Bayesian methods for uncertainty quantification with (complex) nuclear-physics models

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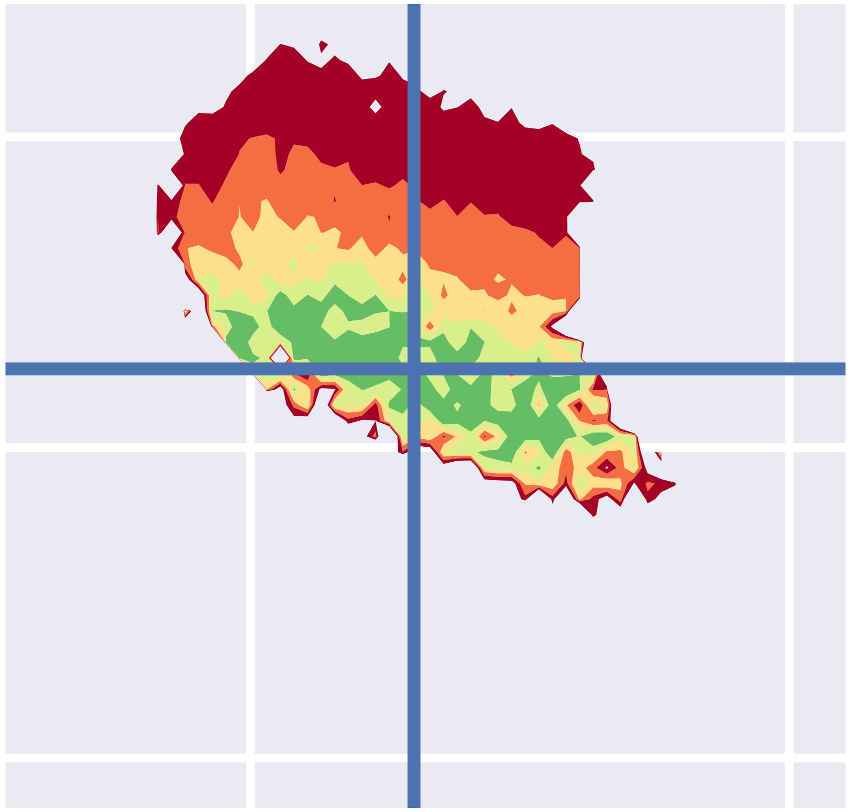

***MITP Topical Workshop*, "Uncertainty quantification in nuclear physics",**
Mainz, June 24-28, 2024

Based on…

1. Z. Sun, et al. *Multiscale physics of atomic nuclei from first principles.* arXiv:2404.00058
2. I. Svensson, et al. *Inference of the low-energy constants in delta-full chiral effective field theory including a correlated truncation error.* Phys. Rev. C 109 (2024) 064003.
3. W.G. Jiang, et al. *Nuclear-matter saturation and symmetry energy within Δ-full chiral effective field theory.* Phys. Rev. C 109 (2024) L061302.
4. W.G. Jiang, et al. *Emulating ab initio computations of infinite nucleonic matter.* Phys. Rev. C 109 (2024) 064314.
5. Y. Kondo, et al. *First observation of 28O.* Nature 620 (2023) 965.
6. D. Gazda, et al. *Nuclear physics uncertainties in light hypernuclei.* Phys. Rev. C 106 (2022) 054001.
7. B. Hu, et al. *Ab initio predictions link the neutron skin of 208Pb to nuclear forces.* Nature Phys. 18, 1196 (2022).
8. T. Djärv, et al. *Bayesian predictions for A=6 nuclei using eigenvector continuation emulators.* Phys. Rev. C 105 (2022) 014005
9. A. Glick-Magid, et al. *Nuclear ab initio calculations of 6He β-decay for beyond the Standard Model studies.* Phys. Lett. B 832 (2022) 137259.

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]
   - Lecture notes: https://cforssen.gitlab.io/learningfromdata/

4. **Multidisciplinary efforts** are being pursued for tackling problems involving complex computer models.
   - See, e.g., the ISNET series [https://isnet-series.github.io/]

Efforts at several *ab initio* frontiers

Open Access

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Emulating *ab initio* computations of infinite nucleonic matter

W. G. Jiang, C. Forssén, T. Djärv, and G. Hagen
Phys. Rev. C **109**, 064314 – Published 12 June 2024

Letter | Open Access

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Nuclear-matter saturation and symmetry energy within Δ-full chiral effective field theory

W. G. Jiang, C. Forssén, T. Djärv, and G. Hagen
Phys. Rev. C **109**, L061302 – Published 12 June 2024

Emulators and Bayesian methods for many-body modelling and predictions

Editors' Suggestion | Open Access

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Inference of the low-energy constants in Δ-full chiral effective field theory including a correlated truncation error

Isak Svensson, Andreas Ekström, and Christian Forssén
Phys. Rev. C **109**, 064003 – Published 18 June 2024

Bayesian inference of χEFT interactions

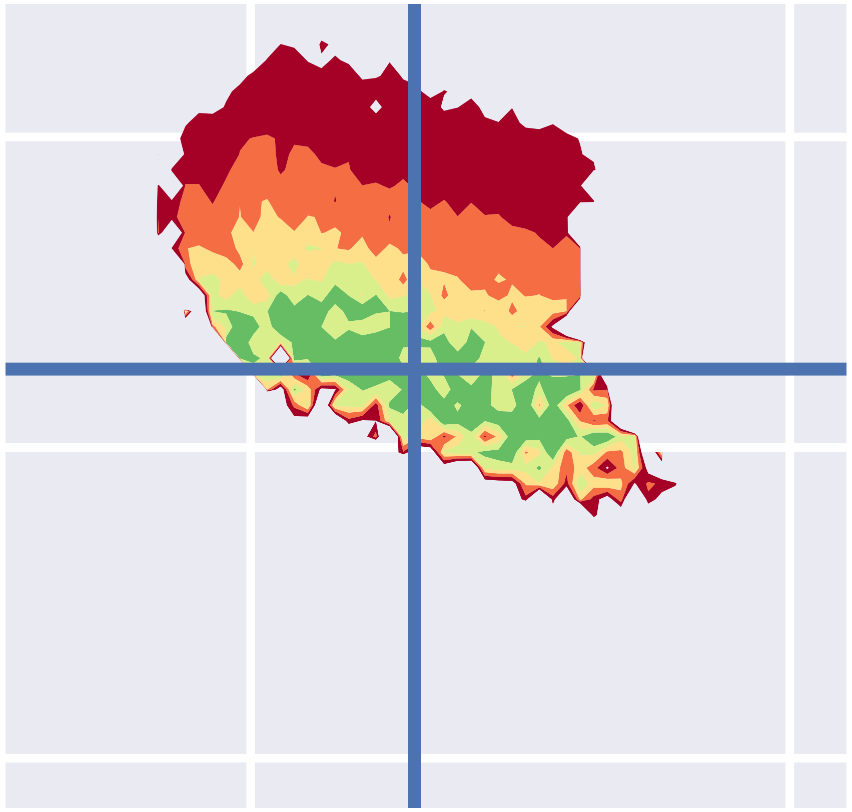
Open Access

Access by Chalmers University of Technology

Perturbative computations of neutron-proton scattering observables using renormalization-group invariant chiral effective field theory up to $\mathrm{N}^3\mathrm{LO}$

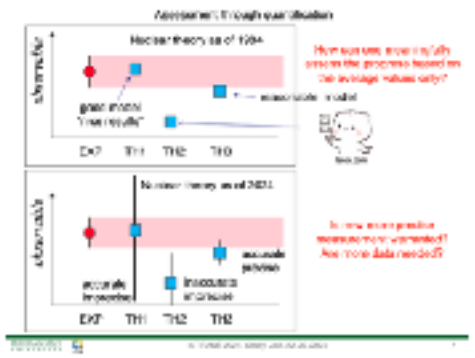
Oliver Thim, Andreas Ekström, and Christian Forssén
Phys. Rev. C **109**, 064001 – Published 3 June 2024

Convergence and RG invariance of χEFT

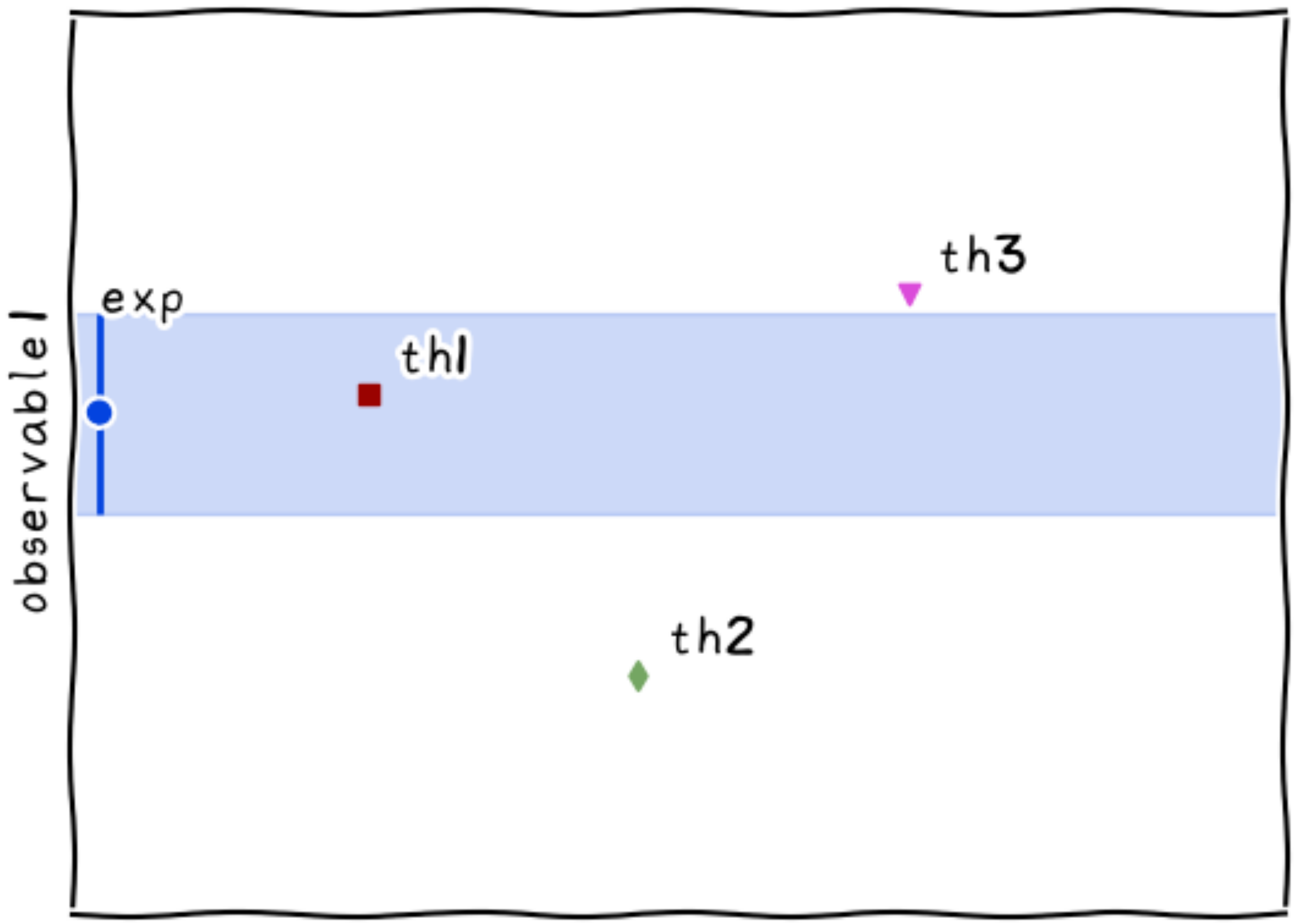


Precision nuclear theory

Data and models

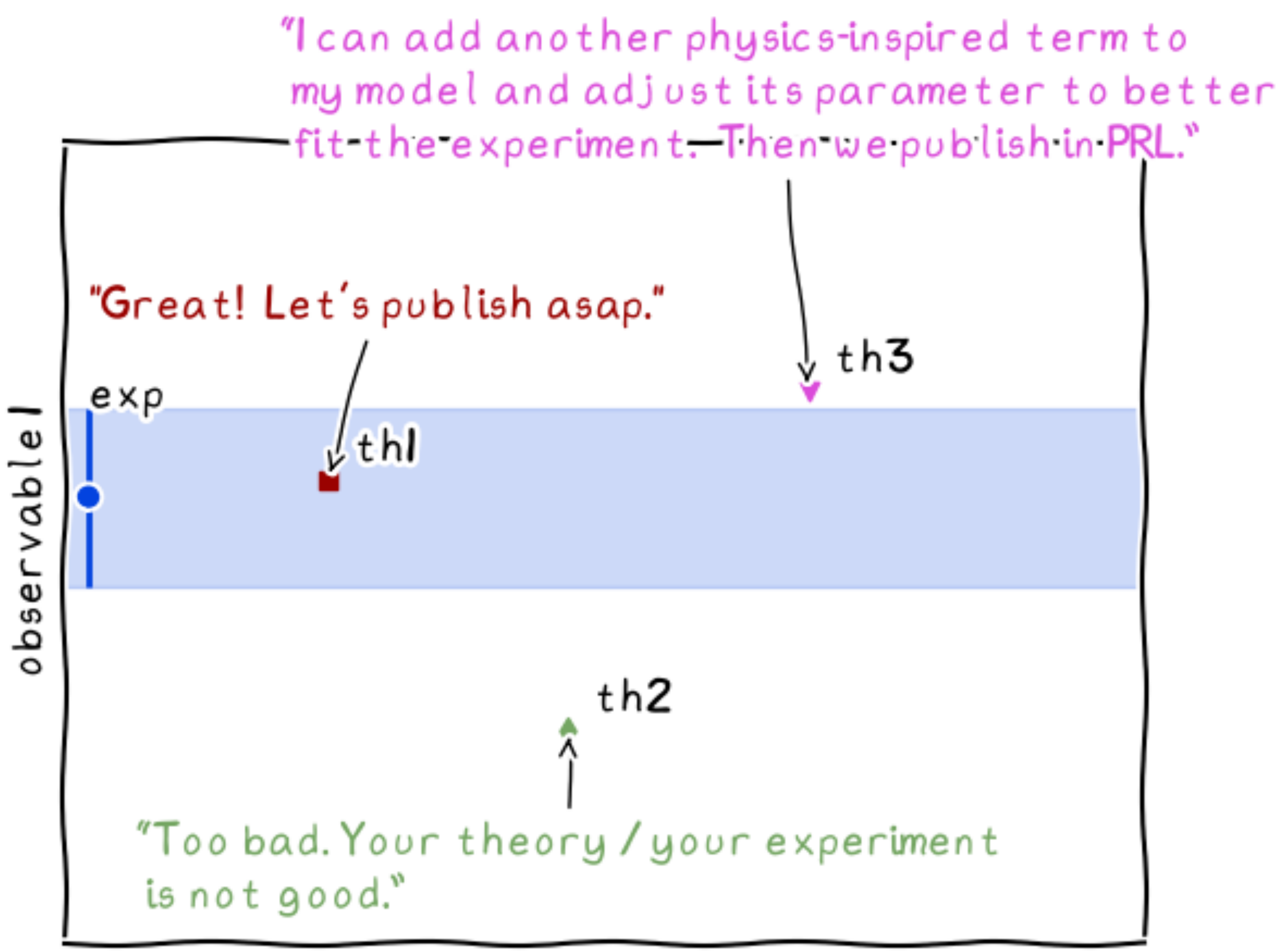


Credit W. Nazarewicz, INTRANS 2024



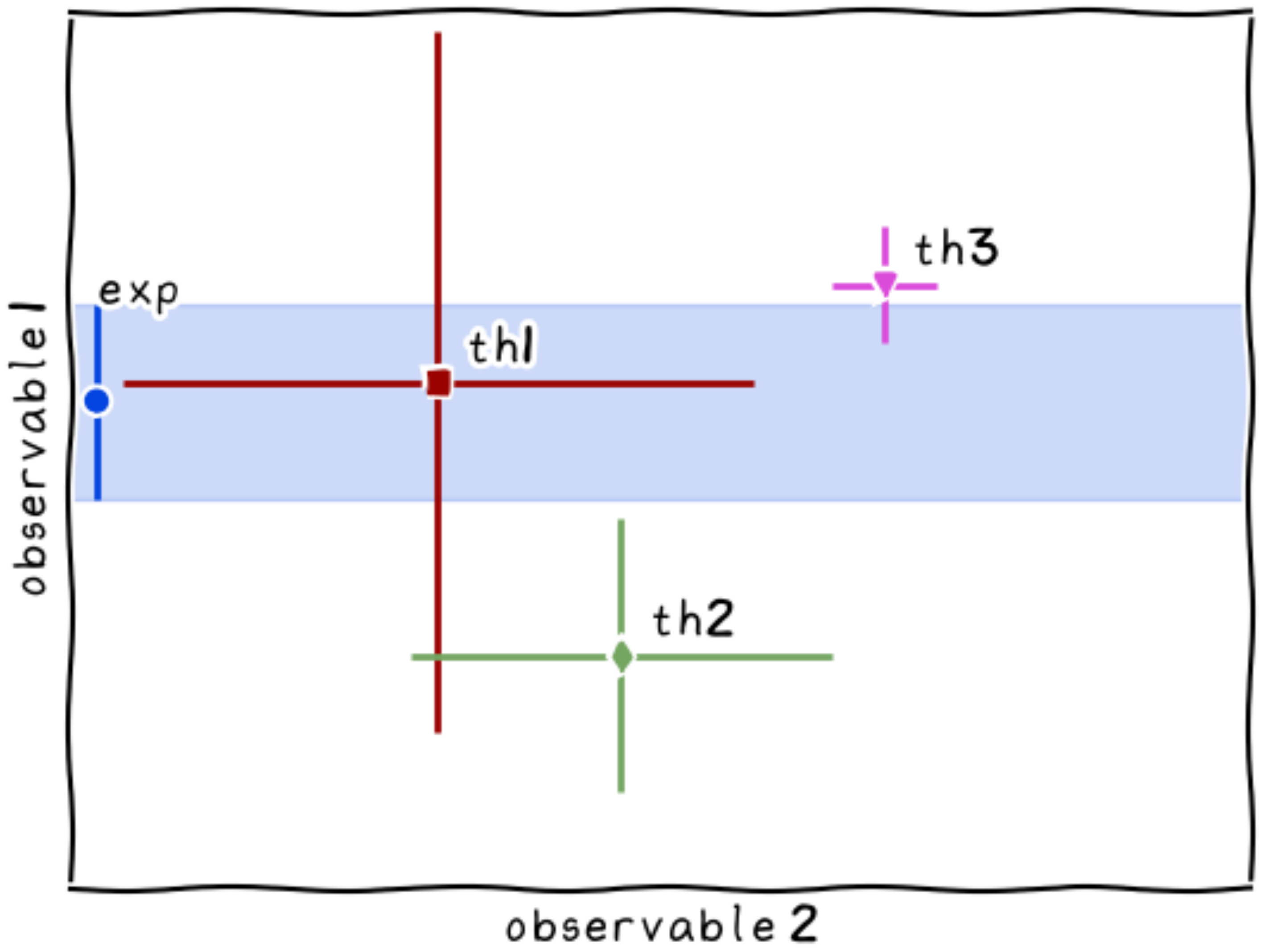
$$y_{\mathrm{exp}} + \delta y_{\mathrm{exp}} = y_{\mathrm{th}}(\boldsymbol{\alpha})$$

More than one observable



$$y_{\mathrm{exp}} + \delta y_{\mathrm{exp}} = y_{\mathrm{th}}(\boldsymbol{\alpha})$$

Assessment through UQ

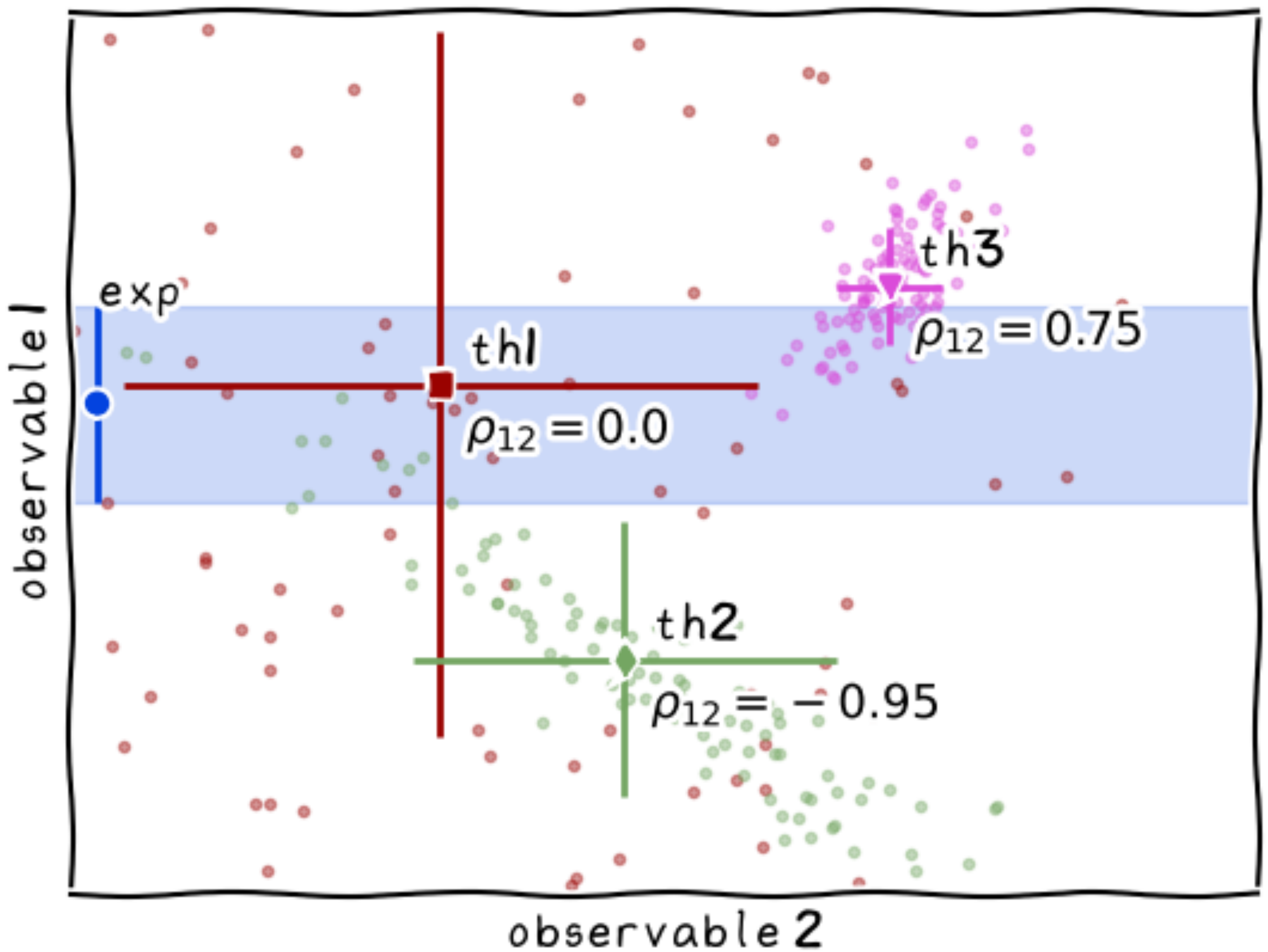


$$y_{\mathrm{exp}} + \delta y_{\mathrm{exp}} = y_{\mathrm{th}}(\boldsymbol{\alpha}) + \delta y_{\mathrm{th}}$$

This is now a **statistical model**

Correlated errors are important

- Theory 1 seems accurate, but very imprecise.
- Theory 2 is in mild tension with the experiment for observable 1, and in strong tension with theory 3.



$$\mathrm{pr}(\delta y_1, \delta y_2) \neq \mathrm{pr}(\delta y_1)\mathrm{pr}(\delta y_2) \quad \text{if } \rho_{12} \neq 0$$

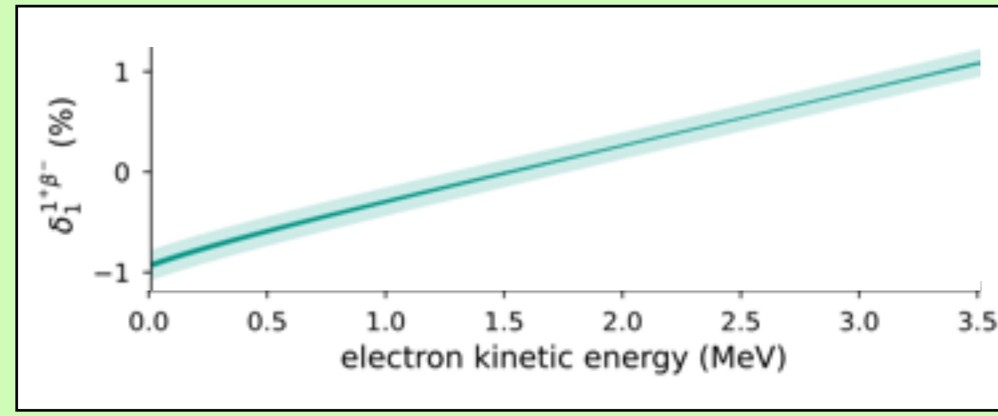
Many relevant errors in ab initio modelling are correlated

Physics predictions with (complex) precision models

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

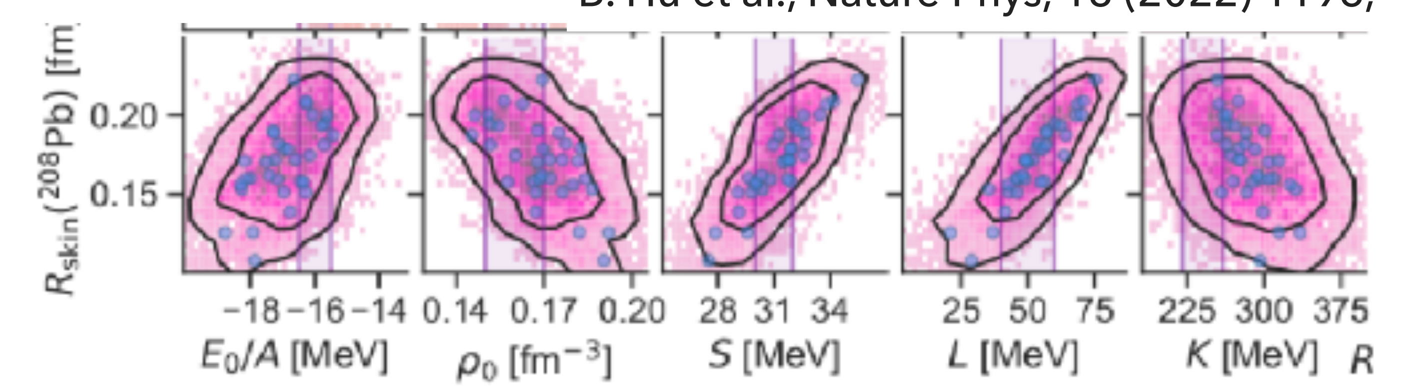
$$\frac{d\omega^{1^+\beta^-}}{dE\,\frac{d\Omega_k}{4\pi}\frac{d\Omega_\nu}{4\pi}} = \frac{4}{\pi^2}\left(E_0-E\right)^2 kEF^-\left(Z_f,E\right)C_{\mathrm{corr}}\left|\langle\|\hat{L}_1^A\|\rangle\right|^2 \times 3\left(1+\delta_1^{1^+\beta^-}\right)\left[1+a_{\beta\nu}^{1^+\beta^-}\vec{\beta}\cdot\hat{\nu}+b_{\mathrm{F}}^{1^+\beta^-}\frac{m_e}{E}\right],$$

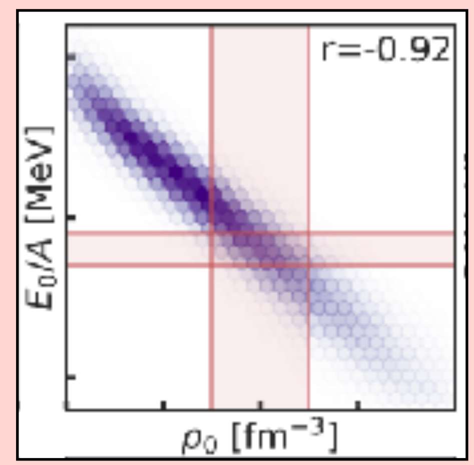
A. Glick-Magid et al., PLB 832 (2022) 137259



Extreme nuclear matter modelling

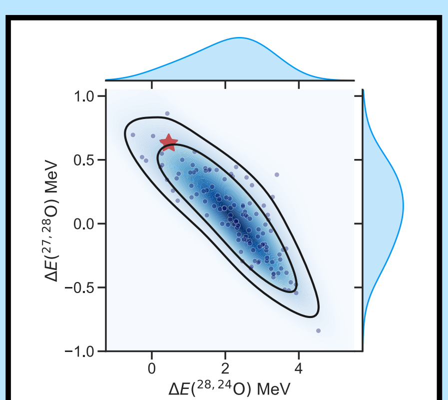
B. Hu et al., Nature Phys, 18 (2022) 1196,





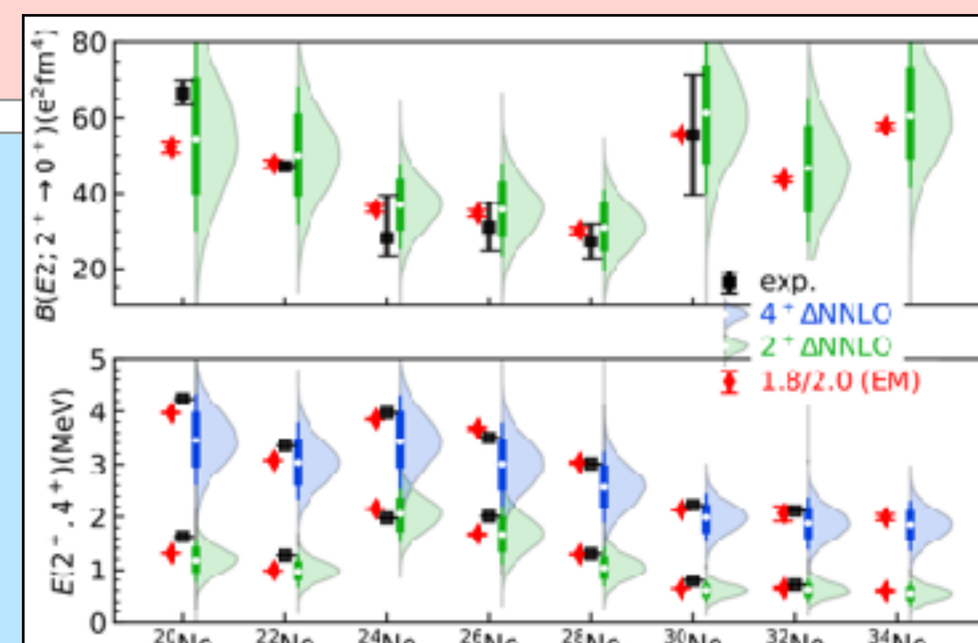
W. Jiang et al., PRC 109 (2024) L061302

Predictive modelling of **rare isotopes**



Z. Sun et al., arXiv 2404.00058

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



Learning from data via Bayes

Model calibration via **Bayes' theorem**

Likelihood Prior

Posterior

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

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.

Statistical modeling (for *ab initio* methods)

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

- Likelihood-free approaches; avoiding full probabilistic modeling.
- Handling of correlated errors; effective data sets and more realistic error quantification.
- Strategic choices of heavy computations; synergies in emulator training.

Bayesian predictive distributions

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

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

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

- Prior checking with "historic" (known) data, are described by the **prior predictive distribution** (important part of model building)

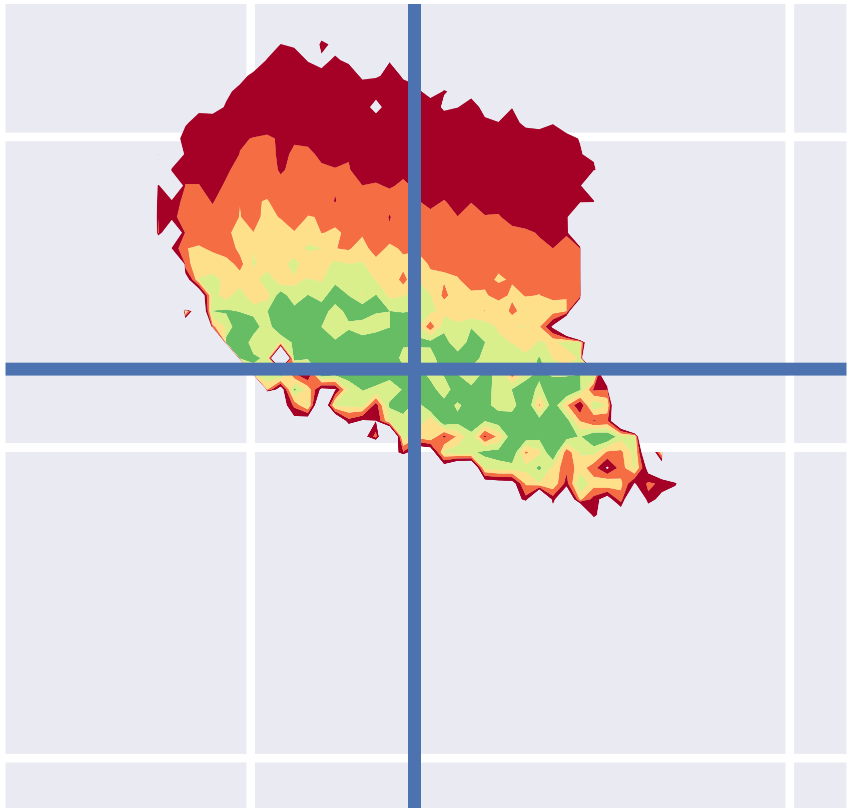
$$\left\{ y(\boldsymbol{\alpha}) : \boldsymbol{\alpha} \sim \mathrm{pr}(\boldsymbol{\alpha} \,|\, I) \right\}$$

- Prior samples filtered by non-implausibility = **History matching**

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

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

B. Hu et al. (Nature Phys. 2022); W. Jiang et al. (PRC 2024)



Error modeling

Ab initio modeling of nuclear systems using chiral EFT

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

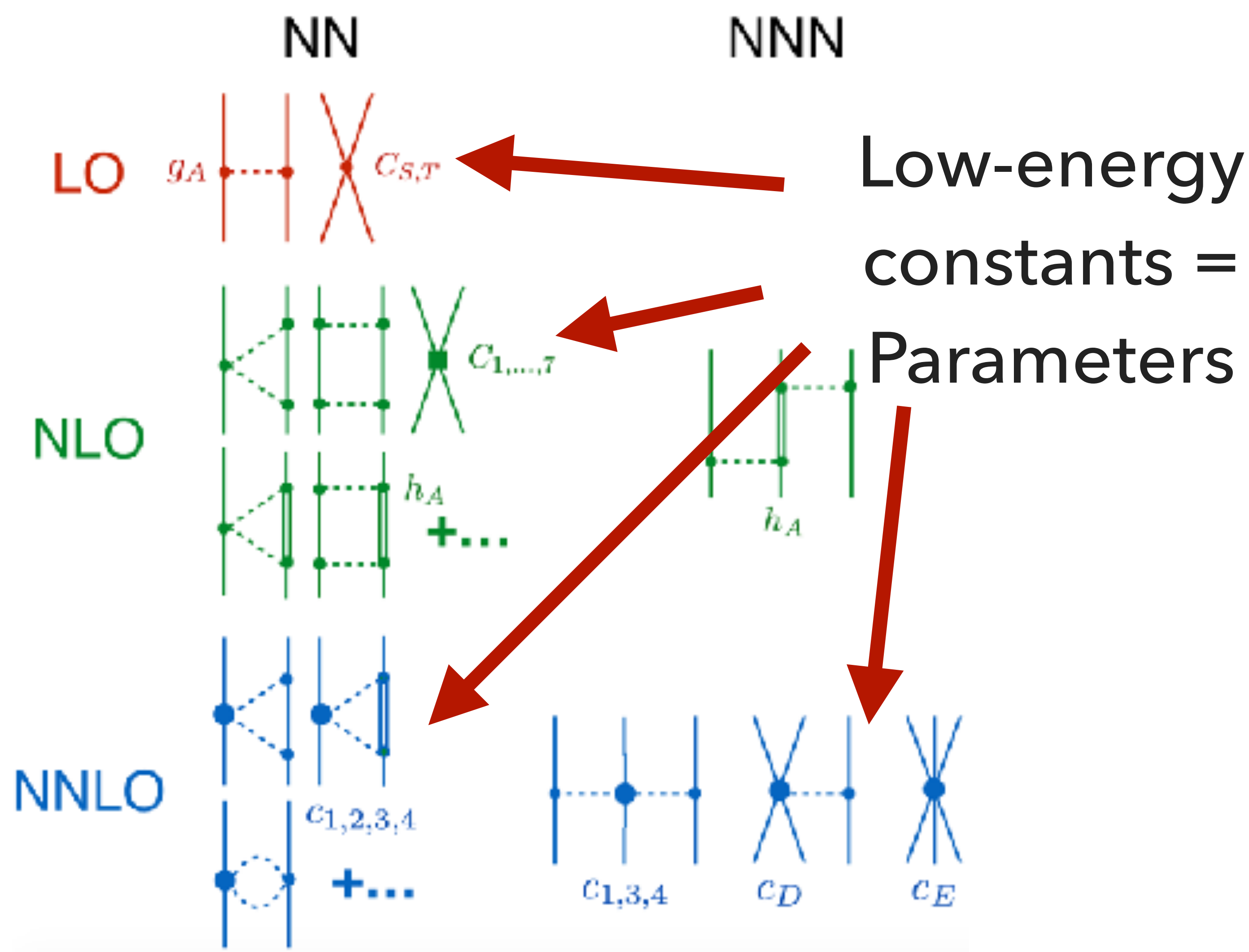
$$\hat{H}(\boldsymbol{\alpha}) = \hat{T} + \hat{V}(\boldsymbol{\alpha})$$

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, …

H. Krebs et al. (2007); E. Epelbaum et al. (2008)
A. Ekström, et al. (2018); W. Jiang, et al. (2020)

Challenge #1: Getting to know your errors

- **EFT truncation errors**
  - **Approach**: study order-by-order results and learn the PDF for expansion coefficients

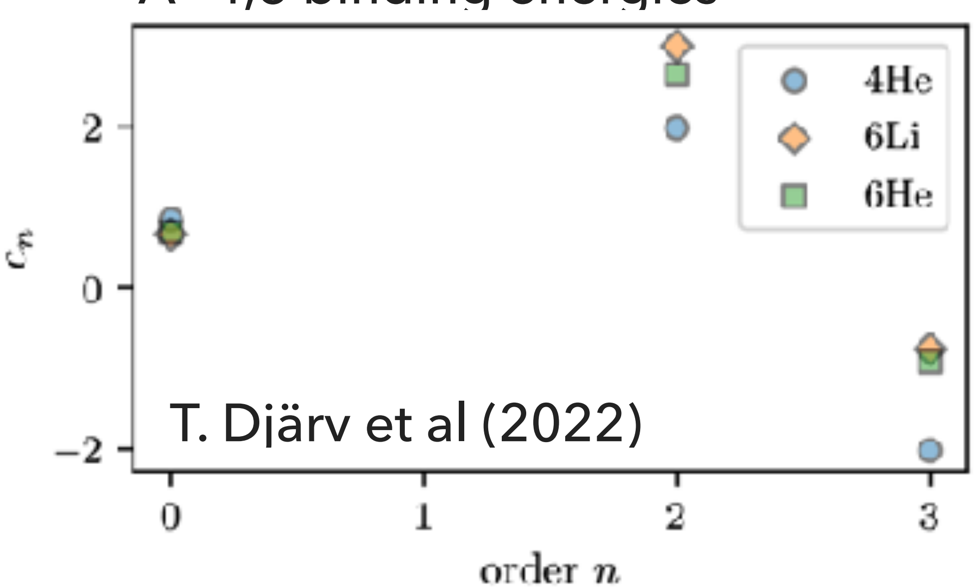
$$y_k = y_{\mathrm{ref}} \sum_{n=0}^{k} c_n Q^n, \quad \delta y_k = y_{\mathrm{ref}} \sum_{n=k+1}^{\infty} c_n Q^n$$

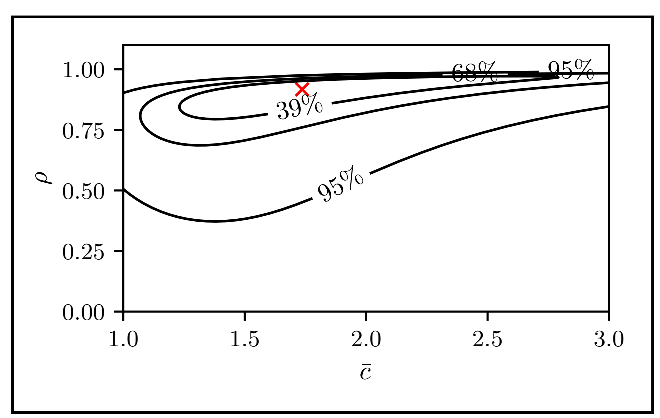
(see Dick's talk)

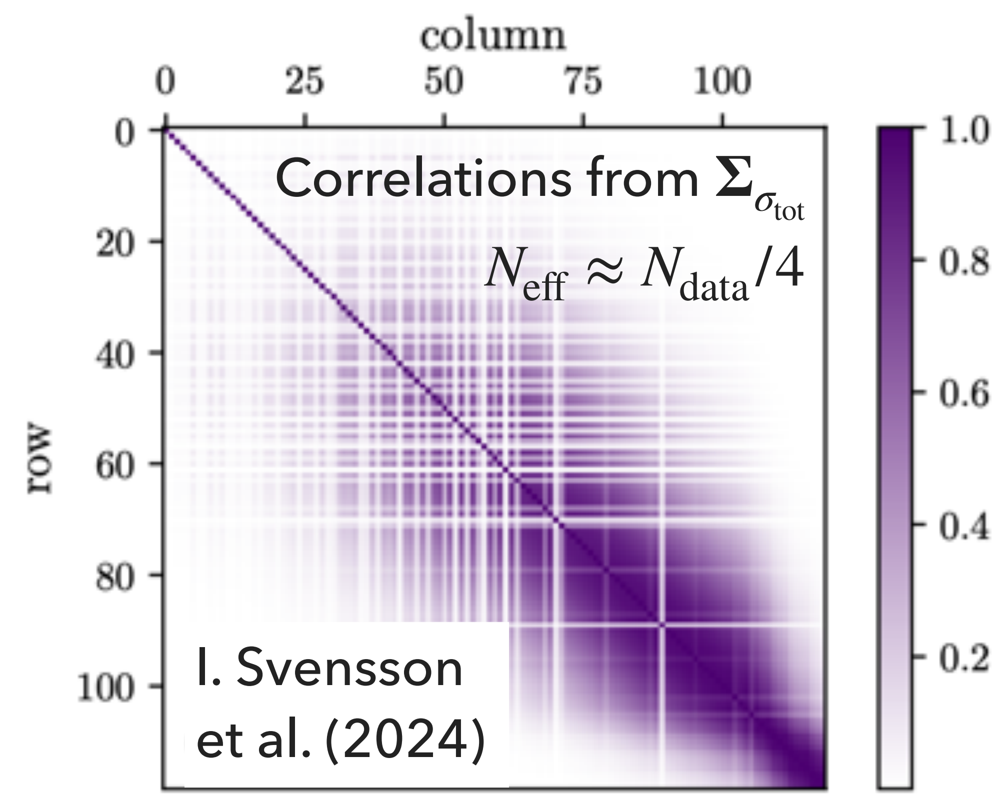
  - **Challenges**: Cutoff dependence, expansion parameter, irregular convergence, correlation structure for *E(A)*, $r_p(A)$, $\sigma(E,\theta)$, *etc*

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

A=4,6 binding energies





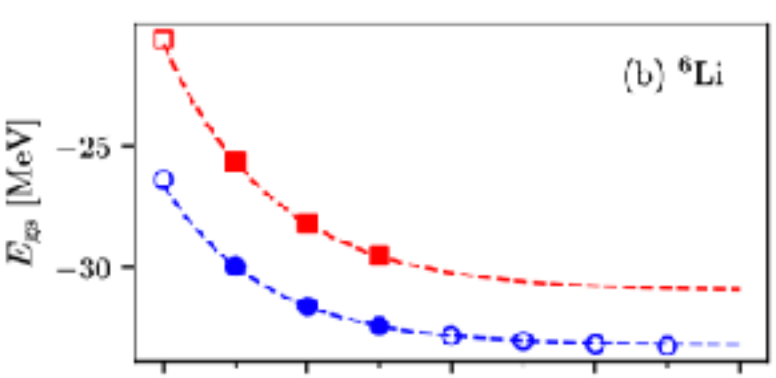


GP modelling for correlated EFT errors in J. Melendez et al (2019) and C. Drischler et al. (2020)

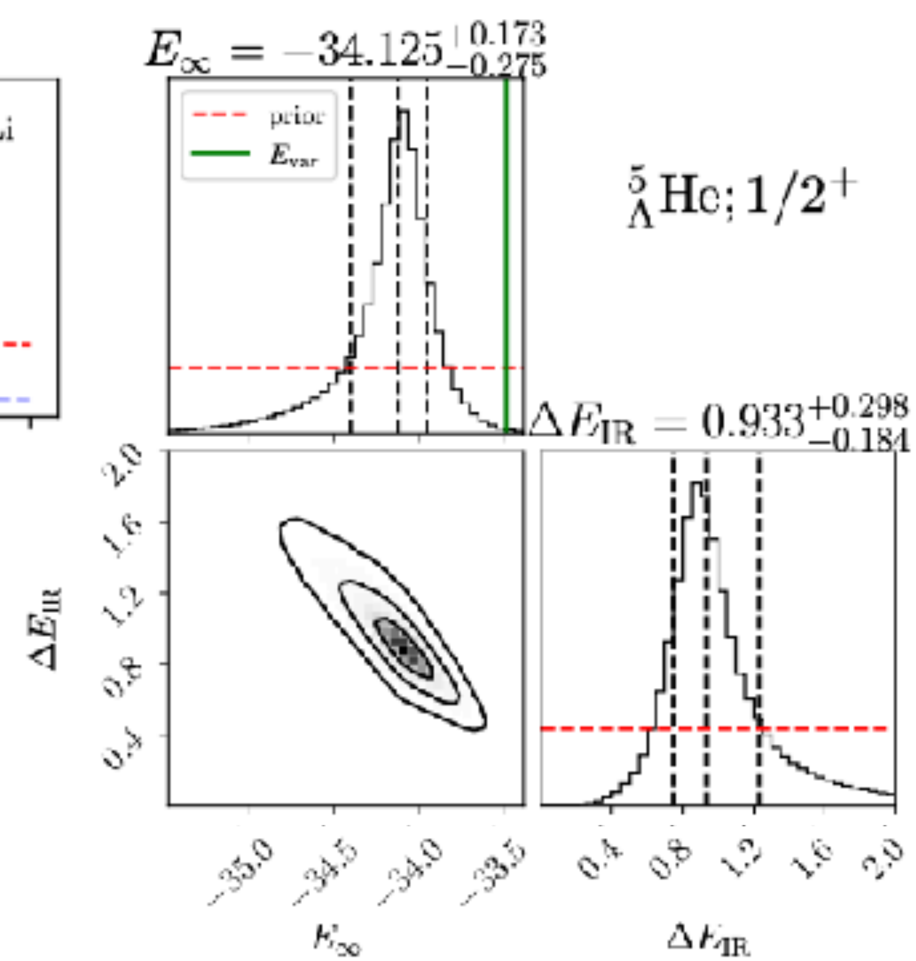
Challenge #1: Getting to know your errors

- **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

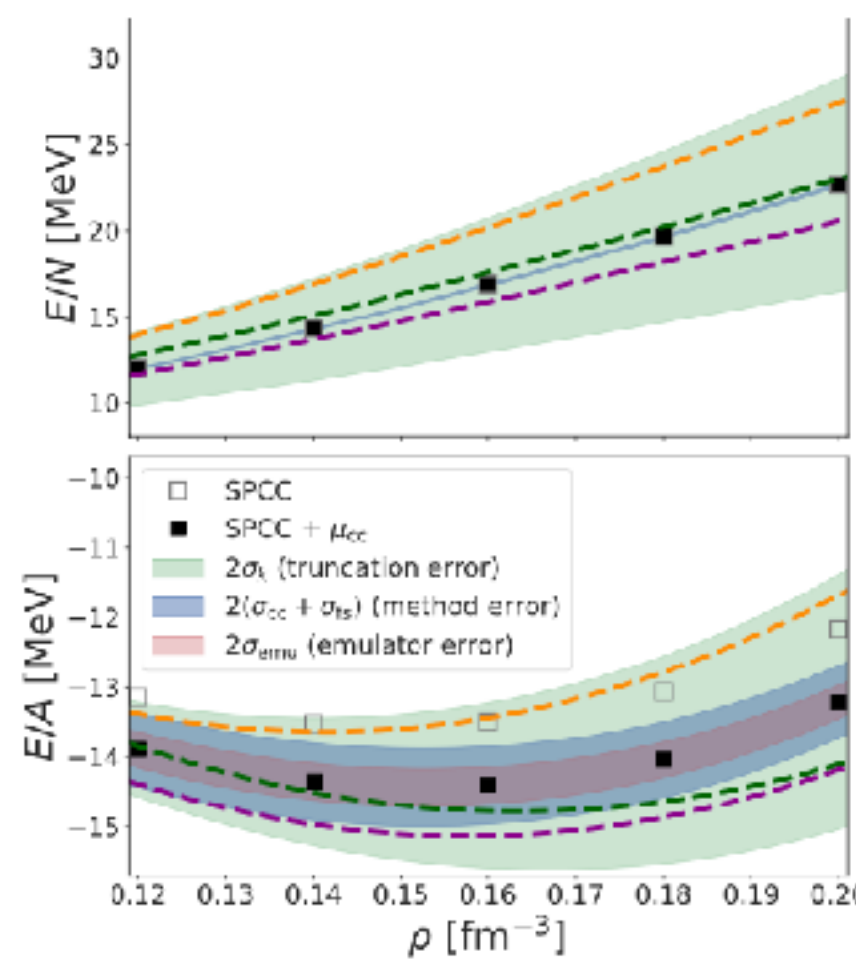
N_{max} extrapolation for NCSM in T. Djärv et al (2022)



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

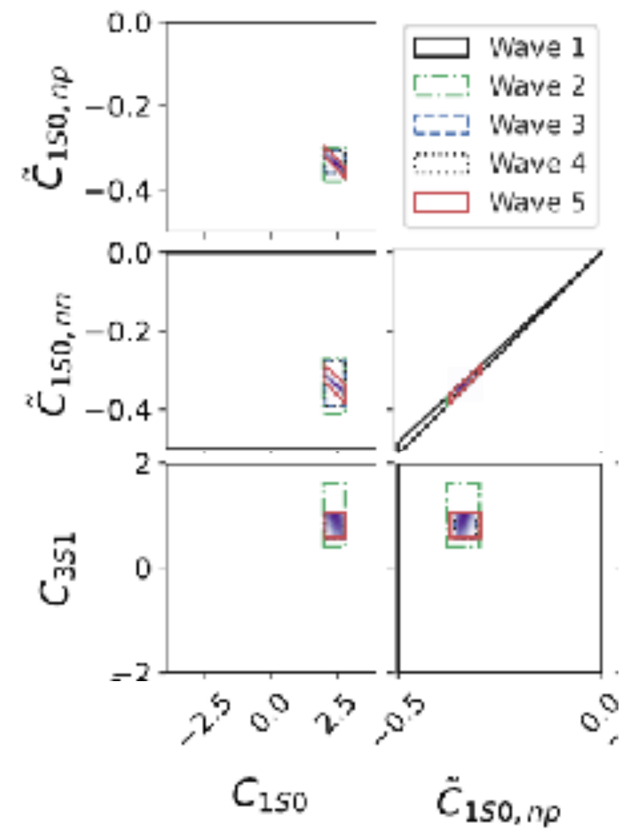


GP modelling for method and model errors in W. Jiang et al (2024)

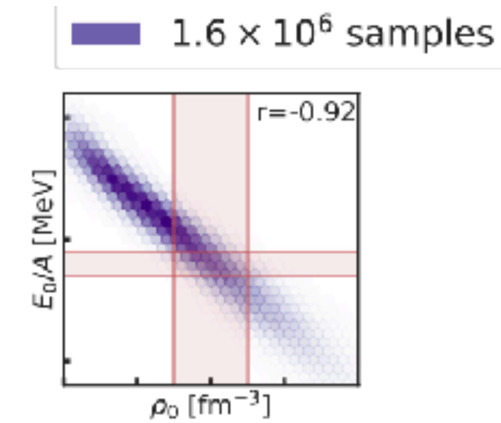


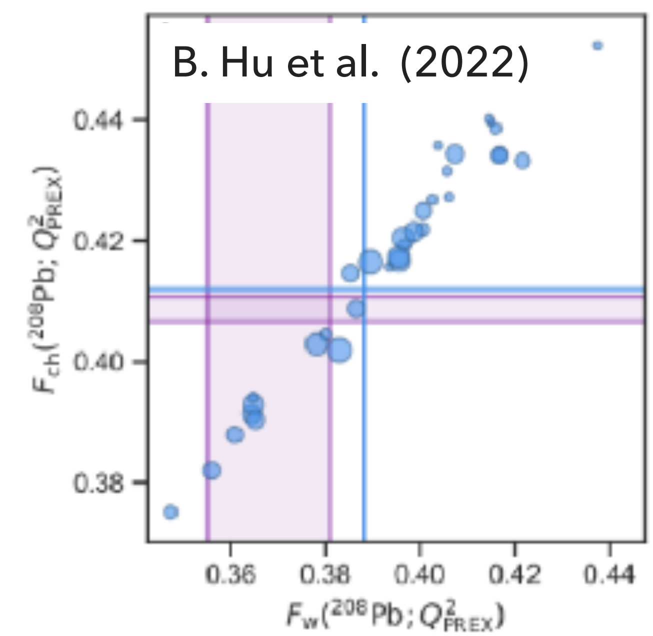
Challenge #2: Parametric uncertainty for high-dim models

- **Likelihood-free methods**
  - History matching allows model exploration without full probabilistic specification (linear Bayes).
  - Should also explore Approximate Bayesian Computation, etc.
- **Posterior sampling**
  - Univariate distributions can often be mapped with relatively few (<100) samples.
  - Make every sample important (HMC renders uncorrelated samples)
  - Posterior updates with importance resampling.
  - Full sampling enabled with emulators.

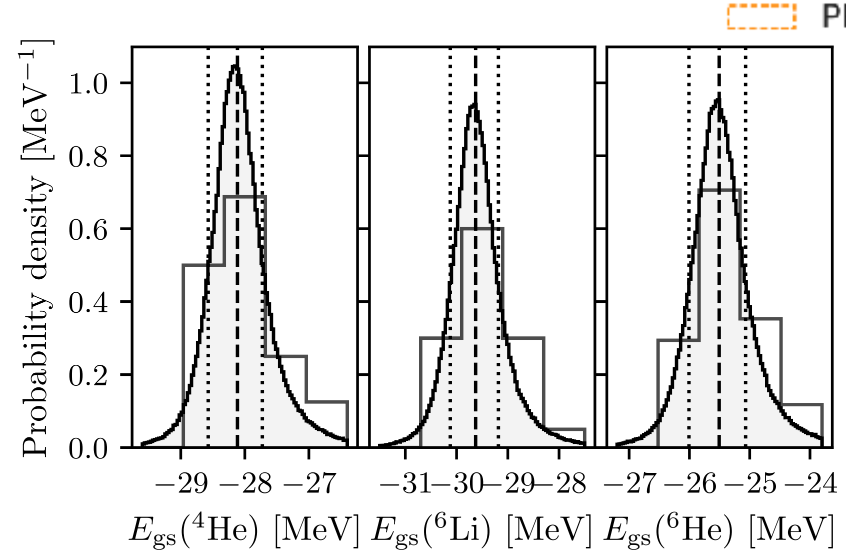


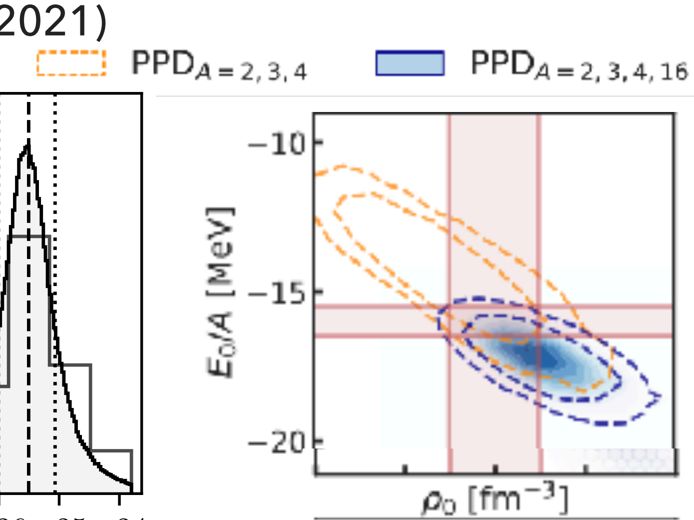
W. Jiang et al. (2024)



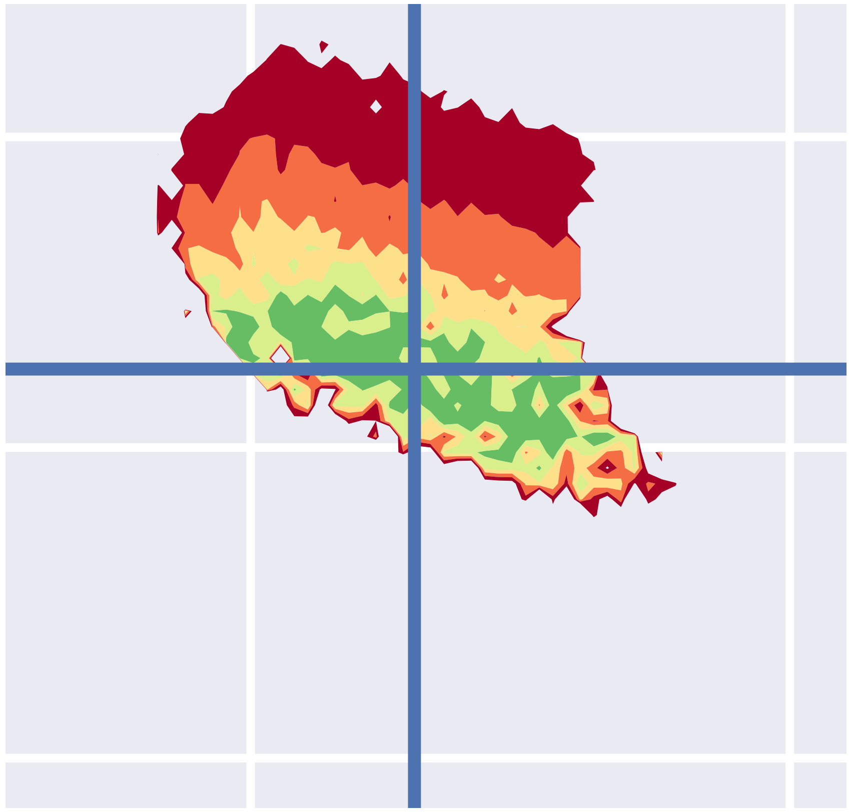


T. Djärv et al PRC (2022)
PPD samples from Wesolowski (2021)





W. Jiang et al. (2024)



Emulators

Emulators

- An **emulator** mimics the simulator output at a reduced computational cost:

$$\boldsymbol{y}(\boldsymbol{\alpha}) \approx \tilde{\boldsymbol{y}}(\boldsymbol{\alpha}) + \delta\tilde{\boldsymbol{y}}$$

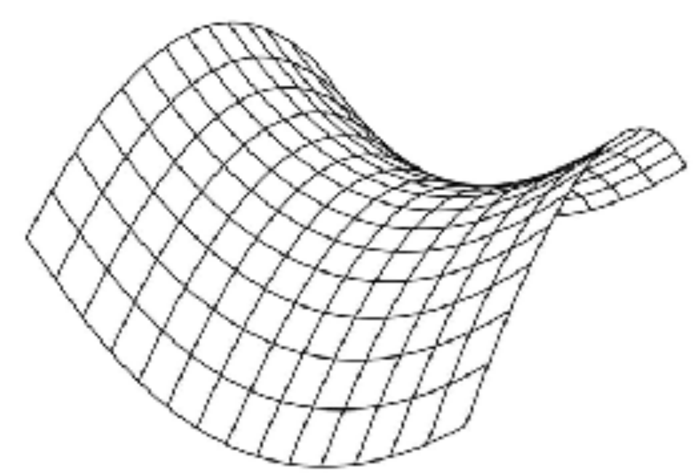
  - A useful emulator is fast and accurate;
  - … with quantified emulator uncertainty.
- Emulators can be non-intrusive (data based)
  - Neural networks, Gaussian processes, etc
- Or intrusive (model based)
  - Translating a high-fidelity model to a low-fidelity one
  - Vast literature on model-order reduction (MOR);
    see, e.g., Melendez et al. (2203.05528) with many refs.

Eigenvector continuation emulators

$$H(\alpha) = H_0 + \alpha H_1$$

continuous parameter

The key insight is that while an eigenvector resides in a linear space with enormous dimensions, the eigenvector trajectory generated by smooth changes of the Hamiltonian matrix is well approximated by a very low-dimensional manifold.

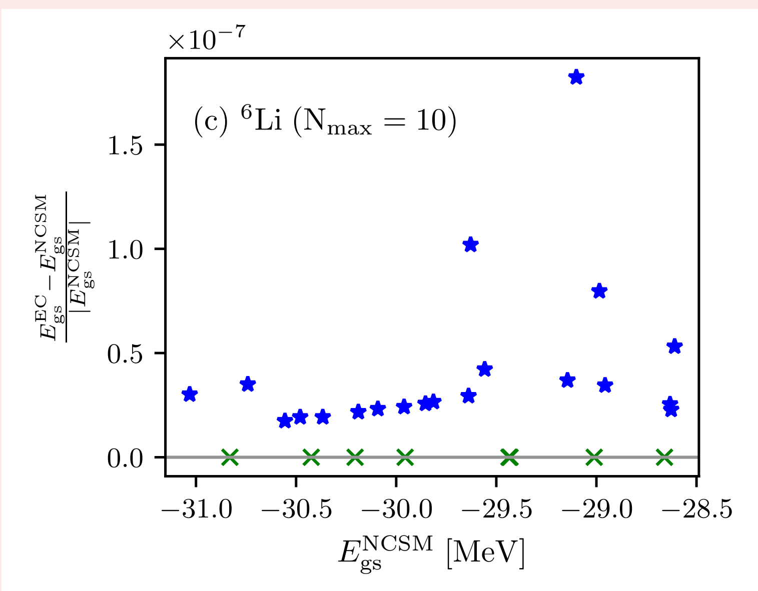


D. Frame, et al. Phys. Rev. Lett. **121**, 032501 (2018)
T. Duguet, et al. arXiv:2310.19419.

Emulator precision and speedup

- **Emulator errors**
  - **Approach**: Cross-validation, EC offers rapid convergence with N_{sub}
  - **Challenges**: Outliers. EC convergence (Sarkar and Lee)

E(^{6}Li)

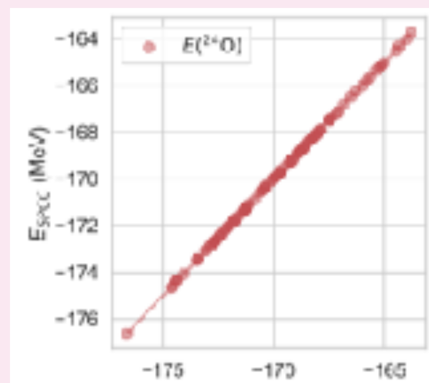


EVC (NCSM M-scheme)

Speedup: 10^7

Djärv et al., (2022)

E(^{24}O)

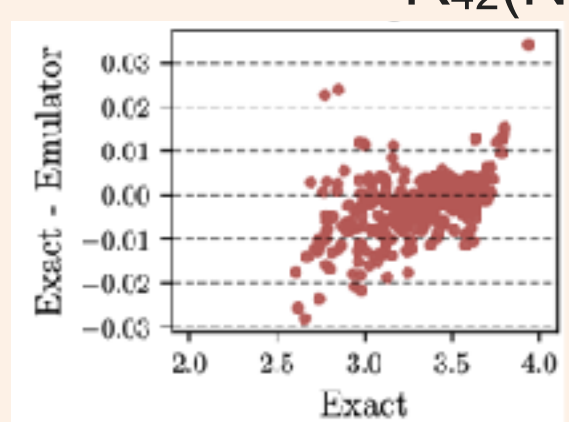


Kondo et al., (2022)

SPCC (CCSDT-3)

Speedup: 10^8

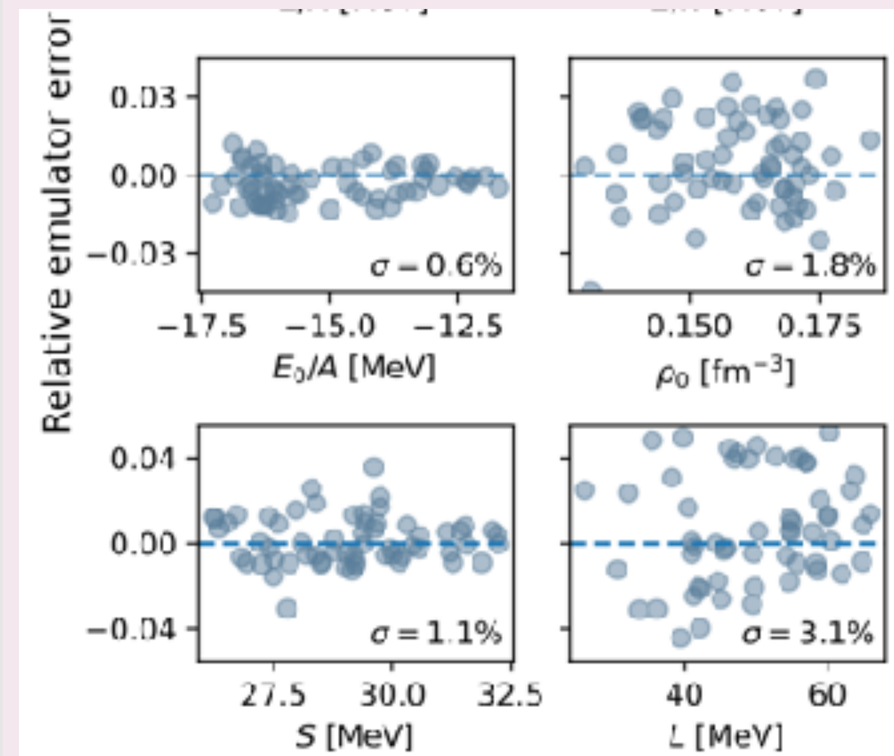
R$_{42}$(Ne,Mg)



HF

Sun et al., (2024)

Infinite nuclear matter



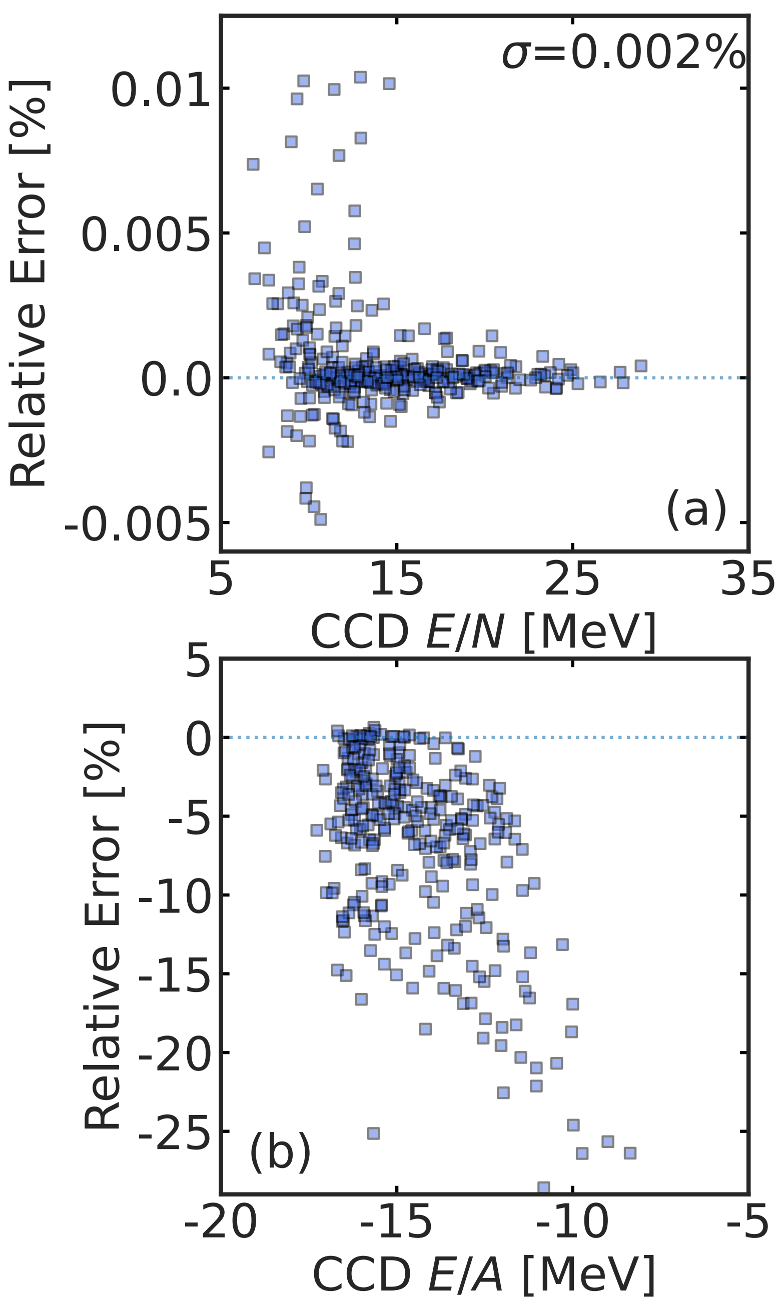
SPCC (CCD k-boxes with A=66,132 at 6 densities)

Speedup: 10^8

Jiang et al., (2024)

Small-batch voting

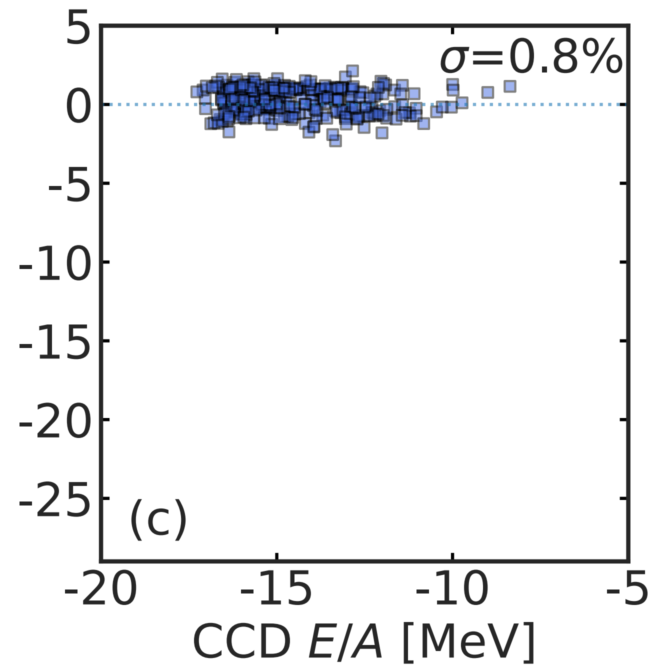
SPCC



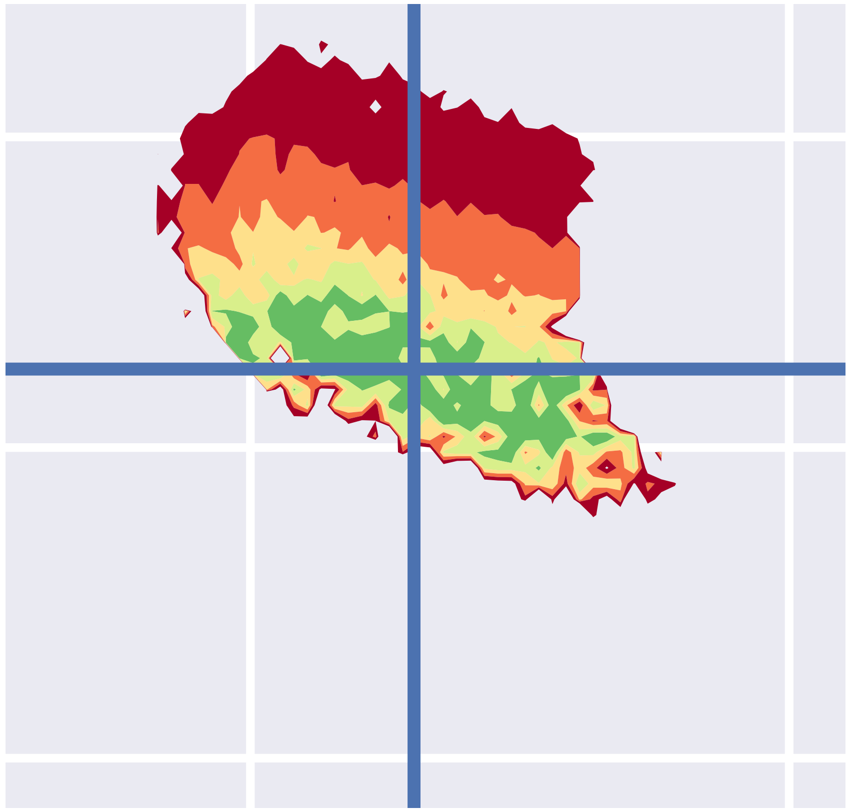
Physical states are stable
w.r.t. subspace variations

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

Create different subspaces from different
batches of training vectors;
Compare the spectra and keep the stable states



SPCC with
small-batch voting



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

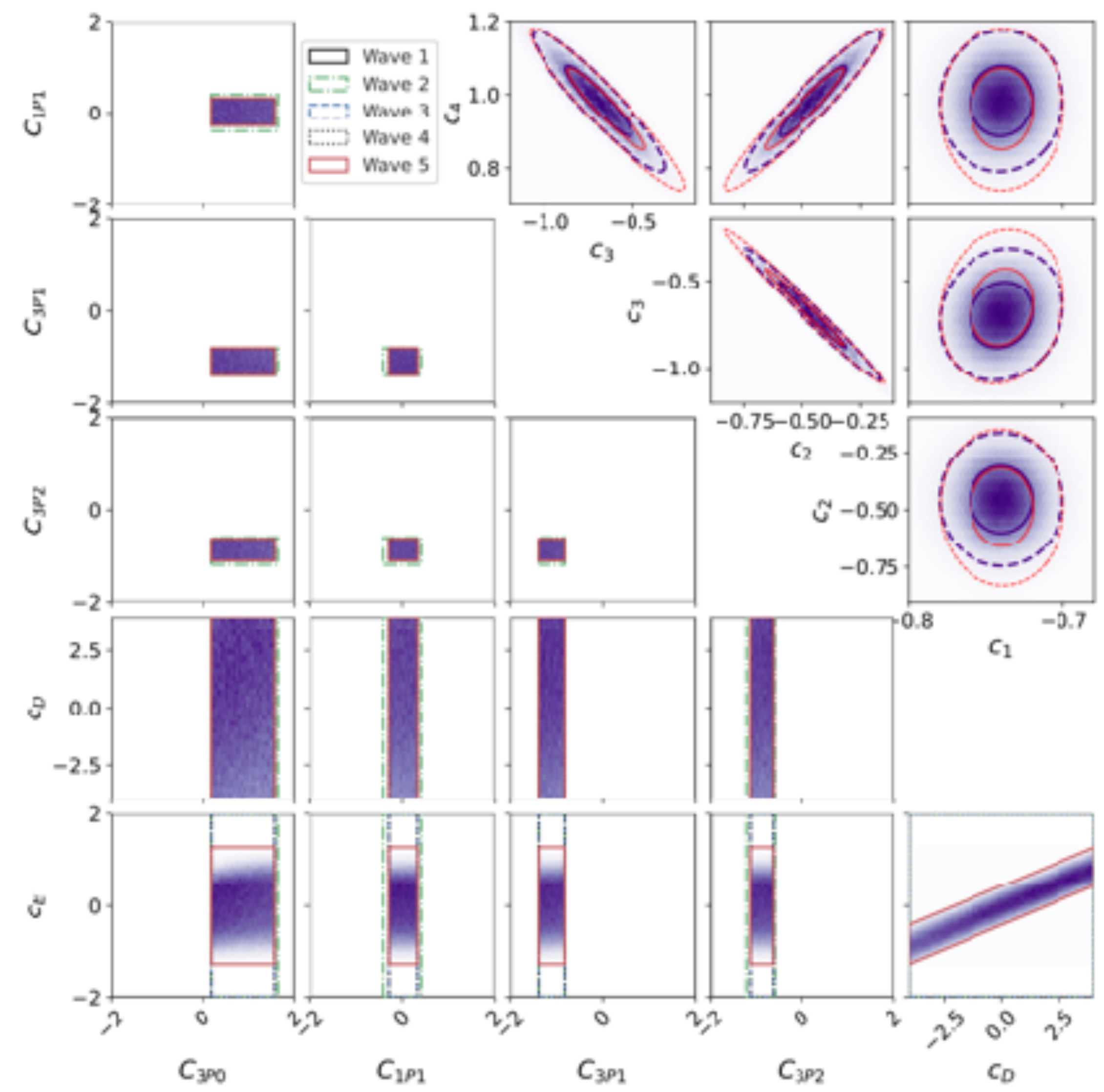
Emergence of nuclear saturation within $\Delta - \chi\mathrm{EFT}$

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

History matching waves

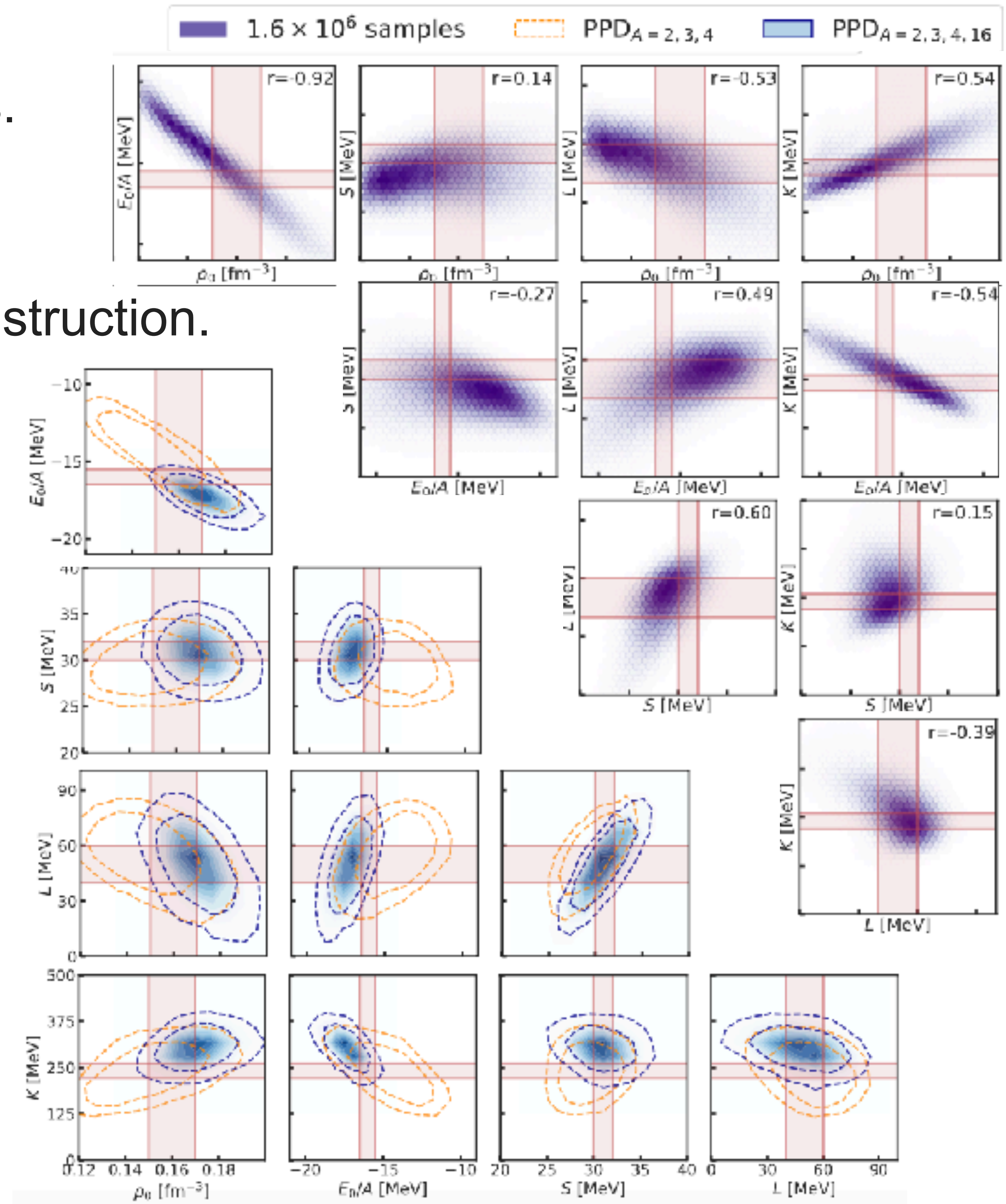
- np S- and P-wave phase shifts at T_{lab}=1, 5, 25, 50, 100, 200 MeV — [wave 1] & [wave 2] & final
- ^{2}H (E, R_p^2, Q), — [wave 3] & [wave 4] & final
- ^{3}H (E), ^{4}He (E, R_p^2) — [wave 4] & final
- Prior for c_1, c_2, c_3, c_4 from a Roy-Steiner analysis of πN data (Siemens 2017)

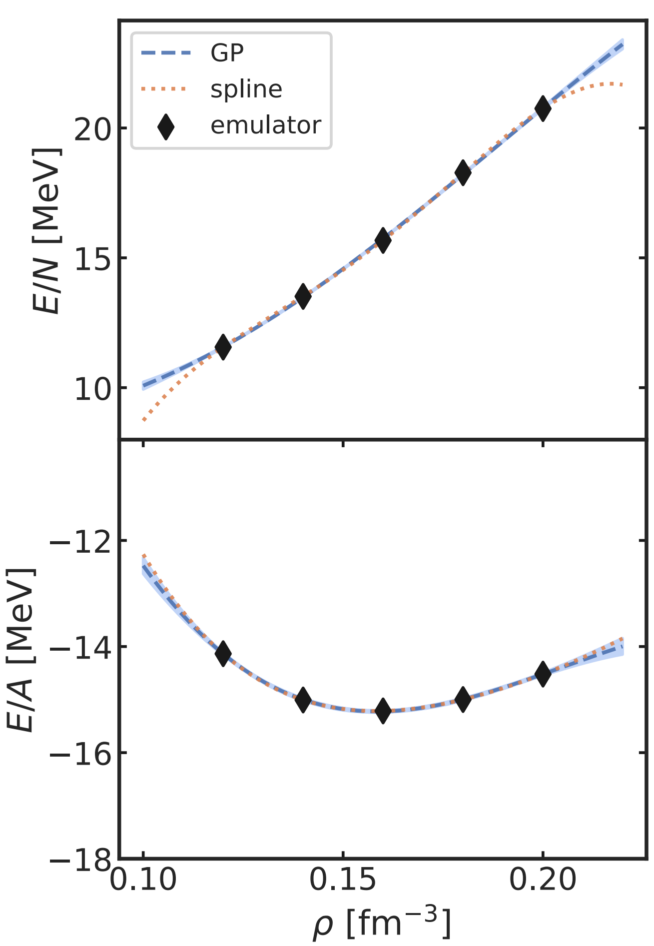
Observable	z	$\varepsilon_{\rm exp}$	$\varepsilon_{\rm model}$	$\varepsilon_{\rm method}$	$\varepsilon_{\rm em}$
$E(^2\mathrm{H})$	-2.2298	0.0	0.05	0.0005	0.001%
$r_p(^2\mathrm{H})$	1.976	0.0	0.005	0.0002	0.0005%
$Q(^2\mathrm{H})$	0.27	0.01	0.003	0.0005	0.001%
$E(^3\mathrm{H})$	-8.4818	0.0	0.17	0.0005	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**.
- 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 / questions**:
  - Finite sample PPDs conditioned on many outputs.
  - Do we understand the convergence of our many-body methods well enough to quantify method errors?
    —benchmarks of different methods and truncation schemes are important.
  - Do we know the EFT convergence well enough to quantify truncation errors?
    —need to revisit leading (and subleading) orders of χEFT and RG invariance