STREAMLINE

SmarT Reduction and Emulation Applying Machine Learning In Nuclear Environments

DOE NP AI/ML
PI Exchange Meeting
November 19 – 20, 2025

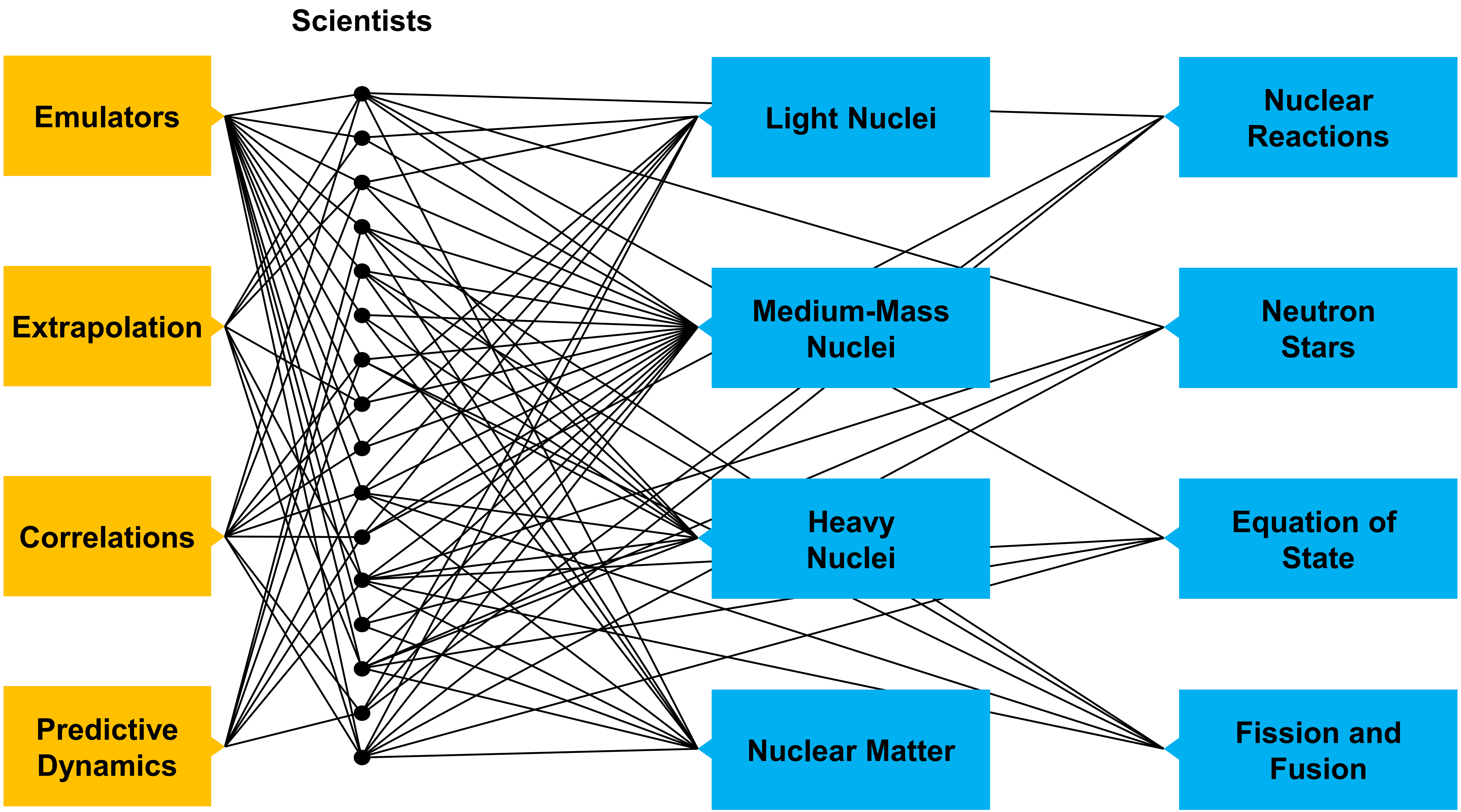
STREAMLINE Collaboration: Machine Learning for Nuclear Many-Body Systems

Principal Investigator: Dean Lee, Facility for Rare Isotope Beams, Michigan State University

Institution	**Investigators** [Co-Investigators*, Senior Personnel†]
Michigan State Univ.	Pablo Giuliani†, Kyle Godbey†, Morten Hjorth-Jensen*, Dean Lee*, Witold Nazarewicz* Xilin Zhang†
Argonne Nat. Lab.	Alessandro Lovato*
Fermilab	Noemi Rocco*
Florida State Univ.	Kévin Fossez*, Jorge Piekarewicz*
North Carolina State Univ.	Sebastian König*
Oak Ridge Nat. Lab.	Gaute Hagen*
Ohio State Univ.	Richard Furnstahl*
Ohio Univ.	Christian Drischler*
Univ. Tennessee	Thomas Papenbrock*

Our team performs research in the areas of fast and accurate emulators, smart model extrapolation, learning correlations in wave functions and operators, and predicting nuclear dynamics, including nuclear fission, and heavy-ion fusion.

Institutions = 9 , PIs + Senior Personnel + Collaborators = 18, Postdocs + Students = 10



STREAMLINE Collaboration Meeting
April 29 – 30, 2025
Argonne National Laboratory

Meeting webpage

YouTube videos of talks

April 29

8:30-9:00	Registration	
9:00-9:15	Ian Cloët (Deputy PHY Division Director)	Welcome to Argonne
9:15-9:30	Dean Lee (FRIB)	Announcements
9:30-10:00	Pablo Giuliani (FRIB)	More on learning equations from data
10:00-10:30	Coffe Break	
10:30-11:00	Patrick Cook (FRIB/MSU)	PMMs for Nonlinear Systems: The Gross-Pitaevskil Equation
11:00-11:30	Danny Jammooa (FRIB/MSU)	PMMs for Euclidean time evolution
11:30-12:00	Benjamin Clark (MSU)	Emulating the Magnus formulation of IMSRG using PMMs
12:00-13:30	Lunch at the Cafeteria	
13:30-14:00	Bryce Fore (ANL)	Investigating the crust of neutron stars with NQS
14:00-14:30	Jane Kim (Ohio)	Excited NQS
14:30-15:00	Alessandro Lovato (ANL)	Hypernuclei with NQS
15:00-15:30	Coffee Break	
15:30-16:00	Simon Sundberg (OSU)	Critical analysis of neural networks in simple nuclear systems
16:00-16:30	Daniel Lay (MSU)	Accelerating DFT simulations for uncertainty quantification
16:30-17:00	Xilin Zhang (MSU)	Nuclear continuum physics and emulations
17:00-18:00	Discussion	
18:00-20:00	Dinner at Wooden Paddle	

April 30

9:00-9:30	Abinhav Giri (Ohio)	Emulators for two-body scattering in momentum space
9:30-10:00	Mudivanselage Nuwan Yapa (FSU)	Towards scalable emulators for many-body resonances
10:00-10:15	Manouchehr Farkhondeh (DOE Program Manager)	Q&A about AI/ML at DOE Nuclear Physics (via Zoom)
10:15-11:00	Coffee Break	
11:00-11:30	Gaute Hagen (ORNL)	Recent advances in emulating coupled cluster calculations
11:30-12:00	Thomas Papenbrock (UT & ORNL)	Emulators tell us about nuclear deformation / Hartree Fock mass models
12:00-12:30	Symposium adjourns	

STREAMLINE Collaboration Progress

All project milestones complete or nearly complete

Projected Date	Task	Milestone
1/31/2024	3.2.1	Theory and development of parametric matrix models
5/31/2024	3.2.2	Proof-of-principle demonstration for greedy algorithm (with error estimates) for two-nucleon scattering with realistic interaction.
8/31/2024	3.2.2	First implementation and testing of three-body scattering emulator for Nd system.
7/31/2024	3.2.3	Implementation of few-body resonance emulators in the Berggren basis
7/31/2024	3.2.4	Initial setup of emulators key nuclei in the “island of inversion” to be studied at FRIB
8/31/2024	4.2.1	Quantified predictions of nuclear properties based on long-range extrapolations for r-process nuclei
6/31/2024	5.1.3	Development of ANN wave functions of A = 40 nuclei
8/31/2024	5.1.4	Light hypernuclei with ANN wave functions
7/31/2024	5.2.1	Unsupervised/supervised learning of alpha clustering in medium-mass nuclei
8/31/2024	5.2.2	Correlations for spectra learned from model-space dependence
1/31/2024	6.1.1	Development of PES emulator for fission using a committee of NNs
8/31/2024	6.1.3	Apply RBs to speed-up nuclear DFT calculations
8/31/2024	6.2.1	Analysis of dynamic modes in TDDFT using time-dependent emulators

Projected Date	Task	Milestone
4/30/2025	3.2.1	Parametric matrix models for neutron separation energies
8/31/2025	3.2.2	Demonstration of extended three-body scattering emulator
8/31/2025	3.2.4	Emulators for key nuclei in the “island of inversion” to be studied at FRIB
8/31/2025	4.2.1	Quantified predictions based on long-range extrapolations for nucleonic phases in the neutron star crust
8/31/2025	4.2.2	Inference of neutron-star radii via smart model extrapolations
8/31/2025	4.2.3	Extrapolations for resonances in few- and many body systems
8/31/2025	5.1.2	Demonstration that RG unitary transformations can be learned
8/31/2025	5.1.3	Demonstration of real-time dynamics for ANN wave functions
8/31/2025	5.2.1	Unsupervised/supervised learning of nuclear matter quantum phases in deformed traps
4/30/2025	5.2.2	Application of ML to nuclear spectra extrapolation with quantified errors based on learned correlations
1/31/2025	5.2.3	Parametric matrix models for ^{8}Be resonances using finite volume energies
4/30/2025	6.1.1	Development of RB for physics-informed/intrusive PES emulation for single nucleus
4/30/2025	6.1.1	Dimensionality reduction investigation of PESs
8/31/2025	6.1.2	Develop and test fission fragment observable emulation from each PES
1/31/2025	6.1.4	Develop framework for ML-directed nuclear EDF determination
1/31/2025	6.1.4	Improvements to the energy density functionals
12/31/2024	6.2.1	Begin development of Neural Implicit Flow emulator for TDDFT

STREAMLINE Collaboration Budget

	FY 2024 ($k)	FY 2025 ($k)	Totals ($k)
a) Funds allocated	605	605	1210
b) Actual costs to date	605	605	1210

WBS or ID#	Institution	Subtotals ($k)
271819	MSU	352
271828	ANL	122
271837	FNAL	124
271823	FSU	187
271870	OSU	90
271873	OU	92
271812	ORNL	71
271846	NCSU	87
271858	UTK	85
Total		1210

STREAMLINE Collaboration Highlights

Team

N. Yapa

K. Fossez

S. König

FSU FLORIDA STATE UNIVERSITY

NC STATE UNIVERSITY

Relevance

Many-body calculations in exotic nuclei are critical for FRIB & astrophysics, but **computationally costly and sometimes unstable** in decaying systems.

Eigenvector continuation (EC) recently emerged as a powerful method to build emulators and perform extrapolations

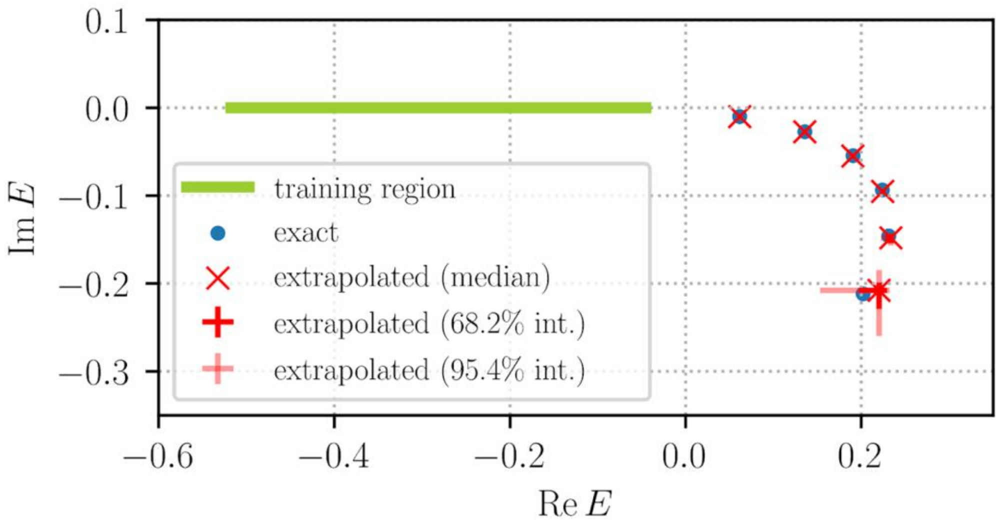
Goal: Generalize EC to complex-energy problems to perform efficient and reliable bound-to-resonance extrapolations in exotic nuclei.

Context

N. Yapa *et al.*, Phys. Rev. C **107**, 064316 (2023), Editor's Suggestion.

New method (pre-STREAMLINE): Complex-augmented EC (CA-EC).

- **Proof-of-concept** for two-body resonances using toy model.
- Method tested using only complex-scaling.



STREAMLINE: Toward realistic applications

- **Scaling of CA-EC to N-body decay** & demonstration in 3-body case.
- **Berggren basis** formulation to improve numerical scalability for N>3.
- **Configuration-interaction** and **lattice formulations** tested.
- First application in **realistic system (^{6}He)**.

N. Yapa *et al.*, Phys. Rev. C **111**, 064318 (2025)

Funding of the STREAMLINE collaboration provided **critical support** to go beyond initial findings.

Current progress

Sequential 5p decay of ^{9}N (observed in 2023)

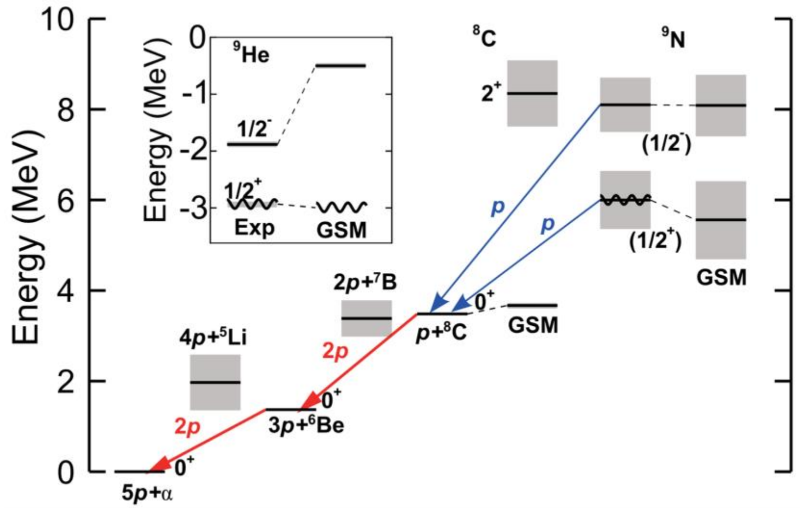
- Six-body resonance, several open decay channels.
- CA-EC with complex-energy Coulomb wave functions.
- Experimental interest.

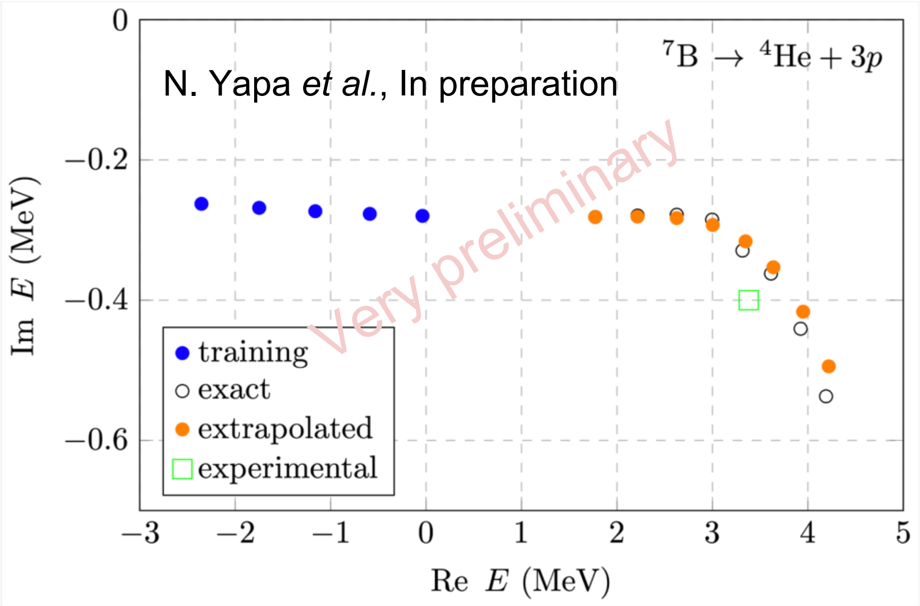
Preliminary results in ^{6}Be and ^{7}B promising.

New directions:

- Parametric matrix models (PMM) for resonances.
- Neural quantum states (NQS) for resonances.

R. J. Charity *et al.*, Phys. Rev. Lett. **131**, 172501 (2023)





Motivation: mining scattering data

Scattering experiments yield invaluable data for calibrating, validating, and improving chiral EFT (and optical models)

Competing formulations of chiral EFT with open questions on issues including

- EFT power counting
- sensitivity to regulator artifacts
- Differing predictions for medium-mass to heavy nuclei

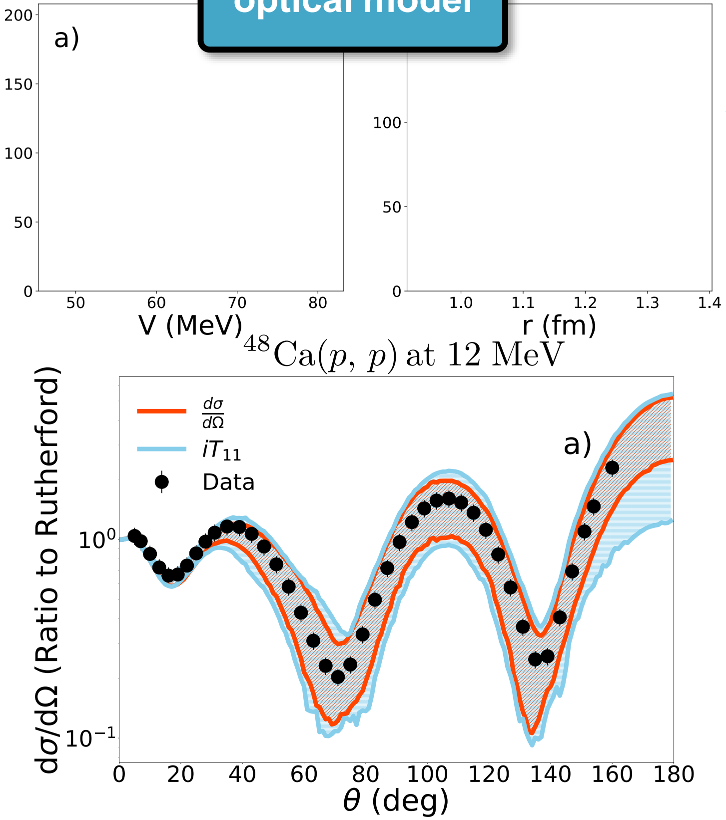
see, *e.g.*, Yang, Ekström *et al.*, arXiv:2109.13303
Furnstahl, Hammer, Schwenk, Few Body Syst. **62**, 72

Bayesian methods have become standard for principled UQ in nuclear physics:

- parameter estimation
- model comparison
- sensitivity analysis
- …

BUQEYE
Chalmers
ISNET

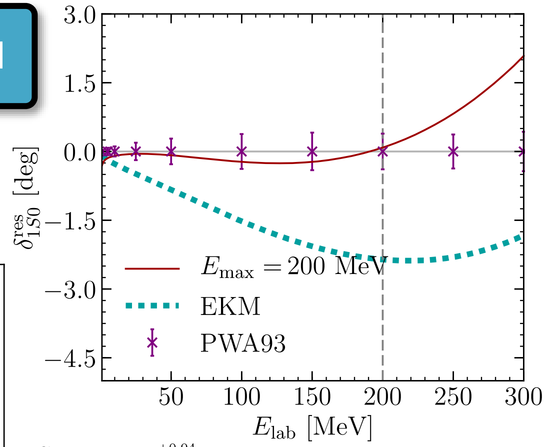
optical model

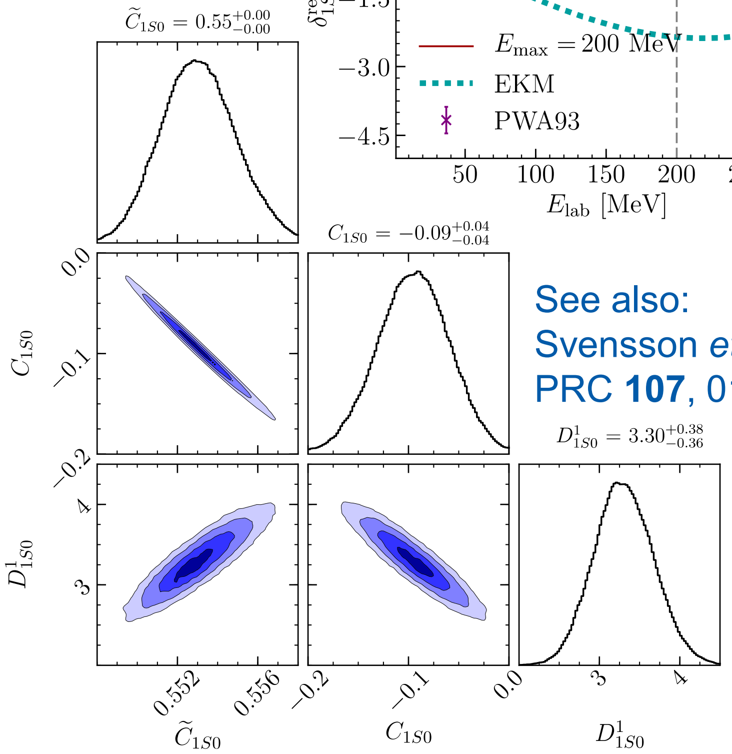


Catacora-Rios, King *et al.*, PRC **104**, 064611

chiral potential

Wesolowski *et al.*, JPG **46**, 045102





See also: Svensson *et al.*, PRC **107**, 014001

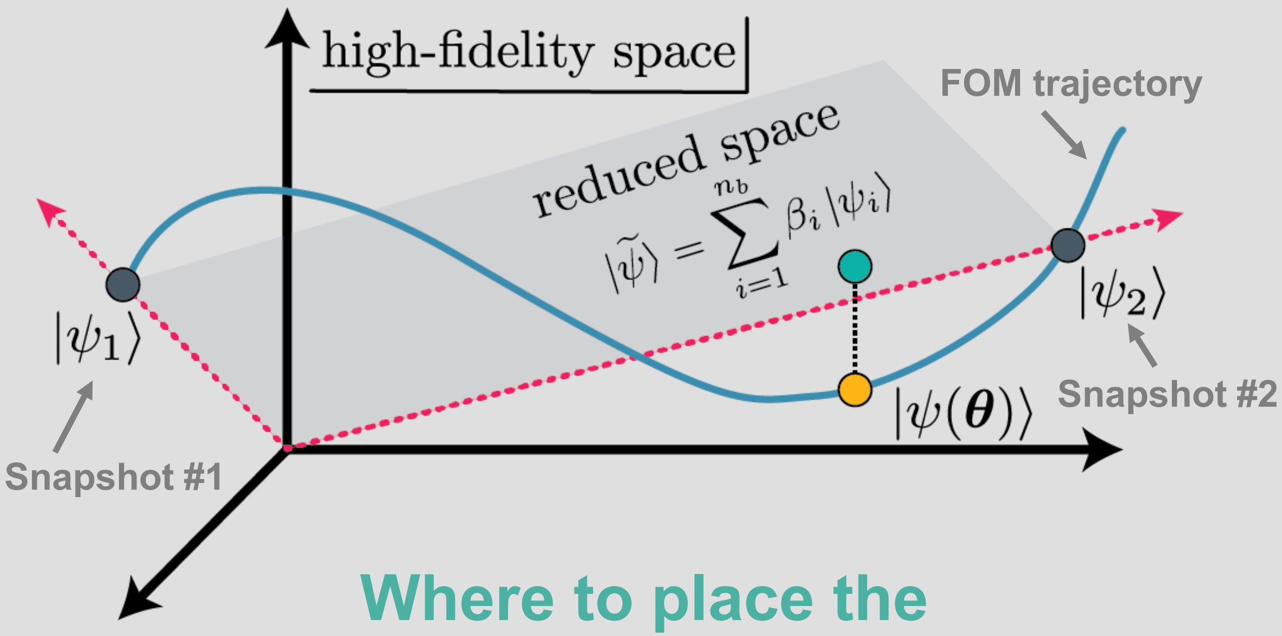
Scattering eqns. (FOM) can be solved accurately in few-body systems.
But: *prohibitively* slow for statistical analyses of $A > 2$ scattering

Construct <u>emulators</u> by removing superfluous information

Emulator basis construction

Maldonado, Drischler, Furnstahl *et al.*, PRC **112**, 024002 (2025)

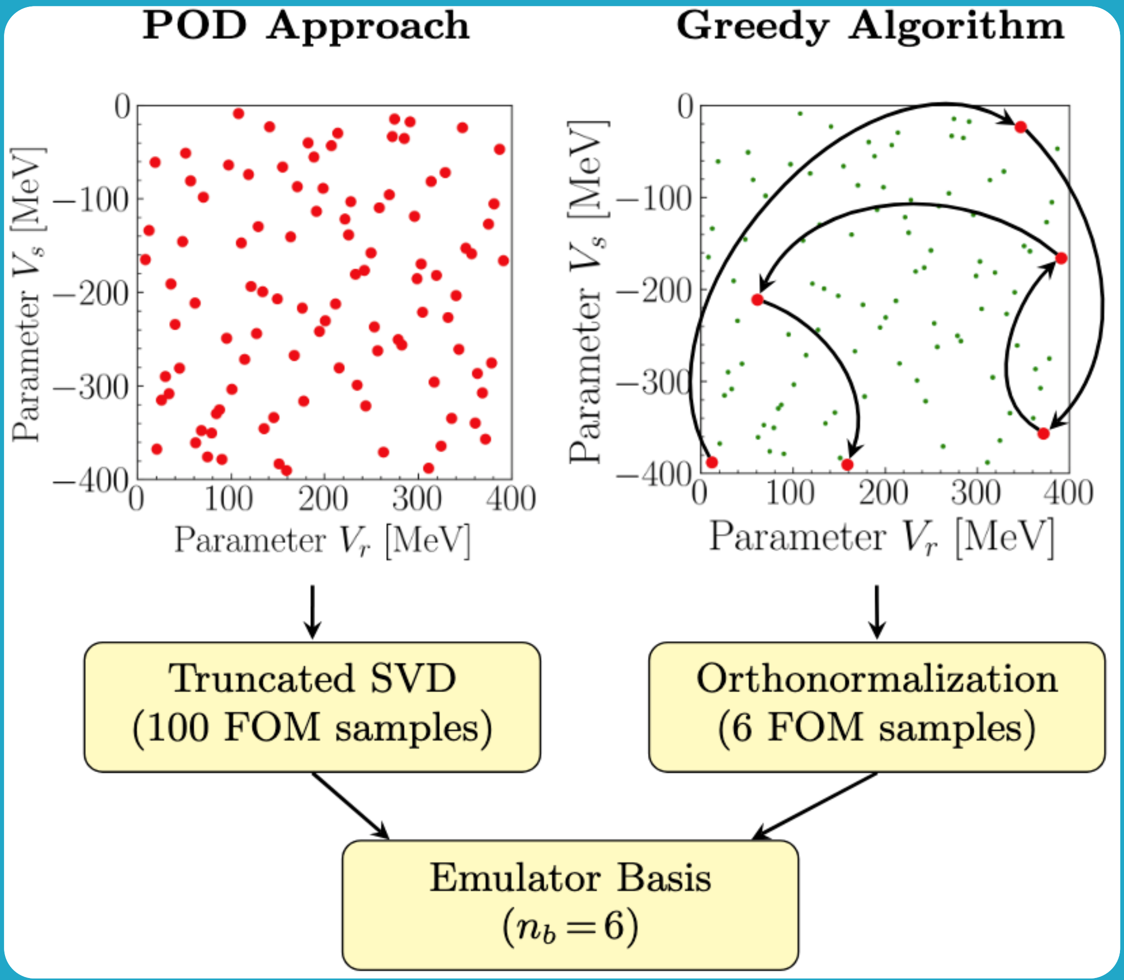
OHIO UNIVERSITY



Where to place the emulator's *snapshots*?

1. **Space-filling sampling** combined with a **Proper Orthogonal Decomposition (POD)**
2. **Active learning** approach based on **error estimation** and a ***greedy algorithm***

See also: Sarkar & Lee, PRR **4**, 023214 ; Bonilla *et al.*, PRC **106**, 054322



The greedy method uses far fewer FOM solutions to construct its basis, iteratively adding snapshots where the (estimated) emulator error is maximum.

Greedy Algorithm in Action (preview)

start with 2 randomly placed initial snapshots

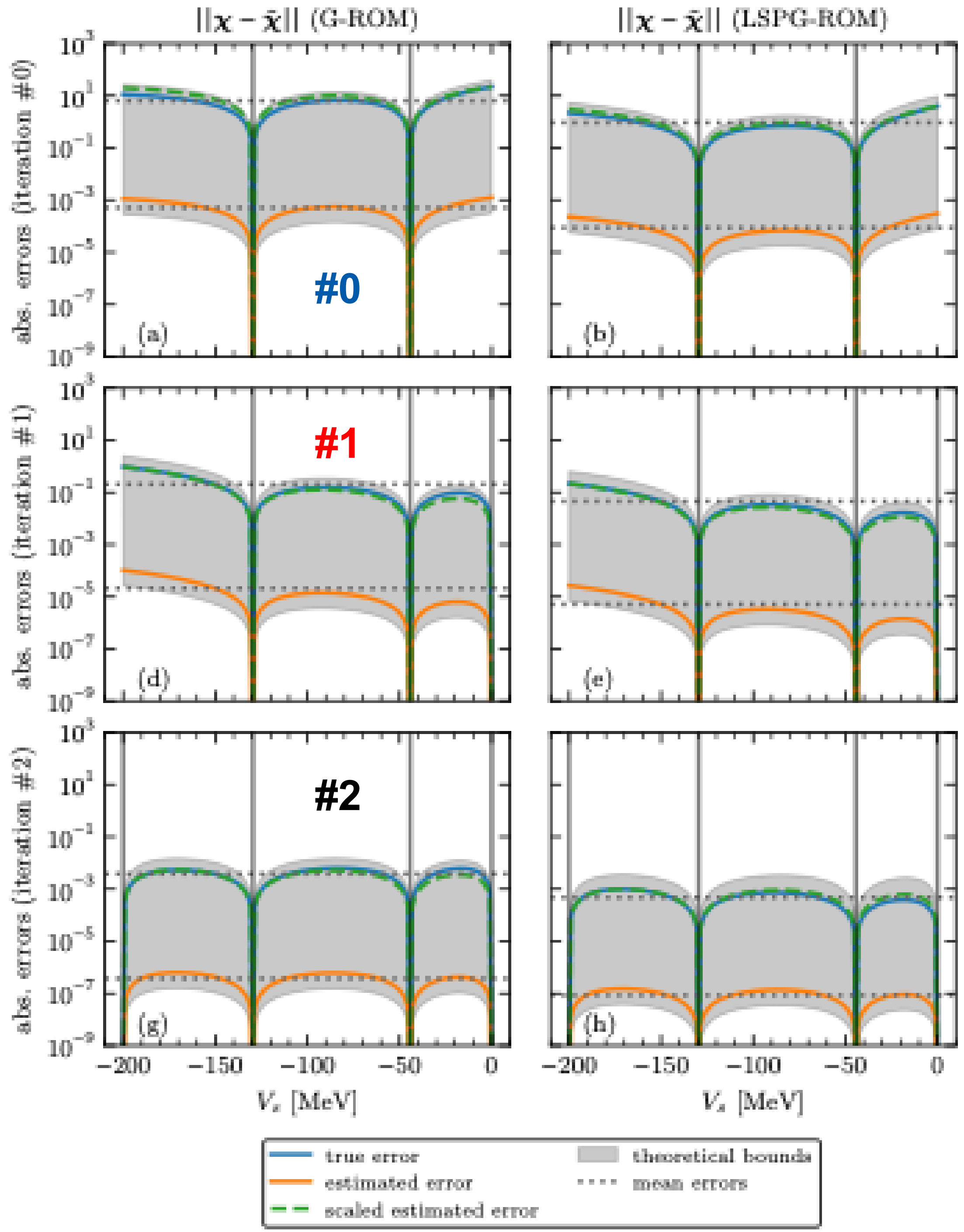
Estimate the emulator error across the parameter space

Place the next snapshot(s) at the location(s) of maximum estimated error

Iterate until the *requested* accuracy is obtained

(1D problem for illustration)

***Greedy* Iteration increasing accuracy**



Extension to coupled channels & momentum space

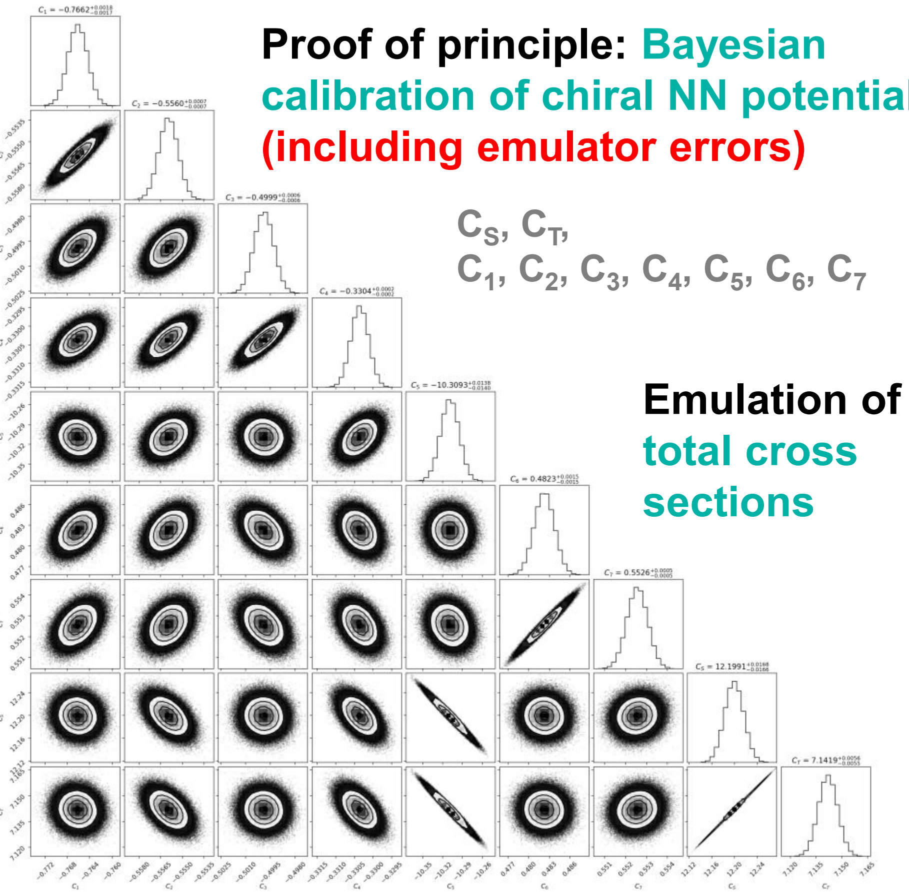
Giri, Kim, Drischler, Elster, Furnstahl *et al.*, in prep.


$$T^{j}_{\ell\ell'}(k,k';E) = V^{j}_{\ell\ell'}(k,k') + \sum_{\ell''}\int_0^\infty dk''\, k''^2 \frac{V^{j}_{\ell\ell''}(k,k'')T^{j}_{\ell''\ell'}(k'',k';E)}{E-E''+i\varepsilon}$$

Lippmann-Schwinger (integral) equation

gives access to a wide range of modern chiral potentials

As before, the greedy algorithm exhibits a fast convergence pattern.



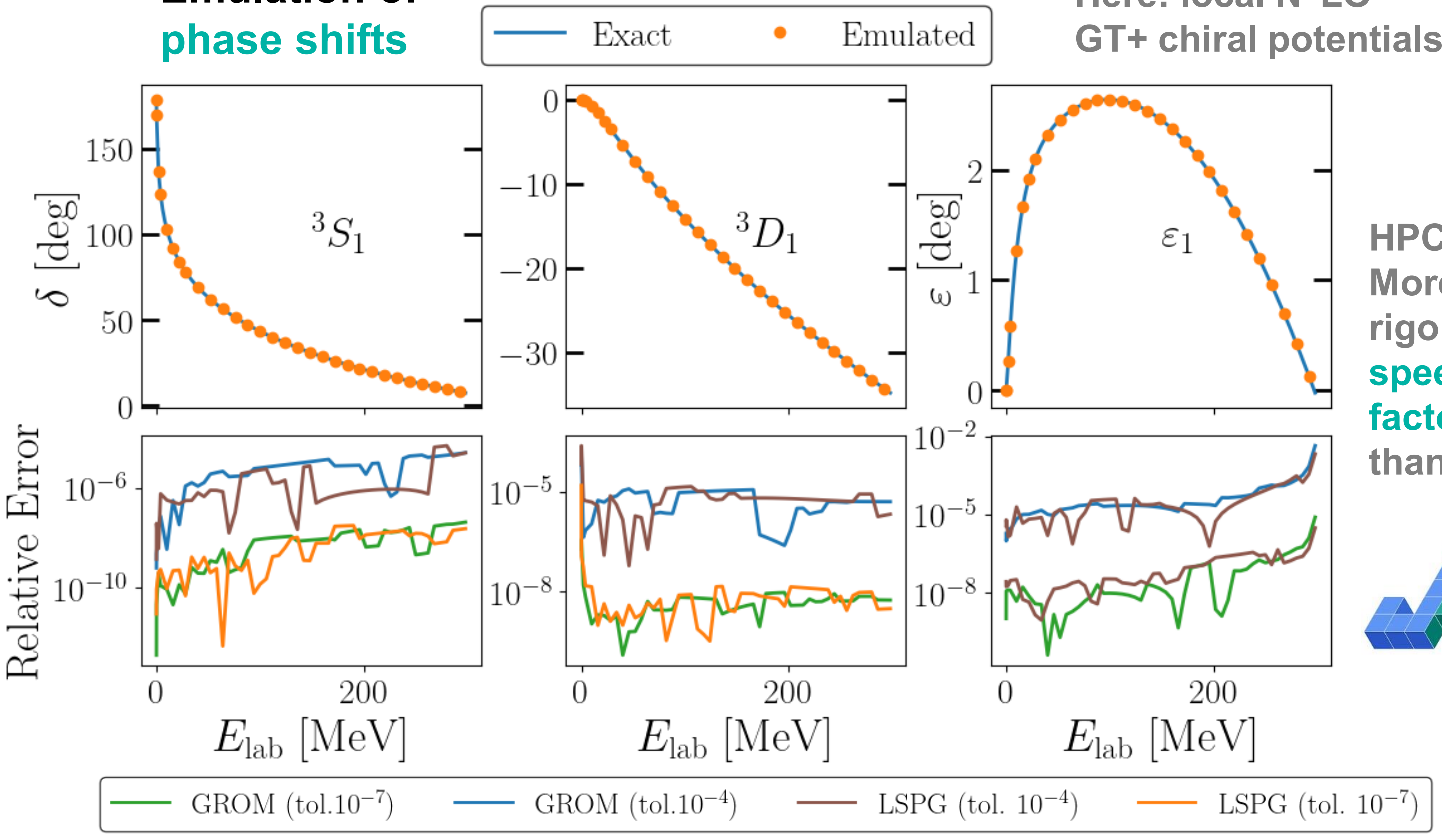
Proof of principle: Bayesian calibration of chiral NN potentials (including emulator errors)

C_S, C_T,
C_1, C_2, C_3, C_4, C_5, C_6, C_7

Emulation of total cross sections

Preliminary results!

Emulation of phase shifts



Here: local N^{2}LO GT+ chiral potentials

HPC: More rigorous speed-up factors thanks to

N-d scattering emulator

Gnech, Zhang, Drischler, Furnstahl et al,, arXiv:2511.01844 and arXiv:2511.10420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Emulate **three-body scattering with greedy snapshot selection**

FOM: KVP for three-body scattering & **hyperspherical harmonics method (linear system)**

$$\mathcal{F}_{a,a'}\left[\Psi^a, \Psi^{a'}\right] \equiv \mathcal{R}_{a,a'} - \left\langle \Psi^{a'} \middle| \hat{H} - E \middle| \Psi^a \right\rangle$$

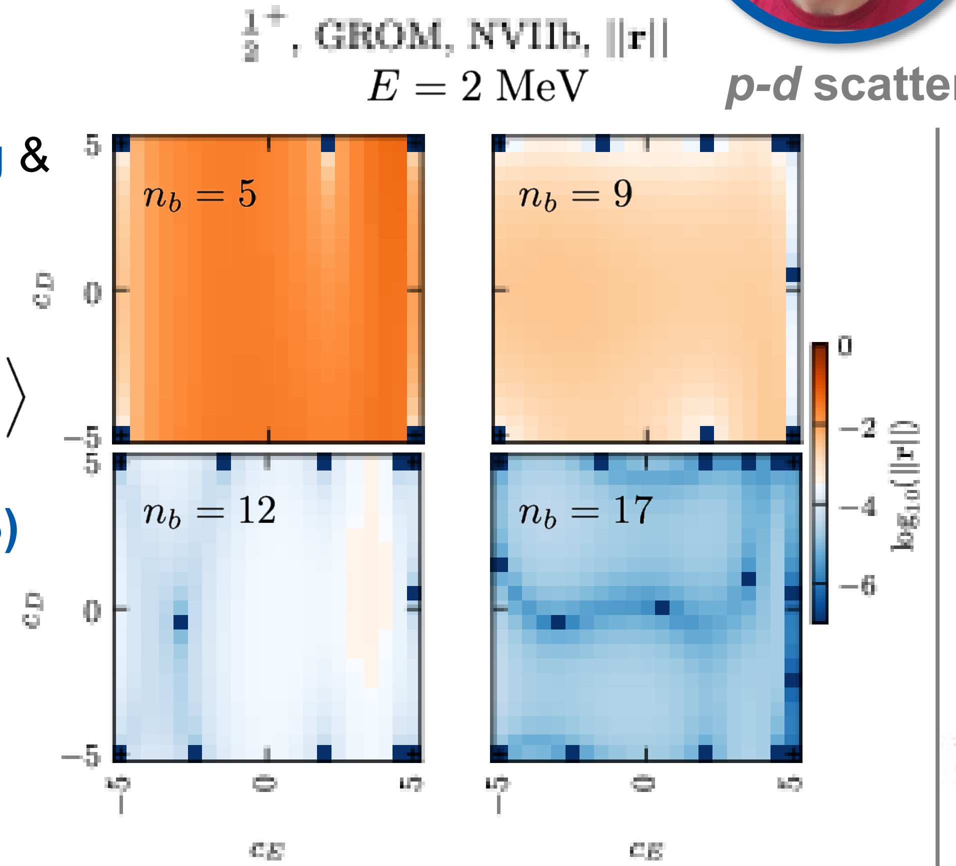
ROM: G-ROM (G) or LSPG-ROM (LS)

So far: ***N-d* scattering *below* the deuteron break-up threshold** with

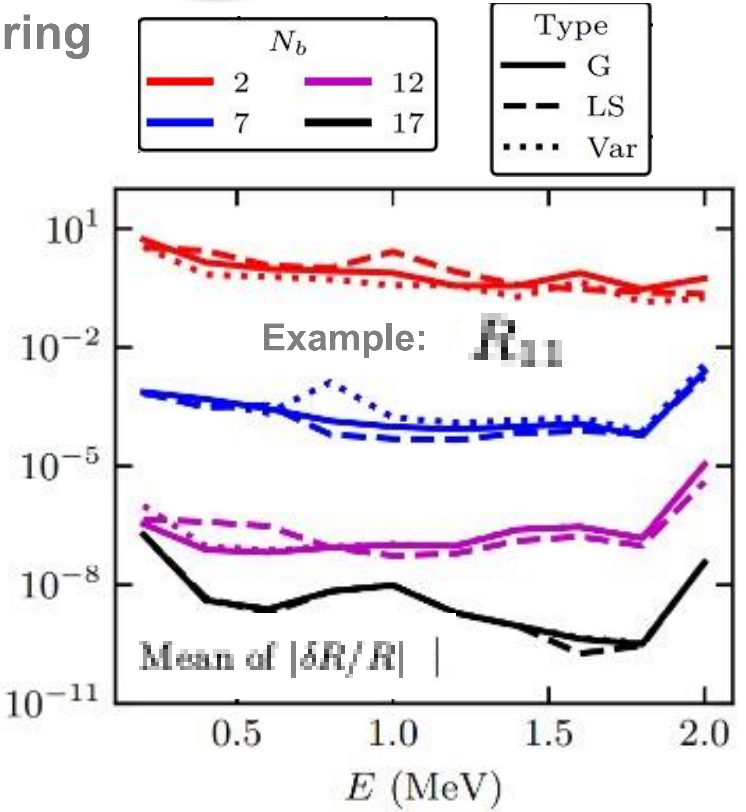
- fixed N^{3}LO NN potential (Norfolk)
- N^{2}LO **3N interactions (c_D, c_E)**

$$|\Psi^a\rangle = \sum_{\xi=1}^{N_A} c_\xi^a |\xi\rangle + \sum_{a'} \left(\delta_{a,a'}|\Omega_{a'}^R\rangle + \mathcal{R}_{a,a'}|\Omega_{a'}^I\rangle\right)$$

FOM trial wave function $a = \{L, S\}$



***p-d* scattering**

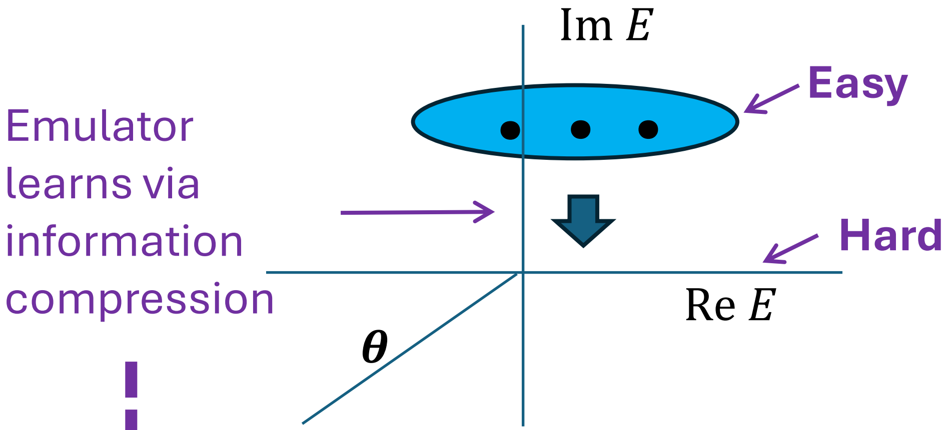


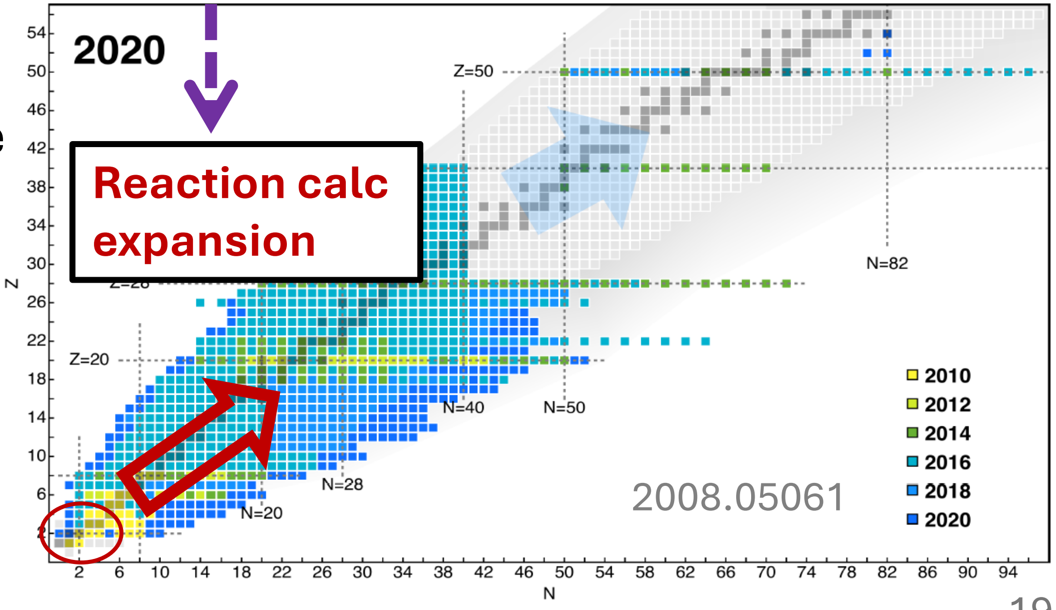
Greedy algorithm: systematic reduction of emulator errors

Needed: extension to cross sections and higher energies is critical for **Bayesian calibration** of chiral 3N interactions

Machine Learning Nuclear Reactions from Imaginary Domain

- Nuclear reaction calculation at complex (imaginary) energy E is similar to bound-state calculation.
- Numerically, it is much easier than its real-E counter part.
- But we need results at real E.
- Emulator learns real-E reaction from easier bound-state-like calculations → expanding reaction calc. in nuclear chart
- Such learning process can be further emulated in the space of other parameters $\boldsymbol{\theta}$ → easy access to the calculations
- Two papers in joint publication at *Physical Review Letters* and *Physical Review C*: Xilin Zhang, 2408.03309, 2411.06712

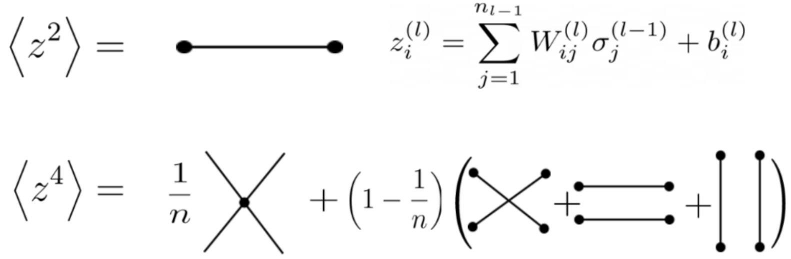




Artificial Neural Network Field Theory for Nuclear Physics

S. Sundberg and R.J. Furnstahl, J. Phys. G (2025, in press)

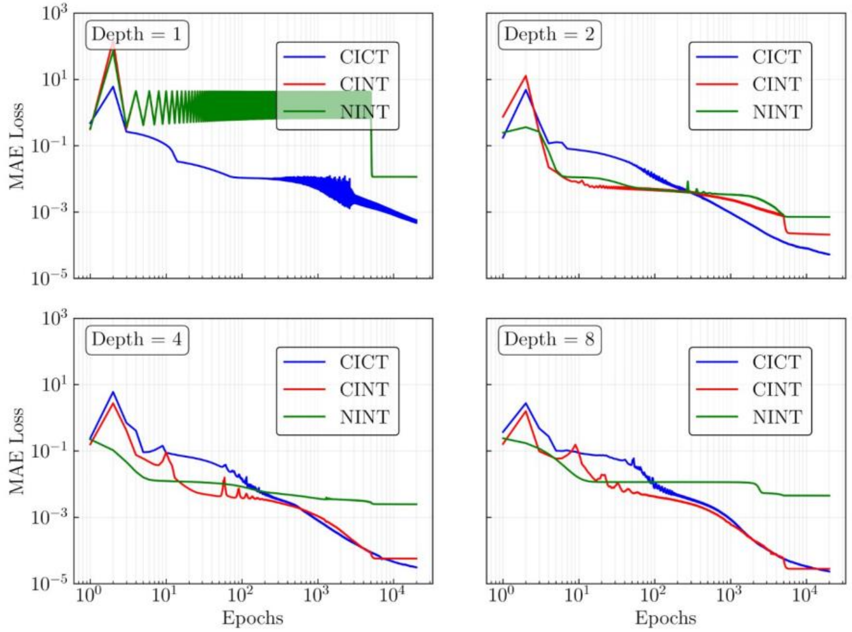
Analogous to path-integral calculations, ANNFT makes tools from Quantum Field Theory applicable to analyzing networks.

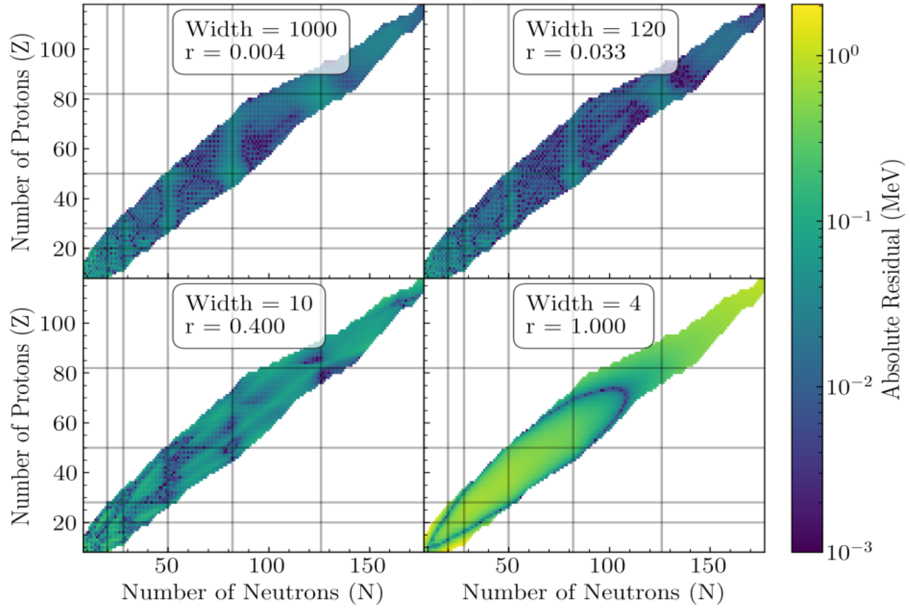


$$z_i^{(l)} = \sum_{j=1}^{n_{l-1}} W_{ij}^{(l)} \sigma_j^{(l-1)} + b_i^{(l)}$$

$$\underbrace{\int d\theta\, P(\theta)\, e^{\int d^dx\, J(x) f(x)}}_{\text{parameter space}} \Longrightarrow Z[J] = \left\langle e^{\int d^dx\, J(x) f(x)} \right\rangle \Longleftarrow \underbrace{\int \mathcal{D}f\, e^{-S[f] + \int d^dx\, J(x) f(x)}}_{\text{function space}}$$

- Artificial Neural Network Field Theory (ANNFT) offers a way of looking inside the black box of neural network behavior.
- Specific values of the initialization and training hyperparameters tune networks to criticality.
- Tuning a network to criticality results stable, understandable networks that offer explanations for common successes and failures in neural networks





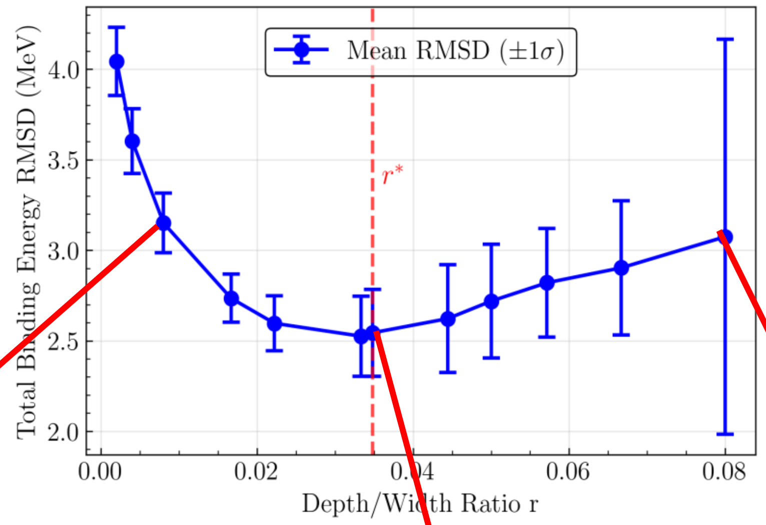
Builds on Roberts, Yaida, Hanin, arXiv:2106.10165 (2021)

ANNFT informed networks (Blue Line) have better loss values than uninformed (Green Line). BE Networks have lower RMSD values.

Gives tools for understanding what choices of network features result in the best learning.

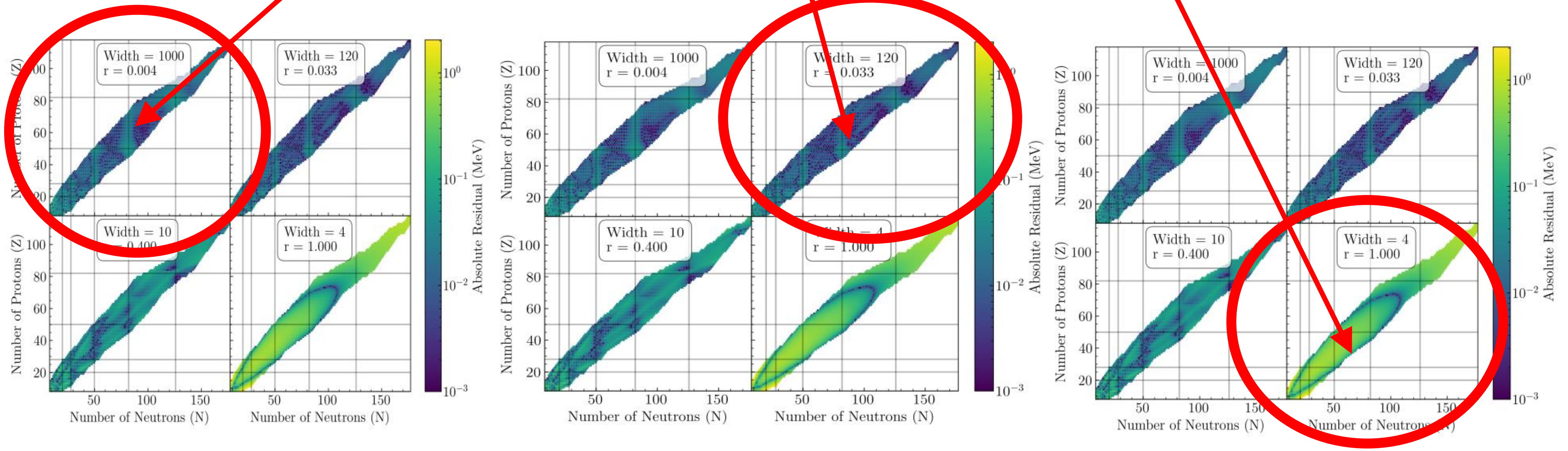
Artificial Neural Network Field Theory for Nuclear Physics

S. Sundberg and R.J. Furnstahl, J. Phys. G (2025, in press)



When tuned to criticality, different regimes of learning appear that are governed by the ratio of depth to width *r*.

To make ANNFT calculations tractable, r should be set to an optimal value *r**



As *r*→0, interactions are turned off, and learning features are lost

For *r* near *r**, interactions are perturbative and features are learned best

As *r* approaches values ≤1, neuron interactions become nonperturbative, and learning is impossible

HYPERNUCLEI WITH NQS

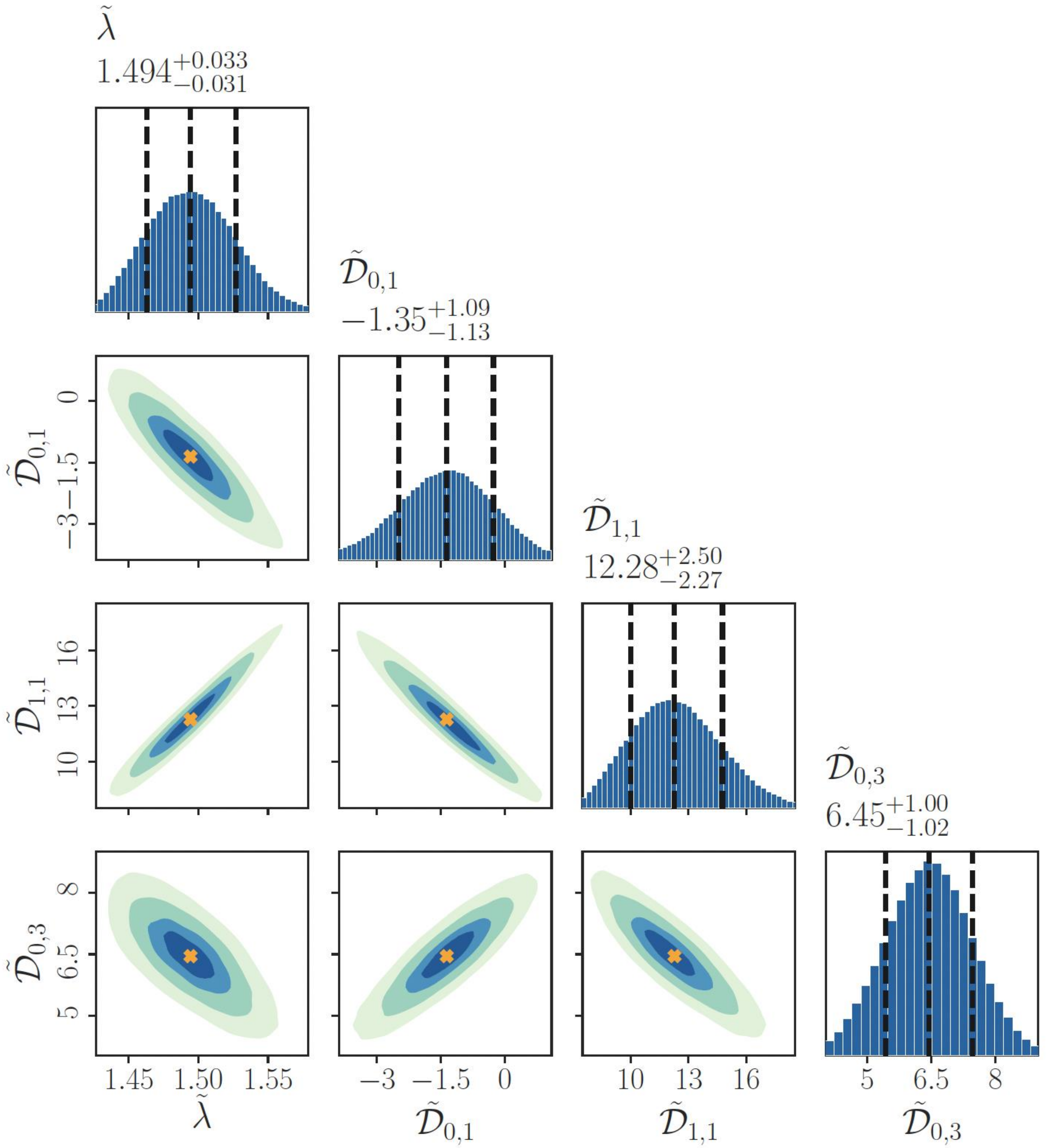
Goal: ab-initio description of hypernuclei with quantified uncertainties

Method: combine gaussian process emulators with neural network quantum states

Results: joint distributions of the LECs (in MeV) and cutoff (in fm⁻¹) entering the three-body NNΛ potential.

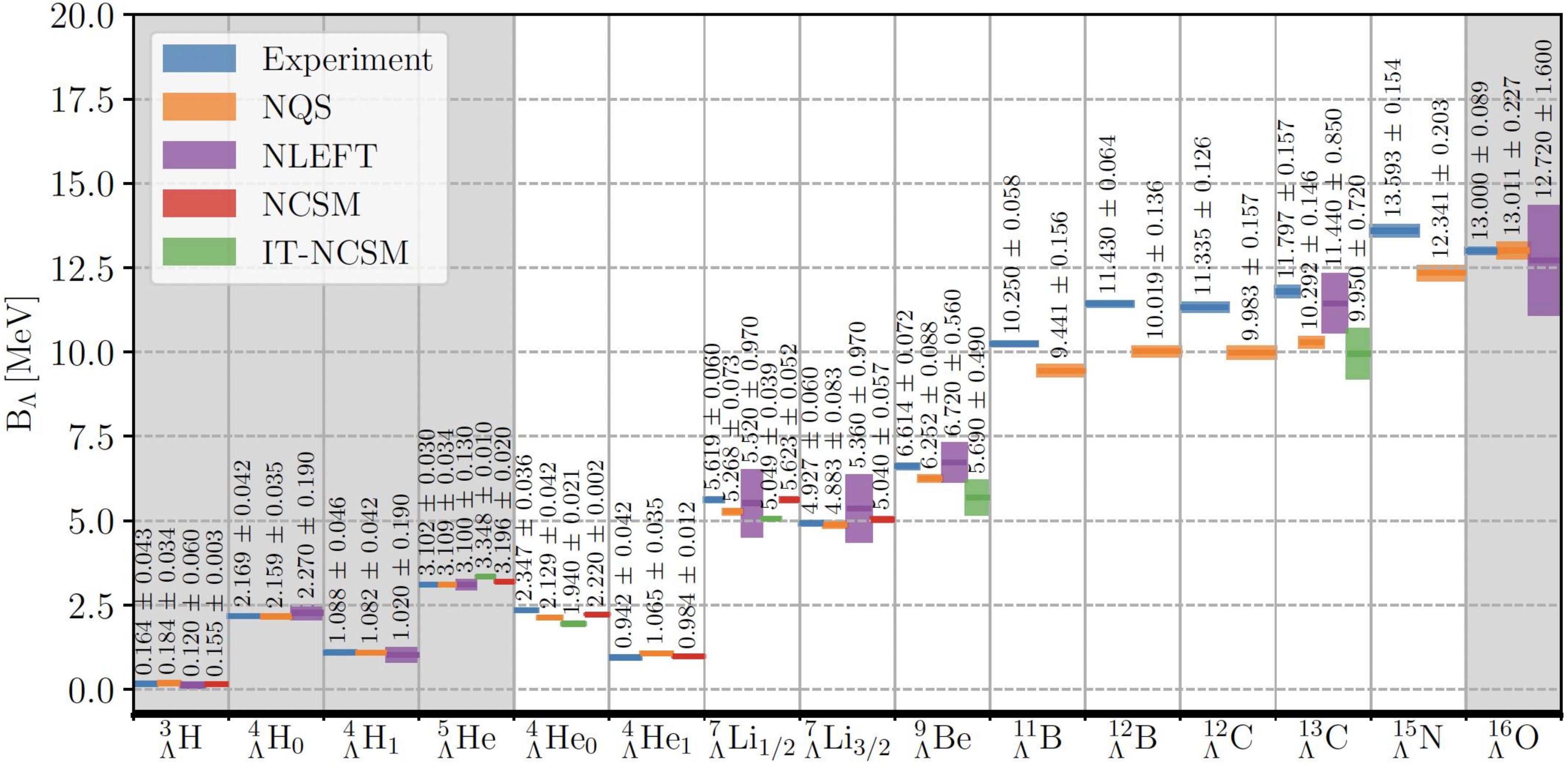
Publication: arXiv:2507.16994 [nucl-th]: (submitted to PRR)

Streamline: A. Lovato (Argonne)
Collaborators: A. Di Donna, F. Pederiva (University of Trento, Italy)



HYPERNUCLEI WITH NQS

Results: excellent agreement with experiments; residual differences likely to be solved including sub-leading contributions in the Hamiltonian



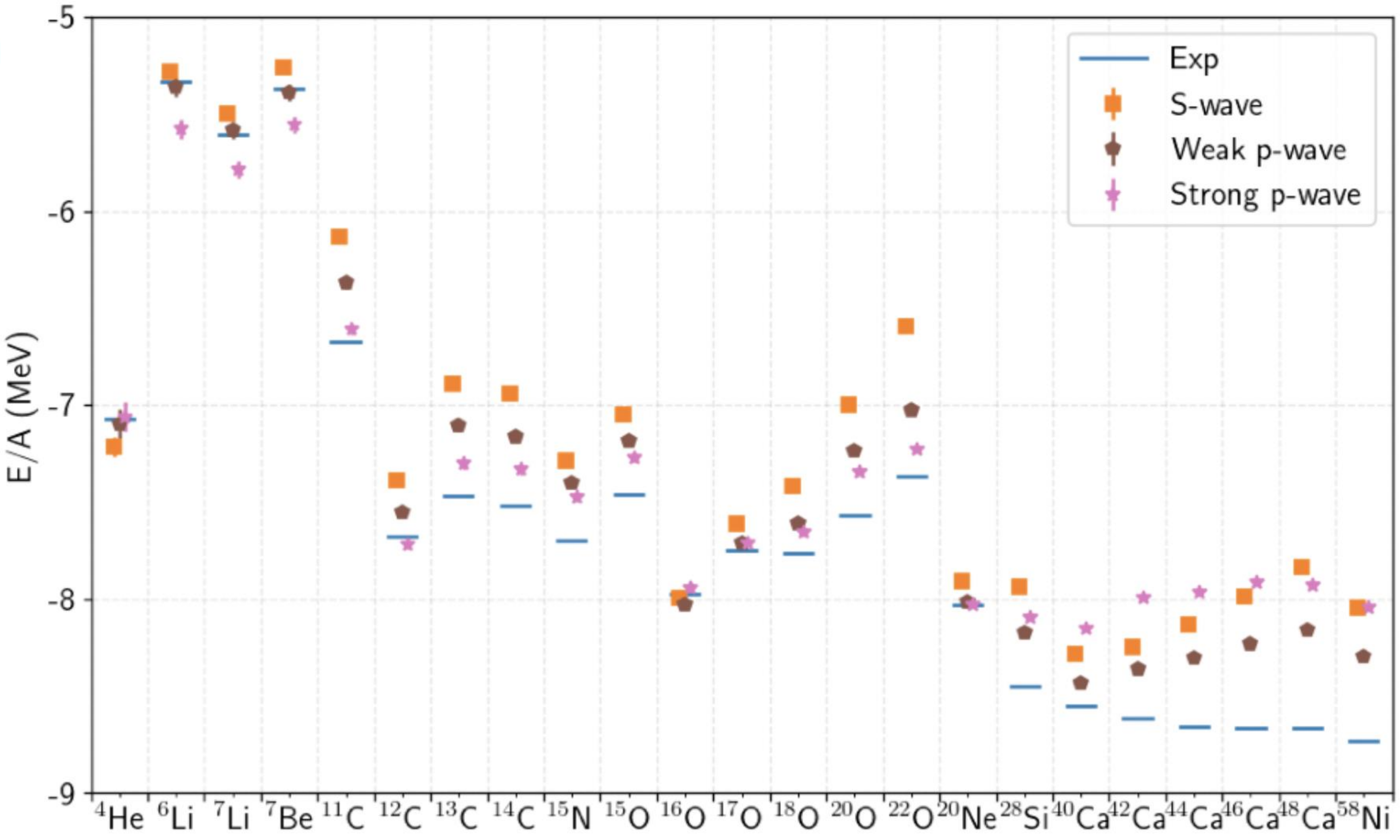
NEURAL WAVE FUNCTION FOR A=40 NUCLEI

Goal: develop a neural wave function to model A=40 nuclei and beyond.

Method: neural Pfaffian ansatz with message-passing neural backflow.

Results: computed ground-state energies and radii for medium-mass nuclei using different interactions (including p-waves).

Streamline: A. Lovato (Argonne), J. Kim (Ohio)
Collaborators: B. Fore (Argonne)



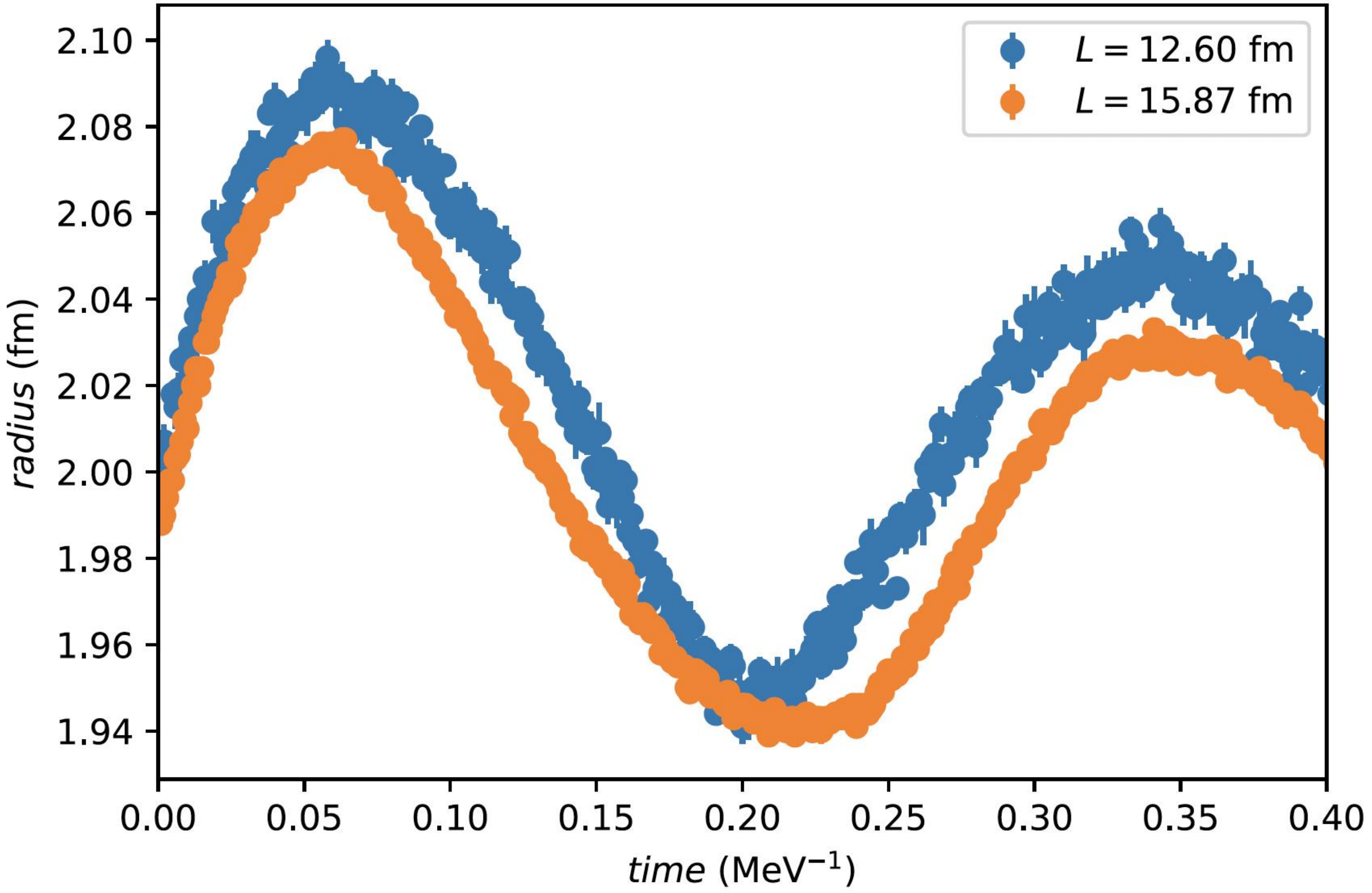
REAL-TIME NUCLEAR DYNAMIC WITH NQS

Goal: compute the quantum real-time dynamics of atomic nuclei.

Method: combine neural quantum states with time-dependent VMC

Results: computed the real-time dynamics of ^{4}He induced by a monopole excitation using periodic-box boundary conditions.

Streamline: A. Lovato (Argonne), N. Rocco (Fermilab), Kyle Godbey (MSU)

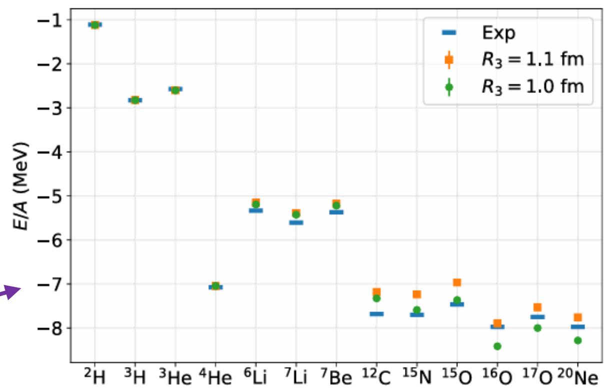


Computing Nuclear Response Function via the Neural-network Quantum State (NQS) method

- NQS: a scientific computing method for quantum many-body studies
- One frontier: computing many-body scattering and reactions
- STREAMLINE members actively developing nuclear NQS
- STREAMLINE project: first NQS computation of nuclear response functions

$$\boxed{\Psi \approx \Psi_{NQS}}$$

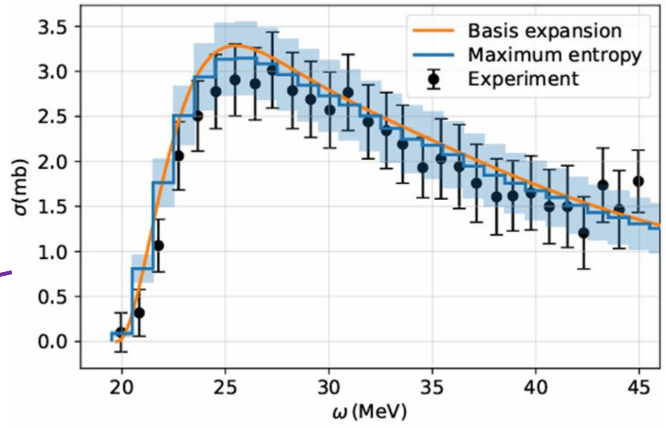
Nuclear ground state



A. Gnech, B. Fore, A. J. Tropiano, and **A. Lovato**, PRL 133, 142501 (2024)

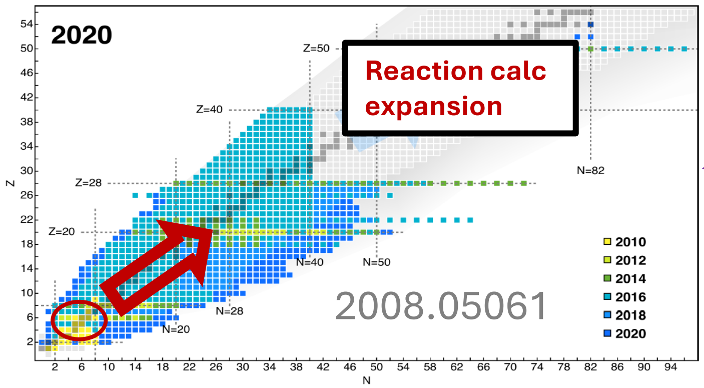
Nuclear continuum state

Photo-disintegration of ^{4}He



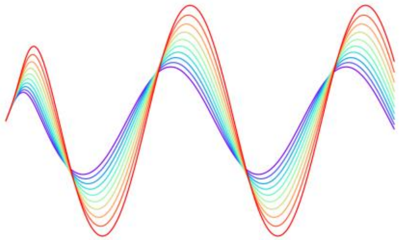
E. Parnes, N. Barnea, G. Carleo, **A. Lovato, N. Rocco and X. Zhang**, arXiv 2504.20195

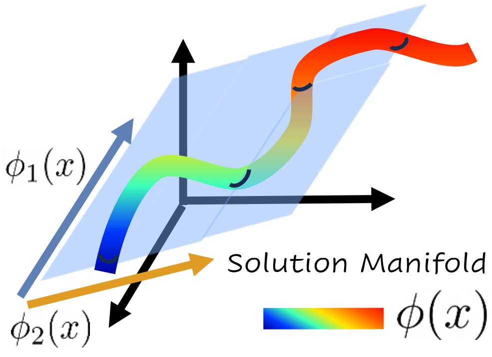
Future!



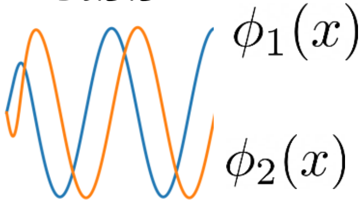
Dimensionality Reduction

Finite element





Reduced Basis



$$\mathcal{H}\phi = E\phi$$

Operator

$$\begin{tikzcd}
\phi(x) \arrow[r, "\mathcal{H}"] \arrow[d, "\text{Compression}"'] & \mathcal{H}\phi(x) \\
\hat{\phi}(x) \arrow[r, "\hat{\mathcal{H}}"] & \hat{\mathcal{H}}\hat{\phi}(x)
\end{tikzcd}$$

$$\langle \phi_j | \mathcal{H} - E | \hat{\phi} \rangle = 0$$

[Galerkin Projection]

$$= \phi_0 + \sum_{k}^{n} a_k \phi_k(x)$$

P. Giuliani

Challenge

1) Because operators are challenging

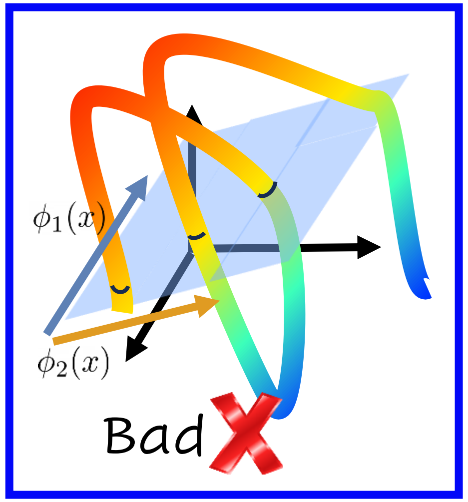
The Woods-Saxon function is defined as

$$f_{\mathrm{WS}}(r, R, a) = \left[1 + \exp\left(\frac{r-R}{a}\right)\right]^{-1}.$$

$\mathcal{H}\phi = E\phi$

Operator

2) Because linear embedding is not good



$\phi(x)$ $\xrightarrow{\mathcal{H}}$ $\mathcal{H}\phi(x)$

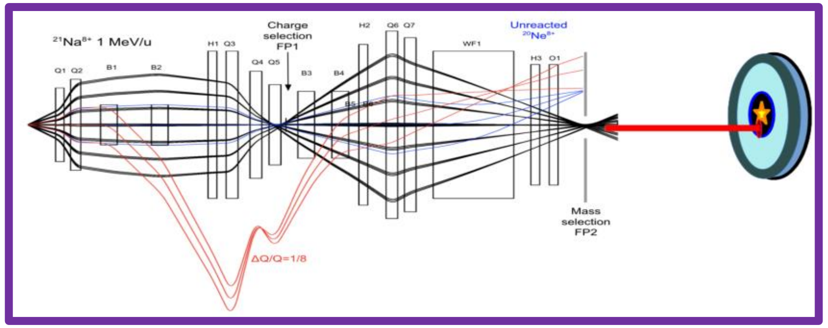
compression

$$\langle \phi_j | \mathcal{H} - E | \hat{\phi} \rangle = 0$$

Galerkin Projection

What if this is **a problem?**

$\hat{\mathcal{H}}$ $\rightarrow$ $\hat{\mathcal{H}}\hat{\phi}(x)$

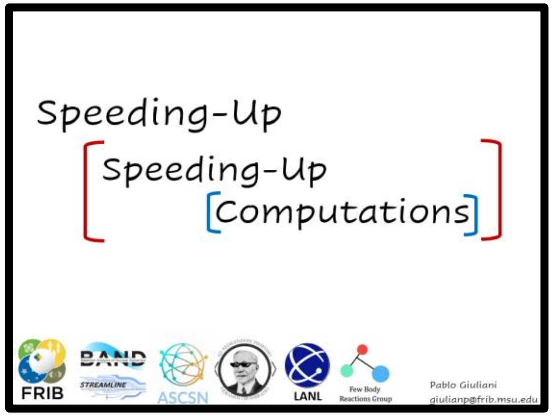


(experimental control)

3) Because there are no equations to project

Solution: Operator Learning

[Pablo talking for an hour on this]()



$$\phi(x) \xrightarrow{\mathcal{H}} \mathcal{H}\phi(x)$$

compression

$$\cancel{\langle \phi_j | \mathcal{H} - E | \hat{\phi} \rangle = 0}$$

~~Galerkin Projection~~

$$\hat{\phi}(x) \xrightarrow{\hat{\mathcal{H}}} \hat{\mathcal{H}}\hat{\phi}(x)$$

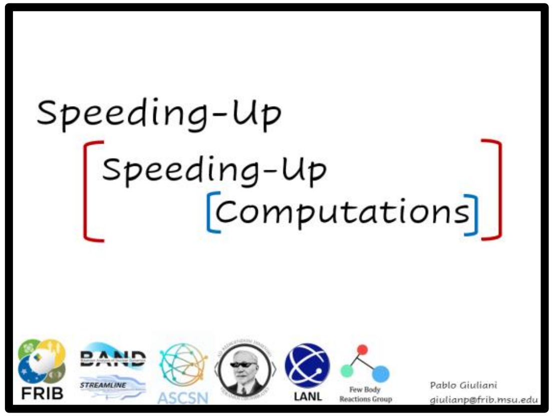
Fit from data inspired by original equations structure

First results show:

- Very easy to set up
- As fast as and more accurate than Galerkin

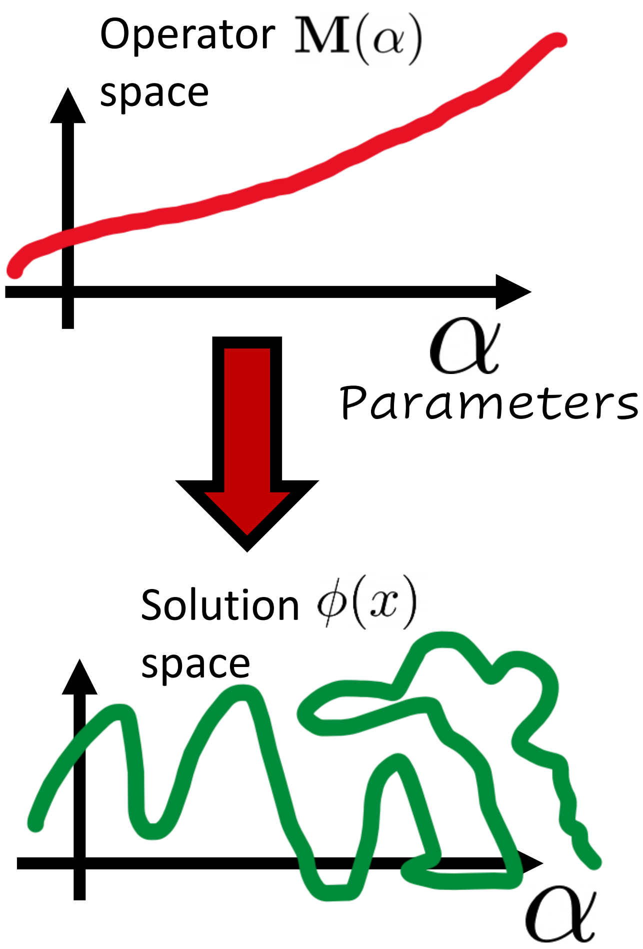
Scientific pipelines

[Pablo talking for an hour on this]



Ideal for STREAMLINING producing emulators for nuclear physics

STREAMLINE
SmarT Reduction and Emulation Applying Machine Learning In Nuclear Environments



Symbolic Regression for Model Discovery

Charge densities are not just proton densities but are close in comparison. **Symbolic regression** is a machine learning method that provides an **explainable AI framework**. These methods give **explicit expressions which can be directly scrutinized** as opposed to other closed-form methods (neural networks, Gaussian processes, etc.).

Once discovered, these expressions open avenues of exploration in the realm of **model emulation, model discovery,** and **direct comparison to experimental data.**.

At MSU, we have tested the method to discover closed form corrections to nuclear charge densities and are currently developing a framework for **data-driven discovery of novel energy density functionals**.

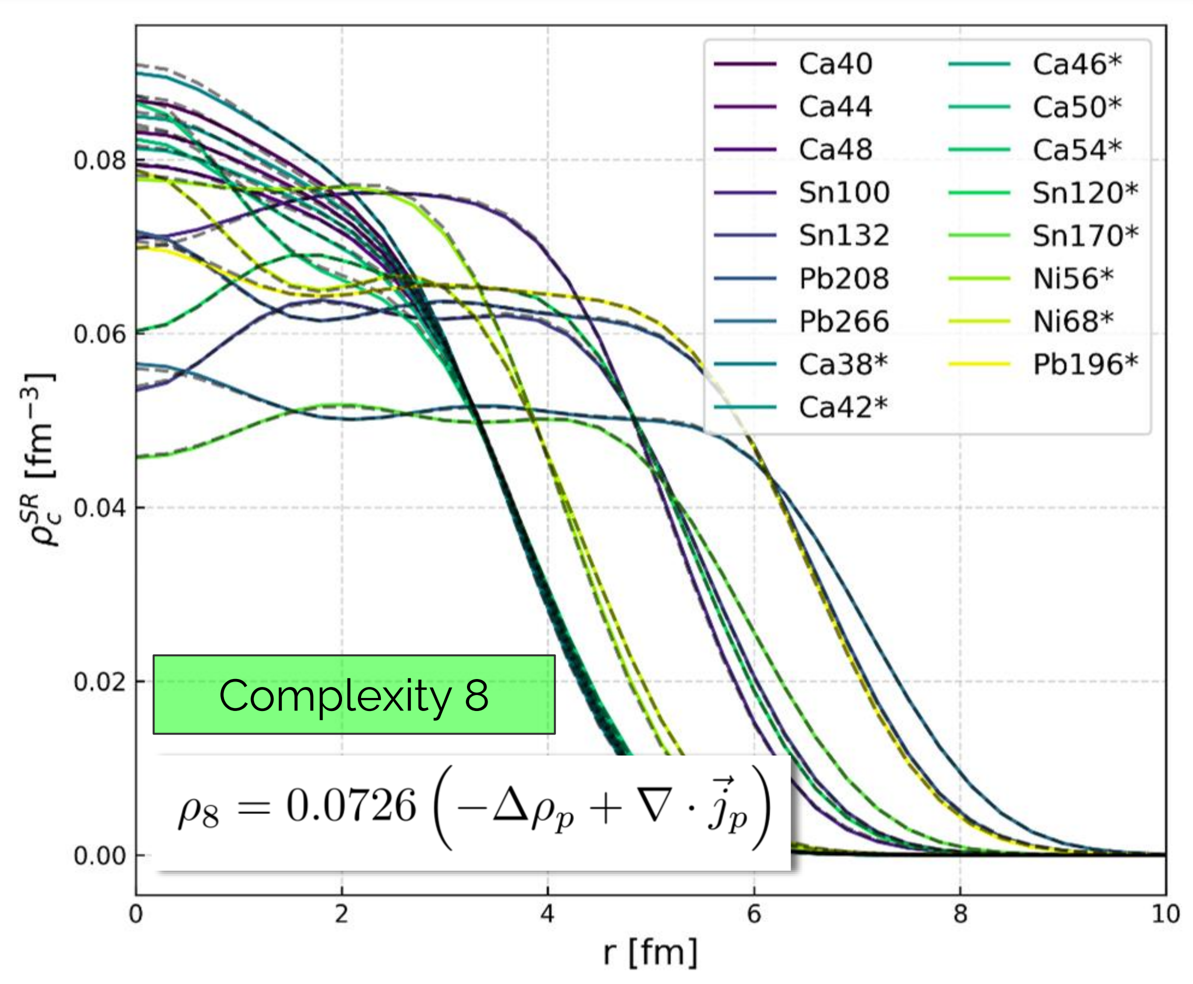
Josh Belieu

with
Kyle Godbey
and
Witek Nazarewicz

Discovering Charge Densities and Radii Corrections

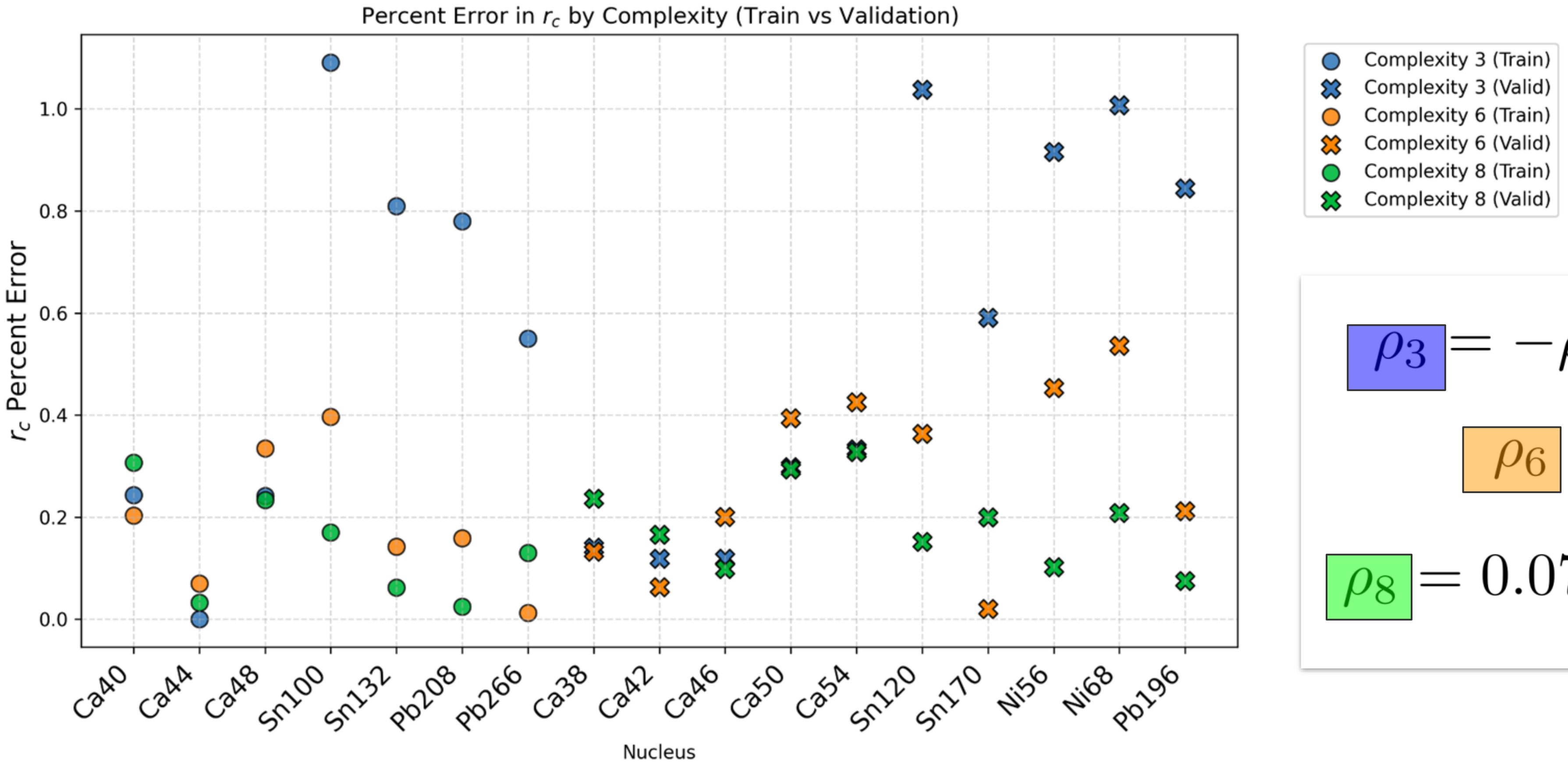
Complexity is a **measure of how complex an expression** is where variables and operations have a complexity of one. **A symbolic regression expression** (misc. colored-solid) with a complexity of 8 is able to **recreate target data** (black-dashed) quite **reliably**.

Validation nuclei are marked with asterisks, training nuclei are unmarked. Training data was generated using SLy4 functional.



Discovering Charge Densities and Radii Corrections

Relatively low complexity expressions give **sub 1% error** in predicted charge radius.

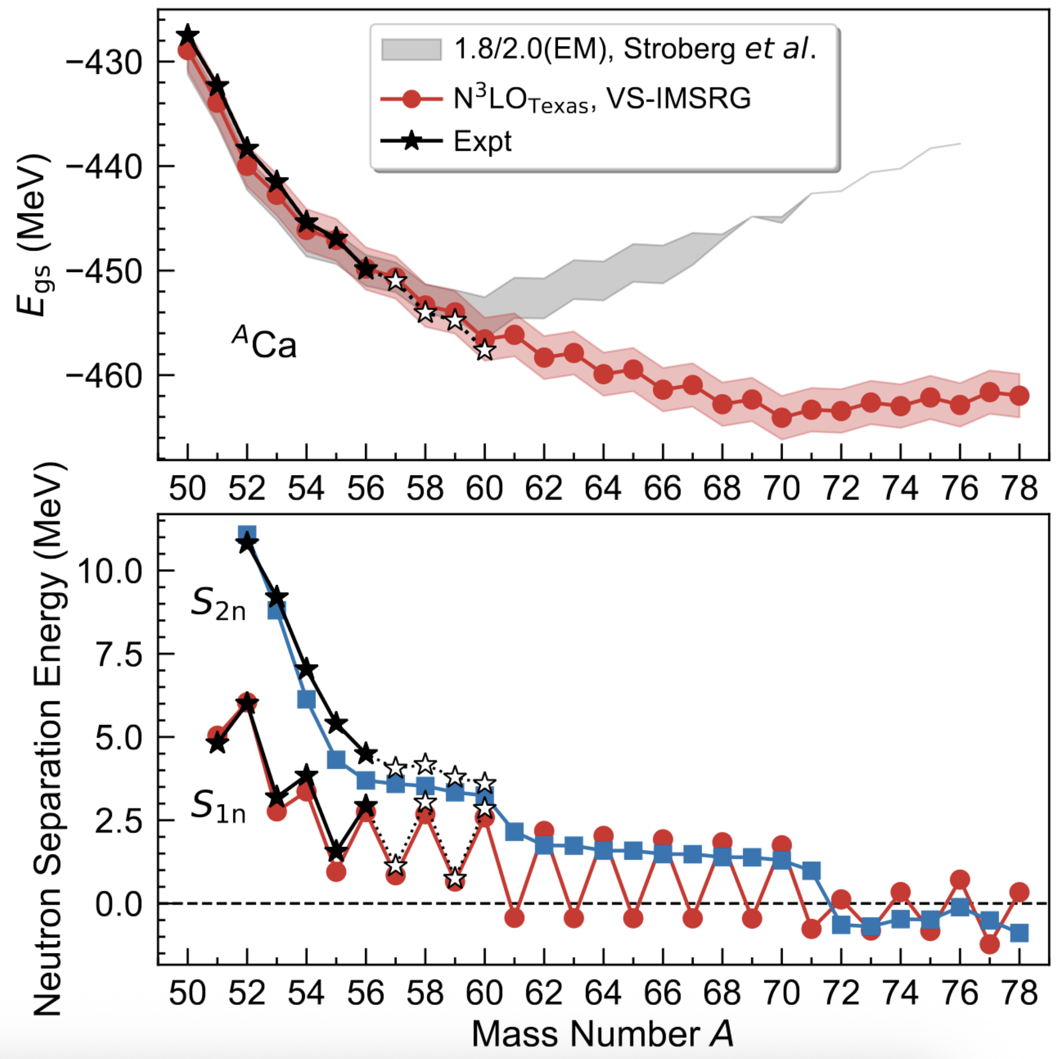


$$\rho_3 = -\rho_p \Delta \rho_p - 7.39 \cdot 10^{-7}$$

$$\rho_6 = -0.0768 \Delta \rho_p$$

$$\rho_8 = 0.0726 \left(-\Delta \rho_p + \nabla \cdot \vec{j}_p \right)$$

Emulators were key in the development of a new interaction from chiral effective field theory



The challenge:

- Ab initio computation found that ^{60}Ca is the most neutron-rich nucleus that the strong force can bind. This is at odds with experimental trends and results from energy density functionals
- Uncertainties in such ab initio computations are large
- Clearly, we need to develop more accurate and precise nuclear interactions

Solution:

- Use reduced-order models ("emulators") to adjust the low-energy coefficients of a new interaction with N^{3}LO terms; this is N^{3}LO$_{\text{Texas}}$

Results:

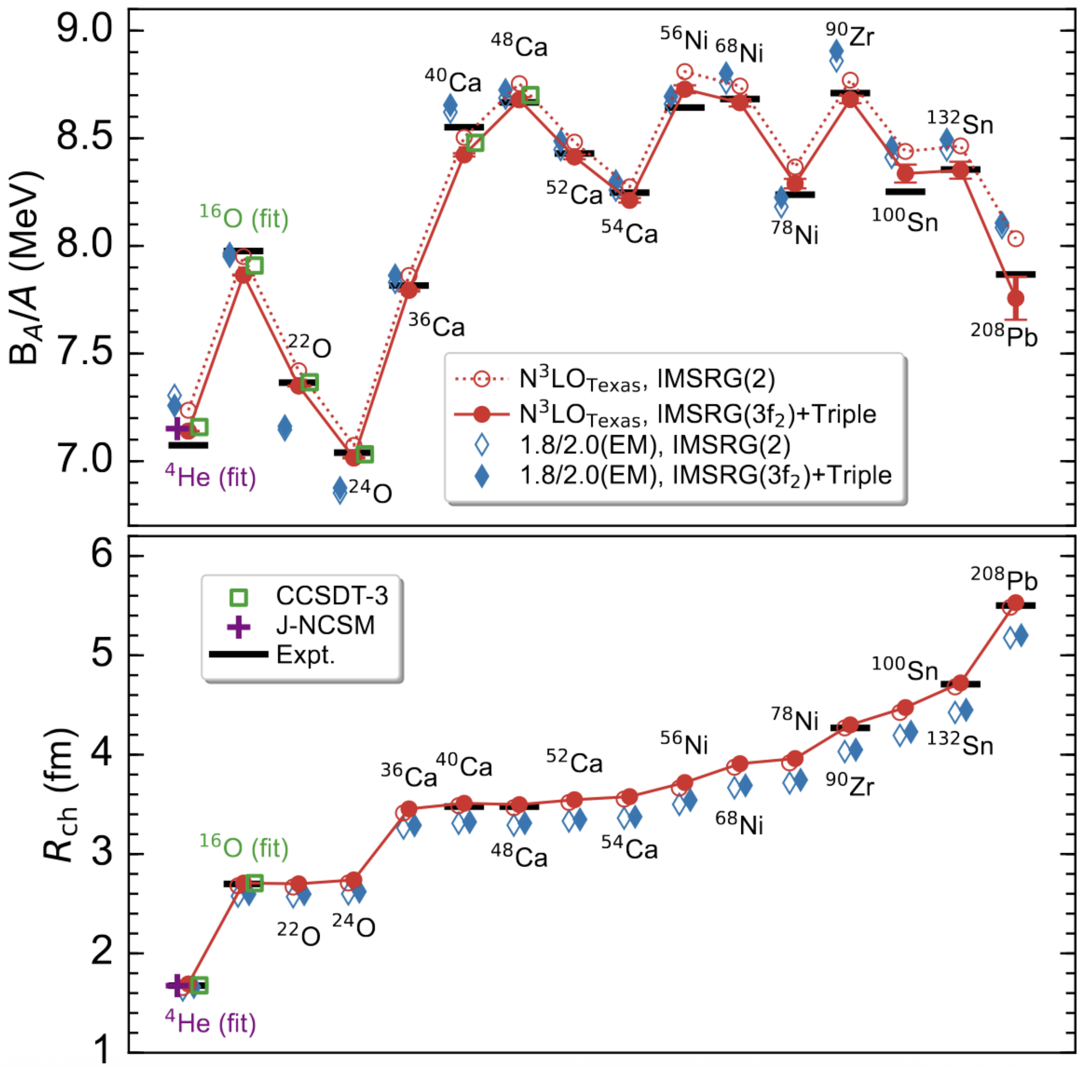
- Calcium isotopes nuclei are now predicted bound
- Top fig.: ground-state energies of calcium nuclei
- Bottom fig.: neutron separation energies

Baishan Hu, A. Ekström, C. Forssén, G. Hagen, W. G. Jiang, T. Miyagi, T. Papenbrock, in preparation

Emulators were key in the development of a new interaction from chiral effective field theory

Results (cont'd):

- Binding energies are accurate for light to heavy nuclei (see top figure)
- Charge radii are accurate for light to heavy nuclei (see bottom figure)



Summary:

- The new interaction N^{3}LO$_{\text{Texas}}$ exhibits accurate saturation properties across the nuclear chart.
- Usage of N^{3}LO terms in the nucleon-nucleon crucial
- This moves the neutron dripline in calcium to about ^{70}Ca.

Baishan Hu, A. Ekström, C. Forssén, G. Hagen, W. G. Jiang, T. Miyagi, T. Papenbrock, in preparation

Parametric matrix models (PMM)

nature communications

Article https://doi.org/10.1038/s41467-025-61362-4

Parametric matrix models

Received: 27 January 2025

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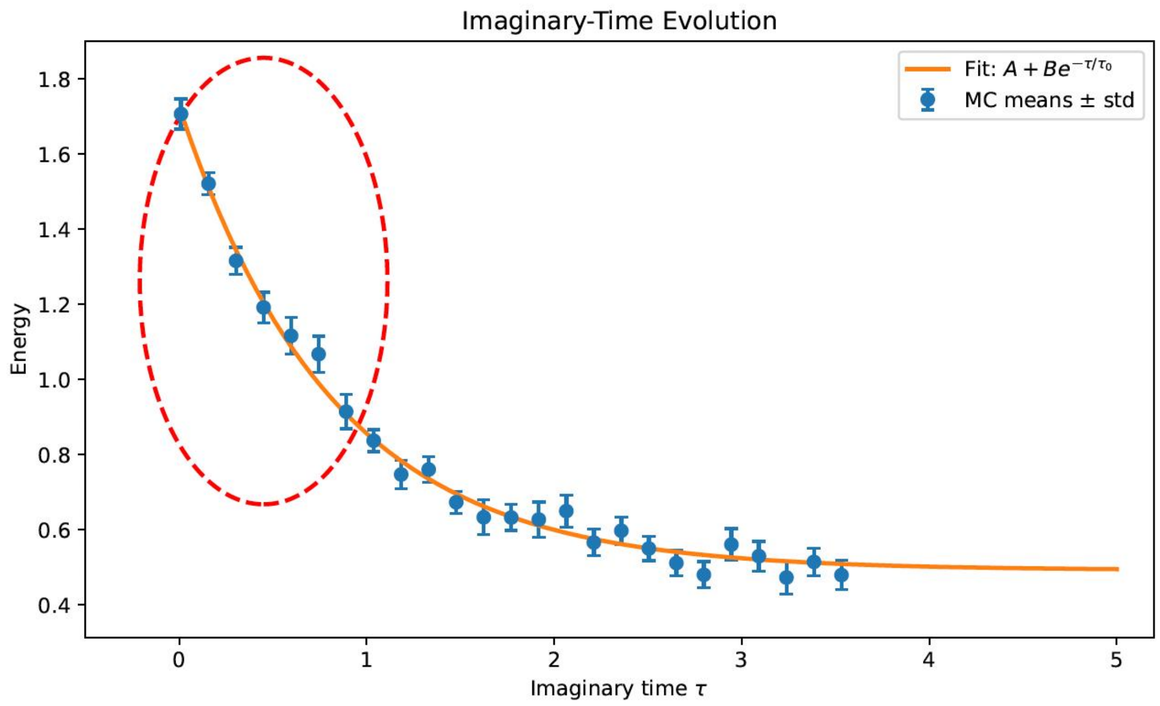
Patrick Cook

Danny Jammooa



$$E(\tau) = \frac{|c_0|^2 E_0 e^{-2E_0\tau/\hbar} + |c_1|^2 E_1 e^{-2E_1\tau/\hbar} + |c_2|^2 E_2 e^{-2E_2\tau/\hbar} + \cdots}{|c_0|^2 e^{-2E_0\tau/\hbar} + |c_1|^2 e^{-2E_1\tau/\hbar} + |c_2|^2 e^{-2E_2\tau/\hbar} + \cdots}$$

Danny Jammooa

Nonperturbative Ground State

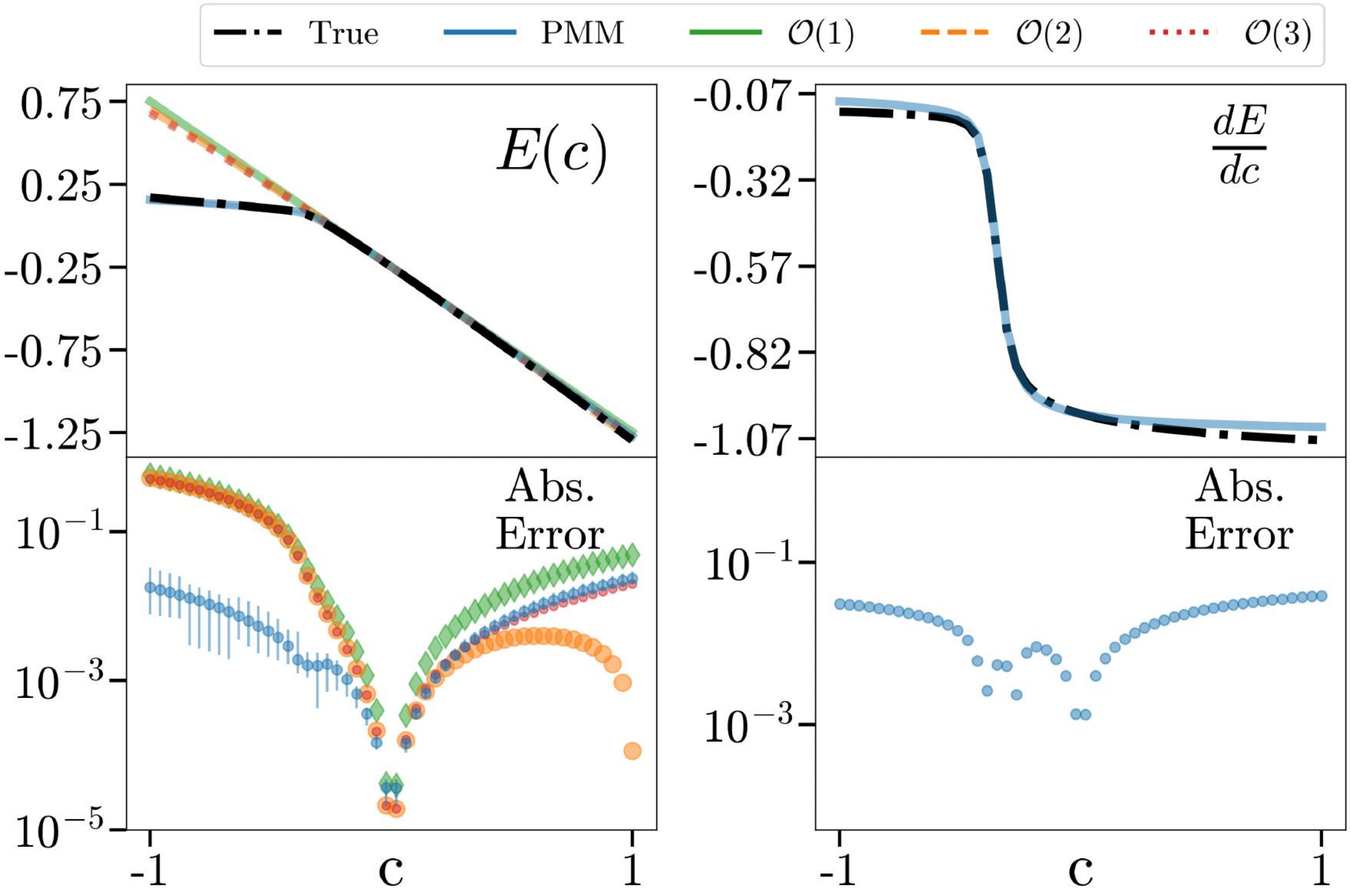
Governing Equations

$$|\psi_i(t)\rangle = e^{-H_0 t/2}|\psi_i(0)\rangle$$
$$\mathcal{M}_{ij}(t_1,t_2) = \langle\psi_i(t_1)|O|\psi_j(t_2)\rangle$$
$$O \in \{H_0, H_I, \rho, R^2\}$$

PMM Equations

$$|\phi_i(t)\rangle = e^{-\underline{M_0} t/2}|\underline{\phi_i}(0)\rangle$$
$$\hat{\mathcal{M}}_{ij}(t_1,t_2) = \langle\phi_i(t_1)|\Delta|\phi_j(t_2)\rangle$$
$$\Delta \in \{\underline{M_0}, \underline{M_I}, \underline{p}, \underline{r}\}$$

- Once PMM is trained on data only as a function of t, can it predict the ground-state energy of $H(c)$ and the expectation of other observables for any c?



True
PMM
$\mathcal{O}(1)$
$\mathcal{O}(2)$
$\mathcal{O}(3)$
$E(c)$
0.75
0.25
-0.25
-0.75
-1.25
$\frac{dE}{dc}$
-0.07
-0.32
-0.57
-0.82
-1.07
Abs. Error
10^{-1}
10^{-3}
10^{-5}
Abs. Error
10^{-1}
10^{-3}
-1
c
1
-1
c
1

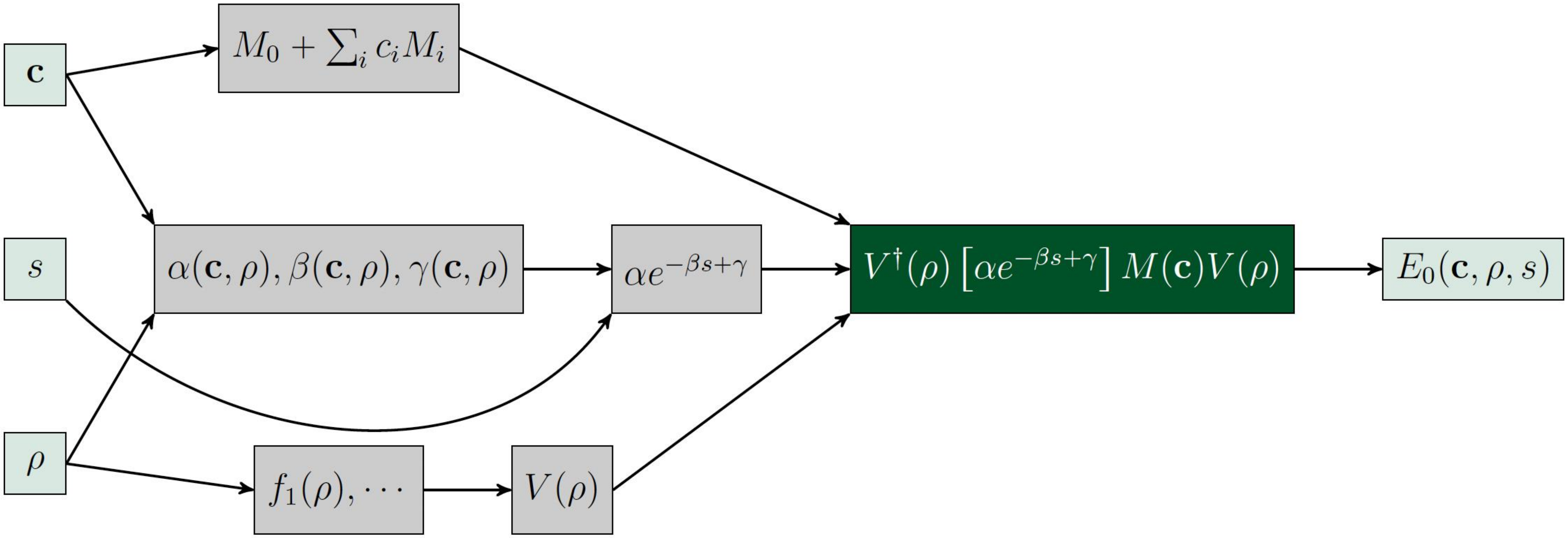
N^3LO IMSRG(2) Calculations of Symmetric Nuclear Matter

$$H(\mathbf{c}\,;\rho,s) = H_0(\rho,s) + \sum_{i=1}^{4} c_i H_i(\rho,s)$$

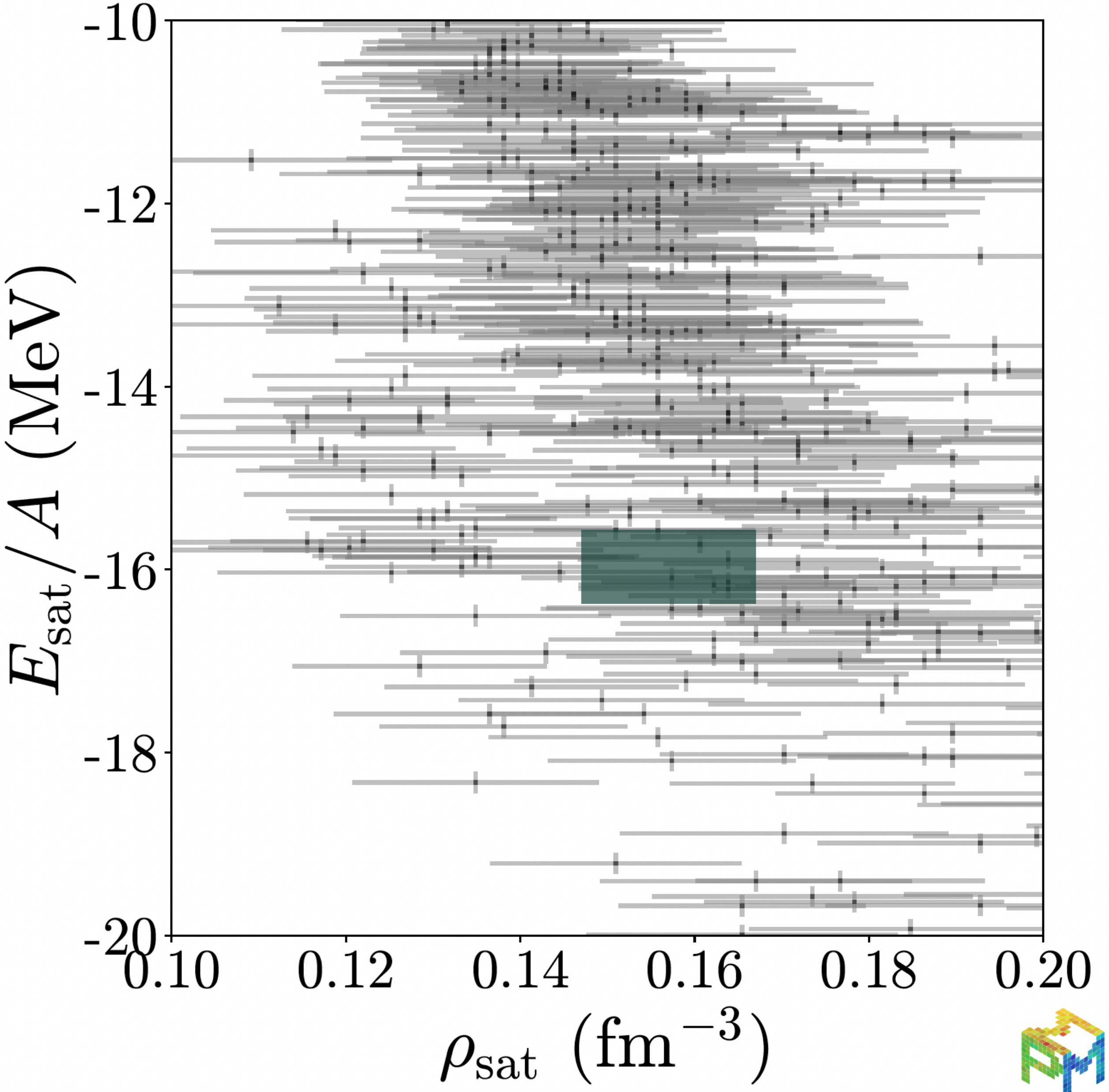
Can we calibrate the 4 LECs $\mathbf{c}$ to reproduce empirical saturation properties?

- Single calculation requires $\sim 10+$ hours on an H100
- Need to sample potentially thousands of LEC sets
- $\sim 50\%$ of flows diverge
- Unknown dependence on flow parameter s
- Basis dependence on density ρ
- Uncertainty quantification

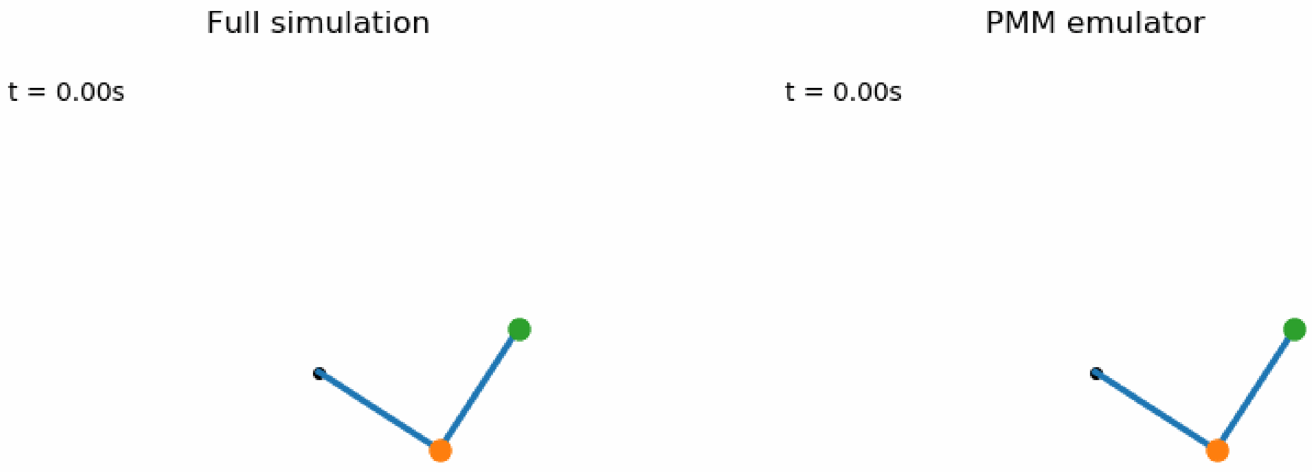
Patrick Cook


$\mathbf{c}$
$M_0 + \sum_i c_i M_i$
s
$\alpha(\mathbf{c}, \rho), \beta(\mathbf{c}, \rho), \gamma(\mathbf{c}, \rho)$
$\alpha e^{-\beta s+\gamma}$
$V^\dagger(\rho) \left[\alpha e^{-\beta s+\gamma}\right] M(\mathbf{c}) V(\rho)$
$E_0(\mathbf{c}, \rho, s)$
ρ
$f_1(\rho), \cdots$
$V(\rho)$

- Average test error ~ 0.1 MeV
- 1000 samples of LECs, ~ 22 minutes on personal PC
- < 1.5 seconds per prediction
- $\sim 10^4\times$ speedup



Double Pendulum



STREAMLINE

SmarT Reduction and Emulation Applying Machine Learning In Nuclear Environments

DOE NP AI/ML
PI Exchange Meeting
November 19 – 20, 2025

Argonne NATIONAL LABORATORY

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