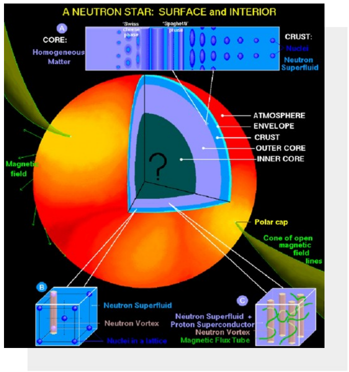
Conformal prediction, neural networks, and emulators for few-body systems

Alex Gezerlis

UNIVERSITY OF GUELPH

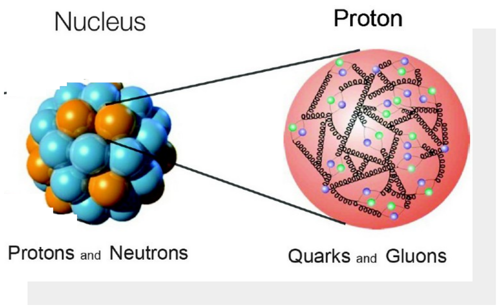
“Next generation *ab initio* nuclear theory” workshop
ECT*, Trento, Italy
July 15, 2025

Outline

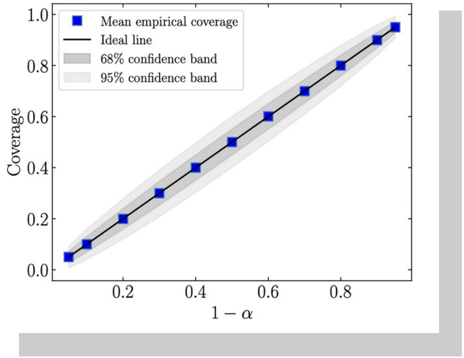


Credit: Dany Page

Motivation

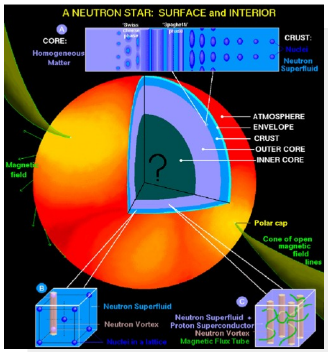


Nuclear methods



Recent results

Outline



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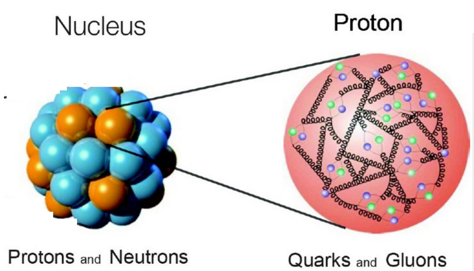
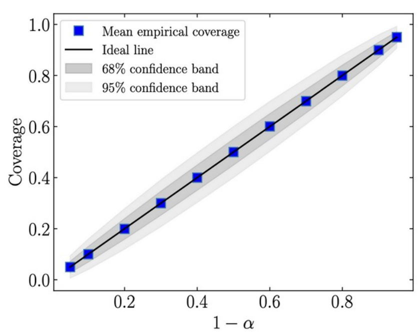


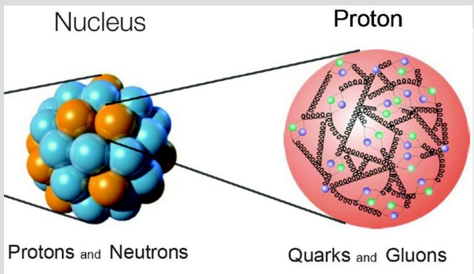
Nuclear methods



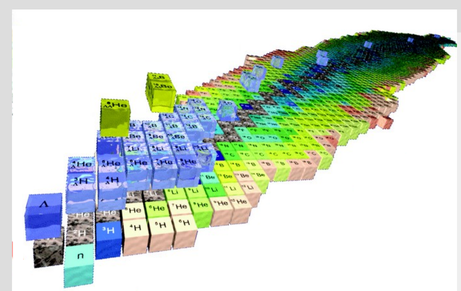
Recent results

Physical systems studied

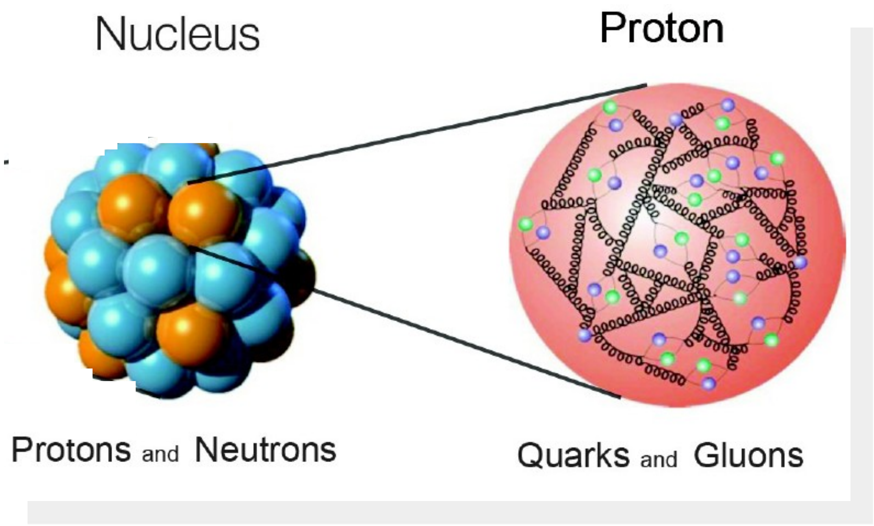
Nuclear forces



Nuclear structure



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

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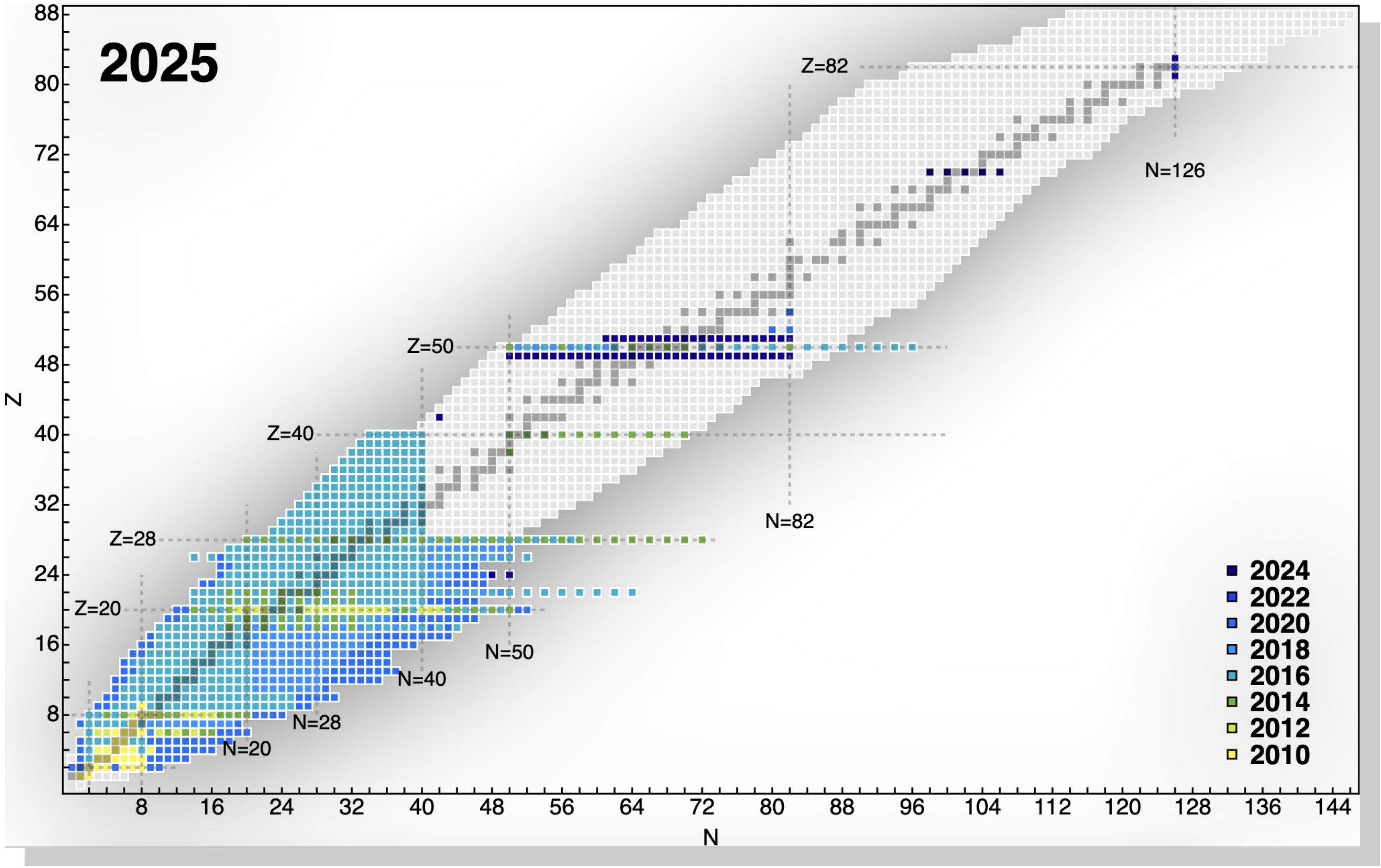
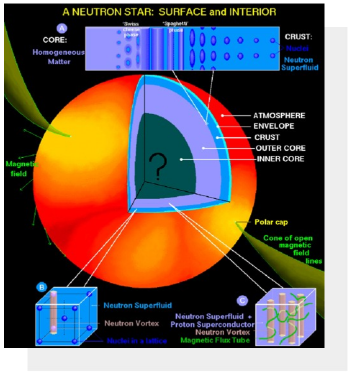


Heiko Hergert's propaganda plot

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

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

Outline



Credit: Dany Page

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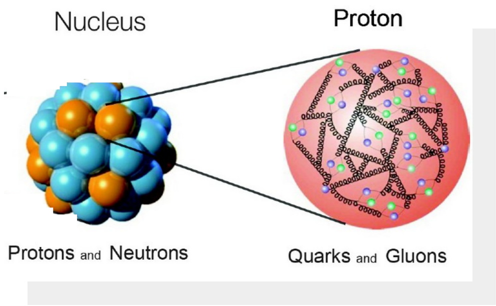
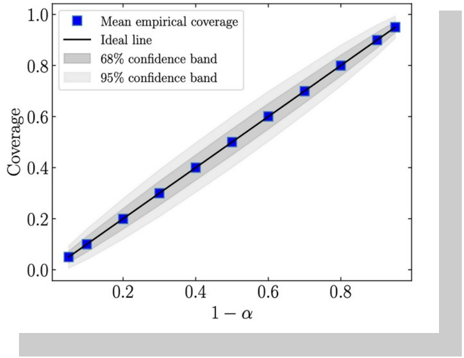


Nuclear methods



Recent results

Nuclear interactions

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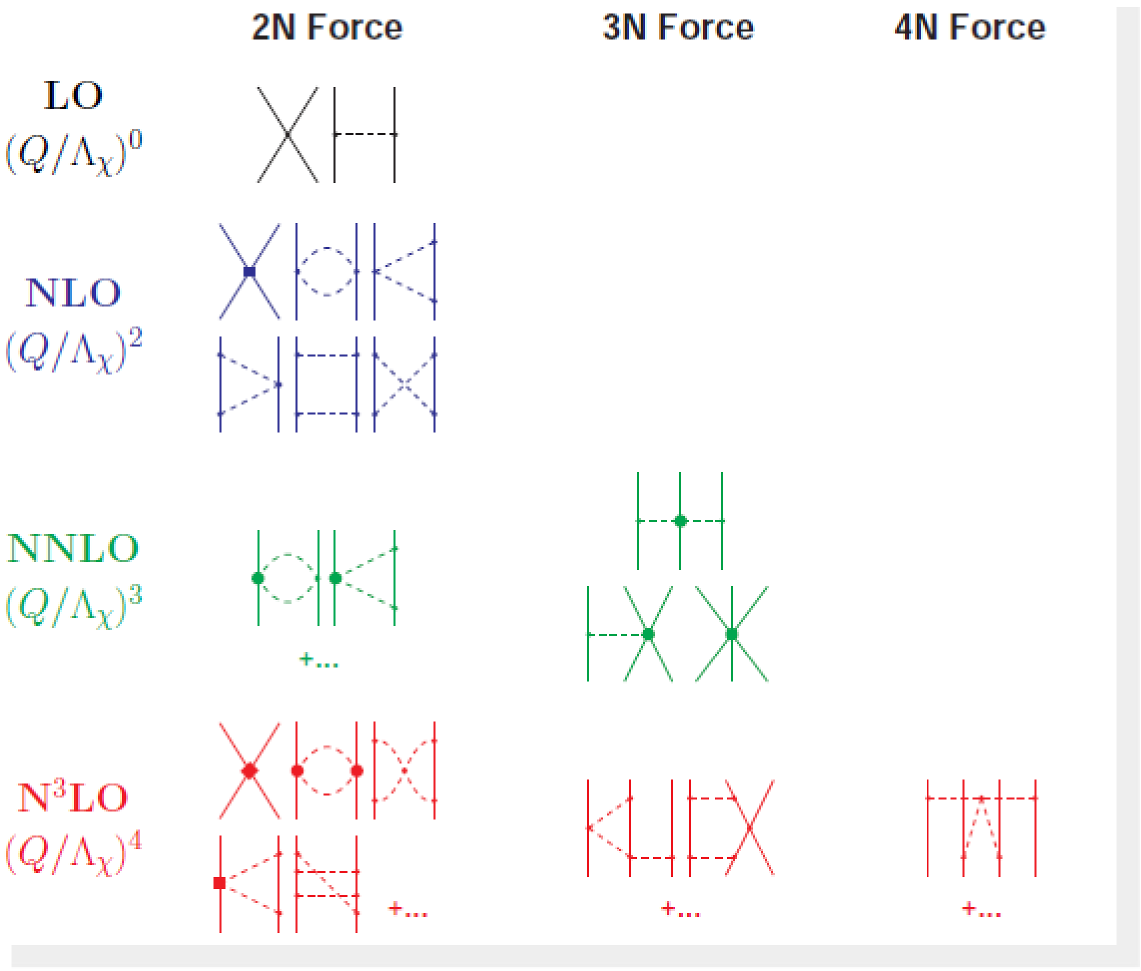


- Attempts to connect with underlying theory (QCD)
- Low-momentum expansion
- Naturally emerging many-body forces
- Low-energy constants from experiment or lattice QCD
- Now available in non-local, local, or semi-local varieties
- Power counting's relation to renormalization actively investigated

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

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

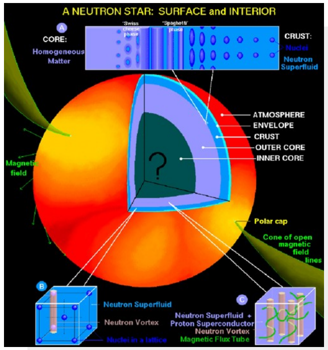
Nuclear many-body problem

$$H\Psi = E\Psi$$

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



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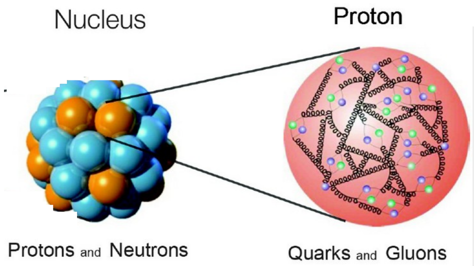
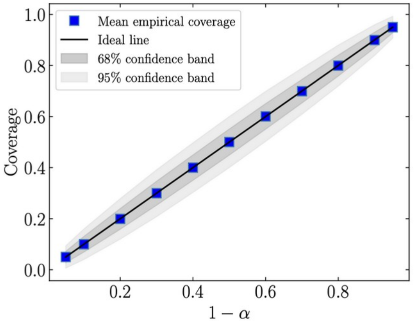


Nuclear methods



Recent results

Recent results

- Conformal prediction for nucleon-nucleon scattering
- Neural-network wave functions for light nuclei
- Emulators for the triton

Conformal prediction for nucleon-nucleon scattering

H. Yousefi Dezdarani, R. Curry, and A. Gezerlis, arXiv:2507:08085

A hint of the philosophy of statistics

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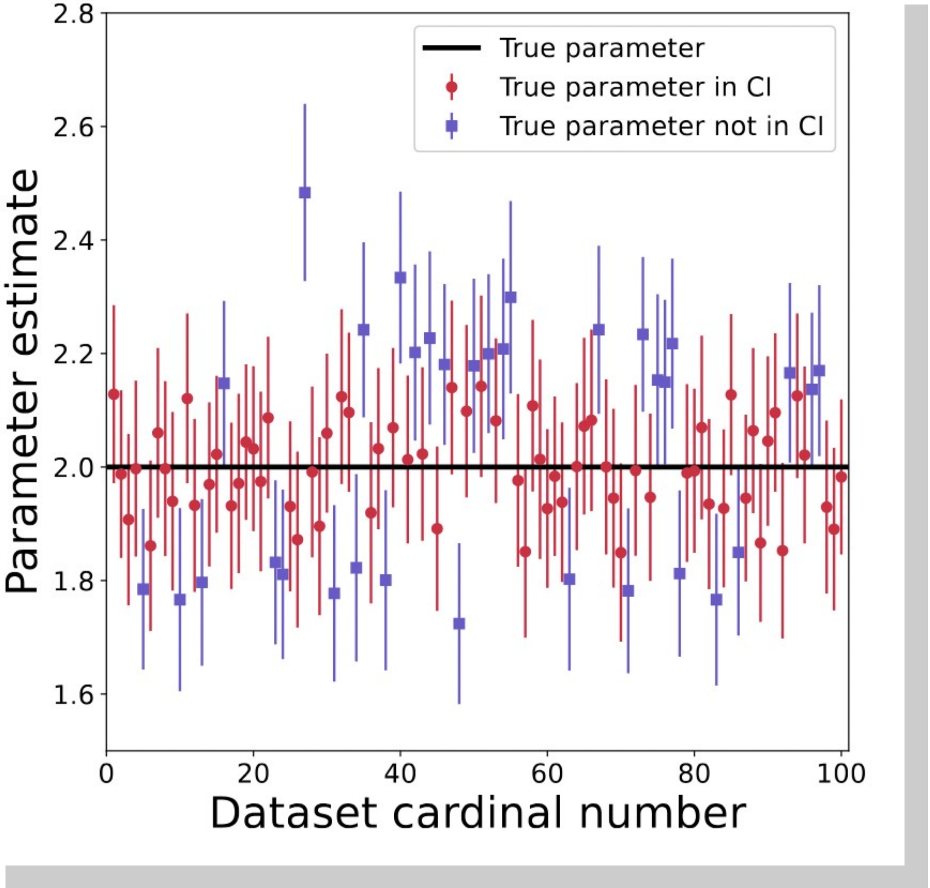
(Frequentist) confidence interval

E.g., maximize likelihood and take an $n\sigma$ 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)

A hint of the philosophy of statistics

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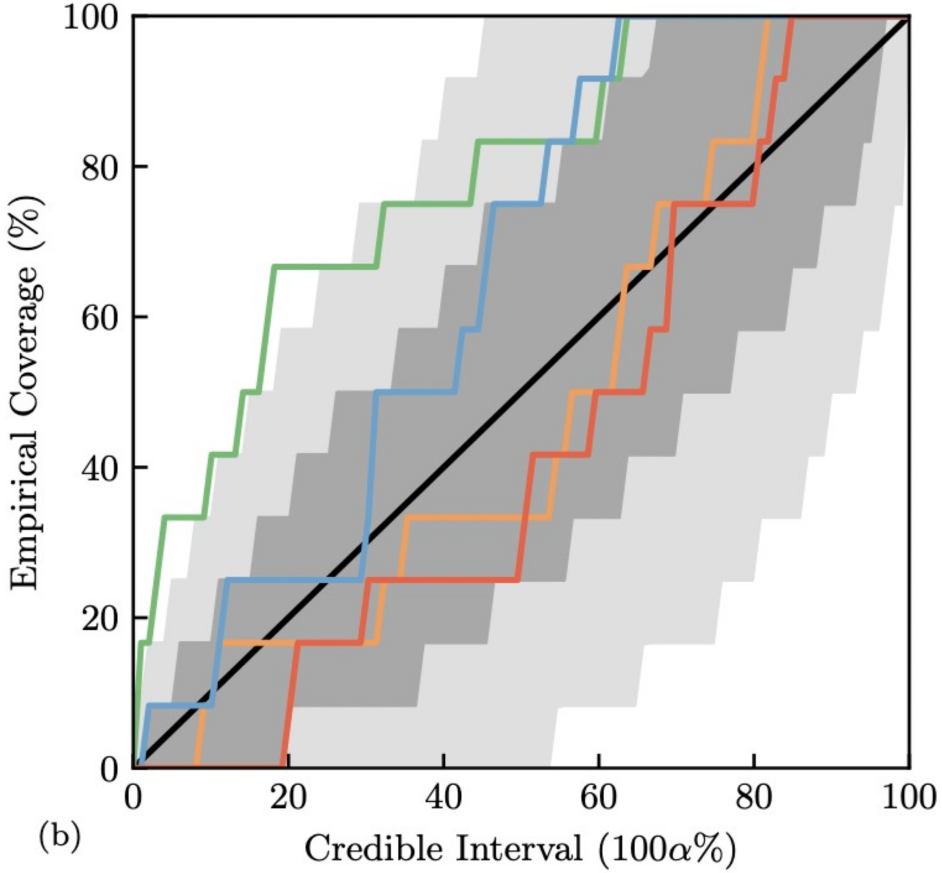
(Bayesian) credible interval

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

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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

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- 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, arXiv:2507:08085

Conformal prediction

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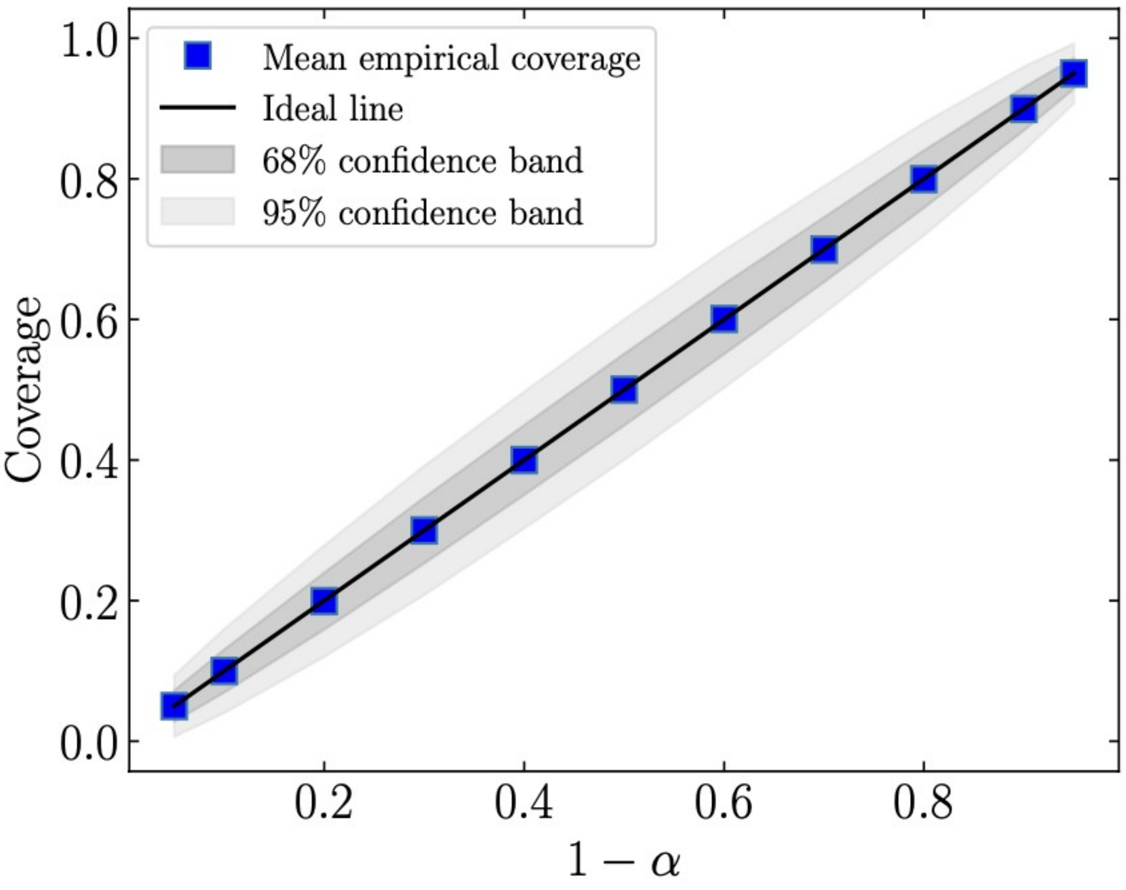
Application: BUQEYE pointwise model

- 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, arXiv:2507:08085

Conformal prediction

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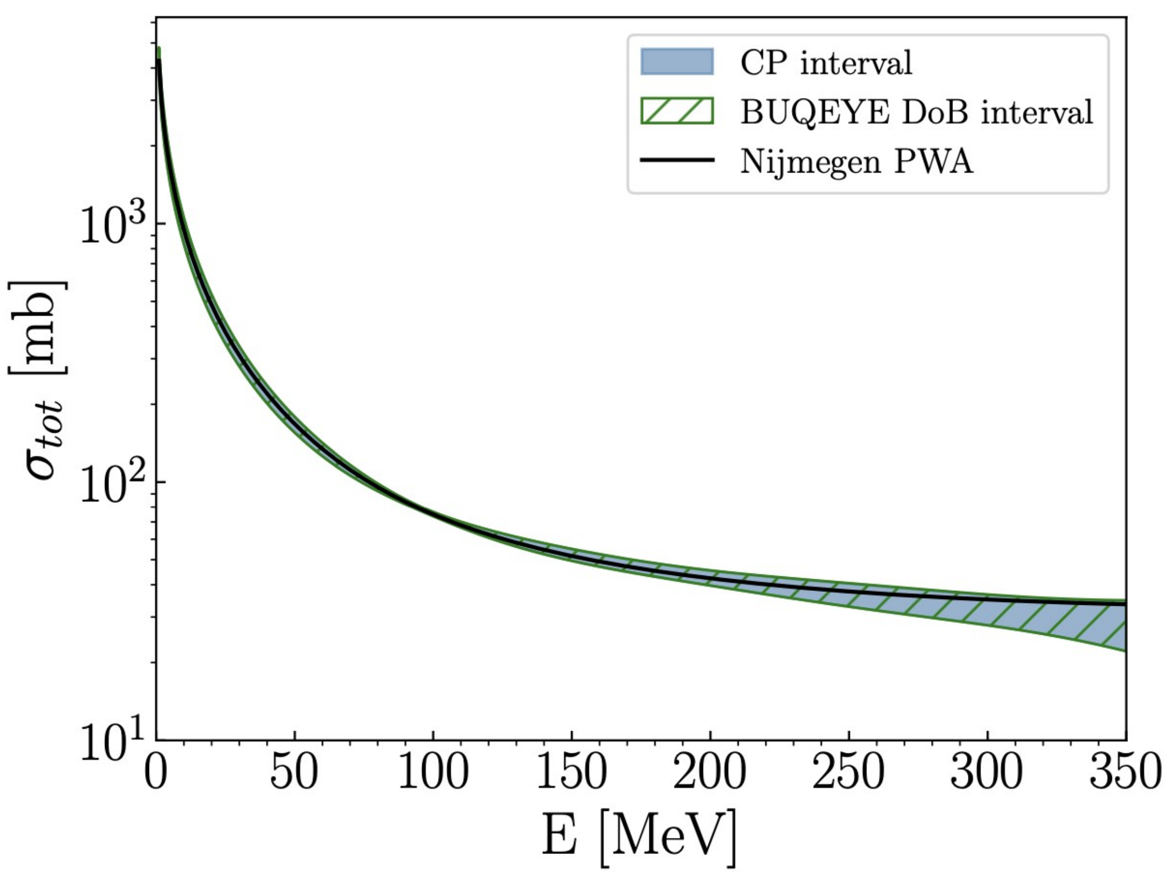
Application: BUQEYE Gaussian-process model

- Two-nucleon total cross section at N^2LO 0.9 fm EKM potential
- BUQEYE's GP is a non-parametric model
- To generate the conformal prediction bands we drew posterior samples using the BUQEYE open-source code



H. Yousefi Dezdarani, R. Curry, and A. Gezerlis, arXiv:2507:08085

Neural-network wave functions for light nuclei

P. Weng, A. Gezerlis, and J. Holt, arXiv:2505.11442

Quantum Monte Carlo in one slide

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Variational Monte Carlo

Encode parameters in trial wave function Ψ_V and use Rayleigh-Ritz principle to minimize expectation value of Hamiltonian

Diffusion Monte Carlo

Project out excited-state contributions, to reach the ground state

$$\Psi(\tau \to \infty) = \lim_{\tau \to \infty} e^{-(\mathcal{H}-E_T)\tau} \Psi_V$$

Earlier work

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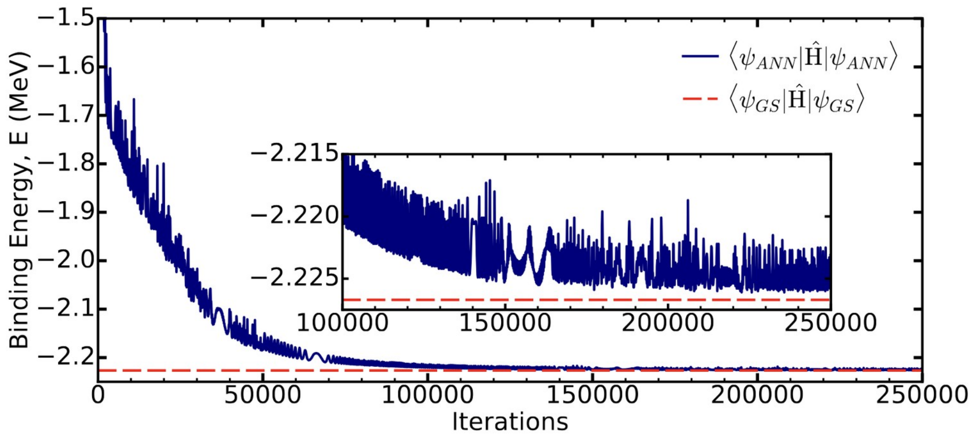
Deuteron



J. W. T. Keeble and A. Rios,
Phys. Lett. B **809**, 135743 (2020)

Light nuclei

	Λ	VMC-ANN	VMC-JS	GFMC	GFMC$_c$
^{2}H	4 fm^{-1}	$-2.224(1)$	$-2.223(1)$	$-2.224(1)$	-
	6 fm^{-1}	$-2.224(4)$	$-2.220(1)$	$-2.225(1)$	-
^{3}H	4 fm^{-1}	$-8.26(1)$	$-7.80(1)$	$-8.38(2)$	$-7.82(1)$
	6 fm^{-1}	$-8.27(1)$	$-7.74(1)$	$-8.38(2)$	$-7.81(1)$
^{4}He	4 fm^{-1}	$-23.30(2)$	$-22.54(1)$	$-23.62(3)$	$-22.77(2)$
	6 fm^{-1}	$-24.47(3)$	$-23.44(2)$	$-25.06(3)$	$-24.10(2)$

C. Adams, G. Carleo, A. Lovato, N. Rocco,
Phys. Rev. Lett. **127**, 022502 (2021)

N.B. Limited to pionless Hamiltonian

Earlier work

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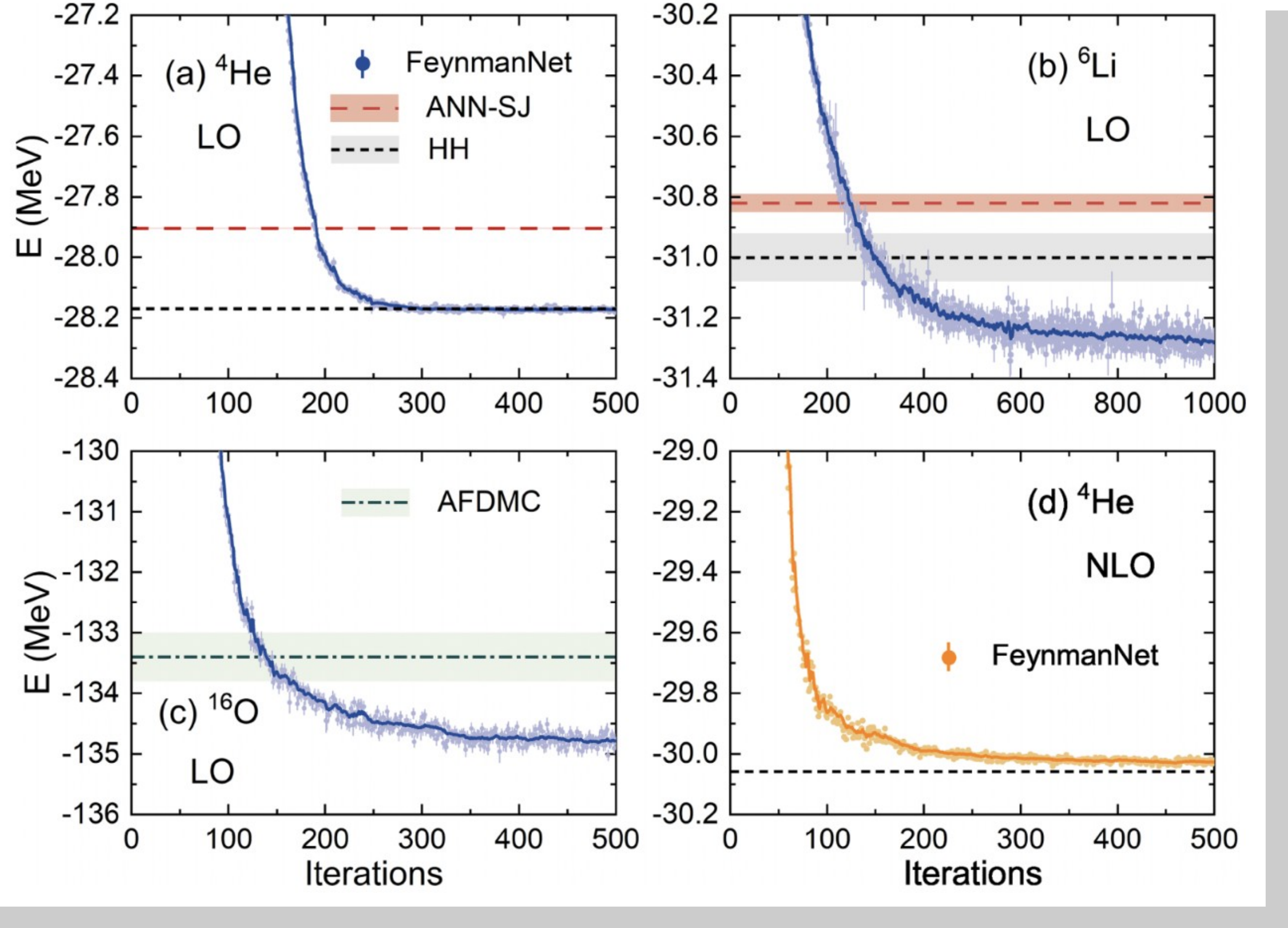
More on light nuclei



Y. L. Yang and P. W. Zhao, Phys. Rev. C **107**, 034320 (2023)

N.B. Also limited to pionless Hamiltonian

Neural networks for light nuclei

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Spin-isospin correlations

$$|\psi\rangle = \mathcal{S}\prod_{i<j}\left(1+\sum_{\mathrm{x}} u_{ij}^{(\mathrm{x})}\hat{O}_{ij}^{(\mathrm{x})}\right) f_{ij}^{(c)}|\Phi\rangle$$

$$|\psi\rangle \to \left(1+\sum_{i<j<k}\sum_{\mathrm{cyc}}\sum_{\mathrm{x}} \epsilon^{(\mathrm{x})}\hat{V}_{ijk}^{(\mathrm{x})}\right)|\psi\rangle$$

for N^2LO chiral Hamiltonian

P. Weng, A. Gezerlis, and J. Holt, arXiv:2505.11442

Neural networks for light nuclei

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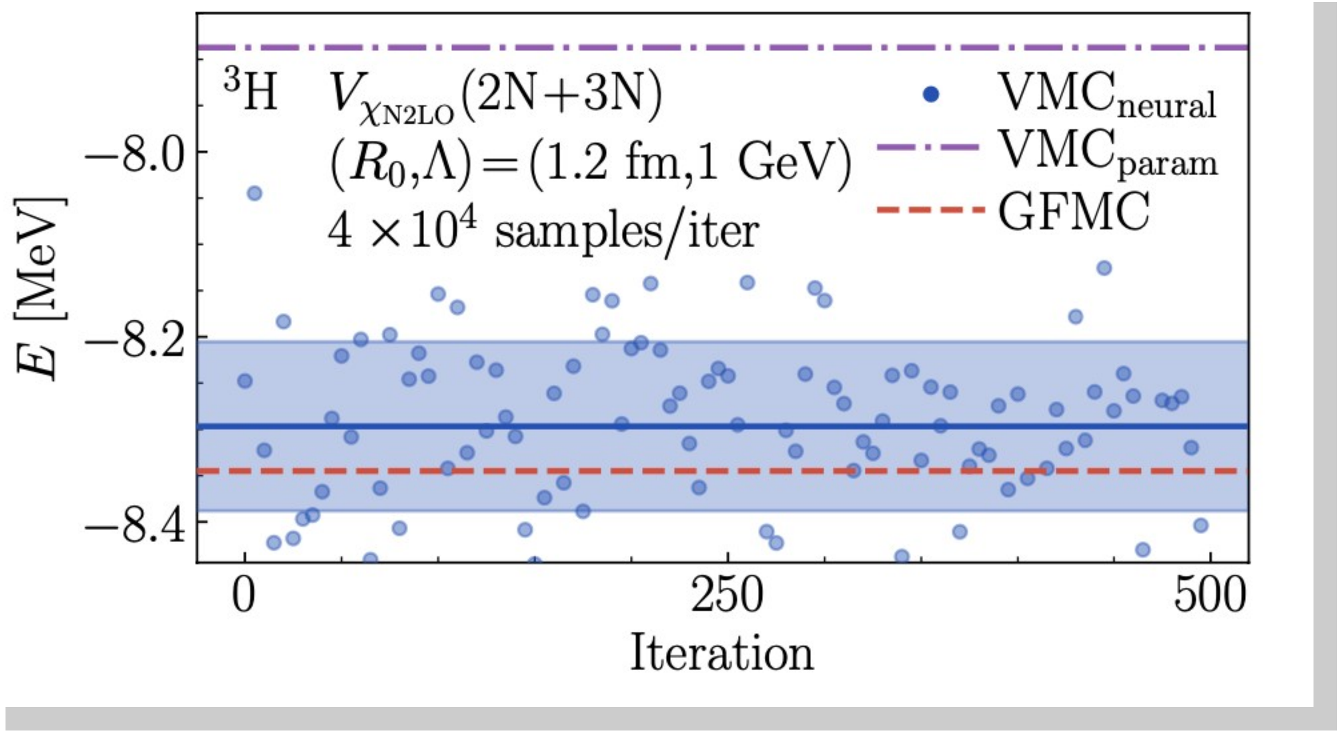
Nearly reproduces GFMC results
already at the VMC level

$E = E_k + V_{\chi N^2LO}(2N)$				
	R_0 [fm]	E_{neural} [MeV]	E_{GFMC} [MeV]	$\lvert\Delta E\rvert/\lvert E_{GFMC}\rvert$
^3H	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%
^2H	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, arXiv:2505.11442

Neural networks for light nuclei

Dramatic improvement over standard/parametric VMC employed before, e.g., AFDMC



P. Weng, A. Gezerlis, and J. Holt, arXiv:2505.11442

Emulators for the triton

R. Curry, A. Gezerlis, K. Hebeler, A. Schwenk, R. Somasundaram, and I. Tews, *in preparation*

Fitting the three-nucleon interaction

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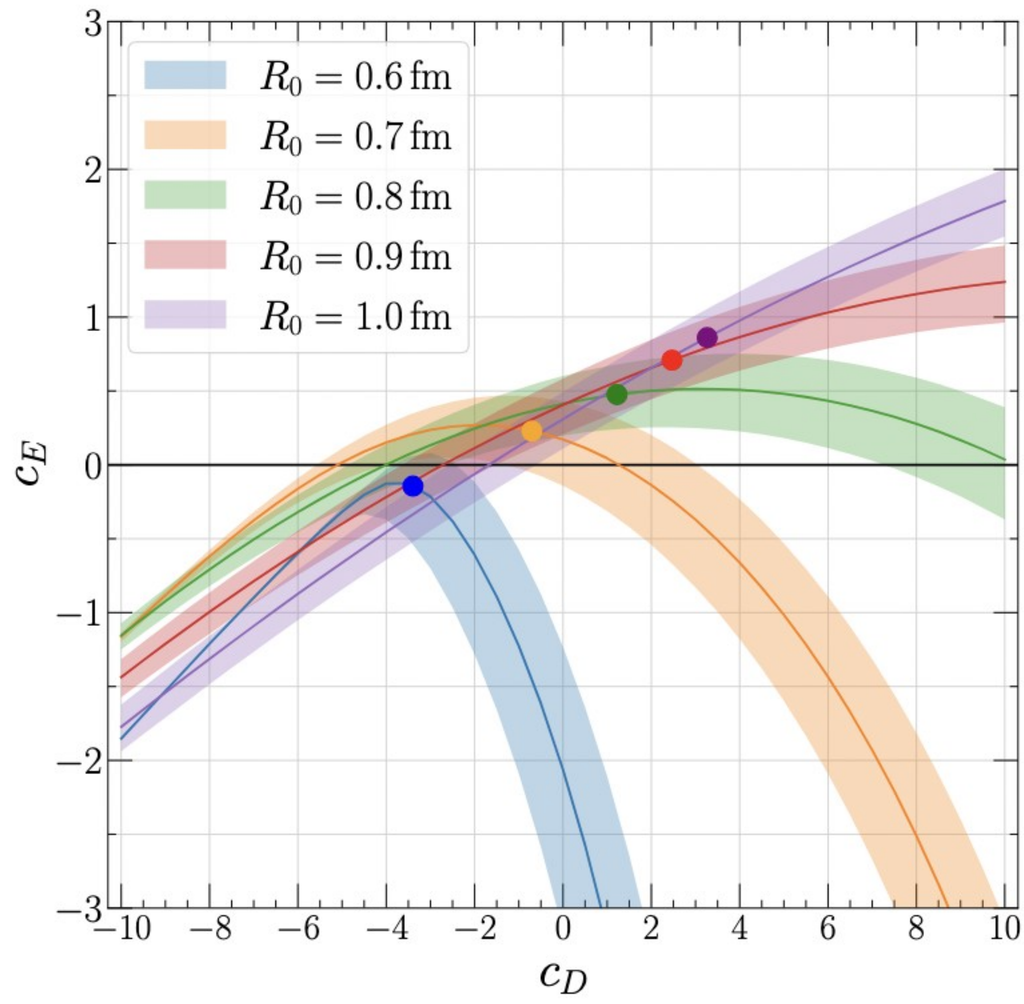
Solve Faddeev equations for triton binding energy to find a curve

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

I'm probably running out of time, so I refer to the previous two talks for a summary of previous applications of emulators to nuclear physics.

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

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

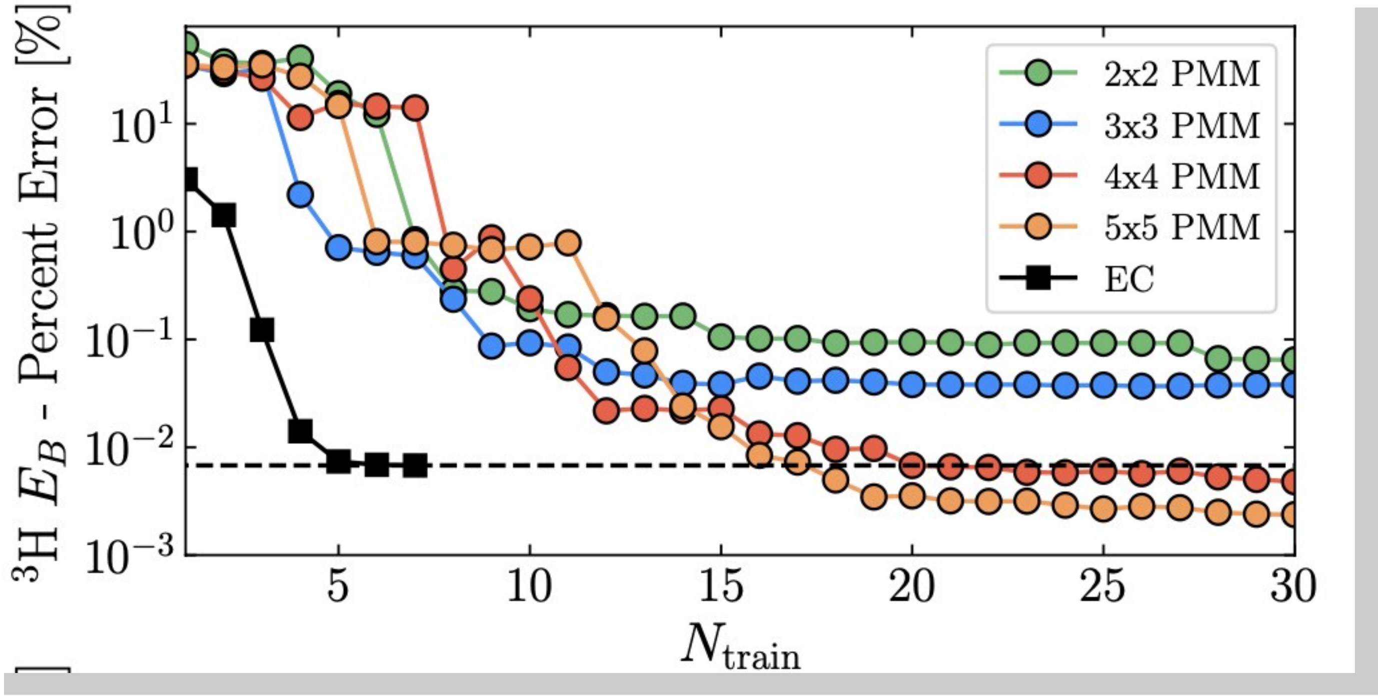
- **Eigenvector continuation (EC)**: Solve within a subspace (leading to generalized eigenvalue problem):

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

Varying the three-nucleon interaction

150 training data points + 75 test data points

New criterion for how to reject linearly dependent new training points



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Varying the three-nucleon interaction

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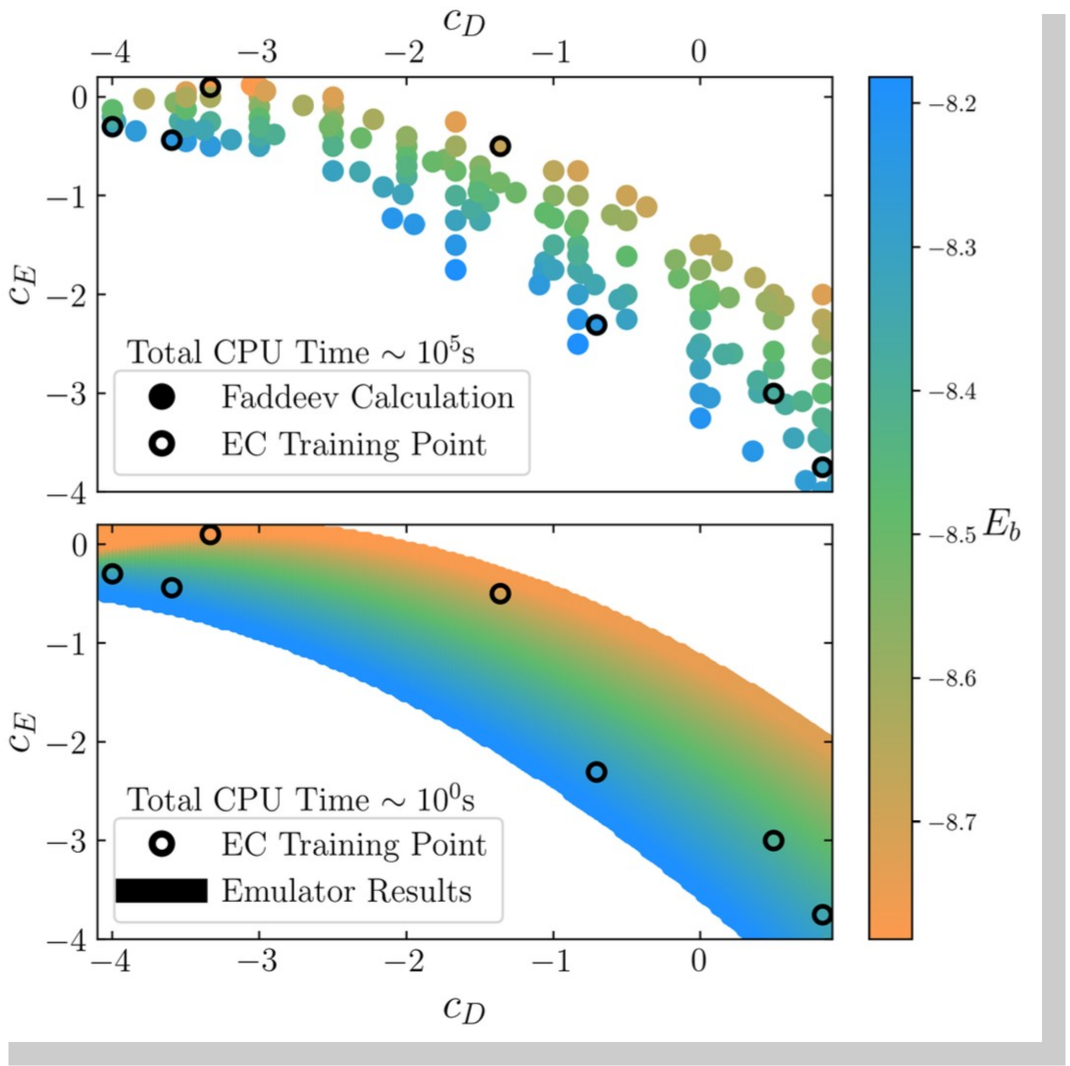
Now that the calculation is so cheap, we can fill out the plot:



R. Curry, A. Gezerlis, K. Hebeler, A. Schwenk, R. Somasundaram, and I. Tews, *in preparation*

Varying the full interaction

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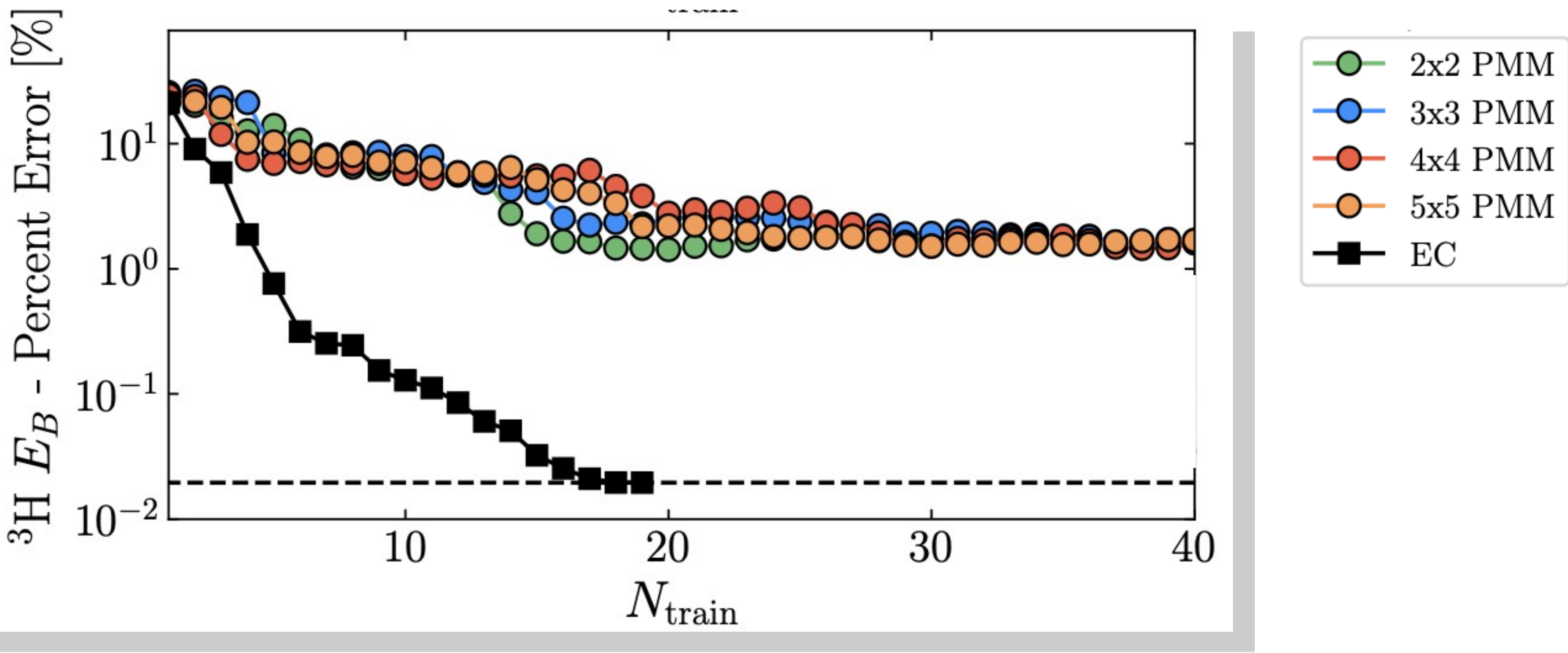
Release the full interaction, leading to 11 matrices:

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



R. Curry, A. Gezerlis, K. Hebeler, A. Schwenk, R. Somasundaram, and I. Tews, *in preparation*

Conclusions

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- We applied conformal prediction to nuclear physics

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

- We used PMM and EC emulators for the three-nucleon problem

Acknowledgments

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Collaborators

Guelph

- Ryan Curry
- Habib Yousefi Dezdarani

Los Alamos

- Rahul Somasundaram
- Ingo Tews

Texas A&M

- Jeremy Holt
- Pengsheng Weng

TU Darmstadt

- Kai Hebeler
- Achim Schwenk

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