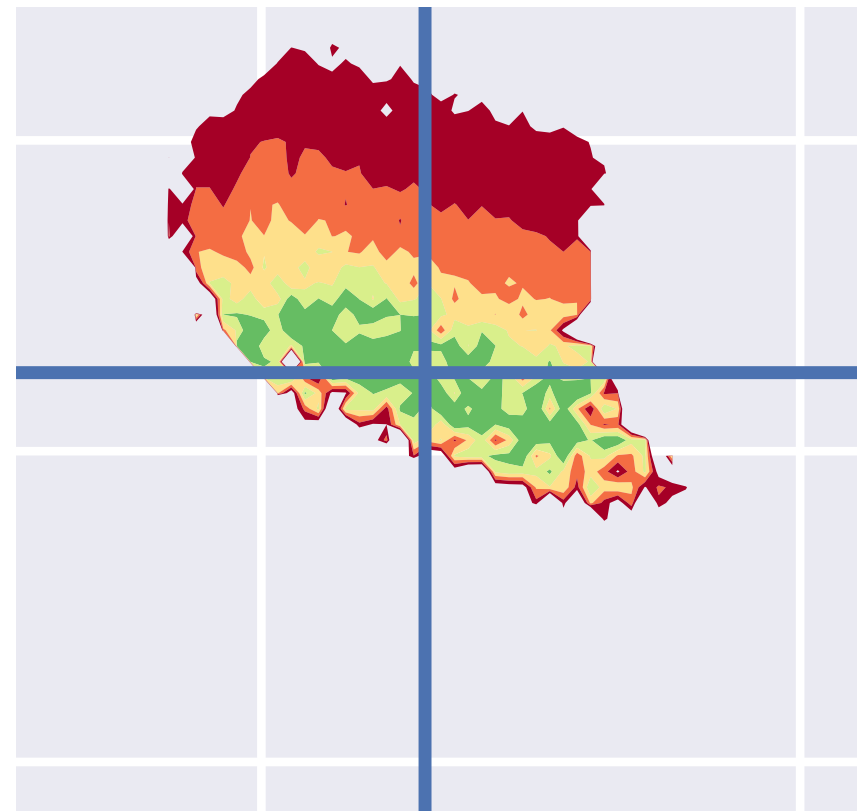


Uncertainty quantification for *ab initio* nuclear modeling

Christian Forssén
Chalmers University of Technology

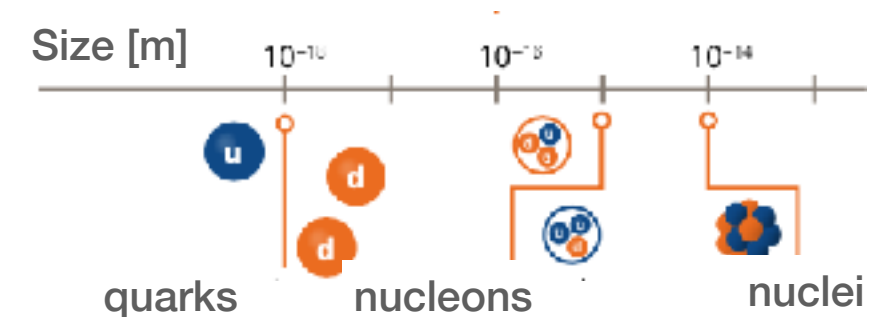


ESNT workshop, “*Theoretical and experimental developments for symmetry-violating nuclear properties*”, Saclay, June 23-27, 2025

Scientific goals in *ab initio* nuclear theory

► Model the strong interaction at low-energy

- At the most fundamental level, the strong interaction is described by Quantum Chromodynamics (QCD);
- Atomic nuclei can presumably be described with relevant low-energy degrees of freedom—nucleons and pions—and residual interactions;
- Effective field theories (EFTs) offer a systematic approach to this problem.
- Specifically: infer low-energy constants (=LECs) of chiral EFT from low-energy observables such as NN scattering phase shifts, few-nucleon observables, etc.

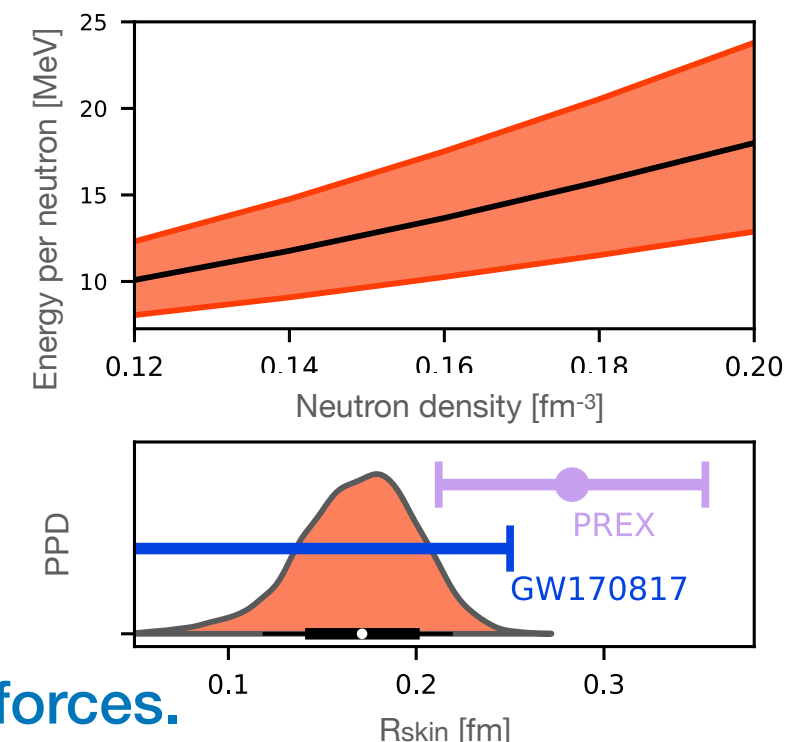


► Universal framework for few- and many-nucleon modeling

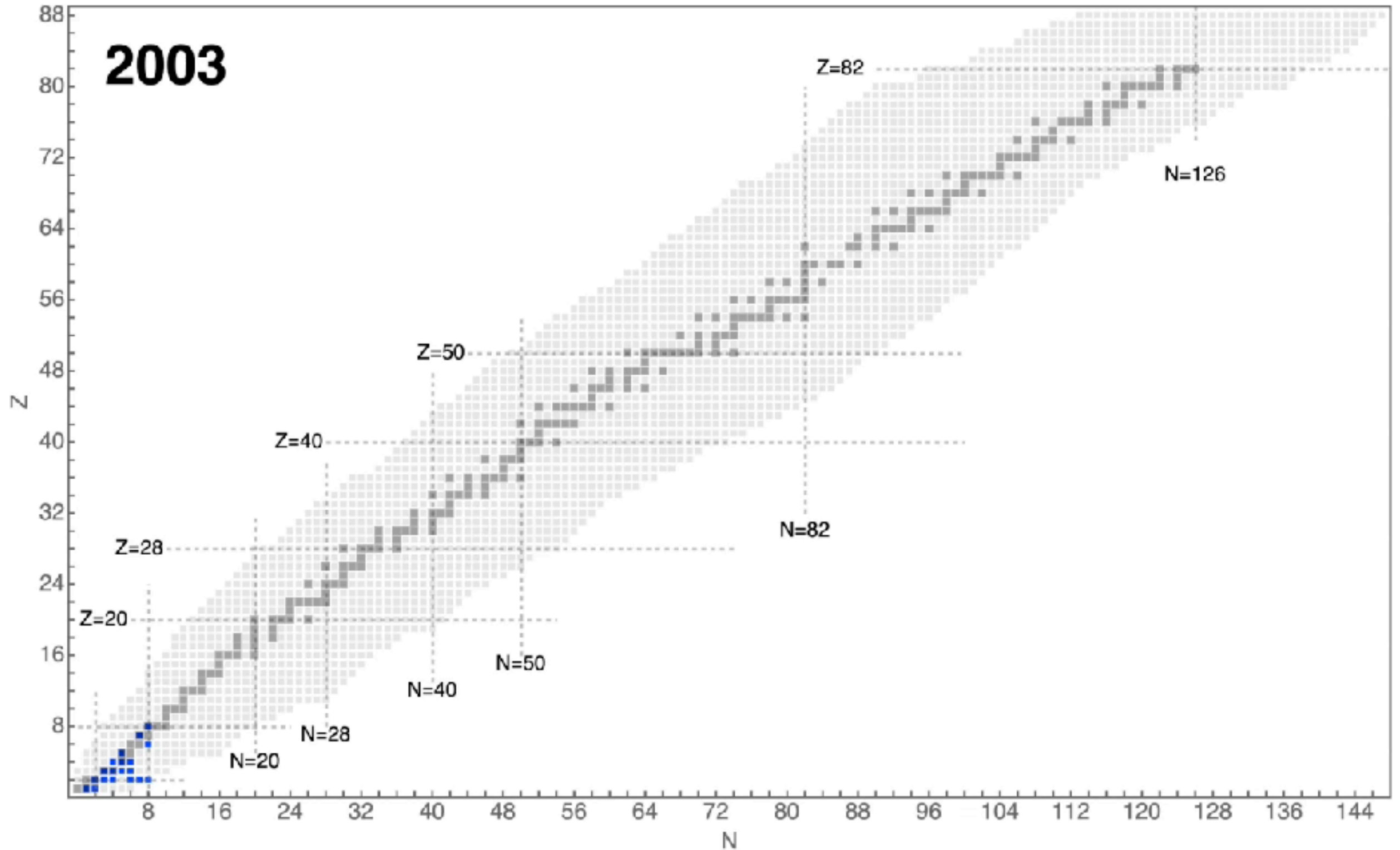
- Universal framework for the modeling of strongly-interacting few- and many-nucleon systems.
- Solving the many-nucleon problem with controlled approximations.

► Predictive power

- Linking nuclear structure and observables to fundamental forces.
- Reliably predict scientifically relevant nuclear observables.

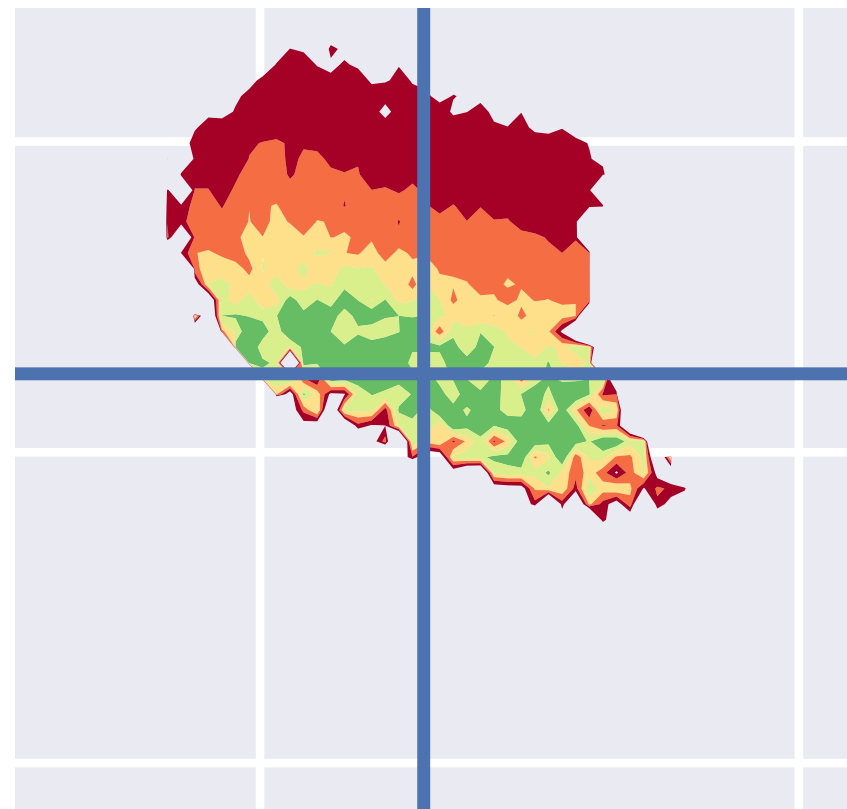


Reach of ab initio nuclear theory



Setting up for this talk

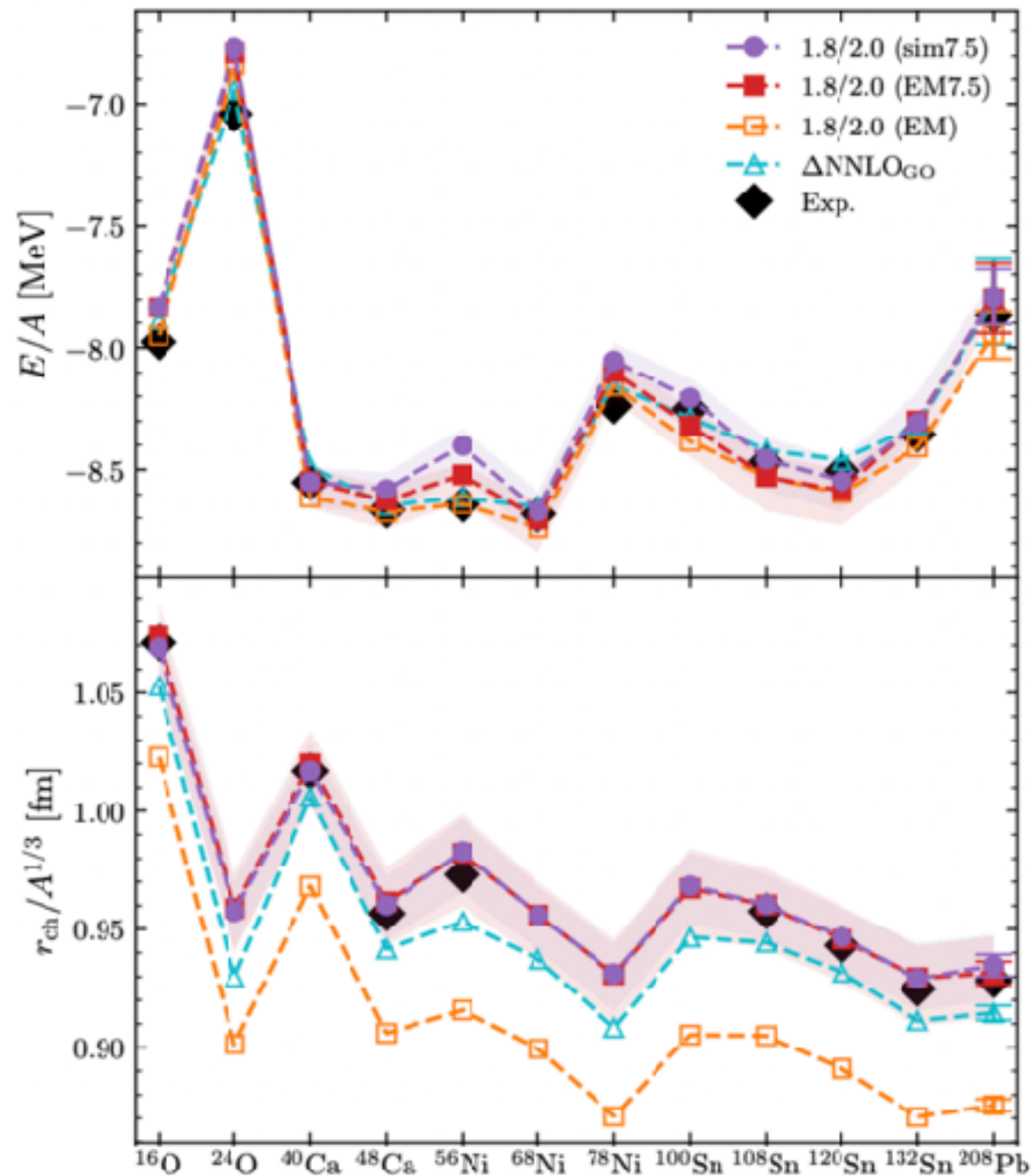
1. The **nucleus is a complex many-body system**. Exact quantitative nuclear models do not exist.
2. While all **models are wrong**, models that know when and how they are wrong are useful. (after G. Box)
3. **Bayesian methods** are particularly useful for assessing uncertainties in nuclear physics. *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 Bugeye 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]
 - Upcoming book by cf, R.J. Furnstahl, D. R. Phillips:
Until then, see 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/>]



***Interlude:* The many-body accuracy of chiral nuclear interactions**

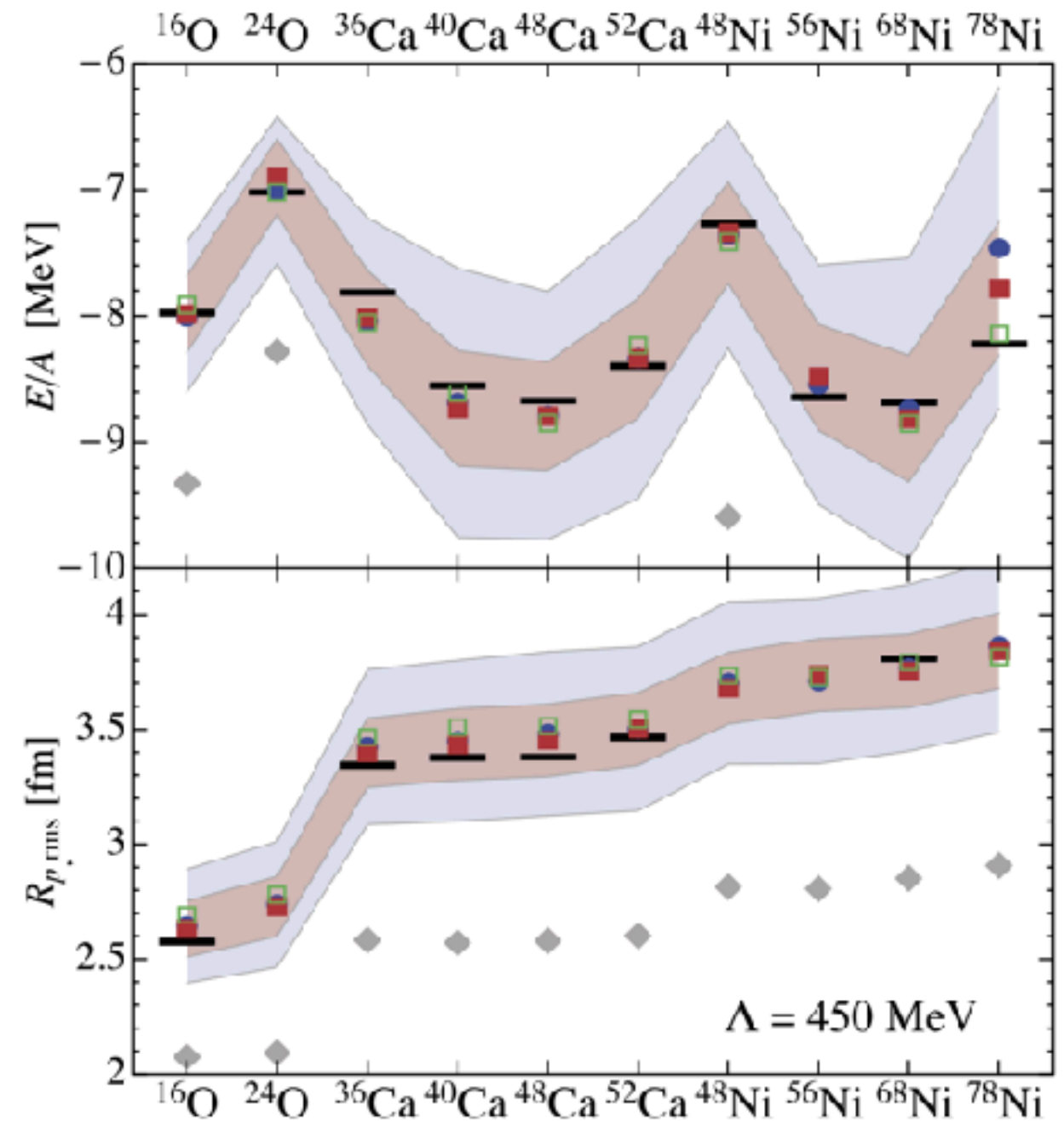
Accuracy: Some interactions work “better” than others

Optimization with 16O energy (and radius)



“Magic interaction” family

P. Arthuis, et al,
arXiv:2401.06675 (2024)



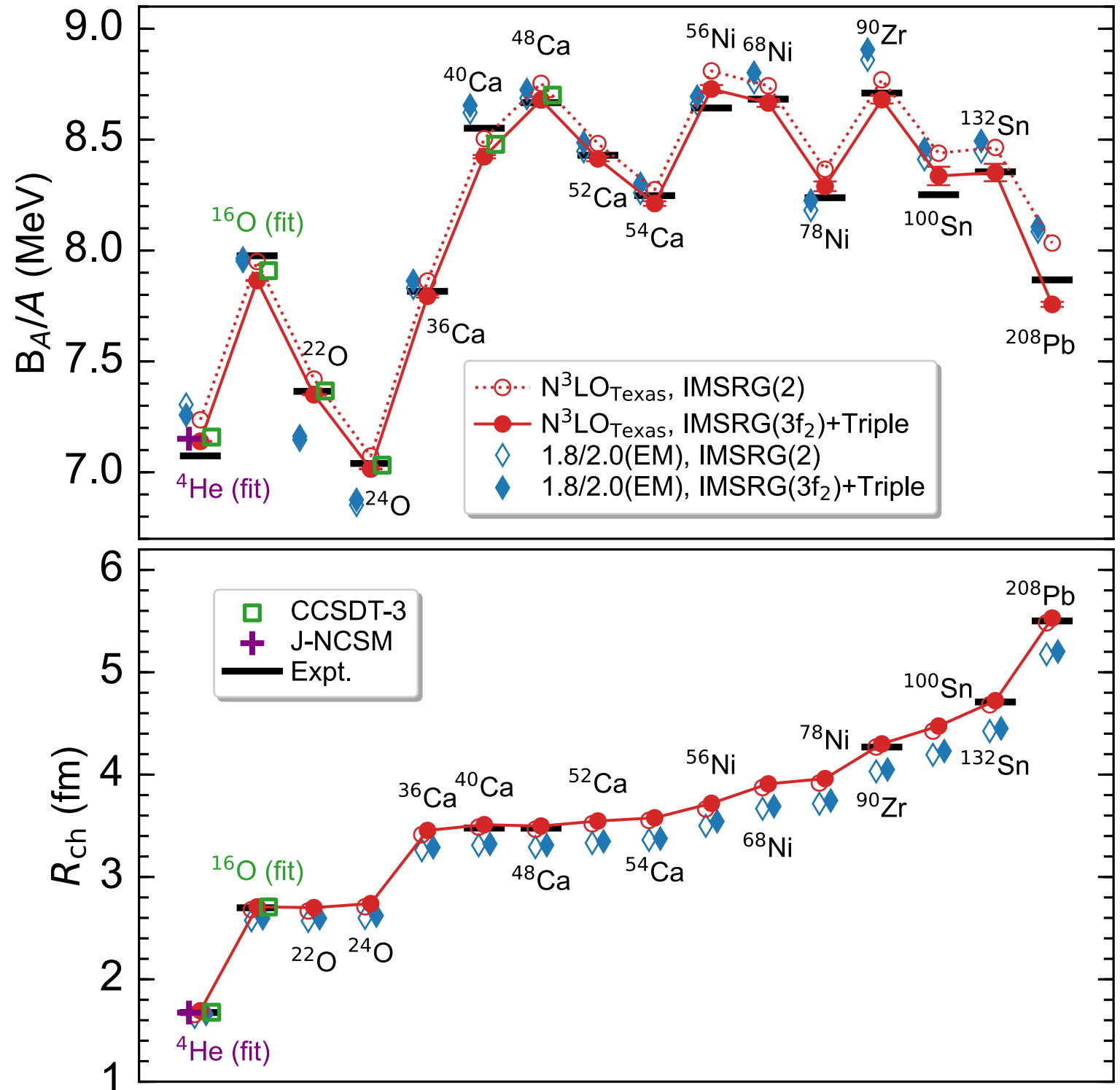
Order-by-order family

T. H  ther et al.,
Phys. Lett. B 808 (2020) 135651

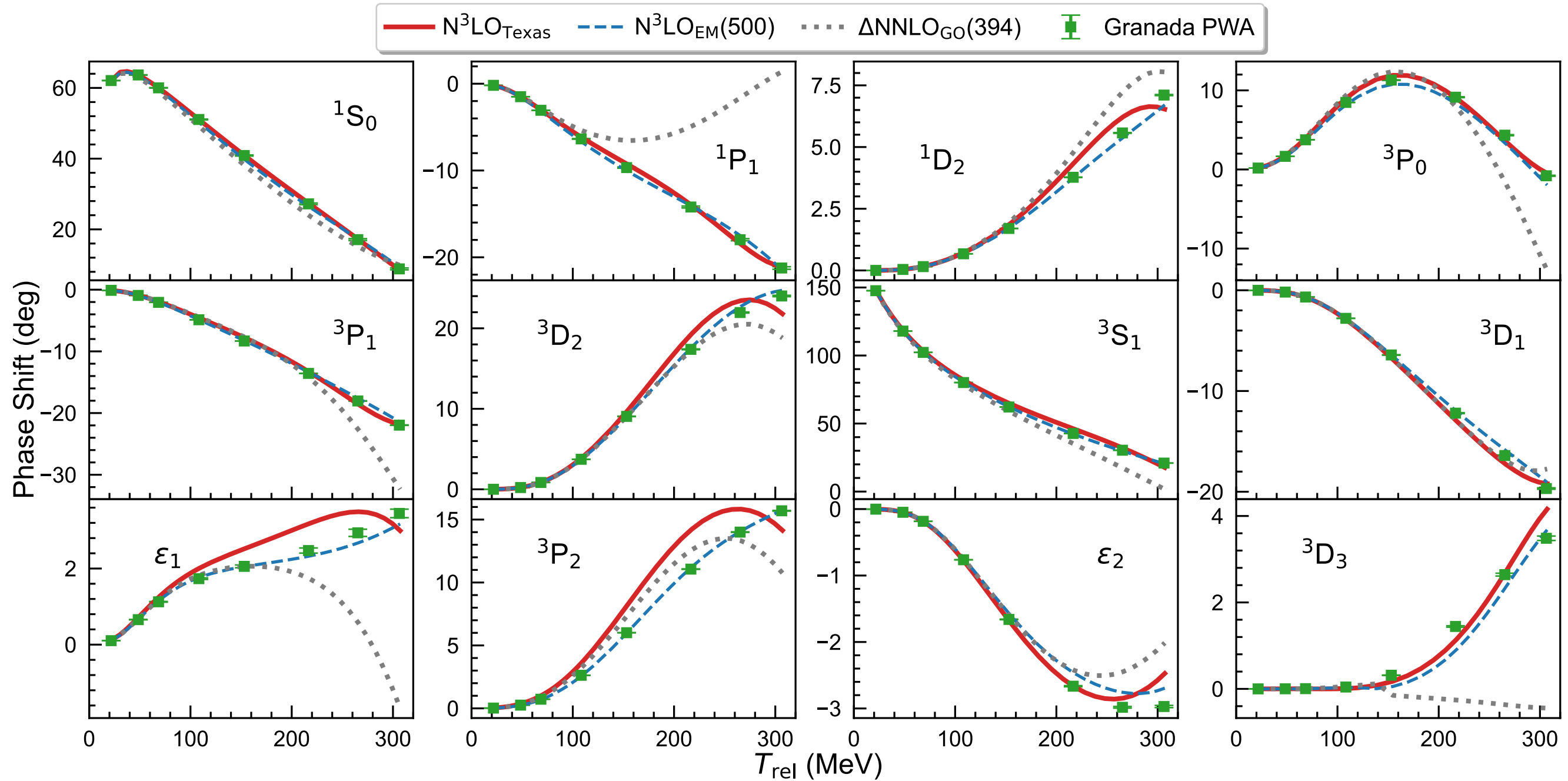
Accuracy: N3LO_{TX} (work in progress)

- ▶ χ EFT at N³LO (NN) + N²LO (3N) with $\Lambda=394$ MeV
- ▶ Manually tuned optimization includes NN observables, ^4He and ^{16}O energy, radius.
- ▶ Enabled by the use of fast & accurate emulators (reduced-order models)

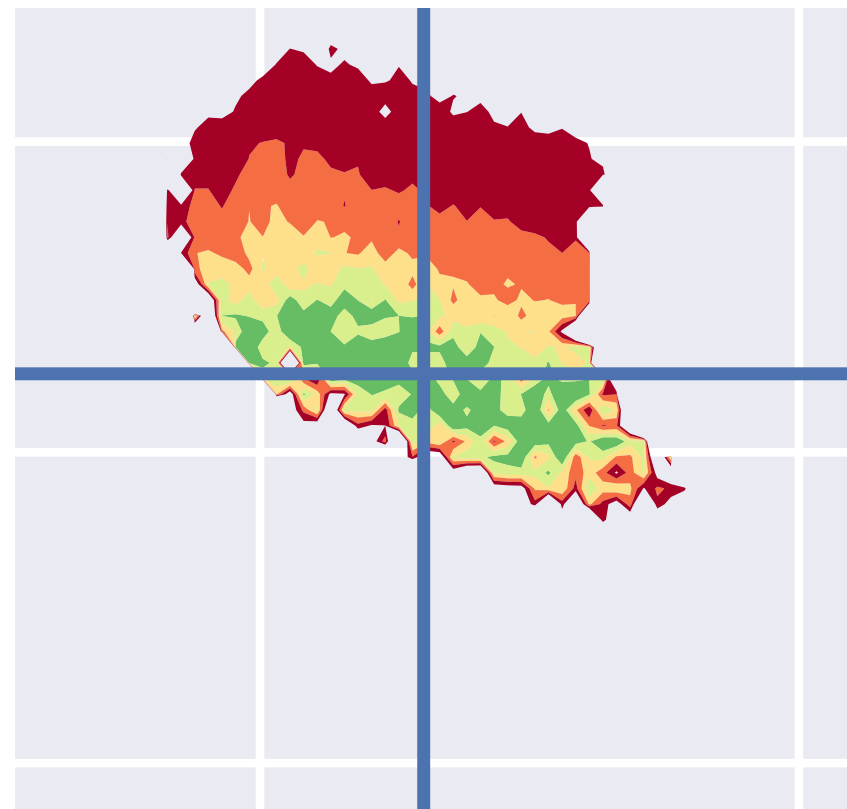
Baishan Hu, Weiguang Jiang,
A. Ekström, cf, G. Hagen. T.
Papenbrock (2025) in prep.



Accuracy: N3LO_{TX} (work in progress)



Baishan Hu, Weiguang Jiang,
A. Ekström, cf, G. Hagen. T.
Papenbrock (2025) in prep.



Precision nuclear theory

From accuracy to precision in *ab initio* theory

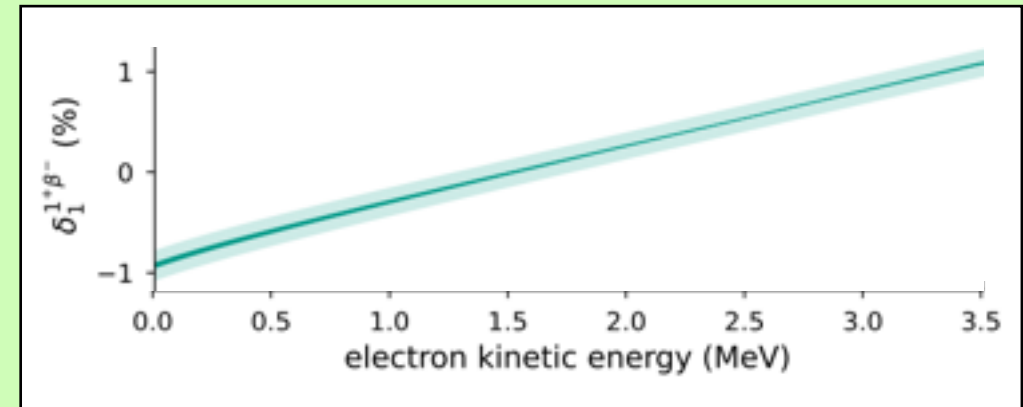
- ▶ Model the strong interaction at low-energy
 - Effective field theories (EFTs) offer a systematic description of this physics.
 - Truncating your EFT implies an understanding of the importance of terms beyond the truncation order.
- ▶ Bayesian parameter estimation and model checking
 - The inference of EFT parameters using low-energy observables.
 - Not only LECs might be of interest. E.g.,
 - The breakdown scale of the EFT
 - Tests of EFT model assumptions
 - Relevant parameters of the error model(s)
- ▶ Predictive power strongly linked to precision
 - Predict scientifically relevant nuclear observables with quantified uncertainties.

Physics predictions with (complex) precision models

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

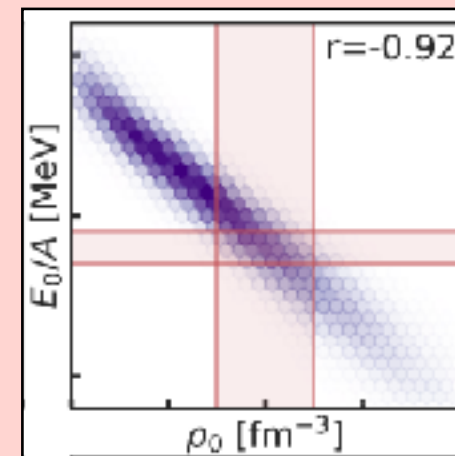
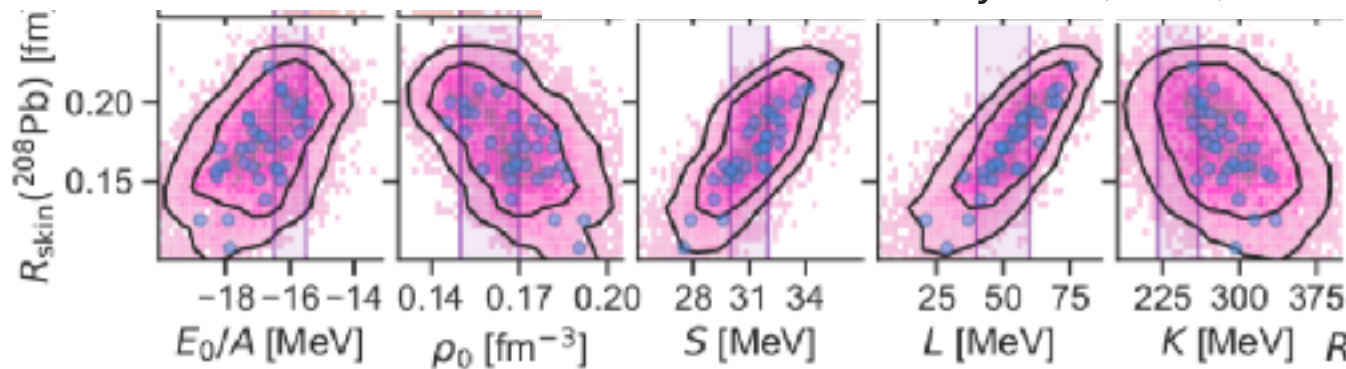
$$\frac{d\omega^{1+\beta^-}}{dE \frac{d\Omega_k}{4\pi} \frac{d\Omega_\nu}{4\pi}} = \frac{4}{\pi^2} (E_0 - E)^2 k E F^-(Z_f, E) C_{\text{corr}} \left| \langle \hat{L}_1^A \rangle \right|^2 \times 3 \left(1 + \delta_1^{1+\beta^-} \right) \left[1 + a_{\beta\nu}^{1+\beta^-} \vec{\beta} \cdot \hat{\nu} +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

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



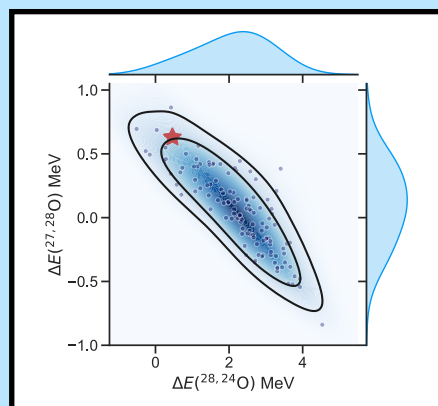
Infinite **nuclear matter** modelling

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



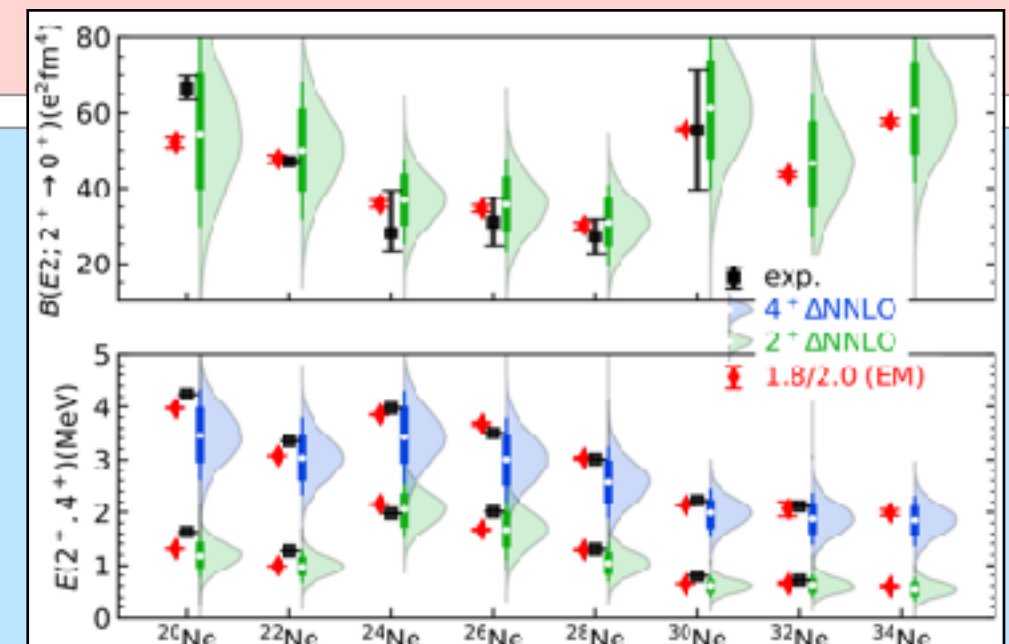
W. Jiang et al., PRC 109 (2024) L061302

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**

$$\text{Posterior} \quad \text{Likelihood} \quad \text{Prior} \\ \text{pr}(\boldsymbol{\alpha} \mid \mathcal{D}, I) = \frac{\text{pr}(\mathcal{D} \mid \boldsymbol{\alpha}, I) \text{pr}(\boldsymbol{\alpha} \mid I)}{\text{pr}(\mathcal{D} \mid I)} \\ \text{Marginal likelihood}$$

- 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.

► Statistical modeling (for *ab initio* methods)

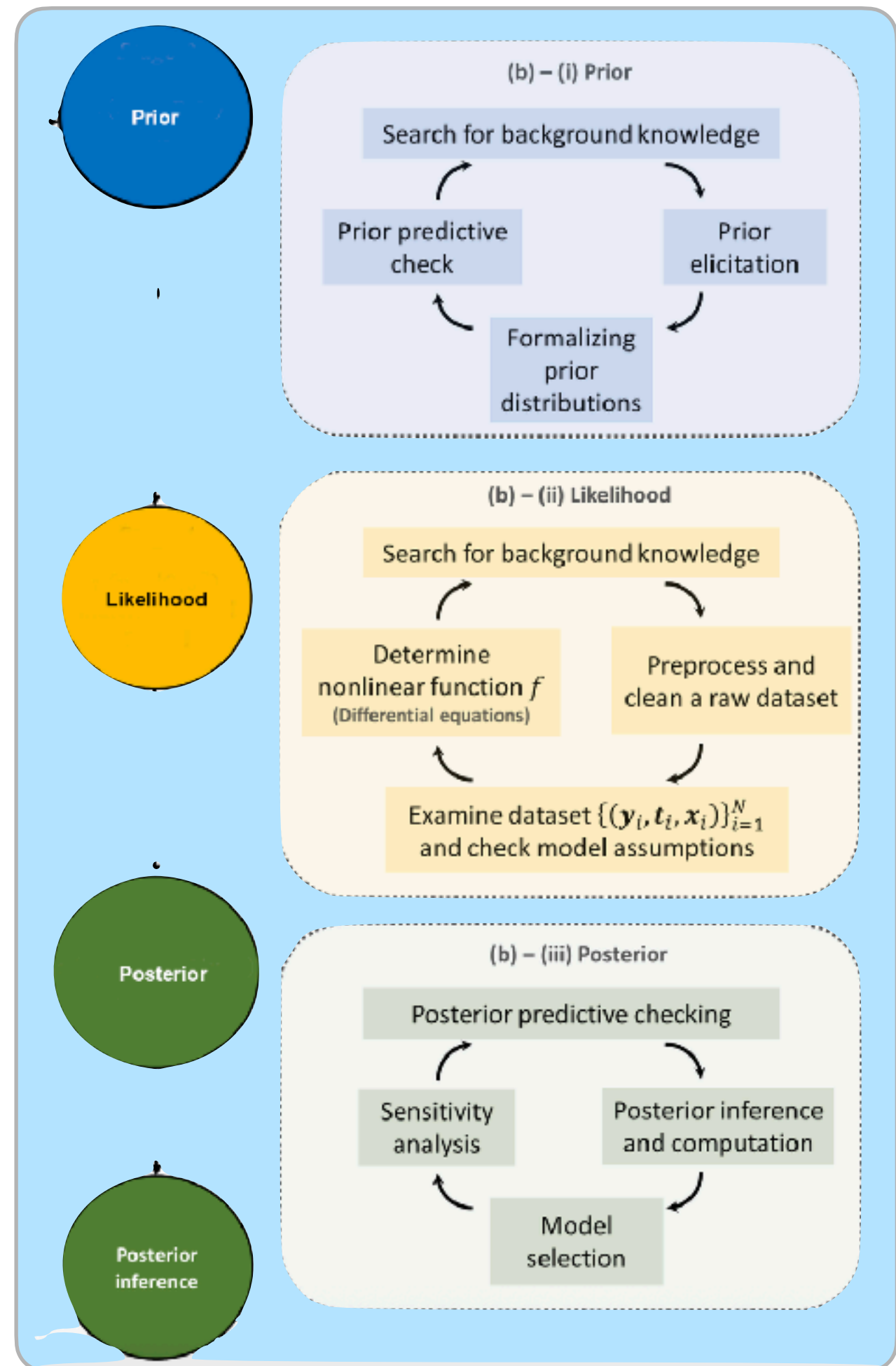
$$y_{\text{exp}} = \tilde{y}(\boldsymbol{\alpha}) + \delta y_{\text{EFT}} + \delta y_{\text{method}} + \delta \tilde{y}_{\text{em}} + \delta y_{\text{exp}}$$

- **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 workflow

Checklist for a sound Bayesian statistical analysis

1. Interact with the experts (i.e., statisticians, applied mathematicians).
2. Incorporate all sources of experimental and theoretical errors.
3. Formulate statistical models for uncertainties.
4. Use as informative priors as is reasonable; test sensitivity to priors.
5. Account for correlations in inputs (type x) and observables (type y).
6. Propagate uncertainties through the calculation.
7. Use model checking to validate our models.



Bayesian predictive distributions

- ▶ Predictions for “future” data, modeled with $y(\alpha)$, are described by the **posterior predictive distribution** (ppd)

$$\{y(\alpha) : \alpha \sim \text{pr}(\alpha \mid \mathcal{D}, I)\}$$

- ▶ We will also introduce **full ppd**:s $\{y(\alpha) + \delta y : \alpha \sim \text{pr}(\alpha \mid \mathcal{D}, I), \delta y \sim \text{pr}(\delta y)\}$

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

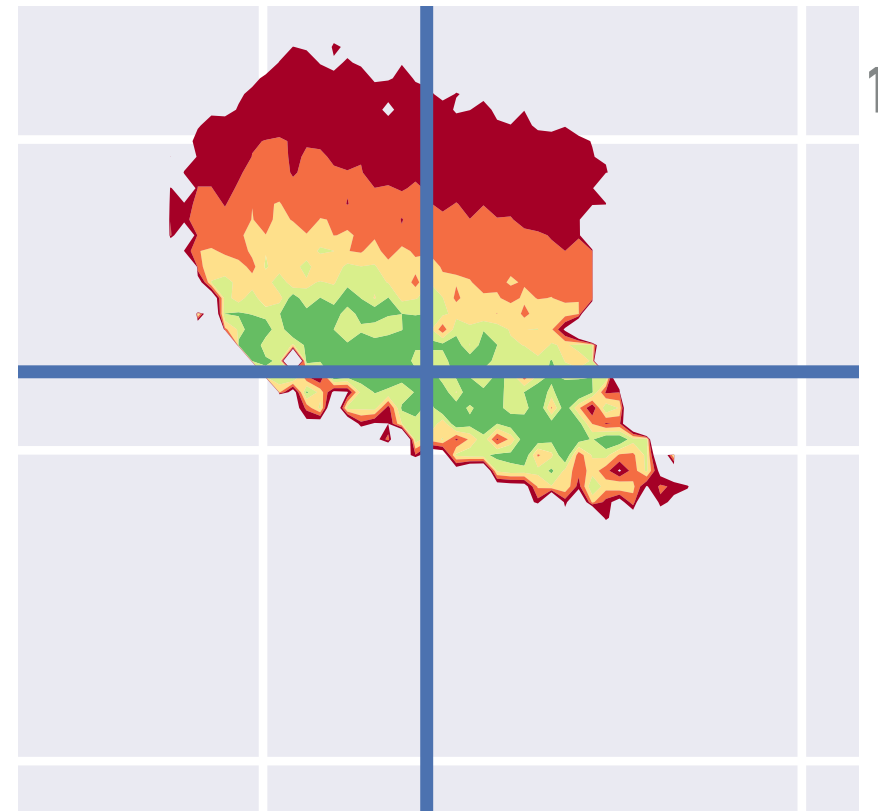
$$\{y(\alpha) : \alpha \sim \text{pr}(\alpha \mid I)\}$$

- ▶ 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

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

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

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

parameters inferred from data.

– **parametric uncertainty**

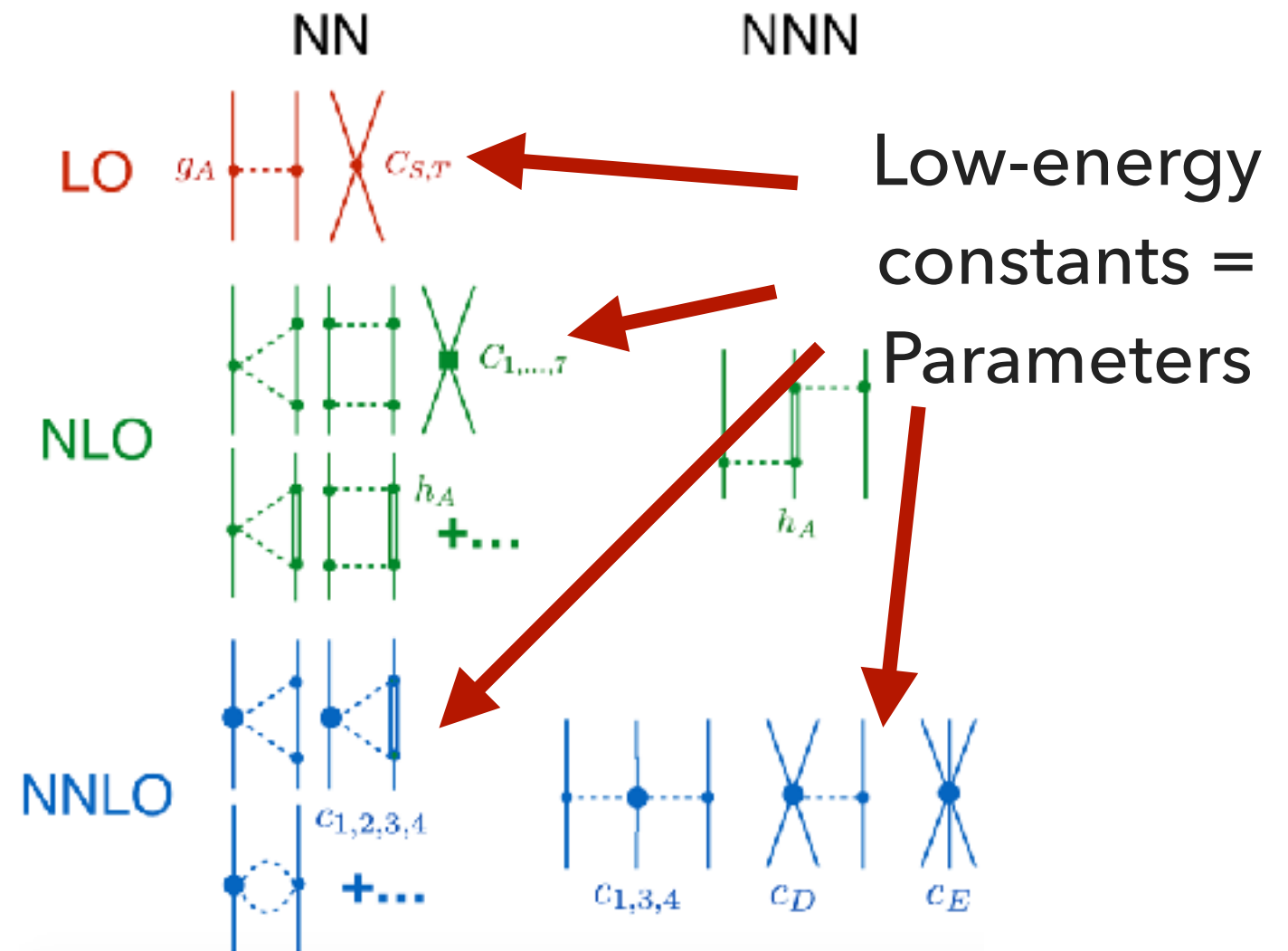
EFT expansion truncated and use of finite regulator cutoff

– **model/EFT truncation error**

many-body solver relies on approximations:

– **many-body error**

χ EFT 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)

Getting to know your errors

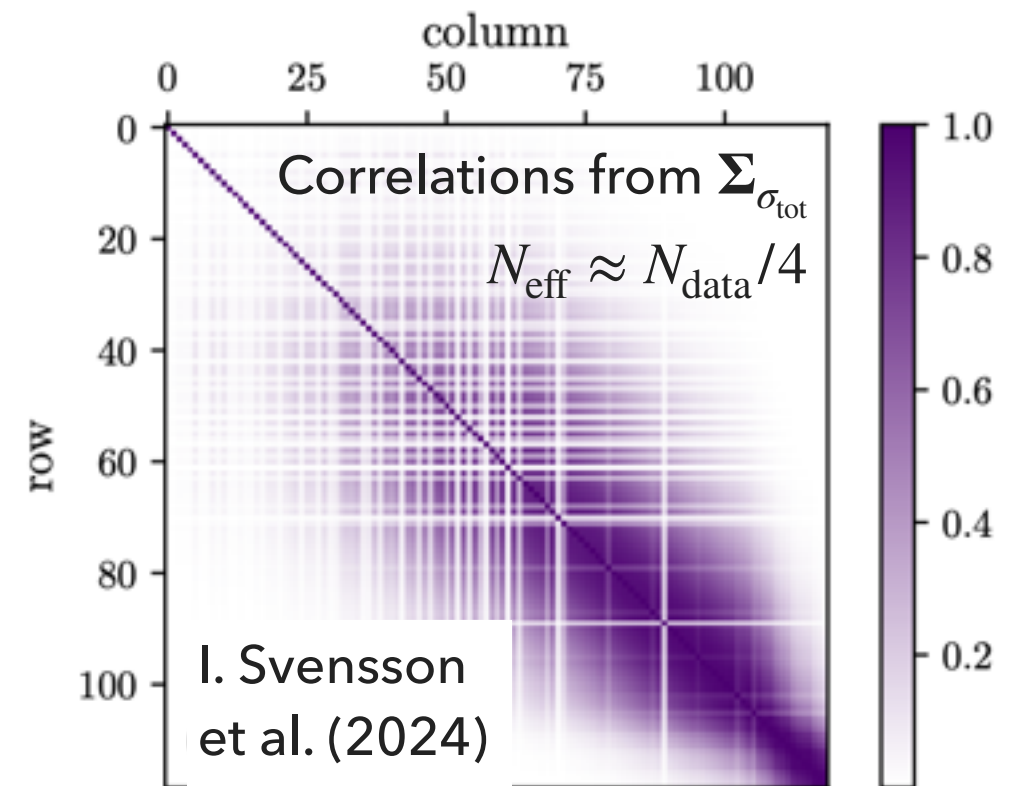
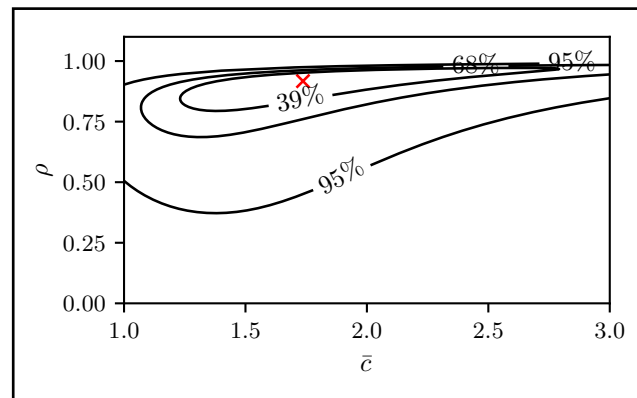
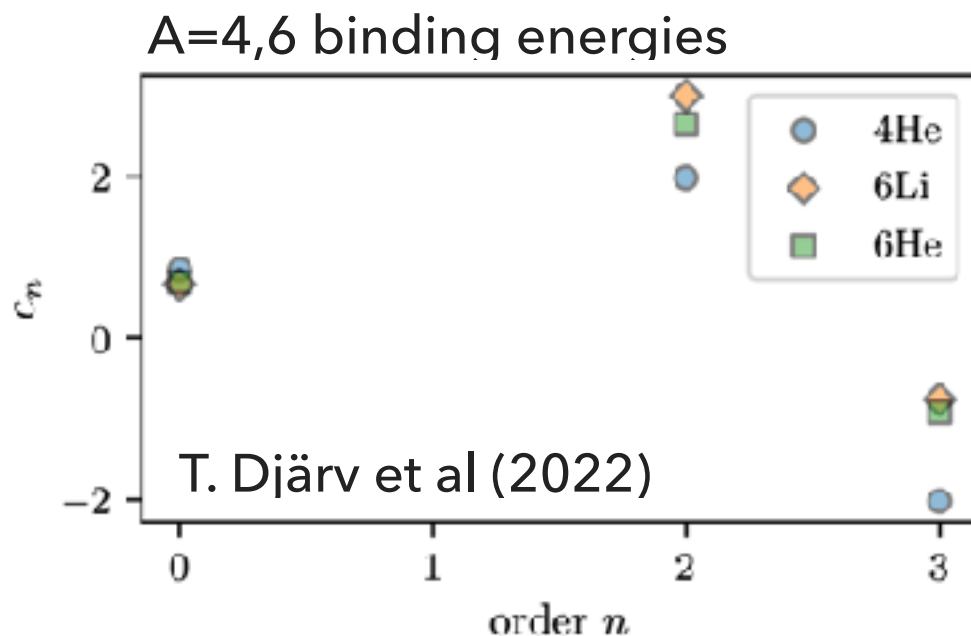
▶ Challenge #1: EFT truncation errors

- ▶ **Approach:** study order-by-order results and learn the PDF for expansion coefficients

$$\mathbf{y}_k = \mathbf{y}_{\text{ref}} \sum_{n=0}^k c_n Q^n, \quad \delta \mathbf{y}_k = \mathbf{y}_{\text{ref}} \sum_{n=k+1}^{\infty} c_n Q^n$$

- ▶ **Challenges:** Correlation structures, cutoff dependence, expansion parameter, irregular convergence patterns

$$\delta \mathbf{y}_k(\vec{x}) = \mathbf{y}_{\text{ref}} \sum_{n=k+1}^{\infty} c_n(\vec{x}) Q^n$$

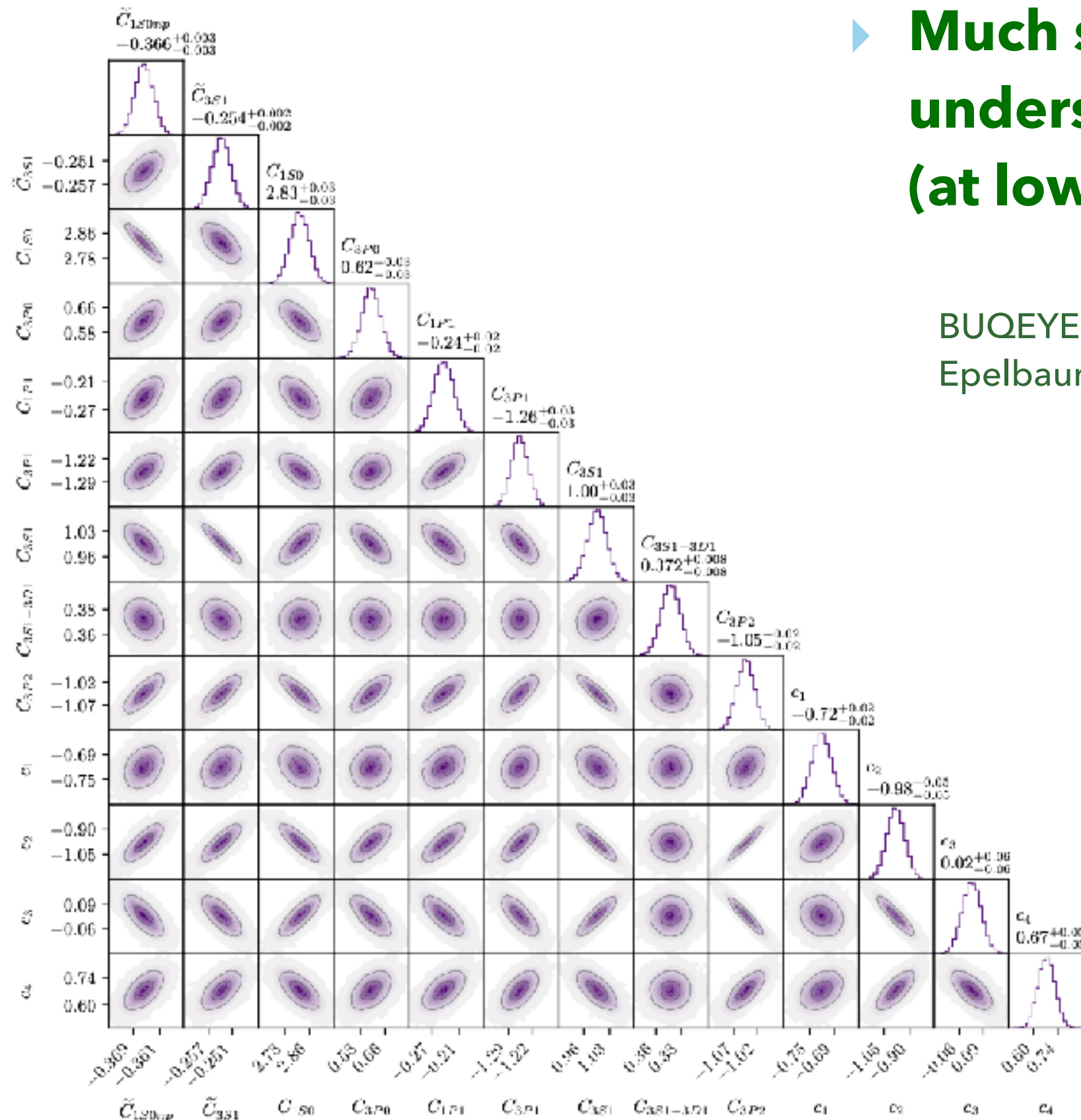


GP modelling for correlated EFT errors in
J. Melendez et al (2019) and C. Drischler et al. (2020)

LEC inference and EFT truncation errors in the NN sector

► **Much studied, and good understanding (at low cutoffs)**

BUQEYE collaboration, Chalmers' group, Epelbaum et al.

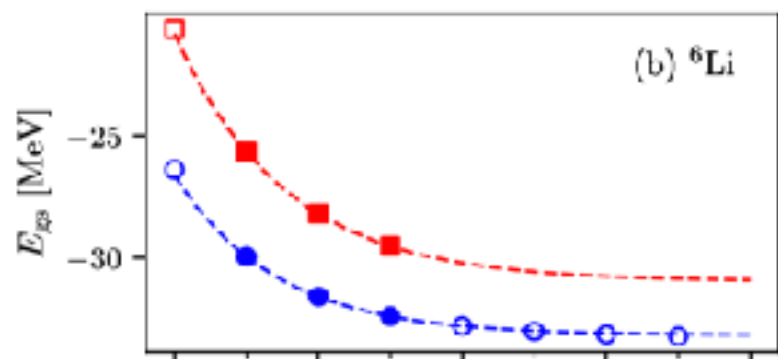


Getting to know your errors

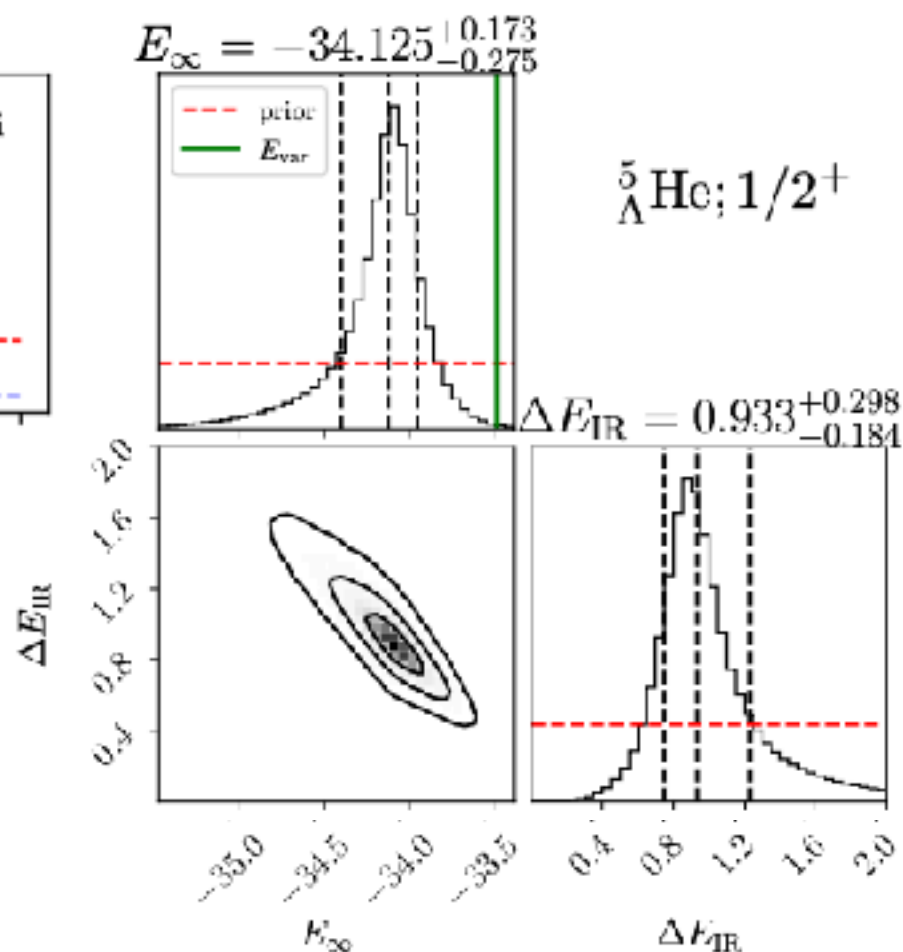
► Challenge #2: Many-body solver errors

- **Approach:** Convergence studies; Method comparisons;
- **Note:** We can incorporate “uncertain” extrapolation, $\mathbb{E}[\delta y_{\text{MB}}] \neq 0$
- **Challenges:** Some approximations might be very difficult to relax;
Non-variational observables/approaches

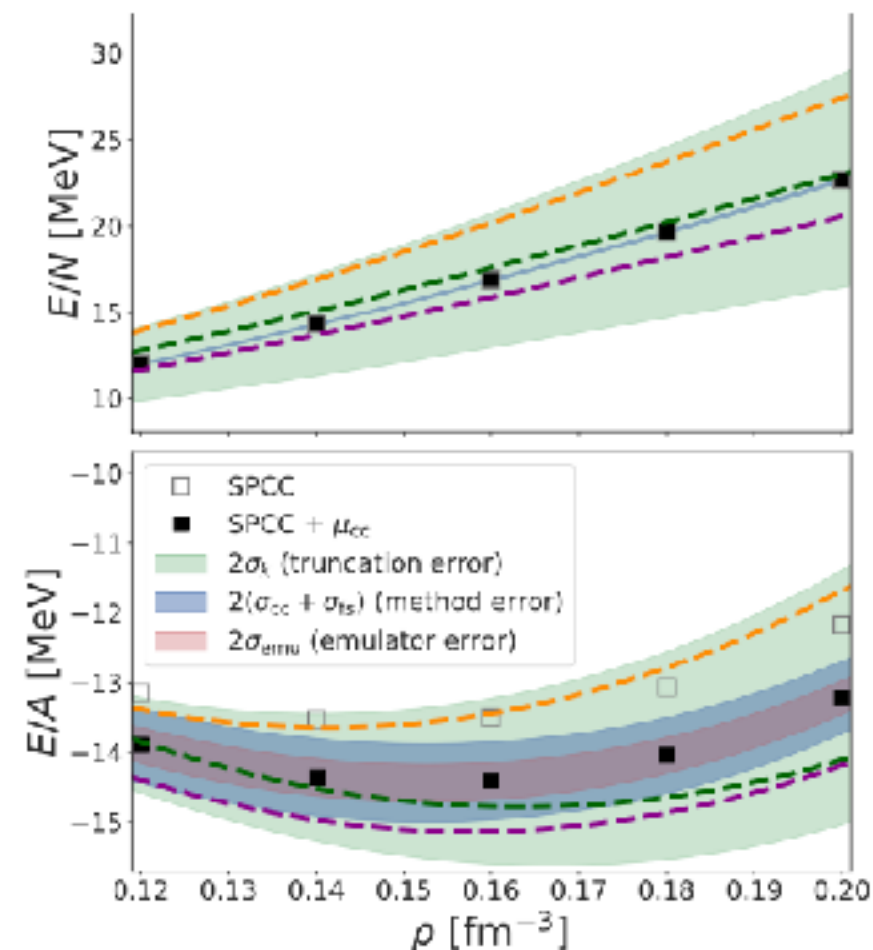
N_{max} extrapolation for NCSM in
T. Djärv et al (2022)



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)



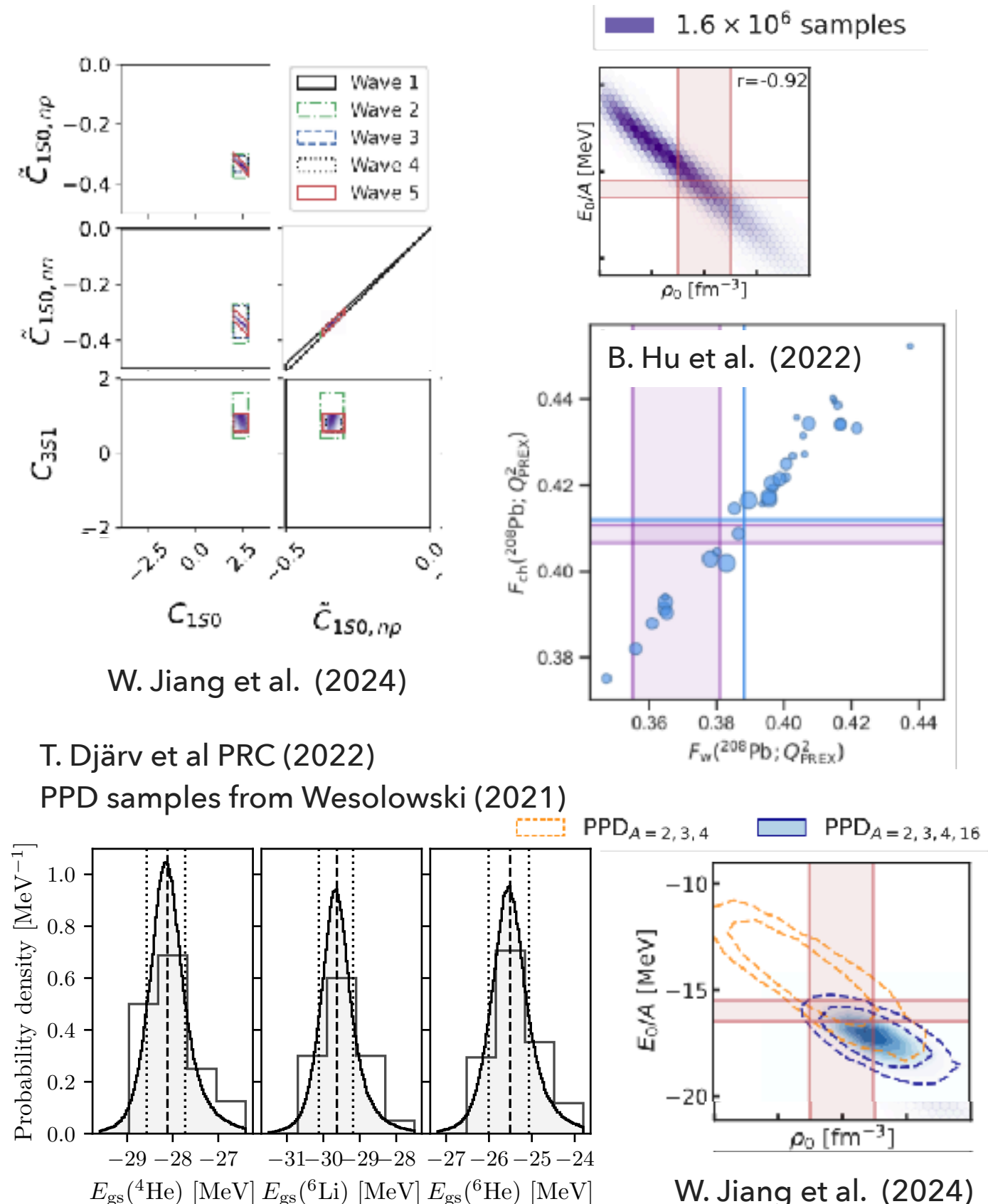
Challenge #3: Parametric uncertainty for high-cost models

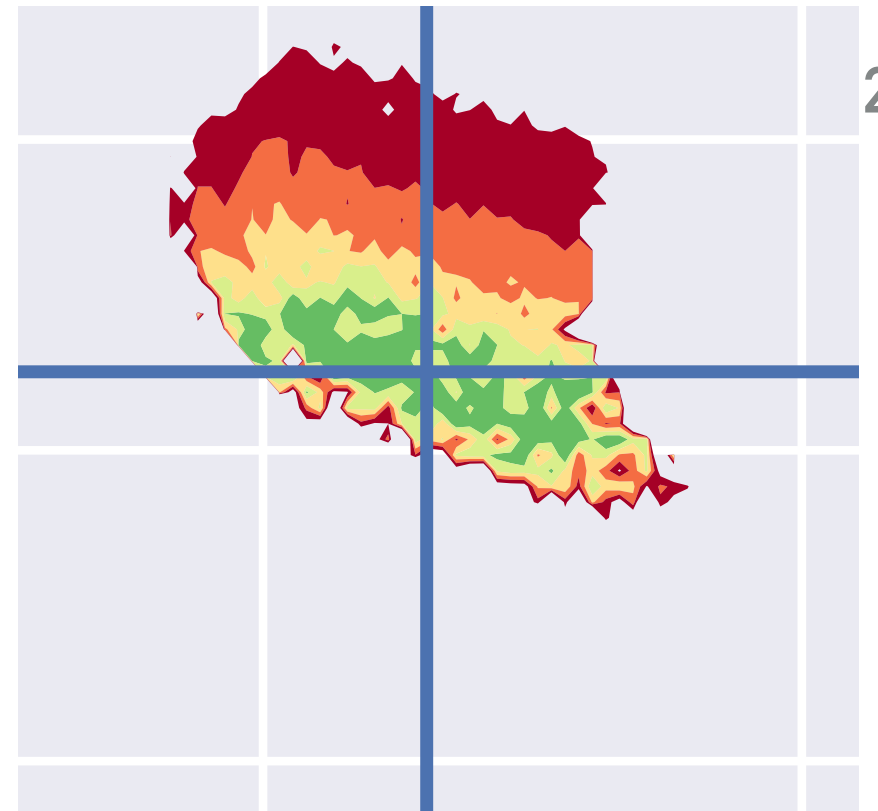
Likelihood-free methods

- 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.





Emulators

Emulators

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

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

- ▶ 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.

Review on projection-based emulators::

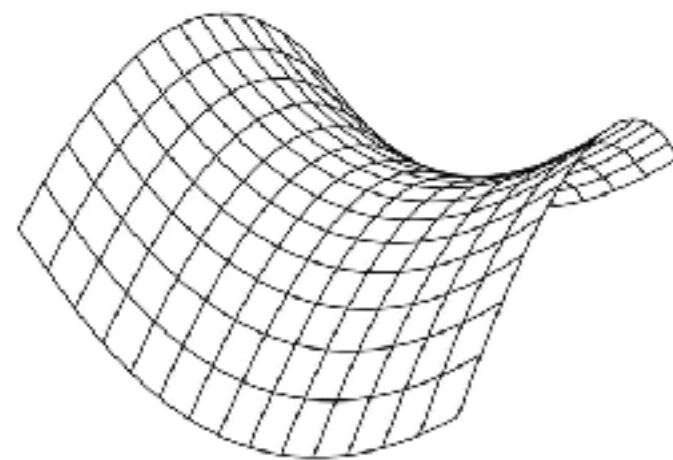
T. Duguet, et al. Rev. Mod. Phys. **96** (2024) 031002

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)

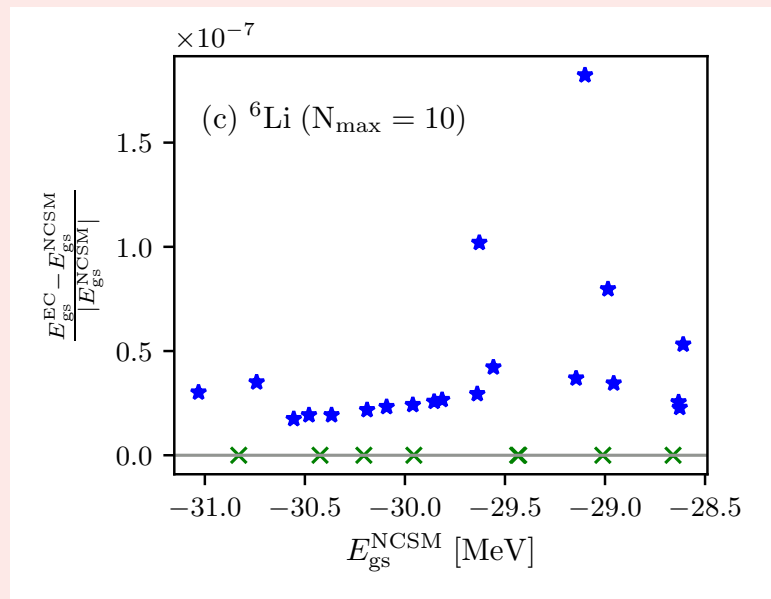
T. Duguet, et al. Rev. Mod. Phys. **96** (2024) 031002

Emulator precision and speedup

► Challenge #4: Emulator errors

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

$E(^6\text{Li})$

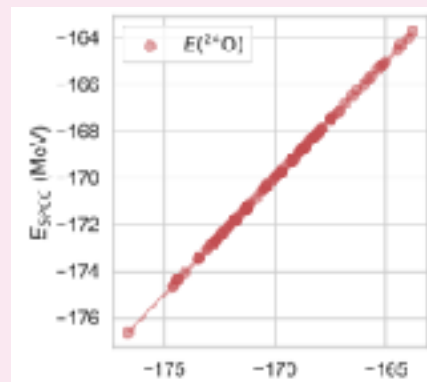


EVC (NCSM M-scheme)

Speedup: 10^7

Djärv et al., (2022)

$E(^{24}\text{O})$

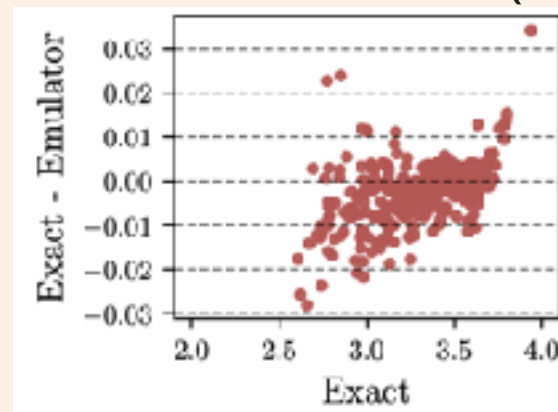


Kondo et al.,
(2022)

SPCC (CCSDT-3)

Speedup: 10^8

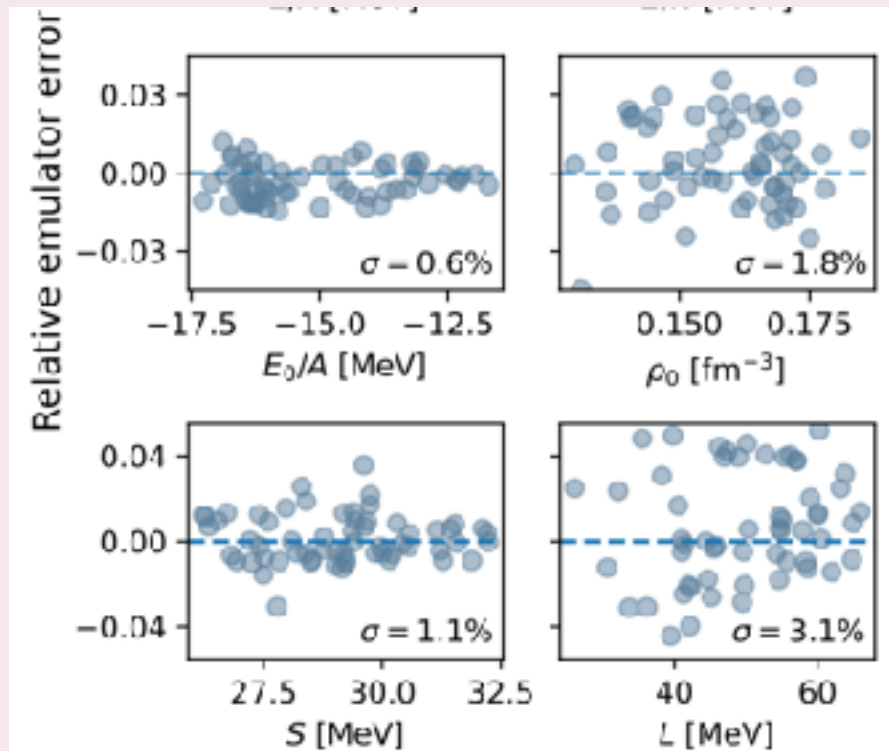
$R_{42}(\text{Ne}, \text{Mg})$



HF

Sun et al., (2024)

Infinite nuclear matter



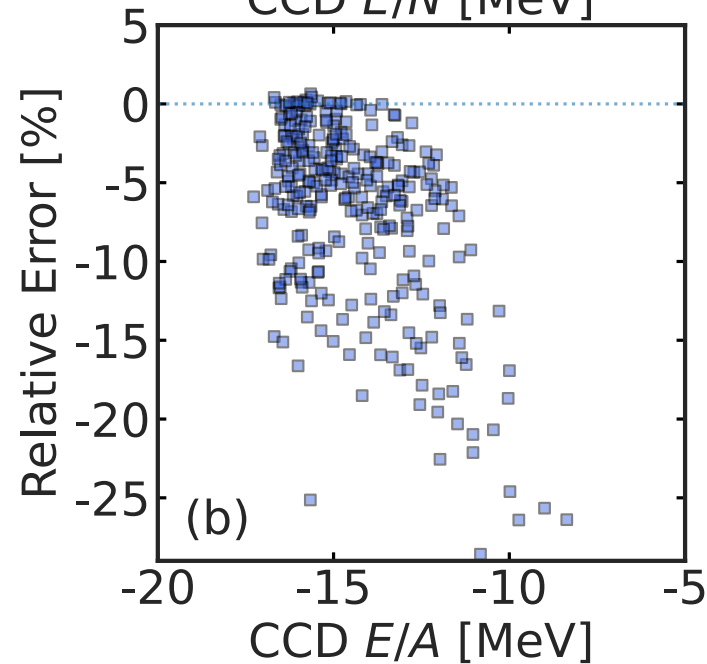
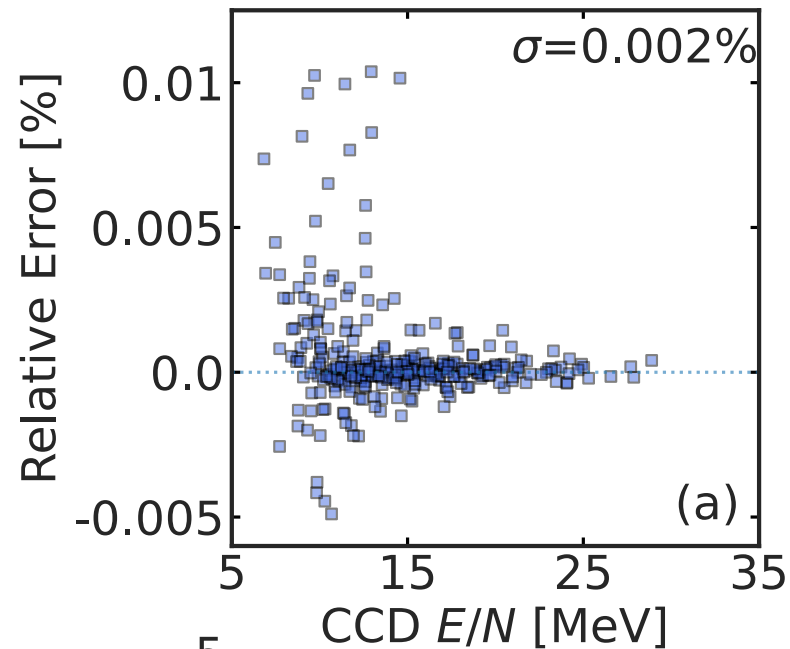
SPCC (CCD k-boxes with
 $A=66, 132$ at 6 densities)

Speedup: 10^8

Jiang et al., (2024)

Small-batch voting

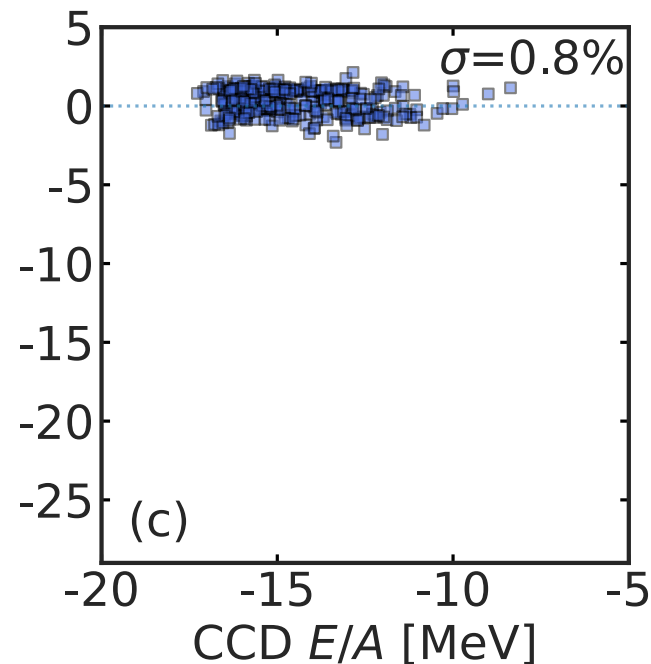
SPCC



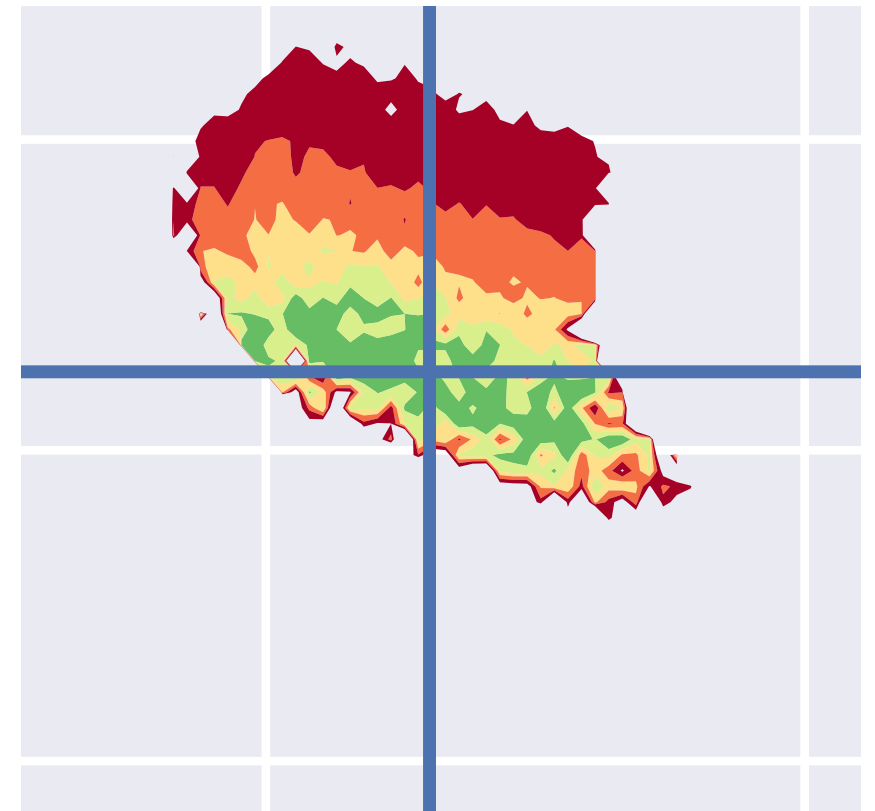
Physical states are stable
w.r.t. subspace variations

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

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 $\Delta - \chi^{\text{EFT}}$

- ▶ χ^{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:
 $\mathcal{D}_{A=2,3,4}$ and $\mathcal{D}_{A=2,3,4,16}$.
- ▶ 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 $T_{\text{lab}}=1, 5, 25, 50, 100, 200$ MeV

[wave 1] & [wave 2] & final

- $^2\text{H} (E, R_p^2, Q),$

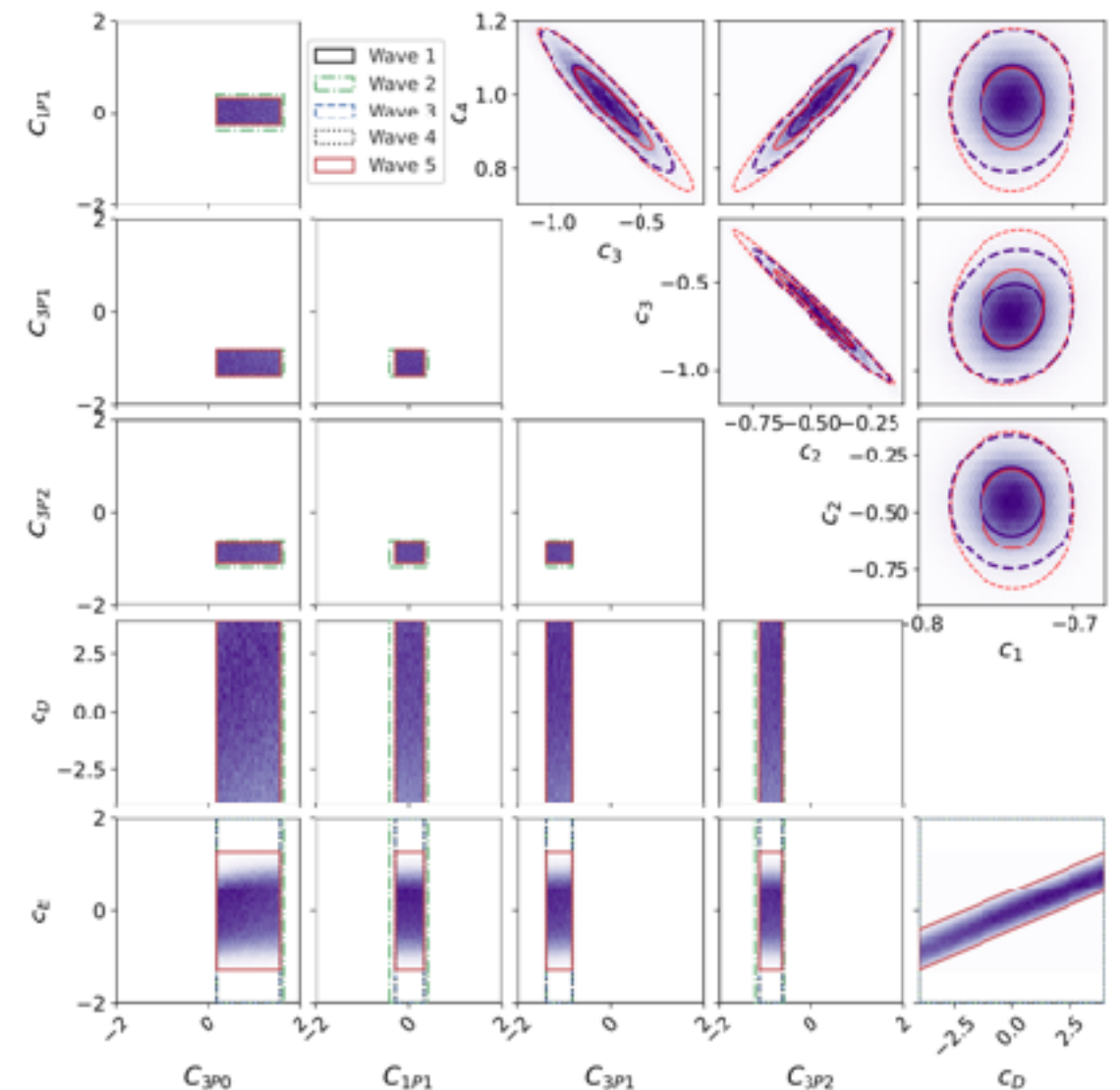
[wave 3] & [wave 4] & final

- $^3\text{H} (E), ^4\text{He} (E, R_p^2)$

[wave 4] & final

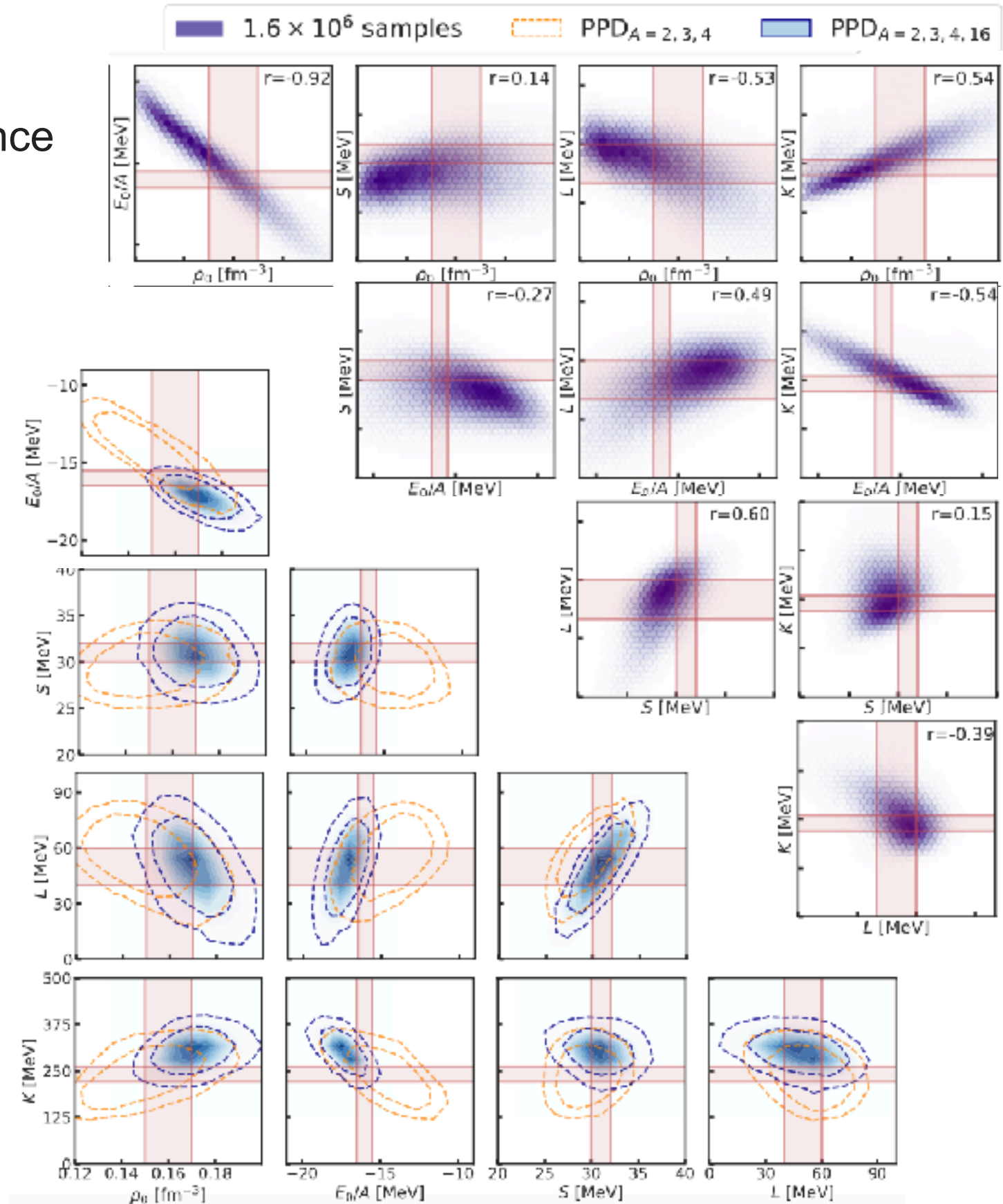
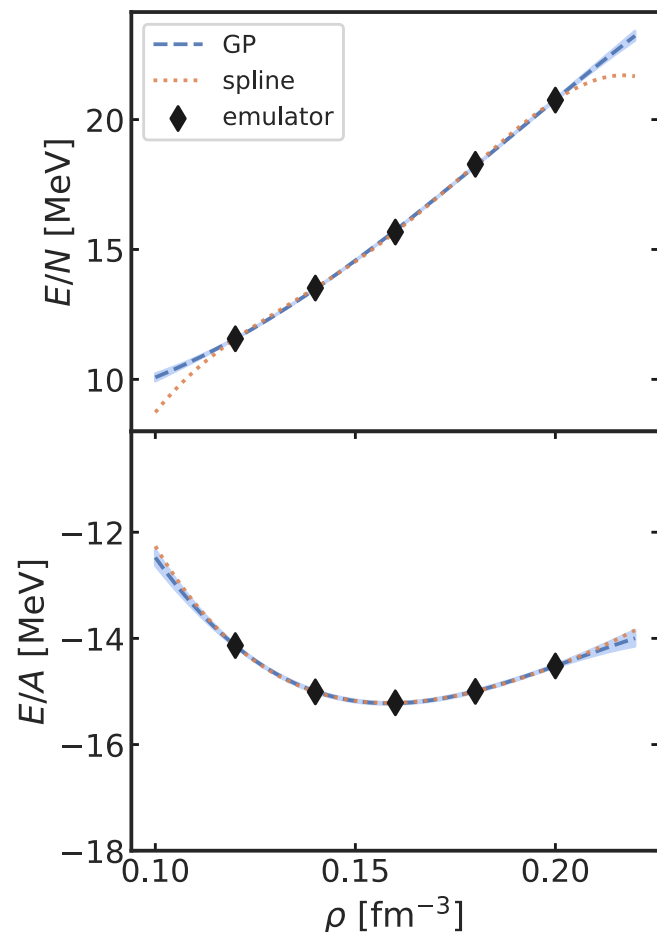
- Prior for c_1, c_2, c_3, c_4 from a Roy-Steiner analysis of πN data (Siemens 2017)

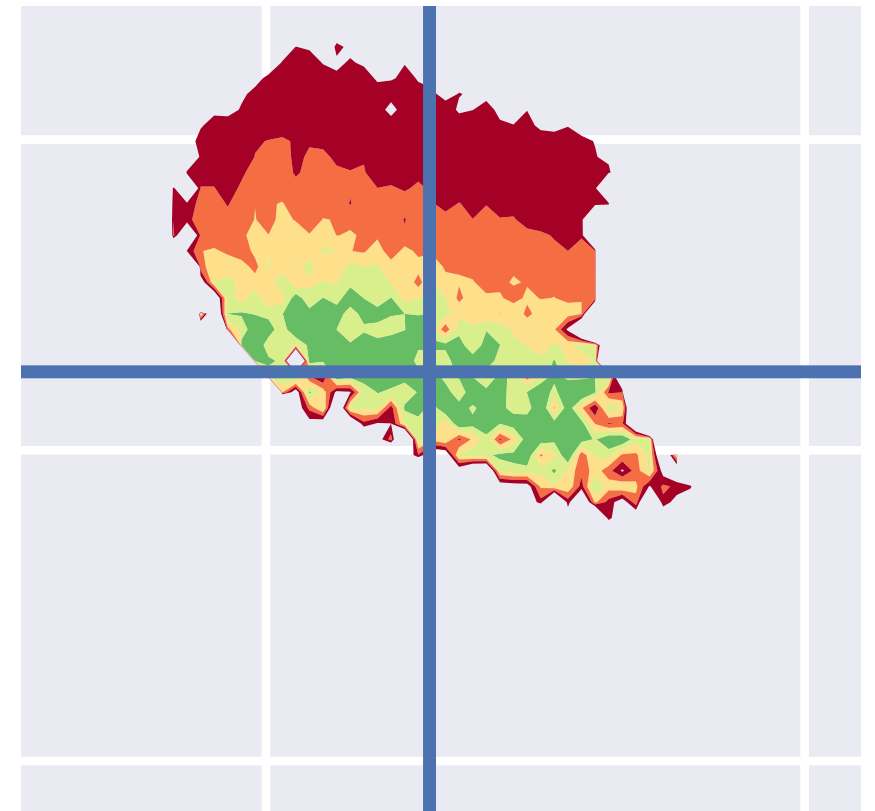
Observable	z	ε_{exp}	$\varepsilon_{\text{model}}$	$\varepsilon_{\text{method}}$	ε_{em}
$E(^2\text{H})$	-2.2298	0.0	0.05	0.0005	0.001%
$r_p(^2\text{H})$	1.976	0.0	0.005	0.0002	0.0005%
$Q(^2\text{H})$	0.27	0.01	0.003	0.0005	0.001%
$E(^3\text{H})$	-8.4818	0.0	0.17	0.0005	0.01%
$E(^4\text{He})$	-28.2956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



Strategic training of NM emulator

- ▶ About 10,000 NI samples.
- ▶ Bayesian PPDs using importance resampling with two different likelihoods ($A=2-4$, $2-16$).
- ▶ Relies on SPCC emulators.
- ▶ Use 64 *most important* samples for emulator construction.





Symmetry-breaking and restoration in *ab initio* modeling of atomic nuclei

Multiscale physics of atomic nuclei from first principles

by Z.H. Sun, A. Ekström, cf, G. Hagen, G.R. Jansen, T. Papenbrock,
Phys. Rev. X **15** (2025) 011028

Octupolar deformation (work in progress)

by M. Heintz, B. Hu, A. Scalesi, A. Ekström, cf, G. Hagen, T. Papenbrock

Ab initio predictions of deformed nuclei

1. **Static correlations**

Included in mean-field reference state through broken symmetries

- ▶ first axially symmetric, but now more general (Alberto Scalesi)

2. **Short-range correlations first**

Include short-range (“dynamical”) correlations via CC method

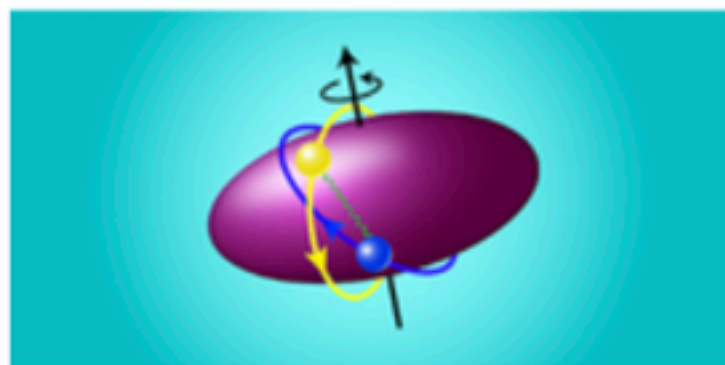
- ▶ captures UV physics; gets most of the binding energy

3. **Long-range correlations next**

Symmetry projection includes collective effects

- ▶ captures IR physics; small contribution to binding; large to structure

Multiscale physics of deformed nuclei

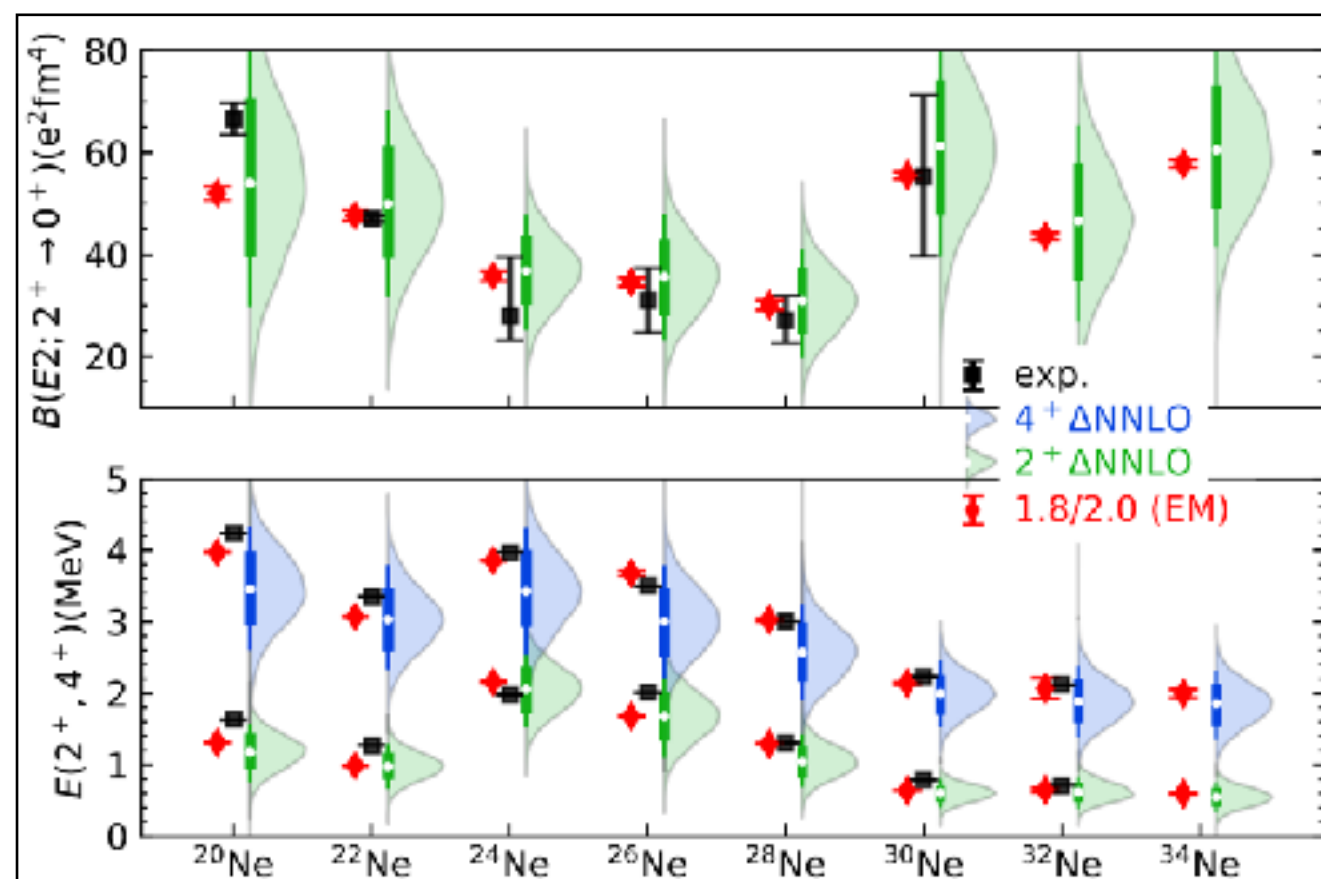
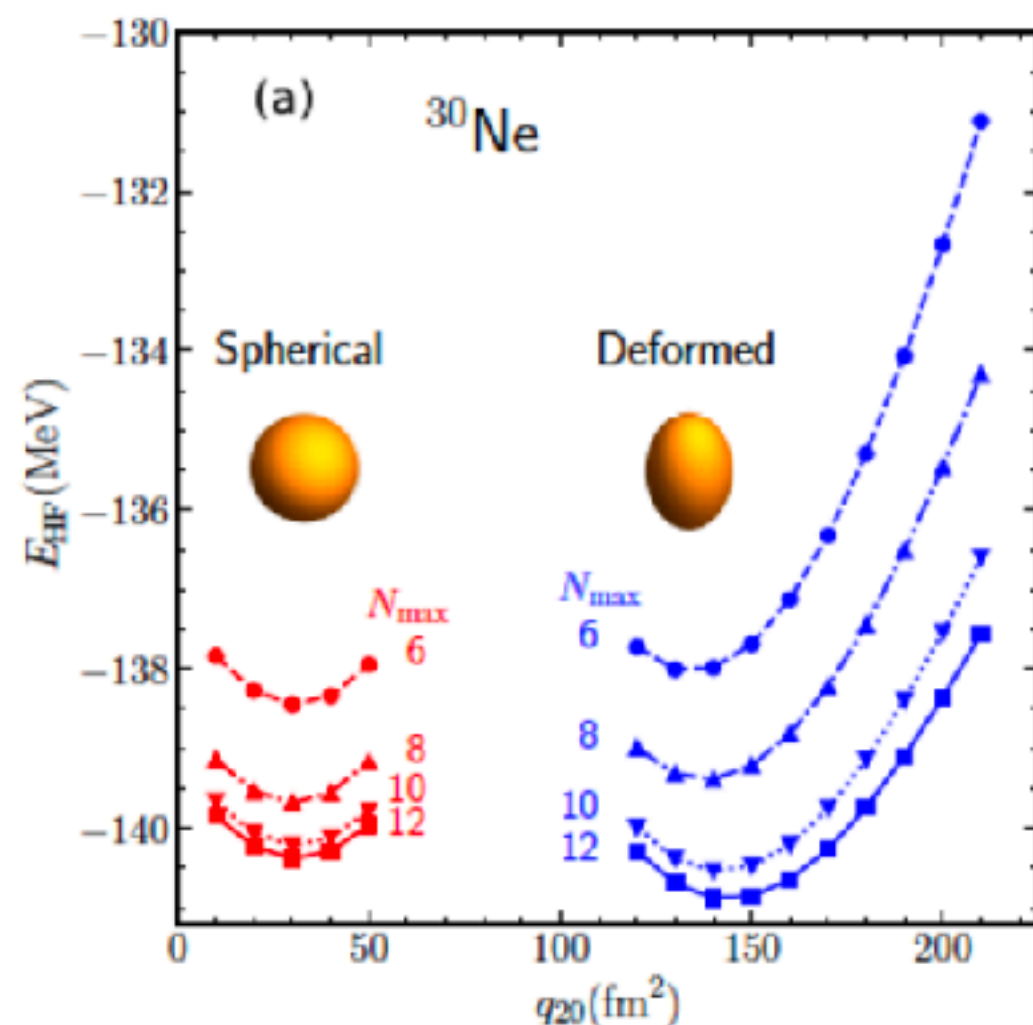


FEATURED IN PHYSICS

Multiscale Physics of Atomic Nuclei from First Principles

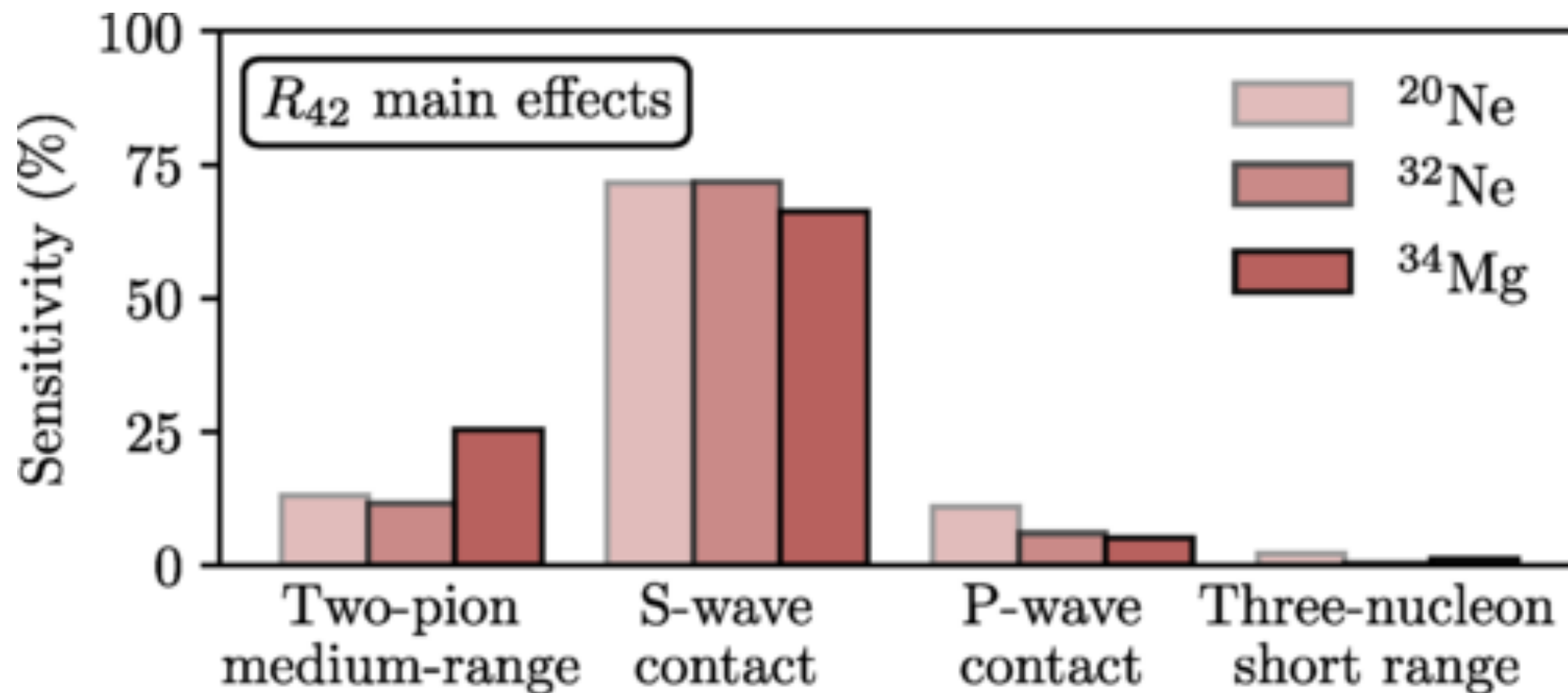
Z. H. Sun, A. Ekström, C. Forssén, G. Hagen, G. R. Jansen, and T. Papenbrock

Phys. Rev. X **15**, 011028 (2025)



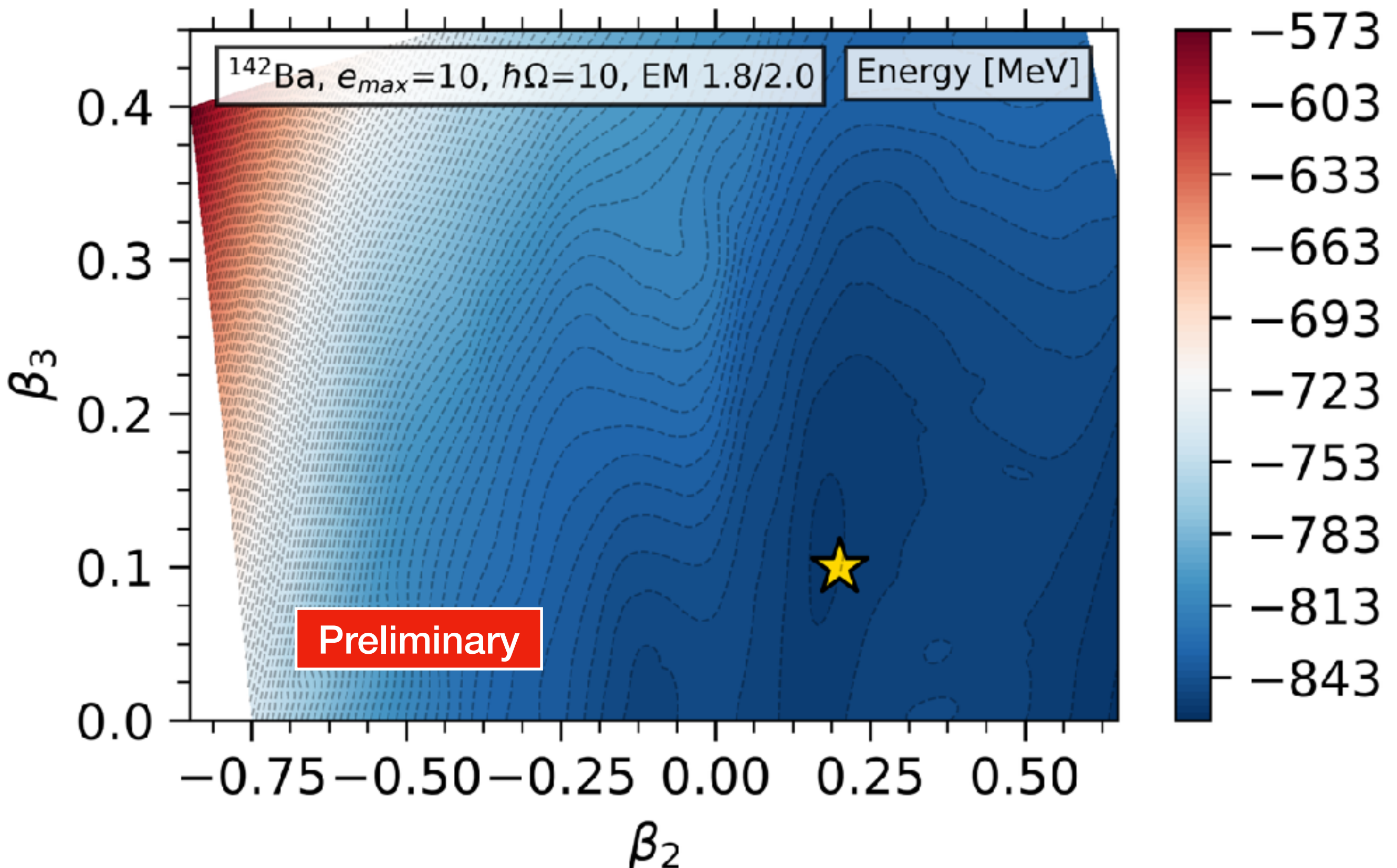
What drives nuclear deformation?

- ▶ Physical insights at mean-field level
- ▶ Global sensitivity analysis based on Hartree-Fock emulators used to compute as a proxy for deformation



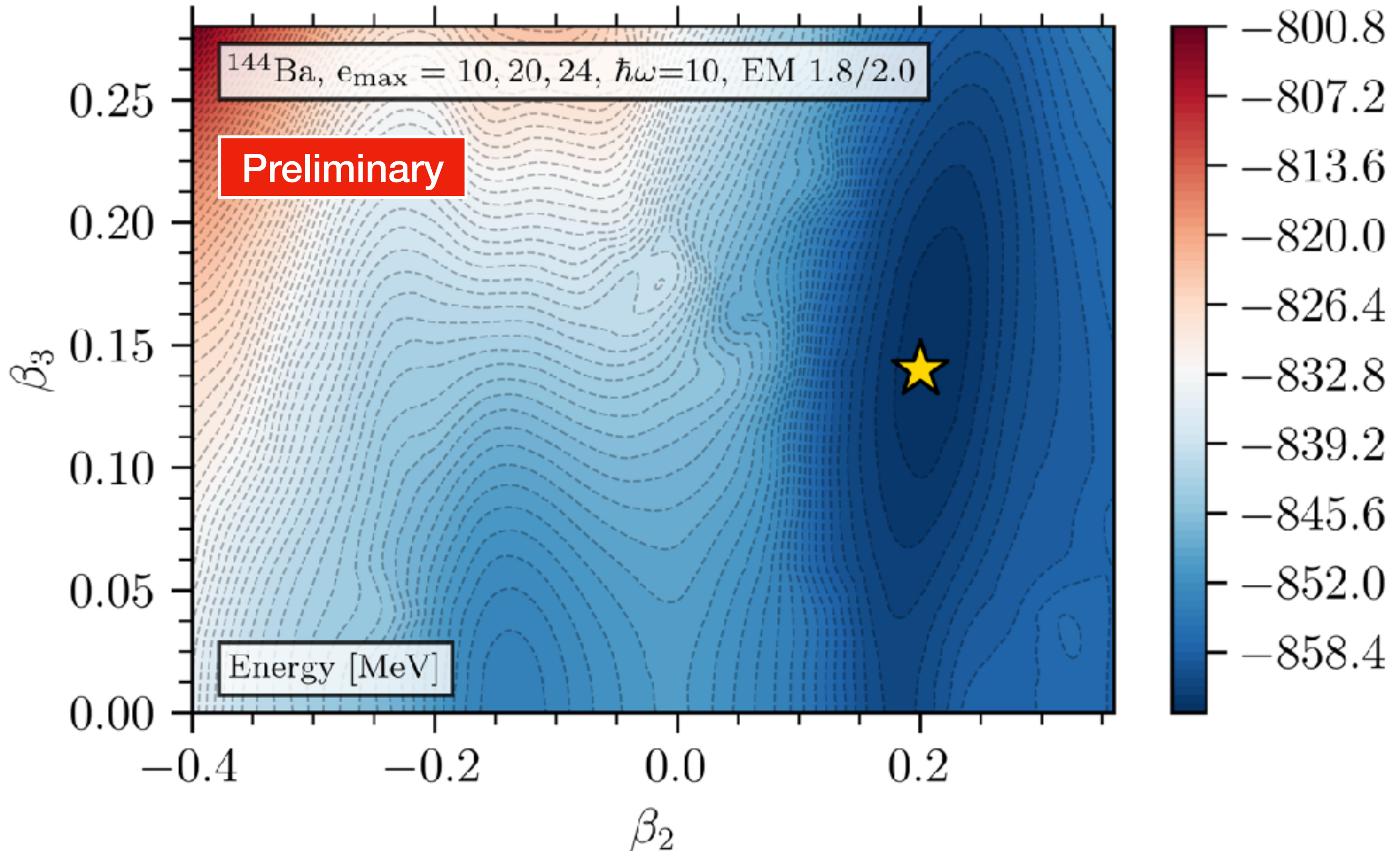
Non-axial deformation in Ba isotopes (work in progress)

A. Scalesi et al.



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Summary and future

- ▶ *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 + χ EFT + Bayesian statistical methods in combination with fast & accurate emulators is enabling **precision nuclear theory**.
- ▶ **Future frontiers of ab initio nuclear structure theory:**
 - ▶ Symmetry-breaking and restoration schemes for open-shell / deformed nuclei.
 - ▶ Efficient handling of many-body forces for converging heavy ($A > 200$) nuclear systems.
 - ▶ Predict scientifically relevant nuclear structure observables across the nuclear chart with quantified uncertainties (e.g. nuclear beta decay observables for BSM searches; ^{225}Ra PT-violating electric dipole moment)