Uncertainty quantification in ab initio nuclear theory

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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:

Overview: physics

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
- ....

A multi-scale problem

Ab initio
Configuration Interaction
Density Functional Theory

Dimensionality of problem increases!!

nucleon 1 fm
nucleus 10 fm
neutron star 20 km
**Ab initio** approach with chiral EFT

<table>
<thead>
<tr>
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<th>NN</th>
<th>NNN</th>
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<tbody>
<tr>
<td>LO ((v=0))</td>
<td><img src="image1" alt="Diagram" /></td>
<td><img src="image2" alt="Diagram" /></td>
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<tr>
<td>NLO ((v=2))</td>
<td><img src="image3" alt="Diagram" /></td>
<td><img src="image4" alt="Diagram" /></td>
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<tr>
<td>NNLO ((v=3))</td>
<td><img src="image5" alt="Diagram" /></td>
<td><img src="image6" alt="Diagram" /></td>
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16 parameters in NN+NNN sector up to \(Q^3\)
Additional 10 from inclusion of piN up to \(Q^4\)

**What data to include?** ...
(in practice governed by)

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

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.

\[ \theta_\star = \arg\min \chi^2(\theta), \quad \chi^2 = \sum_{i}^{N_{\text{data}}} \left( \frac{y_i(\theta) - d_i}{\sigma_i} \right)^2 \]

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

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

Two-nucleon interaction

Pion-nucleon scattering

Three-nucleon interaction

Current

Same LECs appear in various low-energy processes
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 energies of $^3\text{H}$, $^3,^4\text{He}$, $^{14}\text{C}$, $^{16}\text{O}$ As well as binding energies of $^{22,24,25}\text{O}$ and two-nucleon scattering data ($T_{\text{Lab}} < 35$ 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$_{\text{sat}}$
We have carried out a statistical analysis of chiral forces (up to NNLO) in light nuclei
Error budget

\[ \chi^2 = \sum_i^{N_{\text{data}}} \left( \frac{y_i(\theta) - d_i}{\sigma_i} \right)^2 \]

\[ \sigma_{\text{tot}}^2 = \sigma_{\text{exp}}^2 \]

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

\[ + \sigma_{\text{numerical}}^2 \]

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

\[ + \sigma_{\text{method}}^2 \]

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

\[ + \sigma_{\text{model}}^2 \]

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

\[ \sigma_{\text{model},x}^{(\text{amplitude})} = C_x \left( \frac{Q}{\Lambda} \right)^{\nu + 1}, \ x \in \{\text{NN, } \pi\text{N}\} \]
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.

\[
\text{Cov}(A, B) = \mathbb{E}[(\mathcal{O}_A(\alpha) - \mathbb{E}[\mathcal{O}_A(\alpha)]) \times (\mathcal{O}_B(\alpha) - \mathbb{E}[\mathcal{O}_B(\alpha)])]
\]

\[
\approx \sum_{ijkl}^{N_\alpha} \mathbb{E}\left[\left(\tilde{J}_{A,i} x_i + \frac{1}{2} \tilde{H}_{A,ij} x_i x_j - \frac{1}{2} \tilde{H}_{A,ii} \sigma_i^2\right) \times \left(\tilde{J}_{B,k} x_k + \frac{1}{2} \tilde{H}_{B,kl} x_k x_l - \frac{1}{2} \tilde{H}_{B,kk} \sigma_k^2\right)\right]
\]

\[
= \tilde{J}_A^T \Sigma \tilde{J}_B + \frac{1}{2} (\sigma^2)^T (\tilde{H}_A \circ \tilde{H}_B) \sigma^2,
\]

Figure from J. Dobaczewski et al, J. Phys. G 41 (2014) 074001
Linear Correlations at NNLO
Joint probability distributions

(a) $R_{pt-p}(^2H)$ (fm)

$E(^4\text{He})$ (MeV)

-28.4
-28.2
-28.0

(b) $E(^4\text{He})$ (MeV)

-120
-80
-40
0

SIMULTANEOUS OPTIMIZATION

SEPARATE OPTIMIZATION

Ellipses from Gaussians
“Boomerangs” traced numerically

Quadratic propagation

MC sample ($10^5$)

Linear prop.

MC sample ($10^5$)
Predicting cross sections and UQ

neutron – proton integrated cross sections

\[
\text{Total cross section (mb)}
\]

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

\[
\pi^- + p \rightarrow \pi^0 + n \\
(\theta_{\text{cm}} = 41.4^\circ)
\]

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 $T_{\text{Lab}}$ truncations reveal that the constant $C_{\text{NN}}$ doesn’t change much. (However, for NNLOsep $C_{\text{NN}} = 1.6 \text{ mb}^{1/2}$)

The np scattering cross section at 300 MeV ($\text{Exp} = 34.563(174) \text{ mb}$)

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

\[ p + p \rightarrow d + e^+ + \nu_e \]

\[ S(E) = \sigma(E) E e^{2\pi n} \]

\[ \sigma(E) = \int \frac{d^3 p_e}{(2\pi)^3} \frac{d^3 p_\nu}{(2\pi)^3} \frac{1}{2E_e} \frac{1}{2E_\nu} \times \]

\[ 2\pi \delta \left( E + 2m_p - m_d - \frac{q^2}{2m_d} - E_e - E_\nu \right) \]

\[ \frac{1}{v_{rel}} F(Z, E_e) \frac{1}{4} \sum |\langle f | \hat{H}_W | i \rangle|^2 \]
Correlations and cutoff variation

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

\[ S(0) = (4.047^{+0.024}_{-0.032}) \times 10^{-23} \text{ MeV fm}^2 \]

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

\[ \Lambda^2 \text{ trivially correlates with deuteron radius.} \]

\[ \Lambda(E) \sim \int_0^\infty dr \ u_d(r) \chi_0(r; E) \]

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

2B-current proportional to triton weak-decay

\[ S = (4.030 \pm 0.006) \times 10^{-23} \text{ MeV fm}^2 \]

Marcucci et al. PRL 2013

\[ S = (4.01 \pm 0.04) \times 10^{-23} \text{ MeV fm}^2 \]

Adelberger et al. RMP 2011
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.
A Gaussian process is specified by its mean and covariance functions $m(x)$, $k(x,x')$.

We have operated with the standard covariance function

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

\[ E(4\text{He}) \text{ [MeV]} \]

\[ R_{pt-p}^{(2\text{H})} \text{ [fm]} \]

1σ, 2σ

12000 samples
GPM and light nuclei

\[ E(4\text{He}) [\text{MeV}] \]

Model
12000 samples
emulator(100)

10^5 samples
Thank You.