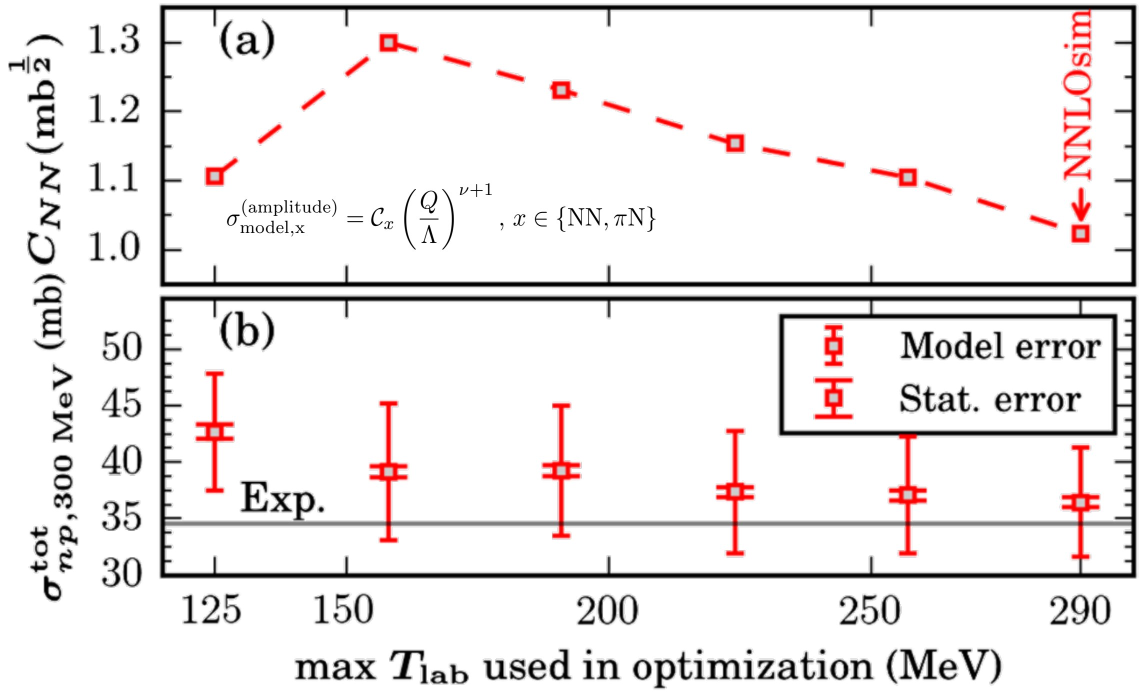


The statistical errors are very small, and the np scattering cross section exhibits an order-by-order convergence with increasing chiral powers

This is not observed for the sequentially optimized potentials

Predicting cross sections

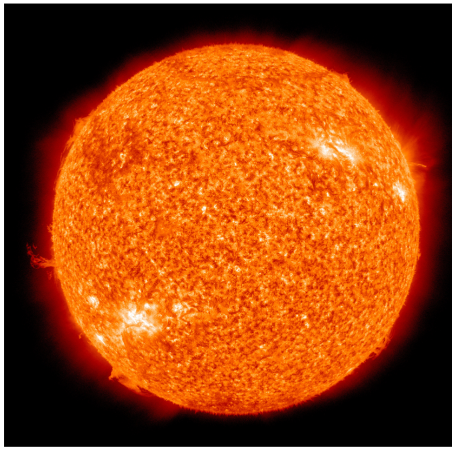
Our procedure for determining the model error is rather stable. Varying the input NN data by means of T_{Lab} truncations reveal that the constant C_{NN} doesn't change much. (However, for NNLOsep C_{NN} = 1.6 $mb^{1/2}$)



The np scattering cross section at 300 MeV (Exp = 34.563(174) mb)

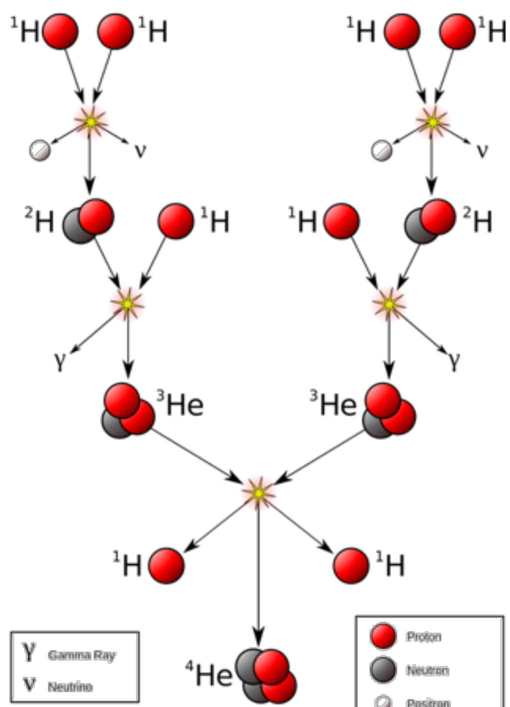
At a particular cutoff, The size of the model error is comparable with the variation due to changing T_{lab}

Proton-proton fusion

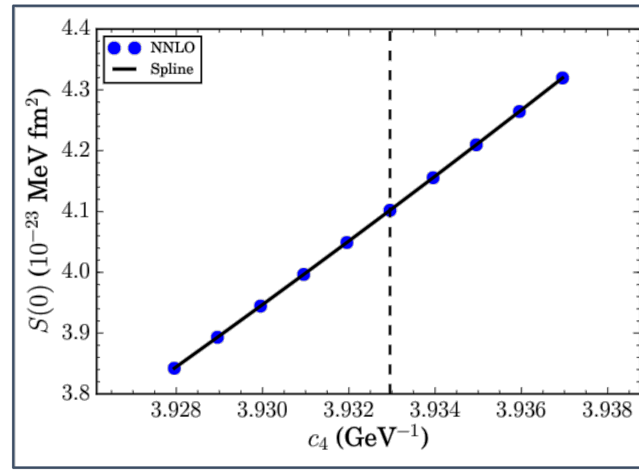


In the core of the Sun, energy is released through sequences of nuclear reactions that convert hydrogen into helium. The primary reaction is thought to be the fusion of two protons with the emission of a low-energy neutrino and a positron.

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

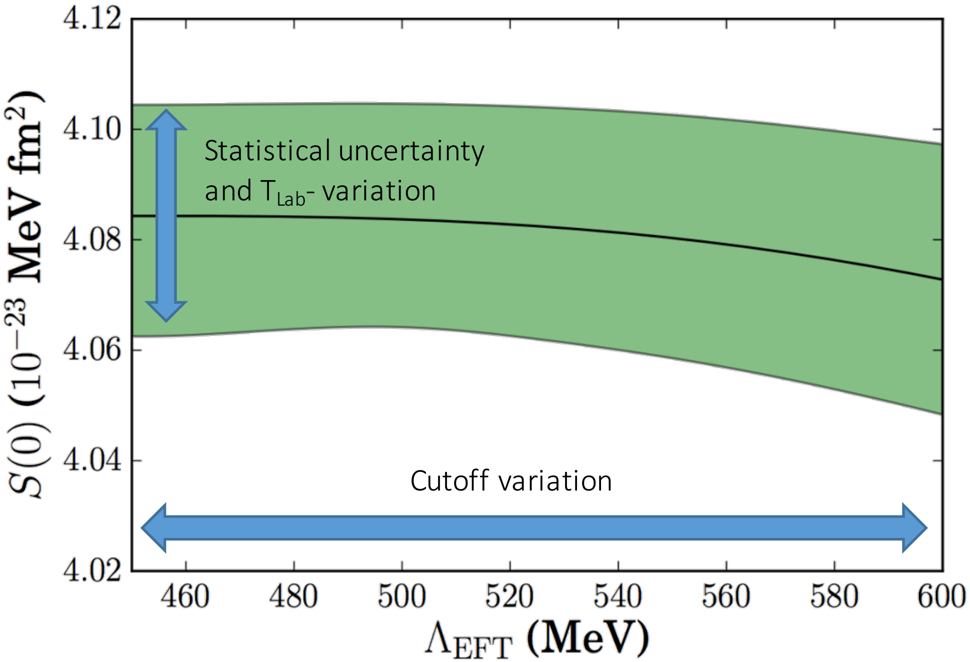


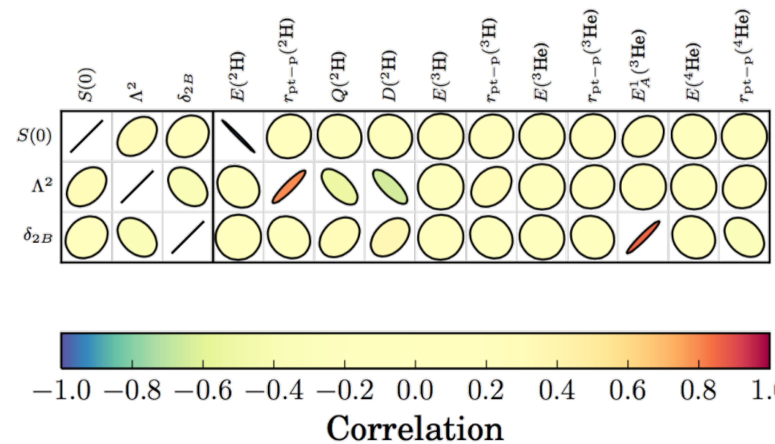
$$S(E) = \sigma(E) E e^{2\pi\eta}$$



$$\sigma(E) = \int \frac{d^3 p_e}{(2\pi)^3} \frac{d^3 p_\nu}{(2\pi)^3} \frac{1}{2E_e} \frac{1}{2E_\nu} \times$$
$$2\pi\delta\left(E + 2m_p - m_d - \frac{q^2}{2m_d} - E_e - E_\nu\right)$$
$$\frac{1}{v_{rel}} F(Z, E_e) \frac{1}{4} \sum |\langle f | \hat{H}_W | i \rangle|^2$$

Correlations and cutoff variation





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

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

Marcucci et al. PRL 2013

$$S = (4.030 \pm 0.006) \times 10^{-23}\ \mathrm{MeV\ fm}^2$$

Adelberger et al. RMP 2011

$$S = (4.01 \pm 0.04) \times 10^{-23}\ \mathrm{MeV\ fm}^2$$

S-factor correlates with deuteron B.E. via Q-value dependence of the phase space

Λ^2 trivially correlates with deuteron radius.

$$\Lambda(E) \sim \int_0^\infty \mathrm{d}r\ u_d(r)\chi_0(r;E)$$

Λ^2 only contains the 1B piece, thus only connects S-wave components. Consequently, larger Λ^2 means smaller deuteron D-state probability and Q-moment

2B-current proportional to triton weak-decay

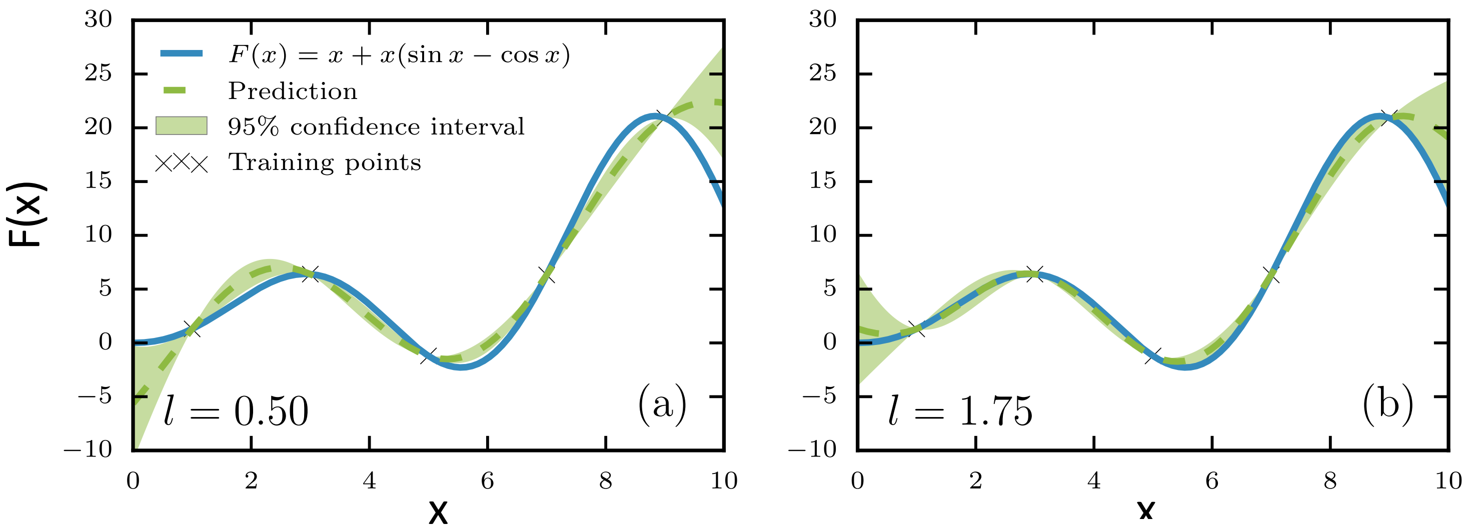
A surrogate for ab initio solutions

The general idea is to circumvent a computationally expensive model. Hopefully we could design an emulator for calibrating the models (ABC?) and exploring uncertainties.

We (=four bachelor students) emulated two-nucleon scattering and few-nucleon systems at next-to-leading order in chiral EFT using Gaussian process modelling.

So far we have only sampled EFT parameters within our covariance matrices. That is, we have only emulated EFT in a very ”smooth” or ”nice” region. But this is still very useful.

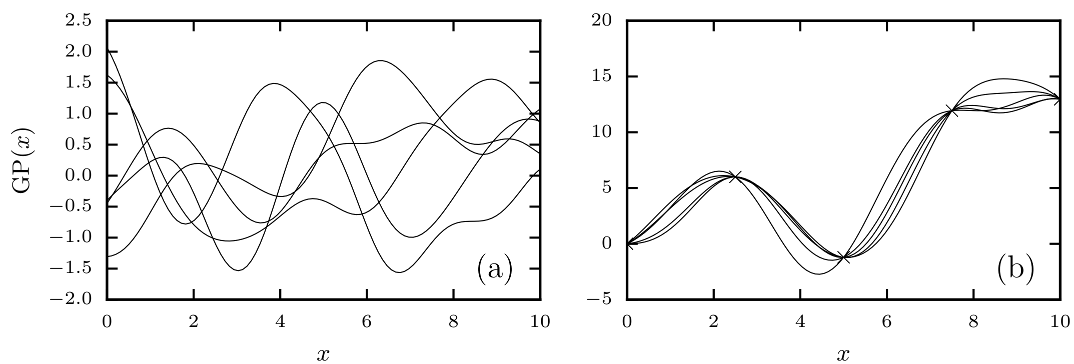
Gaussian Process Modelling



A Gaussian process is specified by its mean and covariance functions m(x), k(x,x')

We have operated with the standard covariance function

$$k(\boldsymbol{x}, \boldsymbol{x}') = e^{-\frac{|\boldsymbol{x}-\boldsymbol{x}'|^2}{2l^2}}$$

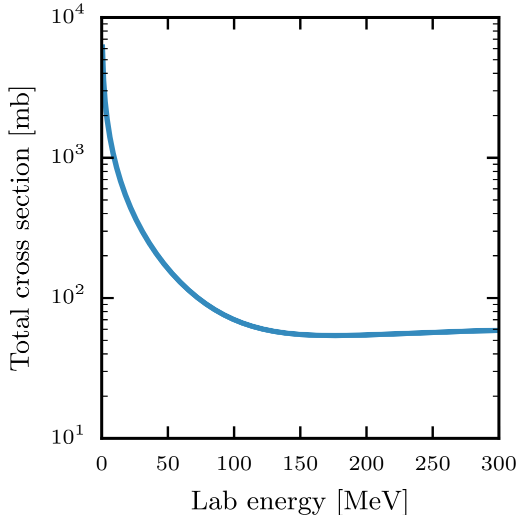


prior

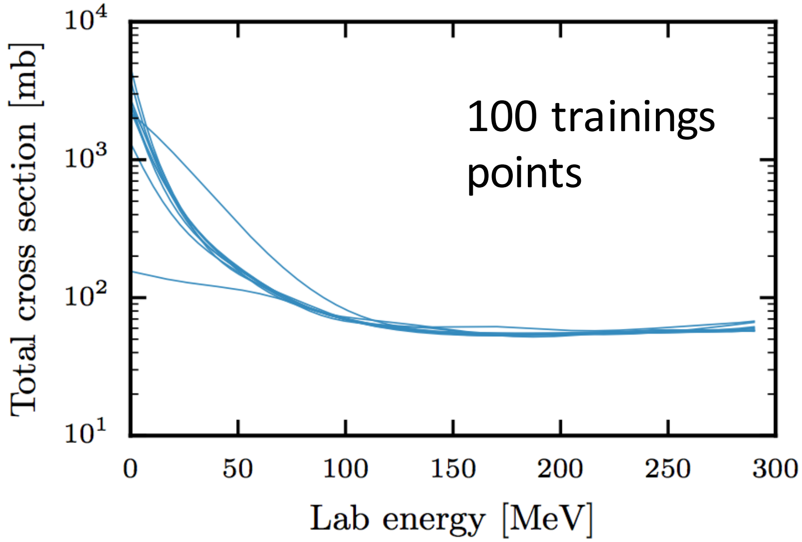
posterior
(prior conditioned on data)

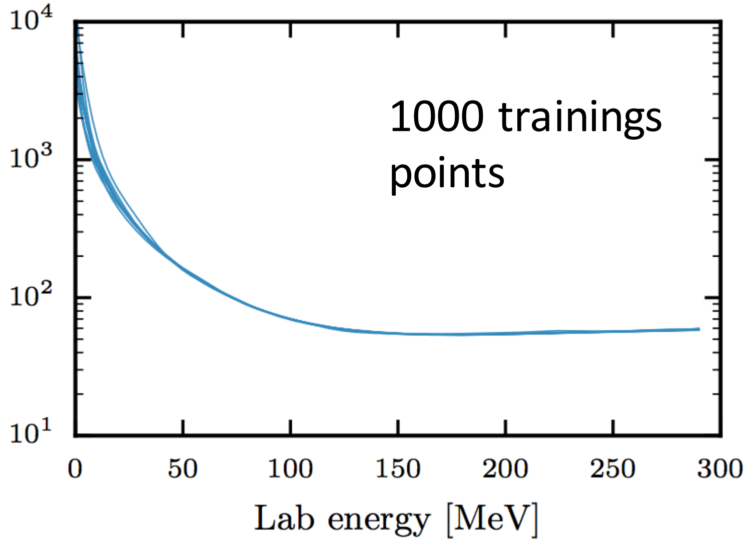
GPM and np cross sections

Goal: construct a GP to emulate the neutron-proton cross section for a set of coupling constants of the chiral EFT and 0.5 < E < 290 MeV

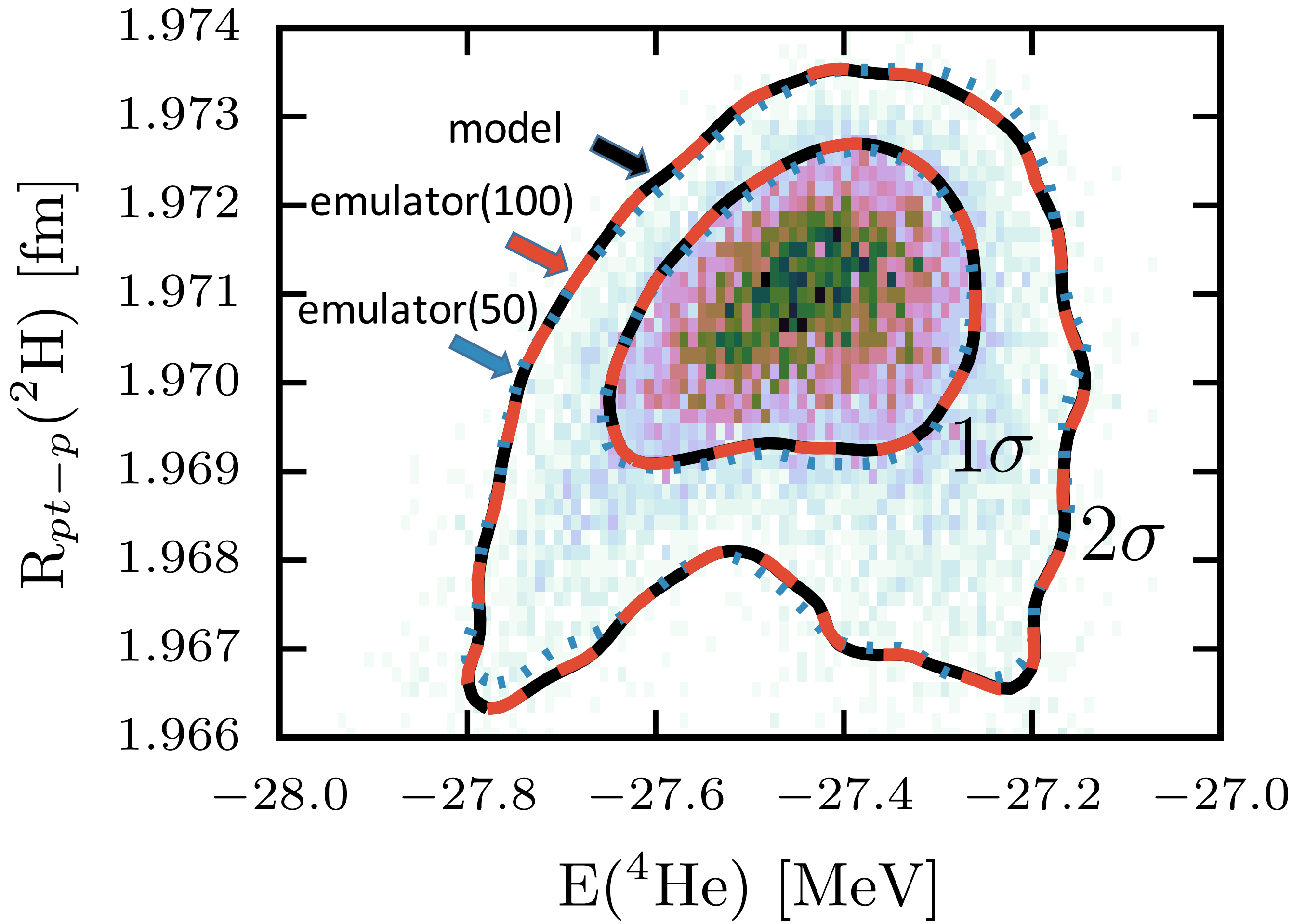


NLO(np) 9 coupling constants + 1 energy



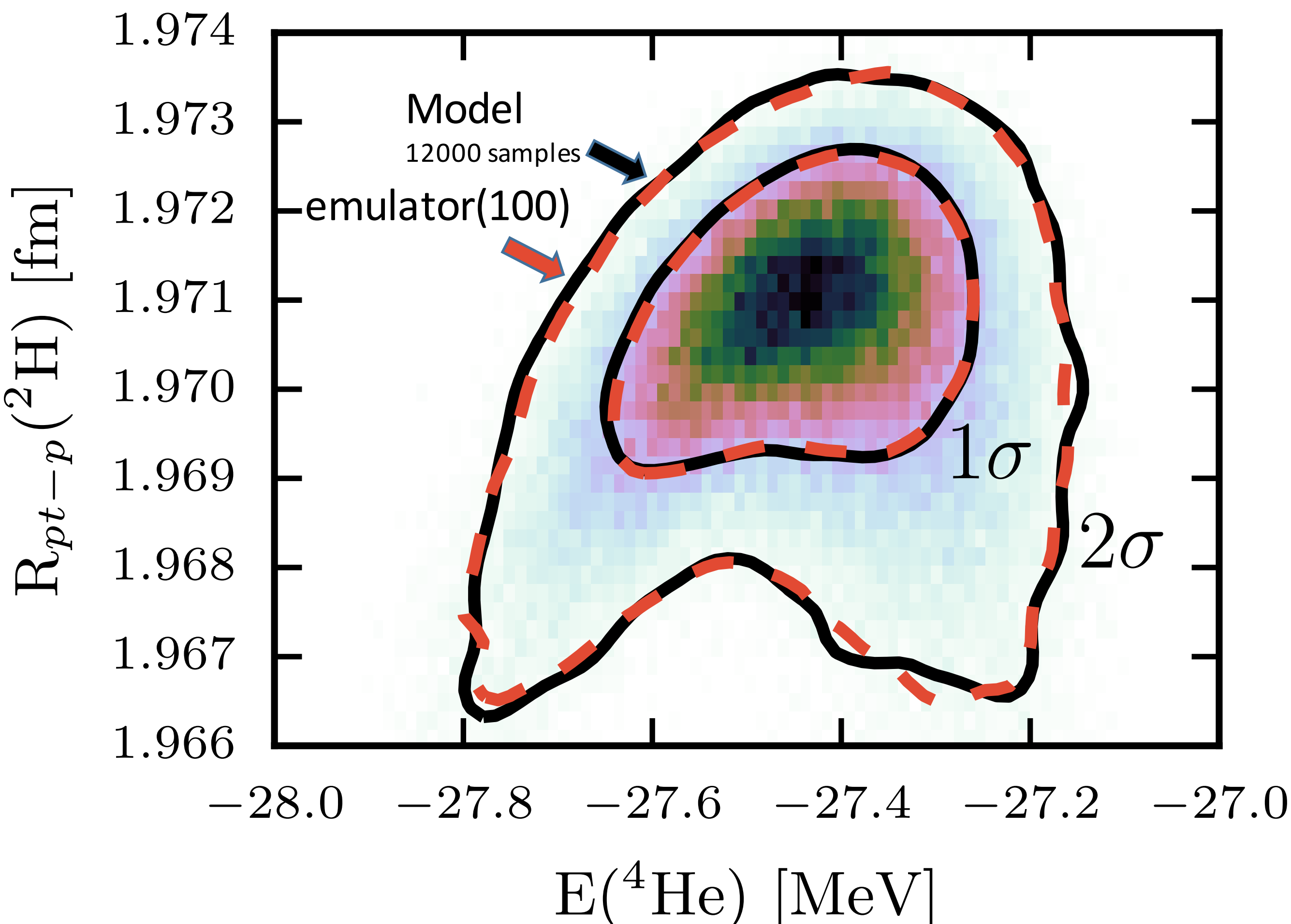


GPM and light nuclei



12000 samples

GPM and light nuclei



10^5 samples

Thank You.