The Virtue of Doubt: Bayesian UQ in *ab initio* nuclear theory

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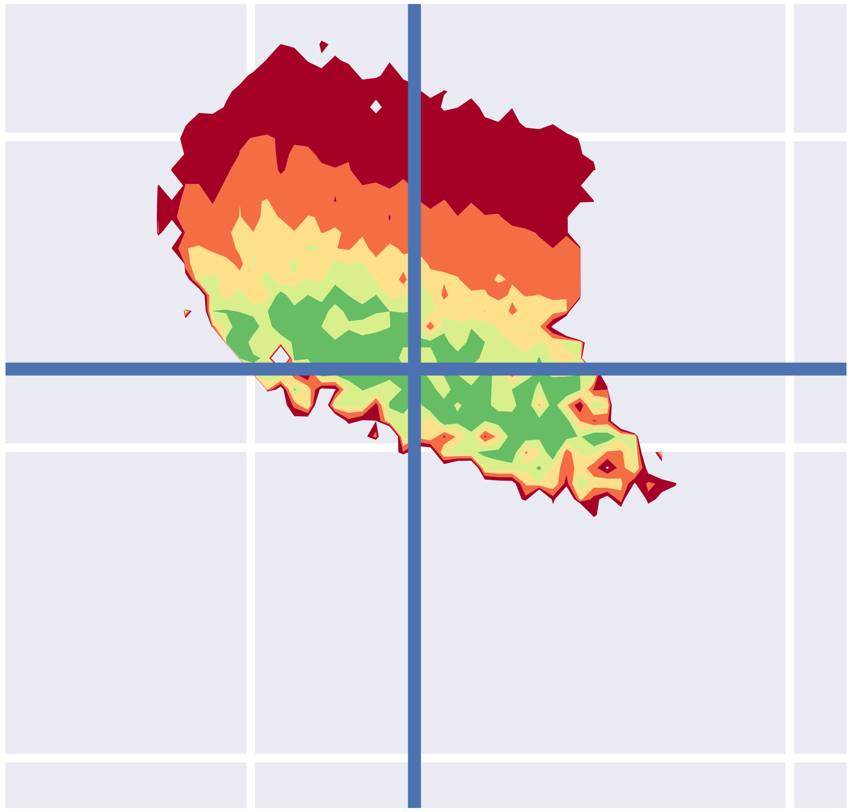
Setting up for this talk

1. The **nucleus is a complex many-body system**. Exact quantitative nuclear models do not exist.

2. While all **models are wrong**, models that know when and how they are wrong are useful. (after G. Box)

3. **Bayesian methods** are particularly useful for assessing uncertainties in nuclear physics. *Ab initio* models have an **inferential advantage**.
   - M. Schindler and D. Phillips [Ann. Phys. 324 (2009) 682]
   - S. Wesolowski, R. Furnstahl, D. Phillips, J. Melendez, C. Drischler and the Buqeye collaboration
   - A. Ekström, cf, I. Svensson, W. Jiang
   - and many others [see, e.g., M. Piarulli, E. Epelbaum, cf (2023) Editorial: Uncertainty quantification in nuclear physics. Front. Phys. 11:1270577]
   - New book (in progress): https://nucleartalent.github.io/LFD_for_Physicists/

4. **Multidisciplinary efforts** are needed when tackling uncertainty quantification for predictions involving complex computer models.
   - See, e.g., the ISNET series [https://isnet-series.github.io/]



Bayesian UQ: ingredients and workflow

Learning from data via Bayes

- Model calibration via **Bayes' theorem**

Posterior, Likelihood, Prior, Marginal likelihood

$$\mathrm{pr}(\boldsymbol{\alpha} \,|\, \mathscr{D}, I) = \frac{\mathrm{pr}(\mathscr{D} \,|\, \boldsymbol{\alpha}, I)\,\mathrm{pr}(\boldsymbol{\alpha} \,|\, I)}{\mathrm{pr}(\mathscr{D} \,|\, I)}$$

- The prior encodes our knowledge about parameter values before analyzing the data
- The likelihood is the probability of observing the data given a set of parameters
- The marginal likelihood (or model evidence) provides normalization of the posterior.
- The posterior is the inferred probability density for the parameters.

Bayesian workflow

Formulate priors before new data is used.

Define a statistical model

Computational challenges:

1. Many model evaluations needed
2. Stationarity of Markov chain
3. Number of effective samples

Enabling technologies

- ✓ Emulators, modeling at different fidelity
- ✓ Advanced sampling
- ✓ History matching

Compute the posterior probabilities.

- Prior checking with the **prior predictive distribution**
  $\{y(\boldsymbol{\alpha}) : \boldsymbol{\alpha} \sim \mathrm{pr}(\boldsymbol{\alpha} \,|\, I)\}$
  where $y(\boldsymbol{\alpha})$ represents the physics model for observable(s) y.
- Model checking with the **posterior predictive distribution**
  $\{y(\boldsymbol{\alpha}) : \boldsymbol{\alpha} \sim \mathrm{pr}(\boldsymbol{\alpha} \,|\, \mathcal{D}, I)\}$
  for known data plotting histograms and summary statistics.

Do model checking

Bayesian workflow

Formulate priors before new data is used.

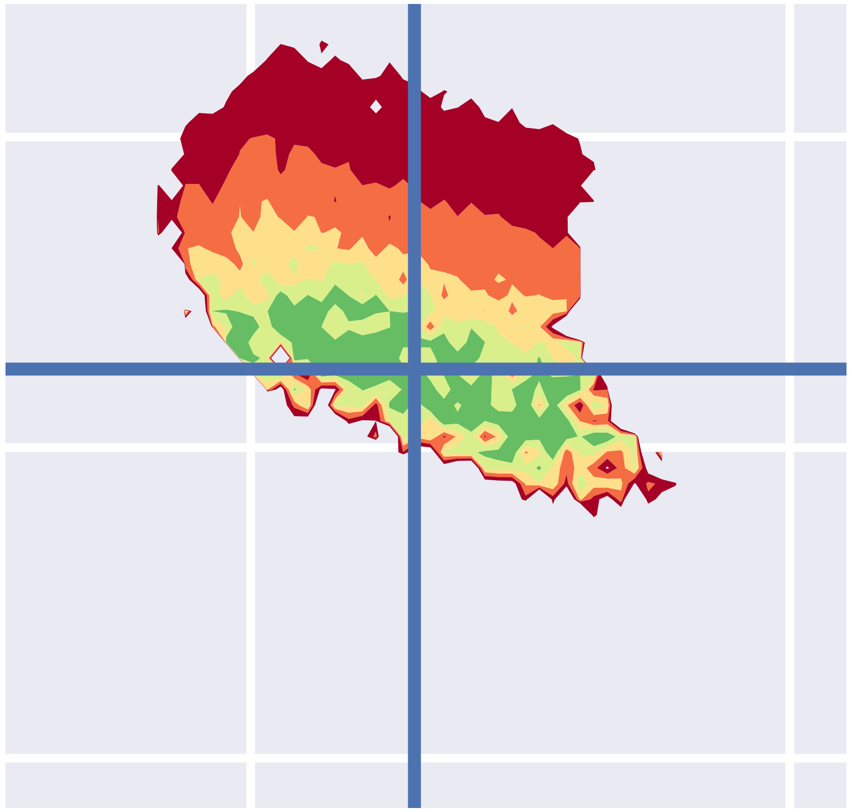
Define a statistical model

Compute the posterior probabilities.

Do model checking

Important choices to be made in the experimentation phase:

1. Noninformative versus informative prior.
2. Input (α) correlations (type x).
3. Constructing the data-generating process—relating the physics model and data—including all errors
4. Output (y) correlations (type y).
5. Formalizing prior and likelihood distributions.



Statistical models in *ab initio* nuclear theory

Ab initio modeling of nuclear systems using chiral EFT

$$\hat{H}|\psi_i\rangle = E_i|\psi_i\rangle$$

$$\hat{H}(\boldsymbol{\alpha}) = \hat{T} + \hat{V}(\boldsymbol{\alpha})$$

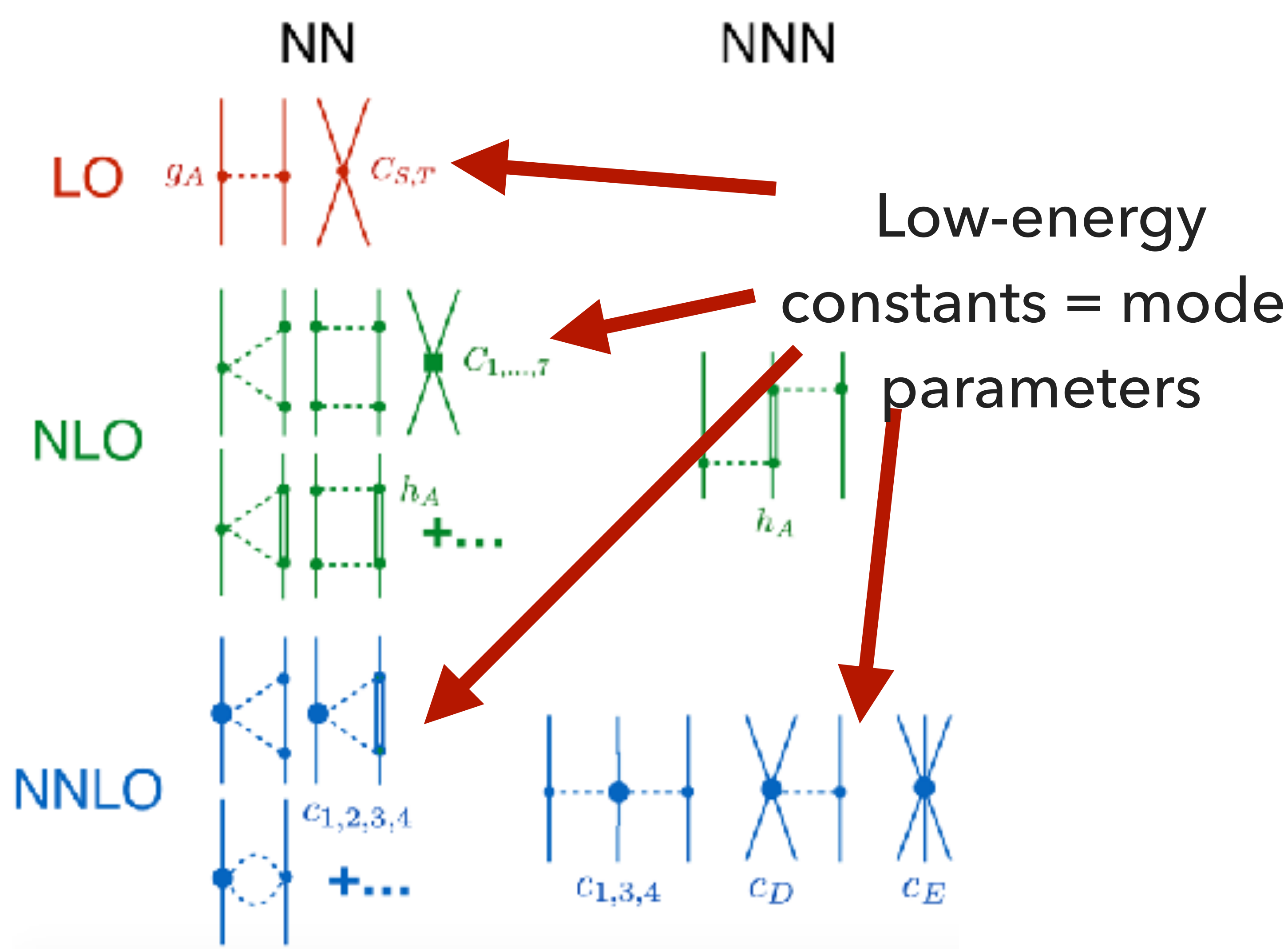
$$O_{ij} = \langle\psi_j|\hat{O}|\psi_i\rangle$$

parameters inferred from data.
– **parametric uncertainty**

EFT expansion truncated
– **model/truncation error**

many-body solver relies on approximations:
– **many-body error**
– **emulator error**

χEFT promises a connection with QCD



Weinberg, van Kolck, Kaiser, Bernard, Meißner, Epelbaum, Machleidt, Entem, ...

Statistical model (relating data and *ab initio* model)

$$y_{\rm exp} = \tilde{y}(\boldsymbol{\alpha}) + \delta y_{\rm EFT} + \delta y_{\rm MB} + \delta\tilde{y}_{\rm em} + \delta y_{\rm exp}$$

Getting to know your errors

Challenge #1: EFT truncation errors

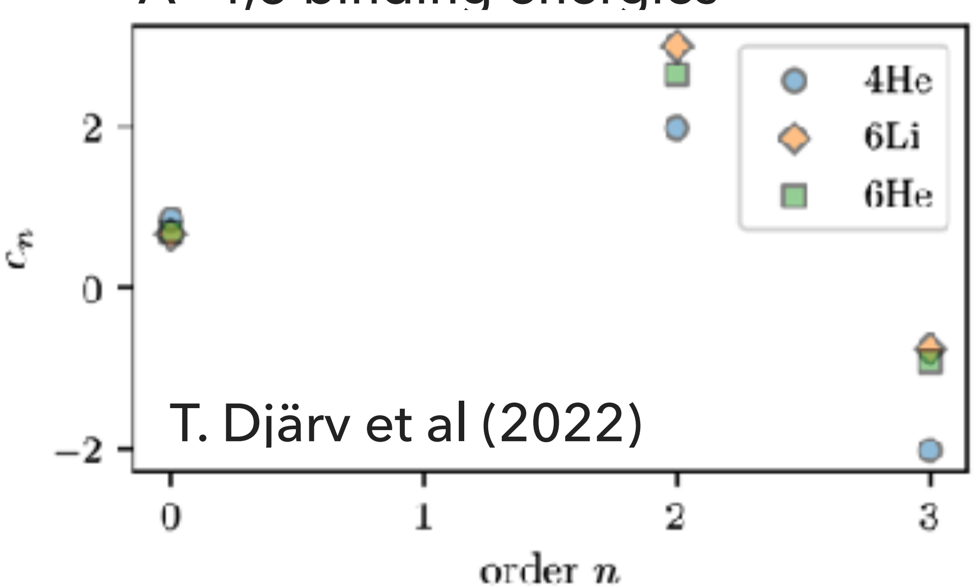
- **Approach**: study order-by-order results, assuming a model for the EFT convergence, learn the PDF for expansion coefficients

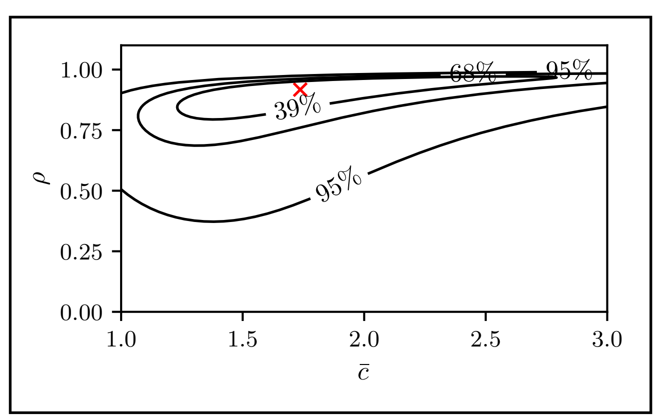
$$y_k = y_{\text{ref}} \sum_{n=0}^{k} c_n Q^n, \quad \delta y_k = y_{\text{ref}} \sum_{n=k+1}^{\infty} c_n Q^n$$

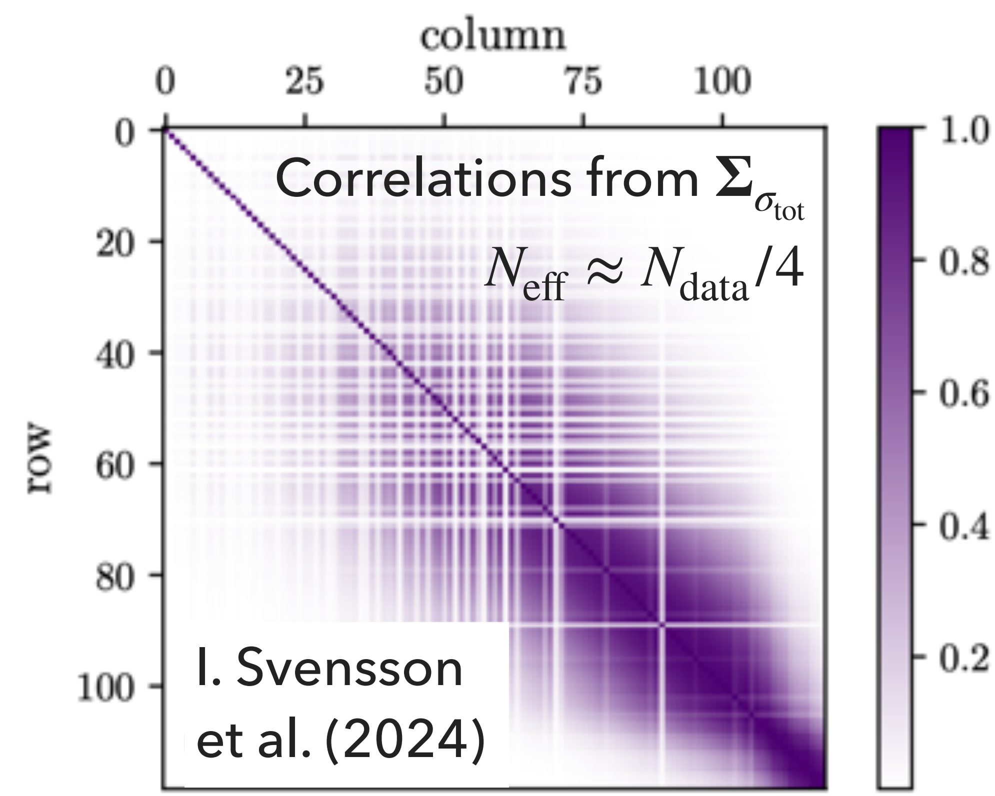
- **Challenges**: Cutoff dependence, expansion parameter, irregular convergence (i.i.d. coefficients), correlation structure for *E(A), r_p(A), **σ**(E,**θ**), etc*

$$\delta y_k(\vec{x}) = y_{\text{ref}} \sum_{n=k+1}^{\infty} c_n(\vec{x}) Q^n$$

A=4,6 binding energies







GP modelling for correlated EFT errors in J. Melendez et al (2019) and C. Drischler et al. (2020)

Getting to know your errors

Emergent symmetries (Challenge #1: EFT truncation errors)

- How do emergent symmetries—such as Wigner SU(4)—affect the EFT convergence pattern for "symmetry-protected" observables?

$$y_k = y_{\mathrm{ref}} \sum_{n=0}^{k} c_n Q^n$$

Transition	Within irrep	Eq. (4)	This work (NCSM) LO	NLO	NNLOopt	$N_{\max}$	VMC [7]
$^3\mathrm{H}(\frac{1}{2}^+) \longrightarrow {}^3\mathrm{He}(\frac{1}{2}^+)$	✓	2.449	2.267	2.332	2.313	18	–
$^6\mathrm{He}(0^+) \longrightarrow {}^6\mathrm{Li}(1^+)$	✓	2.449	2.178	2.259	2.260	14	2.200
$^7\mathrm{Be}(\frac{3}{2}^-) \longrightarrow {}^7\mathrm{Li}(\frac{3}{2}^-)$	✓	2.582	2.301	2.375	2.357	12	2.317
$^7\mathrm{Be}(\frac{3}{2}^-) \longrightarrow {}^7\mathrm{Li}(\frac{1}{2}^-)$	✓	2.309	2.086	2.178	2.175	12	2.157
$^8\mathrm{Li}(2^+) \longrightarrow {}^8\mathrm{Be}(2^+)$	X	0.0	0.018	0.081	0.093	10	0.147
$^8\mathrm{He}(0^+) \longrightarrow {}^8\mathrm{Li}(1^+)$	X	0.0	0.066	0.364	0.335	10	0.386

c_2	c_3
0.3	-0.3
0.4	0.02
0.4	-0.09
0.5	-0.05
-6.1	24.7

($y_{\mathrm{ref}} = y_{\mathrm{LO}}$, $Q = 0.3$)
see also Wesolovski et al. (2021)

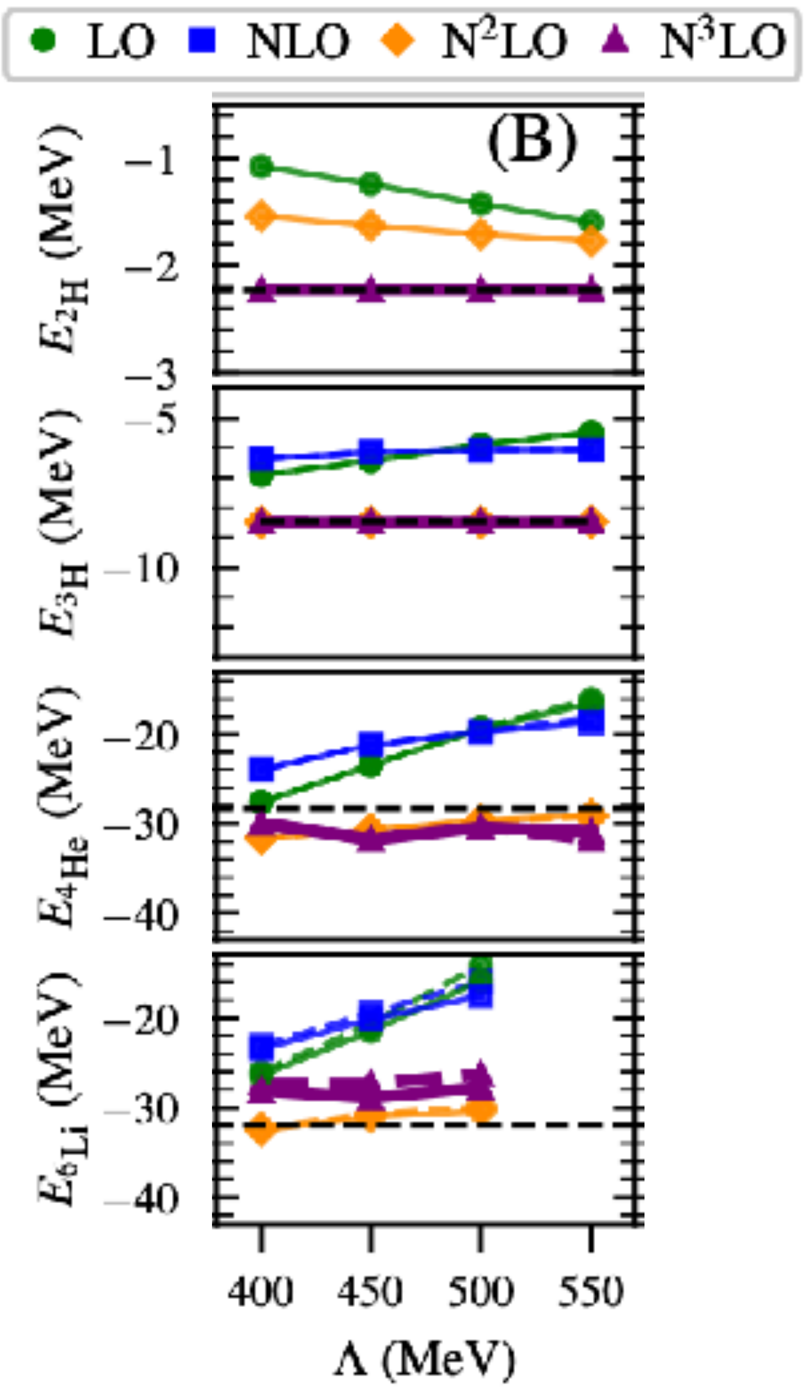
Analytic result in the Wigner SU(4) limit

Simone Li Muli, T. Djärv, cf, D. Phillips
(accepted in Phys. Rev. Lett)

Getting to know your errors

RG invariance (Challenge #1: EFT truncation errors)

- Predictions of observables using Weinberg PC depend on regulator cutoff (= not RG invariant).
- Order-by-order Bayesian inferences at multiple cutoffs are still missing.
- Can an RG-invariant χEFT with partly perturbative pions describe nuclear observables in A>2 systems and provide principled EFT error estimates?
- First, perturbative computations up to A=6 for LO-N3LO.
- Bayesian inference and EFT error analysis should be performed.



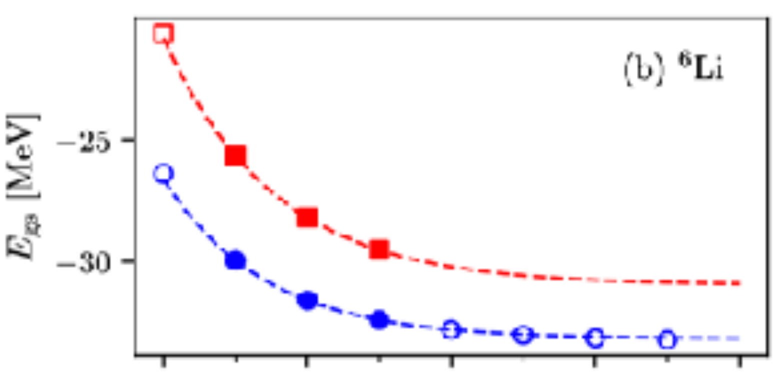
Oliver Thim, A. Ekström, cf, (2026)

Getting to know your errors

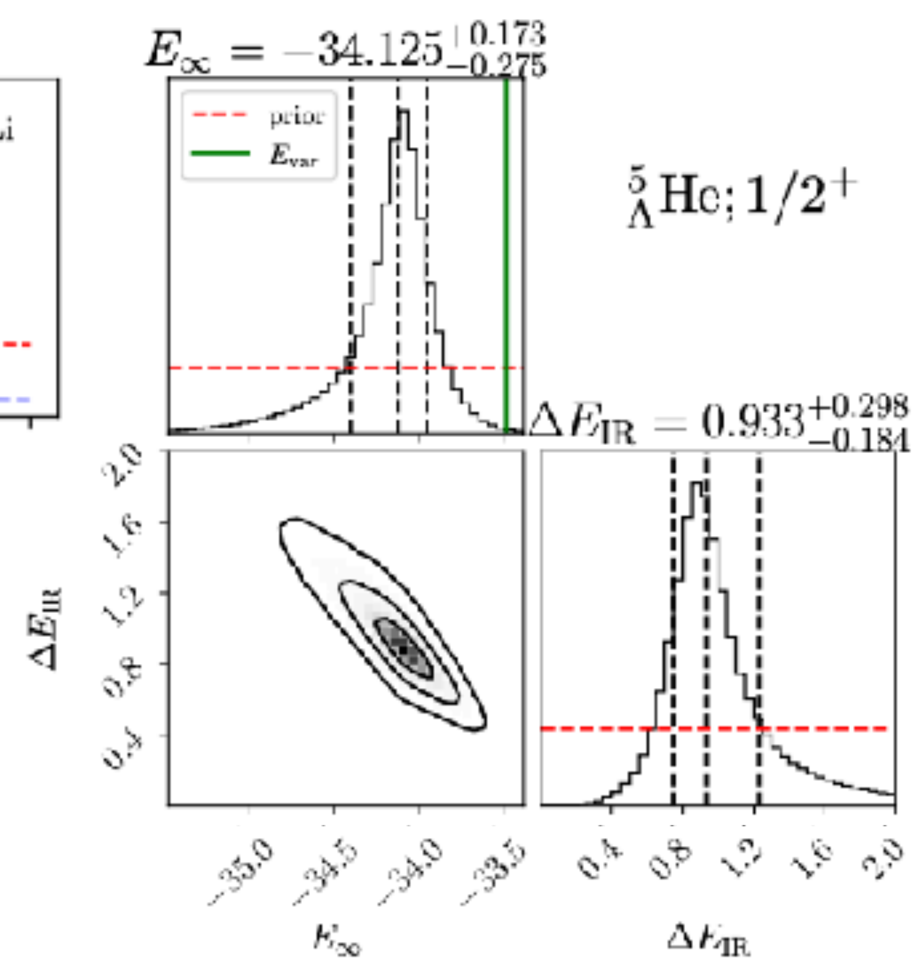
Challenge #2: Many-body solver errors

- **Approach**: Convergence studies; Method comparisons;
- **Note**: We can incorporate "uncertain" extrapolation, $\mathbb{E}[\delta y_{\mathrm{MB}}] \neq 0$; Errors are correlated, should be modeled as such.
- **Challenges**: Some approximations might be very difficult to relax; Non-variational observables/approaches

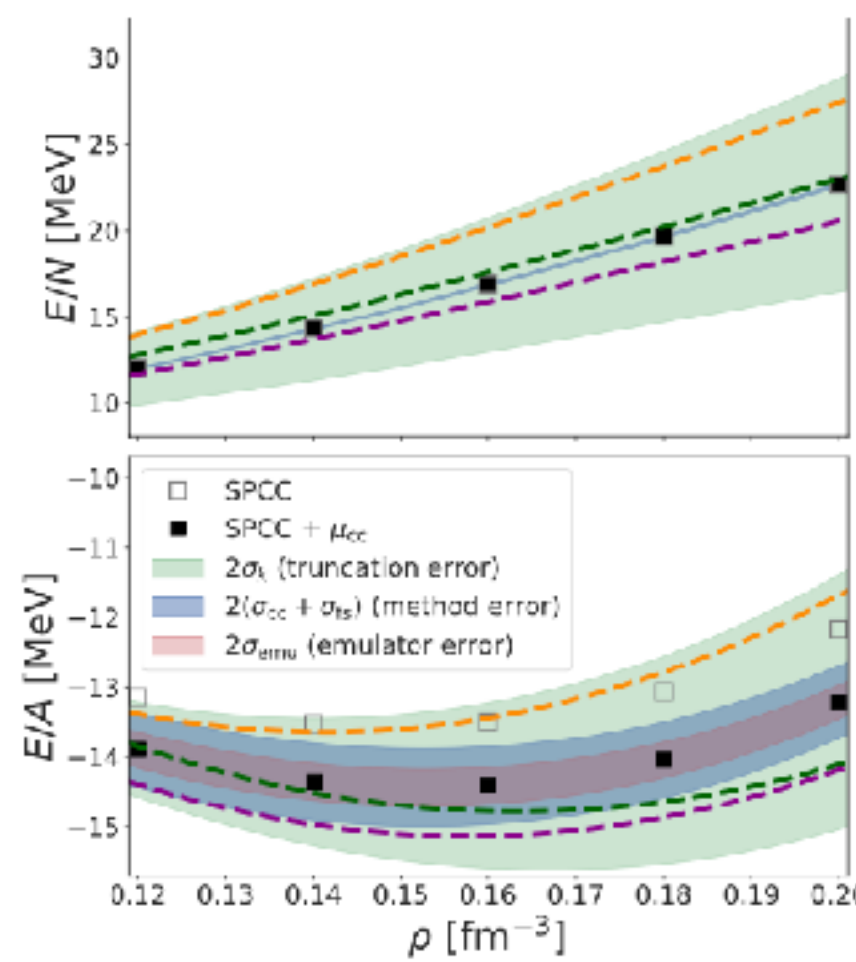
N_{max} extrapolation for NCSM in T. Djärv et al (2022)



Bayesian IR extrapolation for Y-NCSM in D. Gazda et al (2022)



GP modeling for correlated method and model errors in W. Jiang et al (2024)



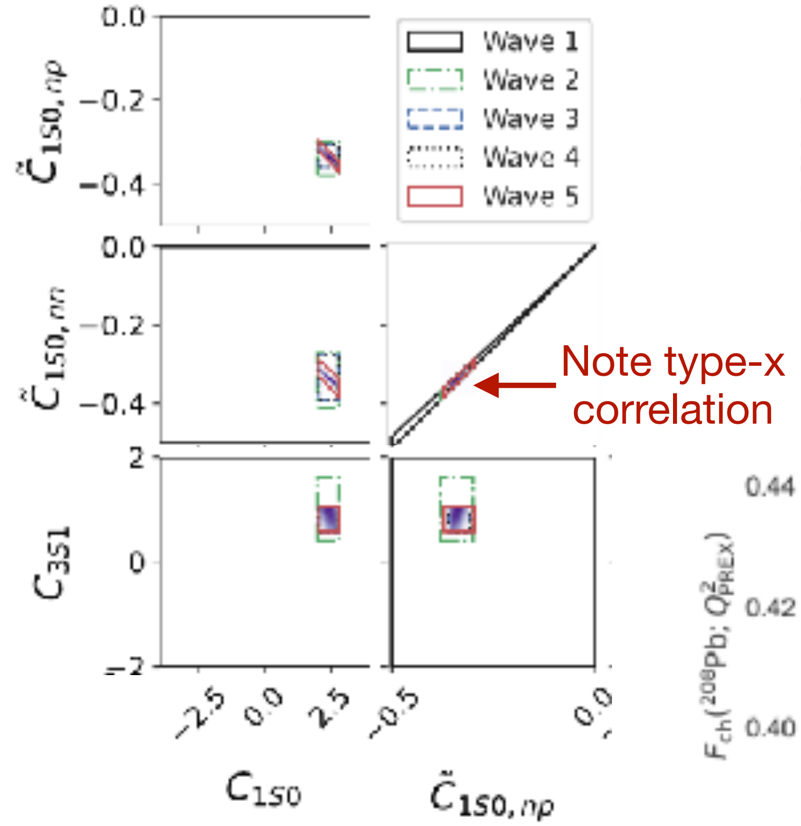
Challenge #3: Parametric uncertainty for high-dim models

Likelihood-free methods

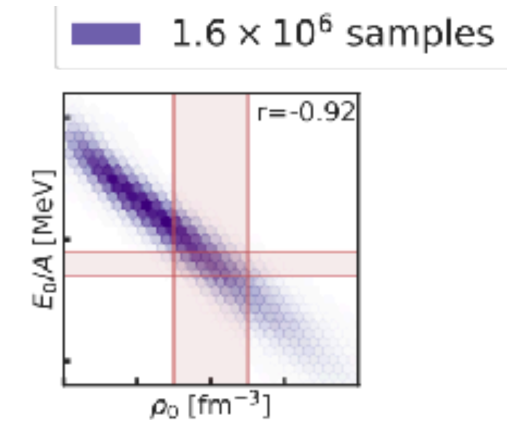
- History matching allows model exploration without full probabilistic specification (linear Bayes).
- Should also explore Approximate Bayesian Computation, etc.

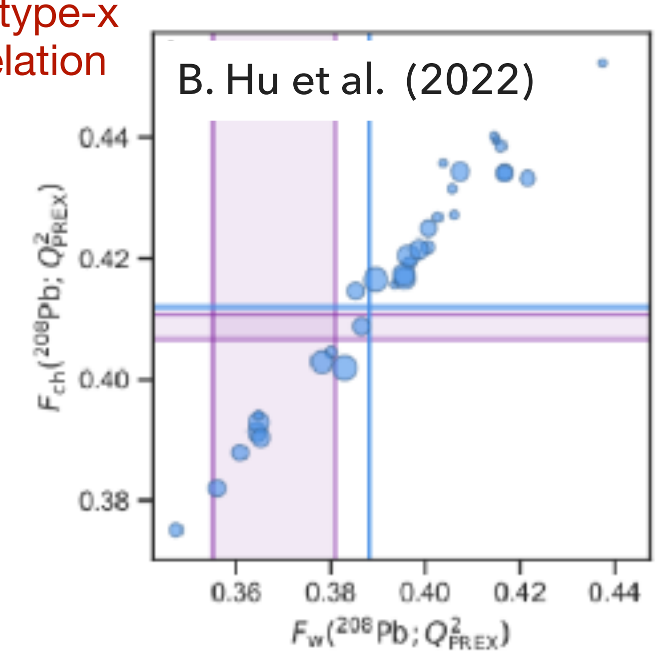
Posterior sampling

- **Marginalized** (univariate) distributions can often be mapped with relatively few (<100) samples.
- Make **every sample count** (HMC renders uncorrelated samples)
- Posterior updates with **importance resampling.**
- Full sampling enabled with emulators.



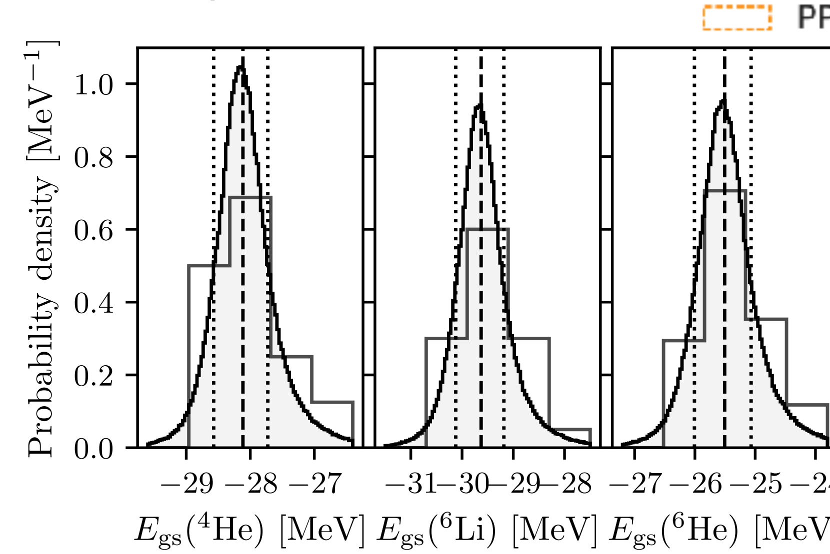
W. Jiang et al. (2024)

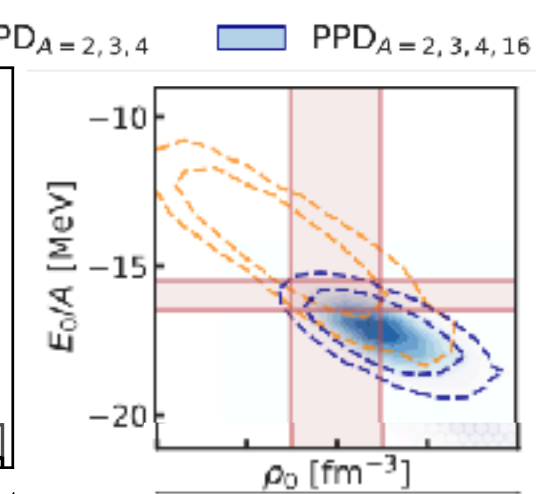




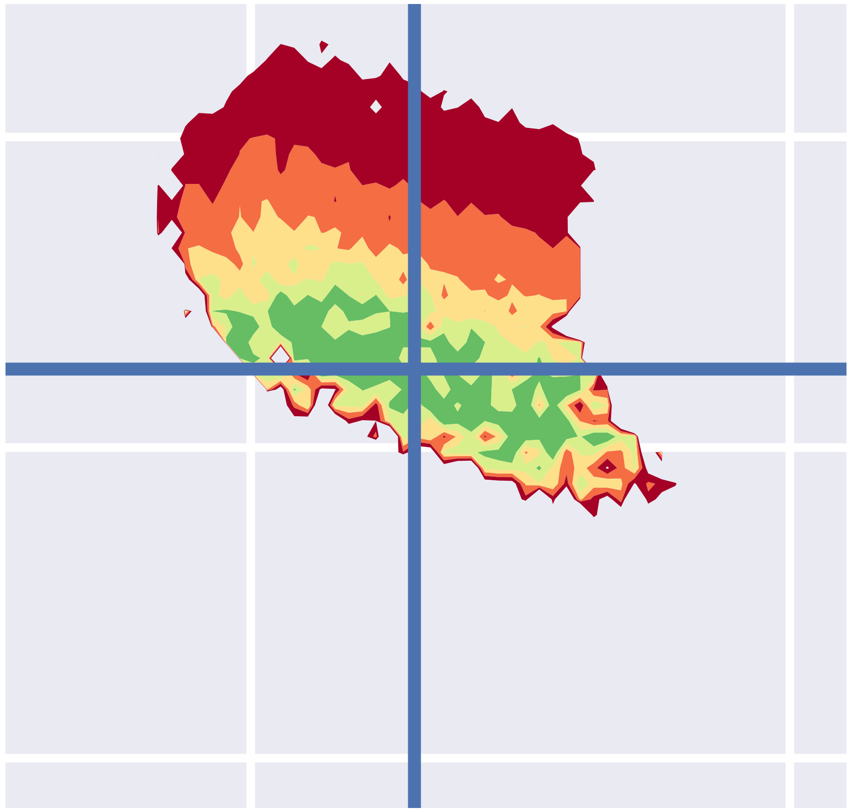
B. Hu et al. (2022)

T. Djärv et al PRC (2022)
PPD samples from Wesolowski (2021)





W. Jiang et al. (2024)



Bayesian UQ in *ab initio* nuclear theory

Nuclear physics research with Bayesian methods

- **Aim #1**: Inference of **nuclear Hamiltonians**
  - Focus on the **inference** process, order-by-order **convergence**, and the information content of **calibration** data.
  - Produce interaction **samples** for subsequent analyses.

- **Aim #2**: **Physics** exploration
  - Perform **sensitivity** analyses and reach for **experimental design**.
  - Expose **limitations** of the physics model, and/or the statistical model

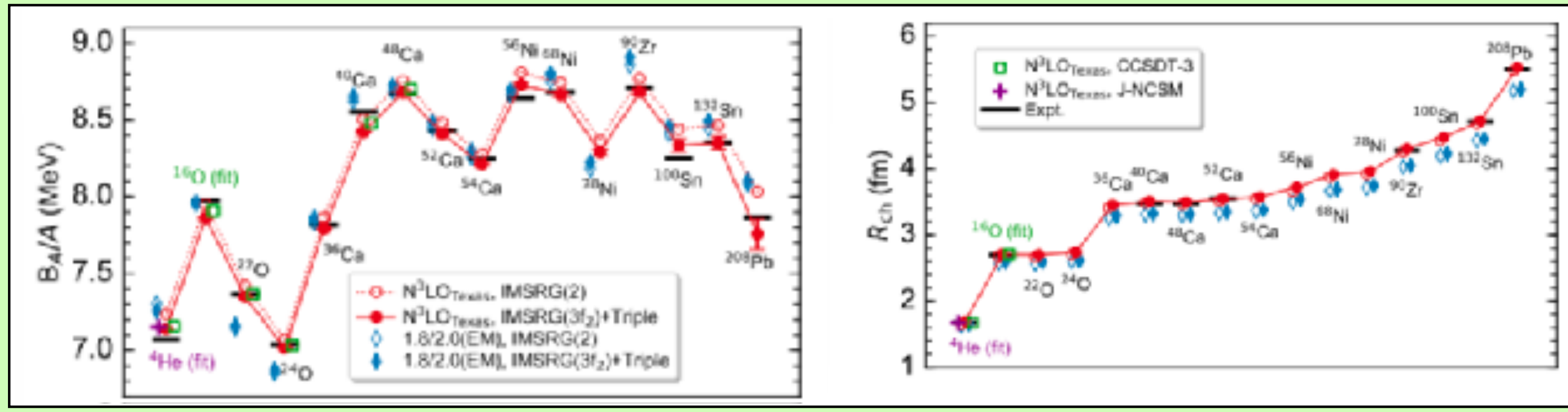
- **Aim #3**: **Predictive** modelling
  - Physics predictions with **propagated uncertainties**.
  - **New physics searches** with nuclear-physics probes.

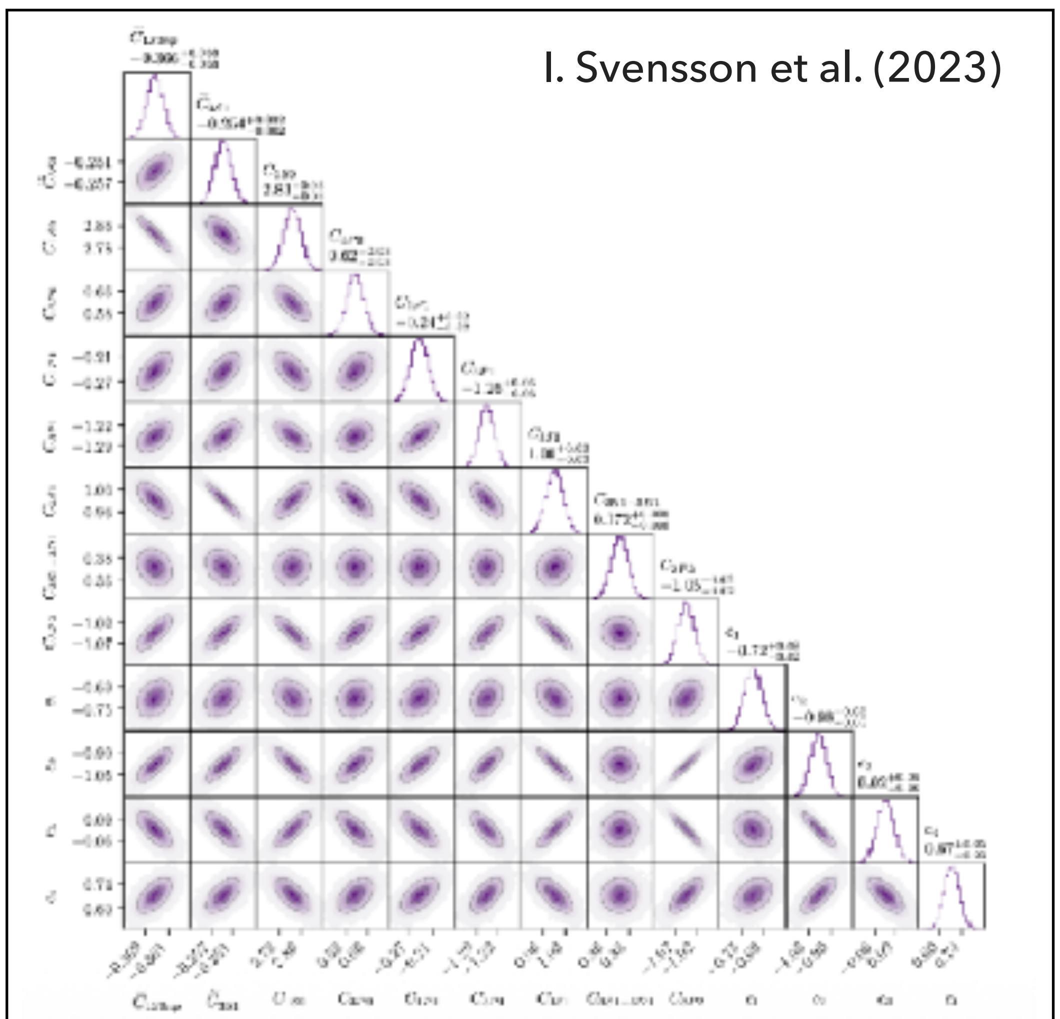
Inference of nuclear Hamiltonians

Why do some optimized interactions "work better" than others?

N³LO$_{TX}$ see G. Hagen's talk

- Calibration protocol
- Promoted terms
- UQ? (both parametric and EFT errors)





I. Svensson et al. (2023)

Bayesian inference in the NN sector

Much studied, and many interesting results

See the BUQEYE collaboration, Chalmers' group, Epelbaum et al.

Several questions remain:

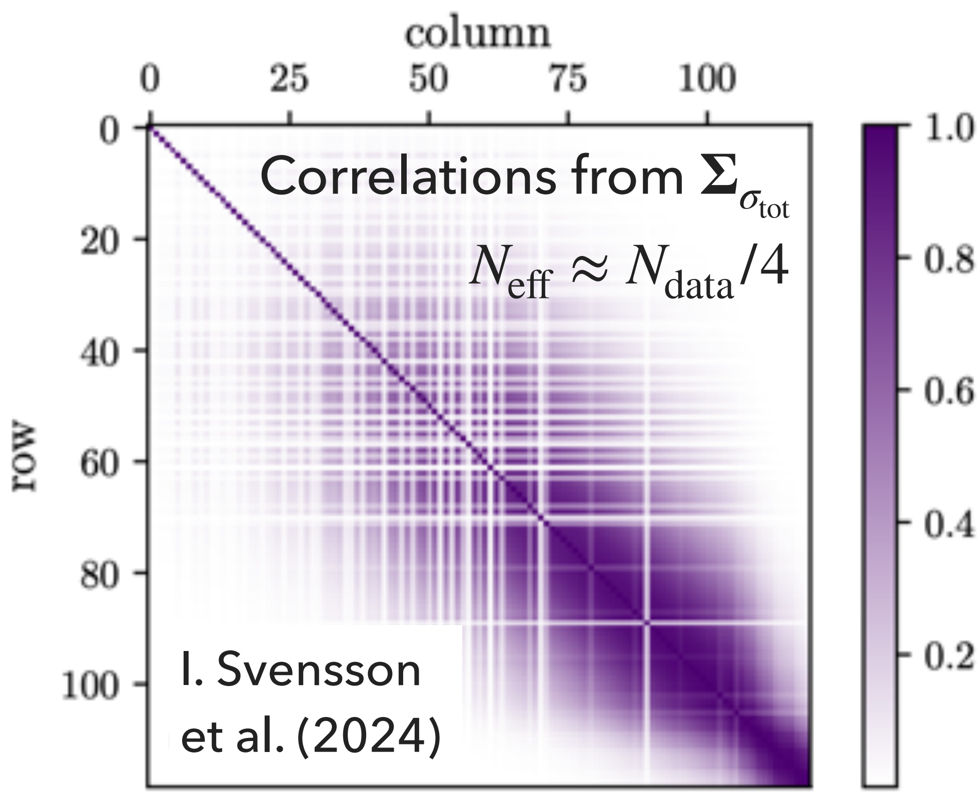
- Performance in many-body predictions
- Simultaneous inference of 3N sector
- EFT convergence pattern
- Correlated EFT errors across observables

Inference of nuclear Hamiltonians

GP modelling for correlated EFT errors

J. Melendez et al (2019), C. Drischler et al. (2020), I. Svensson et al. (2024)

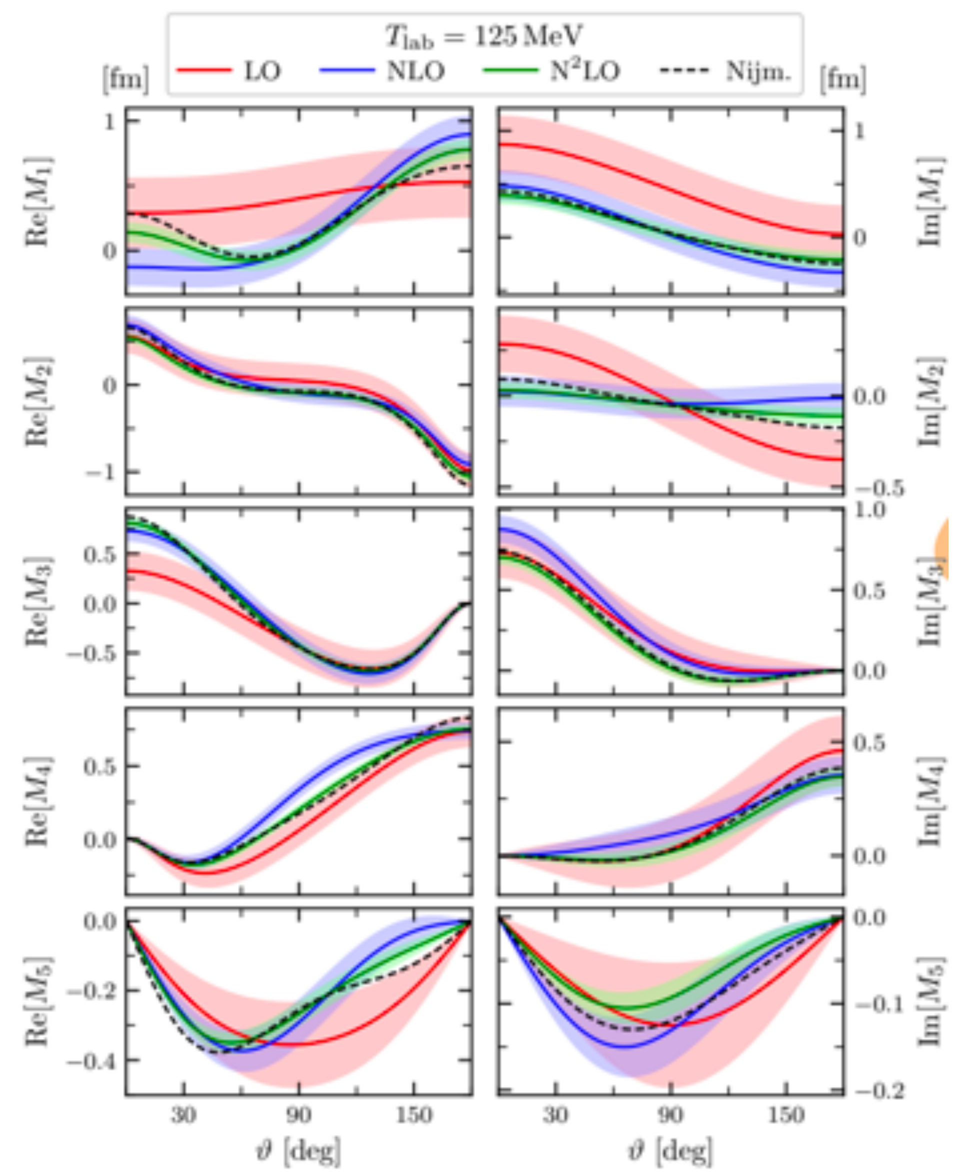
$$\delta y_k(\vec{x}) = y_{\text{ref}} \sum_{n=k+1}^{\infty} c_n(\vec{x}) Q^n$$



EFT errors on scattering amplitude level

See B. McClung et al (2025)

L. Abrahamsson et al. (in preparation).



Inference of nuclear Hamiltonians

GP modelling for correlated EFT errors

J. Melendez et al (2019), C. Drischler et al. (2020), I. Svensson et al. (2024)

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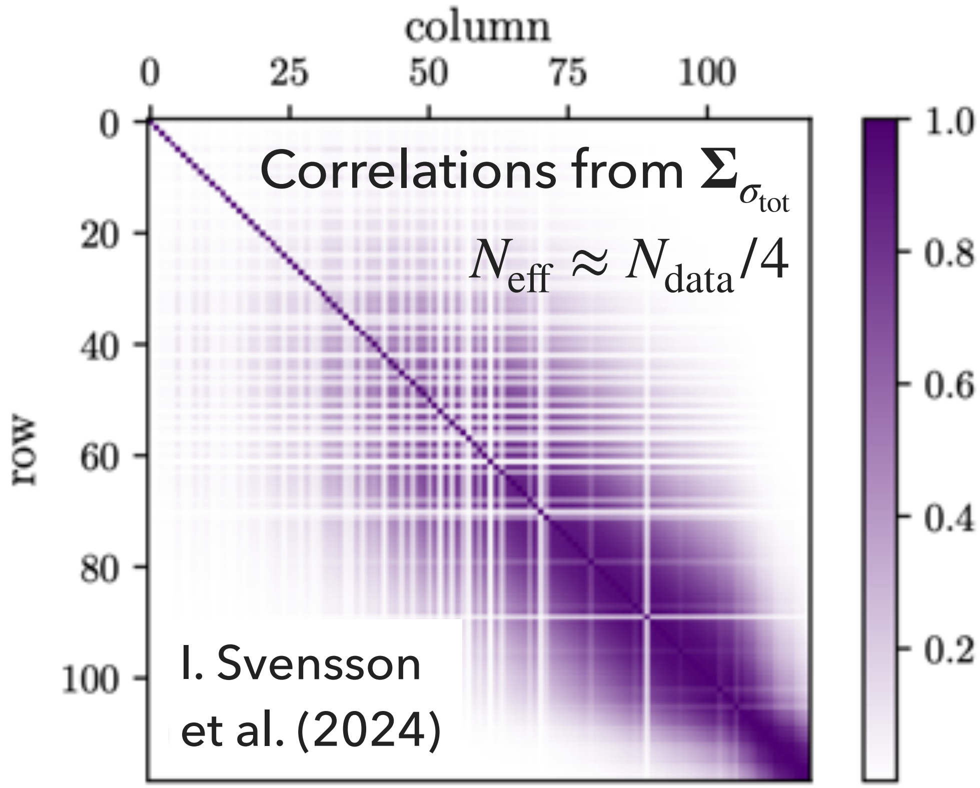

Correlations **within** observable type

EFT errors on scattering amplitude level

See B. McClung et al (2025)

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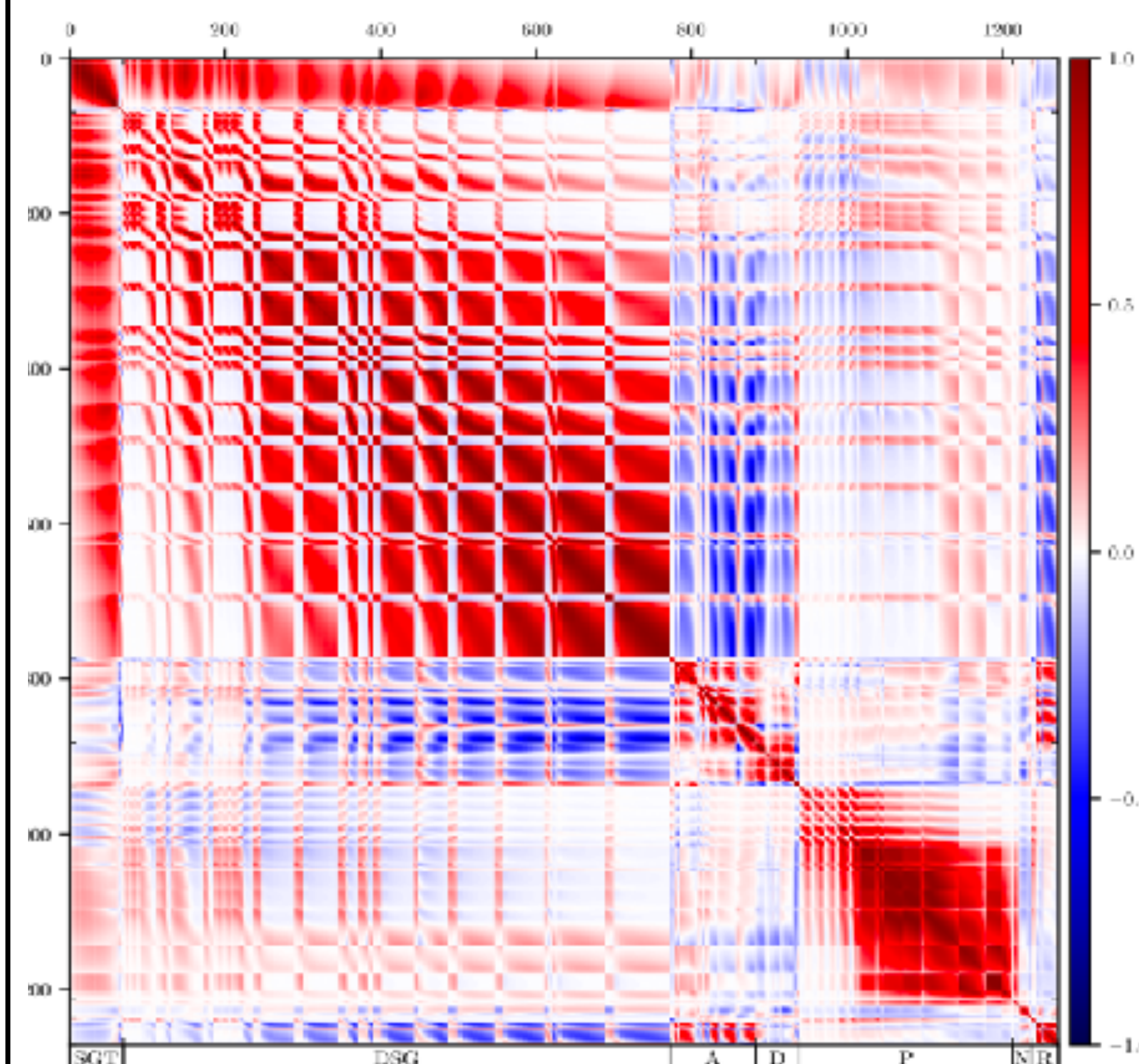
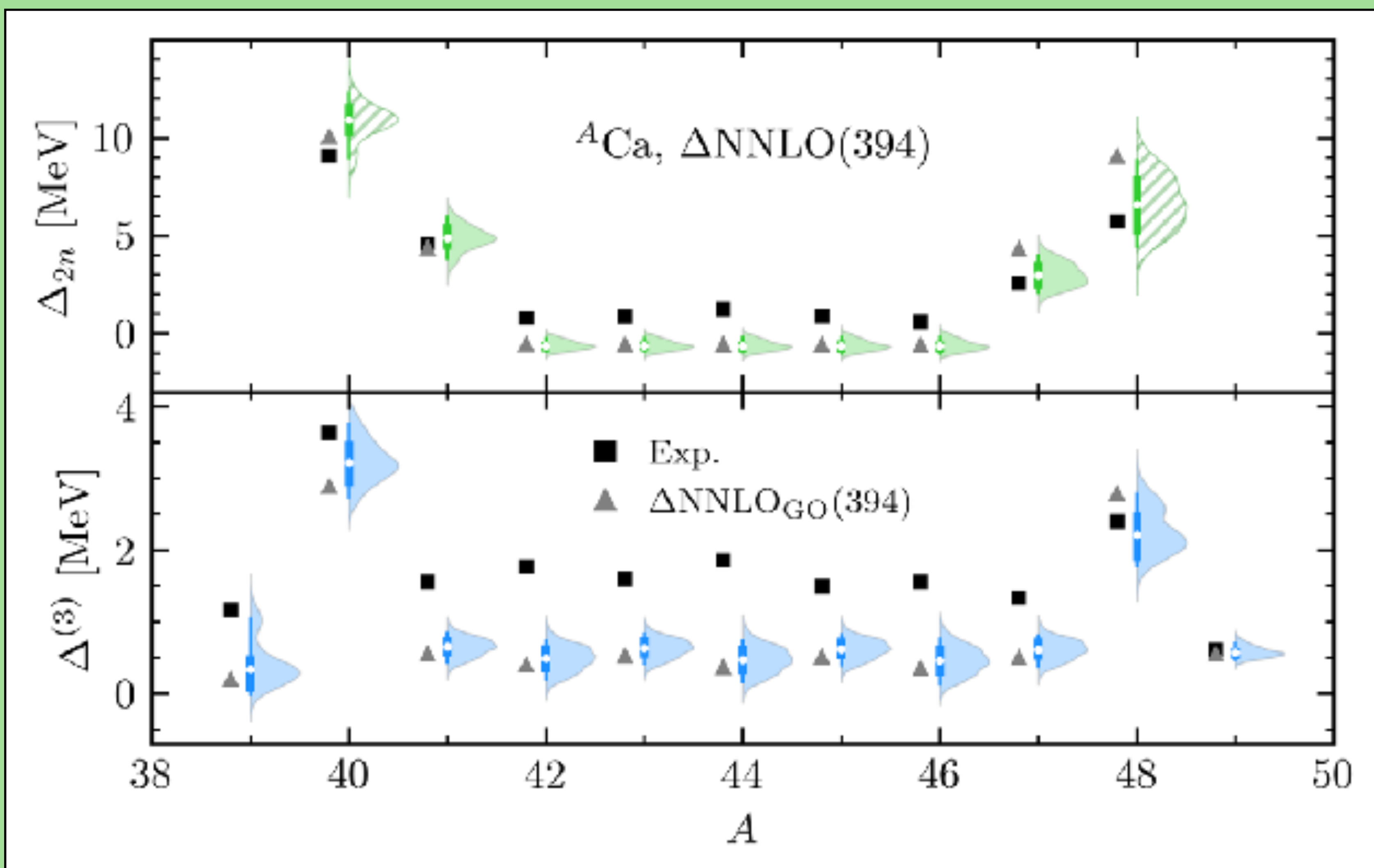


Correlations **between** observable types

Physics exploration

Scientific **tension** requires statements on **precision**

- Might reveal **missing physics**
- **Sensitivity analysis** and experimental design



Example: Superfluidity in calcium isotopes

- History matching allows model exploration using (relatively cheap) HFB.
- Importance resampling gives approximate posterior distribution.
- Tension reveals systematic error due to likely missing many-body correlations.

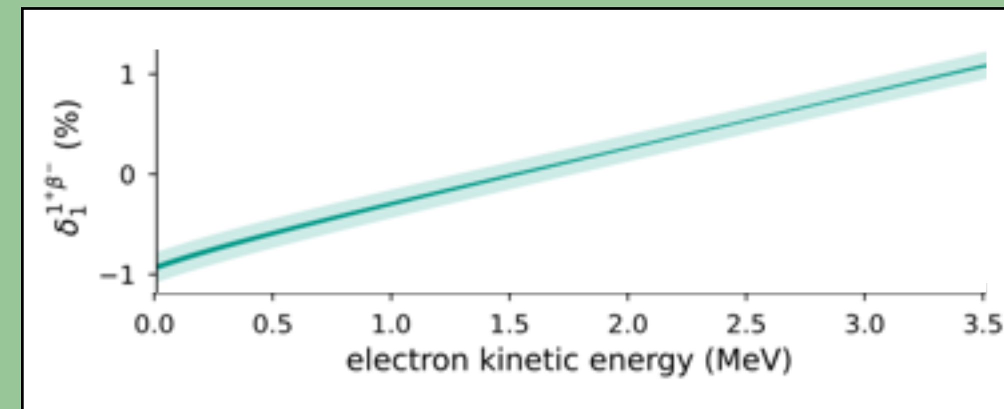
Alberto Scalesi, A. Ekström, cf, G. Hagen (2026)

Predictive modeling

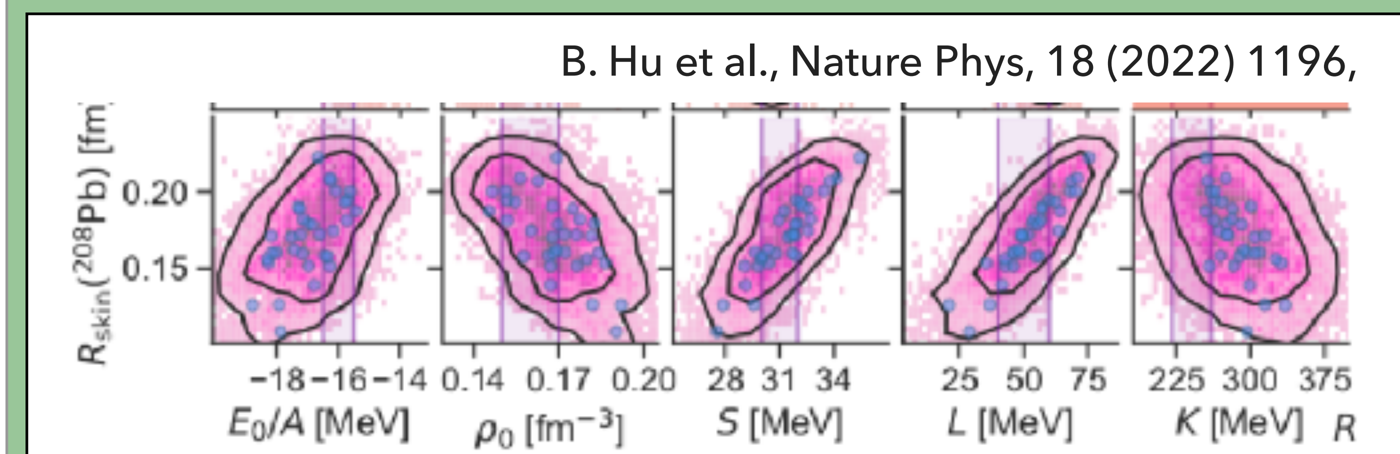
- Searches for **BSM physics** via high-precision beta decay

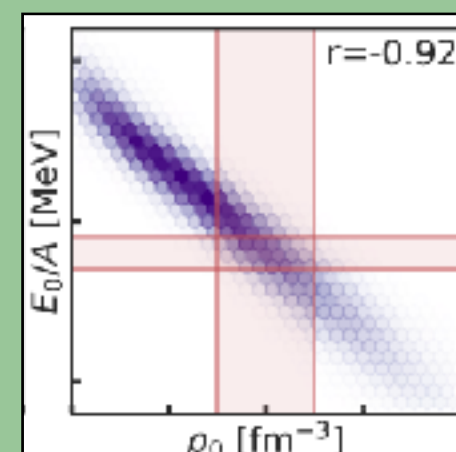
$$\frac{d\omega^{1^+\beta^-}}{dE\frac{d\Omega_k}{4\pi}\frac{d\Omega_\nu}{4\pi}} = \frac{4}{\pi^2}\left(E_0-E\right)^2 kEF^-\left(Z_f,E\right)C_{\mathrm{corr}}\left|\langle\|\hat{L}_1^A\|\rangle\right|^2 \times 3\left(1+\delta_1^{1^+\beta^-}\right)\left[1+a_{\beta\nu}^{1^+\beta^-}\vec{\beta}\cdot\hat{\nu}+b_{\mathrm{F}}^{1^+\beta^-}\frac{m_e}{E}\right],$$

A. Glick-Magid et al., PLB 832 (2022) 137259



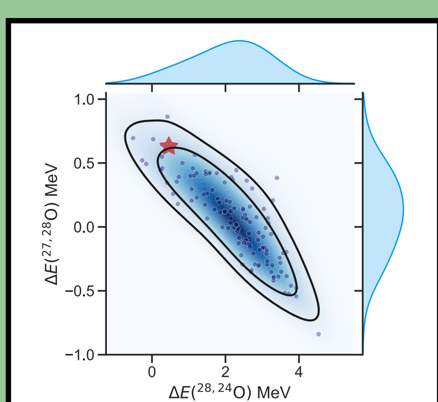
- **Extreme nuclear matter** modelling





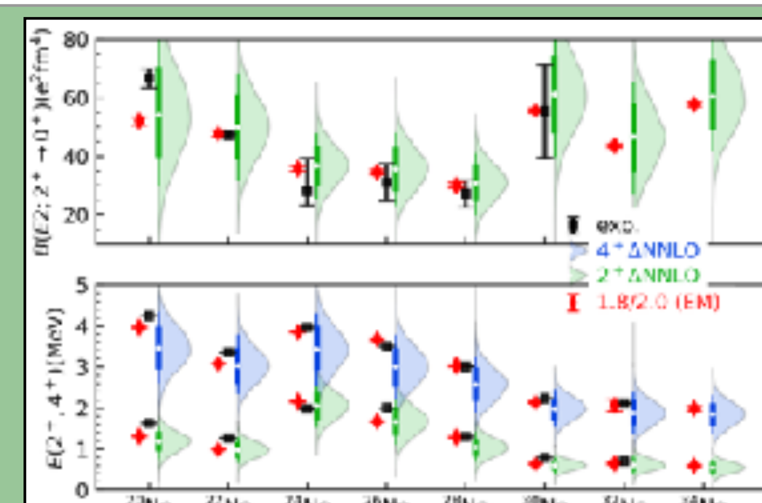
W. Jiang et al., PRC 109 (2024) L061302

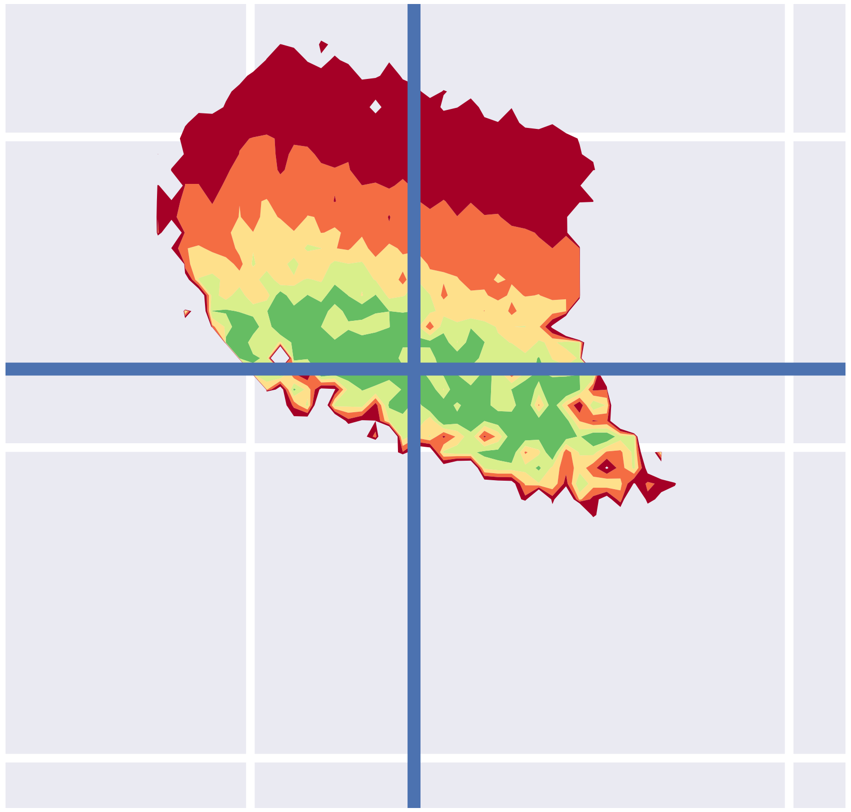
- Predictive modelling of **rare isotopes**



Y. Kondo et al., Nature 620, (2023), 965

Z. Sun et al.,
PRX 15, (2025) 011028,





Emergence of nuclear saturation

Nuclear-matter saturation and symmetry energy within Δ-full chiral effective field theory
by W.G. Jiang, cf, T. Djärv, G. Hagen, **109** (2024) L061302

Emulating ab initio computations of infinite nucleonic matter
by W.G. Jiang, cf, T. Djärv, G. Hagen, **109** (2024) 064314

Emergence of nuclear saturation within $\Delta-\chi$EFT

- χEFT **with explicit** Δ **isobar**.

- Extensive **error model**
(EFT truncation, method convergence, finite-size errors).

- **Iterative history-matching** for global parameter search. Study *ab initio* model performance, and provide a large ($>10^6$) number of non-implausible samples.
    - Implausibility criterion involves only $A \leq 4$ observables.

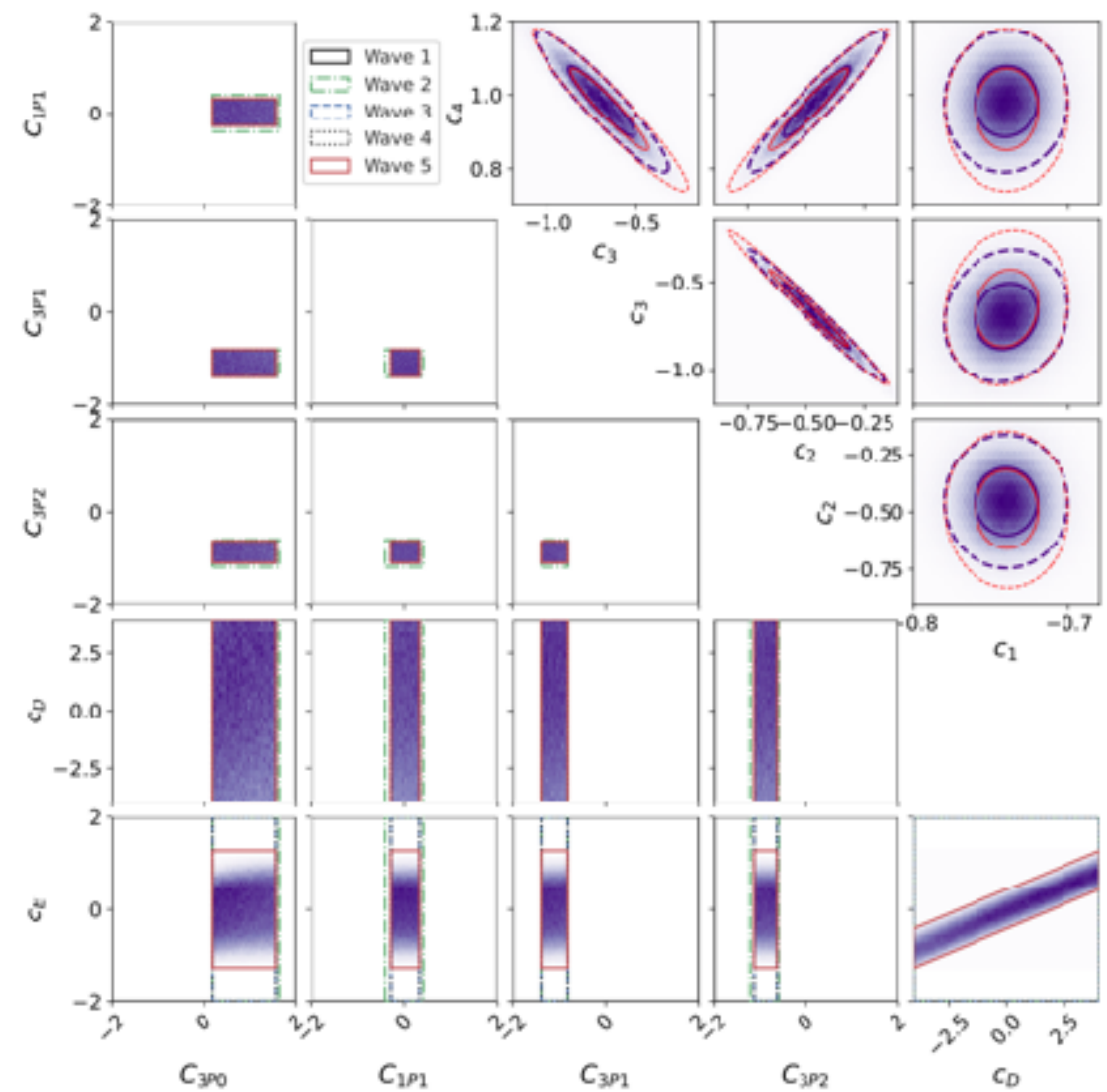
- Bayesian **posterior predictive** distributions for nuclear matter properties.
    - Importance resampling with two different data sets:
$\mathscr{D}_{A=2,3,4}$ and $\mathscr{D}_{A=2,3,4,16}$.

- Relies on sub-space projected coupled cluster (SP-CCD) **emulators** for infinite nuclear matter systems at different densities.

History matching waves

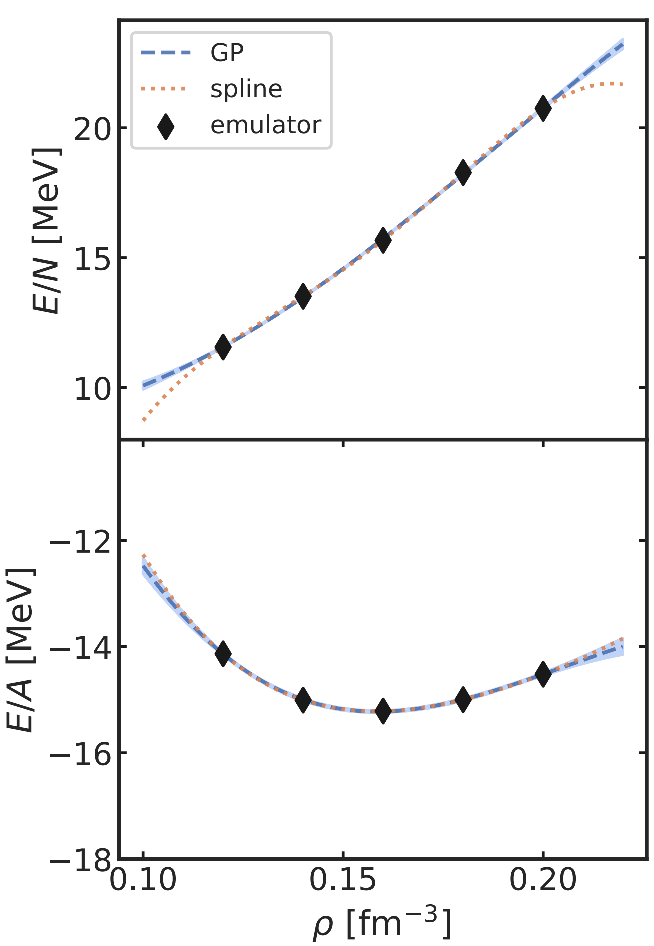
- np S- and P-wave phase shifts at T_{lab}=1, 5, 25, 50, 100, 200 MeV — [wave 1] & [wave 2] & final
- ^{2}H (E, R_p^2, Q), — [wave 3] & [wave 4] & final
- ^{3}H (E), ^{4}He (E, R_p^2) — [wave 4] & final
- Prior for c_1, c_2, c_3, c_4 from a Roy-Steiner analysis of πN data (Siemens 2017)

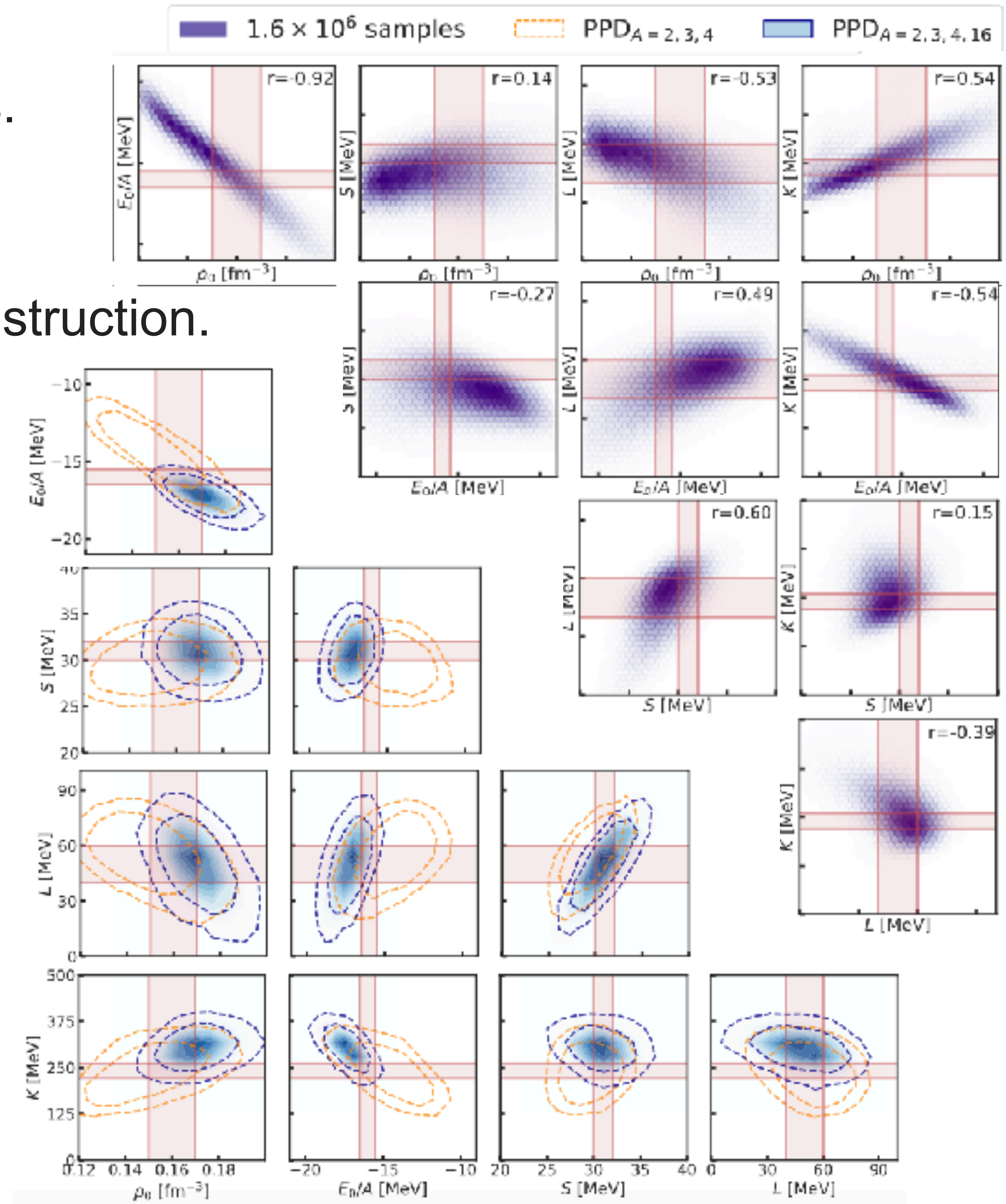
Observable	z	$\varepsilon_{\mathrm{exp}}$	$\varepsilon_{\mathrm{model}}$	$\varepsilon_{\mathrm{method}}$	$\varepsilon_{\mathrm{em}}$
$E(^2\mathrm{H})$	-2.2298	0.0	0.05	0.0005	0.001%
$r_p(^2\mathrm{H})$	1.976	0.0	0.005	0.0002	0.0005%
$Q(^2\mathrm{H})$	0.27	0.01	0.003	0.0005	0.001%
$E(^3\mathrm{H})$	-8.4818	0.0	0.17	0.0005	0.01%
$E(^4\mathrm{He})$	-28.2956	0.0	0.55	0.0005	0.01%
$r_p(^4\mathrm{He})$	1.455	0.0	0.016	0.0002	0.003%



Strategic training of NM emulator

- About 10,000 NI samples.
- Assign likelihood(s).
- Use 64 *most important* samples for emulator construction.
- Decreases errors during resampling,





Summary and outlook

- *The concept of* **tension in science** *relies on statements of uncertainties*
- It is natural to strive for **accuracy** in theoretical modeling; but actual predictive power is more associated with quantified **precision**.
- *Ab initio* methods + χEFT + Bayesian statistical methods in combination with fast & accurate emulators is enabling **precision nuclear theory**.
- Focusing on UQ, my outlook relating to "**Current limitations of nuclear Hamiltonians**" is
  - **Extend the range** of ab initio modeling and emulation; identify **failures** beyond quantified errors. *−benchmarks of different methods and truncation schemes are important.*
  - Make posterior predictions for **high-dimensional models** conditioned on many outputs *−must understand correlation structures of EFT errors.*
  - **Foundational challenge**: Understand EFT convergence to quantify truncation errors. *—revisit leading (and subleading) orders of χEFT, RG invariance, and error models.* *—perform order-by-order Bayesian inference at multiple cutoff values.*