Ab initio computation of ^{208}Pb and the emergence of nuclear saturation

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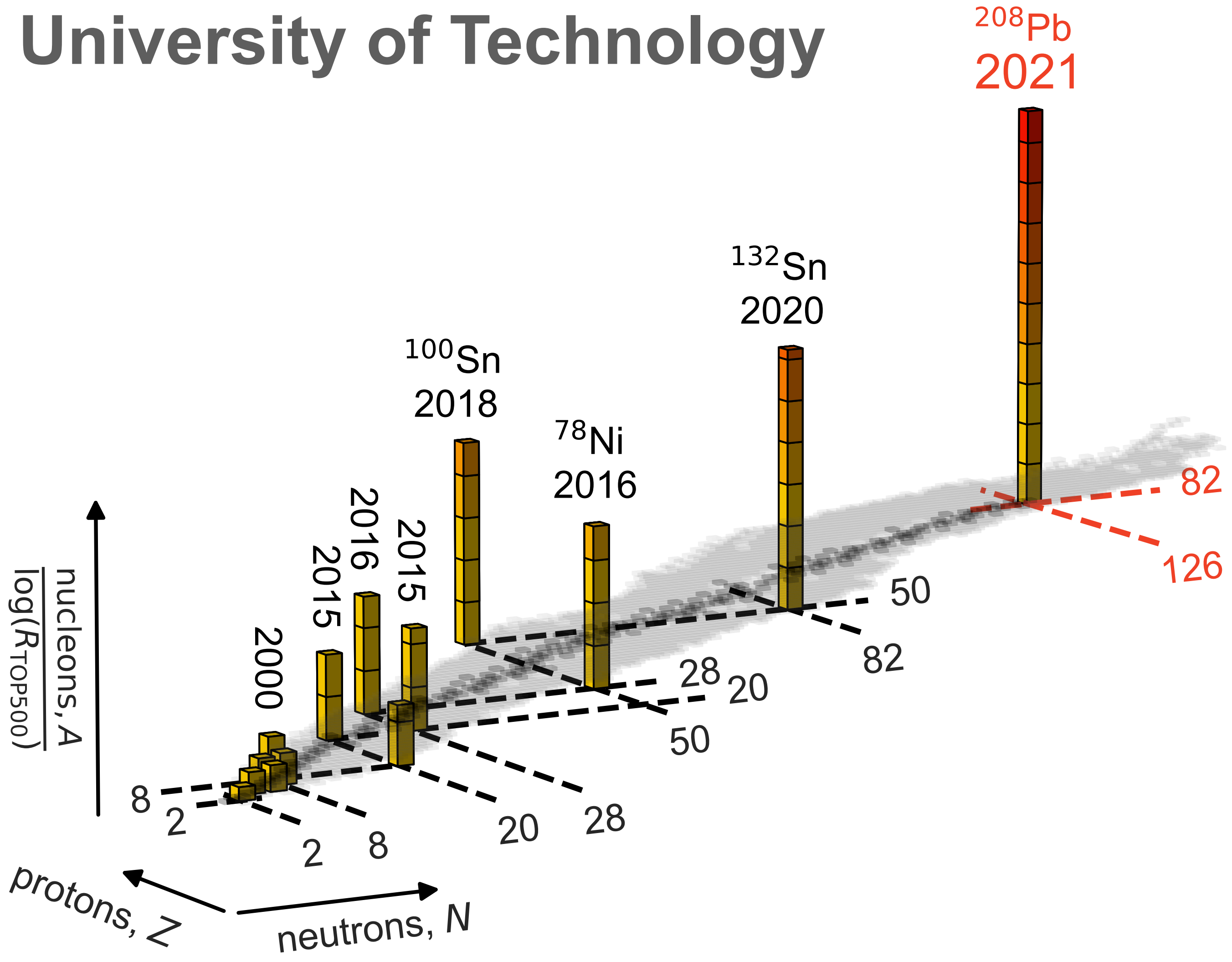


Workshop on Progress in Ab Initio Nuclear Theory, TRIUMF, Vancouver, 2023

Contents of this talk

- Uncertainty quantification for *ab initio* methods
- *Ab initio* computations of ^{208}Pb
- The emergence of nuclear saturation
- Revisiting the leading order of χEFT

Presenting (mainly) work published in:

Ab initio predictions link the neutron skin of ^{208}Pb to nuclear forces
by B. Hu, W.G. Jiang, T. Miyagi, Z. Sun, A. Ekström, cf, G. Hagen, J.D. Holt, T. Papenbrock, S.R. Stroberg, I. Vernon, **Nature Phys. 18, 1196 (2022)**

Emergence of nuclear saturation within Δ-full chiral effective field theory
by W.G. Jiang, cf, T. Djärv, G. Hagen, **arXiv:2212.13203**

Emulating ab initio computations of infinite nucleonic matter
by W.G. Jiang, cf, T. Djärv, G. Hagen, **arXiv:2212.13216**

Bayesian probability updates using Sampling/Importance Resampling
by W.G. Jiang, cf, **Front. Phys. 10:1058809 (2022)**

What is *ab initio* in nuclear theory?

We(*) interpret the *ab initio* method as a "***systematically improvable approach for quantitatively describing nuclei using the finest resolution scale possible while maximizing its predictive capabilities***."

In a nuclear physics context, we let nucleons define the beginning.

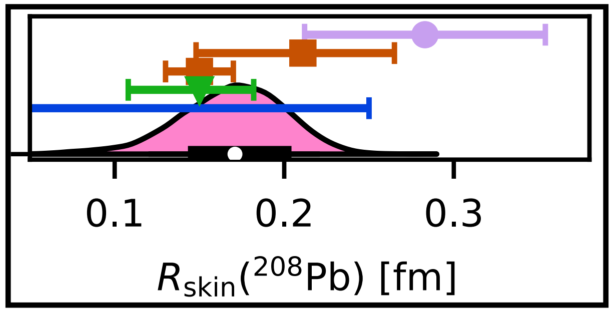
Lattice QCD might one day be the optimal starting point. However, it currently lacks predictive power for describing atomic nuclei.

The systematic aspects of the *ab initio* method creates an inferential advantage.

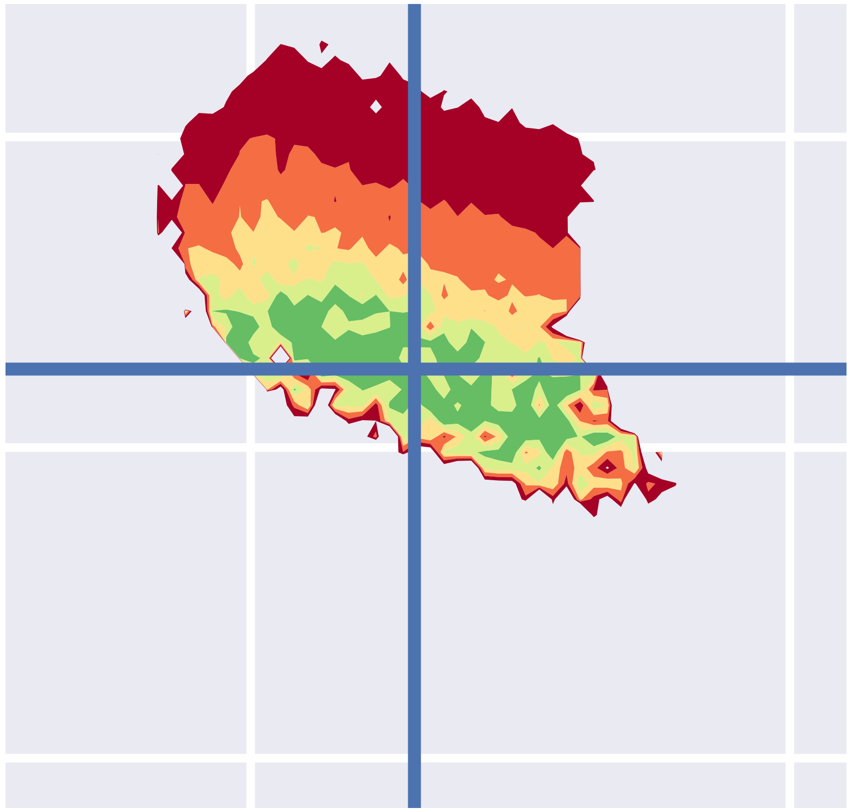
Fine resolution scale

Predictive capability

Systematically improvable



(*)A. Ekström, cf, G.Hagen, G. R. Jansen, W.G. Jiang, and T. Papenbrock, Frontiers in Phys. (2023)



Uncertainty quantification for *ab initio* methods based on EFT

Some terminology

- Data = $\mathcal{D}$,
  Future data = $\mathcal{F}$
- Ultimate goal:

  everything we know/assume

  $$p(\mathcal{F} \,|\, \mathcal{D}, \ldots)$$
- Model checking / validation:
  $$p(\mathcal{D} \,|\, \mathcal{D}, \ldots)$$
  $$p(\mathcal{D}_{\mathrm{val}} \,|\, \mathcal{D}, \ldots)$$
- Experimental observations: $z + \delta z$
  where errors are random variables, e.g., Var$[\delta z_i] = \sigma^2_{\mathrm{exp},i}$
- Often assume Gaussian errors: $p(\delta z \,|\, I) = \mathcal{N}(0, \Sigma)$

Theoretical models

- Theoretical modelling: $\boldsymbol{y}(\boldsymbol{\alpha}) + \delta\boldsymbol{y}$
  with model **parameters** α
- Theoretical errors can have different origin; The inclusion of relevant errors is a prerequisite for precision theory:
  $\delta\boldsymbol{y} = \delta\boldsymbol{y}_{\mathrm{th},1} + \delta\boldsymbol{y}_{\mathrm{th},2} + \ldots$
  Note: there might be an α-dependence in the errors
- **Hard-to-compute** models: $y^{\text{😡}}(\alpha)$
- … might be **emulated** / designed at low fidelity
  $y^{\text{😡}} \rightarrow \tilde{y}^{\text{😀}} + \delta\tilde{y}$

Learning from data via Bayes

- Apply **Bayes' theorem**

$$\underbrace{p(\boldsymbol{\alpha}\,|\,\mathscr{D},I)}_{\text{Posterior}} = \frac{\overbrace{p(\mathscr{D}\,|\,\boldsymbol{\alpha},I)}^{\text{Likelihood}} \cdot \overbrace{p(\boldsymbol{\alpha}\,|\,I)}^{\text{Prior}}}{\underbrace{p(\mathscr{D}\,|\,I)}_{\text{Marginal likelihood}}}$$

  - 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.

- Predictions for "future" data, modeled with y(α), are described by the **posterior predictive distribution** (ppd)

$$\left\{ y(\boldsymbol{\alpha}) : \boldsymbol{\alpha} \sim p(\boldsymbol{\alpha}\,|\,\mathscr{D},I) \right\}$$

  - We will also introduce **full ppd**:s $\left\{ \boldsymbol{y}(\boldsymbol{\alpha}) + \delta\boldsymbol{y} : \boldsymbol{\alpha} \sim p(\boldsymbol{\alpha}\,|\,\mathscr{D},I),\ \delta\boldsymbol{y} \sim p(\delta\boldsymbol{y}) \right\}$

Ab initio modeling of nuclear systems using χEFT

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

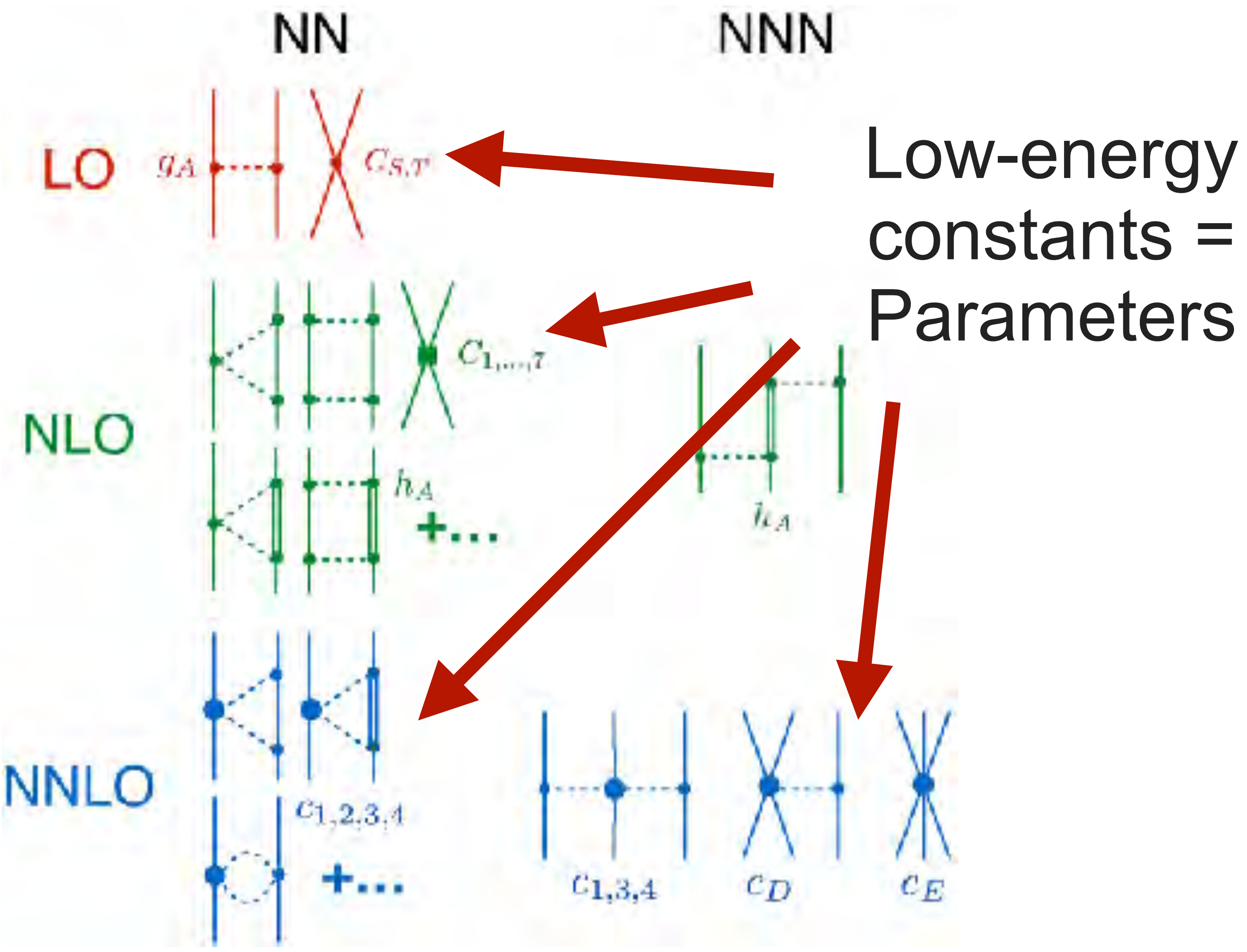
$$\hat{H}(\boldsymbol{\alpha}) = \hat{T} + \hat{V}(\boldsymbol{\alpha})$$

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

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

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

χEFT promises a connection with QCD



Low-energy constants = Parameters

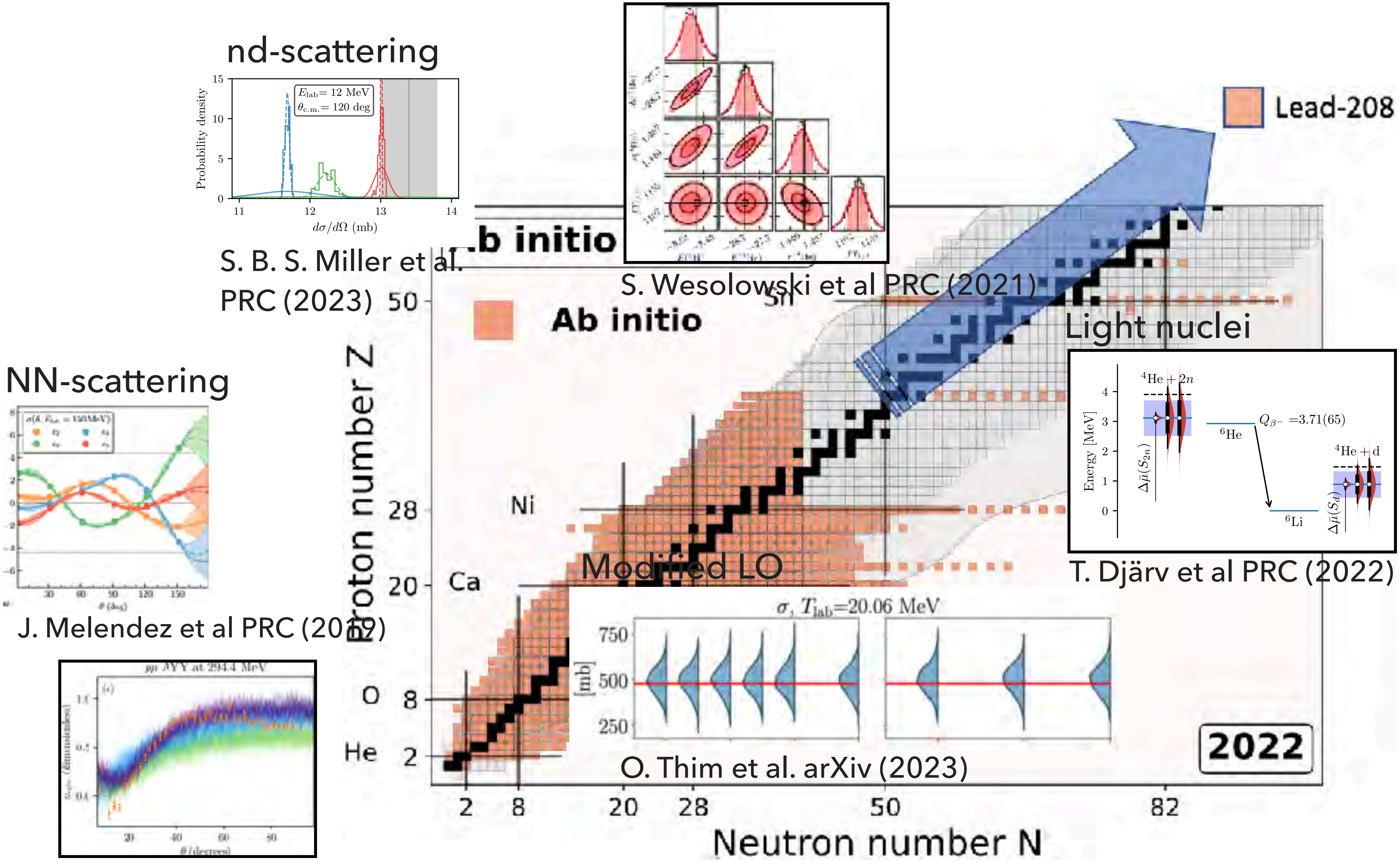
Weinberg, van Kolck, Kaiser, Bernard, Meißner, Epelbaum, Machleidt, Entem, …

A. Ekström, et al. Phys. Rev **C 97**, 024332 (2018)

W. Jiang, et al. Phys Rev **C 102,** 054301 (2020)

Recent UQ progress in χEFT modeling

From light…



nd-scattering

S. B. S. Miller et al. PRC (2023)

Few-nucleon systems

S. Wesolowski et al PRC (2021)

Light nuclei

T. Djärv et al PRC (2022)

NN-scattering

J. Melendez et al PRC (2019)

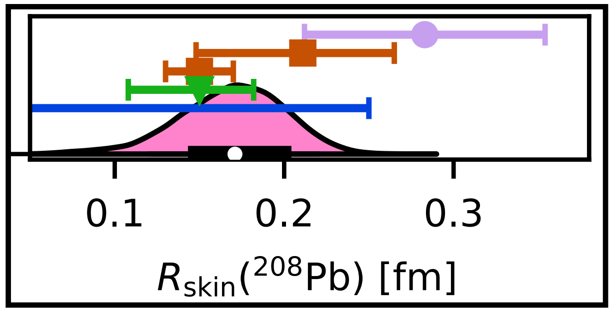
Modified LO

O. Thim et al. arXiv (2023)

I. Svensson et al PRC (2022)

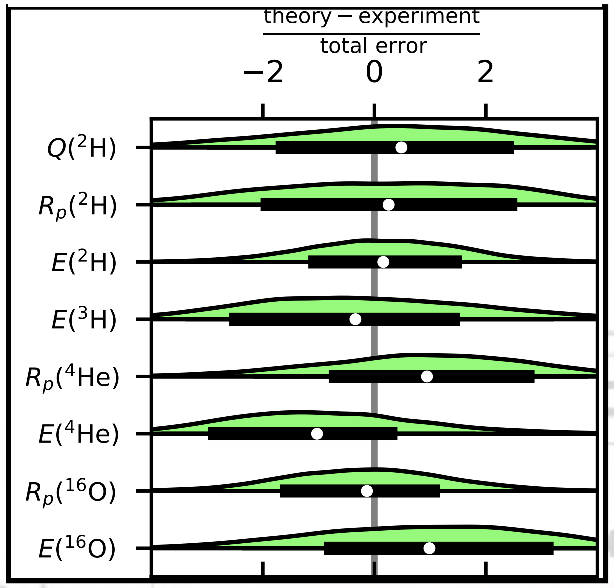
Recent UQ progress in χEFT modeling

… to heavy



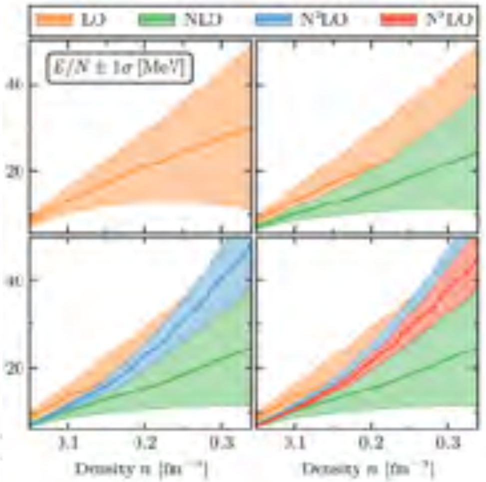
B. Hu et al
Nature Phys. (2022)

History matching



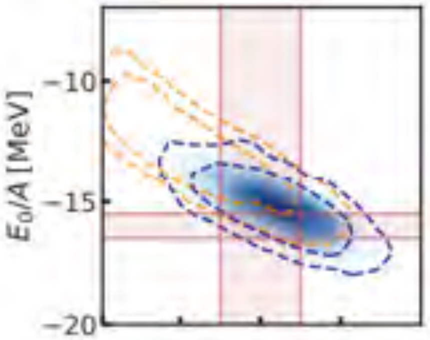
B. Hu et al Nature Phys. (2022)

Nuclear matter EoS (correlated errors)



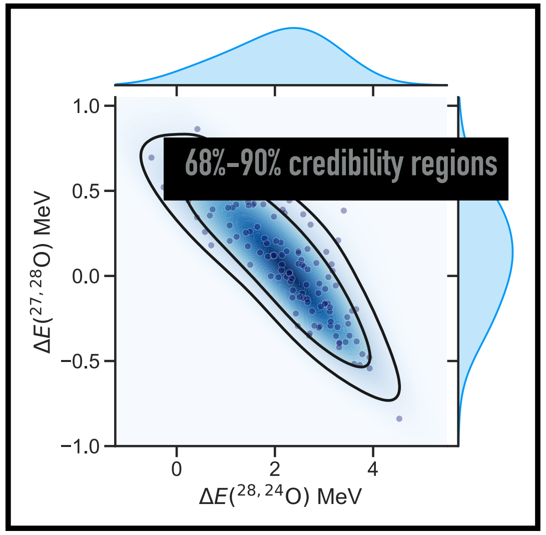
C. Drischler et al PRL,PRC (2020)

(importance resampling)



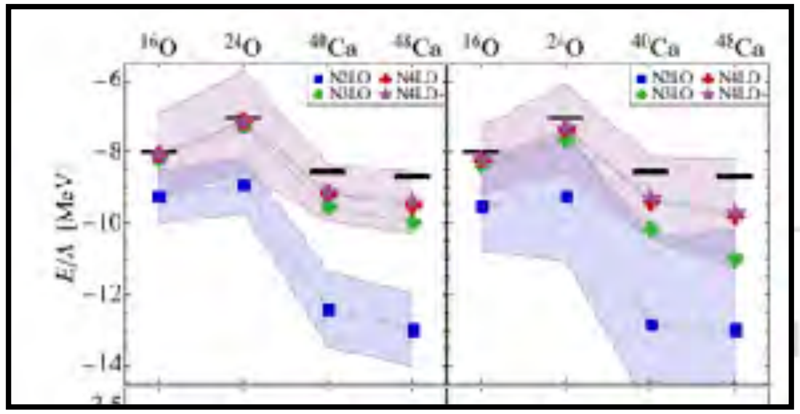
W.G. Jiang et al
Frontiers Phys.,
+ arXiv (2022)

Predicting oxygens



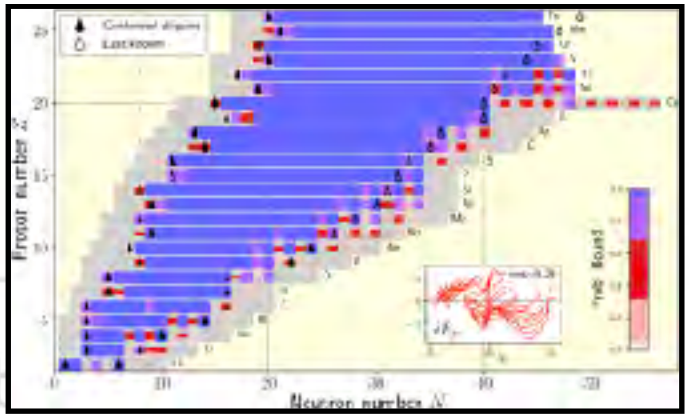
in preparation

Truncation errors/Model checking



P. Maris et al PRC (2022)

Bayesian linear regression



S. R. Stroberg et al PRL (2021)

Current UQ frontiers in *ab initio* nuclear theory

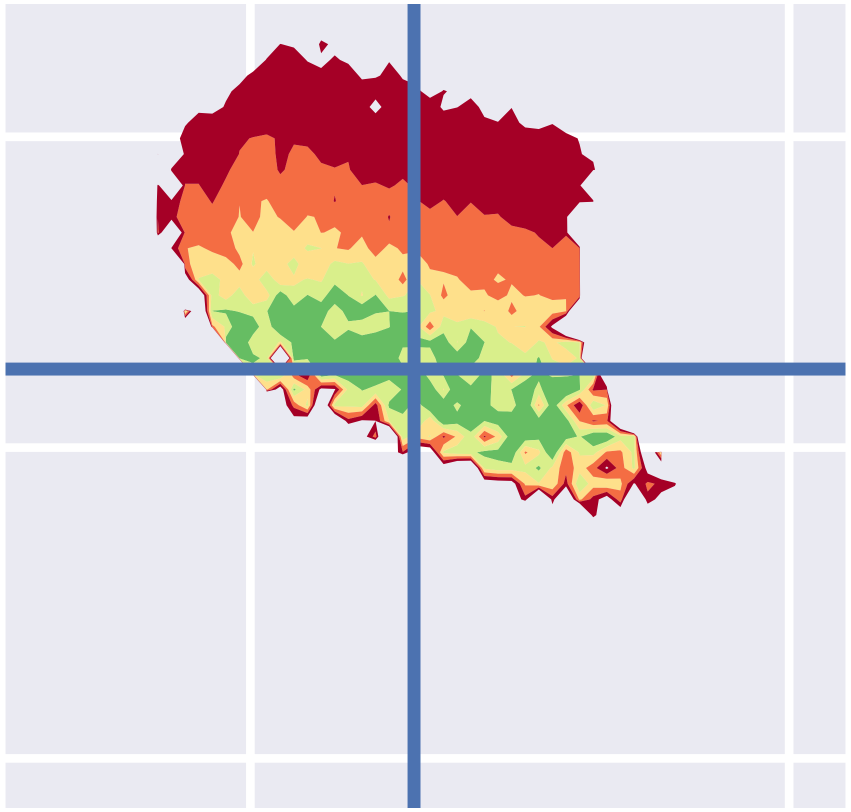
- Getting to know your errors
    - means, variances, and covariances of EFT truncation, many-body method, emulator errors;
    - PDF functional forms;
    - model calibration and validation
- Sampling PDFs without tears
    - emulators, Hamiltonian MC, sampling / importance resampling, …
- Technologies to be explored
    - Model mixing, experimental design, …

See, e.g., Frontiers in Physics volume on
“*Uncertainty Quantification in Nuclear Physics*”

And talks by Ekström, cf, Furnstahl at Hirschegg 2023
https://indico.gsi.de/event/15509/

Ab initio modeling of nuclei and nuclear matter with $\Delta - \chi\mathrm{EFT}$

- $\chi\mathrm{EFT}$ **with Δ isobar** (higher breakdown scale)
- Extensive **error model**
  - EFT truncation, method convergence, finite-size errors.
- **Iterative history-matching** for global parameter search.
  - Easier to claim implausibility than to quantify likelihood.
  - Define implausibility measure using only means and variances.
  - Iteratively remove implausible regions.
- Bayesian **PPDs** for nuclear observables up to ^{208}Pb and for infinite nuclear matter properties.



Ab initio computations of ^{208}Pb

Ab initio predictions link the neutron skin of ^{208}Pb to nuclear forces
by B. Hu, W.G. Jiang, T. Miyagi, Z. Sun, A. Ekström, cf, G. Hagen, J.D. Holt, T. Papenbrock, S.R. Stroberg, I. Vernon, **Nature Phys. 18, 1196 (2022)**

Ab initio computations of ^{208}Pb

We start from a ΔNNLO(394) chiral Hamiltonian. Order by order results provide estimates of the model errors. Pion-nucleon couplings are from a Roy-Steiner analysis.

W. Jiang, et al. Phys Rev **C 102,** 054301 (2020)
M. Hoferichter et al, Phys. Rev. Lett. **115**, 192301 (2015)

Approximately solve the Schrödinger equation in HF basis using Coupled-Cluster, IMSRG, and MBPT methods. Comparisons and domain knowledge provide estimates of the method errors.

G. Hagen, et al. Rep. Prog. Phys. **77**, 096302 (2014)
H. Hergert, et al. Phys Rep. **621** 165 (2016)

3NFs are captured using the NO2B approx. Large emax (=14) and E3max (=28) spaces. For ^{208}Pb, IR extrapolation adds only ~2% to the skin thickness and ~6% to the energy.

T. Miyagai, et al. Phys. Rev. **C 105**, 014302 (2022)

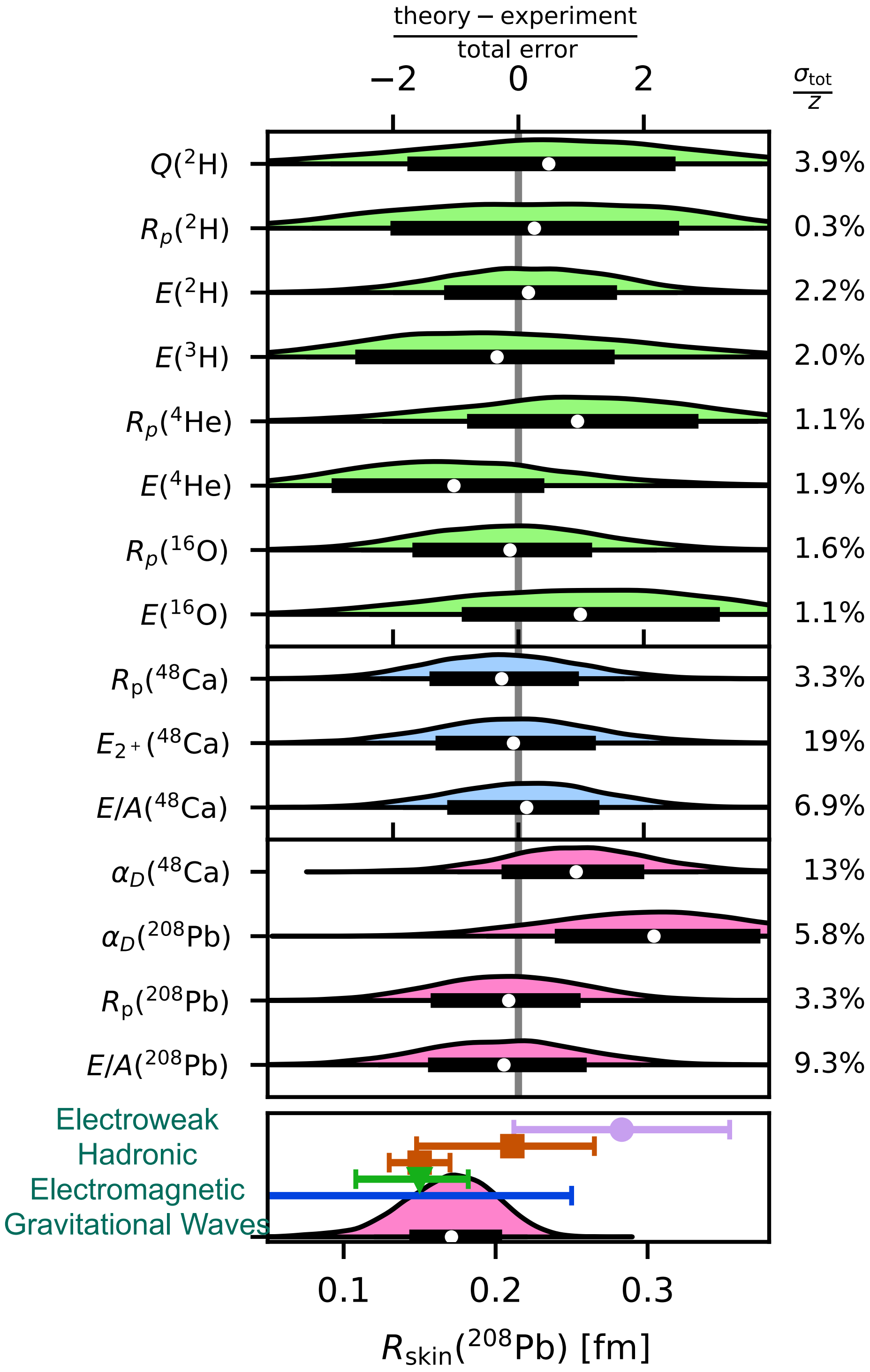
EC-emulators for observables with $A \leq 16$. Validated and trusted to within 0.5%

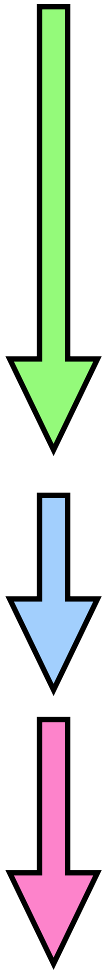
S. König, et al. Phys. Lett. **B 810**, 135814 (2020)
A. Ekström and G. Hagen Phys. Rev. Lett. **123**, 252501 (2019)

Nuclear matter computed using CCD(T) with estimates of the method error from systematics. Conflated with estimates for the model error using a multitask Gaussian Process.

C. Drischler, et. al. Phys. Rev. Lett. **125**, 202702 (2020)

Ab initio predictions link the skin of ^{208}Pb to nuclear forces





History Matching

We explore 10^9 different interaction parameterizations

Confronted with A=2-16 data + NN scattering information

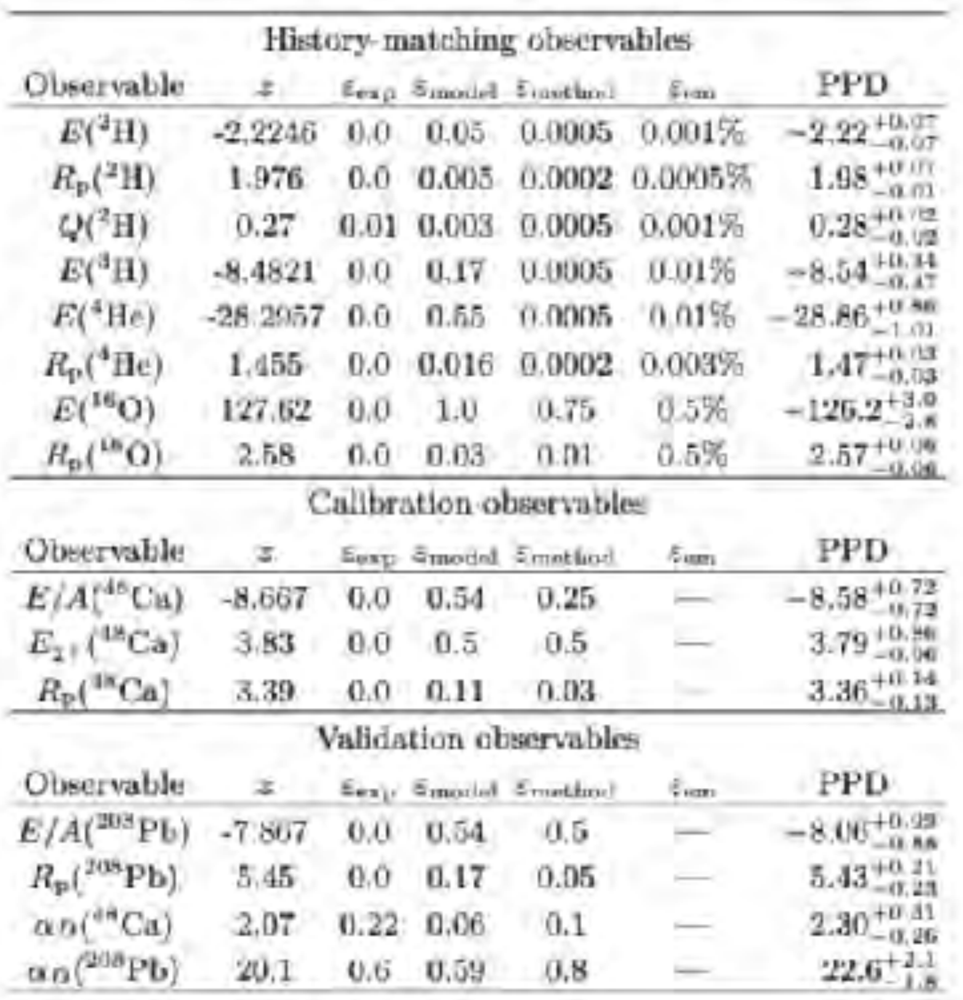
Find 34 non-implausible interactions

Calibration

Importance resampling

Validation

Inspect ab initio model and error estimates



History-matching observables

Observable	z	ε_{exp}	ε_{model}	ε_{method}	ε_{em}	PPD
$E(^2H)$	-2.2246	0.0	0.05	0.0005	0.001%	$-2.22^{+0.07}_{-0.07}$
$R_p(^2H)$	1.976	0.0	0.005	0.0002	0.0005%	$1.98^{+0.01}_{-0.01}$
$Q(^2H)$	0.27	0.01	0.003	0.0005	0.001%	$0.28^{+0.02}_{-0.02}$
$E(^3H)$	-8.4821	0.0	0.17	0.0005	0.01%	$-8.54^{+0.34}_{-0.47}$
$E(^4He)$	-28.2957	0.0	0.55	0.0005	0.01%	$-28.86^{+0.86}_{-1.01}$
$R_p(^4He)$	1.455	0.0	0.016	0.0002	0.003%	$1.47^{+0.03}_{-0.03}$
$E(^{16}O)$	127.62	0.0	1.0	0.75	0.5%	$-126.2^{+3.0}_{-3.8}$
$R_p(^{16}O)$	2.58	0.0	0.03	0.01	0.5%	$2.57^{+0.06}_{-0.06}$

Calibration observables

Observable	z	ε_{exp}	ε_{model}	ε_{method}	ε_{em}	PPD
$E/A(^{48}Ca)$	-8.667	0.0	0.54	0.25	—	$-8.58^{+0.72}_{-0.72}$
$E_{2^+}(^{48}Ca)$	3.83	0.0	0.5	0.5	—	$3.79^{+0.86}_{-0.96}$
$R_p(^{48}Ca)$	3.39	0.0	0.11	0.03	—	$3.36^{+0.14}_{-0.13}$

Validation observables

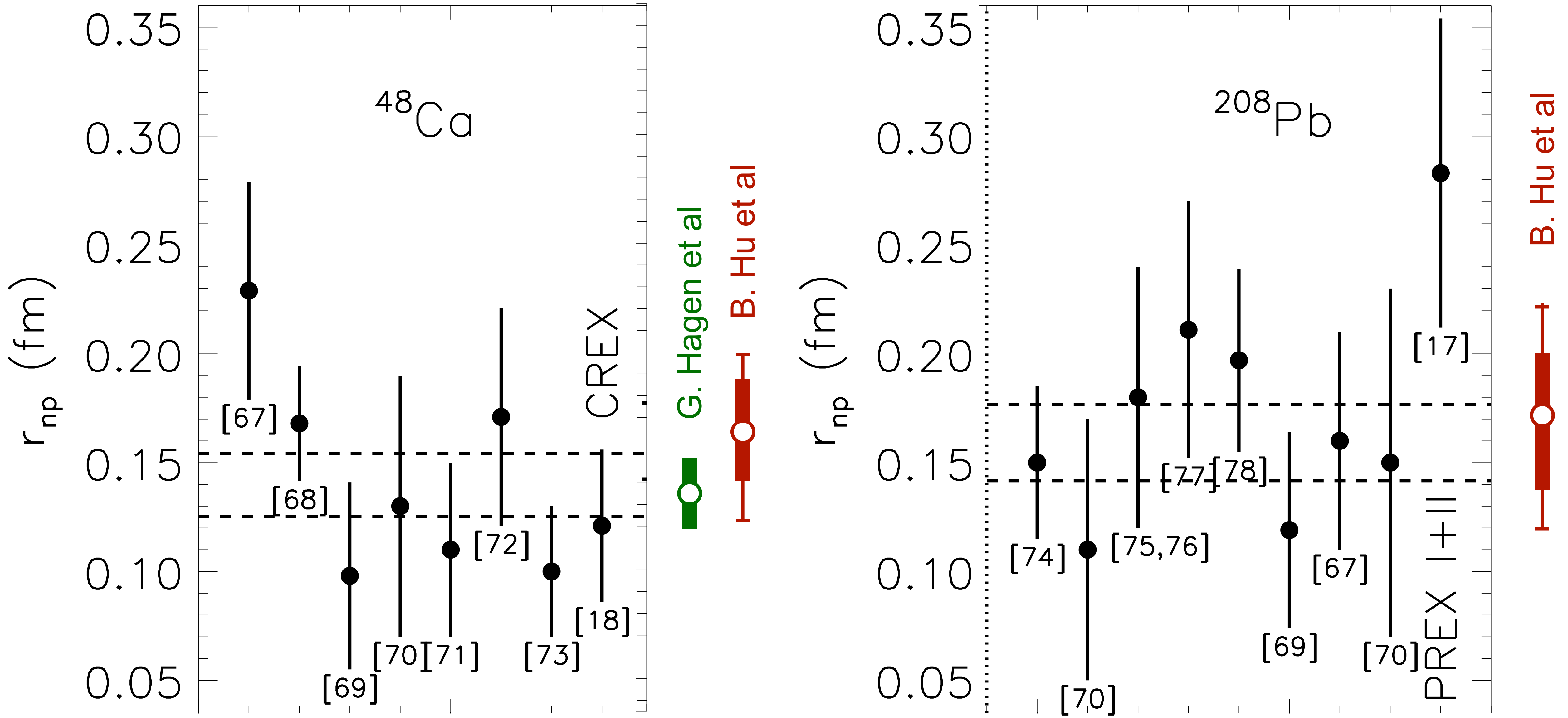
Observable	z	ε_{exp}	ε_{model}	ε_{method}	ε_{em}	PPD
$E/A(^{208}Pb)$	-7.867	0.0	0.54	0.5	—	$-8.06^{+0.29}_{-0.88}$
$R_p(^{208}Pb)$	5.45	0.0	0.17	0.05	—	$5.43^{+0.21}_{-0.23}$
$\alpha_D(^{48}Ca)$	2.07	0.22	0.06	0.1	—	$2.30^{+0.31}_{-0.26}$
$\alpha_D(^{208}Pb)$	20.1	0.6	0.59	0.8	—	$22.6^{+2.1}_{-1.8}$

B. Hu et al (Nature Phys. 2022)

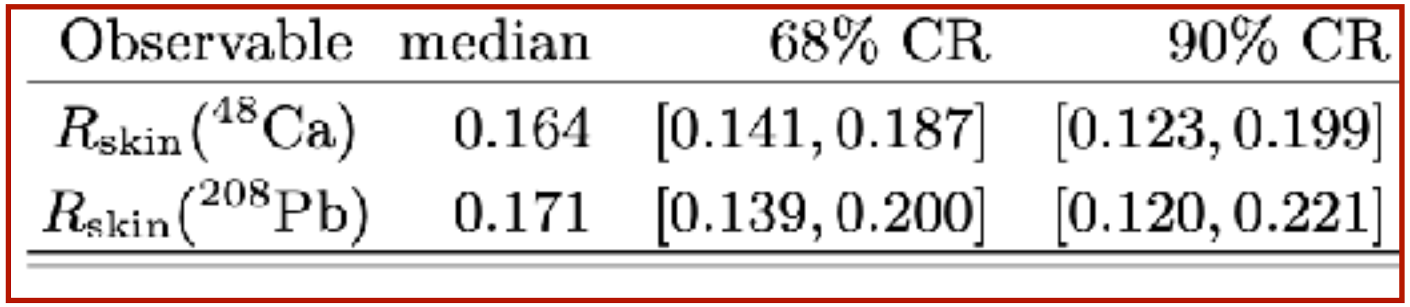
<u>Prediction</u>: small skin thickness 0.14-0.20 fm in mild (1.5 sigma) tension with PREX.

Neutron skin thickness

Constraints on Nuclear Symmetry Energy Parameters
J. Lattimer (2023)



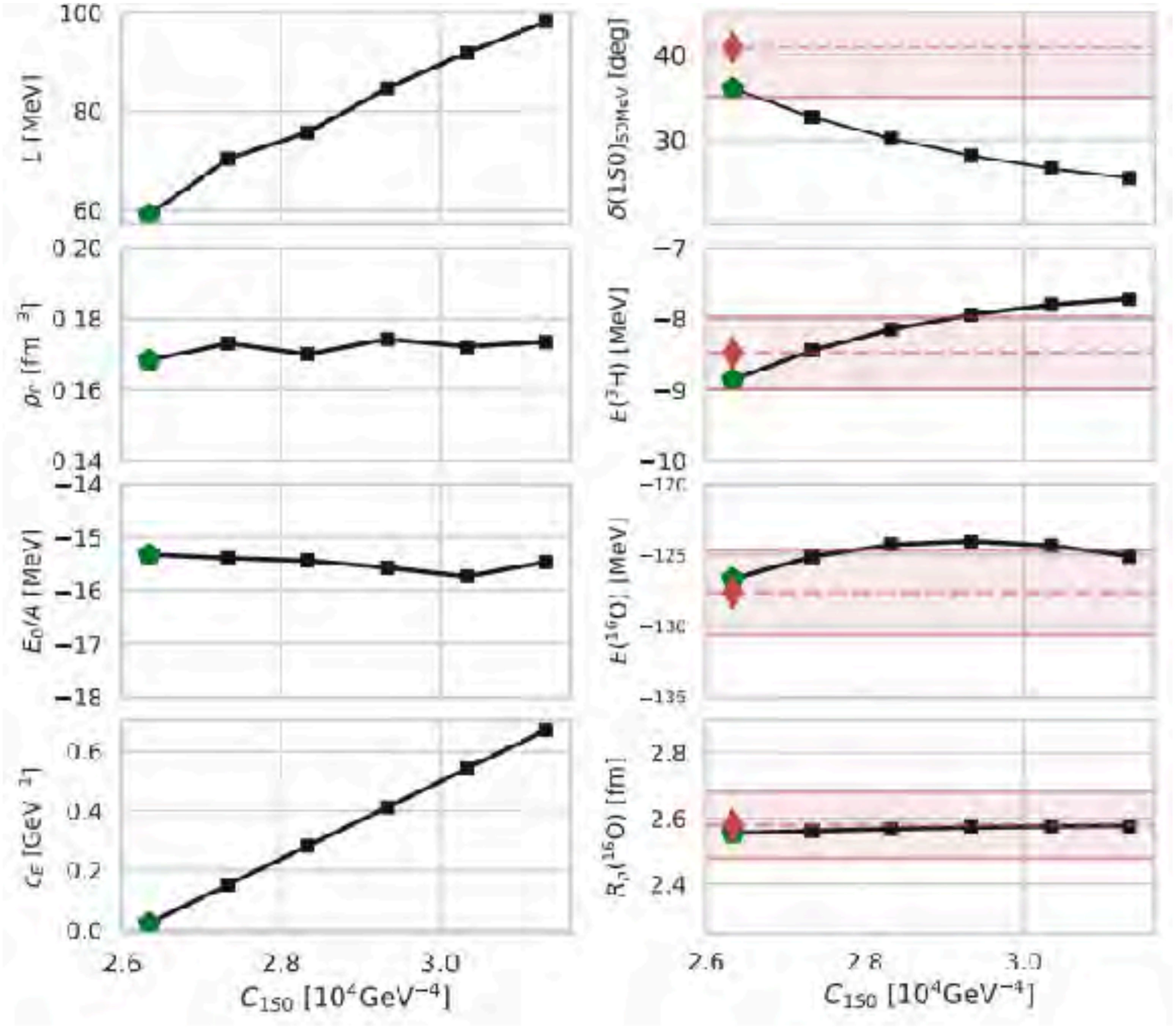
B. Hu et al (Nature Phys. 2022)

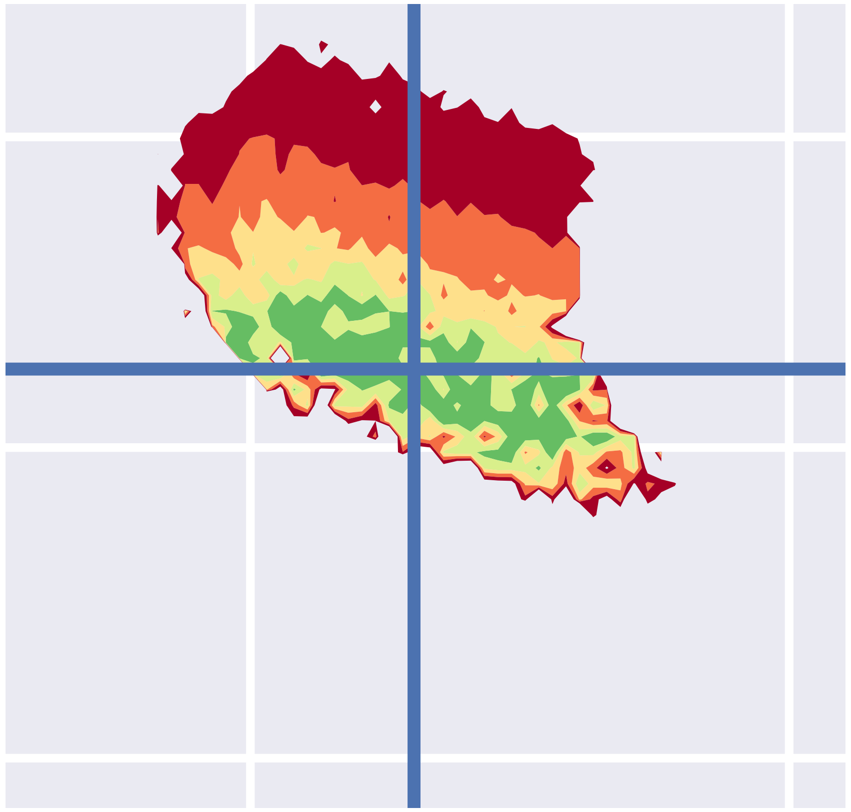


Observable	median	68% CR	90% CR
$R_{\rm skin}(^{48}{\rm Ca})$	0.164	[0.141, 0.187]	[0.123, 0.199]
$R_{\rm skin}(^{208}{\rm Pb})$	0.171	[0.139, 0.200]	[0.120, 0.221]

Why does ab initio predict thin skins?

- Tune C1S0 while adjusting cE to maintain saturation
- Study the effect on various observables. Note *L* & $\delta_{1S0}(50)$





Emergence of nuclear saturation

Emergence of nuclear saturation within Δ-full chiral effective field theory
by W.G. Jiang, cf, T. Djärv, G. Hagen, **arXiv:2212.13203**

Emulating ab initio computations of infinite nucleonic matter
by W.G. Jiang, cf, T. Djärv, G. Hagen, **arXiv:2212.13216**

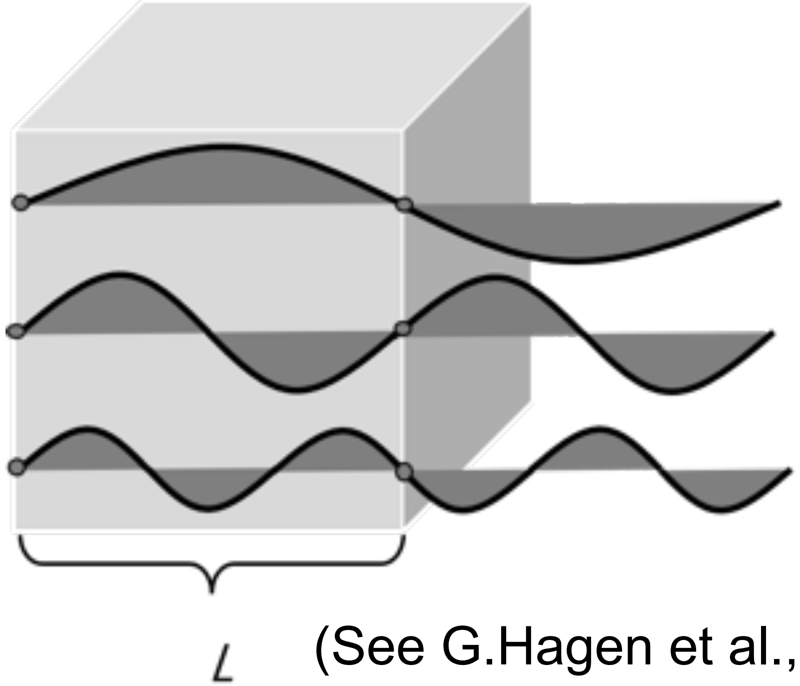
Emergence of nuclear saturation within $\Delta - \chi\mathrm{EFT}$

- $\chi\mathrm{EFT}$ **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.

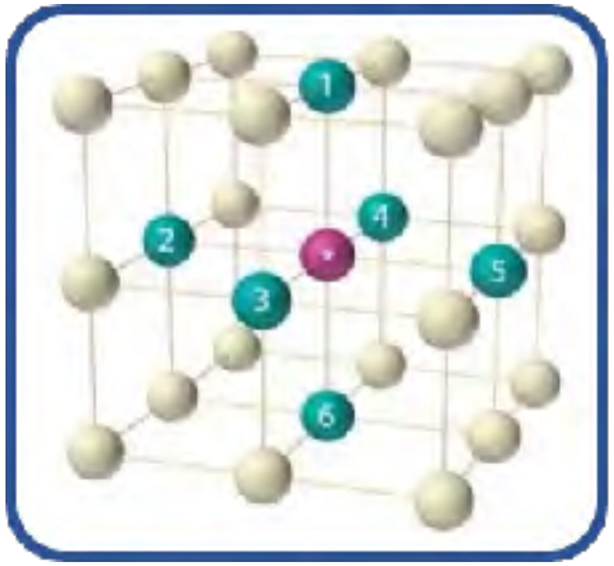
Infinite nuclear matter: computational approach

- Discrete momentum basis states $\psi_k(x) \propto e^{ikx}$
- Cubic lattice in momentum space, (k_x, k_y, k_z)
- $k_n = \dfrac{2\pi n}{L}$, with $n = 0, \pm 1, \pm 2, \ldots \pm n_{\max}$
- Results should converge with increasing $n_{\max}$

- Periodic boundary conditions $\psi_k(x + L) = \psi_k(x)$

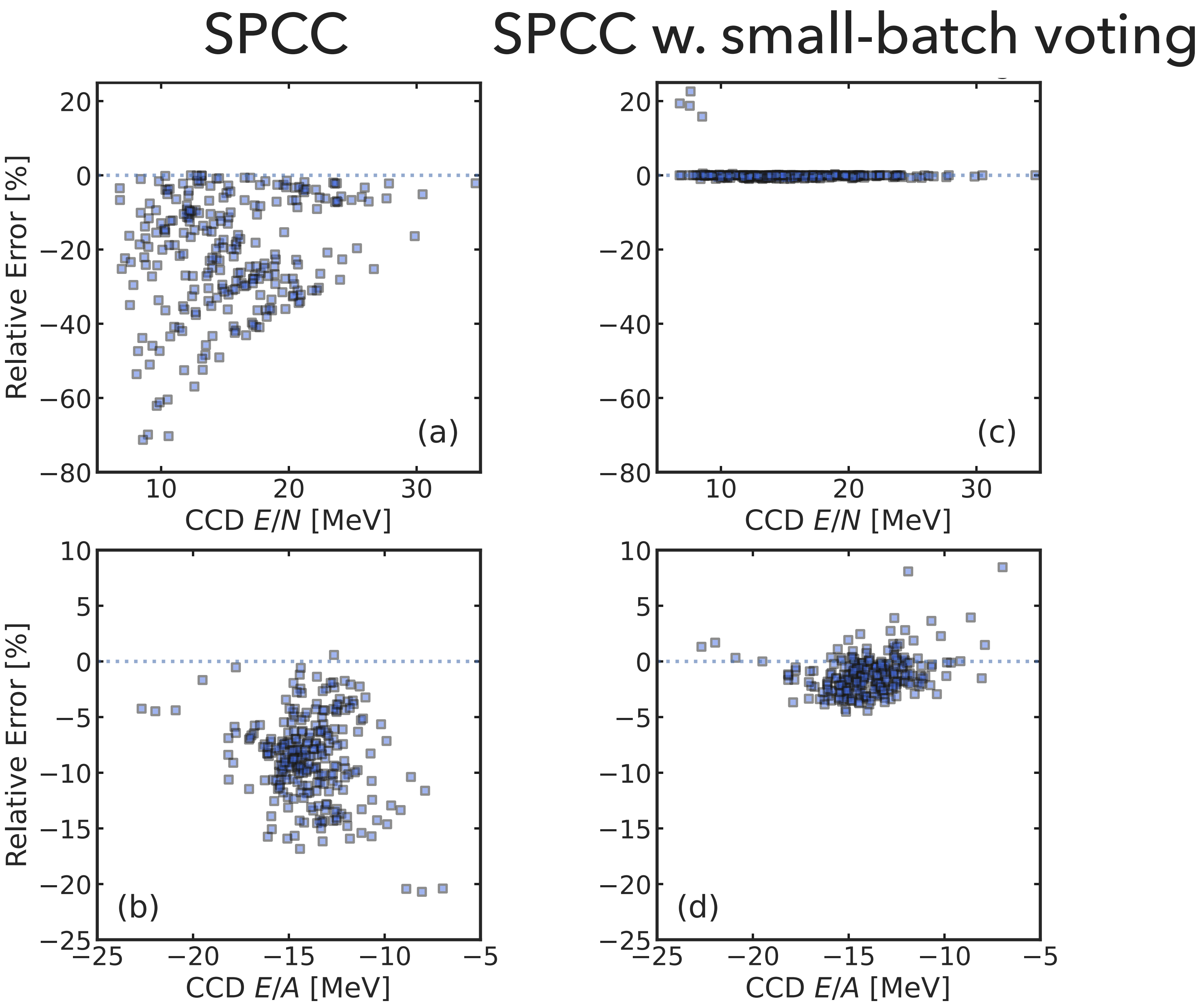


(See G.Hagen et al., 2014)



- The box size (L) and the nucleon number (N) controls the density (ρ)
- Computational challenge ($n_{\max} = 4$):
  - PNM: 1458 orbits with 66 neutrons
  - SNM: 2916 orbits with 132 nucleons

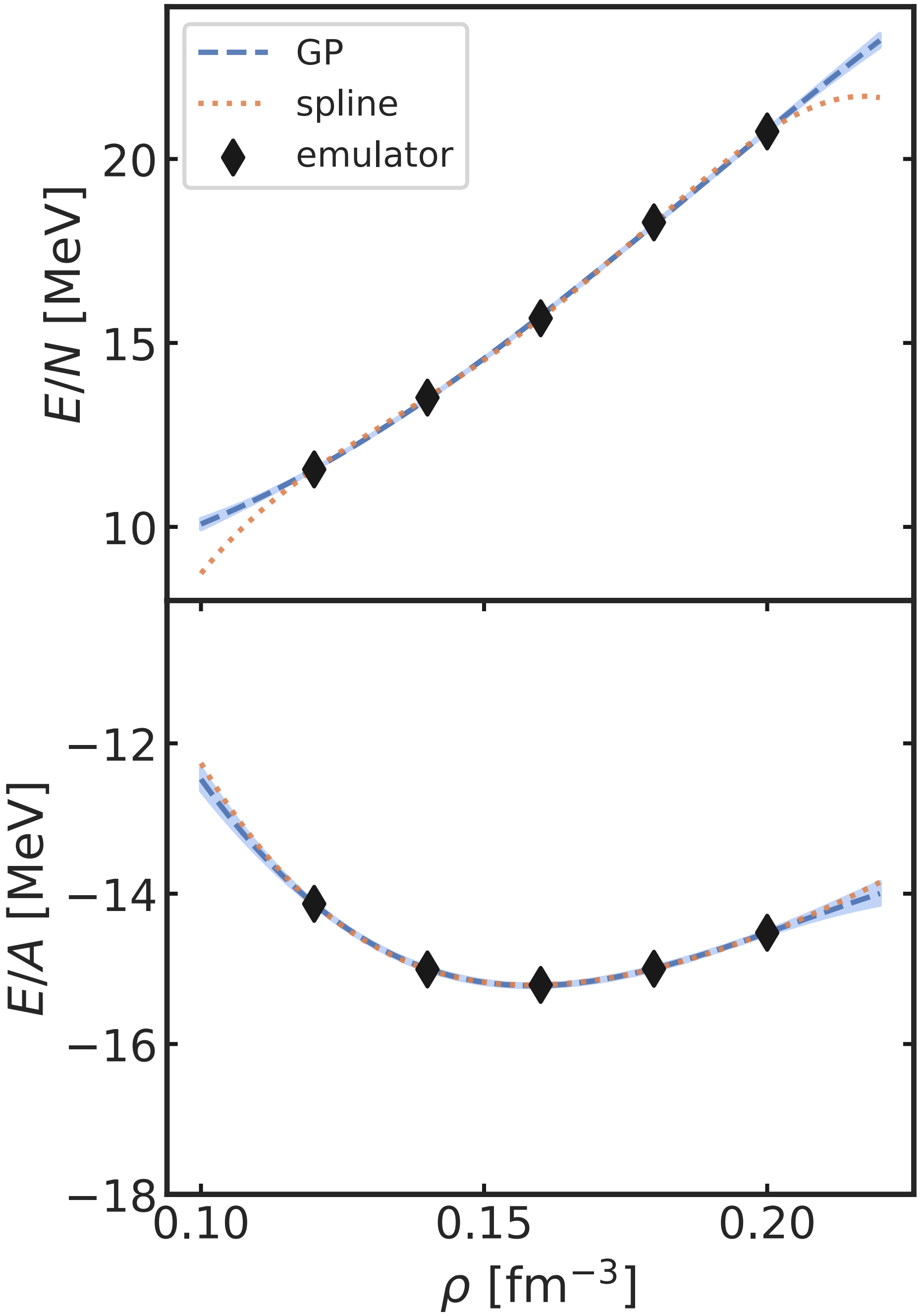
SPCC with small-batch voting

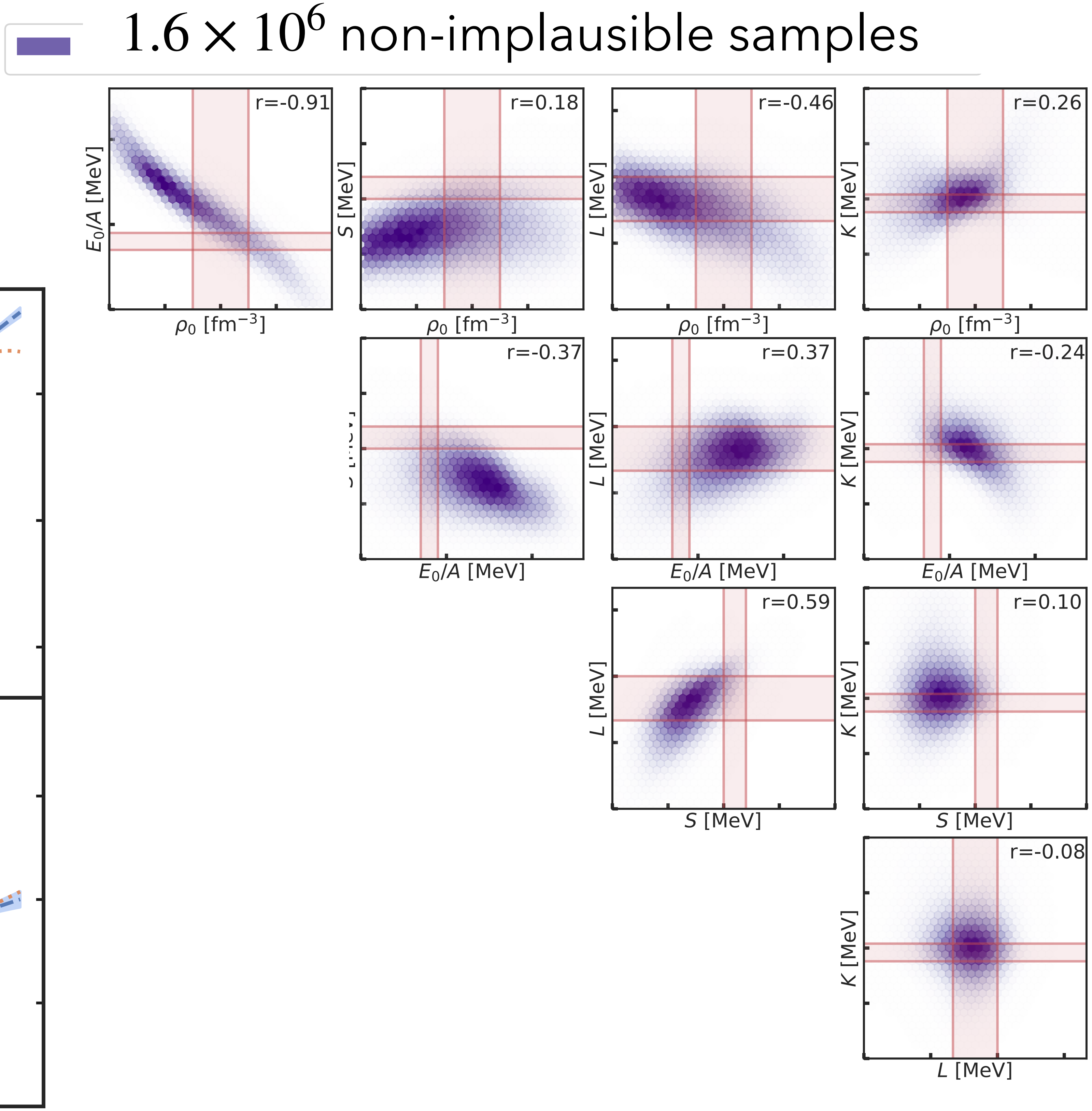


Physical states are stable w.r.t. subspace variations

$$|\Psi(\boldsymbol{\alpha}_\odot)\rangle = e^{T(\boldsymbol{\alpha}_\odot))}|\Phi_0\rangle \approx \sum_{i=1}^{N_{\text{sub}}} c_i^\star |\Psi_i\rangle$$

Correlation study



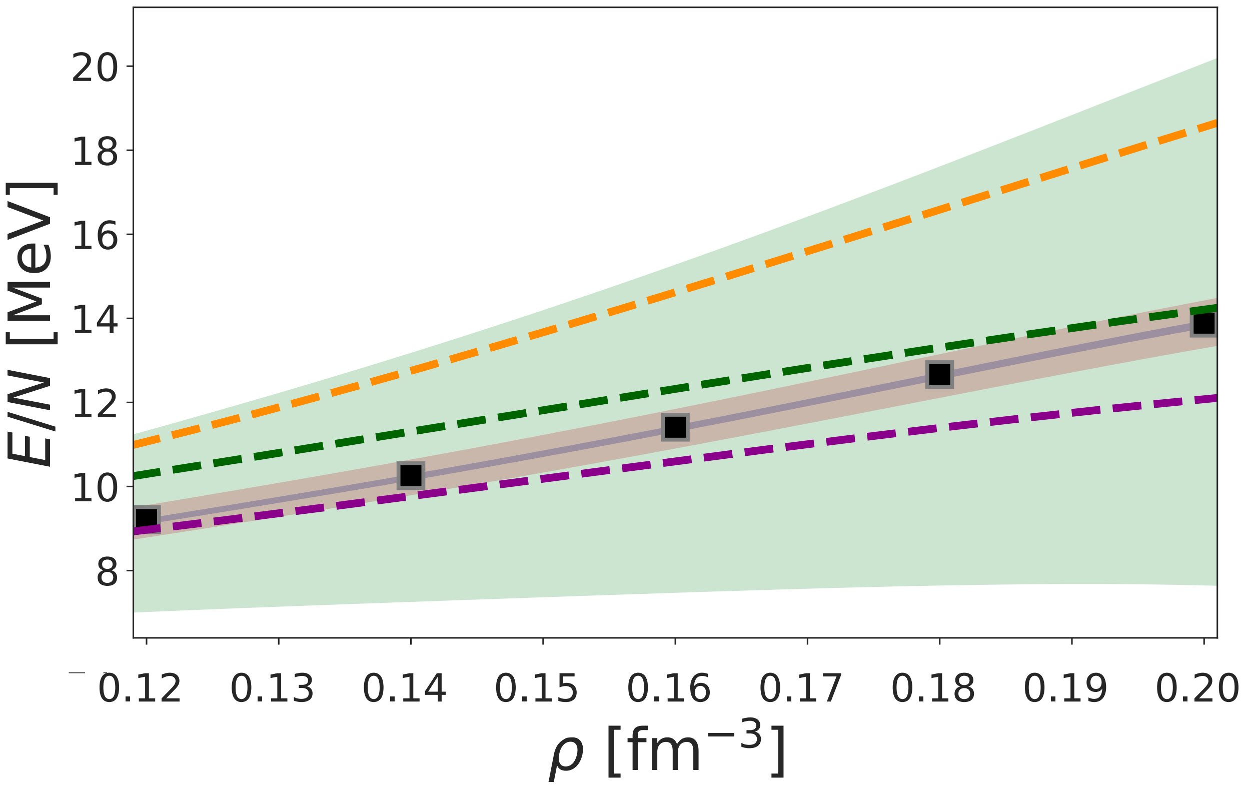


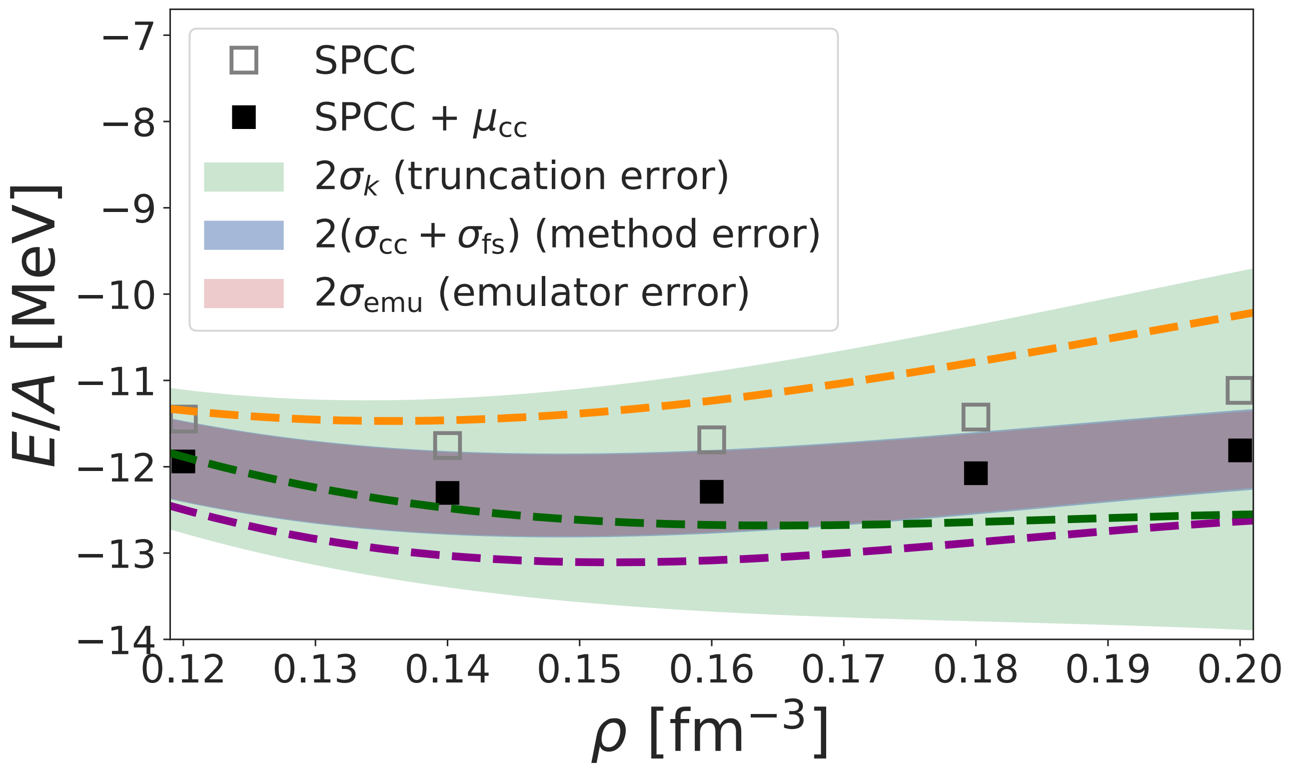
Bayesian machine-learning error model(s)

$$z = \tilde{y}(\boldsymbol{\alpha}) + \delta \boldsymbol{y}_{\text{EFT}} + \delta \boldsymbol{y}_{\text{method}} + \delta \tilde{\boldsymbol{y}}_{\text{em}} + \delta \boldsymbol{y}_{\text{exp}}$$

$$\varepsilon_\kappa(\rho) \mid \bar{c}_\kappa^2, l_\kappa, \sim GP[\mu_\kappa(\rho), \bar{c}_\kappa^2 R_\kappa(\rho, \rho'; l_\kappa)],$$

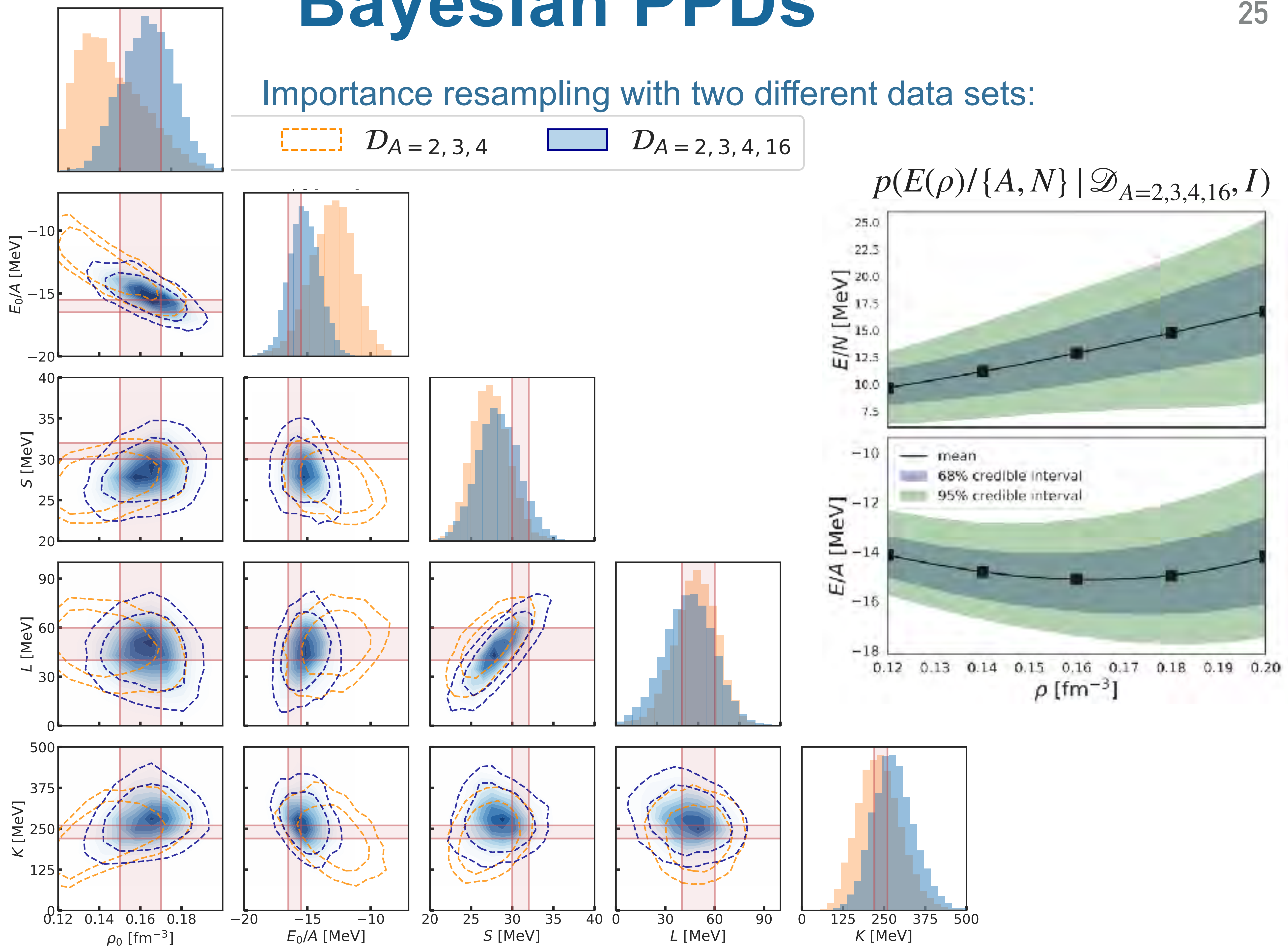
See C. Drischler et al (2020)





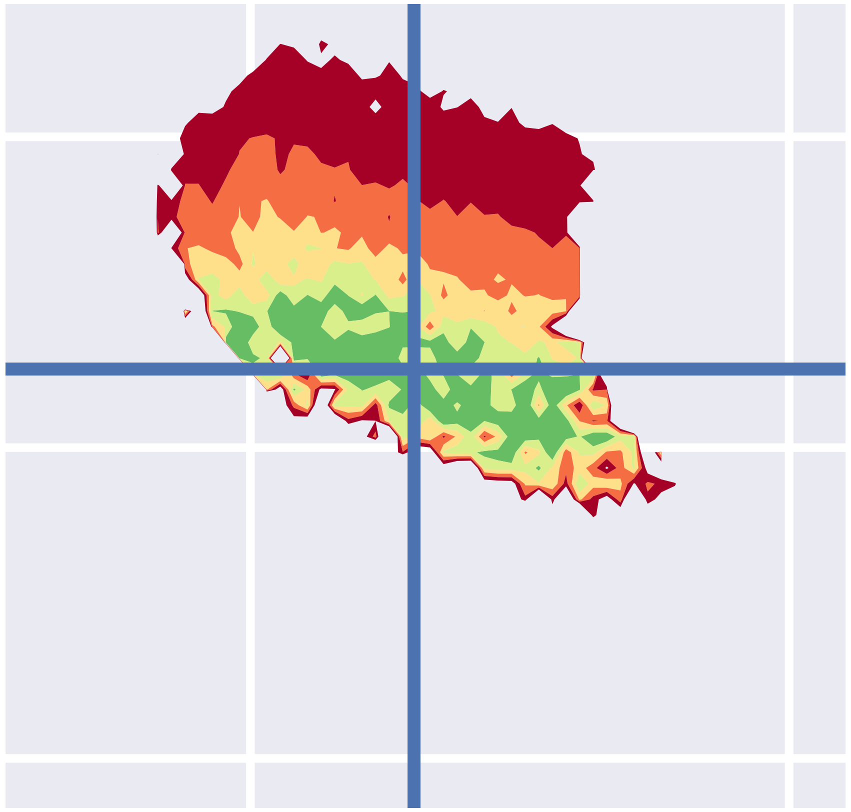
Bayesian PPDs

Importance resampling with two different data sets:



$\mathcal{D}_{A=2,3,4}$ $\mathcal{D}_{A=2,3,4,16}$

$p(E(\rho)/\{A,N\}\,|\,\mathscr{D}_{A=2,3,4,16}, I)$



Revisiting the leading order of χEFT

Power counting in chiral effective field theory and nuclear binding
by C.-J. Yang, A. Ekström, cf, G. Hagen, **Phys. Rev. C 103, 054304 (2021)**

The importance of few-nucleon forces in chiral effective field theory
by C.-J. Yang, A. Ekström, cf, G. Hagen, G. Rupak, U. Van Kolck, **arXiv:2109.13303**

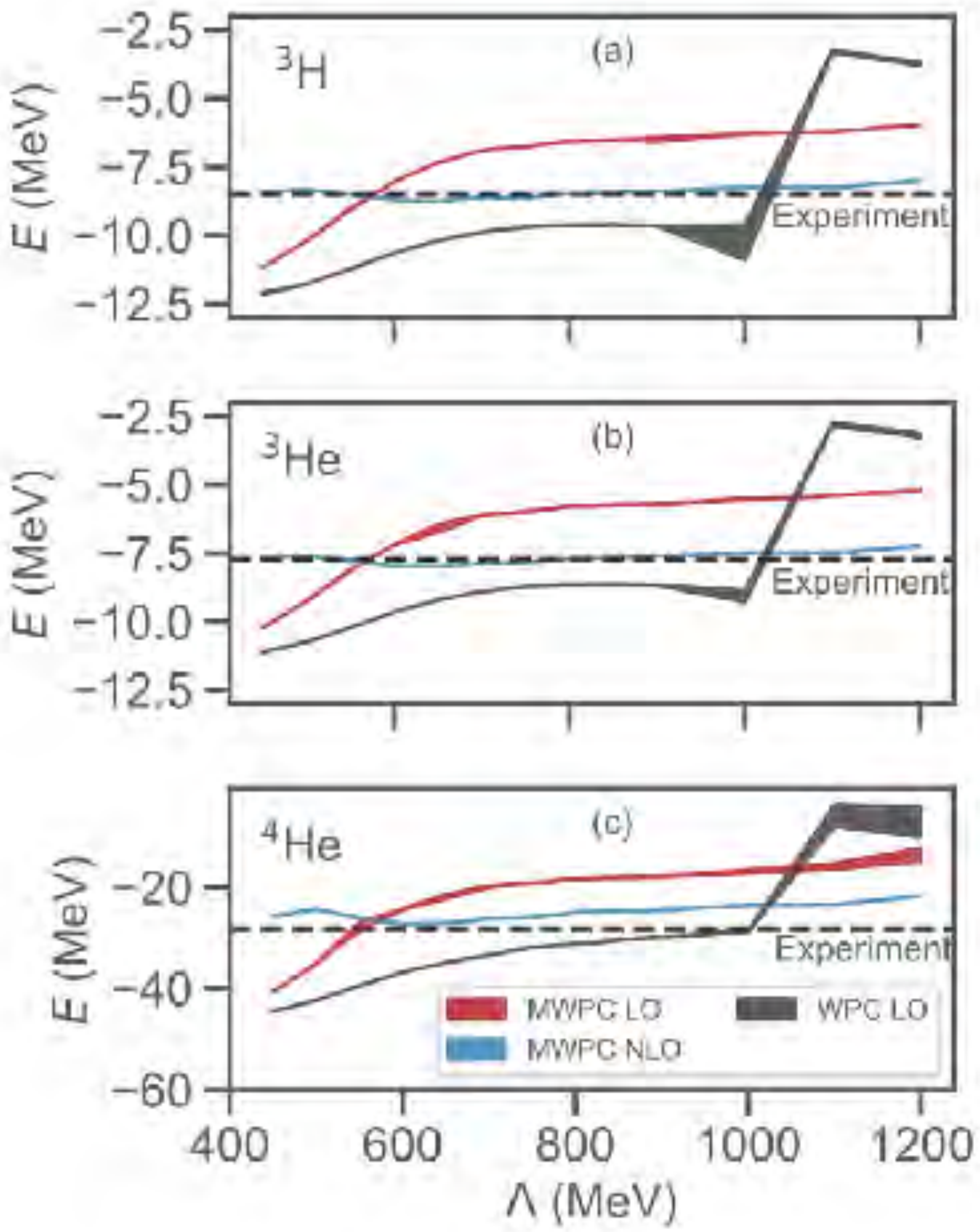
Bayesian Analysis of χEFT at Leading Order in a Modified Weinberg Power Counting
by O. Thim, E. May, A. Ekström, cf, **arXiv:2302.12624**

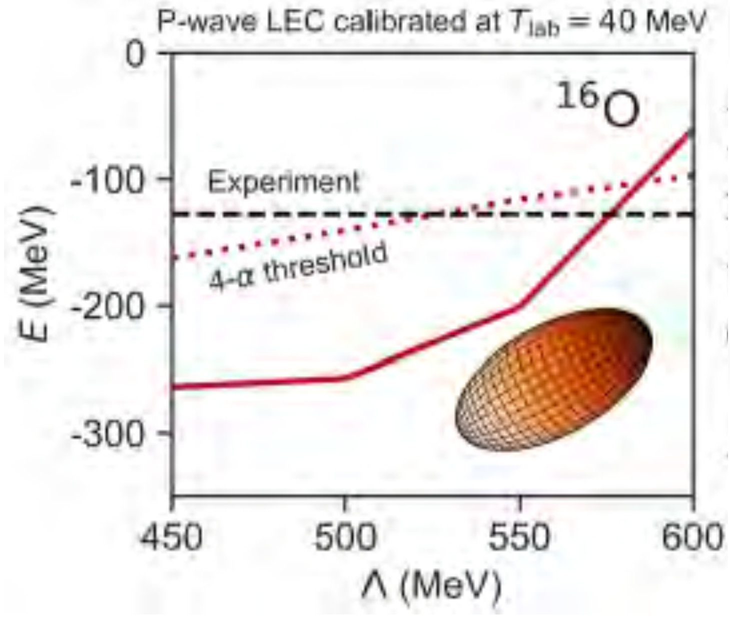
Leading-order nuclear physics?

- Power counting scheme? / RG invariance
- Leading order performance?
  - Full set of NN observables
  - Nuclear binding for A > 4
- Inclusion and importance of subleading physics?

$$V_{\mathrm{LO}}^{\mathrm{WPC}}(\mathbf{p},\mathbf{p}') = -\frac{g_A^2}{4f_\pi^2}\tau_1\cdot\tau_2\frac{(\sigma_1\cdot\mathbf{q})(\sigma_2\cdot\mathbf{q})}{m_\pi^2+\mathbf{q}^2} + \tilde{C}_{^1S_0} + \tilde{C}_{^3S_1}$$

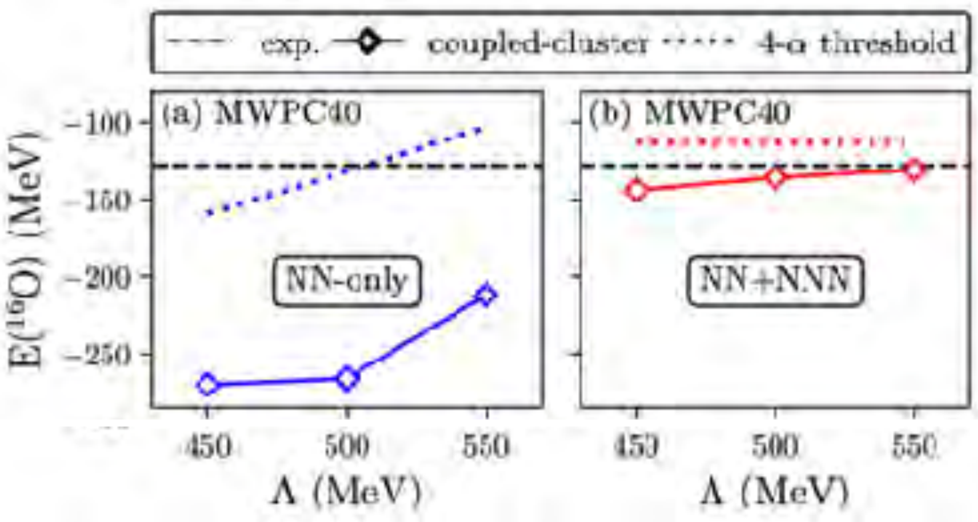
$$V_{\mathrm{LO}}^{\mathrm{MWPC}}(\mathbf{p},\mathbf{p}') = V_{\mathrm{LO}}^{\mathrm{WPC}}(\mathbf{p},\mathbf{p}') + \left(\tilde{C}_{^3P_0} + \tilde{C}_{^3P_2}\right)pp'$$



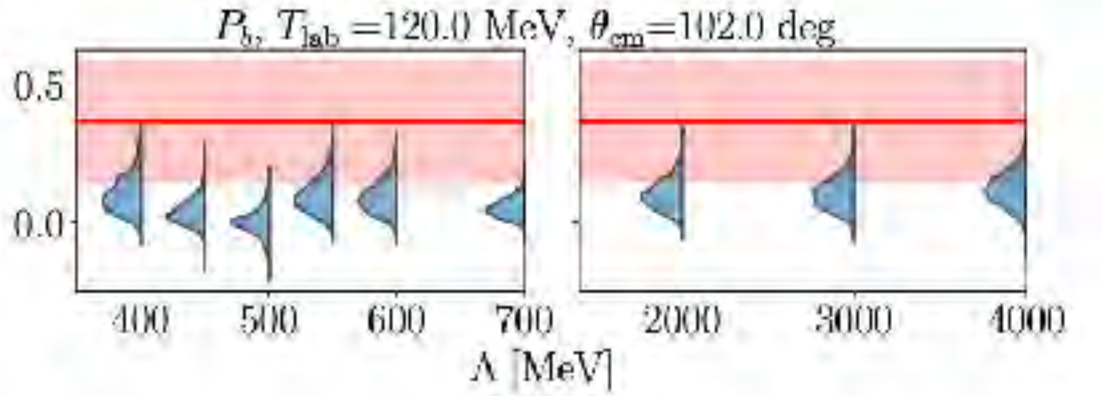


Possible issues (to be revisited)

- LO errors might be misspecified
  - Inference using the full NN data set tends to overestimate EFT errors
- The set of contact terms at LO might not be complete.
- LO might need to be complemented
  - sub-leading pion exchange,
  - many- nucleon interactions



- Fine tuning at LO
  - Revisit χEFT with modified WPC using Bayesian inference methods
  - Need to handle limit cycles, spurious states



See poster by Oliver Thim

Summary and outlook

- *The concept of **tension in science** relies on statements of uncertainties*
- It is natural to strive for **accuracy** in theoretical modelling; 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**.
- We have developed a unified ***ab initio* framework** to link the physics of NN scattering, few-nucleon systems, medium- and heavy-mass nuclei up to ^{208}Pb, and the nuclear-matter equation of state near saturation density.
- **Challenges**:
  - Get to know your uncertainties; sampling without tears.
  - Revisit the leading (and subleading) orders of χEFT