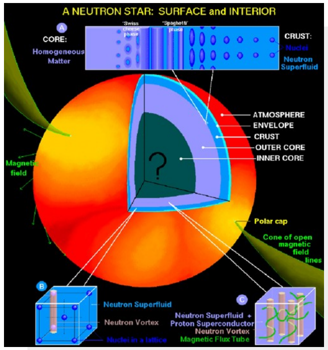
Taking statistical guarantees seriously: emulators and conformal prediction

Alex Gezerlis

UNIVERSITY OF GUELPH

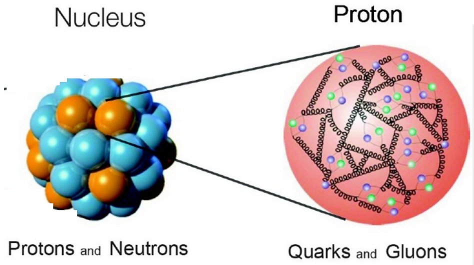
Workshop on Nuclear Hamiltonians for Advancing Nuclear Physics and Beyond
INT, Seattle, WA
May 12, 2026

Outline

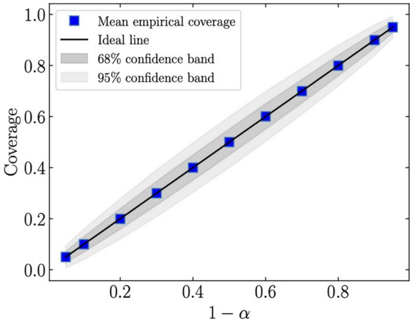


Credit: Dany Page

Motivation



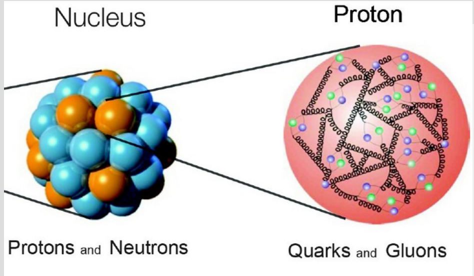
Nuclear methods



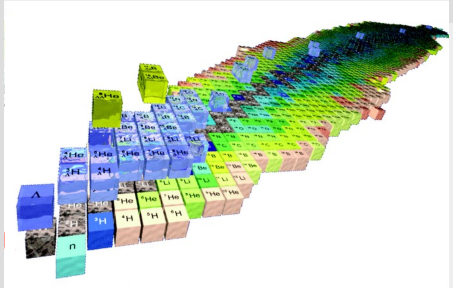
Recent results

Physical systems studied

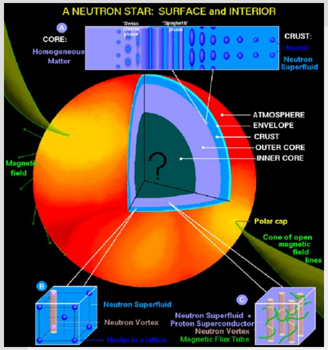
Nuclear forces



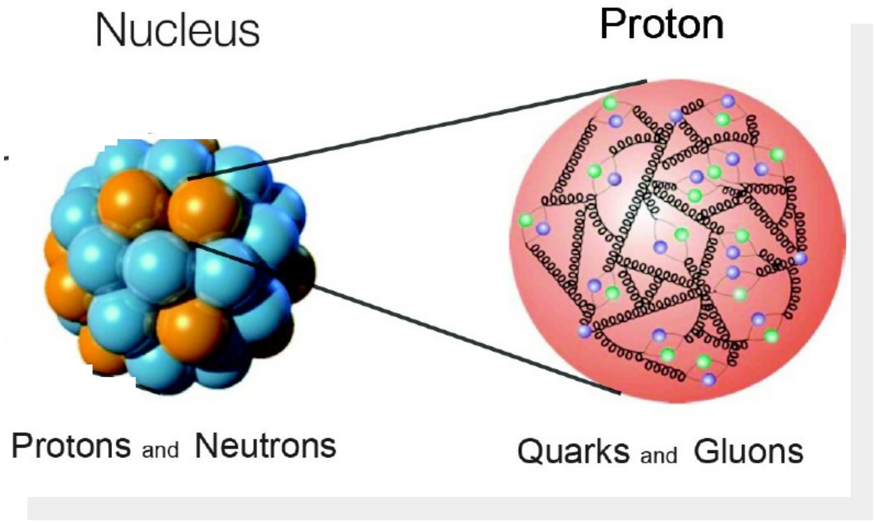
Nuclear structure



Nuclear astrophysics

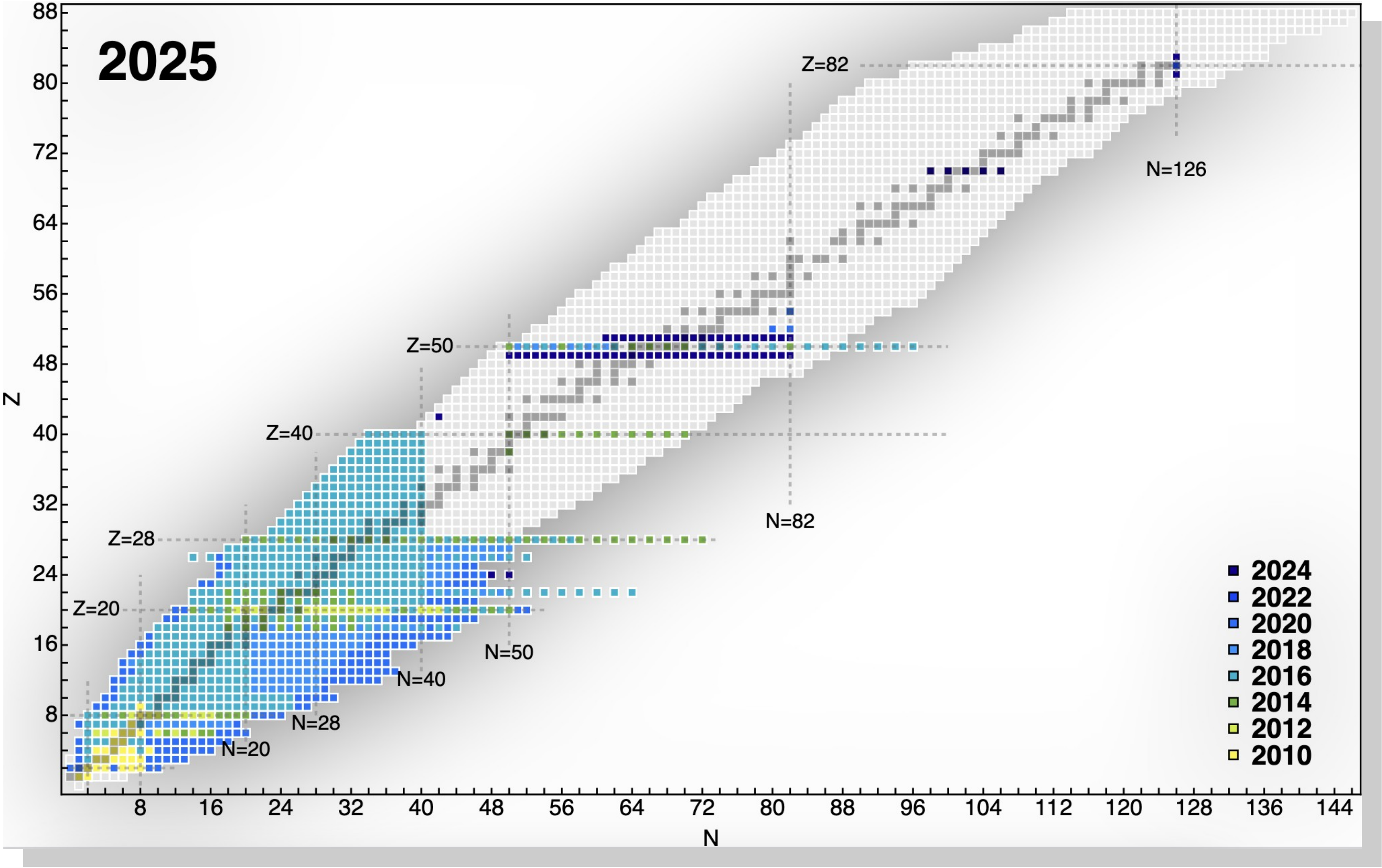


Key system: few nucleons



- No unique nuclear potential
- Preferable to use combination of phenomenological (high-quality) and more modern (conceptually clean) approach
- Desirable to make contact with underlying level
- New era, where practitioners design interactions themselves

Key system: nuclei

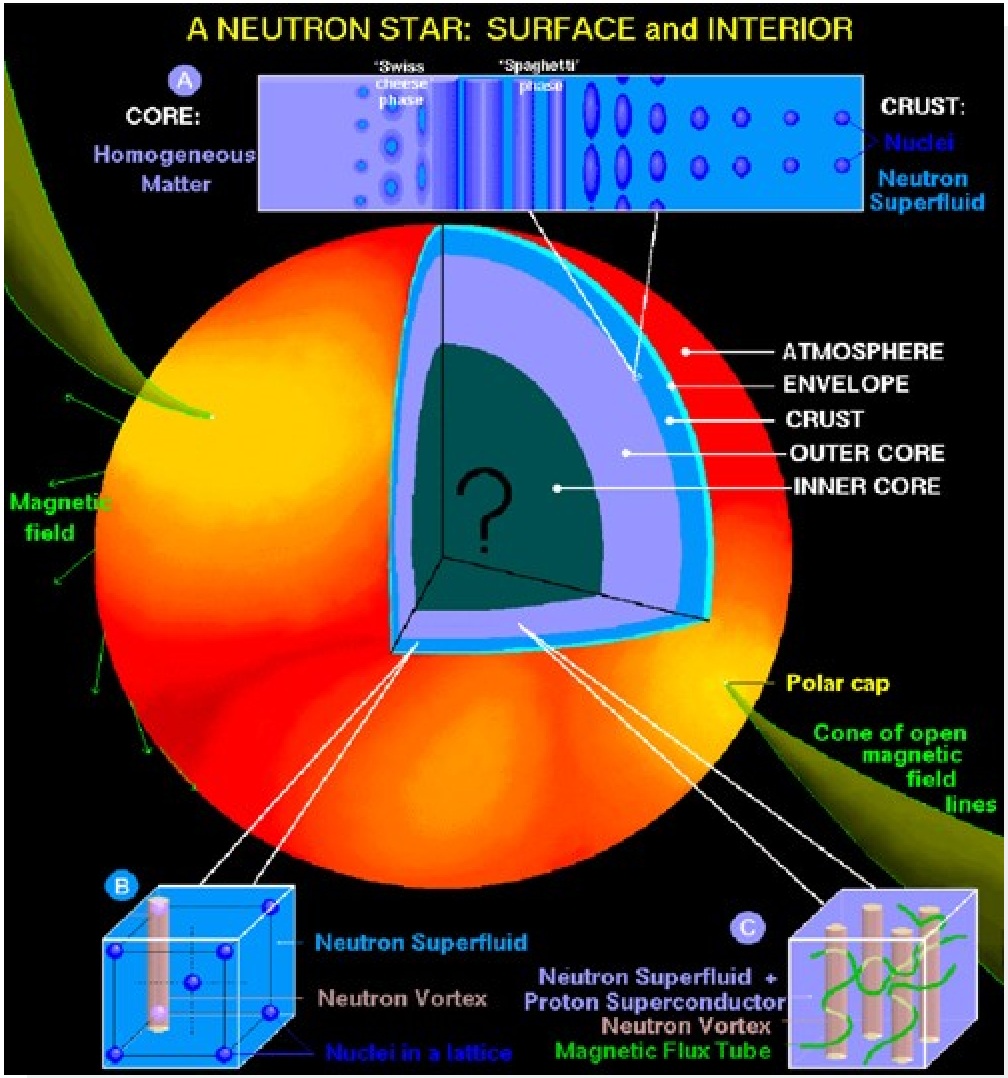


Heiko Hergert's propaganda plot

- Lots of recent progress
- Open-shell nuclei are the current frontier

- Goal is to study nuclei *from first principles* (when possible)

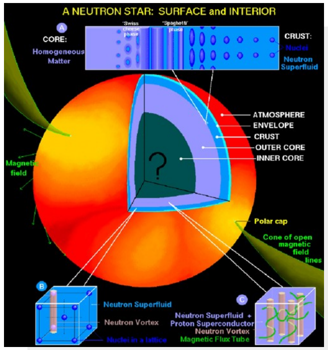
Key system: neutron stars



Credit: Dany Page

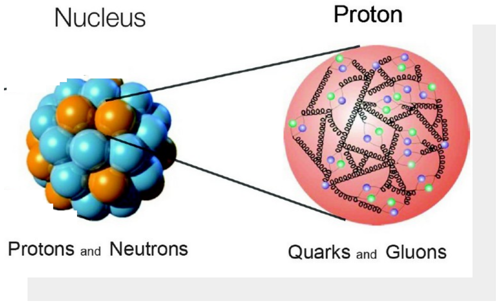
- Ultra-dense: 1.4 solar masses (or more) within a radius of 10 kilometres
- Terrestrial-like (outer layers) down to exotic (core) behaviour
- Observationally probed, i.e., not experimentally accessible
- Goal is to study neutron stars *from first principles* (when possible)

Outline

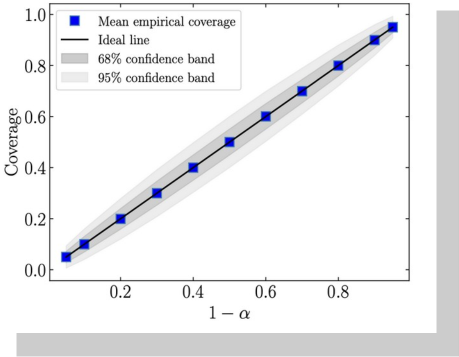


Credit: Dany Page

Motivation

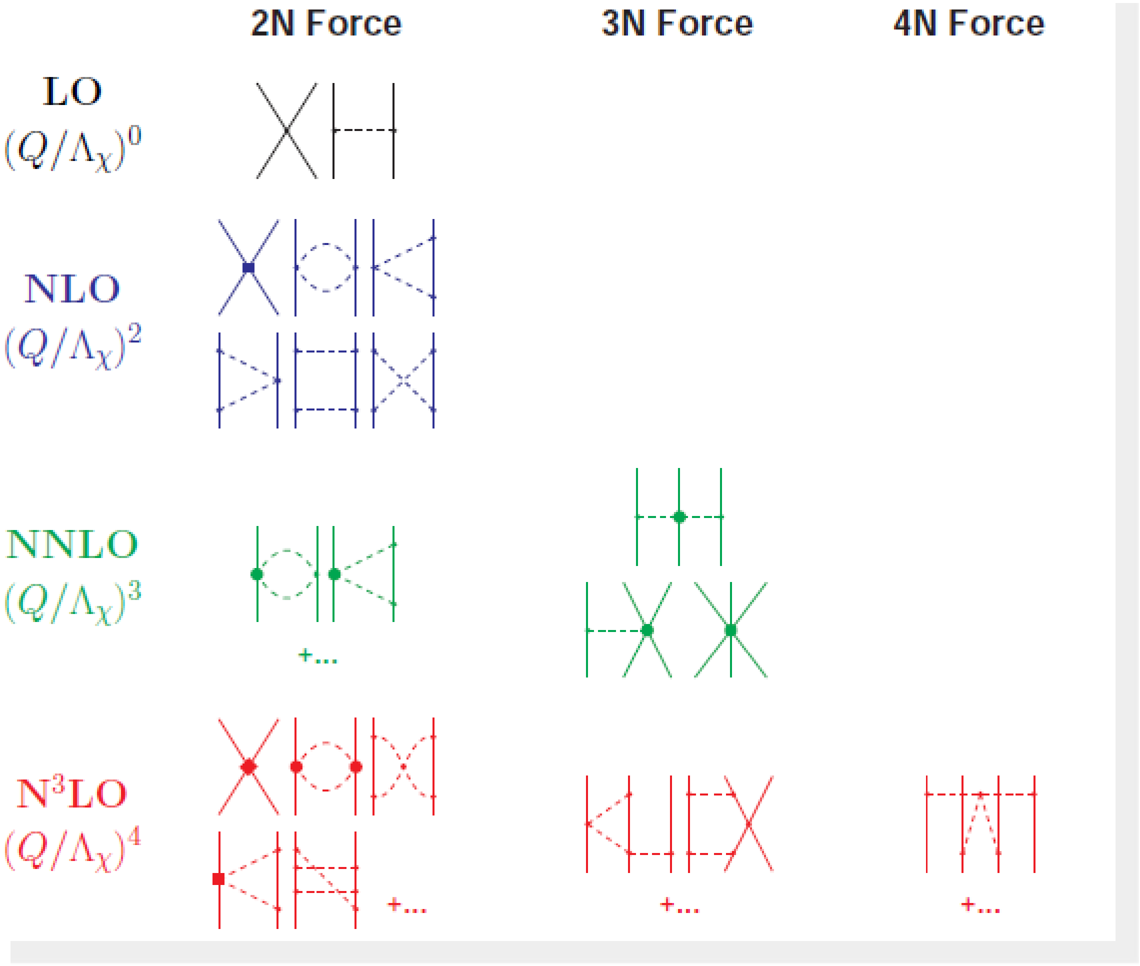


Nuclear methods



Recent results

Nuclear interactions



- Attempts to connect with underlying theory (QCD)
- Low-momentum expansion
- Naturally emerging many-body forces
- Low-energy constants from experiment or lattice QCD
- Now available in non-local, local, or semi-local varieties
- Power counting's relation to renormalization actively investigated

S. Weinberg, U. van Kolck, E. Epelbaum, N. Kaiser ...

But even with the interaction in place, how do you solve the many-body problem?

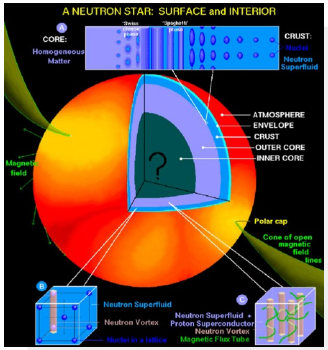
Nuclear many-body problem

$$H\Psi = E\Psi$$

where $$H = \sum_i K_i + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk}$$

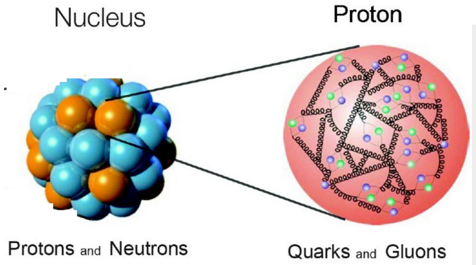
Wave function depends on coordinates, spin projections, and isospin projections, so we are faced with a large number of complex coupled second-order differential equations

Outline

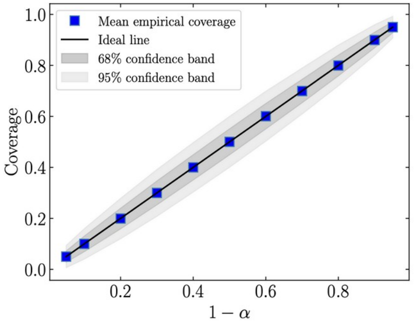


Credit: Dany Page

Motivation



Nuclear methods



Recent results

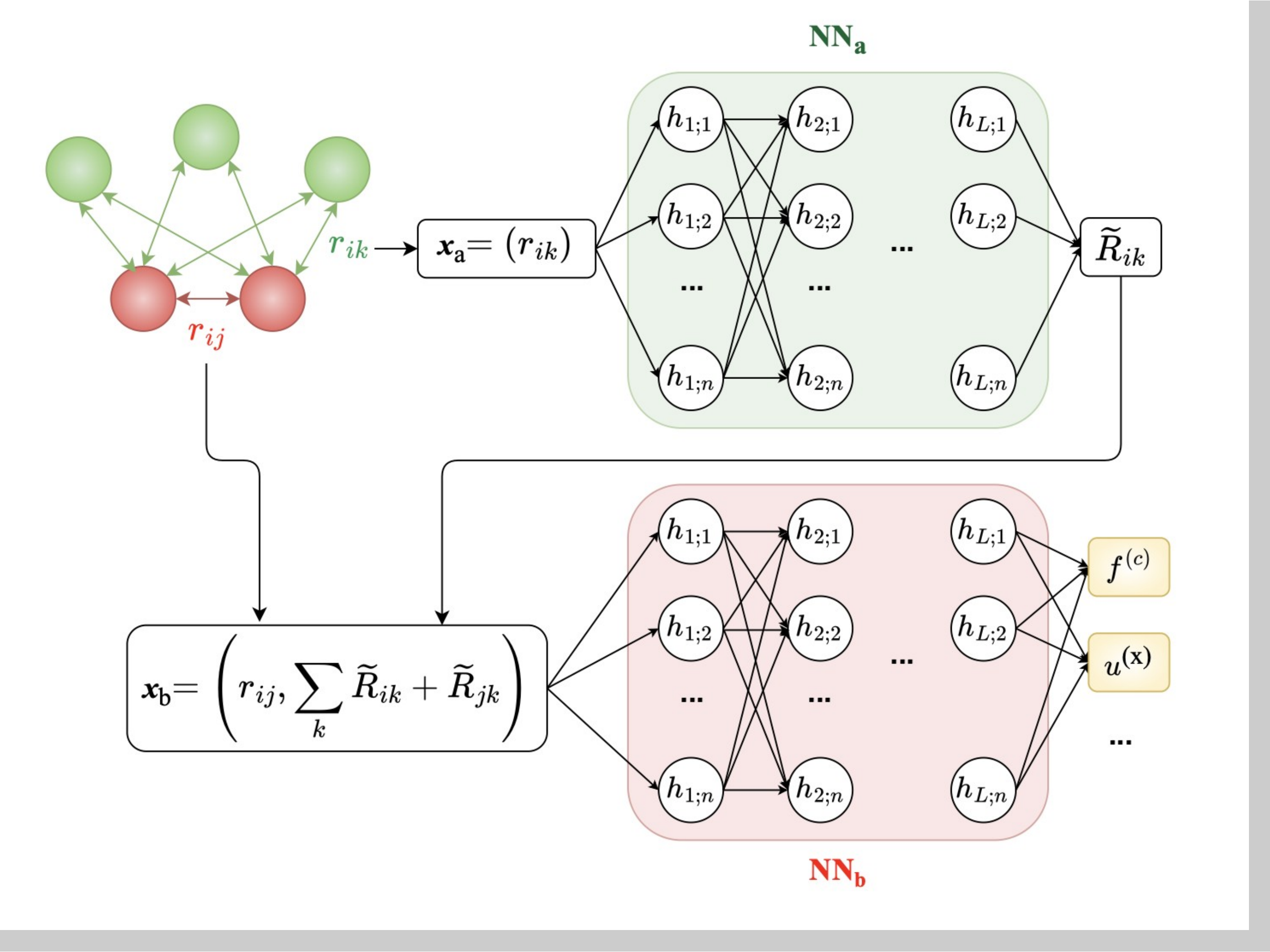
Recent results

- (Neural-network wave functions for light nuclei)
- QMC and emulators for light nuclei
- Conformal prediction for nucleon-nucleon scattering

(Neural-network wave functions for light nuclei)

P. Weng, A. Gezerlis, and J. Holt, Phys. Rev. Lett. **136**, 172502 (2026)

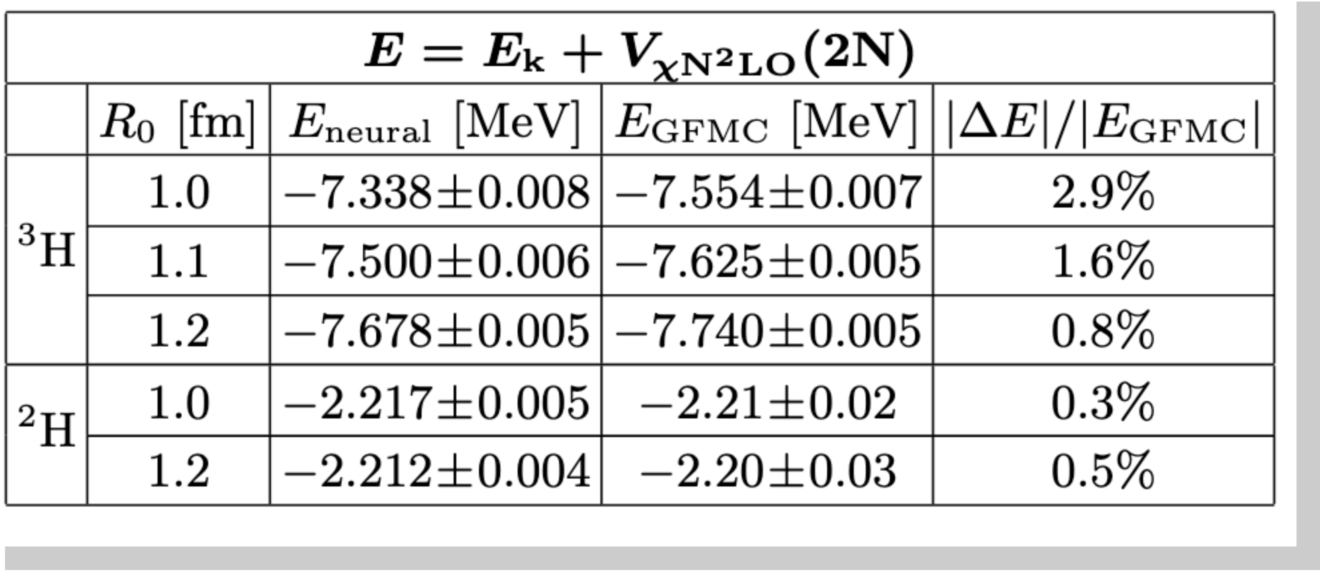
Neural networks for light nuclei



P. Weng, A. Gezerlis, and J. Holt, Phys. Rev. Lett. **136**, 172502 (2026)

Neural networks for light nuclei

Nearly reproduces GFMC results
already at the VMC level



$$E = E_{\mathrm{k}} + V_{\chi \mathrm{N^2LO}}(\mathrm{2N})$$

	R_0 [fm]	E_{neural} [MeV]	E_{GFMC} [MeV]	$\lvert\Delta E\rvert/\lvert E_{\text{GFMC}}\rvert$
^{3}H	1.0	-7.338 ± 0.008	-7.554 ± 0.007	2.9%
	1.1	-7.500 ± 0.006	-7.625 ± 0.005	1.6%
	1.2	-7.678 ± 0.005	-7.740 ± 0.005	0.8%
^{2}H	1.0	-2.217 ± 0.005	-2.21 ± 0.02	0.3%
	1.2	-2.212 ± 0.004	-2.20 ± 0.03	0.5%

P. Weng, A. Gezerlis, and J. Holt, Phys. Rev. Lett. **136**, 172502 (2026)

QMC and emulators for light nuclei

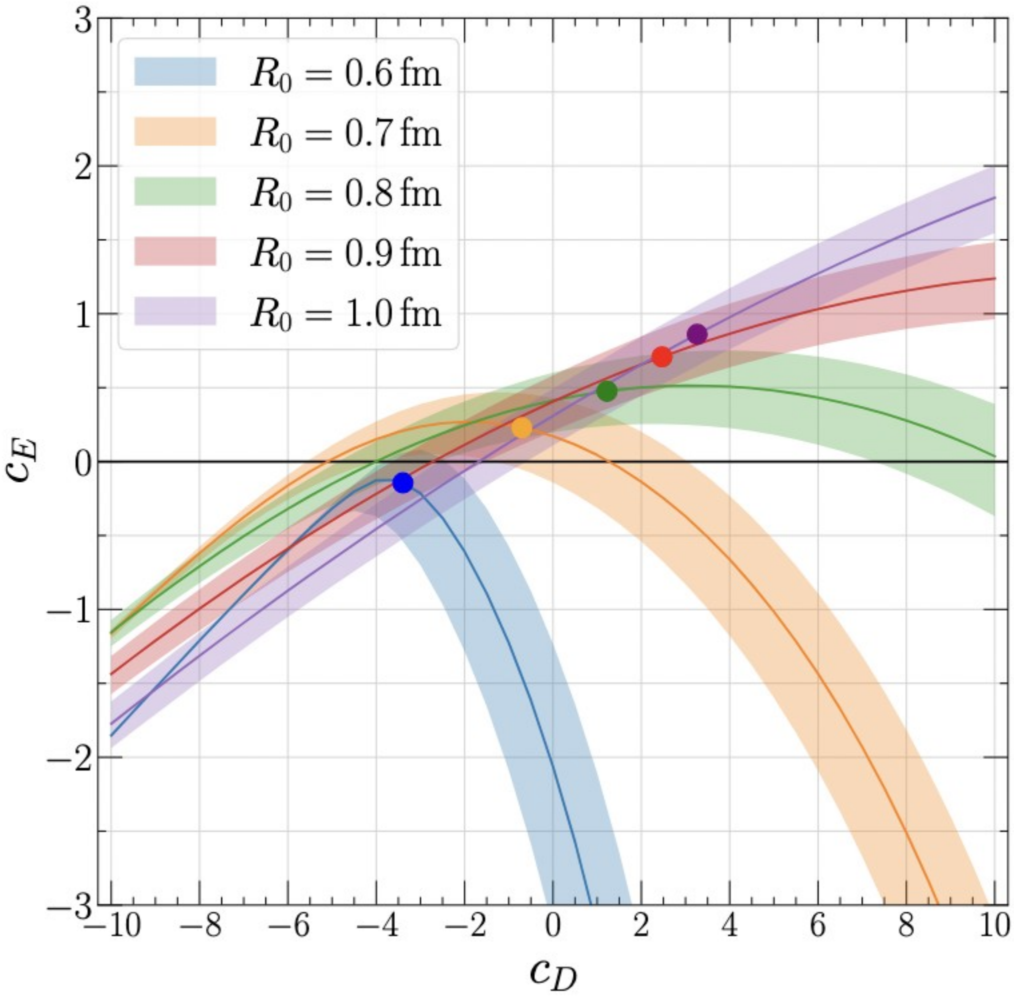
R. Curry, K. Hebeler, S. Gandolfi, A. Gezerlis,
A. Schwenk, R. Somasundaram, and I. Tews,
arXiv:2510.15860

Fitting the three-nucleon interaction

Solve Faddeev equations for triton binding energy to find a curve

Employ triton beta-decay half-life to single out a point (for each interaction)

This process is computationally quite costly



Tews, Somasundaram, Lonardoni, Goettling, Seutin, Carlson, Gandolfi, Hebeler, Schwenk, Phys. Rev. Research **7**, 033024 (2025)

Emulators in one slide

Previous talk introduced applications of emulators to nuclear physics.

- **Parametric Matrix Model (PMM)**: use approximate model with matrices of chosen dimensionality:

$$\hat{H} = H_0 + c_D H_D + c_E H_E$$

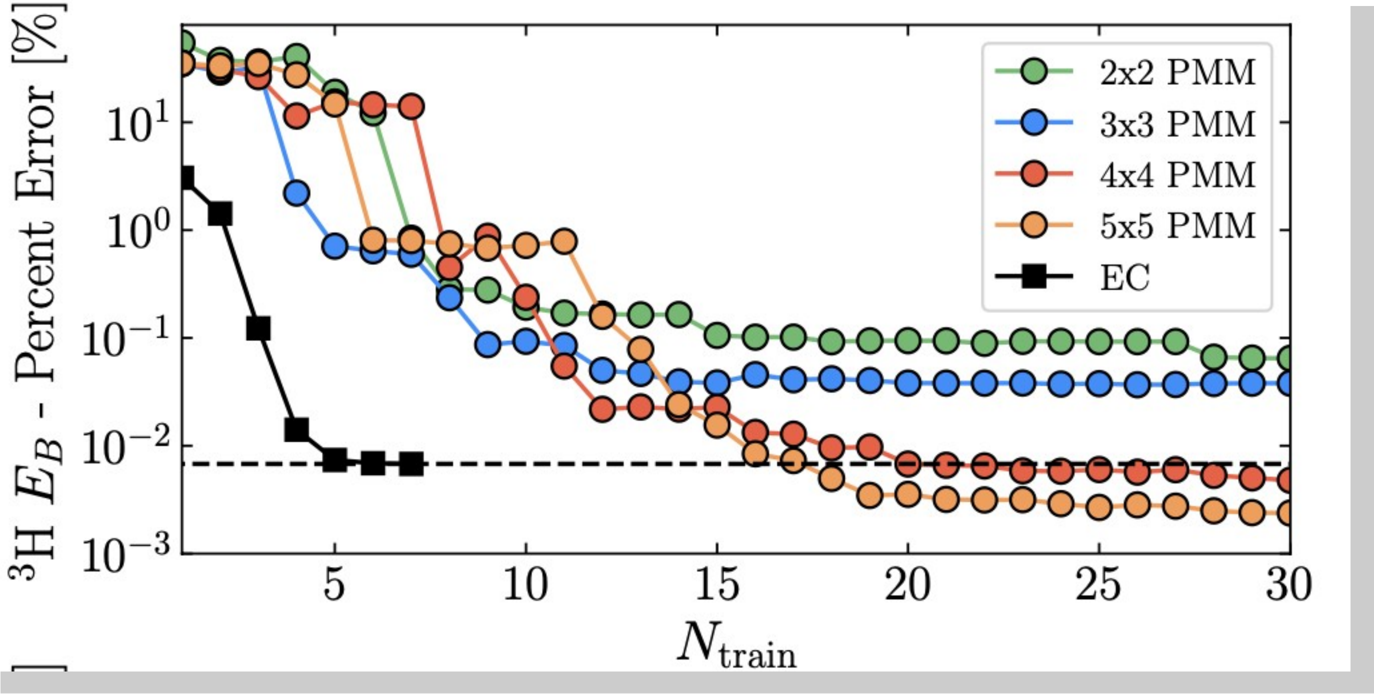
- **Eigenvector continuation (EC)**: Solve within a subspace (leading to generalized eigenvalue problem):

$$\sum_i H \left|\psi_j\right\rangle = E \sum_j \left|\psi_j\right\rangle$$

Varying the three-nucleon interaction

150 training data points + 75 test data points

New criterion for how to reject linearly dependent new training points

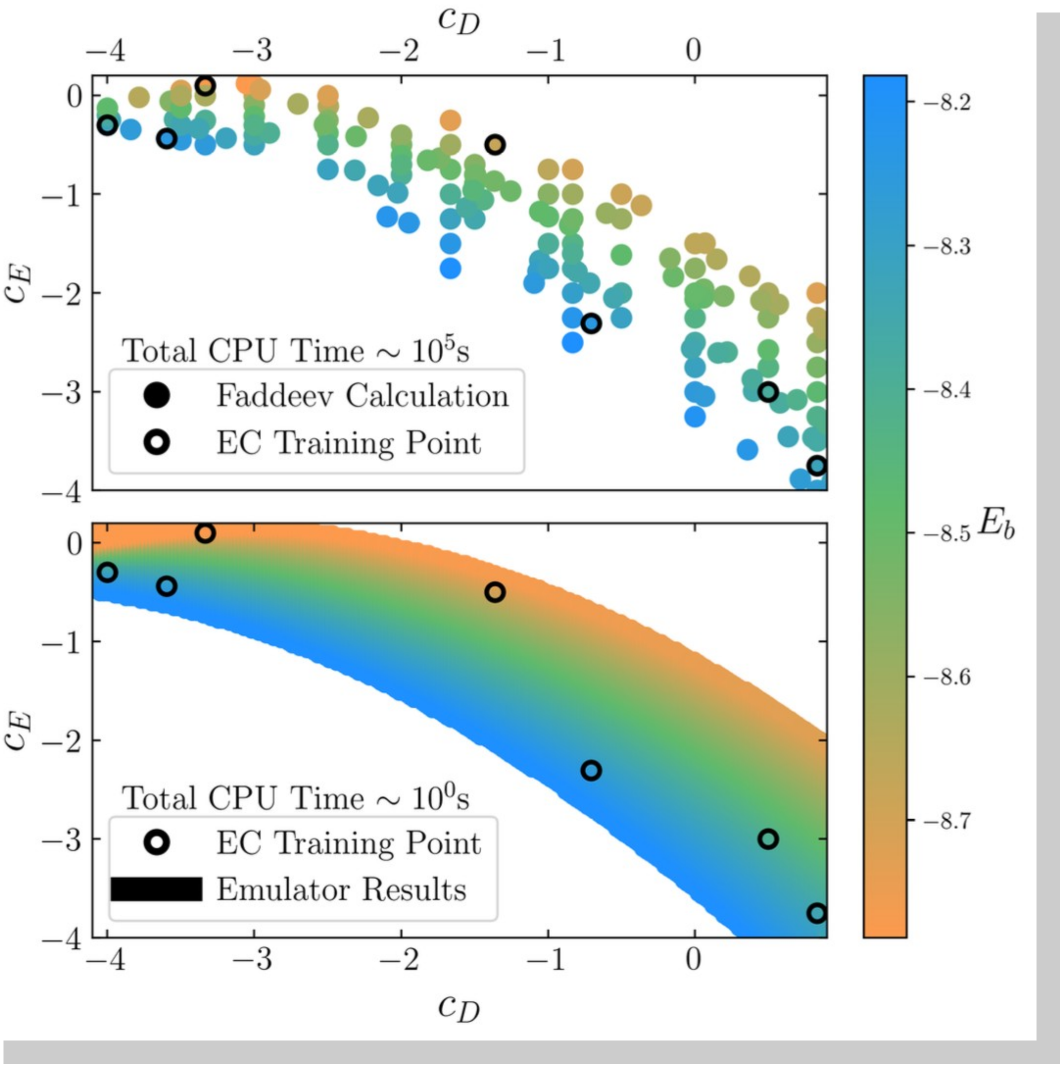


R. Curry *et al*, arXiv:2510.15860

Varying the three-nucleon interaction

UNIVERSITY OF GUELPH

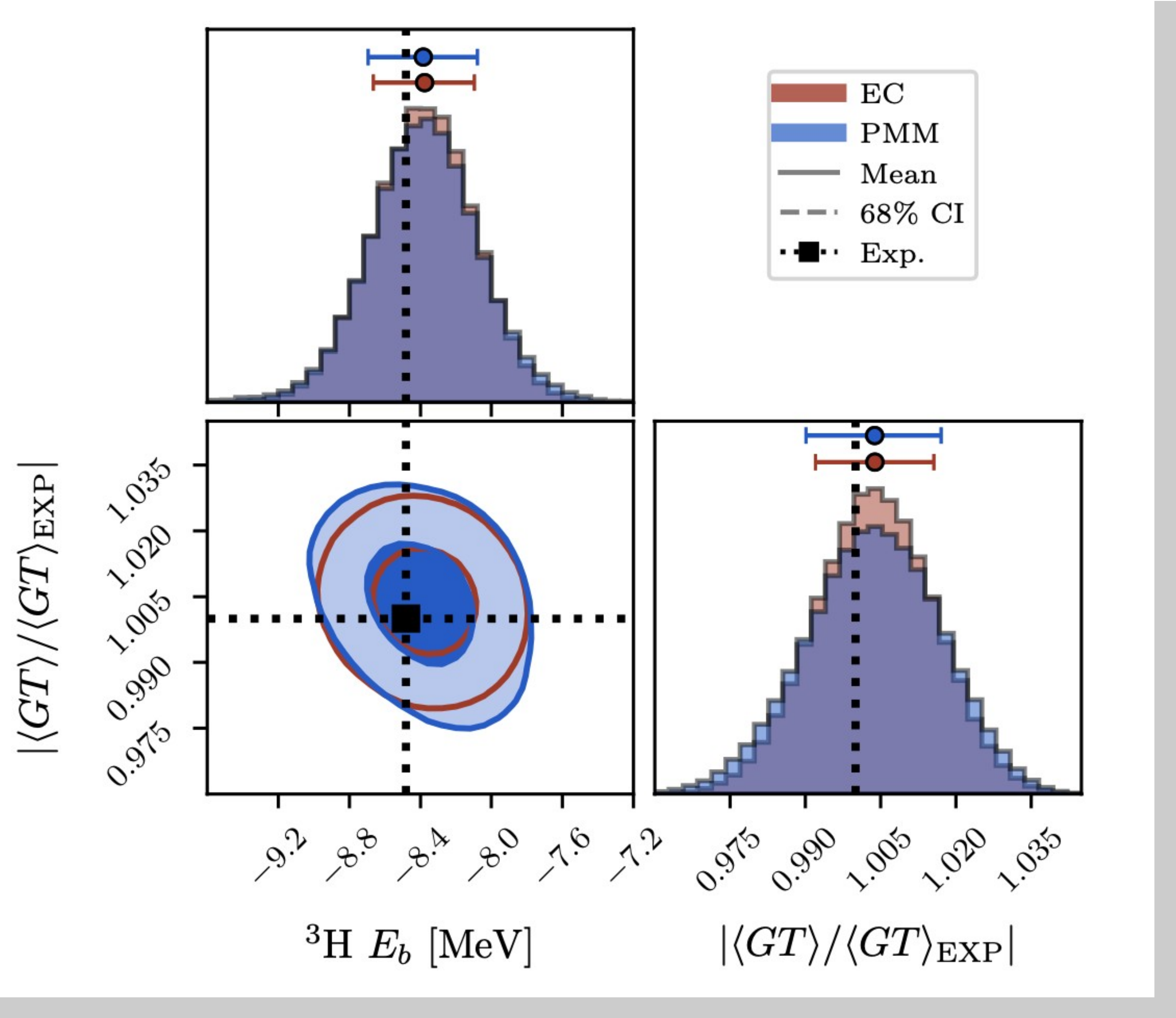
Now that the calculation is so cheap, we can fill out the plot:



R. Curry *et al*, arXiv:2510.15860

Varying the three-nucleon interaction

Posteriors for triton properties:

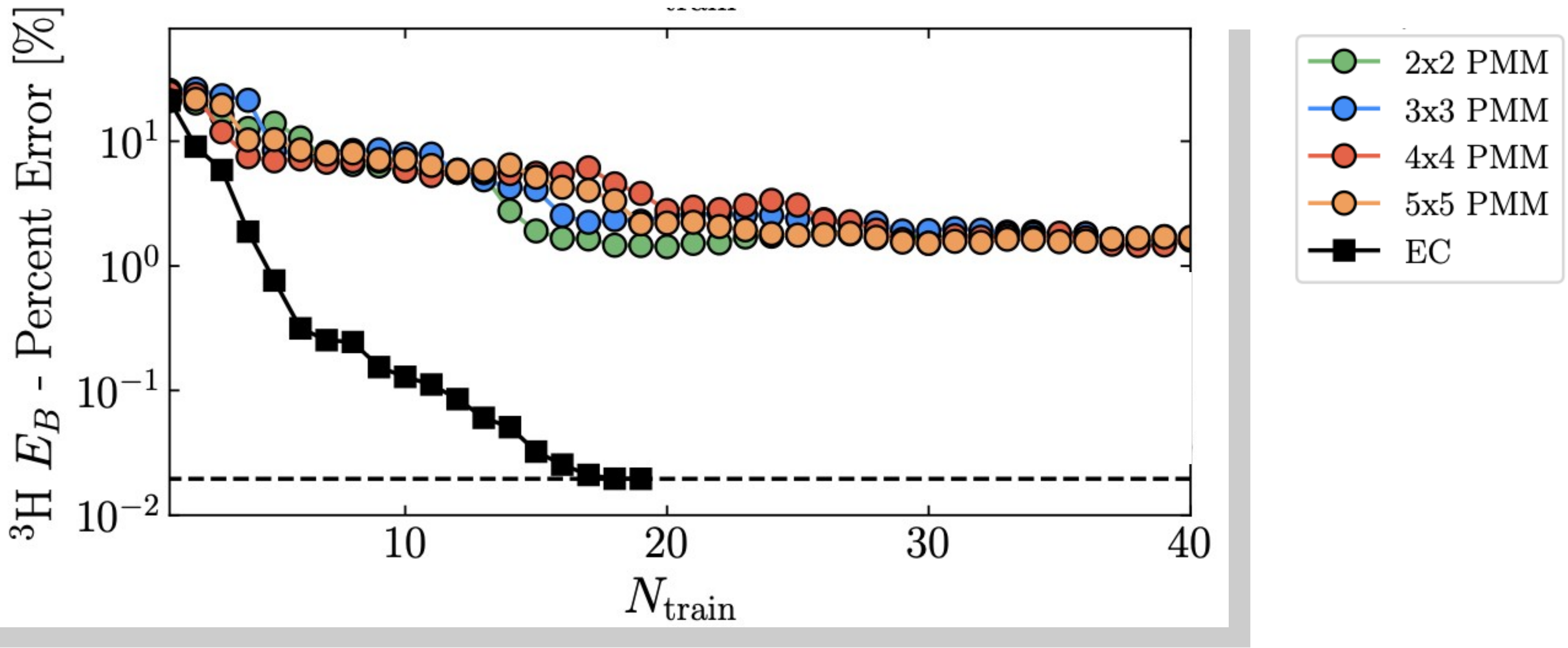


R. Curry *et al*, arXiv:2510.15860

Varying the full interaction

Release the full interaction, leading to 11 matrices:

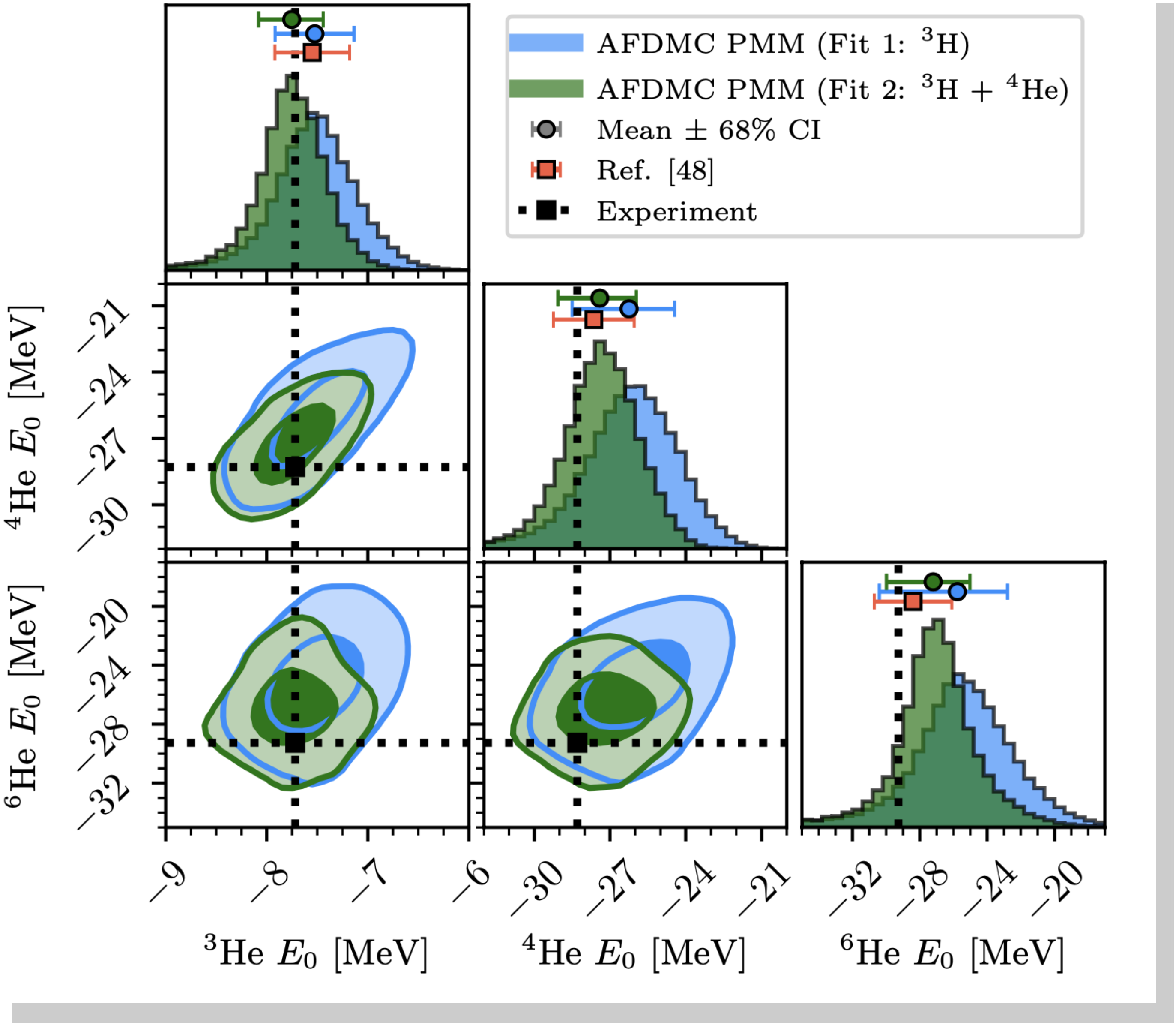
$$\hat{H} = H_0 + c_S H_S + c_T H_T + \sum_{i=1}^{7} c_i H_i + c_D H_D + c_E H_E$$



R. Curry *et al*, arXiv:2510.15860

Varying the full interaction

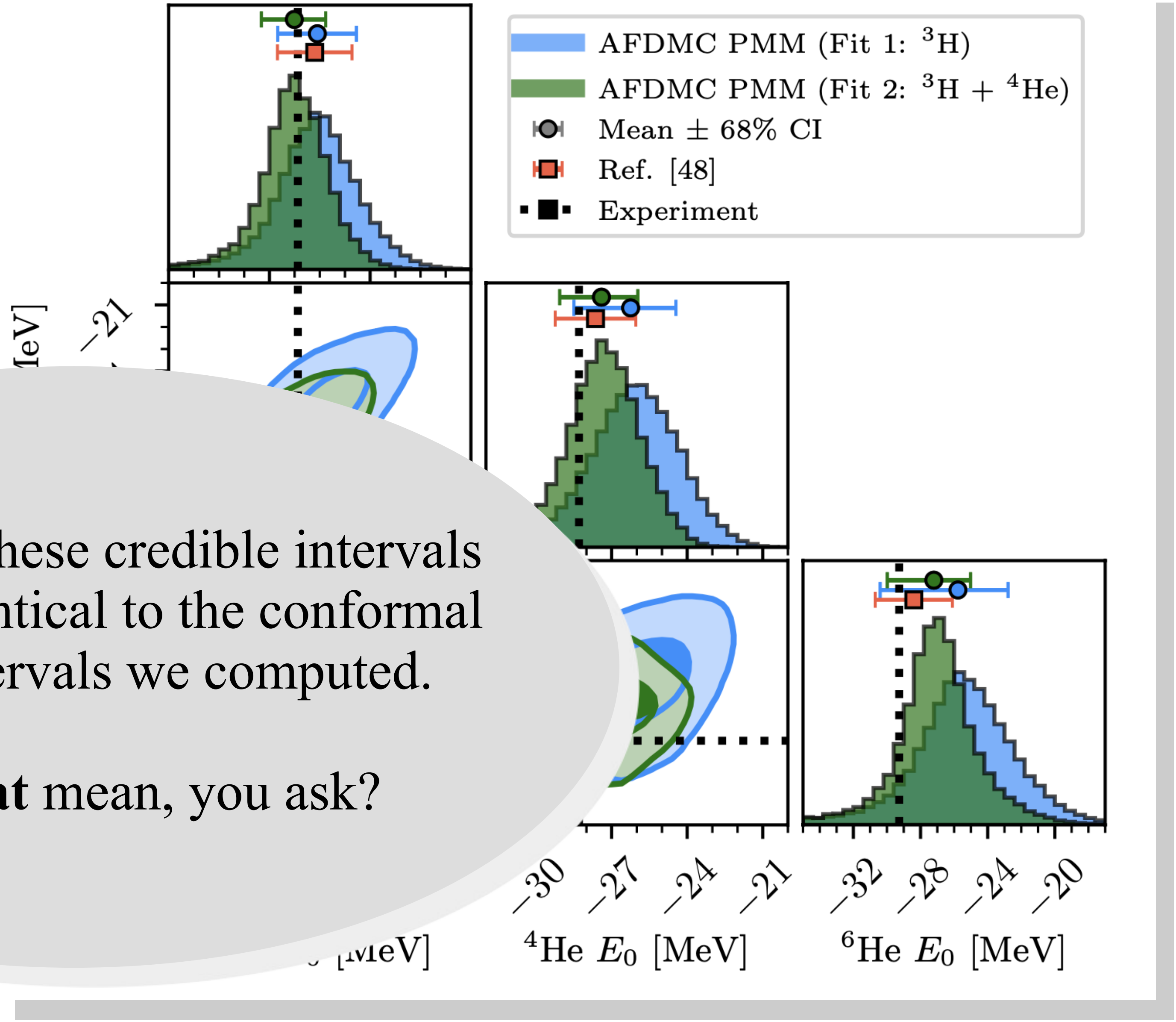
Carry out AFDMC calculations to find:



R. Curry *et al*, arXiv:2510.15860

Varying the full interaction

Carry out AFDMC calculations to find:



Intriguingly, these credible intervals are nearly identical to the conformal prediction intervals we computed.

What does **that** mean, you ask?

R. Curry *et al*, arXiv:2510.15860

Conformal prediction for nuclear physics

H. Yousefi Dezdarani, R. Curry, and A. Gezerlis, Phys. Rev. C, **113**, 014004 (2026)

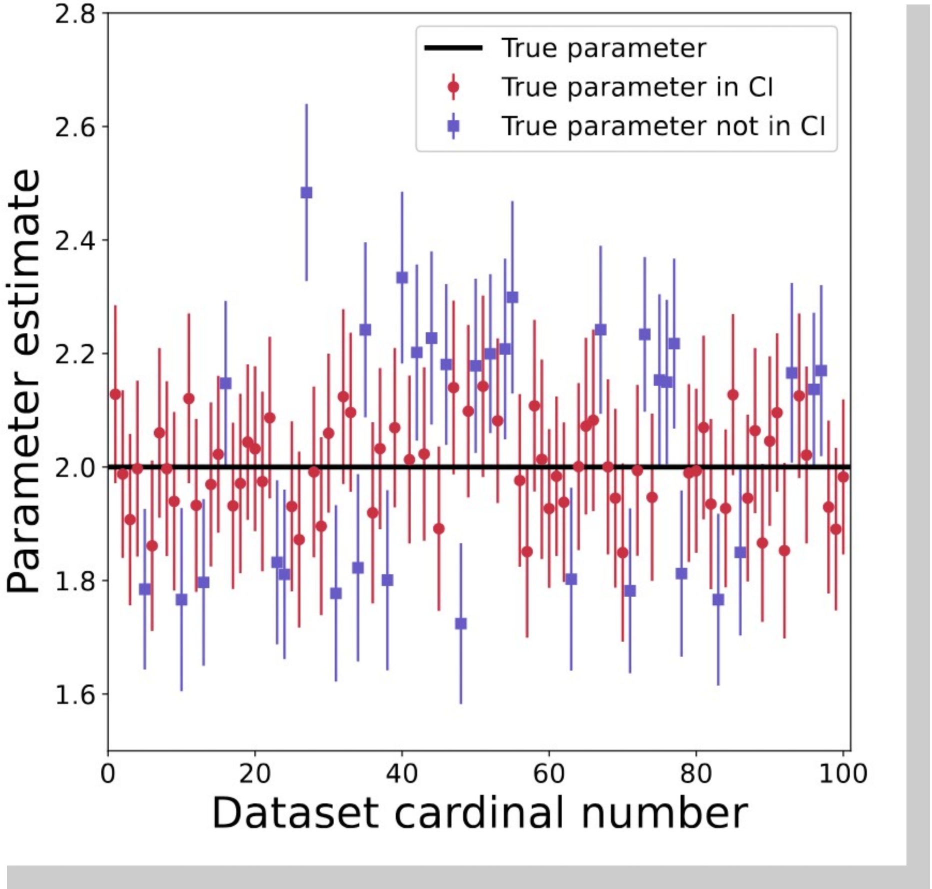
H. Yousefi Dezdarani, R. Curry, C. L. Armstrong, and A. Gezerlis, arXiv:2604.21039

A hint of the philosophy of statistics

(Frequentist) confidence interval

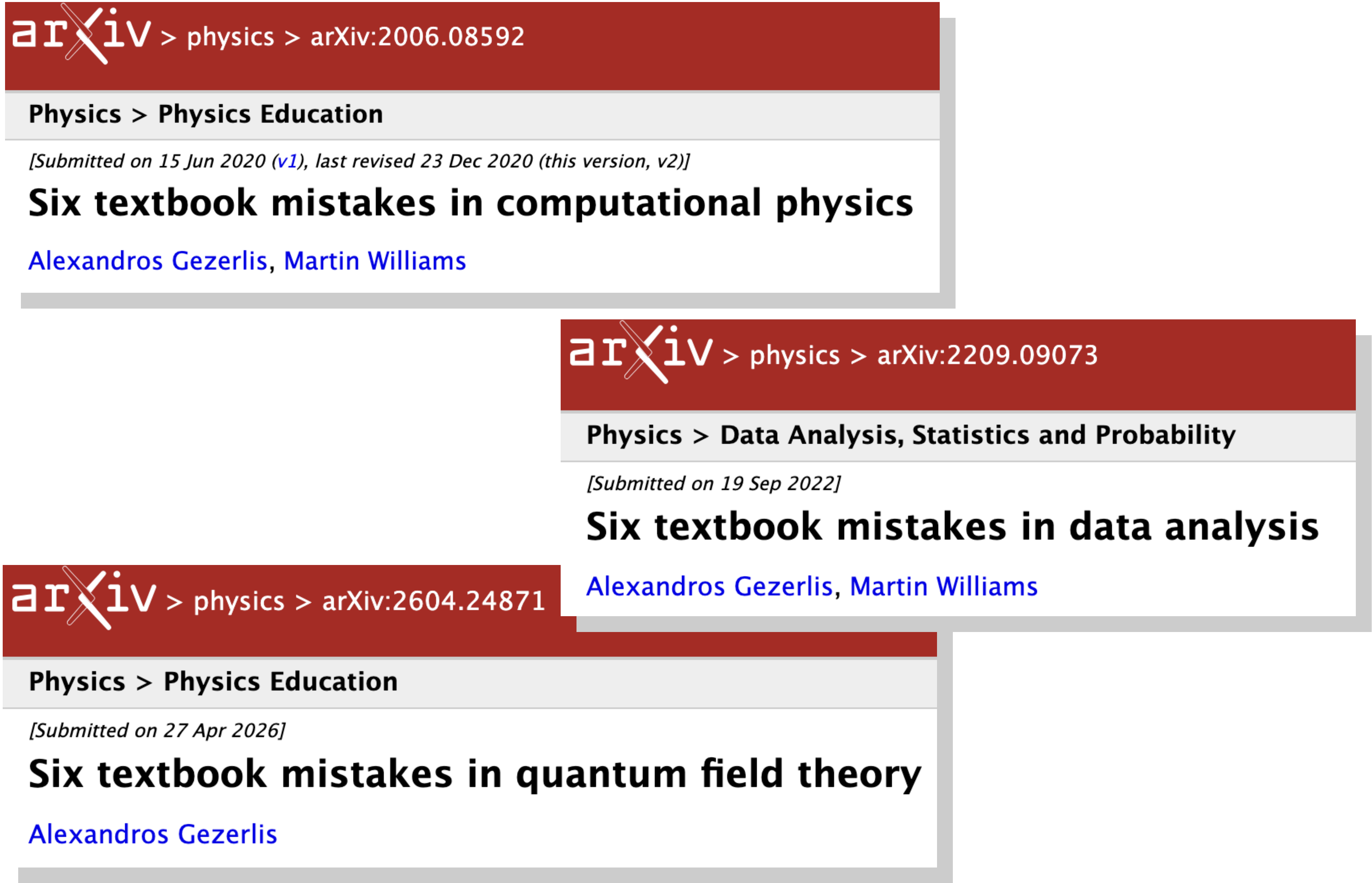
E.g., maximize likelihood and take an *nσ* error bar around that point.

Confidence interval *does not* imply degree of belief about our single dataset, but *does* provide guaranteed coverage across datasets.



A. Gezerlis and M. Williams, Eur. Phys. J Plus **138**, 19 (2023)

My physics-education persona



arXiv > physics > arXiv:2006.08592

Physics > Physics Education

[Submitted on 15 Jun 2020 (v1), last revised 23 Dec 2020 (this version, v2)]

Six textbook mistakes in computational physics

Alexandros Gezerlis, Martin Williams

arXiv > physics > arXiv:2209.09073

Physics > Data Analysis, Statistics and Probability

[Submitted on 19 Sep 2022]

Six textbook mistakes in data analysis

Alexandros Gezerlis, Martin Williams

arXiv > physics > arXiv:2604.24871

Physics > Physics Education

[Submitted on 27 Apr 2026]

Six textbook mistakes in quantum field theory

Alexandros Gezerlis

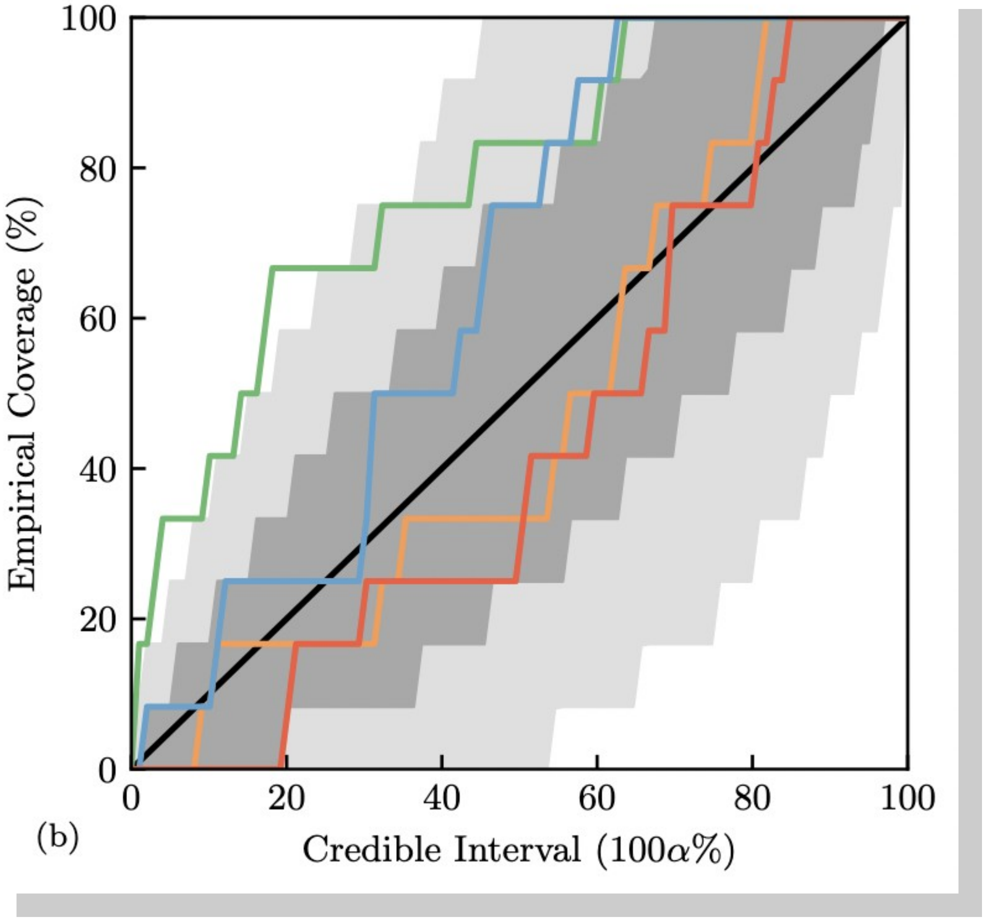
A hint of the philosophy of statistics

(Bayesian) credible interval

E.g., maximize posterior and take an *nσ* error bar around that point.

Credible interval *does* imply degree of belief about our single dataset, but *does not* provide guaranteed coverage across datasets.

N.B. BUQEYE collaboration interprets coverage order-by-order



J. A. Melendez, R. J. Furnstahl, D. R. Phillips, M. T. Pratola, and S. Wesolowski, Phys. Rev. C **100**, 044001 (2019)

A hint of the philosophy of statistics

Summarizing attractive features

- (Frequentist) confidence interval has guaranteed coverage across datasets

- (Bayesian) credible interval combines prior and likelihood to encapsulate degree of belief about our single dataset

A hint of the philosophy of statistics

Summarizing attractive features

- (Frequentist) confidence interval has guaranteed coverage across datasets

- (Bayesian) credible interval combines prior and likelihood to encapsulate degree of belief about our single dataset

Can you get the best of both worlds?

- Yes (*contra* Betteridge's law of headlines)

- Conformal prediction is a tool that post-processes any pre-trained model to produce guaranteed coverage

Conformal prediction

- Distribution-free and model-agnostic uncertainty-quantification method

- Provides finite-sample prediction intervals with guaranteed coverage

- It accomplishes this by employing the quantile function (inverse of the cumulative distribution function) in an ingenious way:

$$C(X_{n+1}) = \left[Q_Y\left(\tfrac{\alpha}{2} \mid X_{n+1}\right) - q,\ Q_Y\left(1 - \tfrac{\alpha}{2} \mid X_{n+1}\right) + q\right]$$

where $q = Q_S(1-\alpha)$

H. Yousefi Dezdarani, R. Curry, and A. Gezerlis, Phys. Rev. C, **113**, 014004 (2026)

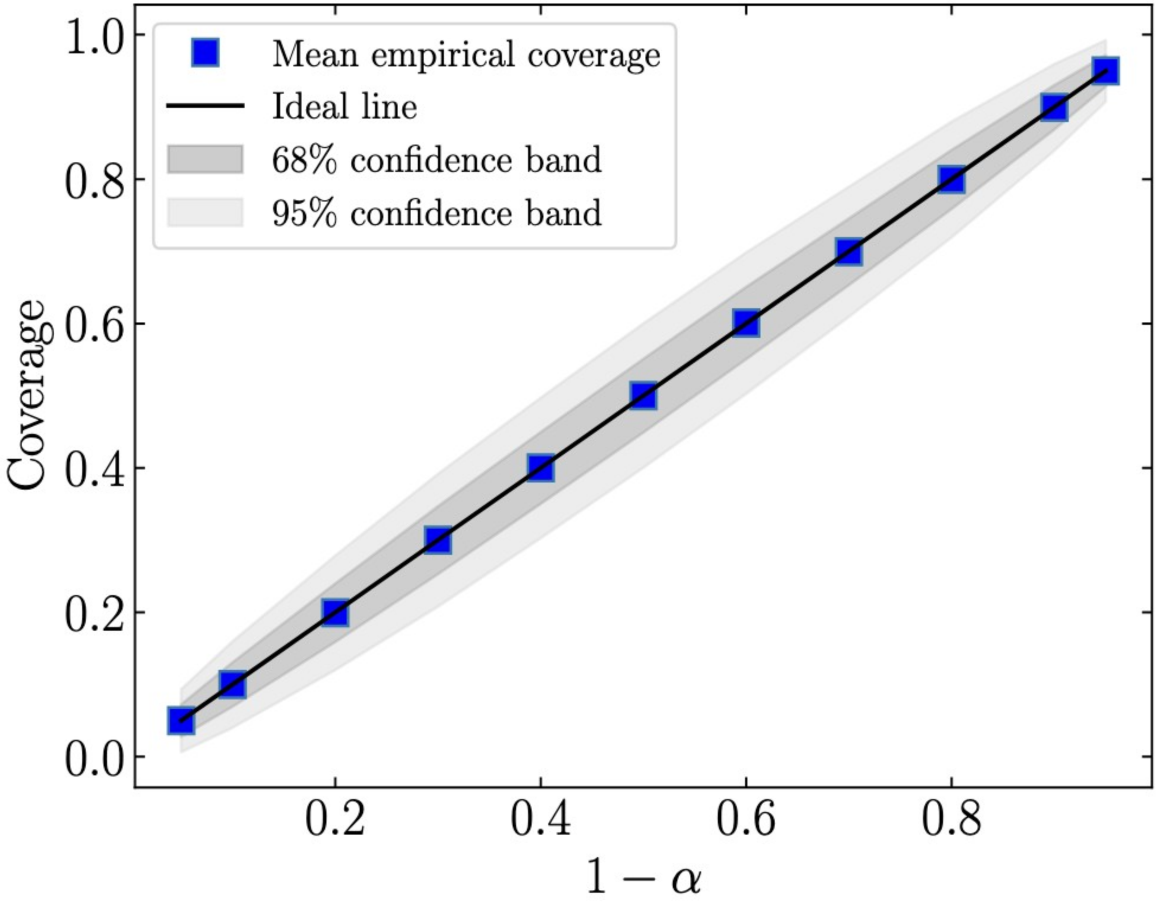
Conformal prediction: scattering

Application: BUQEYE pointwise model

- Two-nucleon total cross section at E = 50 MeV

- Empirical coverage over 4000 independent trials

- There is near-perfect alignment between empirical coverage and ideal line

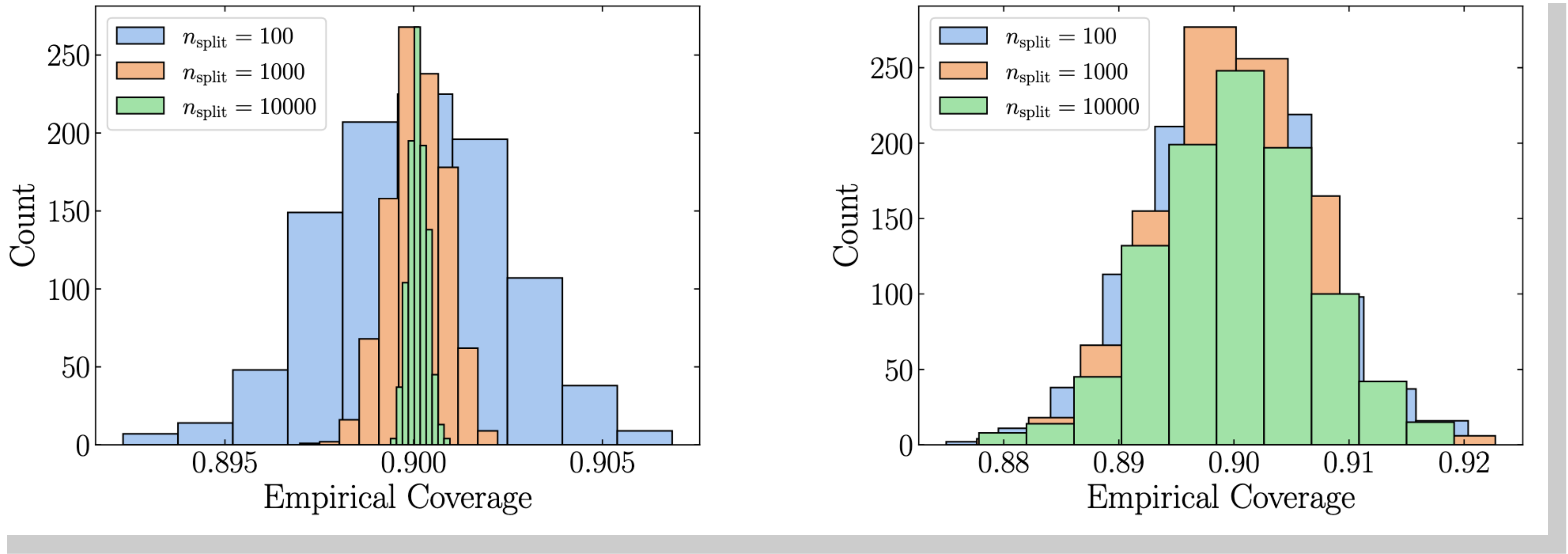


H. Yousefi Dezdarani, R. Curry, and A. Gezerlis, Phys. Rev. C, **113**, 014004 (2026)

Conformal prediction: scattering

Application: BUQEYE Gaussian-process model

We drew posterior samples using the BUQEYE open-source code



conformal

Bayesian

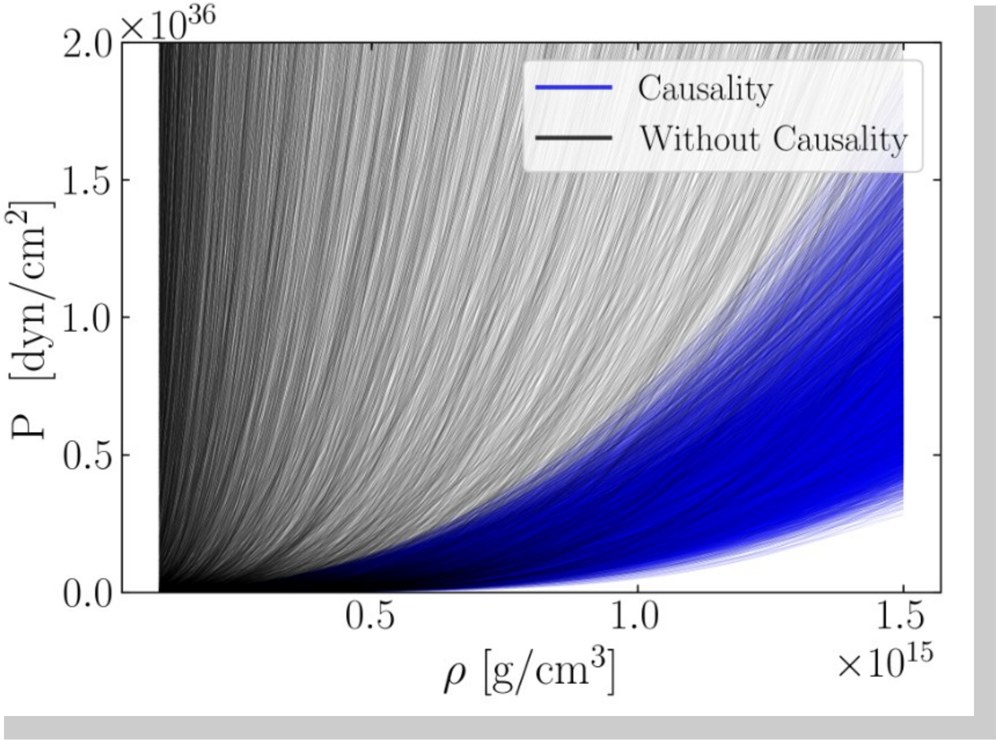
H. Yousefi Dezdarani, R. Curry, and A. Gezerlis, Phys. Rev. C, **113**, 014004 (2026)

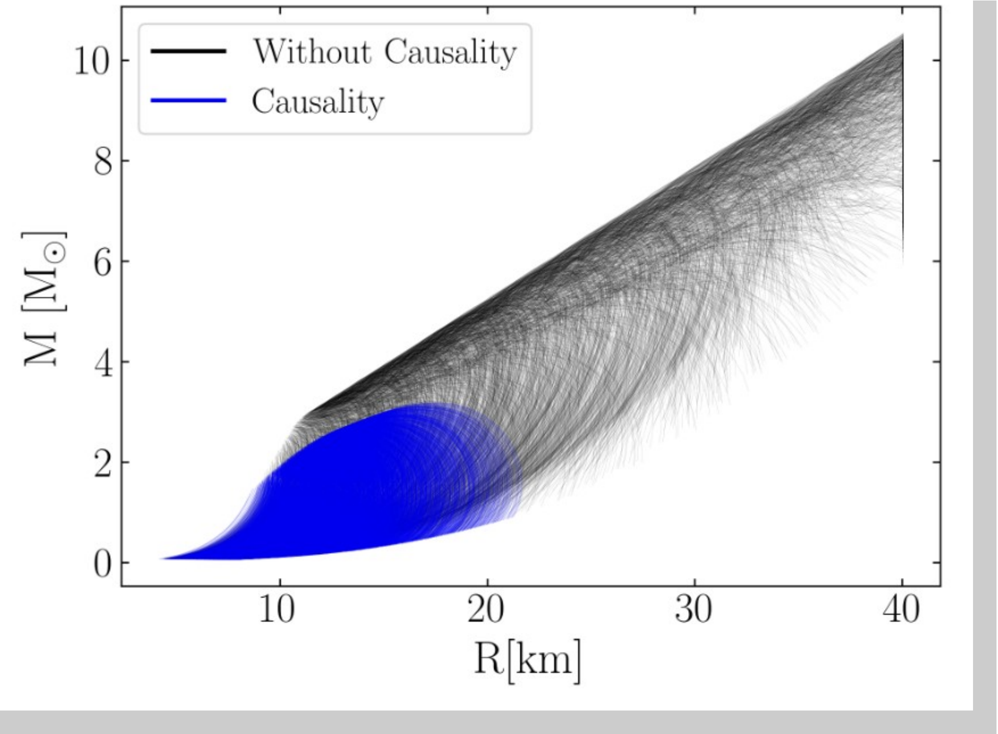
Conformal prediction: neutron stars

Application: TOV equations for polytrope

$$\frac{dP(r)}{dr} = -\frac{G\,m(r)\,\rho(r)}{r^2}\left[1+\frac{P(r)}{\rho(r)c^2}\right]\left[1+\frac{4\pi r^3 P(r)}{m(r)c^2}\right]\left[1-\frac{2Gm(r)}{c^2 r}\right]^{-1}$$

$$\frac{dm(r)}{dr} = 4\pi r^2 \rho(r)$$

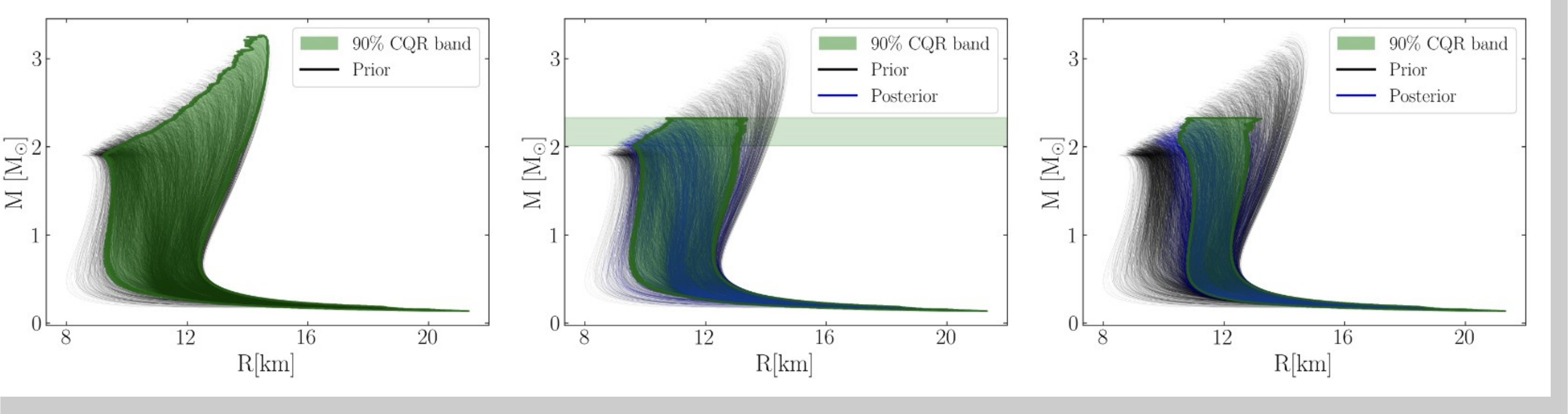




H. Yousefi Dezdarani, R. Curry, C. L. Armstrong, and A. Gezerlis, arXiv:2604.21039

Conformal prediction: neutron stars

Application: multimessenger analysis (NMMA collaboration)



Post-processing carried out using individual EOS samples

T. Dietrich *et al*, Science **370**, 1450 (2020)

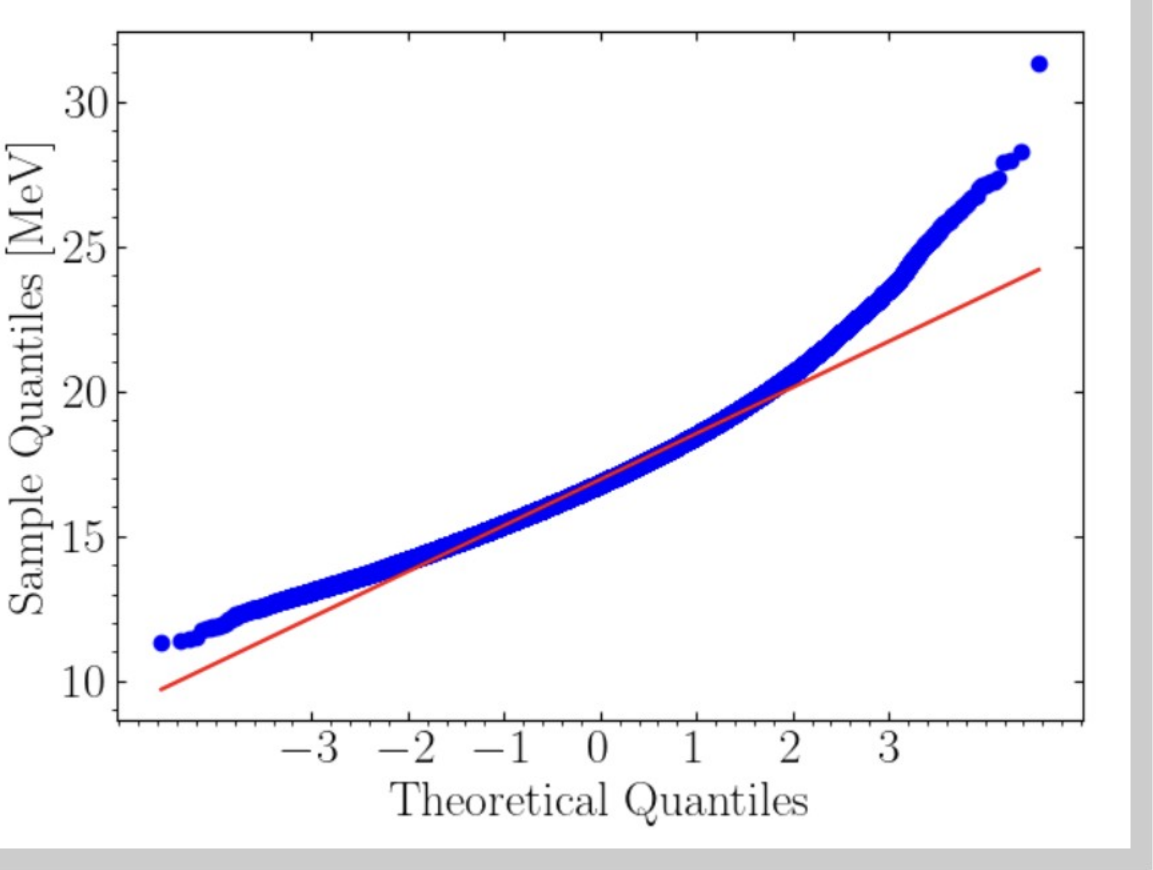
H. Yousefi Dezdarani, R. Curry, C. L. Armstrong, and A. Gezerlis, arXiv:2604.21039

Conformal prediction: neutron stars

Application: QMC neutron matter equation of state (1)

- Deviations from the diagonal reflect a non-normal distribution

- Non-gaussianity motivates use of distribution-free method

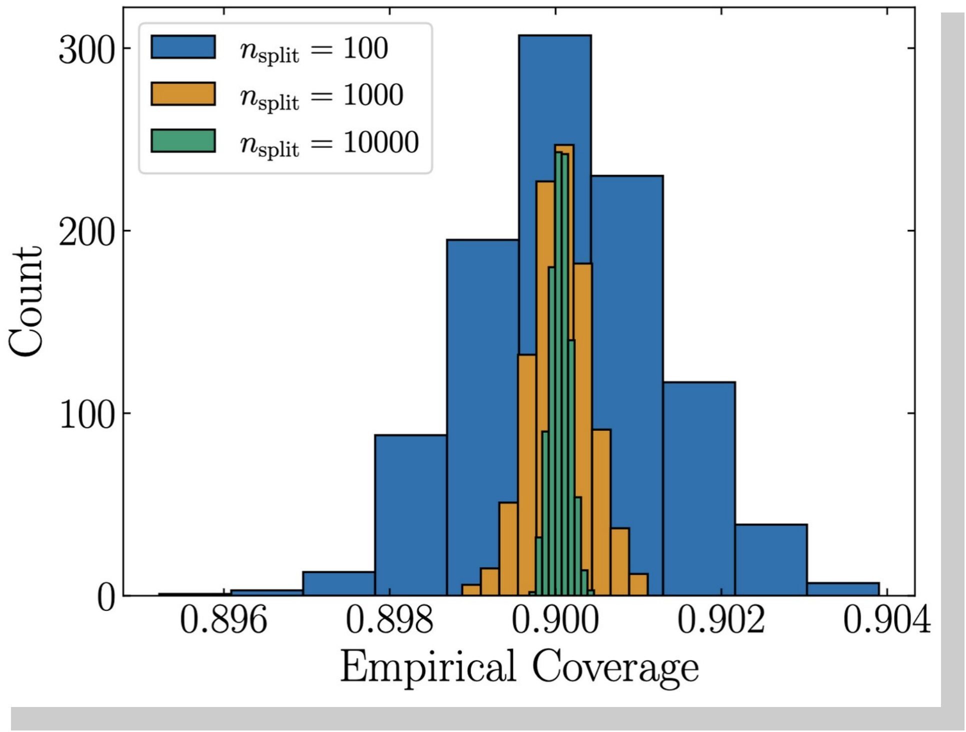


C. L. Armstrong *et al*, Phys. Rev. Lett. **135**, 142501 (2025)

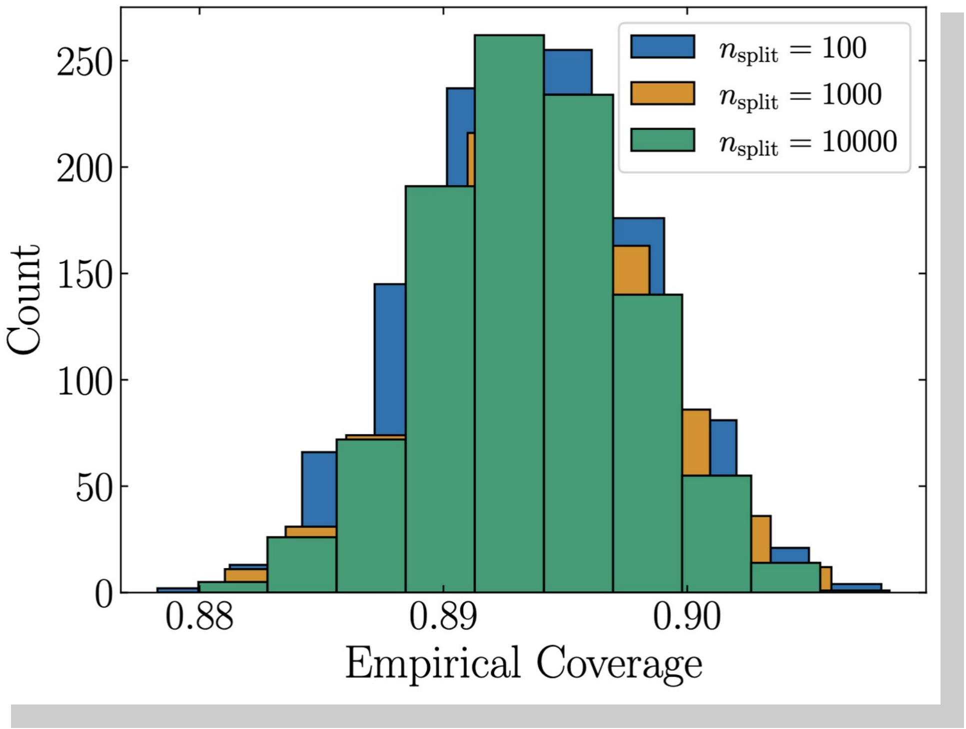
H. Yousefi Dezdarani, R. Curry, C. L. Armstrong, and A. Gezerlis, arXiv:2604.21039

Conformal prediction: neutron stars

Application: QMC neutron matter equation of state (2)



conformal



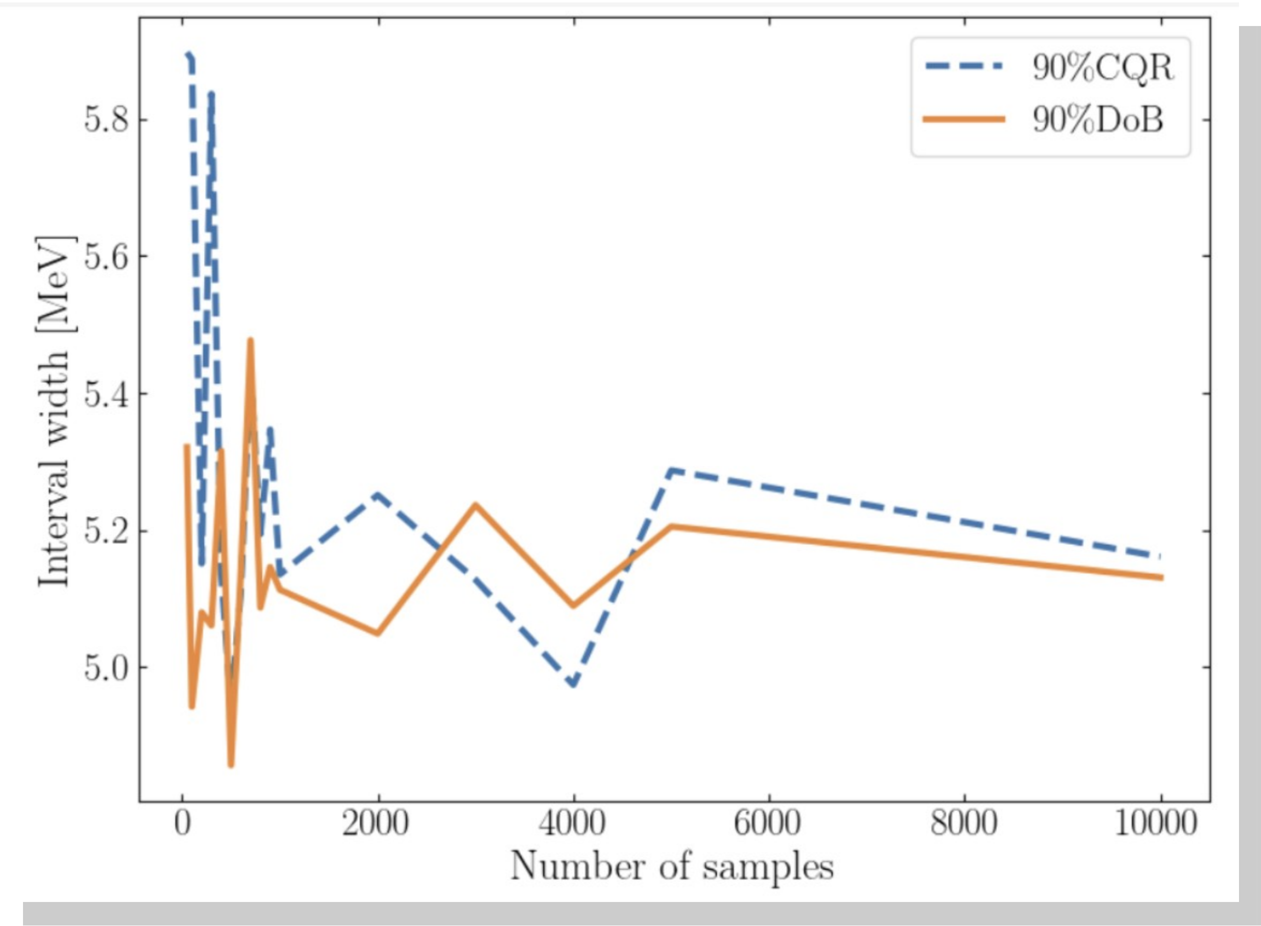
Bayesian

C. L. Armstrong *et al*, Phys. Rev. Lett. **135**, 142501 (2025)

H. Yousefi Dezdarani, R. Curry, C. L. Armstrong, and A. Gezerlis, arXiv:2604.21039

Conformal prediction: neutron stars

Application: QMC neutron matter equation of state (3)



CQR = conformal
DoB = Bayesian

Conformal prediction interval coincides with Bayesian one if you have tons of data

C. L. Armstrong *et al*, Phys. Rev. Lett. **135**, 142501 (2025)

H. Yousefi Dezdarani, R. Curry, C. L. Armstrong, and A. Gezerlis, arXiv:2604.21039

Conclusions

- We used chiral Effective Field Theory interactions in neural-network studies of light nuclei

- We used PMM and EC emulators together with QMC studies of light nuclei

- We applied conformal prediction to nuclear scattering and neutron star EOSs

Bonus slide

- How much should we care about the power counting?
- Do we need to go beyond first-order perturbations?
- How to interface with LGT, practically?

Acknowledgments

Funding

NSERC
CRSNG

INNOVATION.CA
CANADA FOUNDATION FOR INNOVATION | FONDATION CANADIENNE POUR L'INNOVATION

Ontario
MINISTRY OF RESEARCH AND INNOVATION
MINISTÈRE DE LA RECHERCHE ET DE L'INNOVATION

Collaborators

Guelph

- Ryan Curry
- Habib Yousefi Dezdarani

Los Alamos

- Rahul Somasundaram
- Ingo Tews

Michigan State

- Cassandra Armstrong

Texas A&M

- Jeremy Holt
- Pengsheng Weng

TU Darmstadt

- Kai Hebeler
- Achim Schwenk