Precision nuclear theory

The quantification of precision in ab initio nuclear modelling: Computations of ^{208}Pb and the emergence of nuclear saturation in Δ-full χEFT

Christian Forssén, Chalmers University of Technology
Hirschegg, Austria, 2023/01/16

Precision

It is natural to strive for accuracy in theoretical modelling; but actual predictive power is rather associated with precision.

"The concept of tension in science relies on statements of uncertainties"

This presentation is about progress to quantify precision in nuclear theory

Outline

- Uncertainty Quantification for ab initio methods:
  - efforts and challenges
  - highlight Bayesian linear methods; importance resampling

arXiv:2212.13216 [pdf, other] nucl-th

Emulating \emph{ab initio} computations of infinite nucleonic matter

Authors: W. G. Jiang, C. Forssén, T. Djärv, G. Hagen

arXiv:2212.13203 [pdf, other] nucl-th

Emergence of nuclear saturation within Δ--full chiral effective field theory

Authors: W. G. Jiang, C. Forssén, T. Djärv, G. Hagen

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OPEN

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

Baishan Hu[1,11], Weiguang Jiang[2,11], Takayuki Miyagi[1,3,4,11], Zhonghao Sun[5,6,11], Andreas Ekström[2], Christian Forssén[2], Gaute Hagen[1,5,6], Jason D. Holt[1,7], Thomas Papenbrock[5,6], S. Ragnar Stroberg[8,9] and Ian Vernon[10]

ORIGINAL RESEARCH article

Front. Phys., 03 November 2022

Sec. Nuclear Physics

Bayesian probability updates using sampling/importance resampling: Applications in nuclear theory

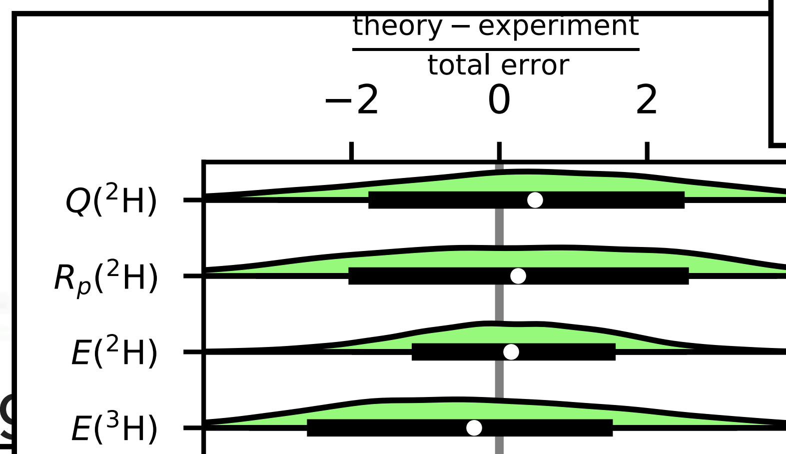
Weiguang Jiang* and Christian Forssén

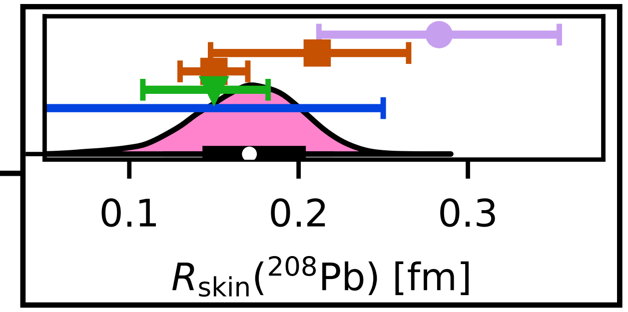
Recent UQ progress

Breakthroughs in

- effective field theory
- many-body methods
- Bayesian approaches
- emulator technology
- statistical learning

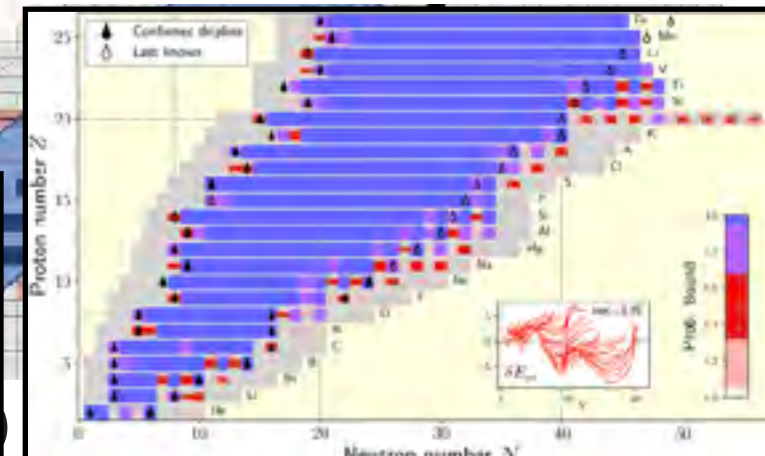
History matching





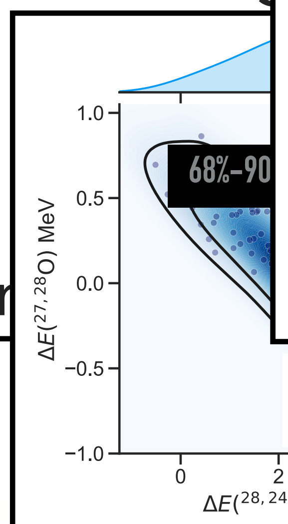
B. Hu et al Nature Physics (2022)

Bayesian linear regression

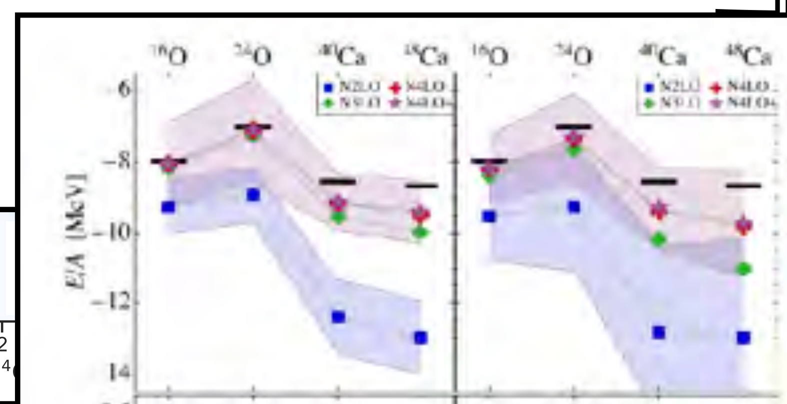


S. R. Stroberg et al PRL (2021)

Predicting



Truncation errors

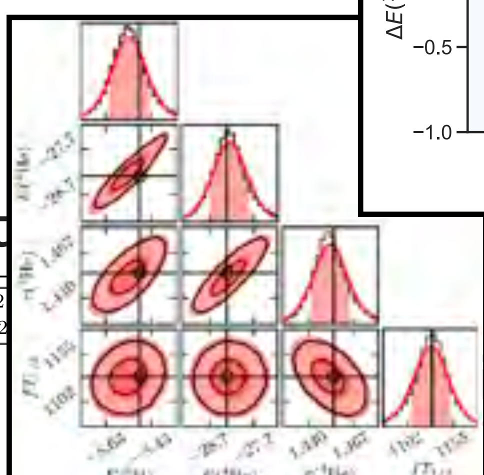


in prep.

P. Maris et al arXiv (2022)

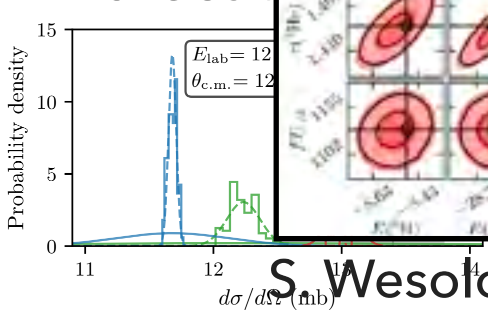
Light nuclei

Few-nucleon

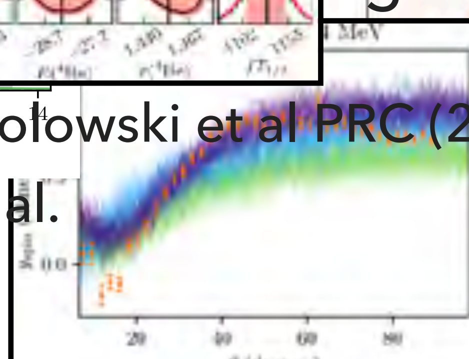


S. Wesolowski et al PRC (2021)

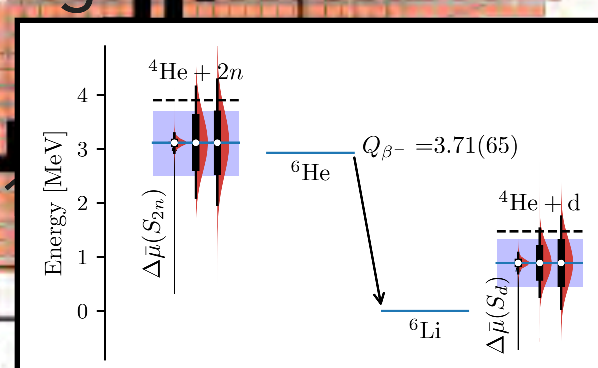
nd-scat



S. B. S. Miller et al.
(2022, arXiv)

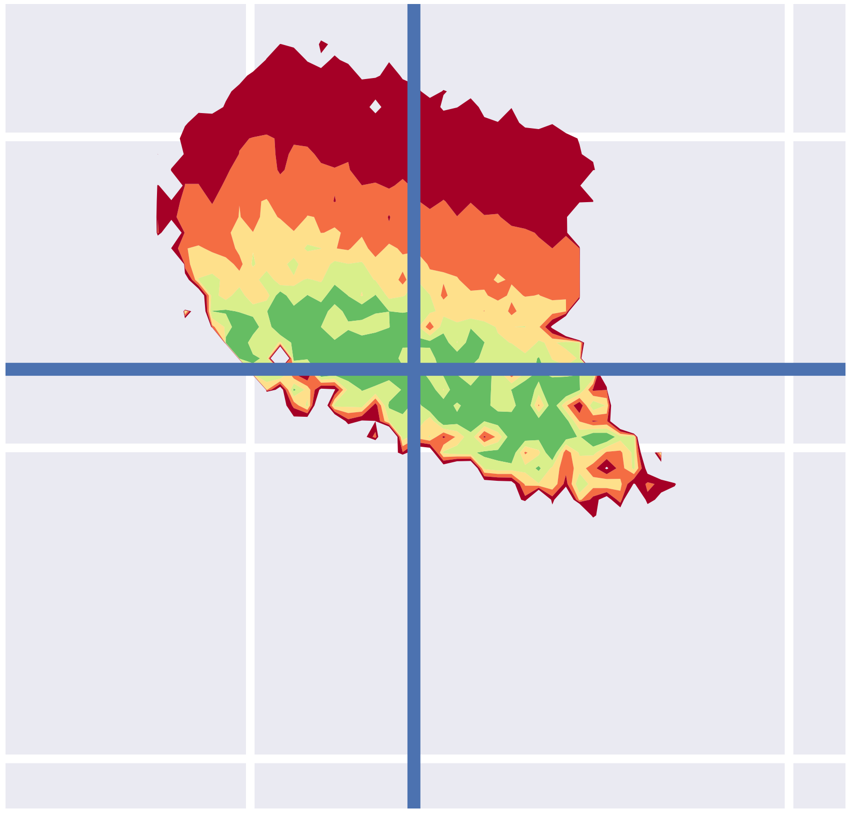


I. Svensson et al PRC (2022)



T. Djärv et al PRC (2022)

8
50
82
2022
Neutron number N



UQ FOR AB INITIO METHODS

Some terminology

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

Theoretical models

- Theoretical modelling: $\boldsymbol{y}(\boldsymbol{\alpha}) + \delta \boldsymbol{y}$
  with model **parameters** $\boldsymbol{\alpha}$

- Theoretical errors can have different origin; The inclusion of relevant errors is a prerequisite for precision theory:
  $\delta \boldsymbol{y} = \delta \boldsymbol{y}_{\mathrm{th,source1}} + \delta \boldsymbol{y}_{\mathrm{th,source2}} + \ldots$

- **Hard-to-compute** models: $y^{😡}(\boldsymbol{\alpha})$

- … might be **emulated** / designed at low fidelity
  $y^{😡} \to \tilde{y}^{😀} + \delta\tilde{y}$

- Note: there might be an $\boldsymbol{\alpha}$-dependence in the errors.

Learning from data via Bayes

- Apply **Bayes' theorem**

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

  - 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)

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

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

Ab initio modeling of nuclear systems using chiral EFT

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

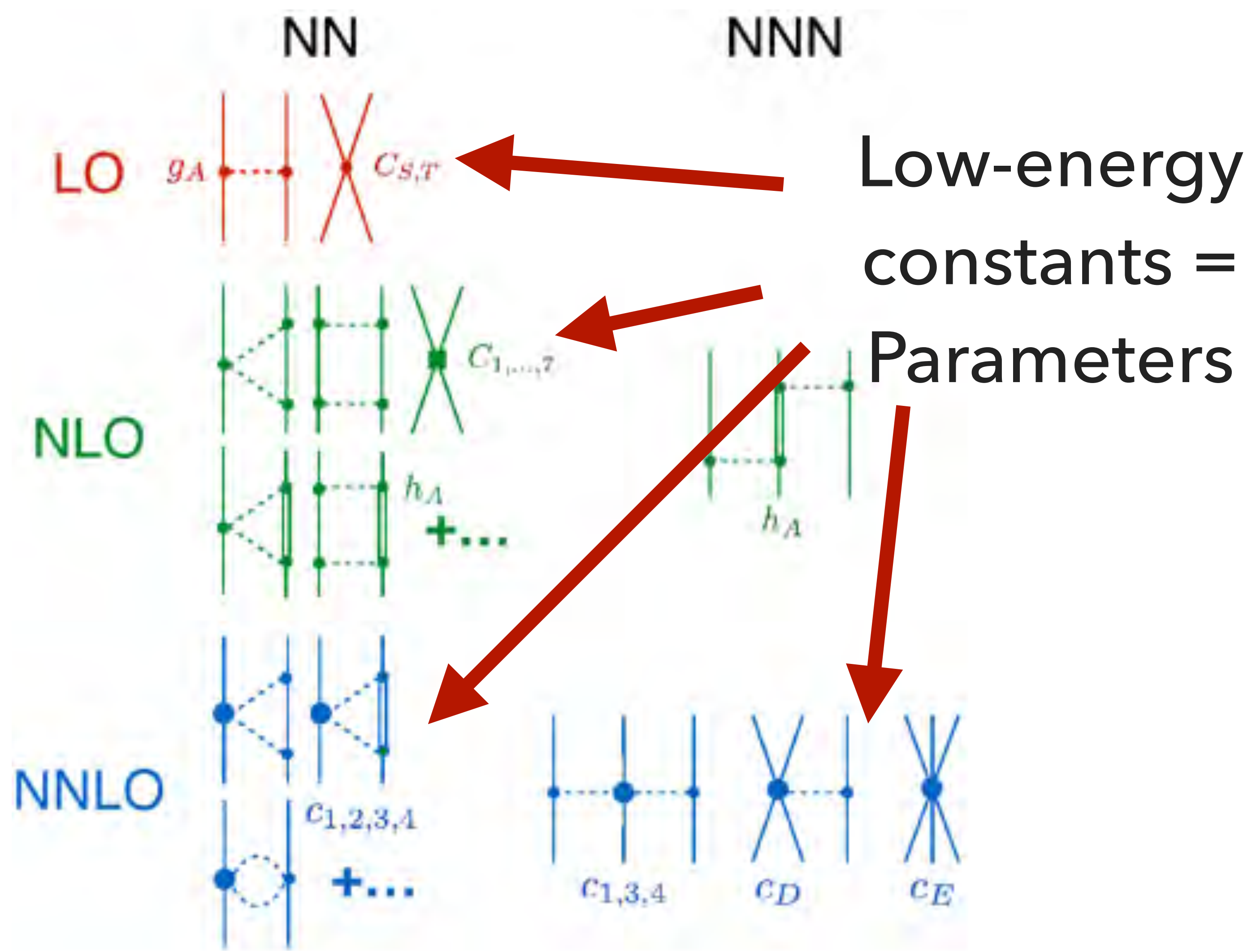
$$\hat{H}(\boldsymbol{\alpha}) = \hat{T} + \hat{V}(\boldsymbol{\alpha})$$

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

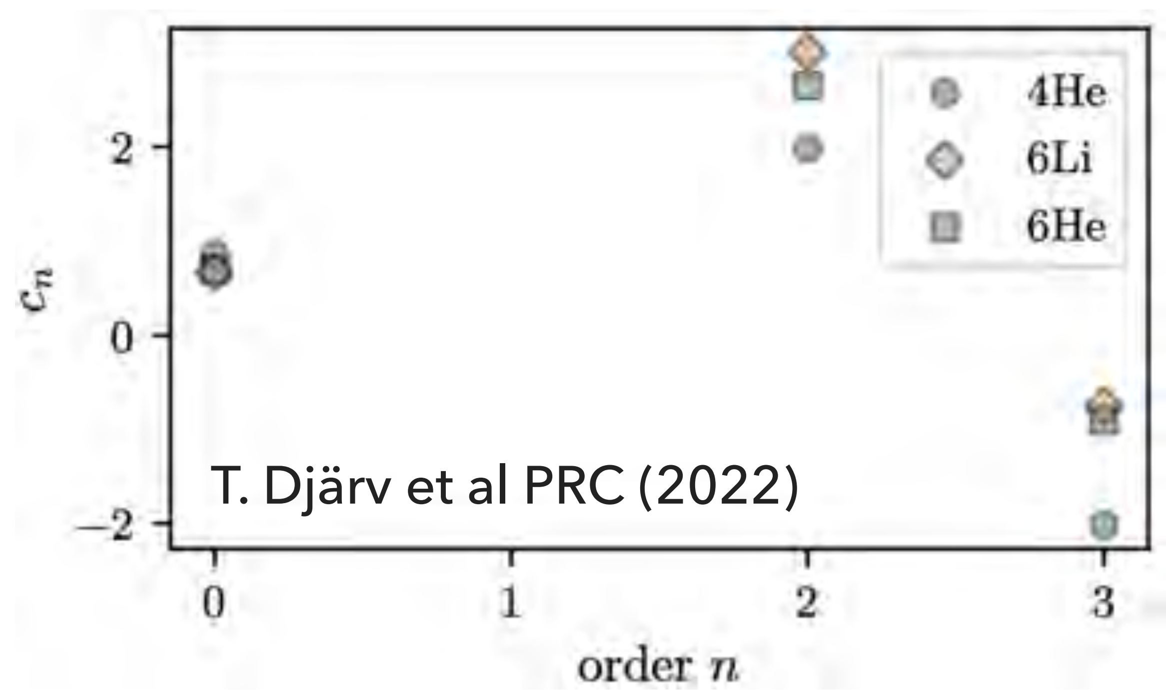


Weinberg, van Kolck, Kaiser, Bernard, Meißner, Epelbaum, Machleidt, Entem, …

A. Ekström, et al. Phys. Rev **C 97**, 024332 (2018)
W. Jiang, et al. Phys Rev **C 102,** 054301 (2020)

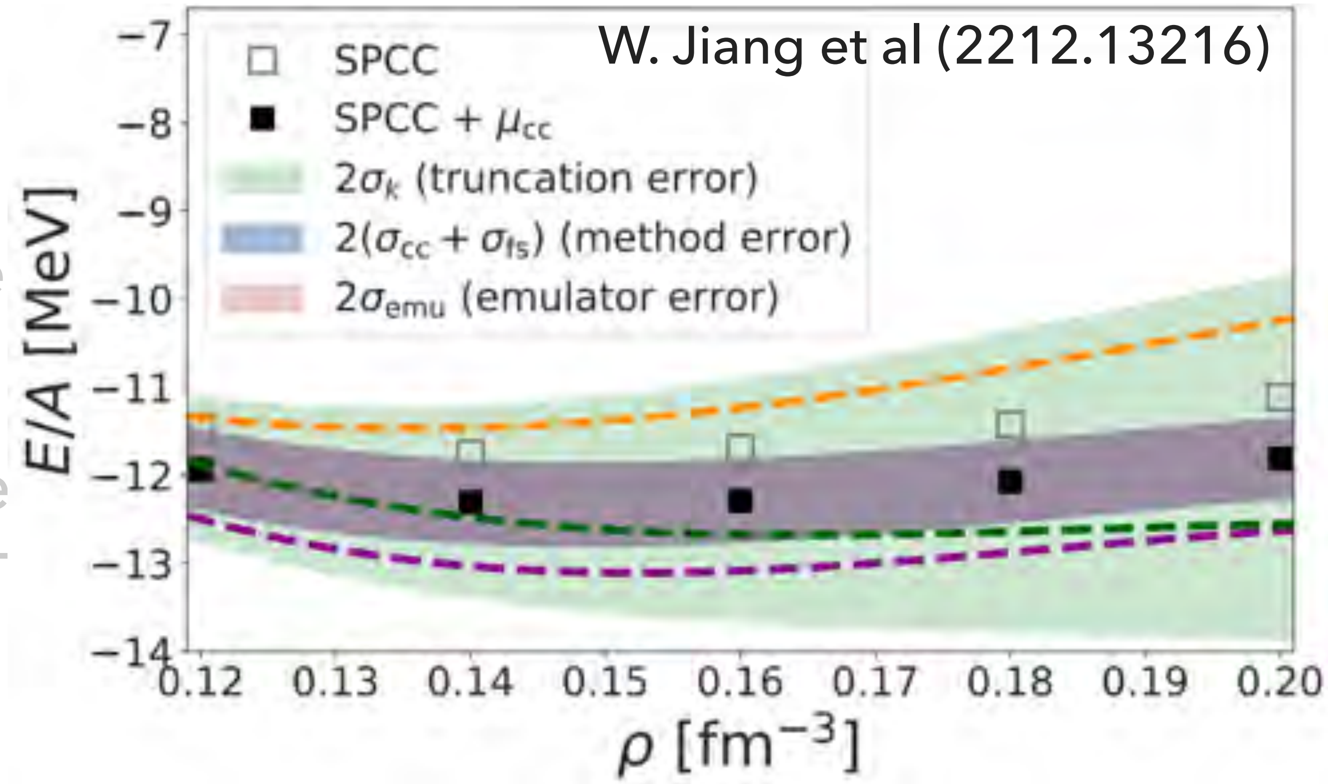
Challenge #1: Getting to know your errors

- **EFT truncation errors**
  - **Approach**: study order-by-order results and learn the PDF for expansion coefficients
    $$y_k = y_{\rm ref}\sum_{n=0}^{k} c_n Q^n, \quad \delta y_k = y_{\rm ref}\sum_{n=k+1}^{\infty} c_n Q^n$$
    (see Dick's talk)
  - **Challenges**: Cutoff dependence, expansion parameter, irregular convergence, correlation structure (e.g., are EFT errors for *E(A)*, r_p*(A)* correlated?),



Challenge #1: Getting to know your errors

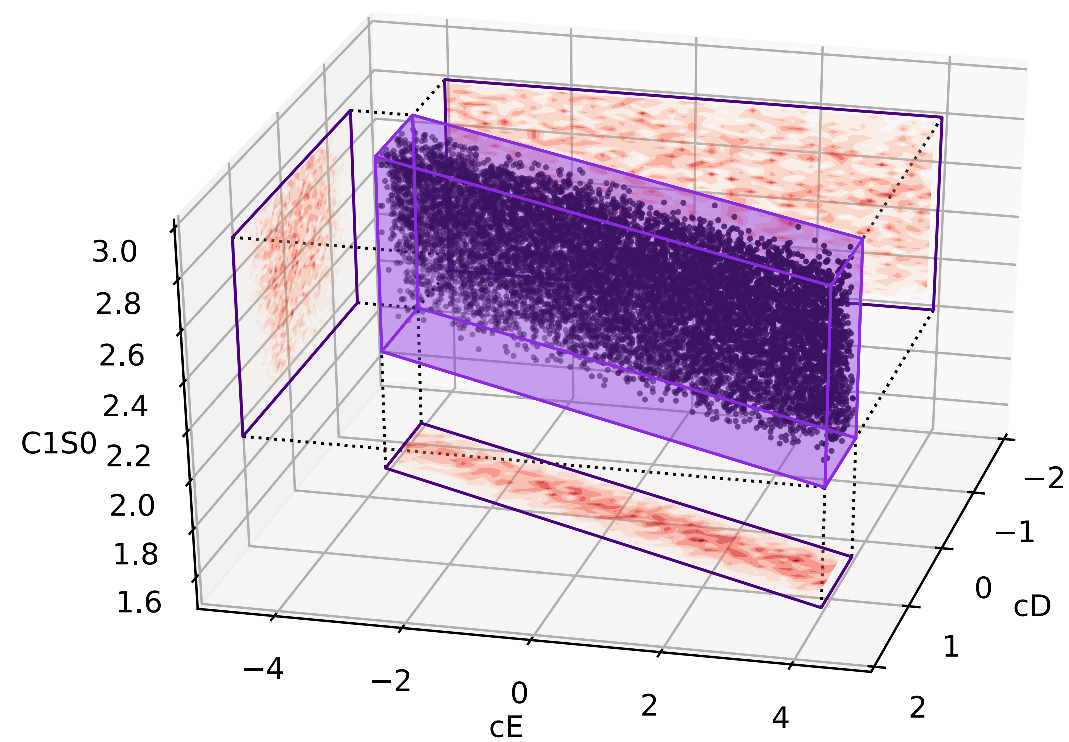
- **EFT truncation errors**
  - **Approach**: study orde oefficients (see Dick's talk)
  - **Challenges**: Cutoff de n structure (e.g., are EFT



- **Many-body errors**
  - **Approach**: Convergence studies; Method comparisons;
  - **Note**: We can incorporate "uncertain" extrapolation, $\mathbb{E}[\delta y_{\mathrm{MB}}] \neq 0$
  - **Challenges**: Some approximations might be very difficult to relax; Non-variational observables/approaches
- **Emulator errors**
  - **Approach**: Cross-validation, EC offers rapid convergence with N_{sub}
  - **Challenges**: Outliers. EC convergence (Sarkar and Lee)

Challenge #2: A PDF is more than just a mean and a variance

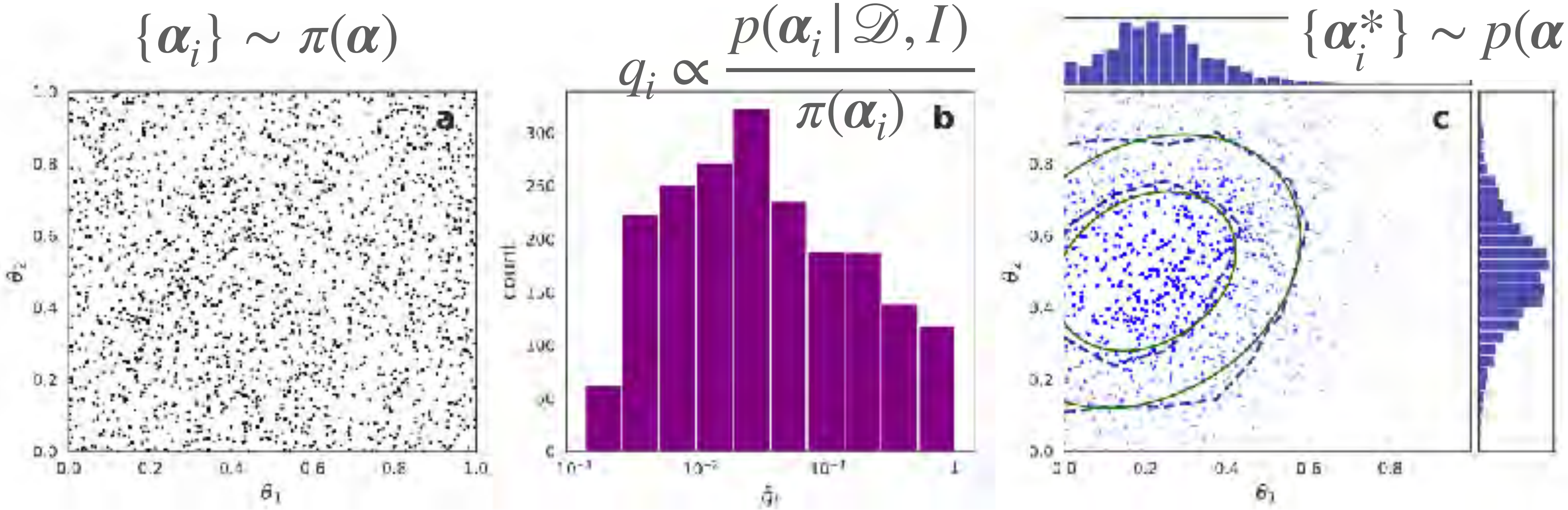
- A PDFs is not uniquely defined by its mean and variance! Consider also covariances (dependencies) and functional forms.
- Marginalization over nuisance parameters (such as the EFT breakdown scale) tends to introduce heavier tails.
- Still, Bayesian linear methods (only means and variances) can be very useful
  - Easier to claim non-implausibility than to quantify likelihood
    $\Theta_{\rm NI}(\boldsymbol{\alpha})$ versus $p(\mathscr{D}\,|\,\boldsymbol{\alpha}, I) \equiv \mathscr{L}(\boldsymbol{\alpha})$
  - Define implausibility measure (using only means and variances)
  - Idea of History Matching:
    Iteratively remove regions with $\Theta_{\rm NI}(\boldsymbol{\alpha}) = 0$

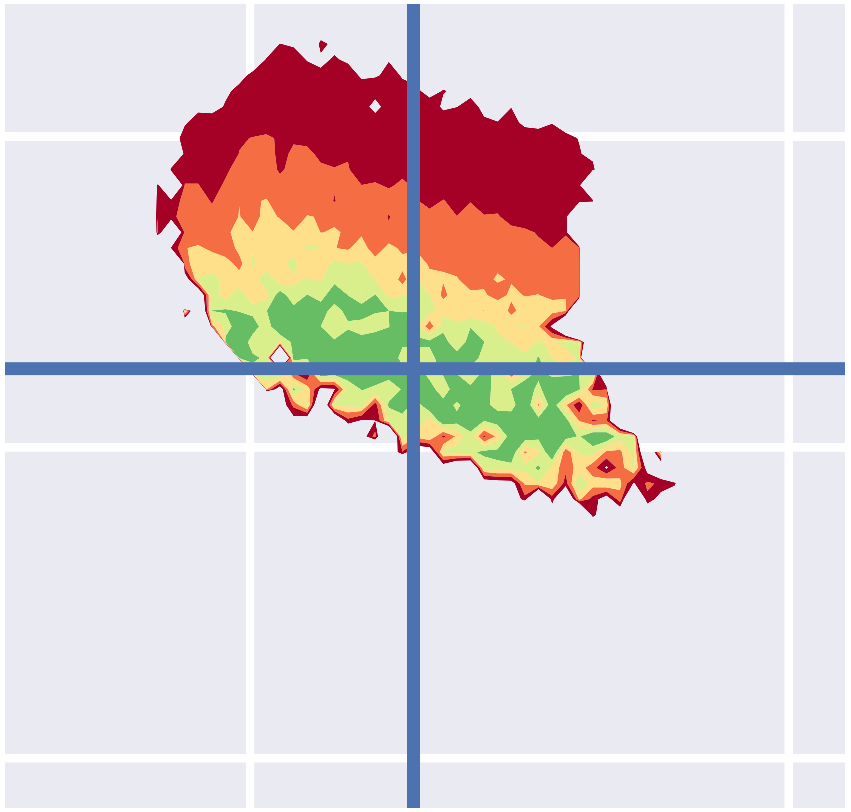


Challenge #3: Sampling without tears

- MCMC **sampling is costly**;
  - might appear unsurmountable when involving costly models
- Random walks suffer from **correlated samples** $\Rightarrow$ wasted CPU-h
  - If possible, try ***Hamiltonian Monte Carlo*** (see Andreas' talk)
- Bayesian **updating**: $p(\boldsymbol{\alpha}\,|\,\mathscr{D}_1, \mathscr{D}_2, I) \approx N p(\mathscr{D}_2\,|\,\boldsymbol{\alpha}, I) p(\boldsymbol{\alpha}\,|\,\mathscr{D}_1, I)$
- **Importance resampling**
  [Jiang and Forssén (2210.02507), Rubin (1988), Smith and Gelfand (1971)]

$\{\boldsymbol{\alpha}_i\} \sim \pi(\boldsymbol{\alpha})$ $\quad$ $q_i \propto \dfrac{p(\boldsymbol{\alpha}_i\,|\,\mathscr{D}, I)}{\pi(\boldsymbol{\alpha}_i)}$ $\quad$ $\{\boldsymbol{\alpha}_i^*\} \sim p(\boldsymbol{\alpha}\,|\,\mathscr{D}, I)$





EMERGENCE OF NUCLEAR SATURATION

arXiv:2212.13216 [pdf, other] nucl-th

Emulating \emph{ab initio} computations of infinite nucleonic matter

Authors: W. G. Jiang, C. Forssén, T. Djärv, G. Hagen

arXiv:2212.13203 [pdf, other] nucl-th

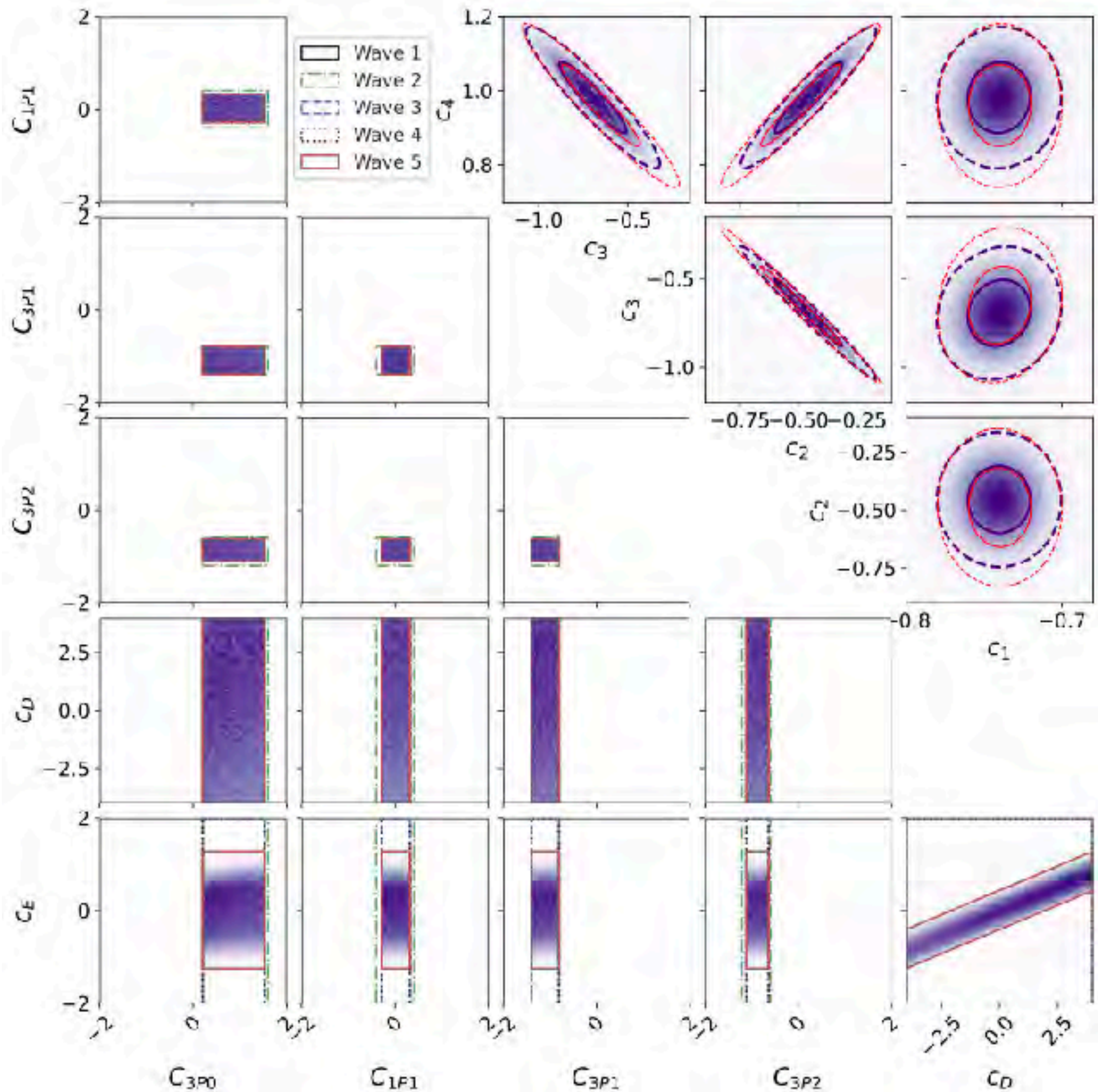
Emergence of nuclear saturation within Δ--full chiral effective field theory

Authors: W. G. Jiang, C. Forssén, T. Djärv, G. Hagen

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

- 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: iterative parameter volume reduction



History matching:

I. Vernon, et al. (Bayesian Anal., 2010)

I. Vernon, et al. (BMC Systems Biology, 2018)

B. Hu et al. (Nature Phys., 2022)

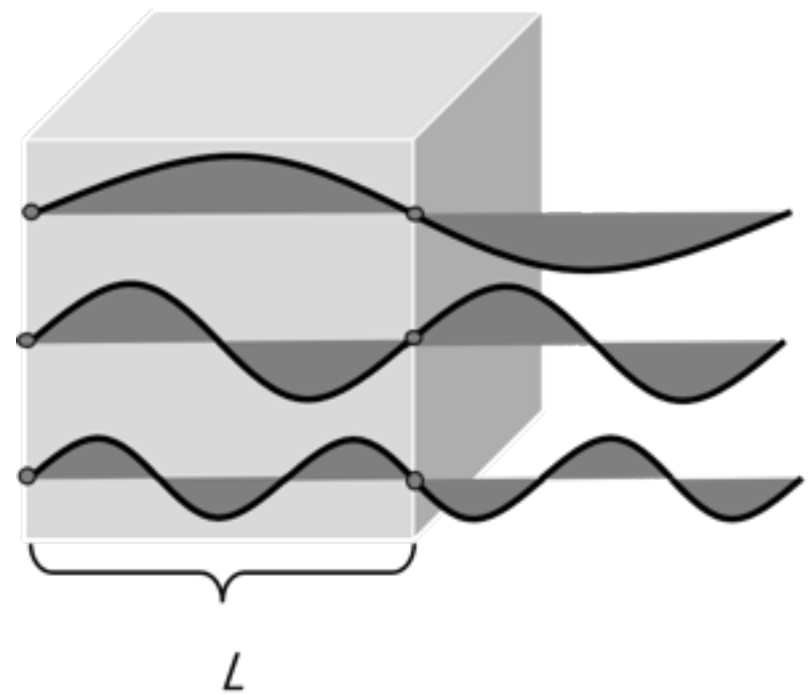
$$I_M^2(\alpha) \equiv \max_{z_i \in \mathcal{Z}} \frac{\left| \mathbb{E}\left[\tilde{f}_i(\alpha)\right] - z_i \right|^2}{\mathrm{Var}\left[\tilde{f}_i(\alpha) - z_i\right]}$$

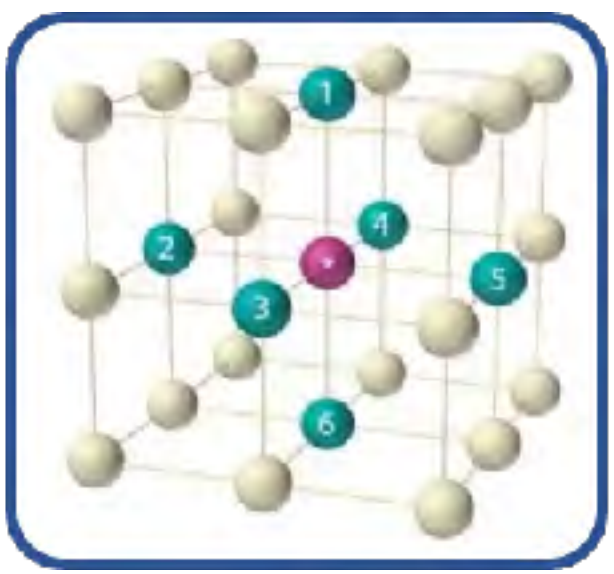
$$I_M(\alpha) > c_M$$

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 $n_{\max}$

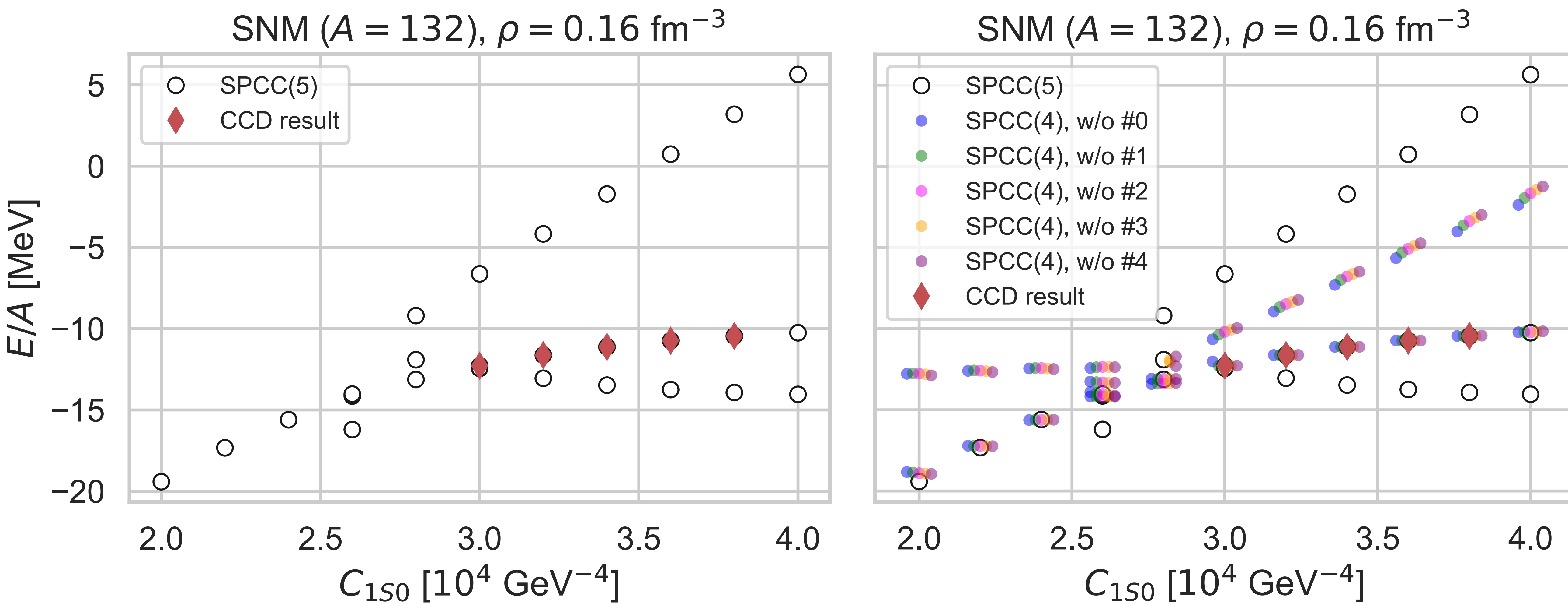
- Periodic boundary conditions
  $\psi_k(x + L) = \psi_k(x)$





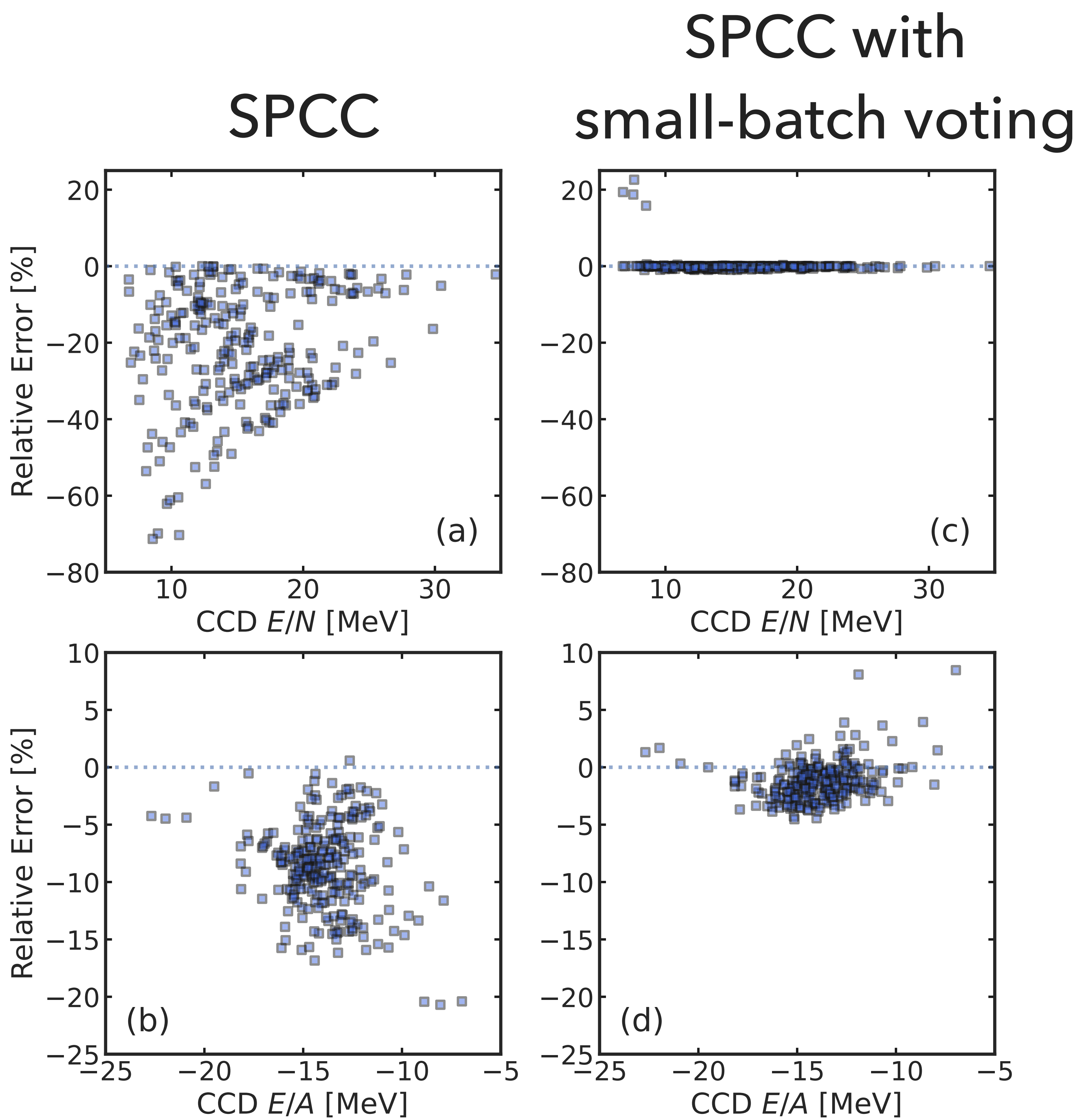
- The box size (L) and the nucleon number (N) controls the density (ρ)
- Computational challenge ($n_{\max} = 4$):
  - PNM: 1458 orbits with 66 neutrons
  - SNM: 2916 orbits with 132 nucleons

SPCC nuclear-matter emulators (1-dim example)

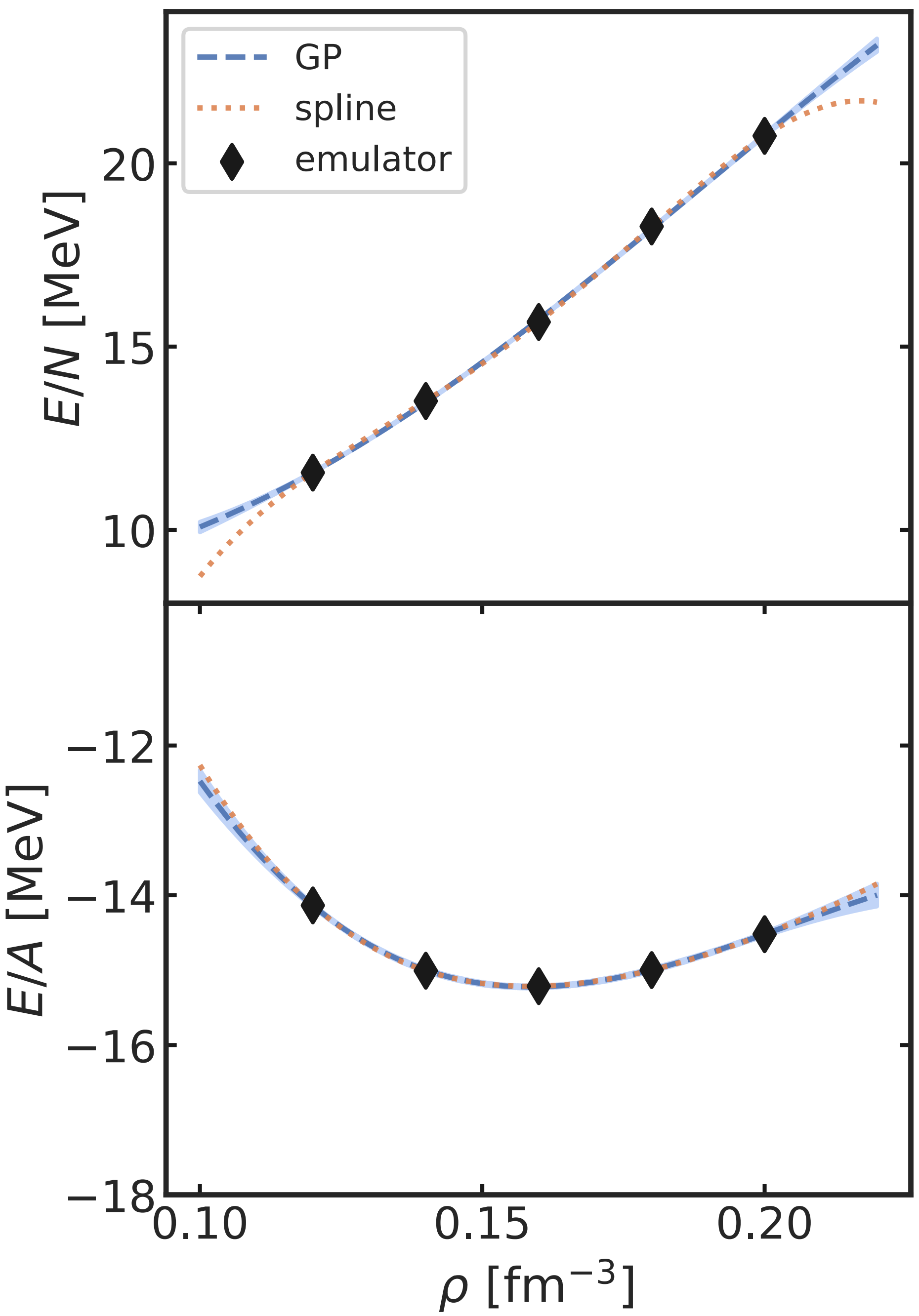


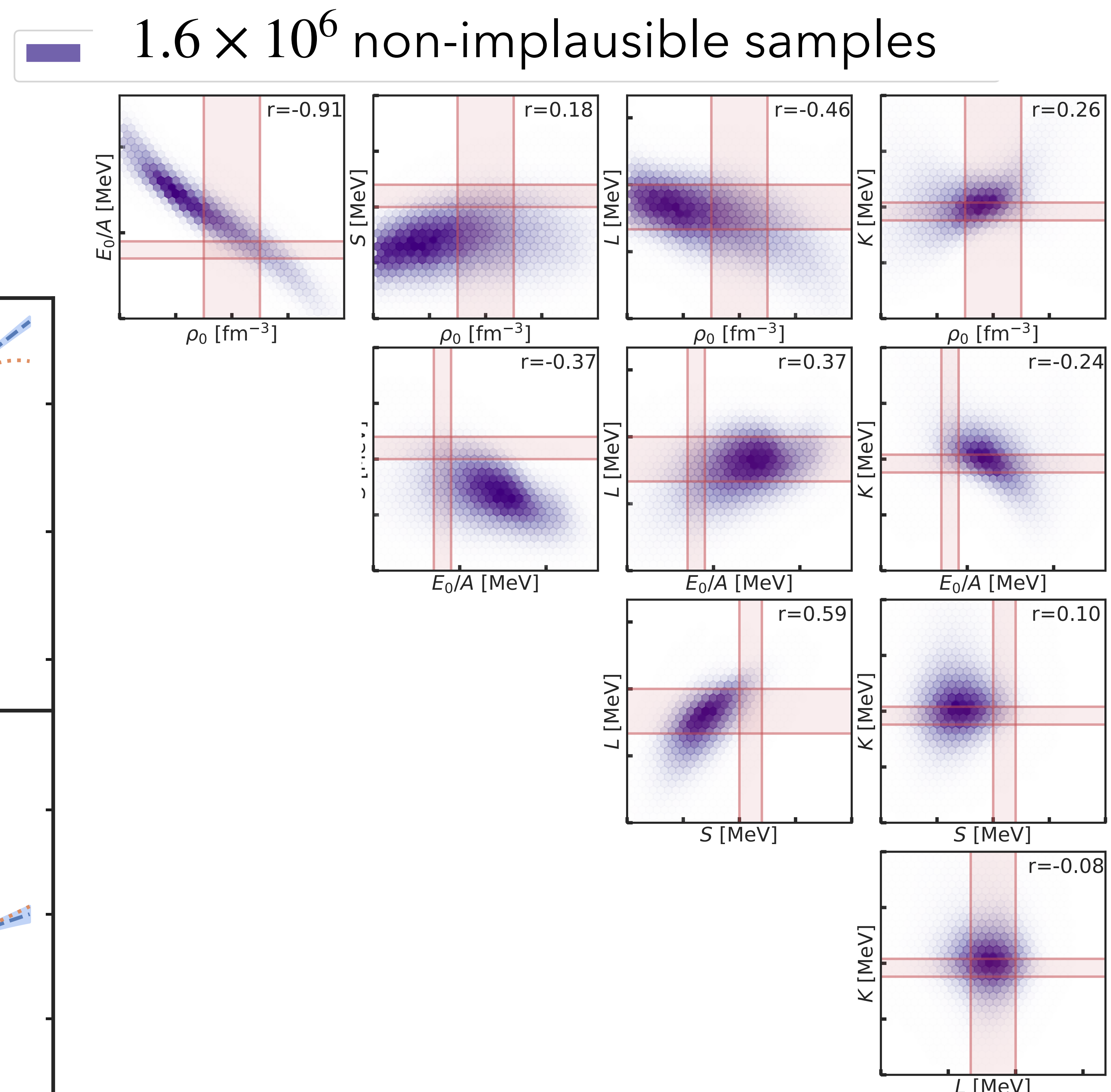
$$|\,\Psi(\boldsymbol{\alpha}_{\odot})\rangle = e^{T(\boldsymbol{\alpha}_{\odot})}\,|\,\Phi_0\rangle \approx \sum_{i=1}^{N_{\rm sub}} c_i^{\star}\,|\,\Psi_i\rangle$$

Small-batch voting



Correlation study



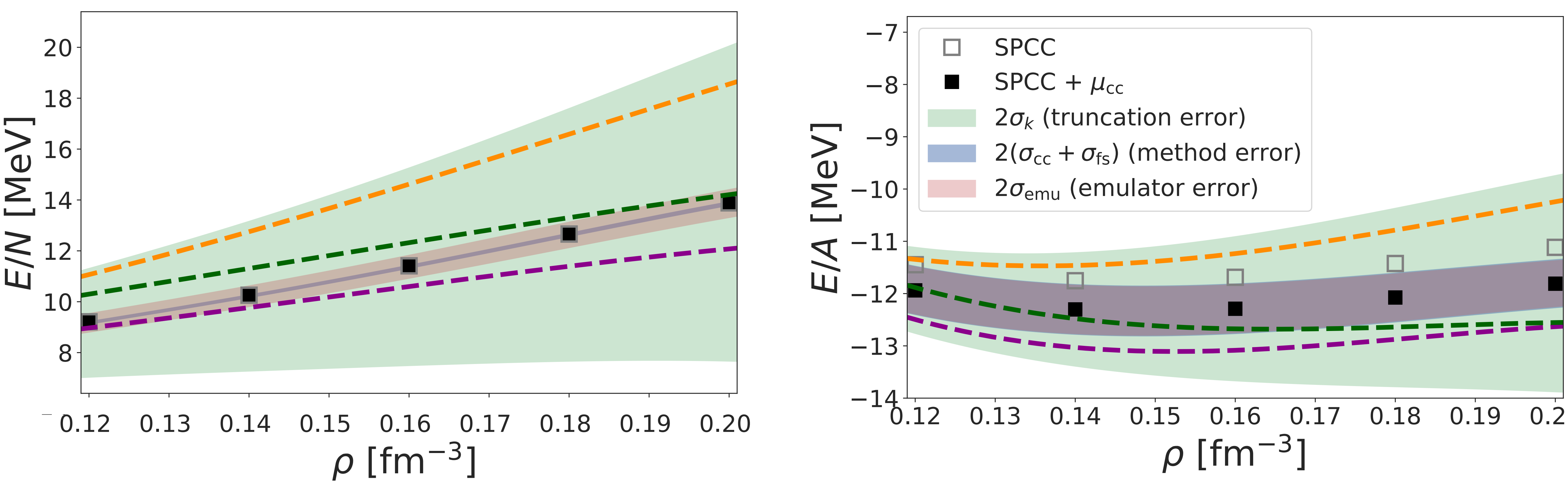


Bayesian machine-learning error model(s)

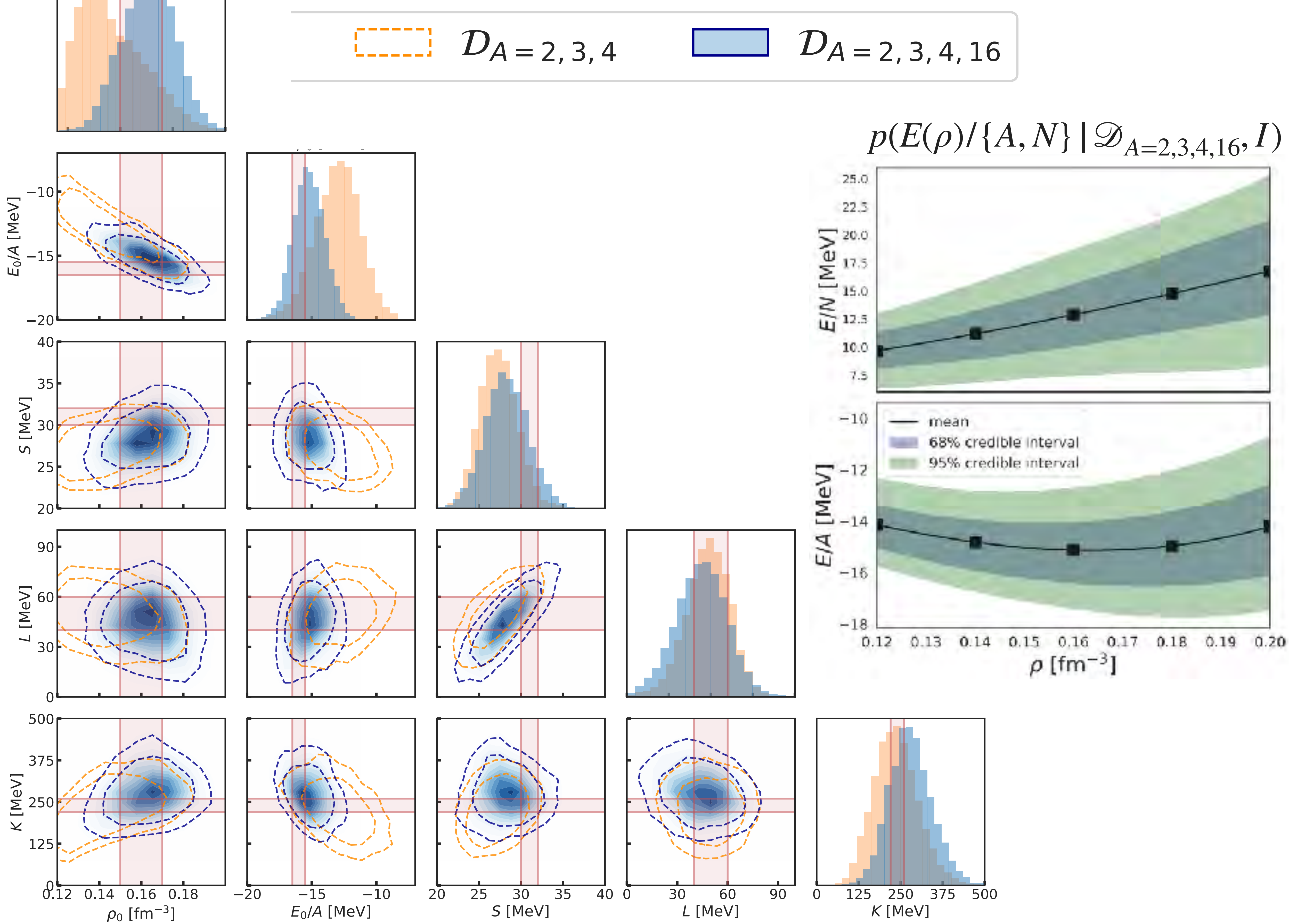
$$z = \tilde{y}(\boldsymbol{\alpha}) + \delta \boldsymbol{y}_{\mathrm{EFT}} + \delta \boldsymbol{y}_{\mathrm{method}} + \delta \tilde{\boldsymbol{y}}_{\mathrm{em}} + \delta \boldsymbol{y}_{\mathrm{exp}}$$

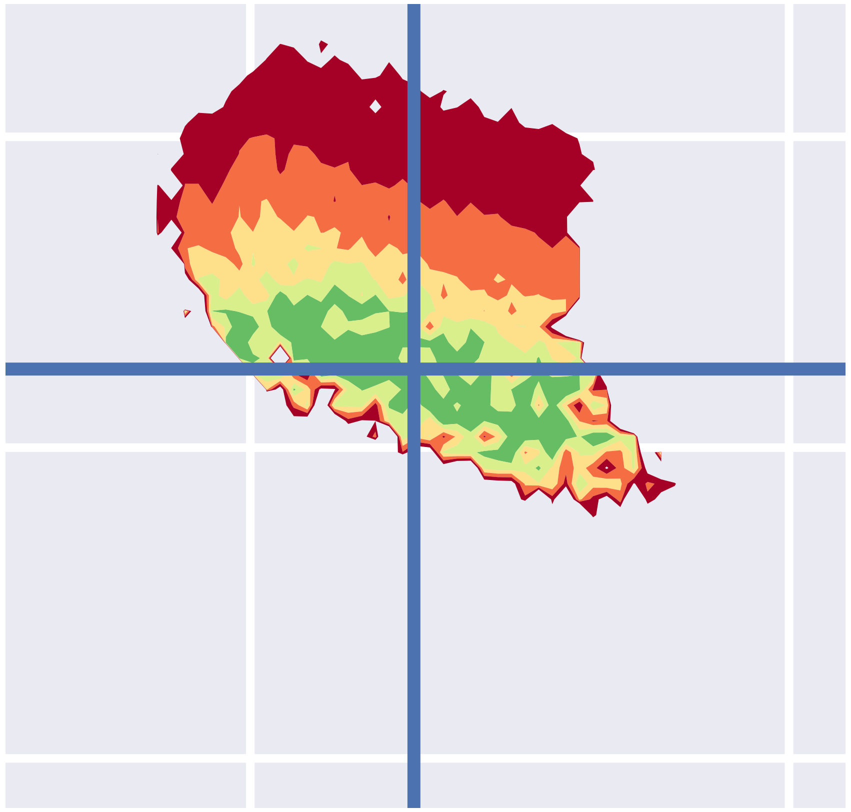
$$\varepsilon_\kappa(\rho) \mid \bar{c}_\kappa^2, l_\kappa, \sim GP[\mu_\kappa(\rho), \bar{c}_\kappa^2 R_\kappa(\rho, \rho'; l_\kappa)],$$

See C. Drischler et al (2020)



Bayesian PPD





^{208}PB NEUTRON SKIN

nature physics

ARTICLES

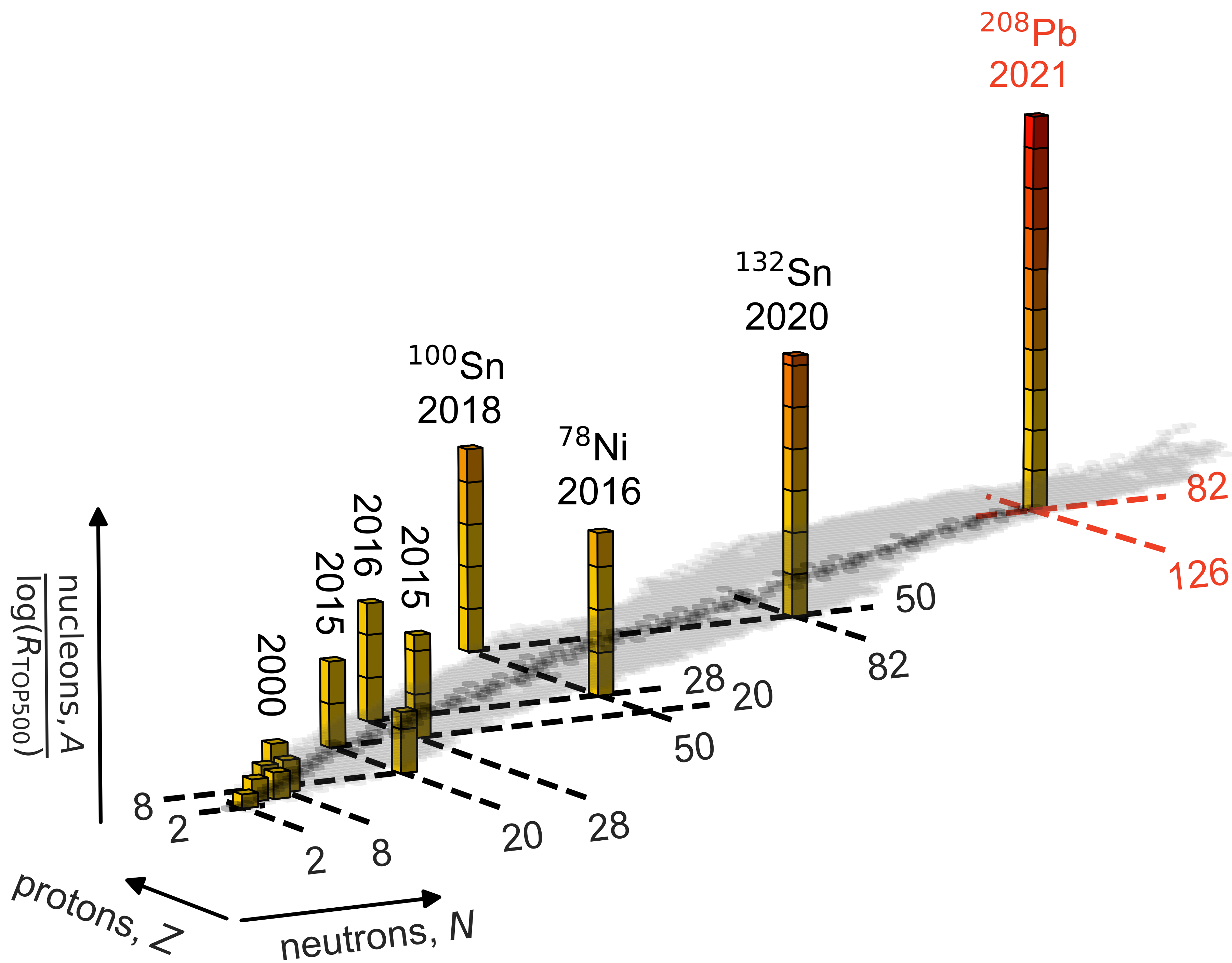
https://doi.org/10.1038/s41567-022-01715-8

OPEN

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

Baishan Hu[1,11], Weiguang Jiang[2,11], Takayuki Miyagi[1,3,4,11], Zhonghao Sun[5,6,11], Andreas Ekström[2], Christian Forssén[2] ✉, Gaute Hagen[1,5,6], Jason D. Holt[1,7], Thomas Papenbrock[5,6], S. Ragnar Stroberg[8,9] and Ian Vernon[10]

Trend of realistic ab initio computations



B. Hu et al (Nature Phys. 2022)

See Takayuki's talk

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

- $\chi\mathrm{EFT}$ **with explicit Δ isobar** (higher breakdown scale)
- 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 finite number of non-implausible samples.
- Bayesian **posterior predictive** distributions for nuclear observables up to ^{208}Pb and for infinite nuclear matter properties.

Trend of realistic ab initio computations

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.

M. Hoferichter et al, Phys. Rev. Lett. **115**, 192301 (2015)

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

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.

See Takayuki's talk

H. Hergert, et al. Phys Rep. **621** 165 (2016)

G. Hagen, et al. Rep. Prog. Phys. **77**, 096302 (2014)

3NFs are captured using the NO2B approx. Large emax & E3max spaces (14 & 28 in lead-208) yield near model-space convergence. For lead-208: 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%

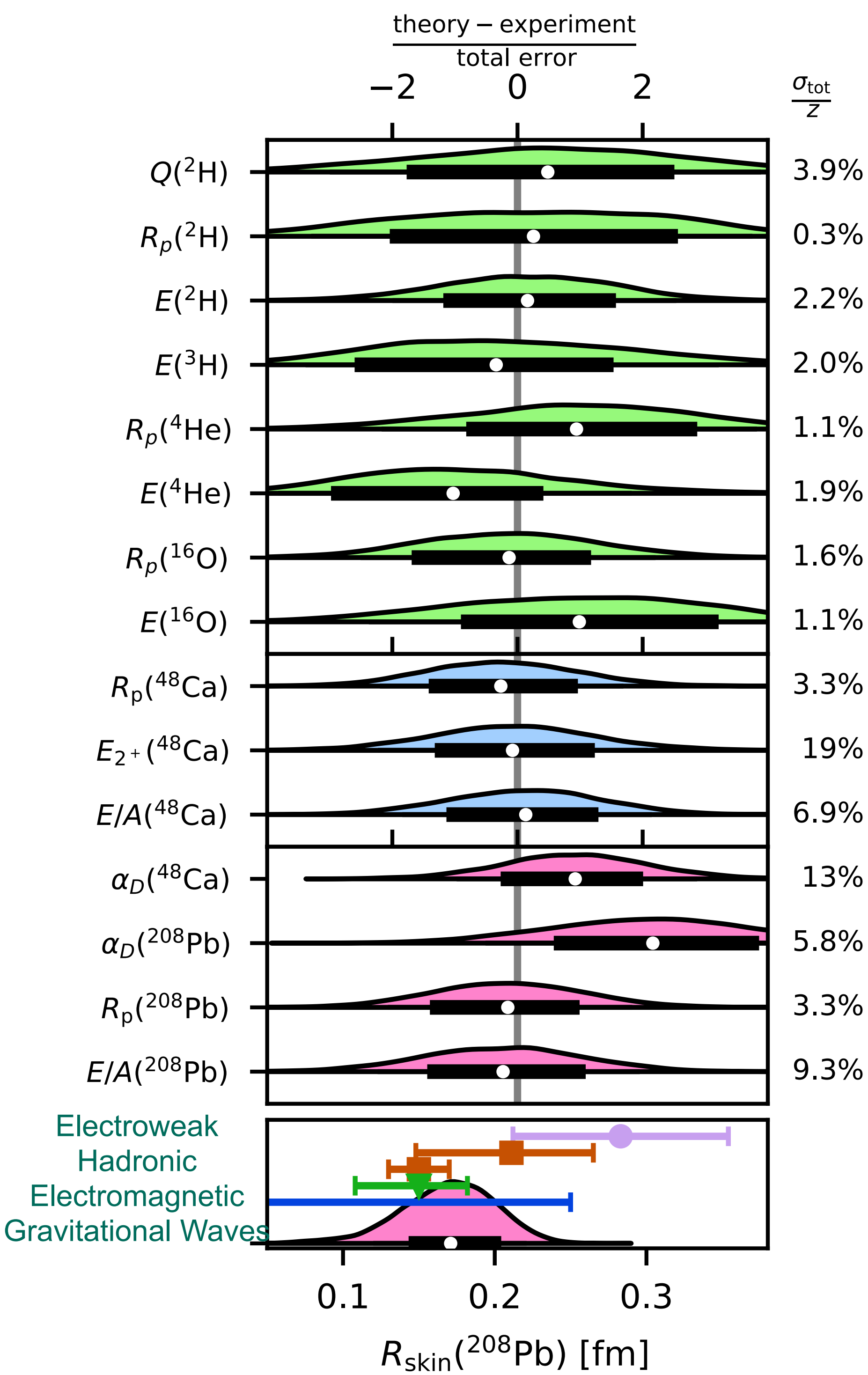
A. Ekström and G. Hagen Phys. Rev. Lett. **123**, 252501 (2019)

S. König, et al. Phys. Lett. **B 810**, 135814 (2020)

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 lead-208 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
$E(^2\mathrm{H})$	-2.2246	0.0	0.05	0.0005	0.001%	$-2.22^{+0.07}_{-0.07}$
$R_p(^2\mathrm{H})$	1.976	0.0	0.005	0.0002	0.0005%	$1.98^{+0.01}_{-0.01}$
$Q(^2\mathrm{H})$	0.27	0.01	0.003	0.0005	0.001%	$0.28^{+0.02}_{-0.02}$
$E(^3\mathrm{H})$	-8.4821	0.0	0.17	0.0005	0.01%	$-8.54^{+0.34}_{-0.37}$
$E(^4\mathrm{He})$	-28.2957	0.0	0.55	0.0005	0.01%	$-28.86^{+0.86}_{-1.01}$
$R_p(^4\mathrm{He})$	1.455	0.0	0.016	0.0002	0.003%	$1.47^{+0.03}_{-0.03}$
$E(^{16}\mathrm{O})$	127.62	0.0	1.0	0.75	0.5%	$-126.2^{+3.0}_{-2.8}$
$R_p(^{16}\mathrm{O})$	2.58	0.0	0.03	0.01	0.5%	$2.57^{+0.09}_{-0.06}$

Calibration observables

Observable	z	ε_{exp}	ε_{model}	ε_{method}	ε_{em}	PPD
$E/A(^{48}\mathrm{Ca})$	-8.667	0.0	0.54	0.25	—	$-8.58^{+0.72}_{-0.72}$
$E_{2^+}(^{48}\mathrm{Ca})$	3.83	0.0	0.5	0.5	—	$3.79^{+0.90}_{-0.96}$
$R_p(^{48}\mathrm{Ca})$	3.39	0.0	0.11	0.03	—	$3.36^{+0.14}_{-0.13}$

Validation observables

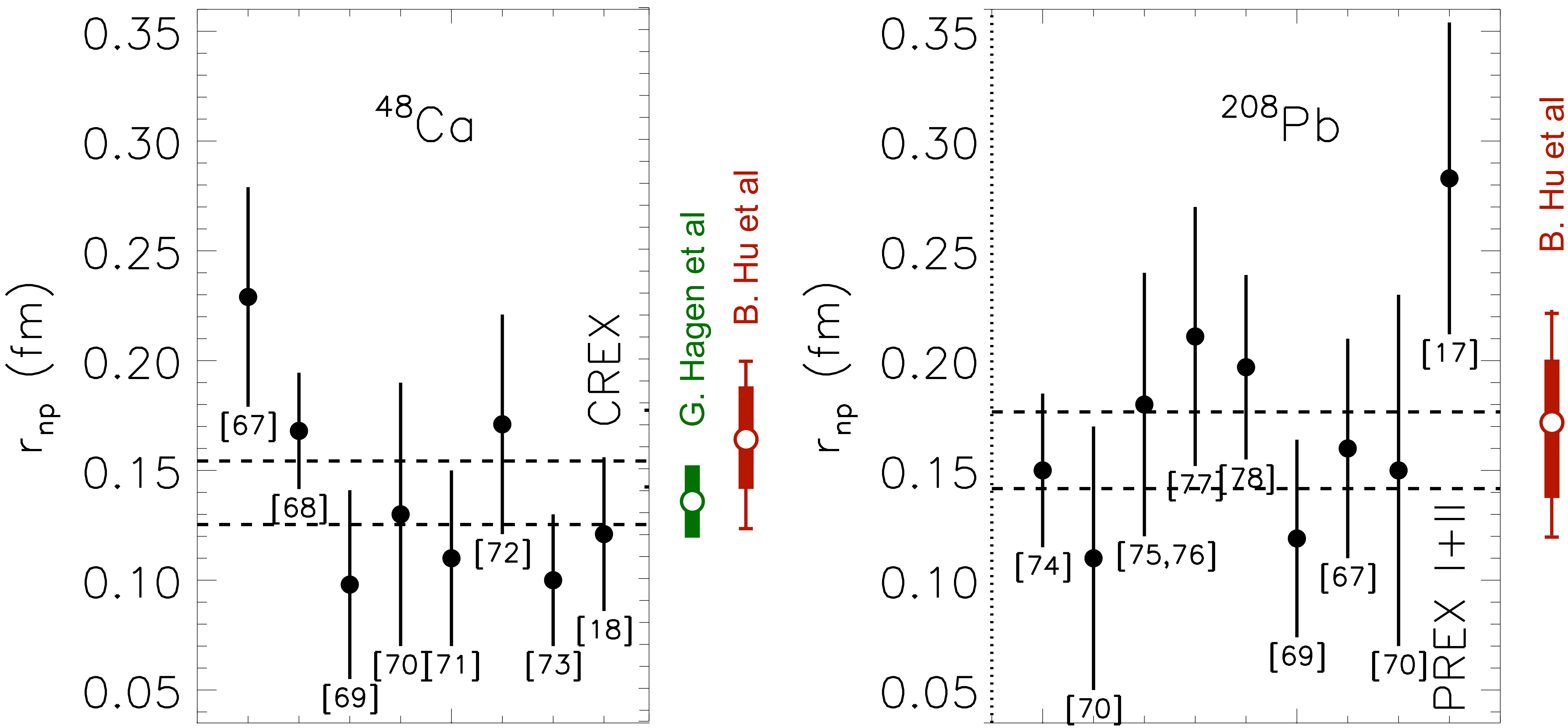
Observable	z	ε_{exp}	ε_{model}	ε_{method}	ε_{em}	PPD
$E/A(^{208}\mathrm{Pb})$	-7.867	0.0	0.54	0.5	—	$-8.06^{+0.99}_{-0.88}$
$R_p(^{208}\mathrm{Pb})$	5.45	0.0	0.17	0.05	—	$5.43^{+0.21}_{-0.23}$
$\alpha_D(^{48}\mathrm{Ca})$	2.07	0.22	0.06	0.1	—	$2.30^{+0.31}_{-0.26}$
$\alpha_D(^{208}\mathrm{Pb})$	20.1	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)

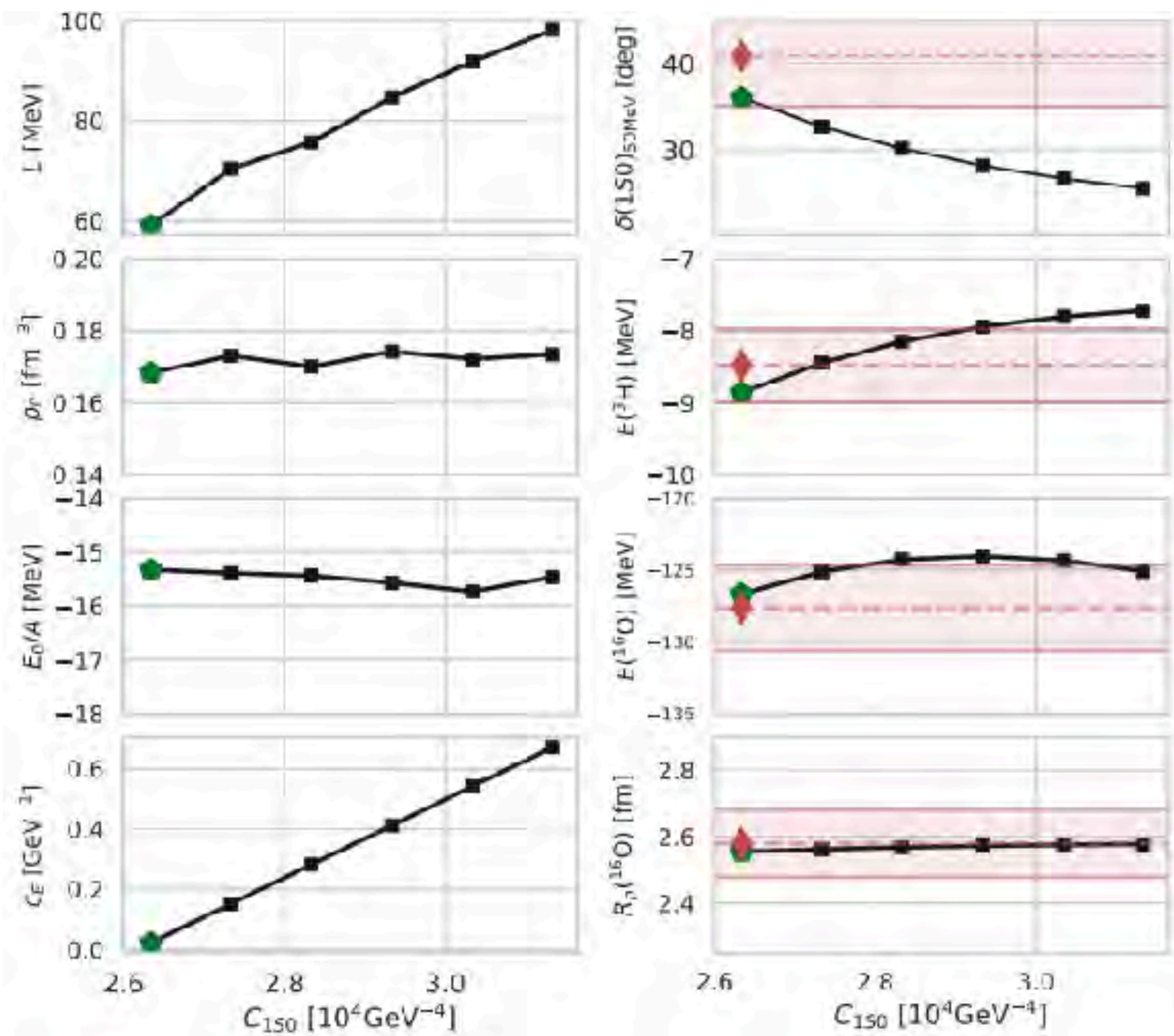


B. Hu et al (Nature Phys. 2022)

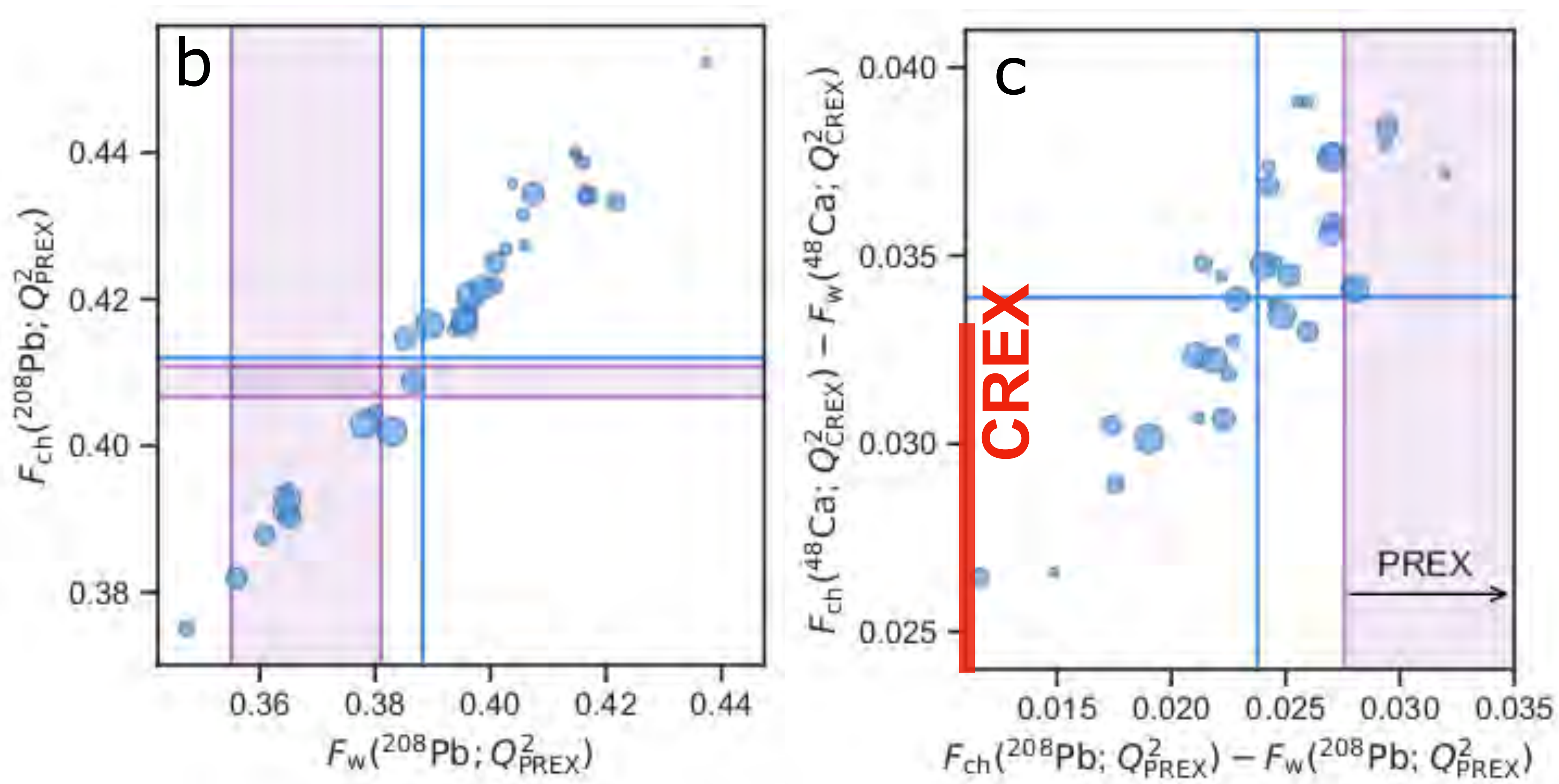
Observable	median	68% CR	90% CR
$R_{\rm skin}(^{48}\rm Ca)$	0.164	[0.141, 0.187]	[0.123, 0.199]
$R_{\rm skin}(^{208}\rm Pb)$	0.171	[0.139, 0.200]	[0.120, 0.221]

Why does ab initio predict thin skins?

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



Electric and weak form factors



B. Hu et al (Nature Phys. 2022)

- *"The concept of tension 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**.
- **Opportunity**: 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 nucleon–nucleon scattering, few-nucleon systems, medium- and heavy-mass nuclei up to lead-208, and the nuclear-matter equation of state near saturation density.
- **Challenge**: Get to know your uncertainties; sampling.