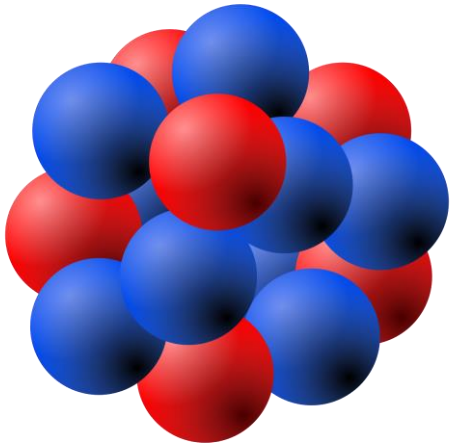
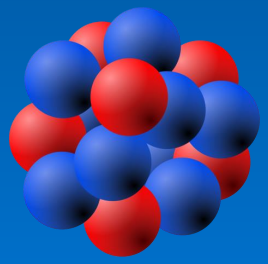
Outline

- Motivation
- History matching
- Nuclear matter emulator
- Non-implausible predictions
- Bayesian inference



Linking finite nuclei with nuclear matter through nuclear forces



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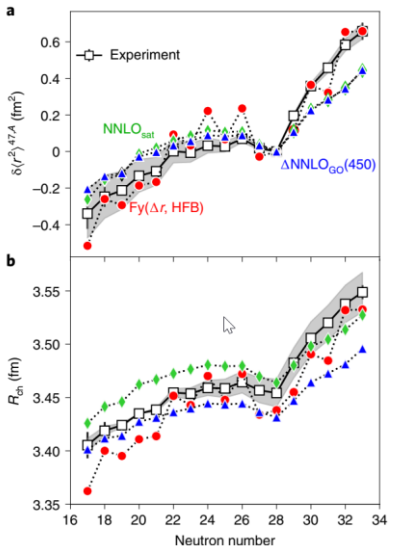
Nucleonic systems linked by nuclear forces

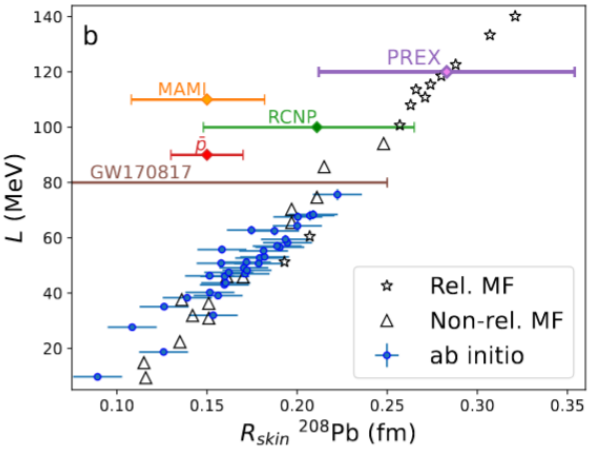
- Precision test of Standard Model (SM) and beyond

High precision experiments, accurate theoretical predictions with quantified uncertainties

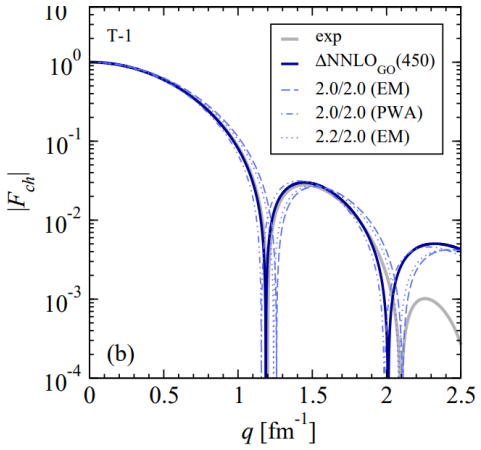
- What can the theoretical nuclear structure study provide?



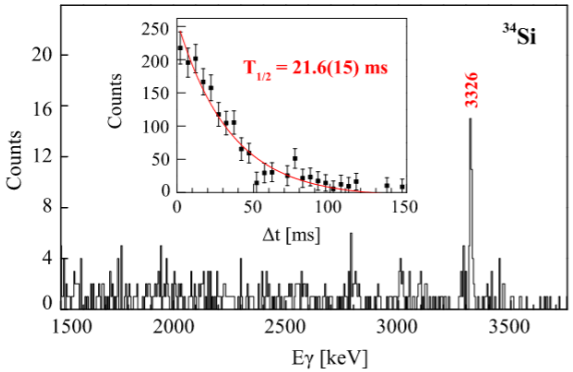
radii



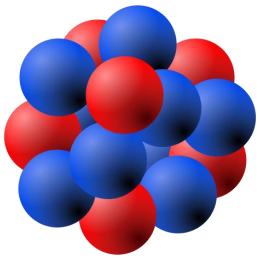
neutron skin thickness

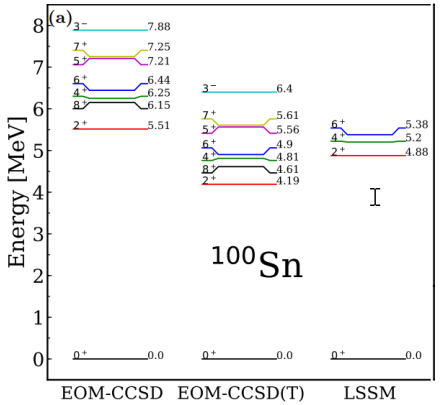


form factors



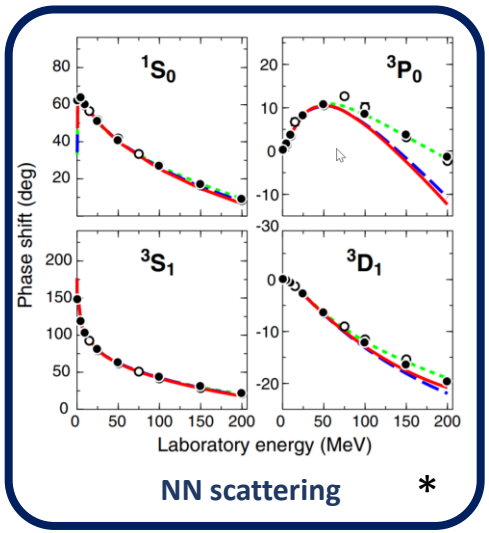
transition probability, half-life



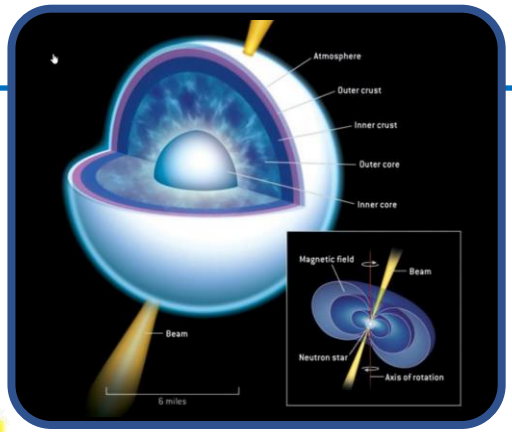


spectra

Nucleonic systems linked by nuclear forces



NN scattering *



neutron star

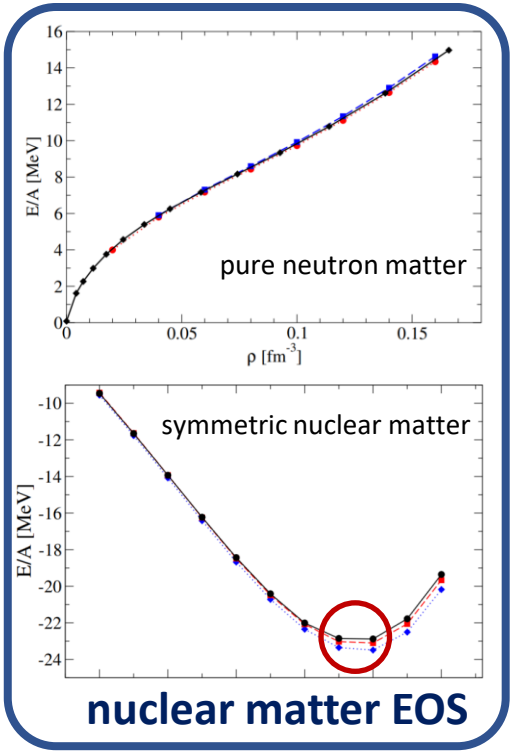
Z

N

NN scattering

Few-body sector

from few-body sector to many-body systems



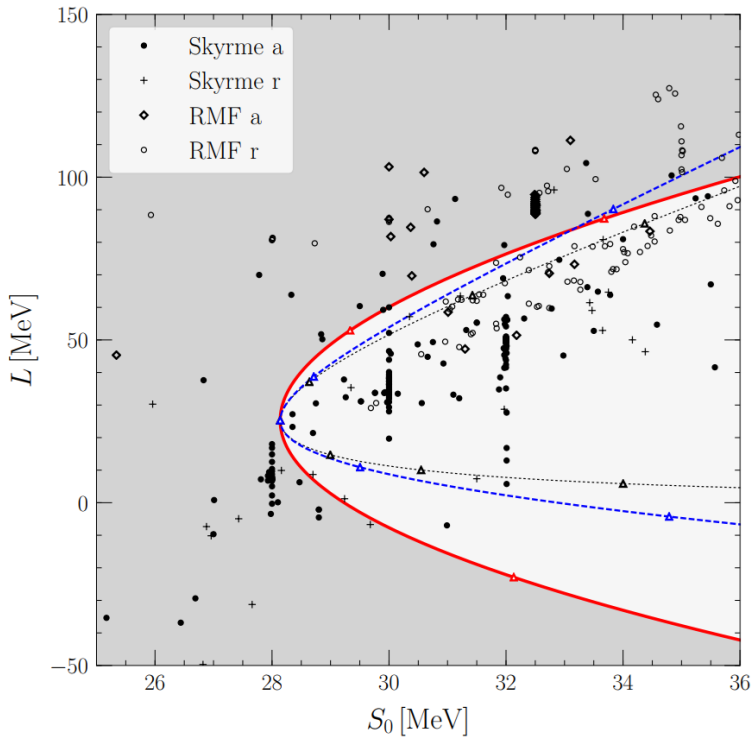
nuclear matter EOS

* A. Ekström, G. Baardsen, C. Forssén, G. Hagen, M. Hjorth-Jensen, et al. Phys. Rev. Lett. 110, 192502 (2013).

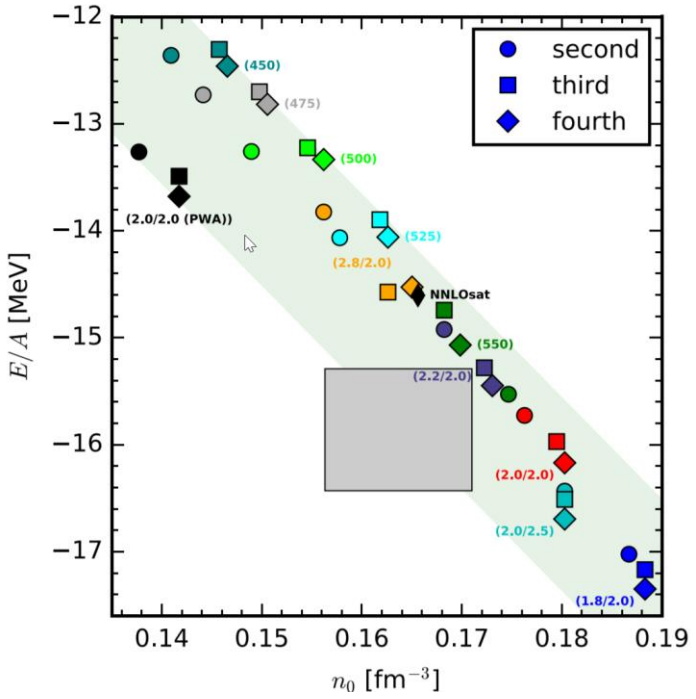
Interaction models

- Phenomenological interactions (like Skyrme and Gogny) with density functional theory (DFT)
- Realistic interaction models based on chiral effective field theory (EFT) combined with ab initio many-body methods

Complex interaction model, limited calibration data → risk of overfitting



Different mean field potentials *

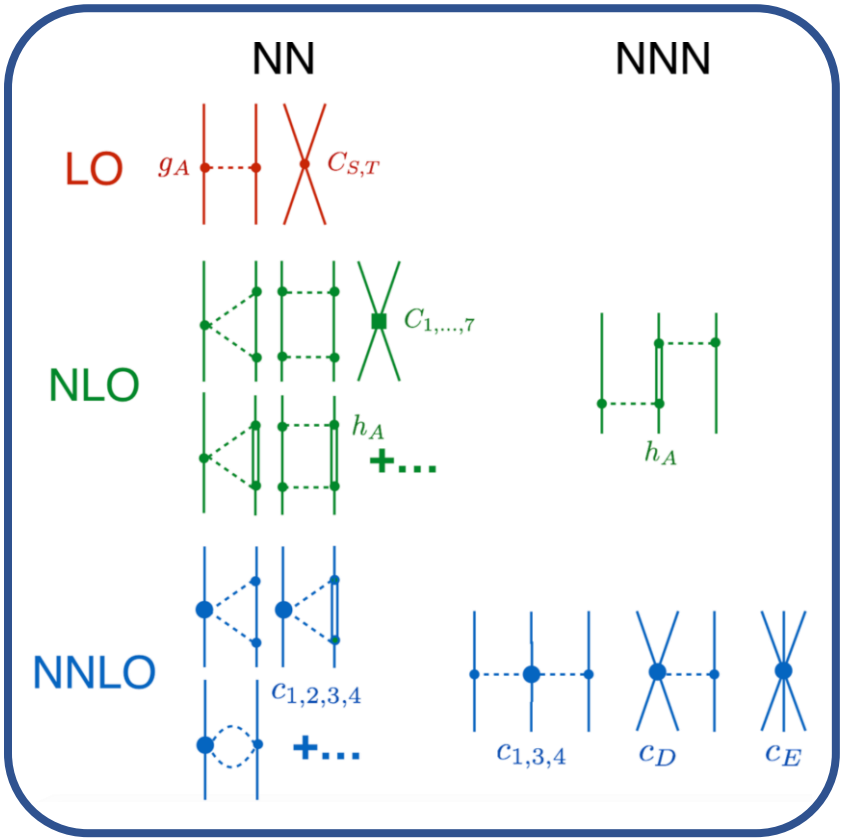


Different chiral potentials **

*Tews, Ingo, et al. "Symmetry parameter constraints from a lower bound on neutron-matter energy.", The Astrophysical Journal 848.2 (2017)

** C. Drischler, K. Hebeler, and A. Schwenk, "Chiral interactions up to next-to-next-to-next-to-leading order and nuclear saturation," Phys. Rev. Lett. 122, 042501 (2019).

Delta-full chiral EFT



- explicit inclusion of Δ-isobar
- Δ couples strongly to the πN system.
- $\delta M \equiv M_\Delta - M_N \approx 293\text{MeV}$
- roughly twice the pion mass (M_π)
- With **17** parameters (low energy constants) at NNLO

Increases EFT breakdown scale

***ab initio* many-body methods**

A-scaling

exponential : no-core shell model (NCSM)

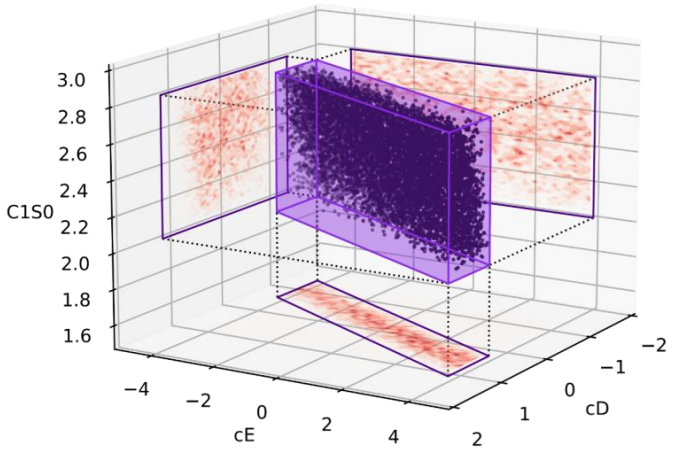
polynomial : Coupled-cluster method (CC)

Chiral interactions are parameterized by low energy constant (LECs)

S. Weinberg, R. Machleidt, V. Bernard, E. Epelbaum, U. van Kolck, U.G. Meißner, *et al.*

Linking models to reality

- A robust statistical approach known as iterative history matching*
- Philosophy: removing implausible parameter domains iteratively
- Enabling technology: fast emulators for predicting many-body observables



different parameterization of interaction samples

implausibility measure

non-implausible samples 😎

implausible samples

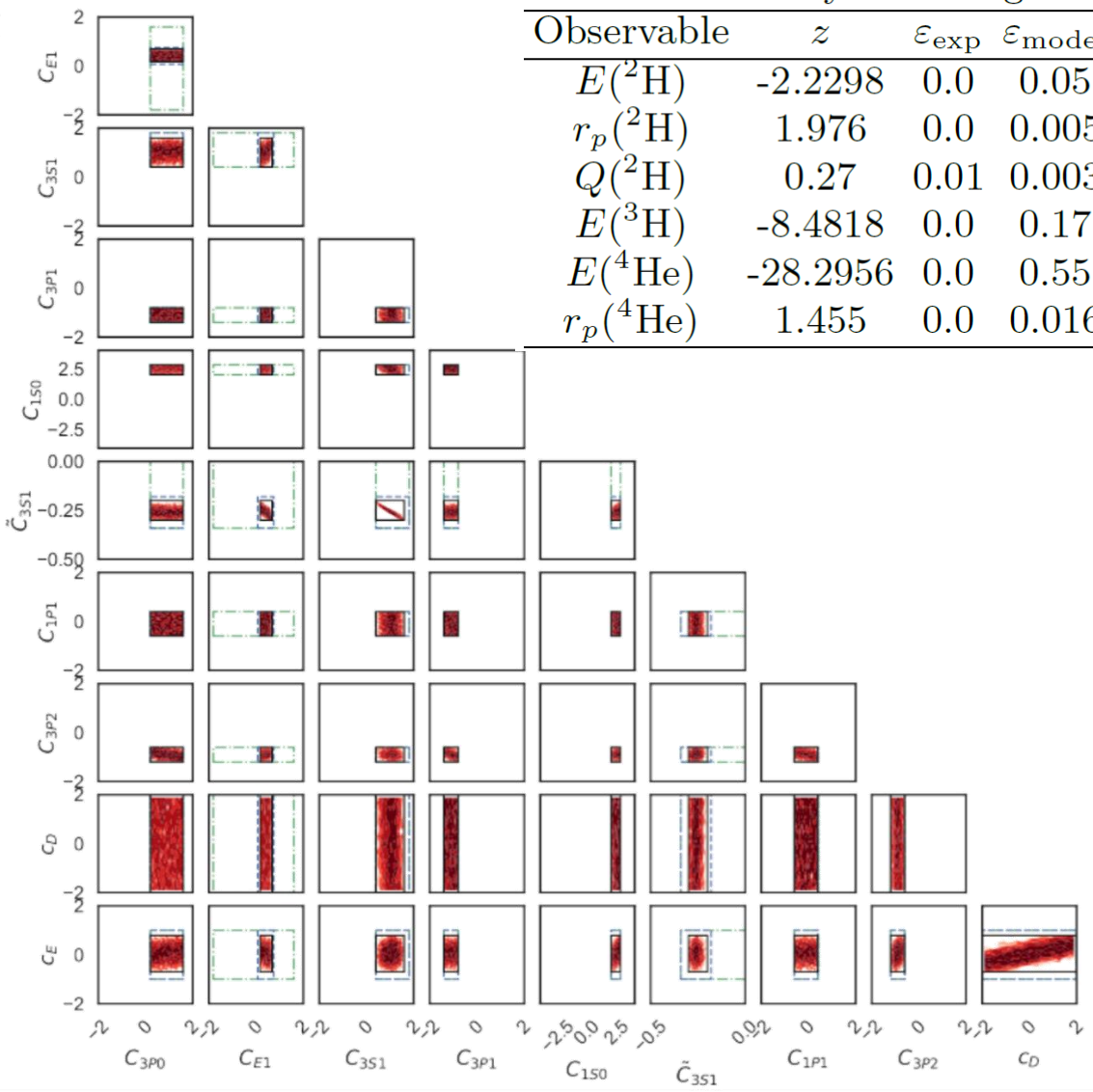
reality | theoretical predictions | experimental errors | theoretical errors

$$y = y_{\mathrm{th}}(\theta) + \varepsilon_{\mathrm{exp}} + \varepsilon_{\mathrm{model}} + \varepsilon_{\mathrm{method}} + \varepsilon_{\mathrm{emu}}$$

*Vernon, I., Goldstein, M. , Bower, R. Statist. Sci. 29, 81 (2014).
Edwards, T.L., Brandon, M.A., Durand, G. *et al. Nature* **566,** 58–64 (2019). B. S. Hu*, *et al*. arXiv:2112.01125

History matching

a



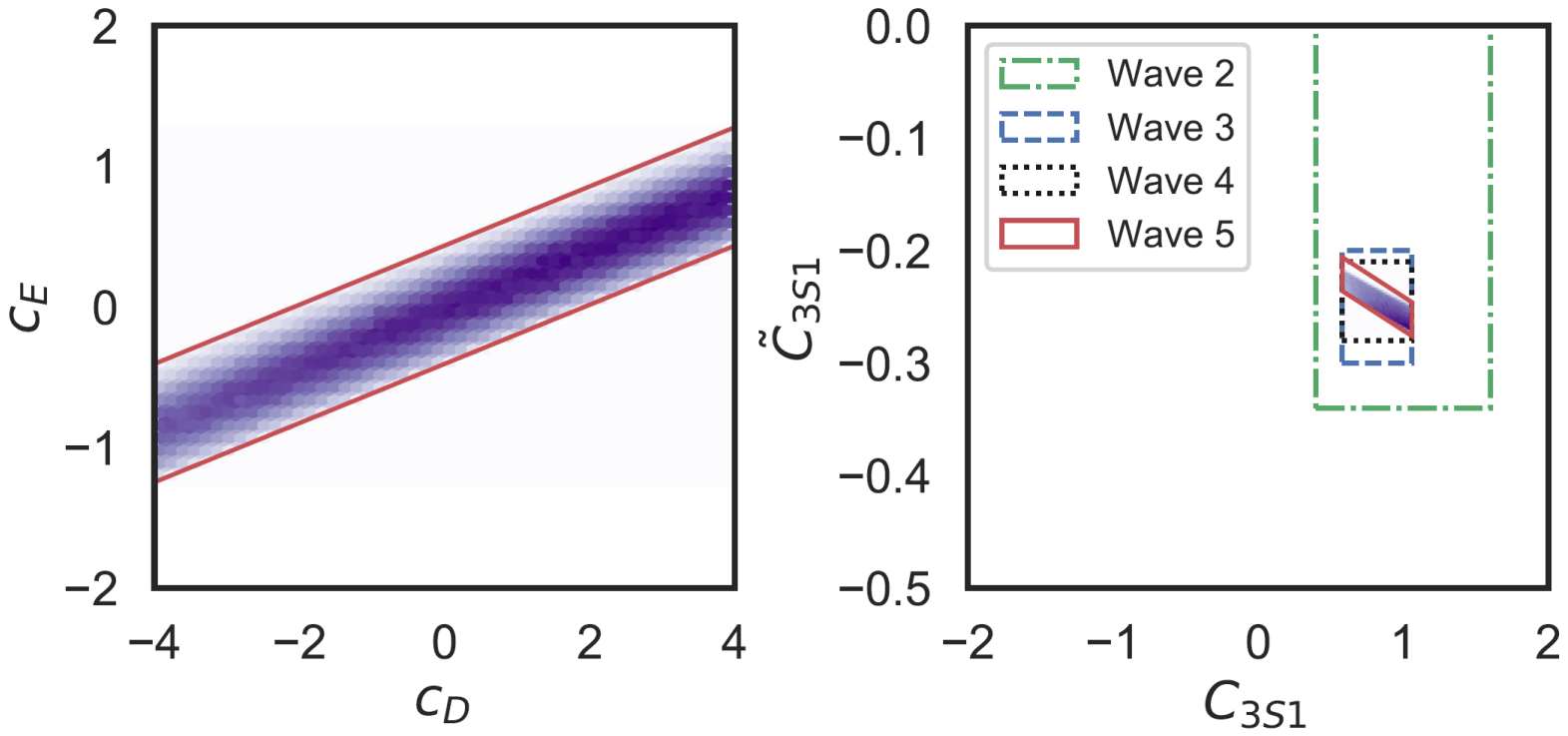
History-matching observables

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

- waves 1 and 2: nucleon-nucleon scattering phase shifts up to laboratory energy of 200 MeV
- waves 3: energy, radius, and quadrupole moment of ^{2}H
- waves 4 and 5: the energies and radii of ^{2}H, ^{3}H, and ^{4}He

History matching

- strongly correlated LEC pairs
- parameter domain reduced by a factor of 10^7
- Only linear combination of contact 3NFs LECs c_D and c_E are constrained by ^{3}H, ^{4}He binding energies and radii

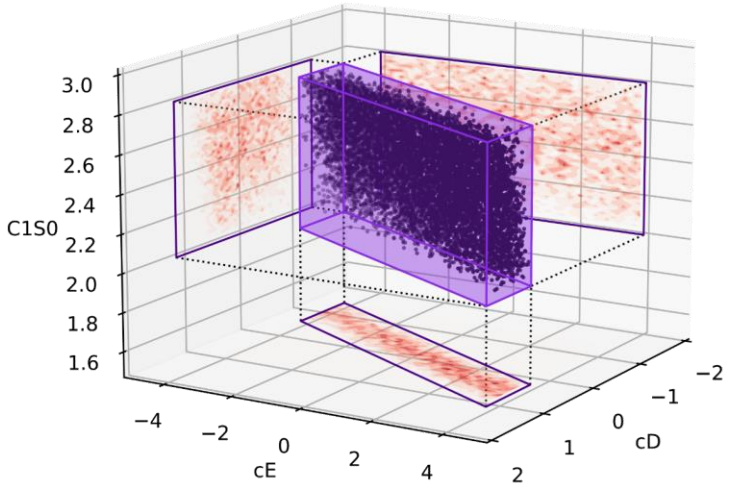


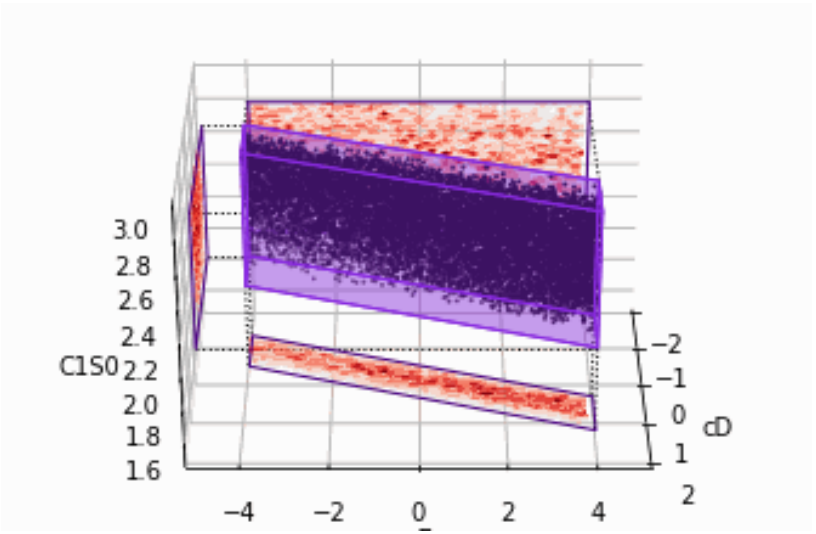
History matching

- Visualization of the history matching procedure in the projected 3D LECs space.

- All non-implausible samples are held within the NI domain. We found no disconnected regions outside.

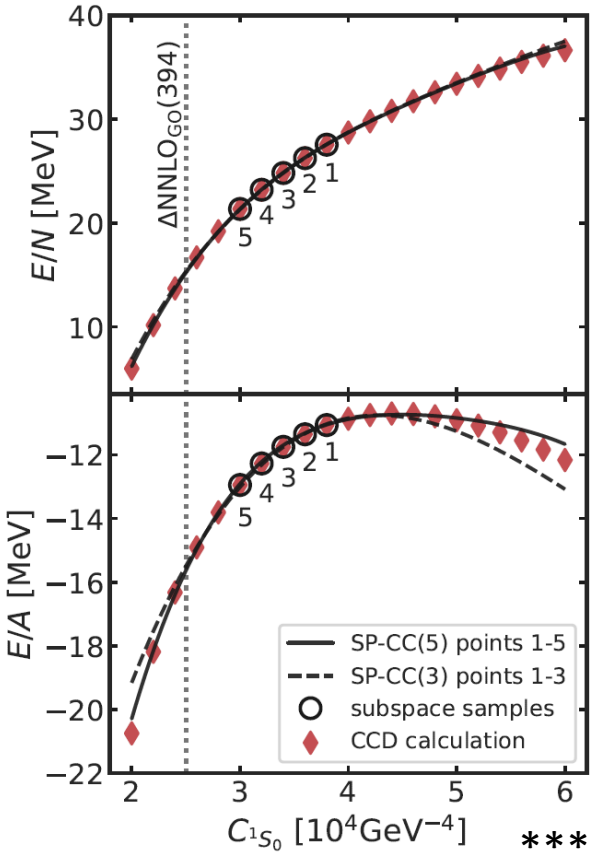
- This domain can not be further reduced by more HM iterations.





Emulators for many-body observables

- Eigenvector continuation*: accurate emulation of many-body observables with enormous speedup
- Subspace-projected coupled-cluster (SPCC)**, non-Hermitian Hamiltonian
- a new algorithm: small-batch voting to cure the spurious state problem
- Allowed us to construct emulators for nuclear matter observables

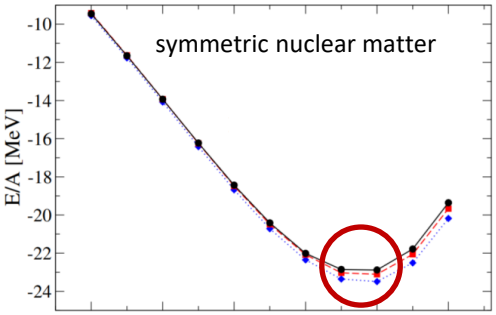


- eg: symmetric nuclear matter (full CCD ~200 CPU-hour) vs (emulator ~2ms)
- Emulator enables 10^6 — 10^8 times acceleration

*D. Frame, R. He, I. Ipsen, D. Lee, D. Lee, and E. Rrapaj, Phys. Rev. Lett. 121, 032501 (2018)
**A. Ekström and G. Hagen, Phys. Rev. Lett. 123, 252501 (2019)

***Exploring non-implausible nuclear-matter predictions with delta-full chiral interactions, W. G. Jiang, et al (in Preparation)

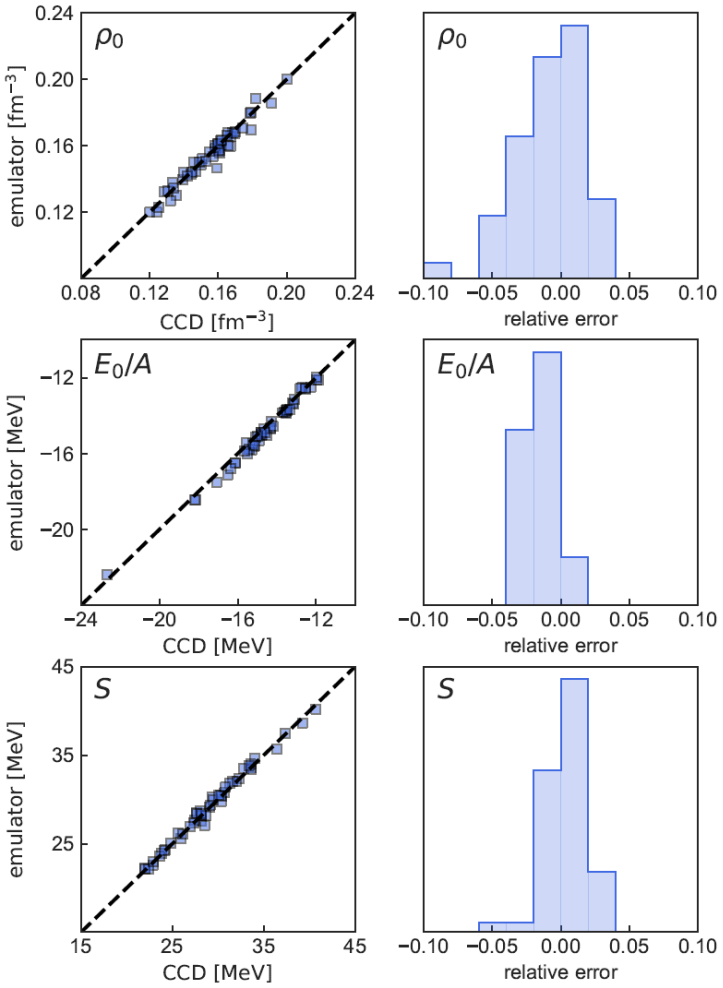
Nuclear matter emulator



saturation properties

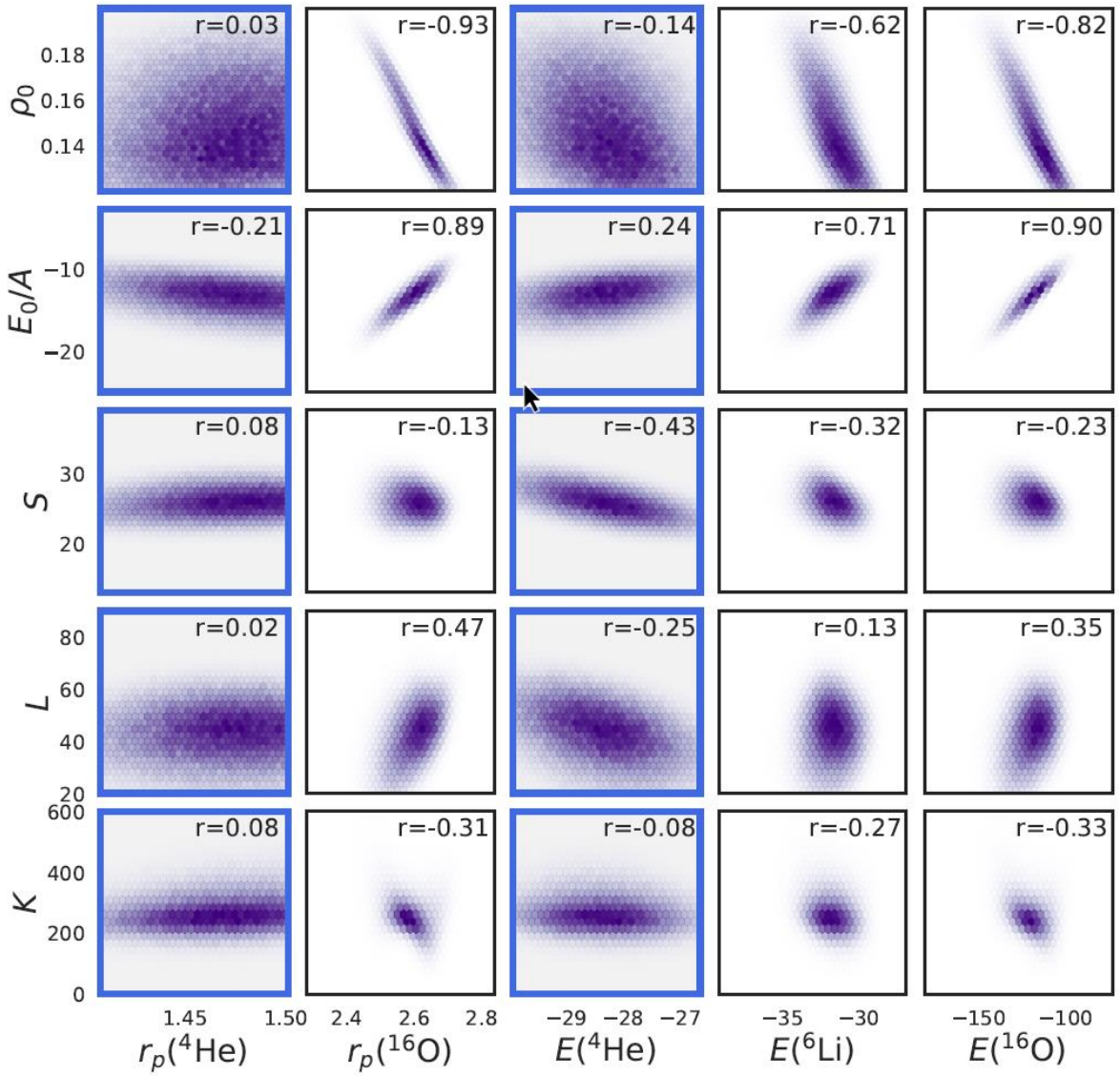
- Target nuclear matter saturation properties:
- Saturation density ρ_0
- Saturation energy E_0/A
- Symmetry energy *S*

- Others: Slope *L,* Incompressibility *K*



Emulator validation

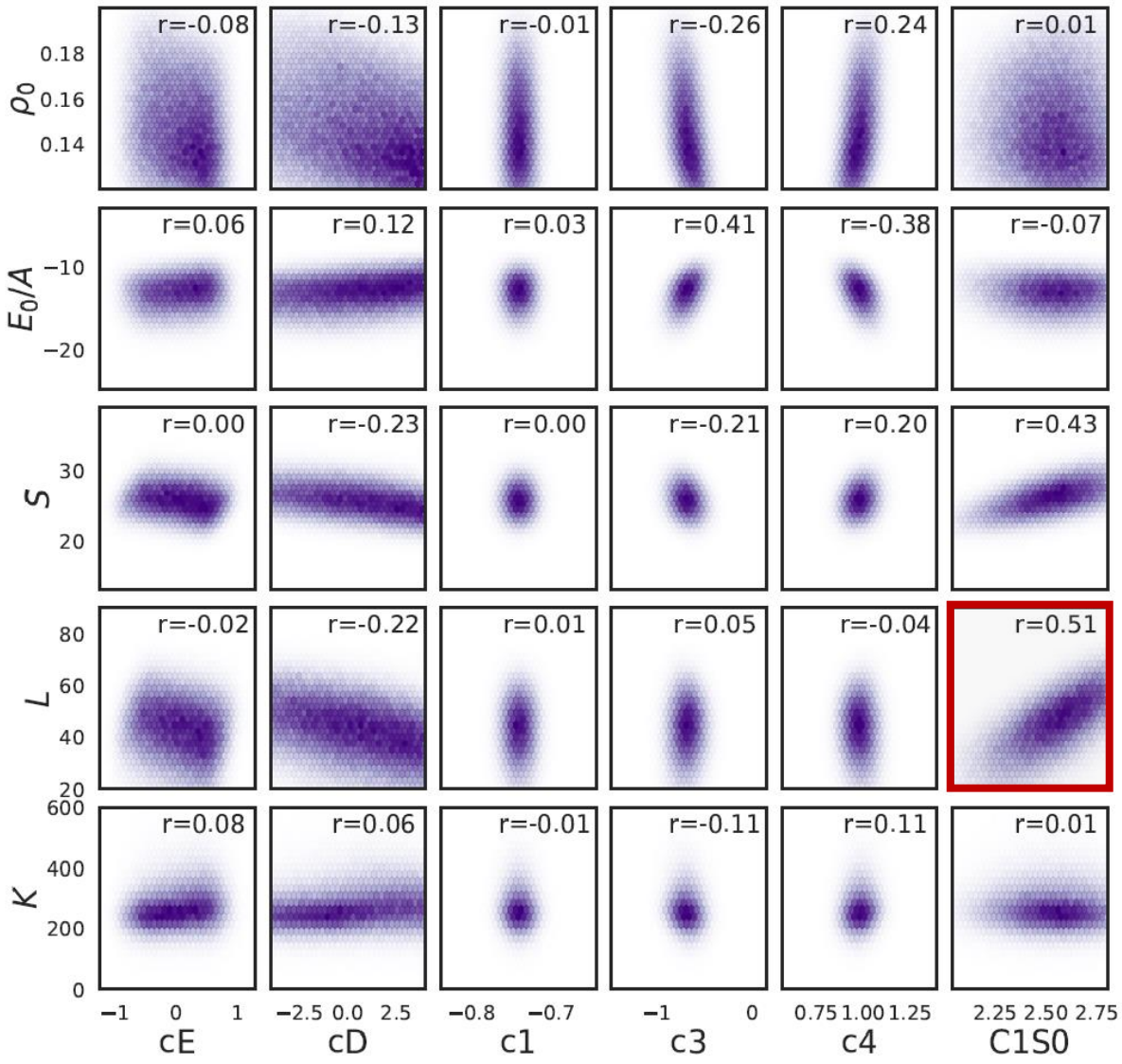
Non-implausible predictions of DNNLO

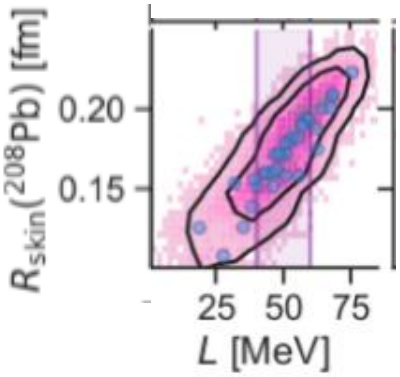


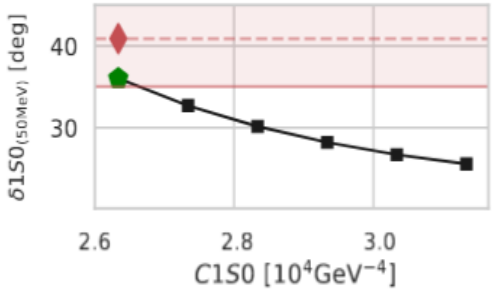
- Correlation structure between NM saturation properties and selected finite nuclei observables for 1.6 $\times 10^6$ non-implausible interactions.
- Note that only ^{6}Li and ^{16}O observables are predictions.
- Strong correlation between ^{16}O and NM observable.
- The correlation structure is determined by the design of the interaction model.

Non-implausible predictions of DNNLO

scattering phase shift ← → LECs ← → neutron skin







B. S. Hu*, *et al*. arXiv:2112.01125

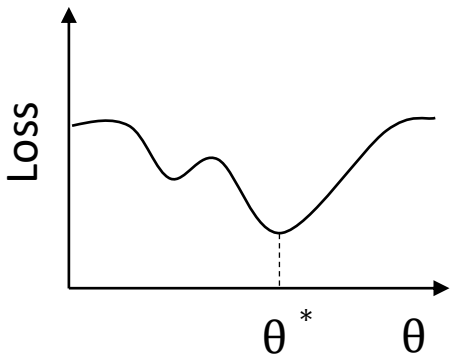
Bayesian Inference

Optimization

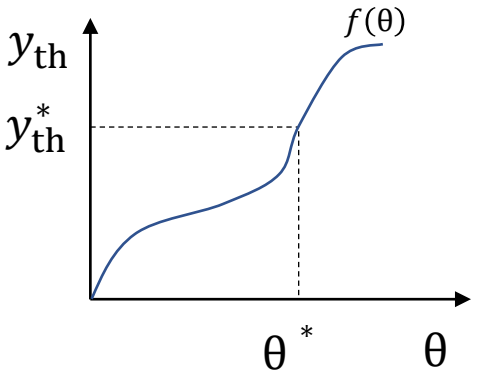
Loss function: χ^2

$$\chi^2=\sum_i^n \frac{(O_i^{\text{th}}(\theta)-O_i^{\text{exp}})^2}{\sigma_i^2}$$

Minimize the loss function



give one prediction for target observable

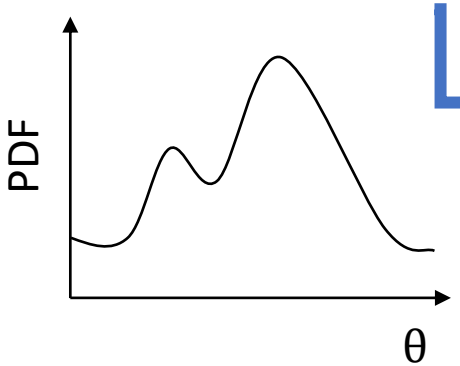


$y_{\text{th}} = f(\theta)$, expectation value of the target observable

Bayesian Inference

posterior probability density function (PDF) of θ

$$\text{PDF} = \text{pr}(\theta \mid \mathfrak{D}) \propto L(\mathfrak{D} \mid \theta)\,\text{pr}(\theta)$$



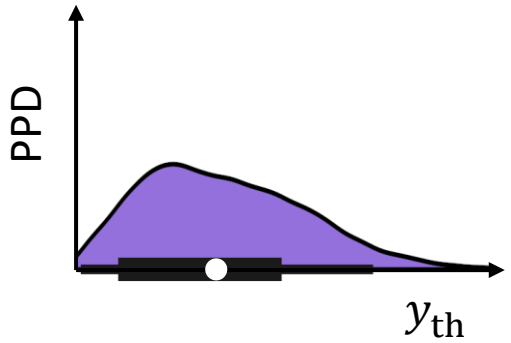
likelihood function:
e.g. non-correlated Gaussian

$$L=\exp\left(-\sum_i^n \frac{(O_i^{\text{th}}(\theta)-O_i^{\text{exp}})^2}{\sigma_i^2}\right) \cdot \prod_i^n \left(\frac{1}{2\pi\sigma_i^2}\right)^{1/2}$$

Generate the model prediction computed over likely values of θ drawn from its PDF, sampling is usually needed

$$\text{PPD} = \{y_{\text{th}}(\theta) : \theta \sim \text{pr}(\theta \mid \mathfrak{D})\}$$

posterior predictive distribution (PPD)



Probabilistic distributions of predictions

Calibration observables

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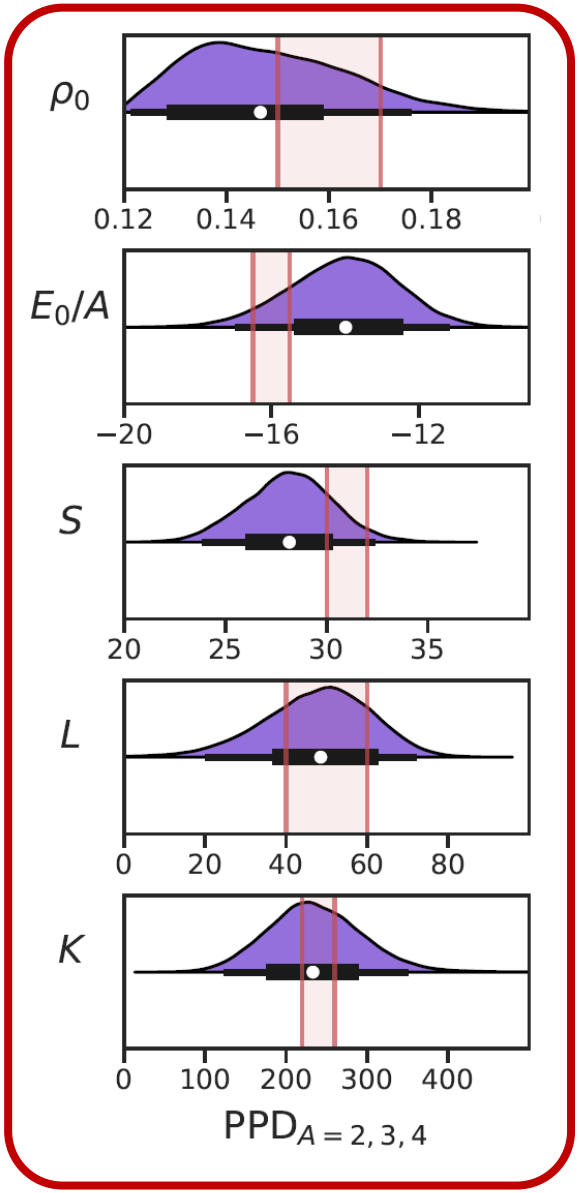
$r_p(^4\text{He})$	1.455	0.0	0.016	0.0002	0.003%

- Non-implausible interactions are calibrated with $\mathfrak{D}_{A=2,3,4}$
- ρ_0, E_0/A and S for $\text{PPD}_{A=2,3,4}$ deviate significantly from the empirical region.
- Significant asymmetry in ρ_0 directions, hints of a bimodality.



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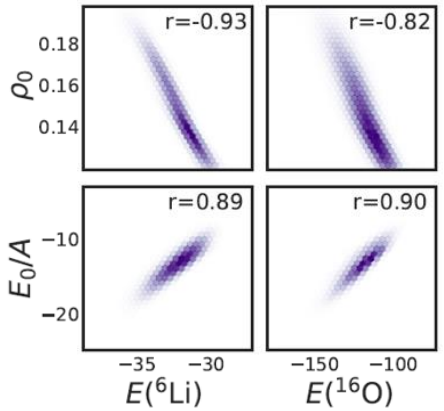
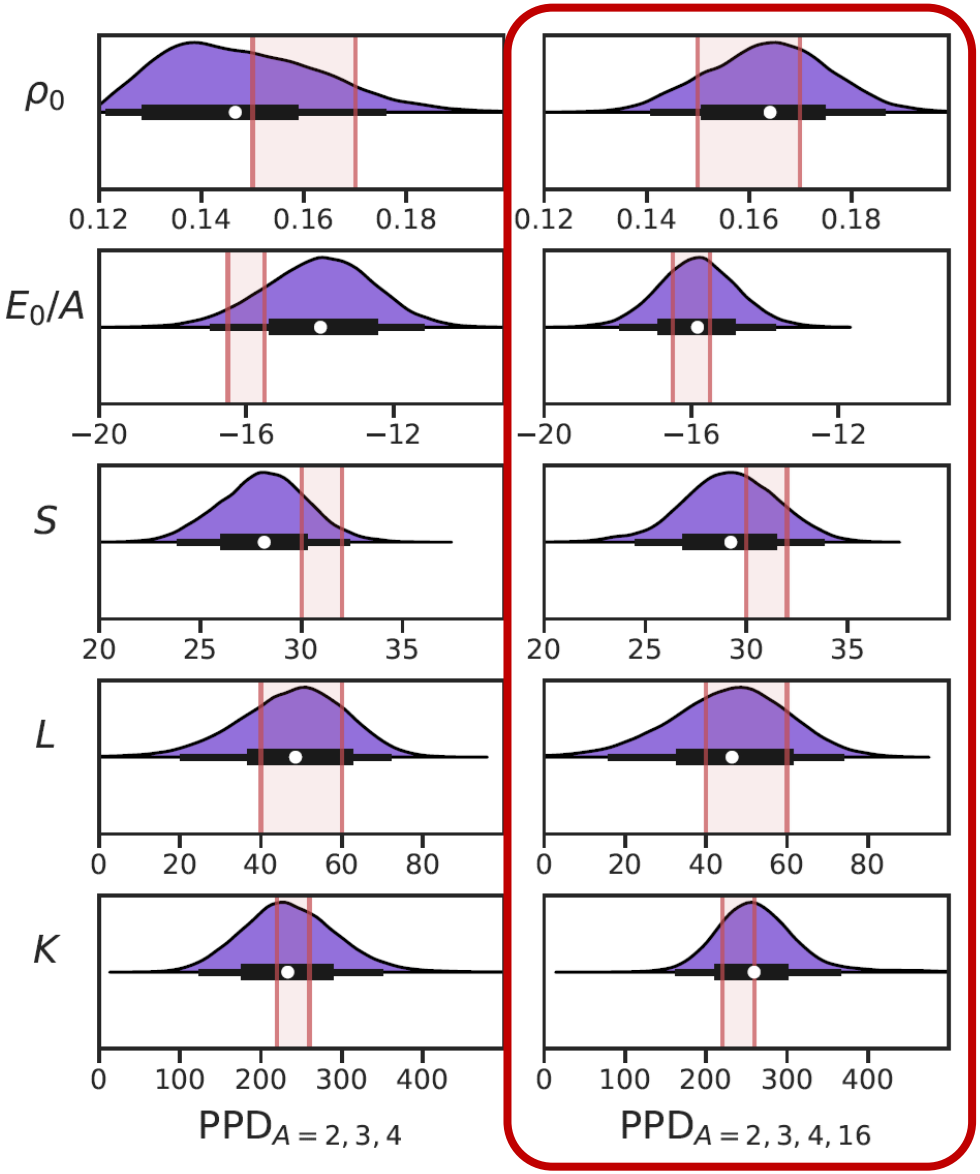
$r_p(^4\text{He})$	1.455	0.0	0.016	0.0002	0.003%
$E(^{16}\text{O})$	-127.62	0.0	1.00	0.75	0.5%
$r_p(^{16}\text{O})$	2.58	0.0	0.03	0.01	0.5%

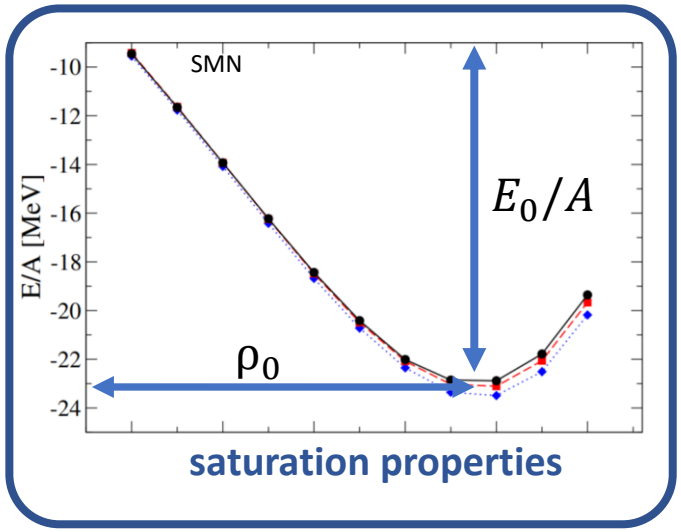
- Non-implausible interactions are calibrated with $\mathcal{D}_{A=2,3,4,16}$
- The correlation structure provides important constraints

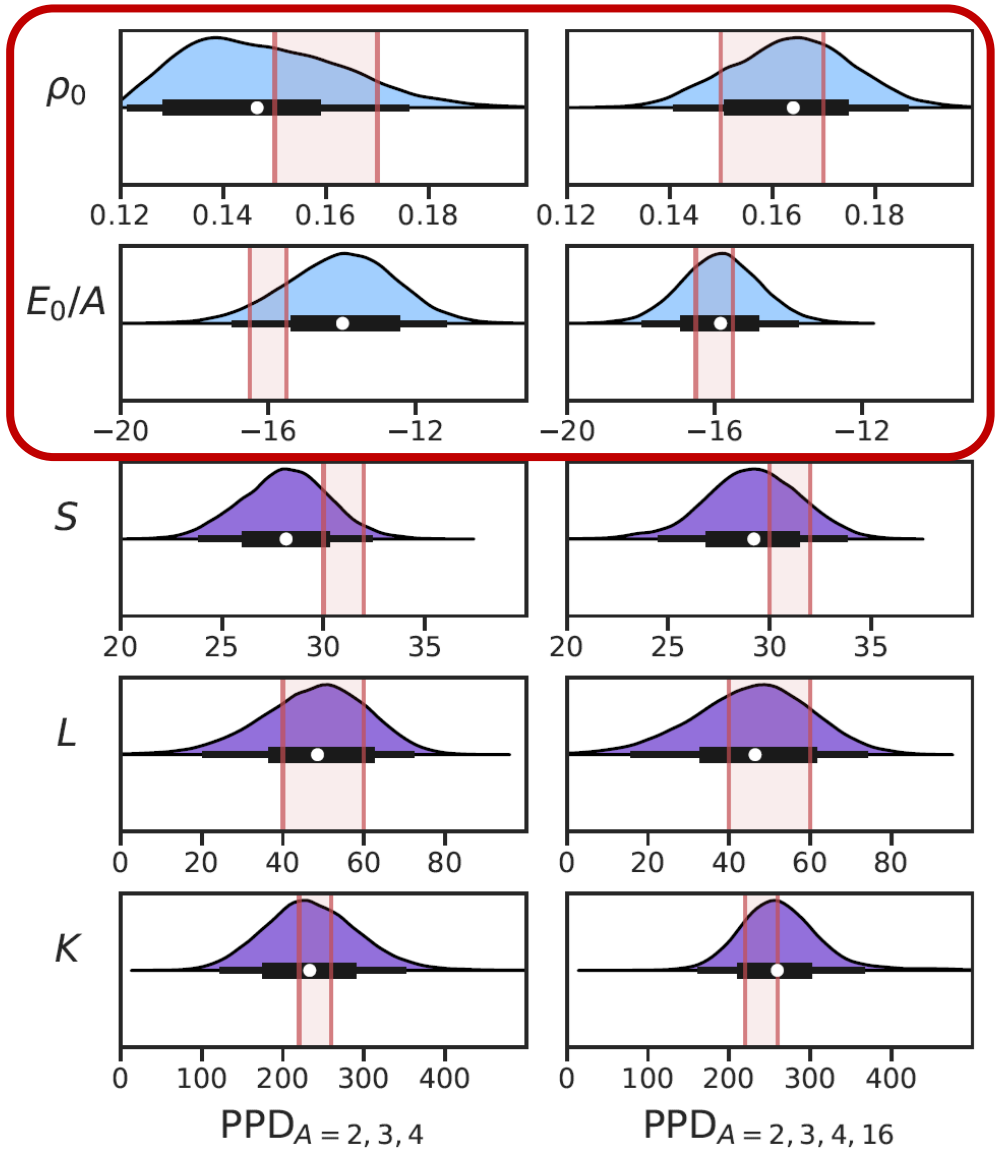




Comparison of two PPDs generated by sampling over two different PDFs of the LECs

Probabilistic distributions of predictions





- Position and shape of the mode can be altered depending on the choice of calibration observables.

- Samples from the tail region of $\mathrm{PPD}_{A=2,3,4}$ correspond largely to the mode of $\mathrm{PPD}_{A=2,3,4,16}$.

Comparison of two PPDs generated by sampling over two different PDFs of the LECs

Bayesian machine learning error model

- Prediction of each interaction consist of:

Theoretical predictions	emulator predictions	truncation errors	CC method errors	emulator errors

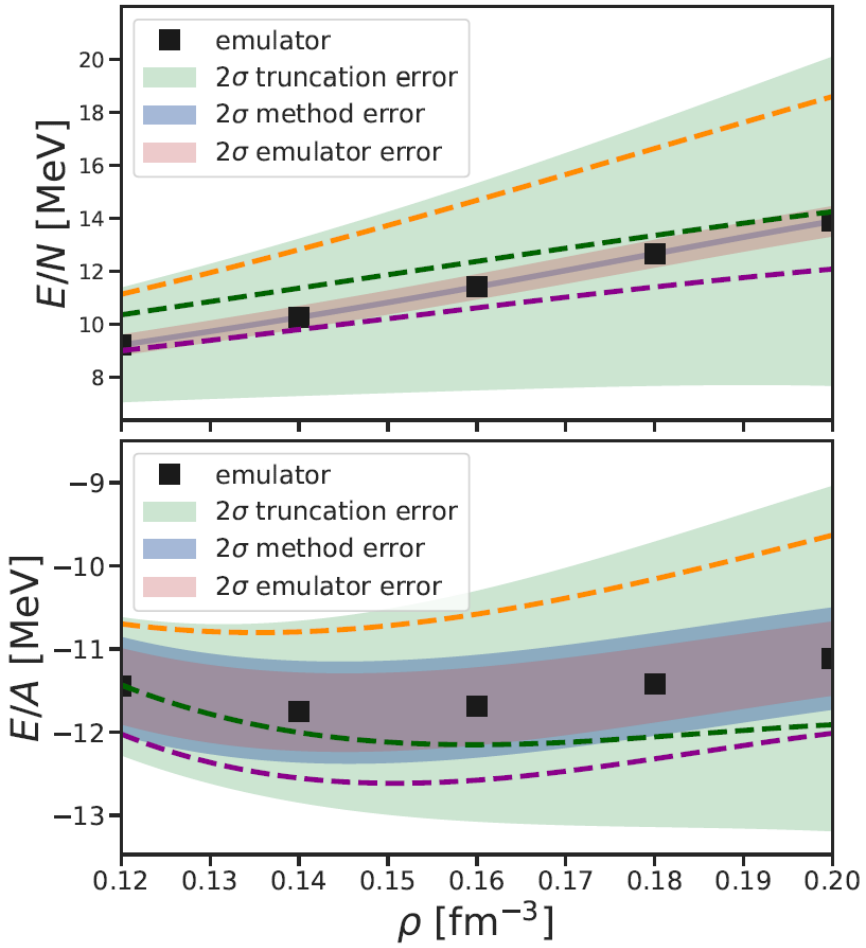
$$y = y_k(\rho) + \varepsilon_k(\rho) + \varepsilon_{\text{method}}(\rho) + \varepsilon_{\text{emu}}(\rho)$$

- Multitask Gaussian processes are trained to describe the distribution of different sources of errors

$$\varepsilon_k(\rho) \mid \bar{c}^2, l, Q \sim GP[0, \bar{c}^2 R_{\varepsilon_k}(\rho, \rho'; l)]$$

- Correlations between PNM and SNM truncation errors

$$\begin{bmatrix} \varepsilon_{k,\text{pnm}} \\ \varepsilon_{k,\text{snm}} \end{bmatrix} \sim N\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} \right)$$

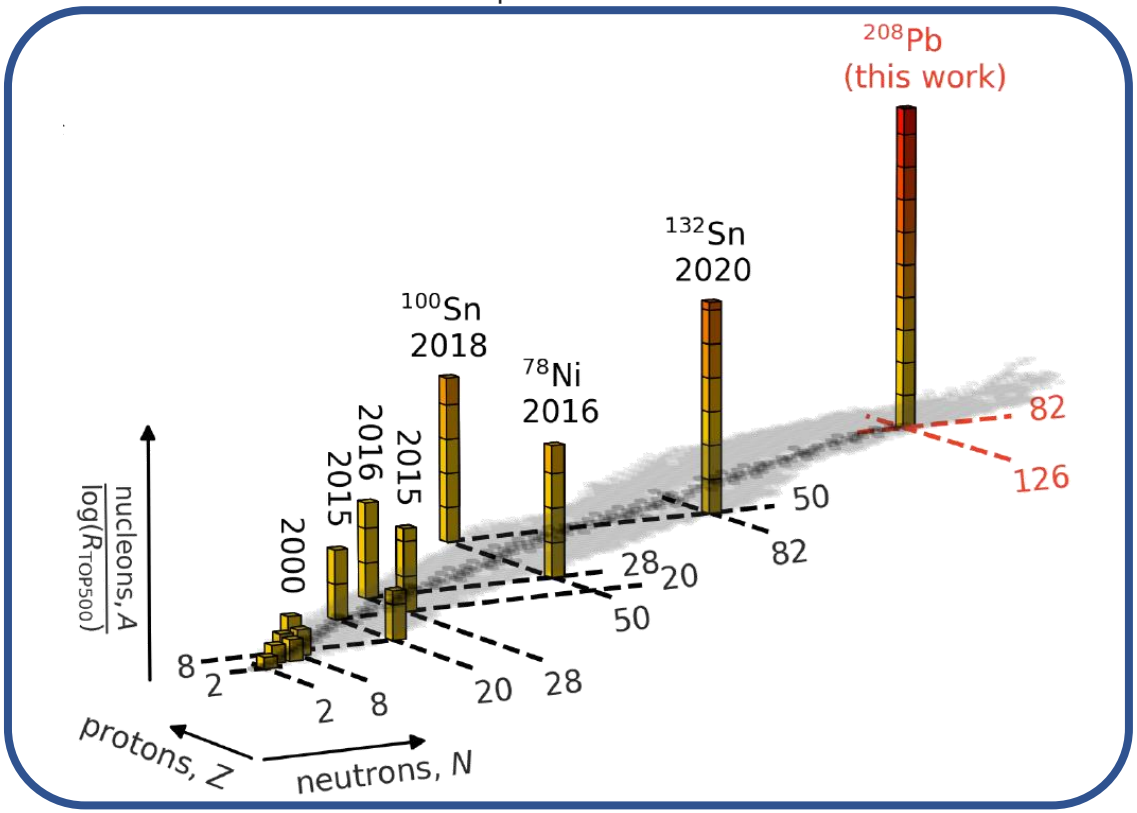


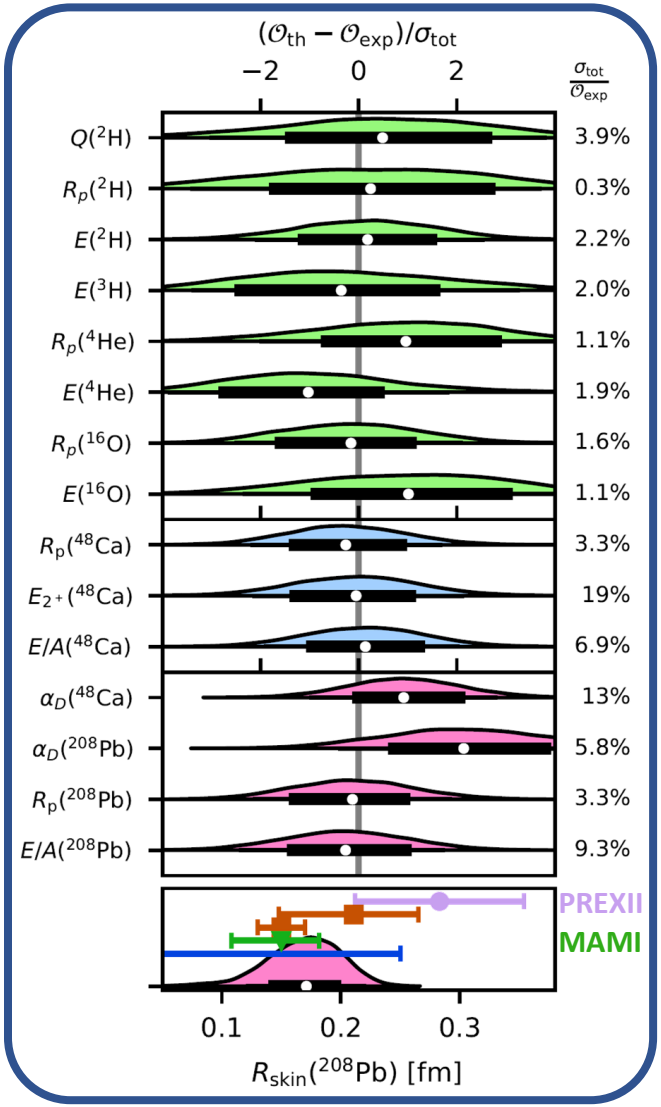
* C Drischler, R. J. Furnstahl, J. A. Melendez, and D. R. Phillips, Phys. Rev. Lett. 125, 202702 (2020)

Linking neutron skin of ^{208}Pb to nuclear forces

- First *ab initio* calculation of ^{208}Pb
- History matching framework enables robust predictions of the skin with quantitative theoretical error estimation. $R_{skin}(^{208}Pb) = 0.14 - 0.20$ fm

scales of *ab initio* computation effort vs Moore's law





B. S. Hu*, *et al*. arXiv:2112.01125

Summary

- We presented a unified statistical framework linking the interaction model and different many-body systems.

- Combining the present (previous) developed NM (finite nuclei) emulators and history matching we studied 1.6×10^6 non-implausible interaction samples in a huge LEC domain.

- This study reveals the correlations between different many-body systems and that our predictions for heavy systems are sensitive to the choice of low-energy constraints (indicate possible multimodality in the predictive distribution).

Thank you!

Collaborators:
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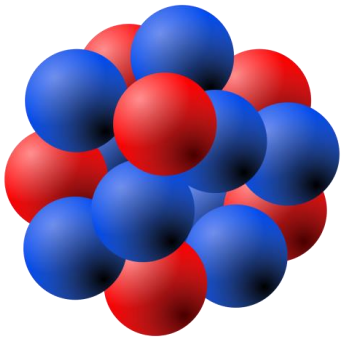
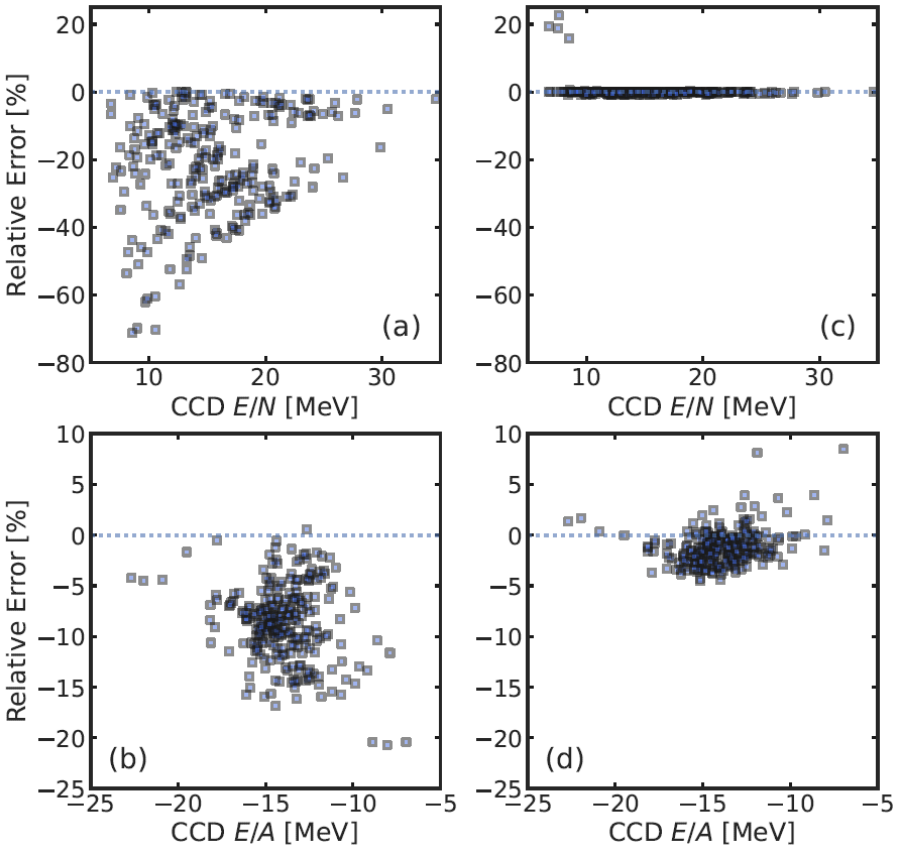
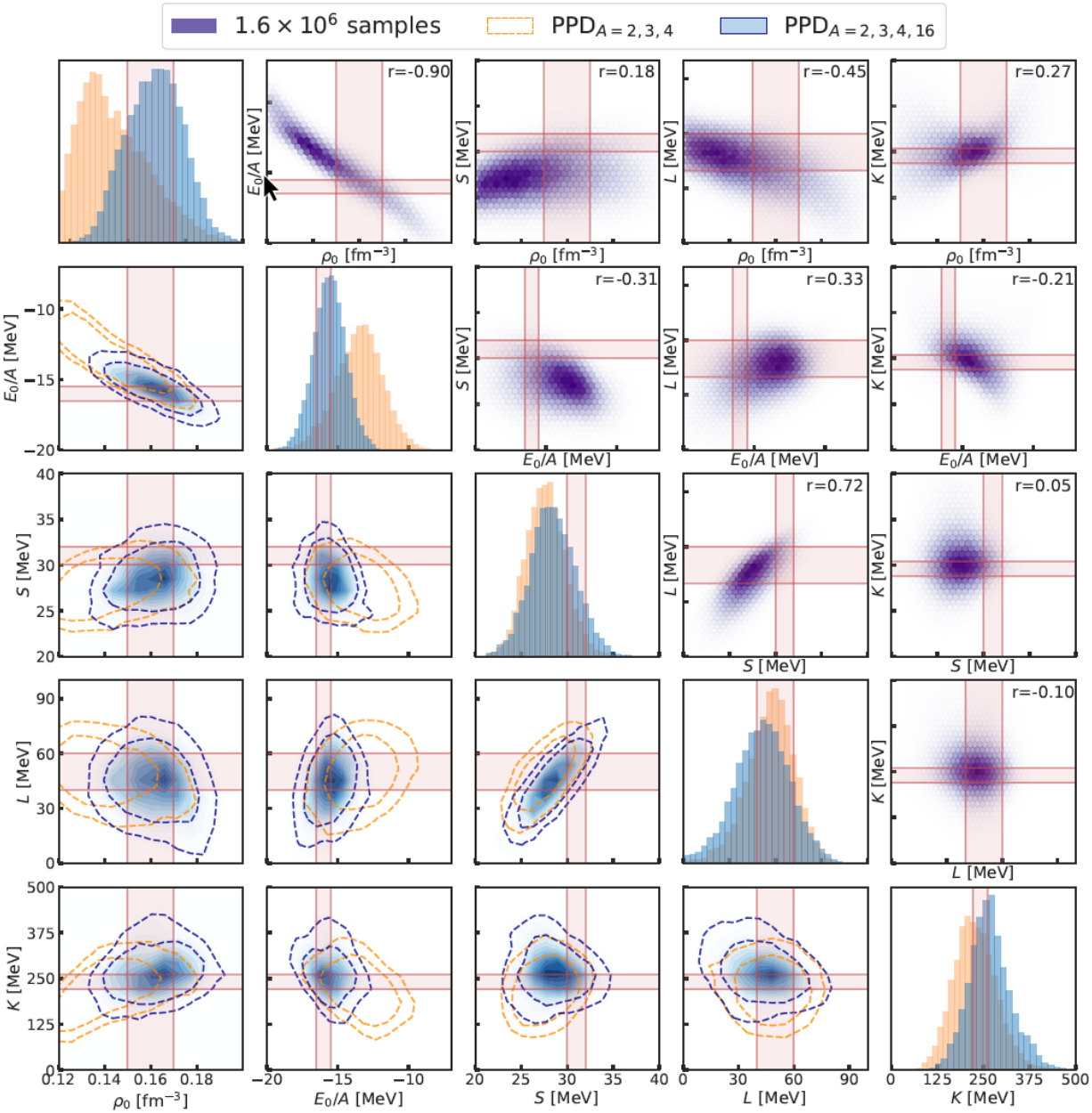


Small-batch voting

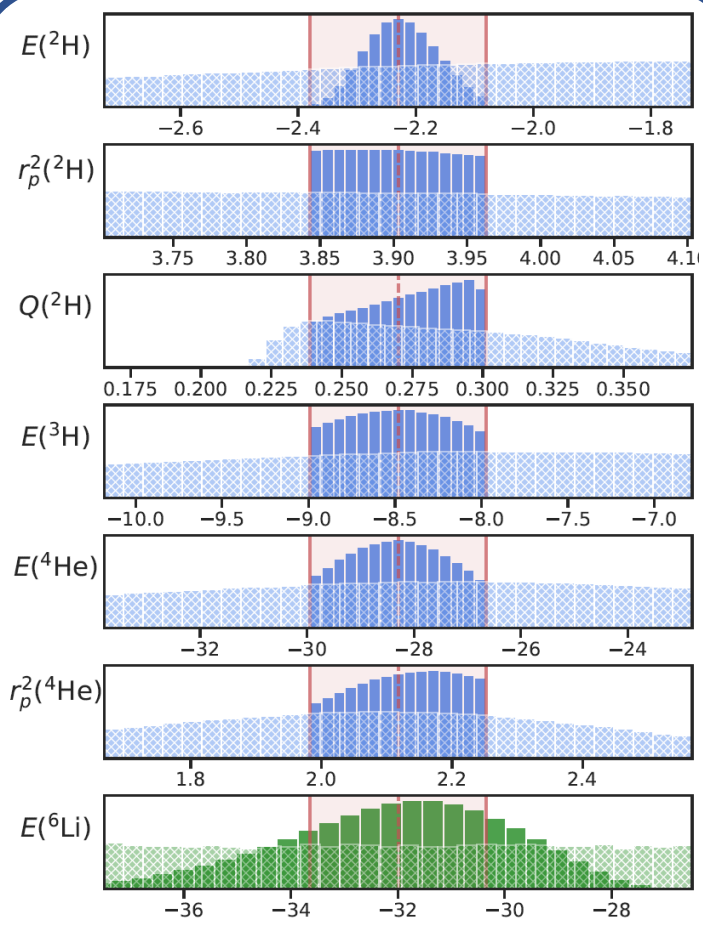


Highlight I: new interaction ΔNNLO$_{GO}$

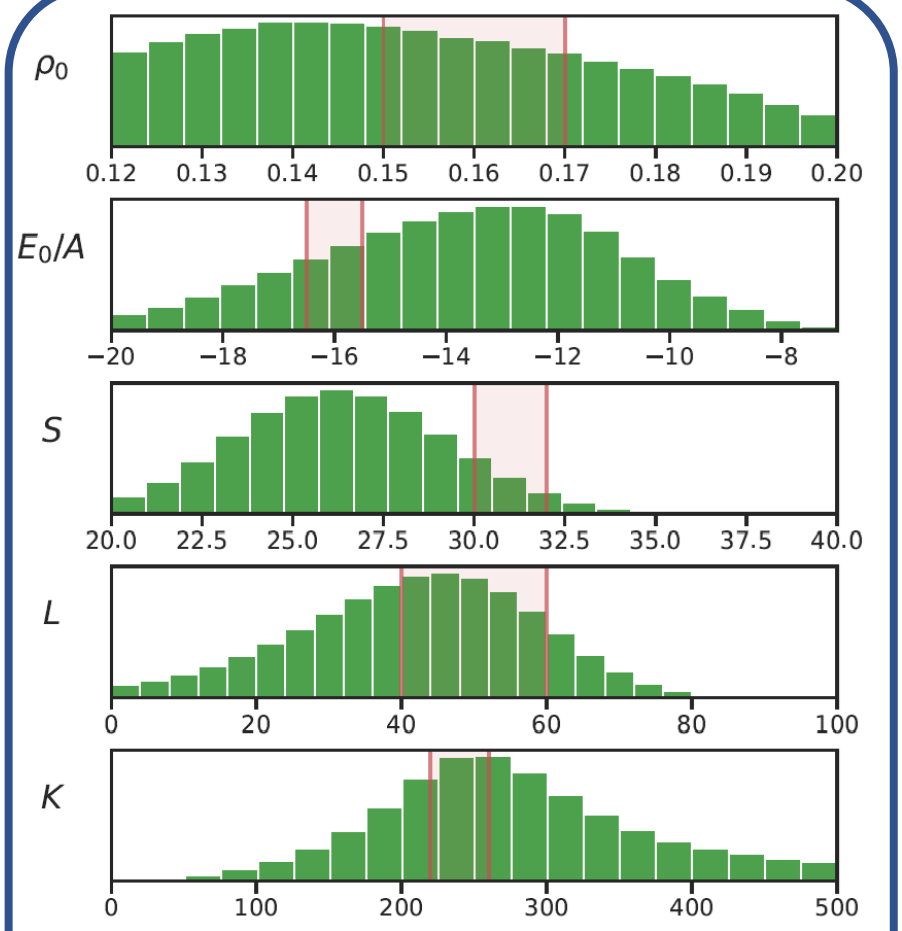


Results

1.6 x 10^6 Non-implausible interactions



few-body system (A=2-6)



NM observables