STREAMLINE

SmarT Reduction and Emulation Applying Machine Learning In Nuclear Environments

DOE NP AI/ML
PI Exchange Meeting
December 4-5, 2024
Gaithersburg, MD

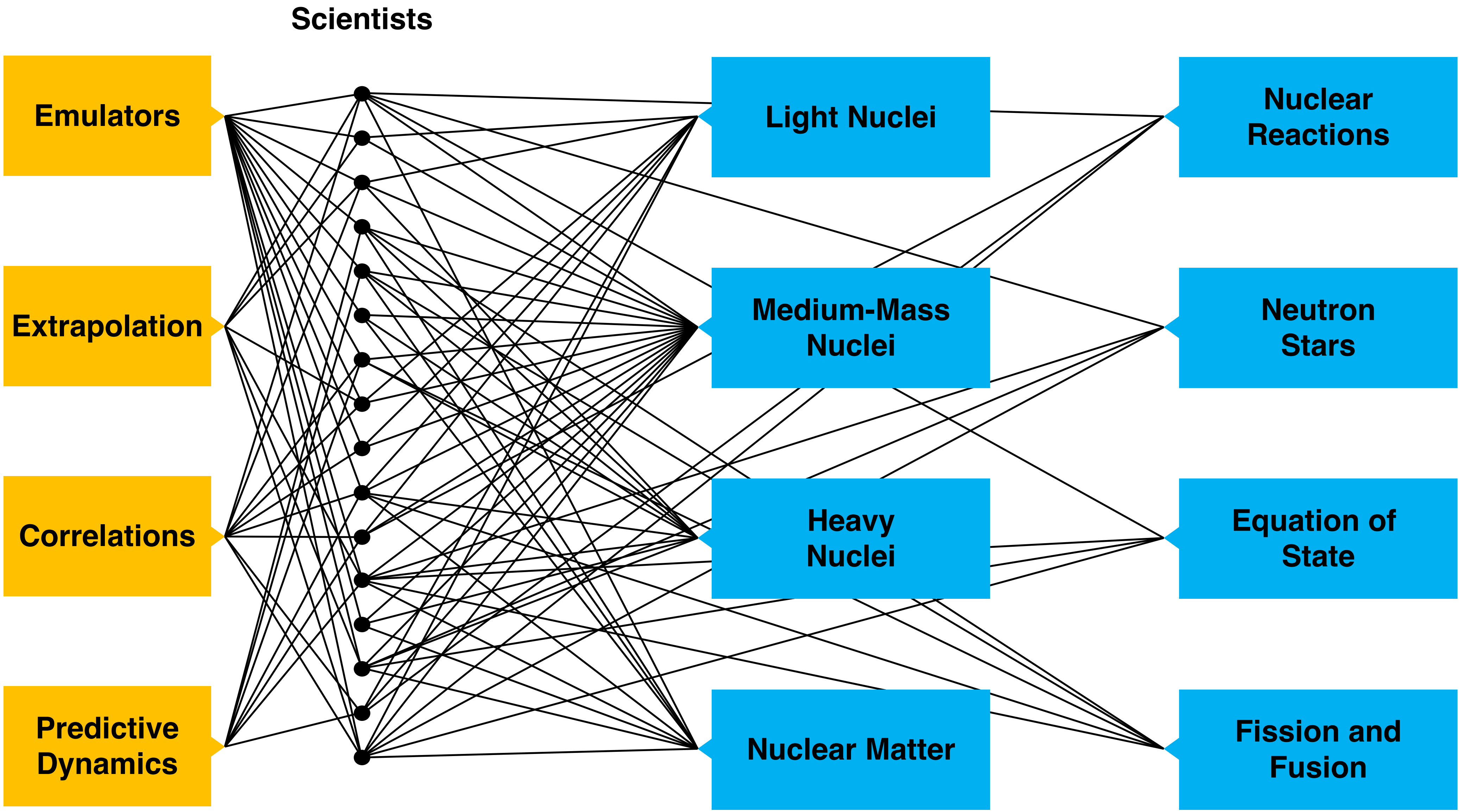
***STREAMLINE* Collaboration: Machine Learning for Nuclear Many-Body Systems**

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 will perform 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 = 13



STREAMLINE Collaboration Meeting

May 9-10, 2024, at FRIB

PROGRAM

Thursday, May 9 in FRIB 1221

8:30 - 8:45 AM	Registration	
8:45 - 8:50 AM	Thomas Glasmacher (FRIB Director)	Welcome to FRIB
9:00 - 9:15 AM	Dean Lee (FRIB)	Announcements
9:15 - 9:30 AM	Manouchehr Farkhondeh (DOE Program Manager)	Q&A about AI/ML at DOE Nuclear Physics (via Zoom)
9:30 - 10:00 AM	Daniel Lay (FRIB)	Neural network emulation of spontaneous fission
10:00 - 10:30 AM	Kyle Godbey (FRIB)	Emulation Prospects For Time Dynamics
10:30 - 11:00 AM	Coffee Break	
11:00 - 11:30 AM	Chinmay Mishra (UTK)	A Nuclear Mass-Model Rooted in Chiral Effective Field Theory
11:30 - 12:00 noon	Simon Sundberg (OSU)	Criticality Analysis of Artificial Neural Networks in Nuclear Physics
12:00 - 1:30 PM	Lunch at Snyder Phillips Cafeteria	
1:30 - 2:00 PM	Danny Jammooa (FRIB)	Parametric Matrix Models for Scientific Computing
2:00 - 2:30 PM	Patrick Cook (FRIB)	Parametric Matrix Models for General Machine Learning
2:30 - 3:00 PM	Pablo Giuliani (FRIB)	Beyond projections: Learning reduced equations from data
3:00 - 3:30 PM	Coffee Break	
3:30 - 4:10 PM	Daniel Lee (Cornell Tech)	Geometry and Latent Signal Representations in Machine Learning
4:10 - 5:00 PM	Morten Hjorth-Jensen (Oslo)	Mathematics of discriminative and generative deep learning, from deep neural networks to diffusion models
5:00 - 5:30 PM	Discussion	
6:00 - 8:00 PM	Dinner at Pizza House	

Friday, May 10 in FRIB 1221

8:30 - 9:00 AM	Joshua Maldonado (Ohio)	A Greedy Emulator for Nuclear Two-Body Scattering
9:00 - 9:30 AM	Christian Drischler (Ohio)	A Bayesian mixture model approach to quantifying the empirical nuclear saturation point
9:30 - 10:00 AM	Nuwan Yapa (FSU)	Emulators for Unbound Nuclei
10:00 - 10:30 AM	Coffee Break	
10:30 - 11:00 AM	Jane Kim (Ohio)	Variational methods with neural networks
11:00 - 11:30 AM	Alessandro Lovato (Argonne)	Hypernuclei with neural network quantum states
11:30 - 12:00 noon	Xiiln Zhang (FRIB)	Emulators for quantum continuum states
12:00 - 12:30 PM	Discussion	
12:30 PM	Symposium Adjourns	

STREAMLINE Collaboration Progress

On schedule: All first-year and early second year 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	151	756

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

S. König N. Yapa K. Fossez


NC STATE UNIVERSITY

FSU FLORIDA STATE UNIVERSITY

Relevance

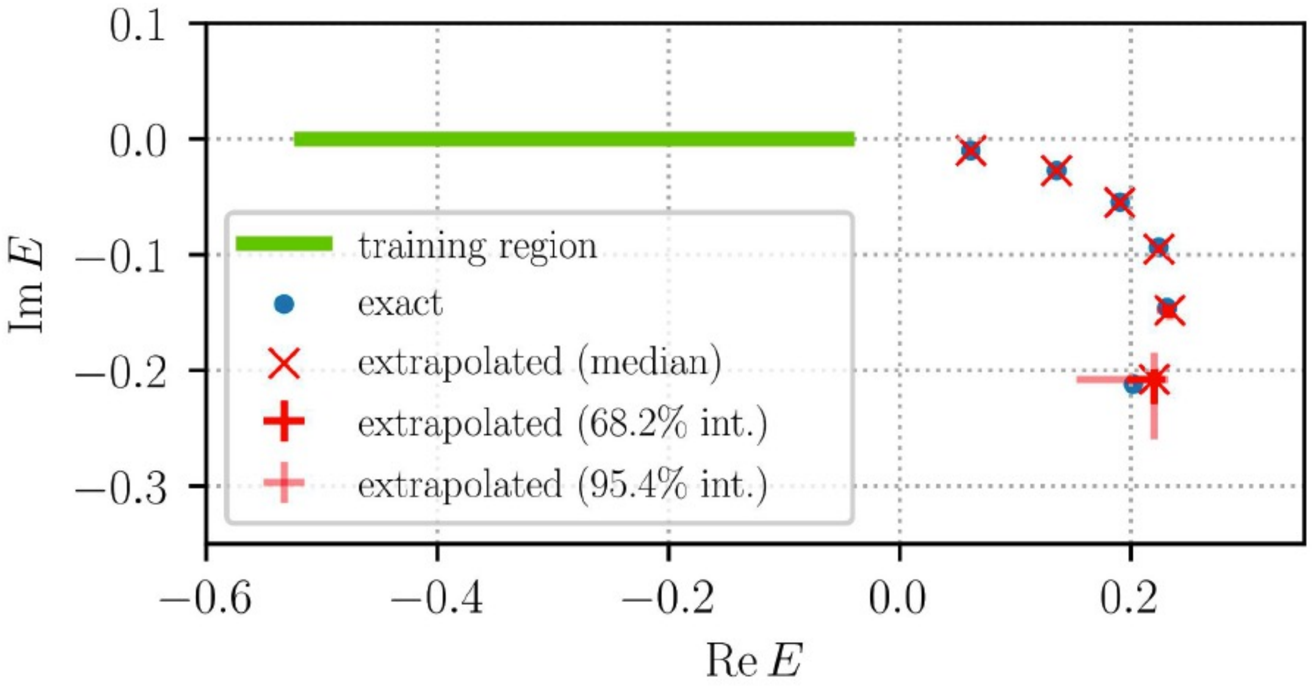
Many-body calculations in exotic nuclei are critical for FRIB & astrophysics, but **computationally costly and sometimes unstable** in decaying systems.

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 (pre-STREAMLINE)

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



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

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

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

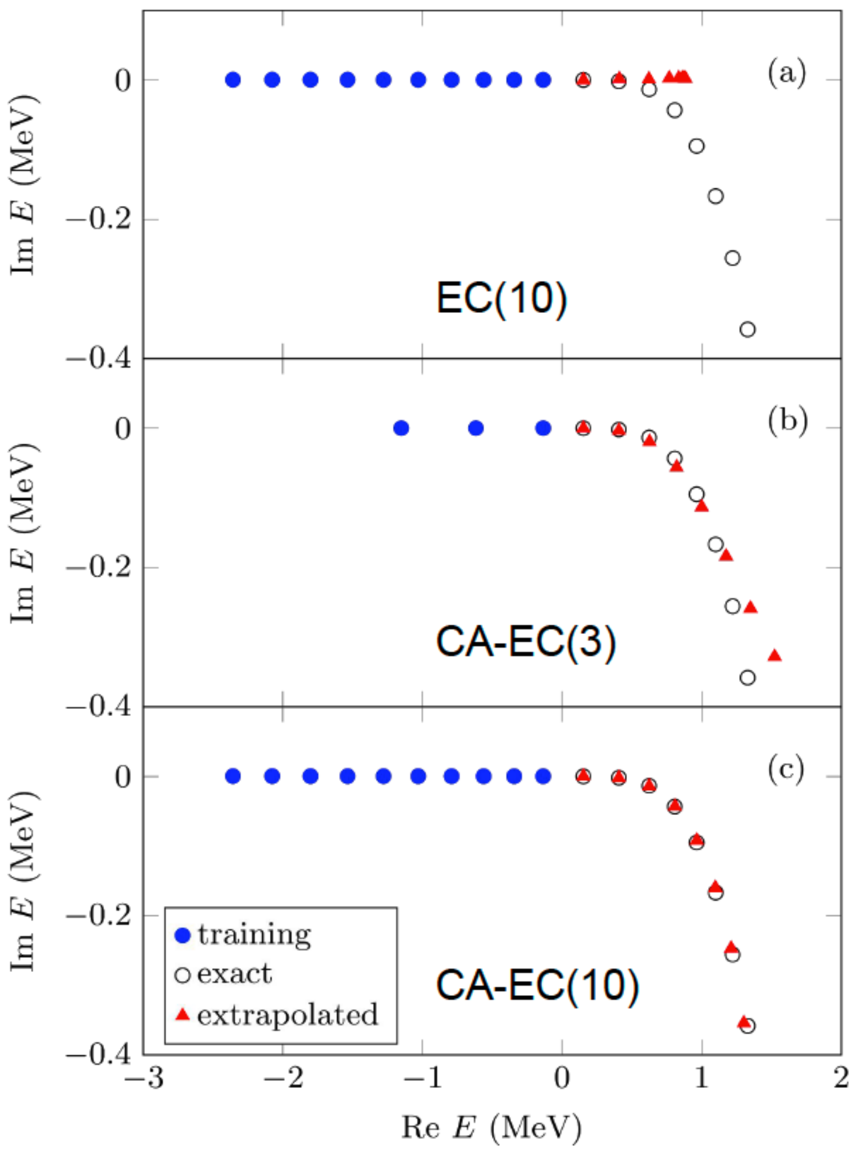
Achievements & Future Directions

- **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 (6He)**.

Currently working towards an ambitious realistic case recently observed (5p decay of 9N).

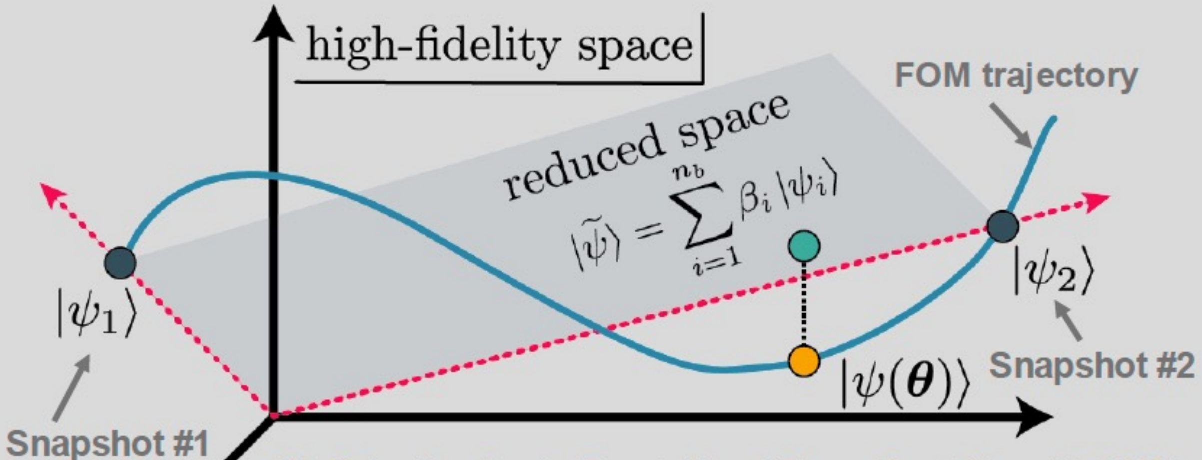
New directions identified based on developments within the STREAMLINE collaboration.

N. Yapa *et al.*, Submitted to Phys. Rev. C



Emulator training

Maldonado, CD, Furnstahl *et al.*, in prep.
Josh Maldonado's Master's thesis (2024)

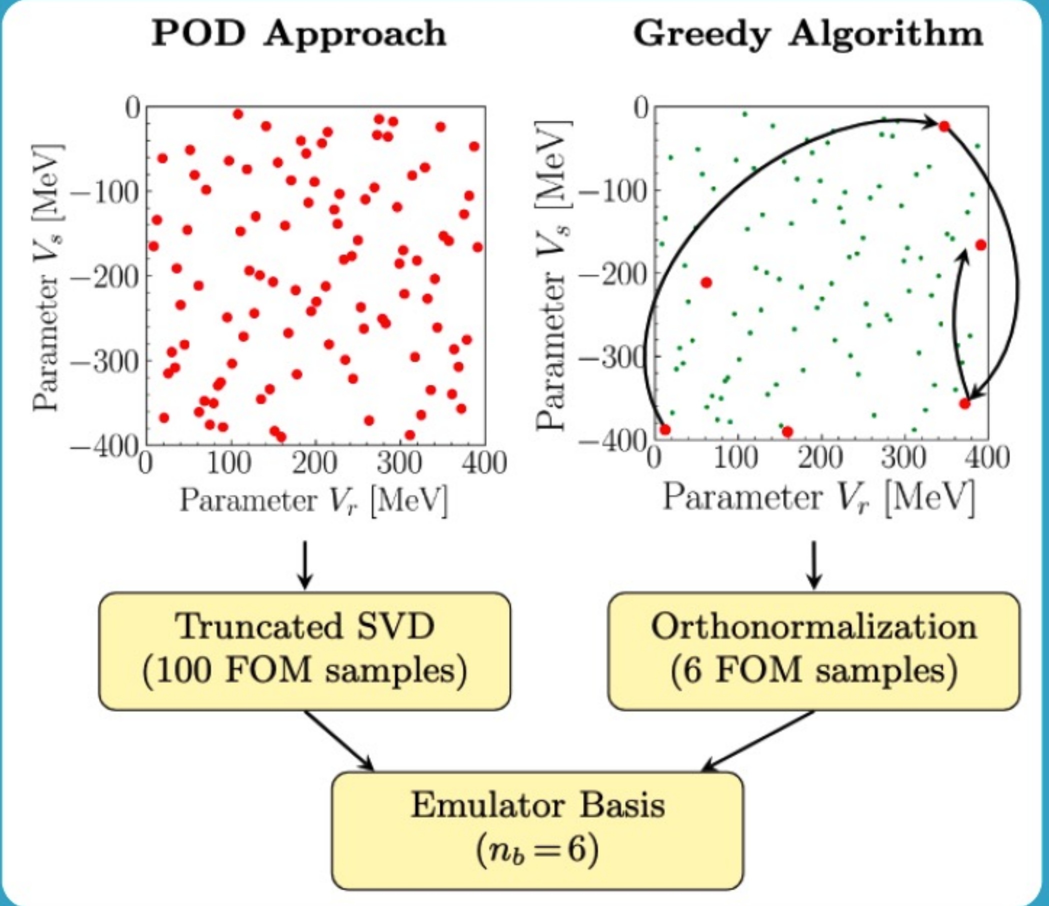


CD, Melendez, Garcia, Furnstahl, and Zhang, Front. Phys. **10**, 92931

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.

Active learning emulators

Maldonado, CD, Furnstahl *et al.*, in prep.
Josh Maldonado's Master's thesis (2024)

STREAMLINE demonstrated that an **active learning approach to snapshot selection** allows for the construction of fast & accurate emulators for **two-body scattering**.

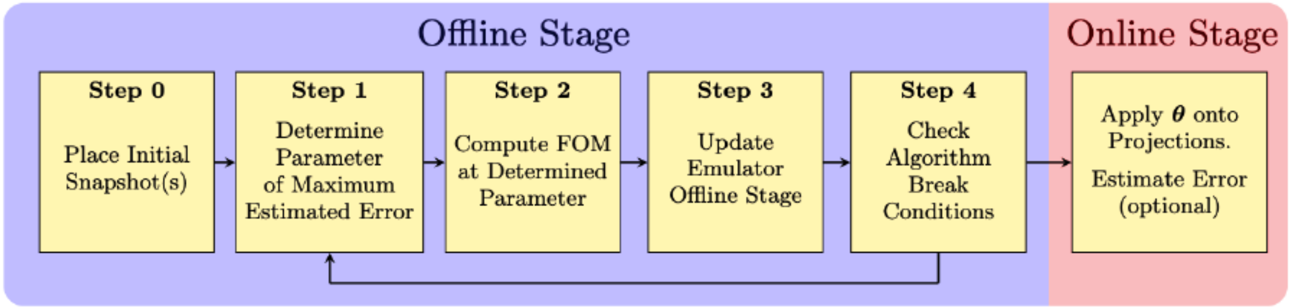
This is a **warm-up for three-body scattering**, where active learning is critical to keep calculations tractable.

A **greedy algorithm iteratively refines the emulator basis** in the training stage, placing training points where the emulator's error is estimated to be maximum.

Includes estimation of emulator errors.

Tested with **chiral potentials** commonly used in quantum Monte Carlo calculations of finite nuclei & infinite matter.

Extension to coupled channel & momentum space in progress



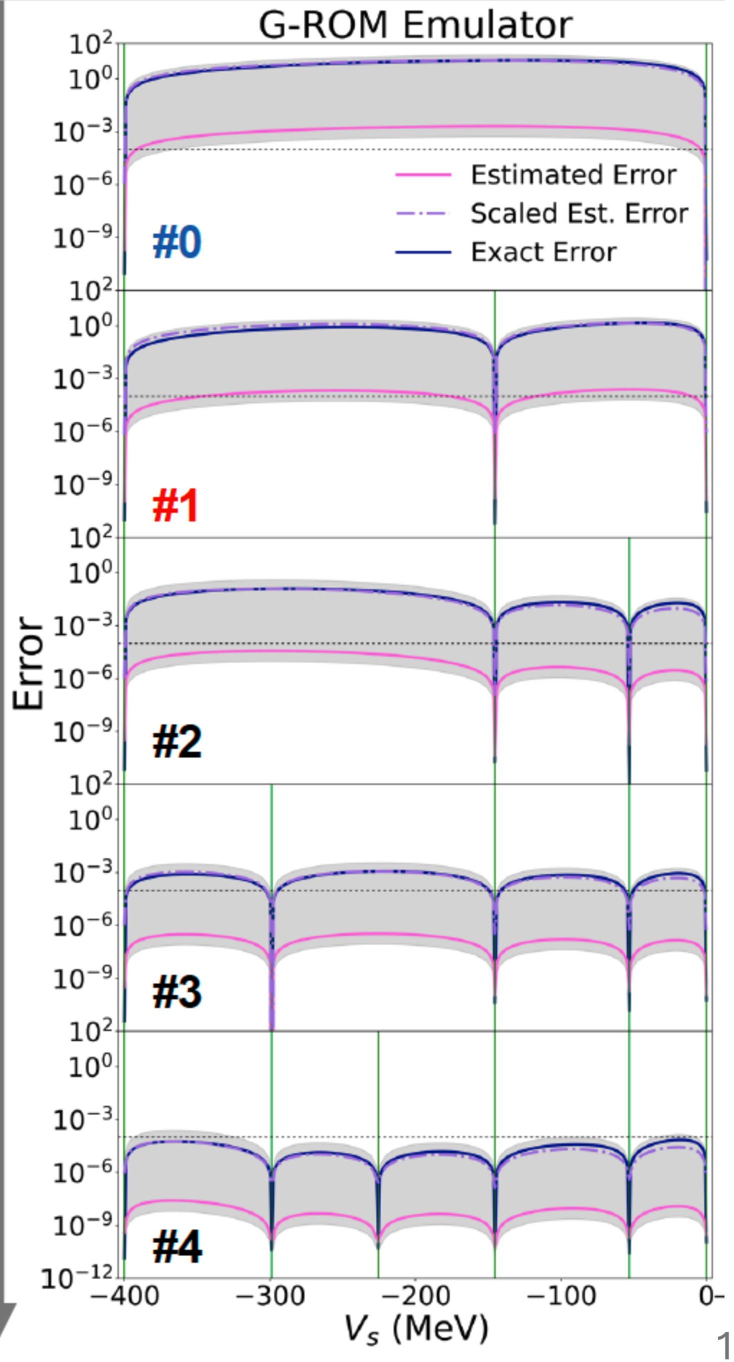
start with 2 randomly placed initial snapshots

Estimate the emulator error across the parameter space

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

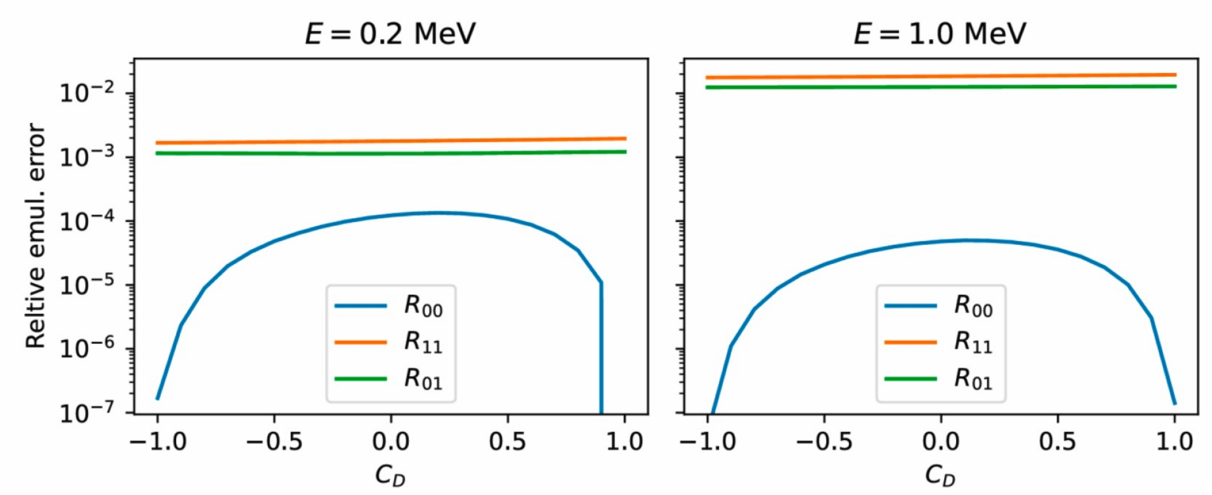
Iterate until the *requested* accuracy is obtained

***Greedy* Iteration increasing accuracy**



Reduced-basis-method-based emulator for nucleon-deuteron scattering

- Emulating $[E - H(\boldsymbol{\theta})]|\psi(\theta)\rangle = 0$ w/ real E in the $\boldsymbol{\theta}$-parameter space
- Nd emulator →
  - Emulation computing costs: milliseconds and 10s MB
  - χEFT calibration in the Bayesian statistics framework
  - Fundamental inputs for modern nuclear ab initio calculations
  - Coupling with the NSF-funded Bayesian Analysis of Nuclear Dynamics (BAND) collaboration
- Preliminary results for R-matrix: χEFT (Norfolk interaction model IIa*); varying 3b int. C_D; two training pts $C_D = -1, 1$; $\frac{1}{2}^+$ channel w/ s and d waves
- To implement new emulation technologies (greedy algorithms) soon



STREAMLINE
SmarT Reduction and Emulation Applying Machine Learning In Nuclear Environments



Jlab/ODU

Pisa group



Criticality analysis for artificial neural networks in nuclear physics

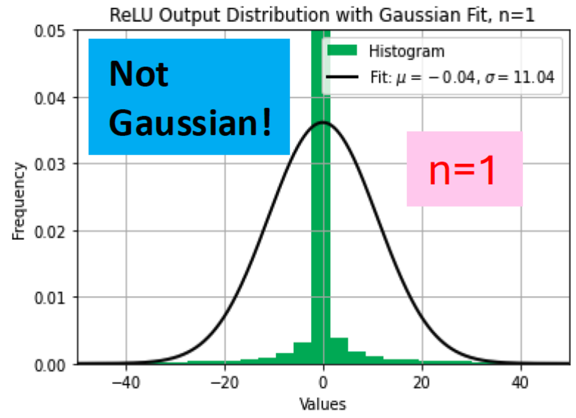
STREAMLINE: Simon Sundberg and Dick Furnstahl (OSU)

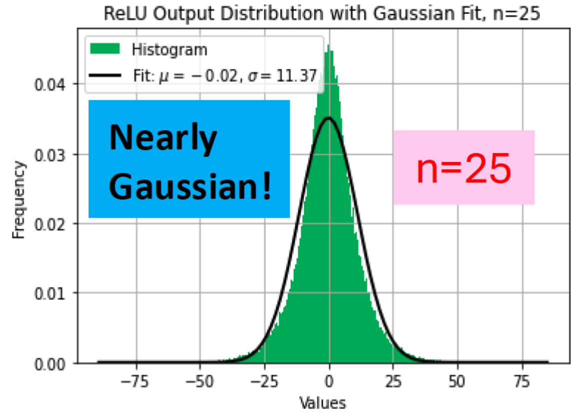
- What ANN architecture/initalization for nuclear applications is best?
- **STREAMLINE:** Adapt *Theory of Deep Learning* (Roberts, Yaida, Henin)
- Exploits ideas from effective theories and the renormalization group

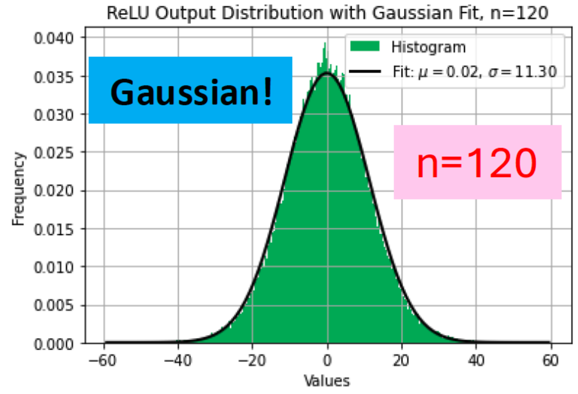
Ensembles of NNs ➔ **Distributions over random functions** 🡐 Path integrals in field theory (FT)

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

- Expand about large width (n) limit; when n → ∞ ➔ Gaussian (see figures)
- Use field theory-inspired organization of correlators
- Take small ratio of depth-to-width (= *r*) for controlled perturbative expansion
- Model complexity is determined by *r*, not number of model parameters
- Apply criticality analysis to initialization and learning to avoid gradient issues



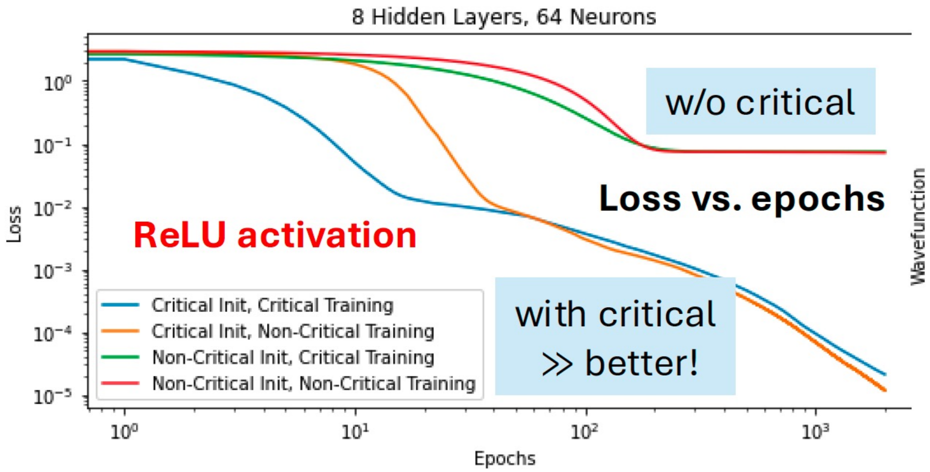


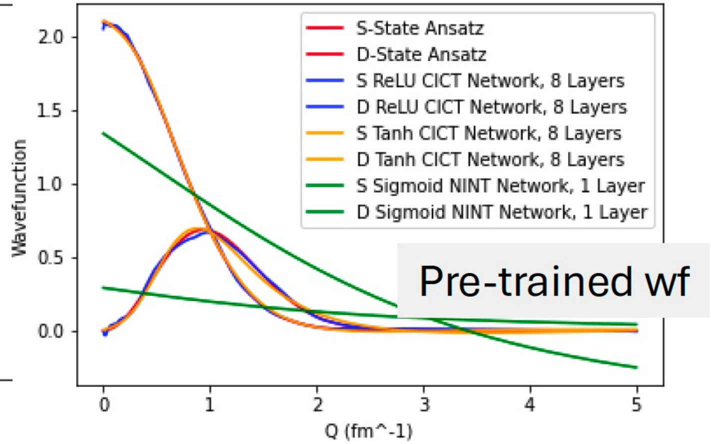


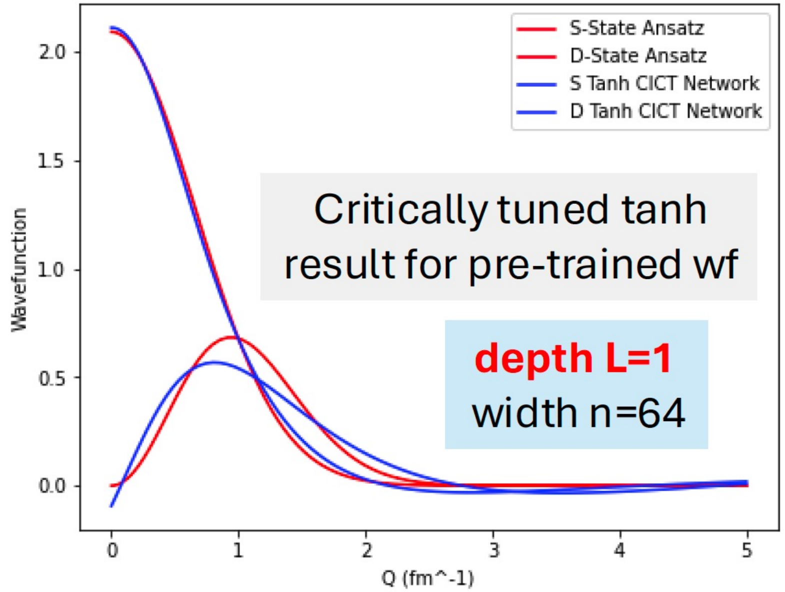
Criticality analysis for artificial neural networks in nuclear physics

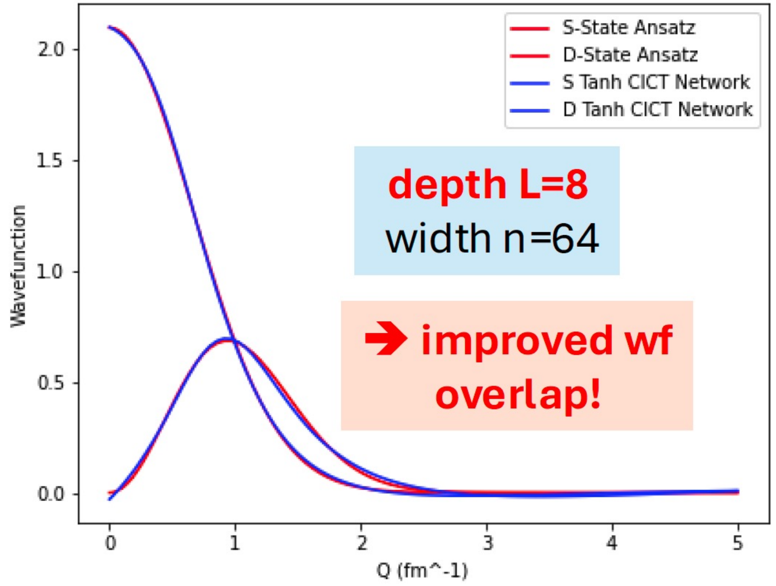
STREAMLINE: Simon Sundberg and Dick Furnstahl (OSU)

- Test case for criticality analysis: learning variational wave functions for the deuteron recently explored by Rozalén Sarmiento et al.
- They favored shallow depth L=1,2 and sigmoid activation function.



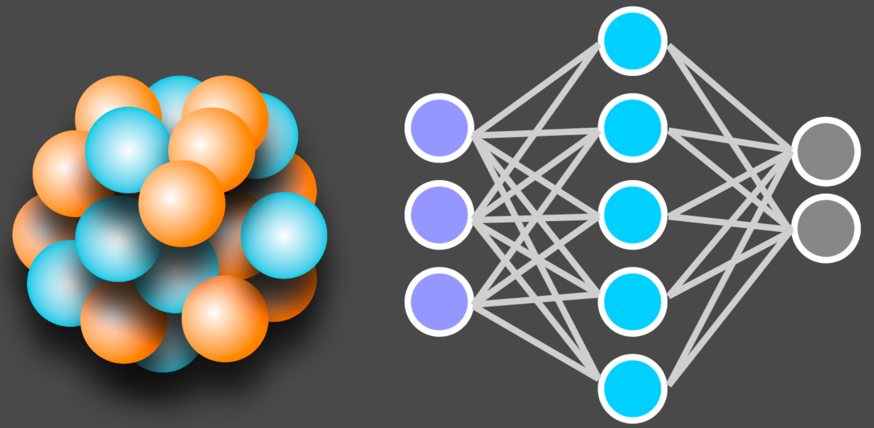






- **First stage:** pre-train the ANN to a variational ansatz, exploring different architectures and activation functions, testing impact of tuning the initialization and learning rate to criticality (above).
  - Sigmoid bad (no fixed point), tanh and ReLU good (above)
  - When critically tuned, improvement with depth (right)
- **In progress:** use variational energy to refine pre-trained network.

STREAMLINE NQS PROGRESS



ALESSANDRO LOVATO

Argonne NATIONAL LABORATORY

HYPERNUCLEI WITH NQS

Goal: achieve an accurate description of hypernuclei and hyper-nuclear matter.

Method: neural wave function ansatz for modeling Λ-hypernuclei

Achievements: ground-state energies in excellent agreement with experimental data

Impact: guide the experimental program and contribute solving the *hyperon puzzle*

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

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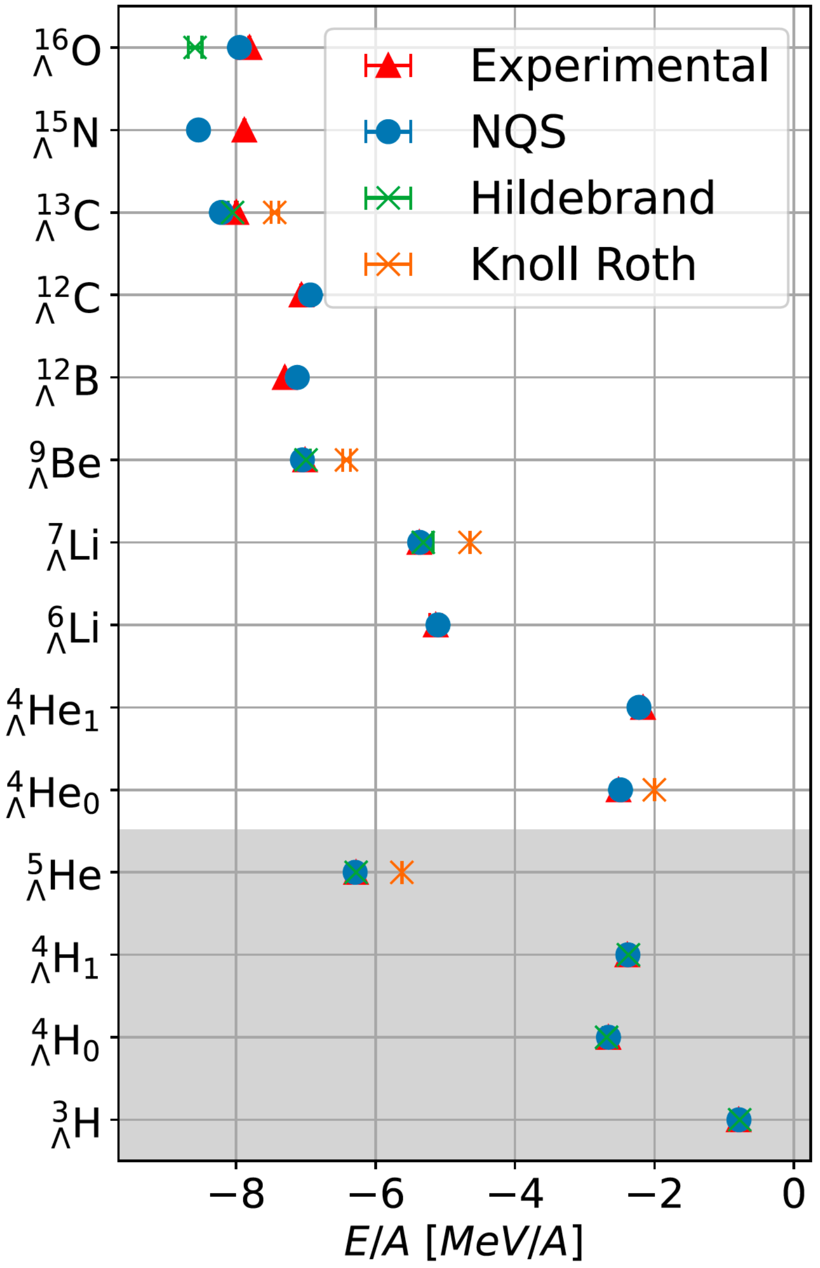


NEURAL WAVE FUNCTION FOR A=40 NUCLEI

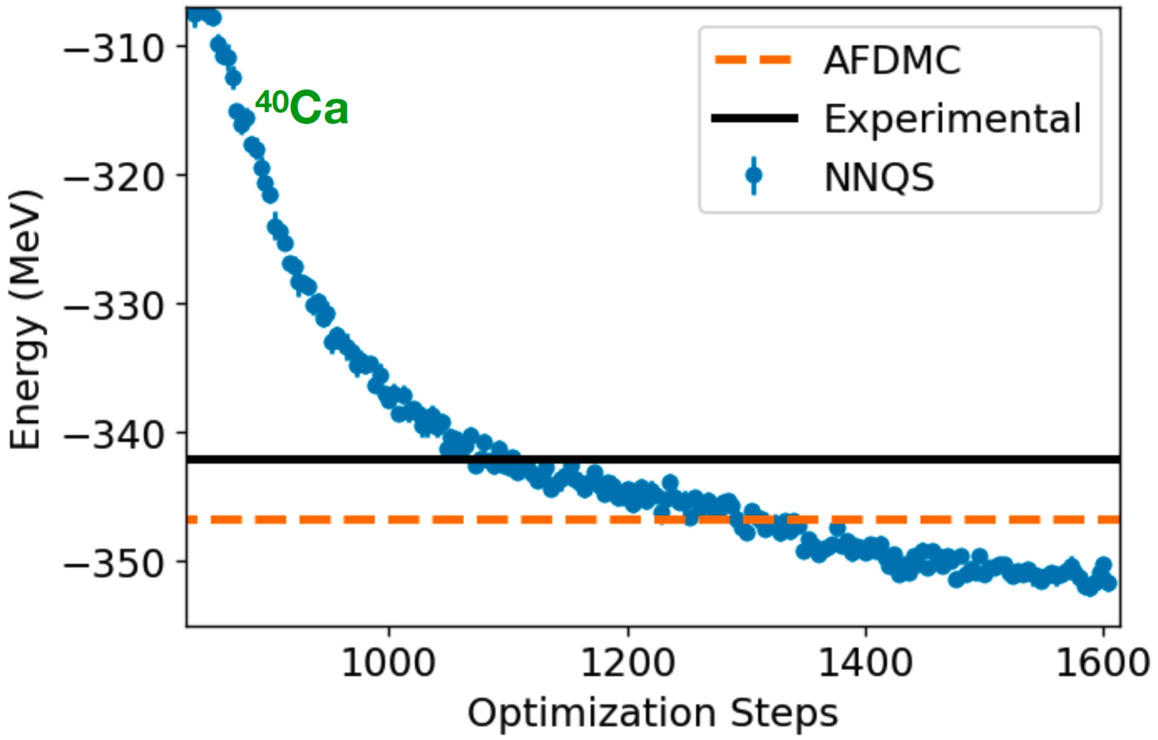
Goal: develop a neural wave function suitable to model A=40 nuclei.

Method: leverage the Pfaffian ansatz, which exhibit favorable scaling with A.

Achievements: Better ground-state energies of ^{40}Ca than the AFDMC method

Impact: achieve a high-resolution description of medium-mass nuclei

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



3

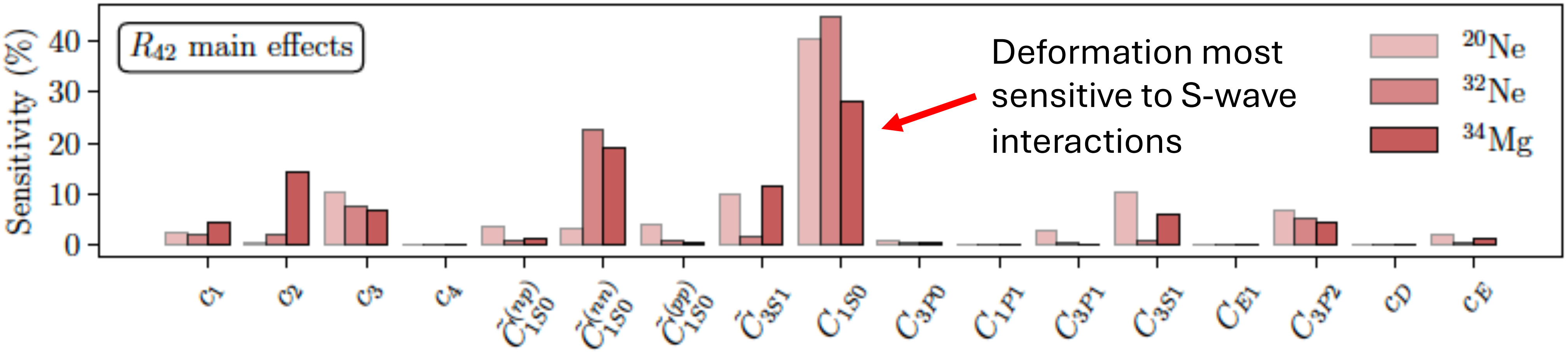
What drives nuclear deformation?

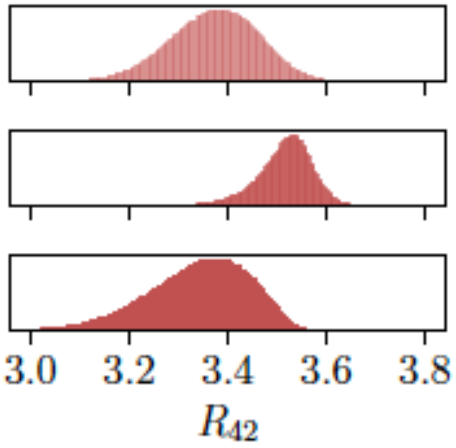
Objective:

- Find how nuclear interactions from effective field theories of quantum chromodynamics yield deformed nuclei
- Tie energy ratio $R_{42} \equiv E(4^+)/E(2^+)$ in ^{20}Ne, ^{32}Ne and ^{34}Mg to low-energy constants

Procedure:

- Global sensitivity analysis ("main effect") based on Hartree-Fock emulators used to compute R_{42}





$R_{42} = \frac{10}{3} \approx 3.33$ indicates a rigid rotor

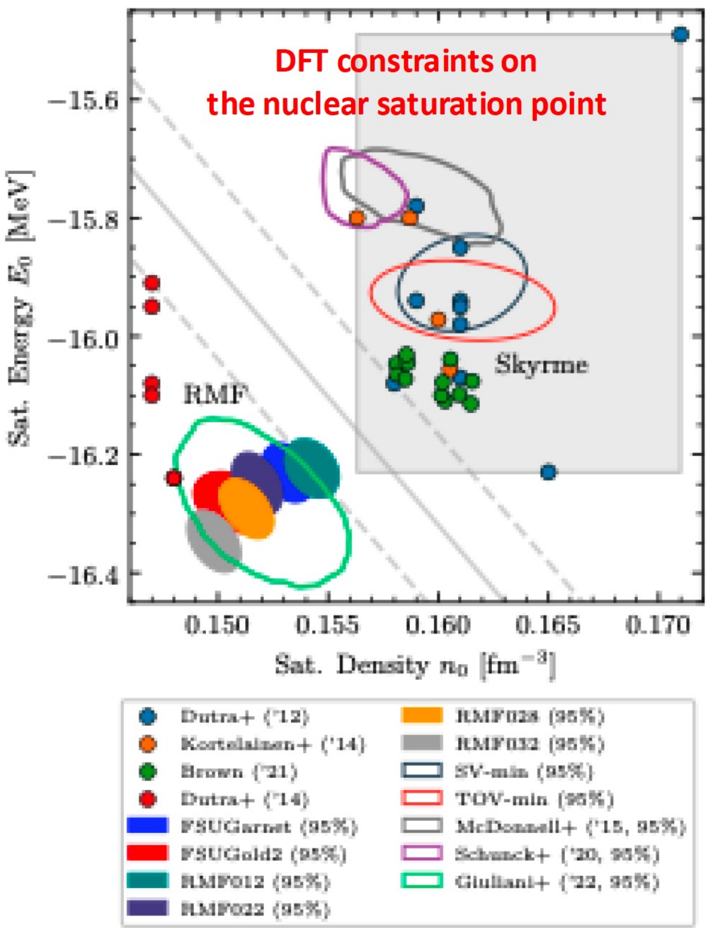
Accomplishments:

- Created emulators for "island-of inversion nuclei" ^{32}Ne and ^{34}Mg
- For the first time provided high-resolution picture of what drives nuclear deformation
- Deformation mostly sensitive to short-range s-wave interactions and pion nucleon couplings
- Paper Zhonghao Sun et al., arXiv:2404.00058

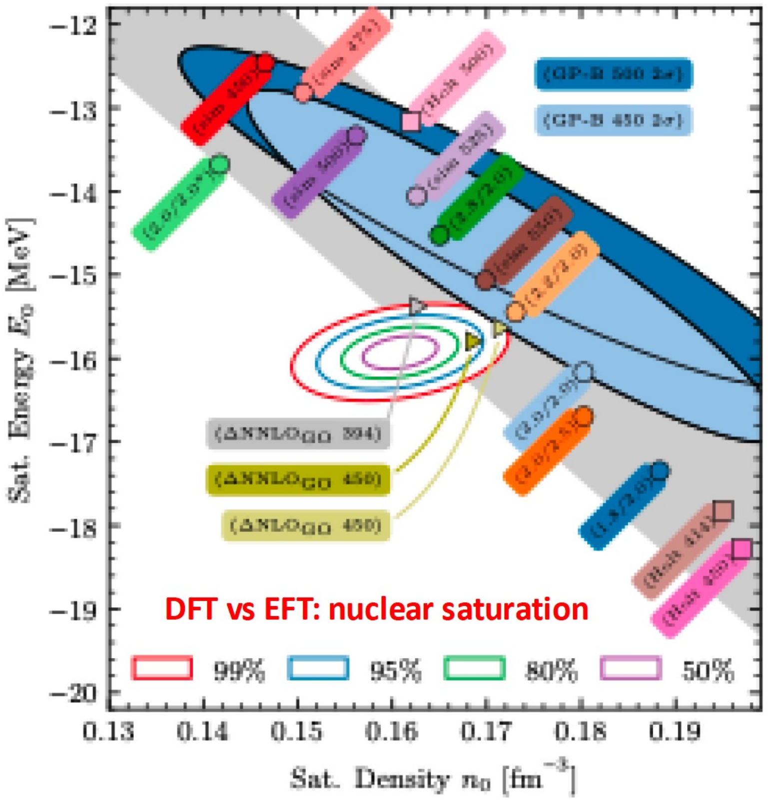
A Bayesian mixture model approach to quantifying the *empirical* nuclear saturation point

Drischler, Giuliani, Bezoui, Piekarewicz, and Viens, Phys. Rev. C **110**, 044320.

Goal: rigorous benchmarks of saturation properties of chiral NN+3N interactions (using Skyrme & RMF models)

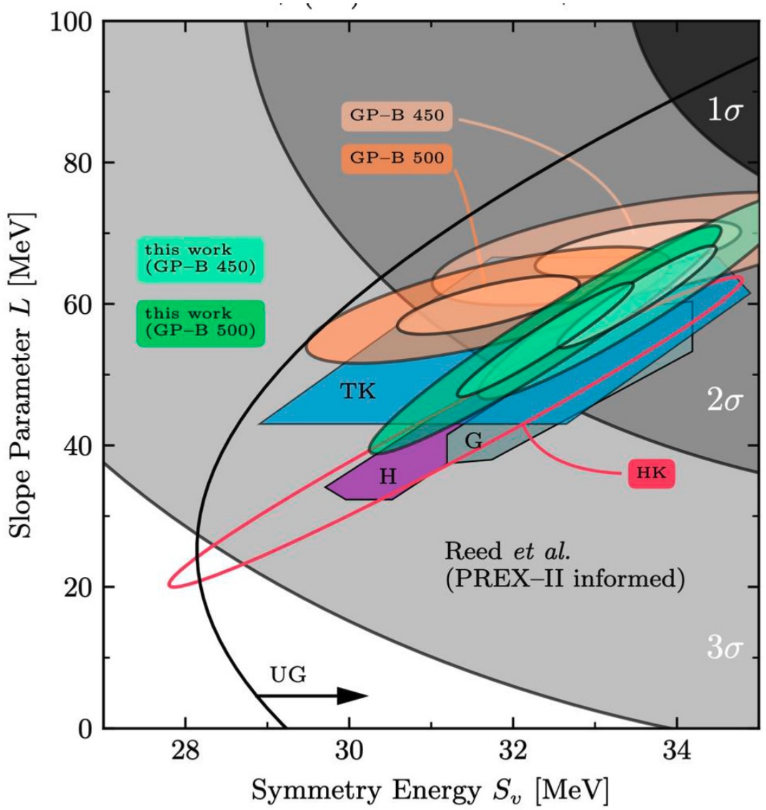


Skyrme and relativistic mean field (RMF) models constrain (n_0, E_0) **tightly**, but when multiple DFT constraints are considered together, they are clearly inconsistent: **not all DFT predictions can be both precise and accurate simultaneously** (left figure).



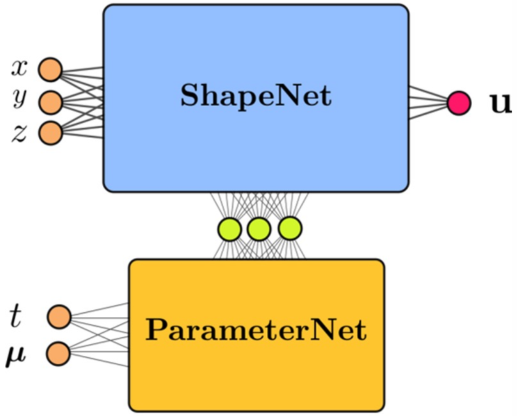
We developed a **Bayesian hierarchical model that estimates the true empirical saturation point by mixing multiple DFT constraints**. This results in a posterior distribution for the empirical saturation point that enables statistically meaningful benchmarks of microscopic interactions in terms of nuclear saturation (center figure).

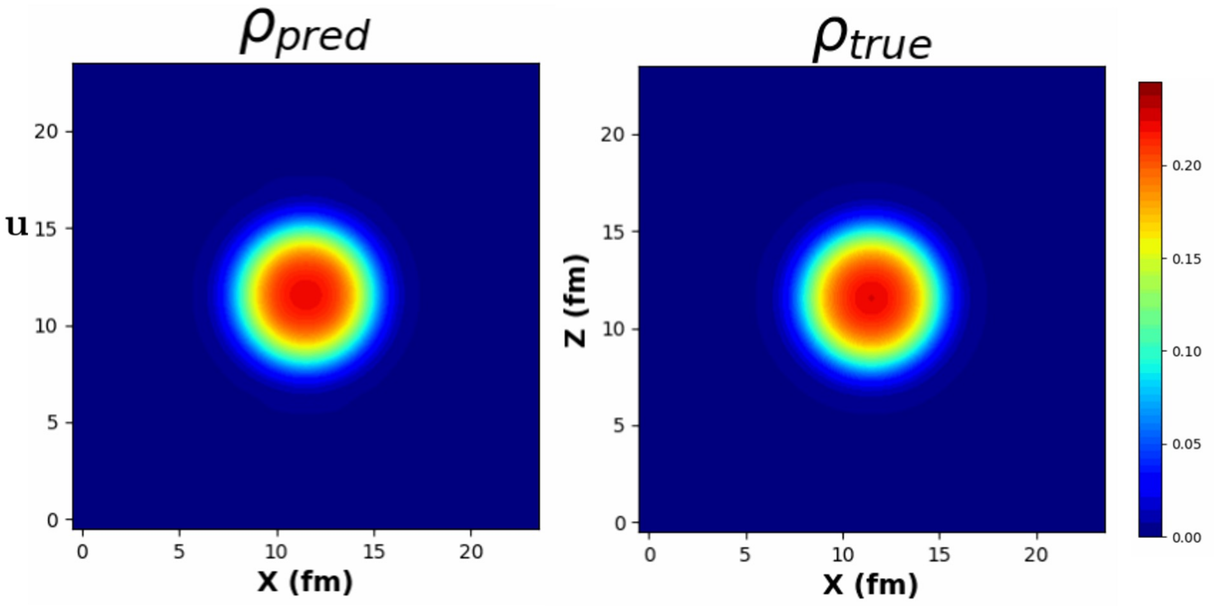
We also derived **tight constraints on the nuclear symmetry energy and its slope parameter at the saturation density** using microscopic calculations of the pure neutron matter EOS (right figure).



MICHIGAN STATE UNIVERSITY SROP SUMMER RESEARCH OPPORTUNITIES PROGRAM

Neural Implicit Flow for time dynamics





Vibrating Calcium

High Fidelity

$$
\begin{aligned}
H_S(\boldsymbol{r}) = {} & \frac{\hbar^2}{2m}\tau + \frac{1}{2}t_0\left(1+\frac{1}{2}x_0\right)\rho^2 - \frac{1}{2}t_0\left(\frac{1}{2}+x_0\right)\left[\rho_p^2+\rho_n^2\right] + \frac{1}{4}\left[t_1\left(1+\frac{1}{2}x_1\right)+t_2\left(1+\frac{1}{2}x_2\right)\right](\rho\tau-\boldsymbol{j}^2) \\
& -\frac{1}{4}\left[t_1\left(\frac{1}{2}+x_1\right)-t_2\left(\frac{1}{2}+x_2\right)\right](\rho_p\tau_p+\rho_n\tau_n-\boldsymbol{j}_p^2-\boldsymbol{j}_n^2) - \frac{1}{16}\left[3t_1\left(1+\frac{1}{2}x_1\right)-t_2\left(1+\frac{1}{2}x_2\right)\right]\rho\nabla^2\rho \\
& +\frac{1}{16}\left[3t_1\left(\frac{1}{2}+x_1\right)+t_2\left(\frac{1}{2}+x_2\right)\right](\rho_p\nabla^2\rho_p+\rho_n\nabla^2\rho_n) \\
& +\frac{1}{12}t_3\left[\rho^{\alpha+2}\left(1+\frac{1}{2}x_3\right)-\rho^{\alpha}(\rho_p^2+\rho_n^2)\left(x_3+\frac{1}{2}\right)\right] \\
& +\frac{1}{4}t_0x_0\boldsymbol{s}^2-\frac{1}{4}t_0(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2)+\frac{1}{24}\rho^{\alpha}t_3x_3\boldsymbol{s}^2-\frac{1}{24}t_3\rho^{\alpha}(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2) \\
& +\frac{1}{32}(t_2+3t_1)\sum_q \boldsymbol{s}_q\cdot\nabla^2\boldsymbol{s}_q-\frac{1}{32}(t_2x_2-3t_1x_1)\boldsymbol{s}\cdot\nabla^2\boldsymbol{s} \\
& +\frac{1}{8}(t_1x_1+t_2x_2)(\boldsymbol{s}\cdot\boldsymbol{T}-\boldsymbol{J}_{\mu\nu}^2)+\frac{1}{8}(t_2-t_1)\sum_q(\boldsymbol{s}_q\cdot\boldsymbol{T}_q-\boldsymbol{J}_{q\mu\nu}^2) \\
& -\frac{t_4}{2}\sum_{qq'}(1+\delta_{qq'})[\boldsymbol{s}_q\cdot\nabla\times\boldsymbol{j}_{q'}+\rho_q\boldsymbol{\nabla}_{\mu\nu}\cdot\boldsymbol{J}_{\mu\nu}]
\end{aligned}
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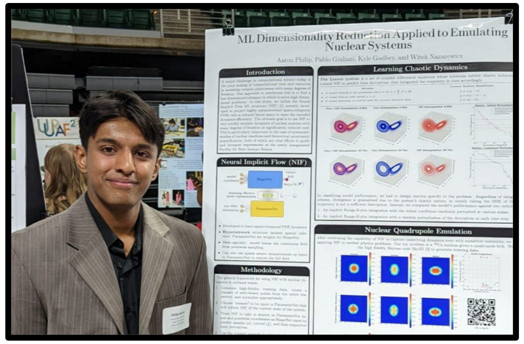
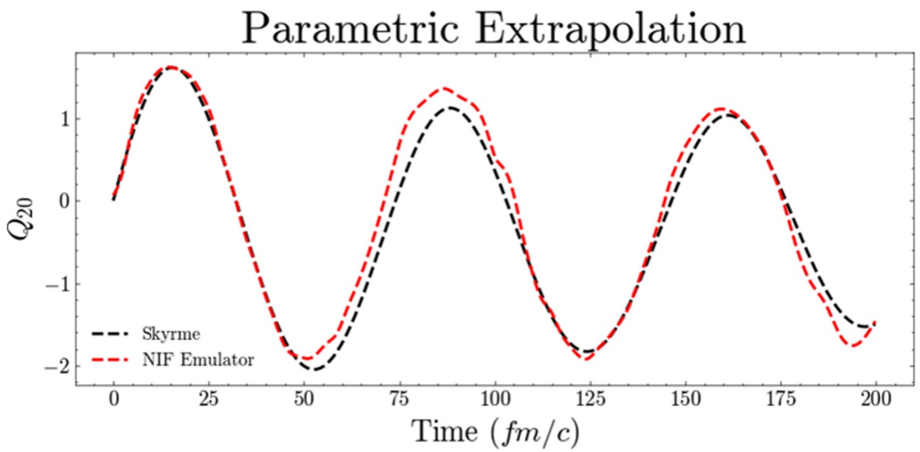
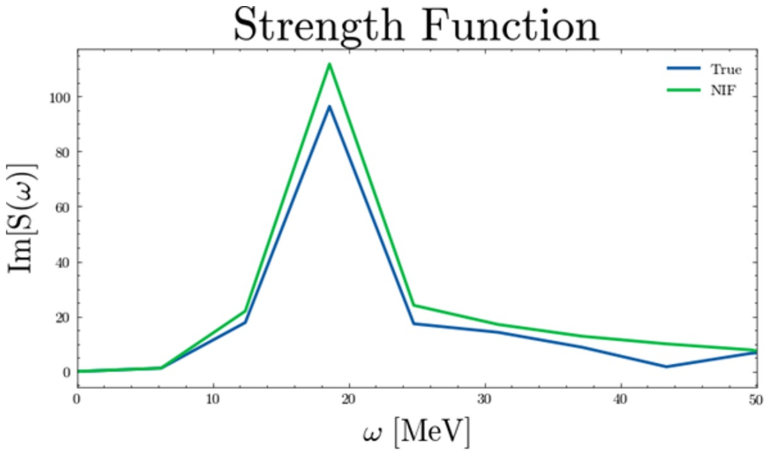


Aaron P.
Pablo G.
Kyle G.
Witek N.

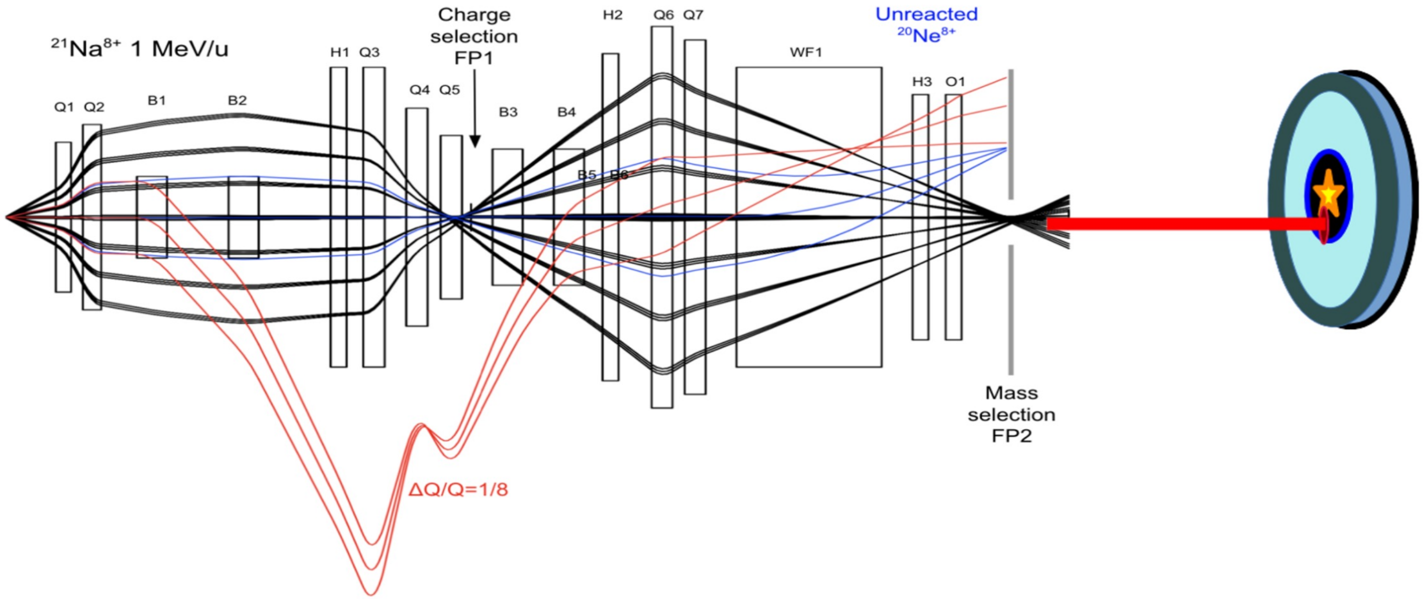




Beam control

Transport matrix
M as a function of
current I

$$\hat{M}(I) = M_0 + \sum_k a_k(I) M_k$$



~ 3,000 faster than high fidelity

Efficient Emulation of the SECAR beam

Dimensionality Reduction in
Nuclear Physics
Presented by ASCSN

# of Bases	Emulation Time (to FP1)	Max Position Error (x)	Max angular Error (ax)
3	(9.7 ± 0.3) ms*	1 μm	1 nrad
10	(10.9 ± 0.6) ms*	0.01 μm	7.5 prad
15	(12.1 ± 0.2) ms*	0.7 nm	0.3 frad

Genetic programming

Discovering reduced order model equations of many-body quantum systems using genetic programming: a technical report

Illya Bakurov,[1] Pablo Giuliani,[2] Kyle Godbey,[2] Nathan Haut,[3] Wolfgang Banzhaf,[1] and Witold Nazarewicz[2,4]

1) Find good reduced coordinates

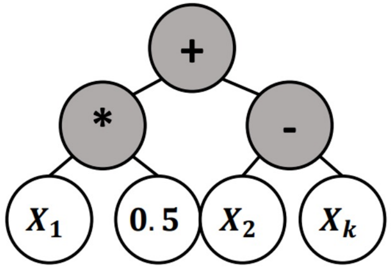
Linear embedding

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

2) Find equations from data

$$\hat{\rho}(x;\alpha) = \sum_{k}^{n} a_k(\alpha)\rho_k(x)$$

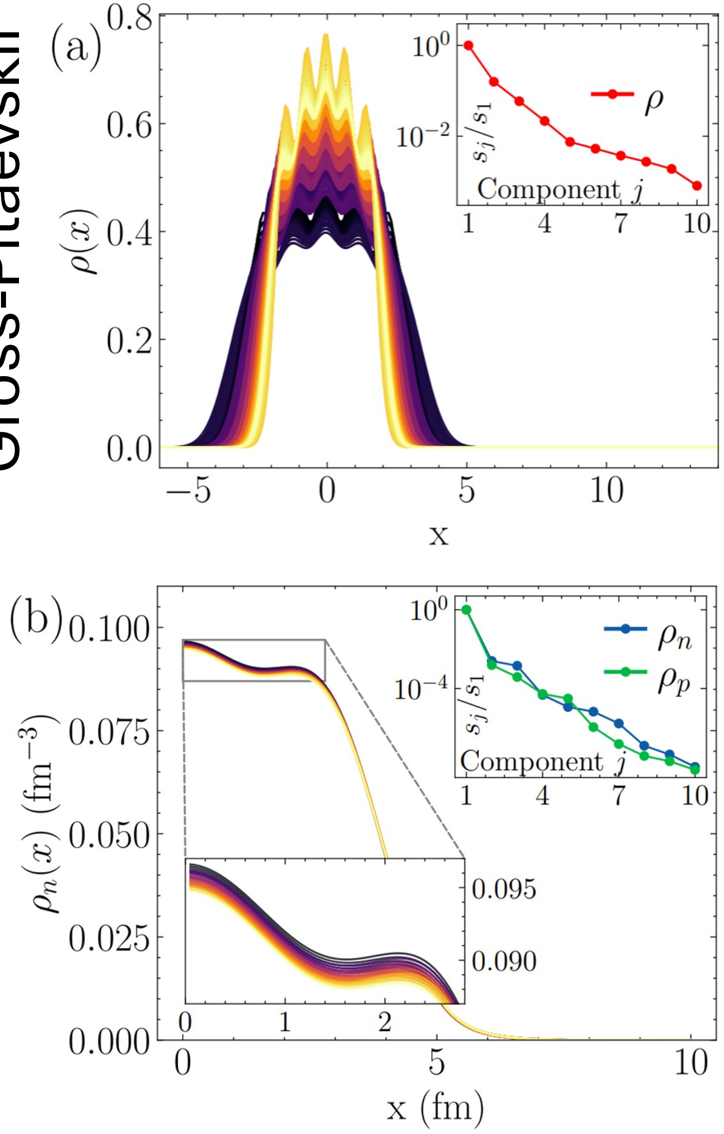
$$\boldsymbol{f_i = X_1 * 0.5 + X_2 - X_k}$$



10,000 speed-up!

Modified Gross-Pitaevskii

Skyrme DFT

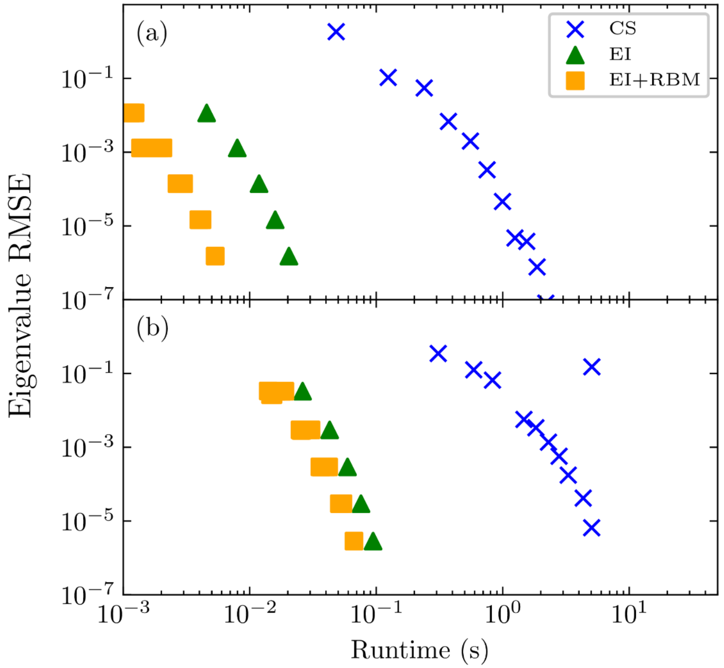


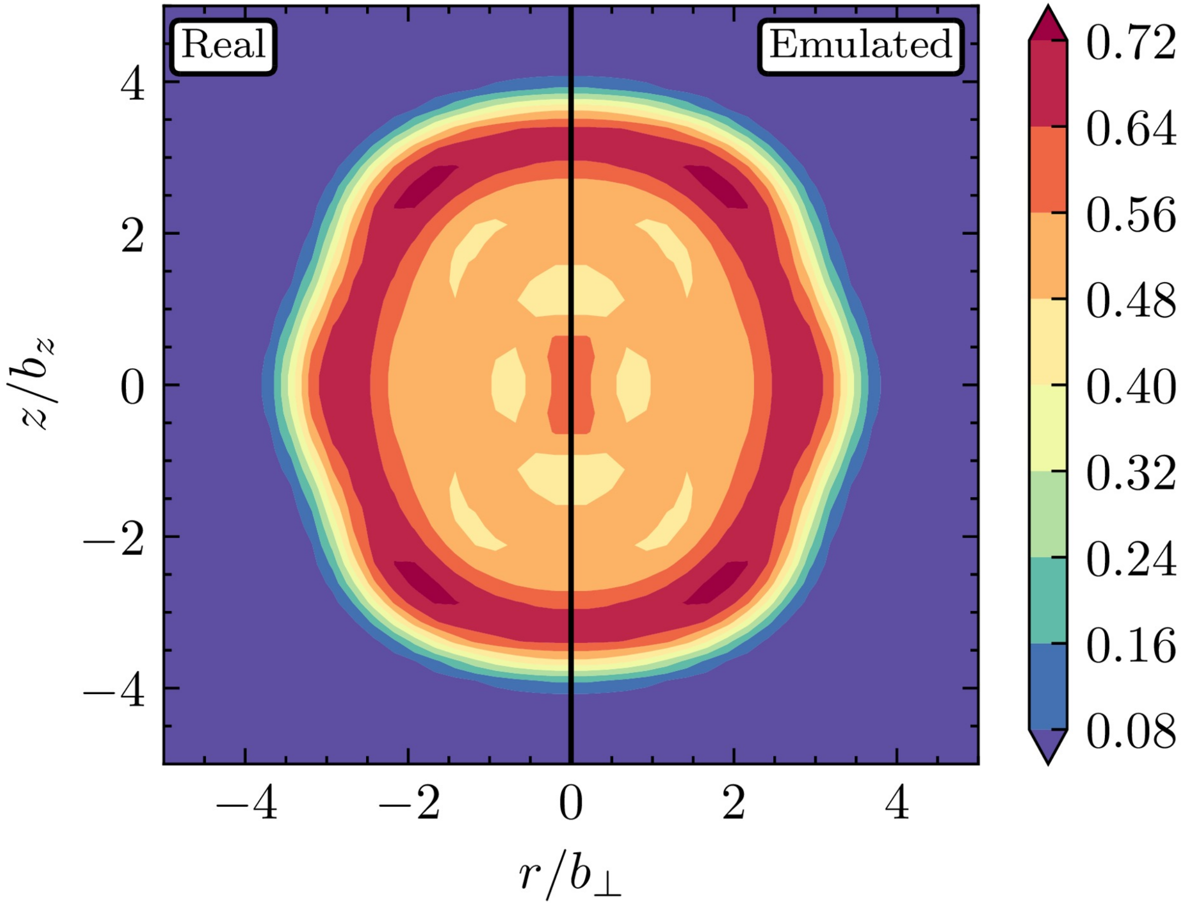
Application to Axial HFB with Realistic Functional

Order-of-magnitude speedup obtained in axial HFB calculations (CAT plot for toy model)

Localization functional reproduced with negligible error, suggesting usefulness for downstream applications (e.g. fission)

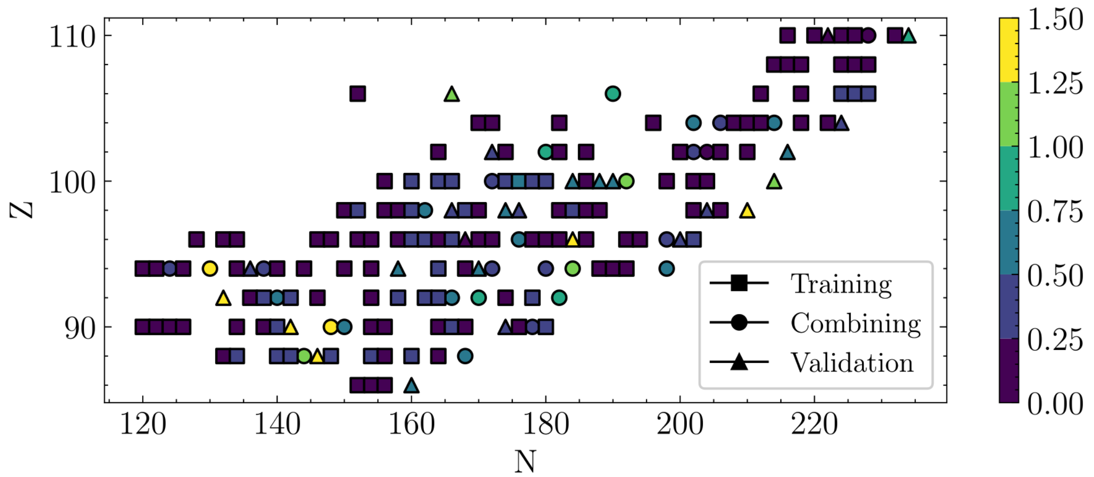
Paper in preparation



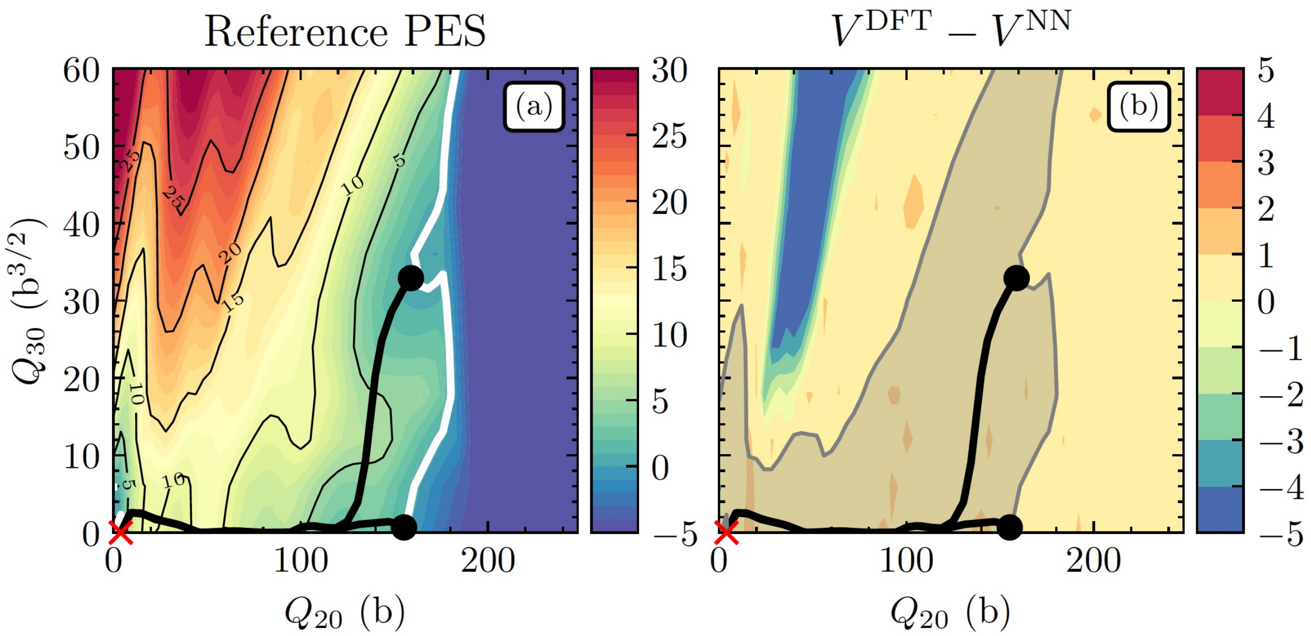


Neural network emulation of spontaneous fission

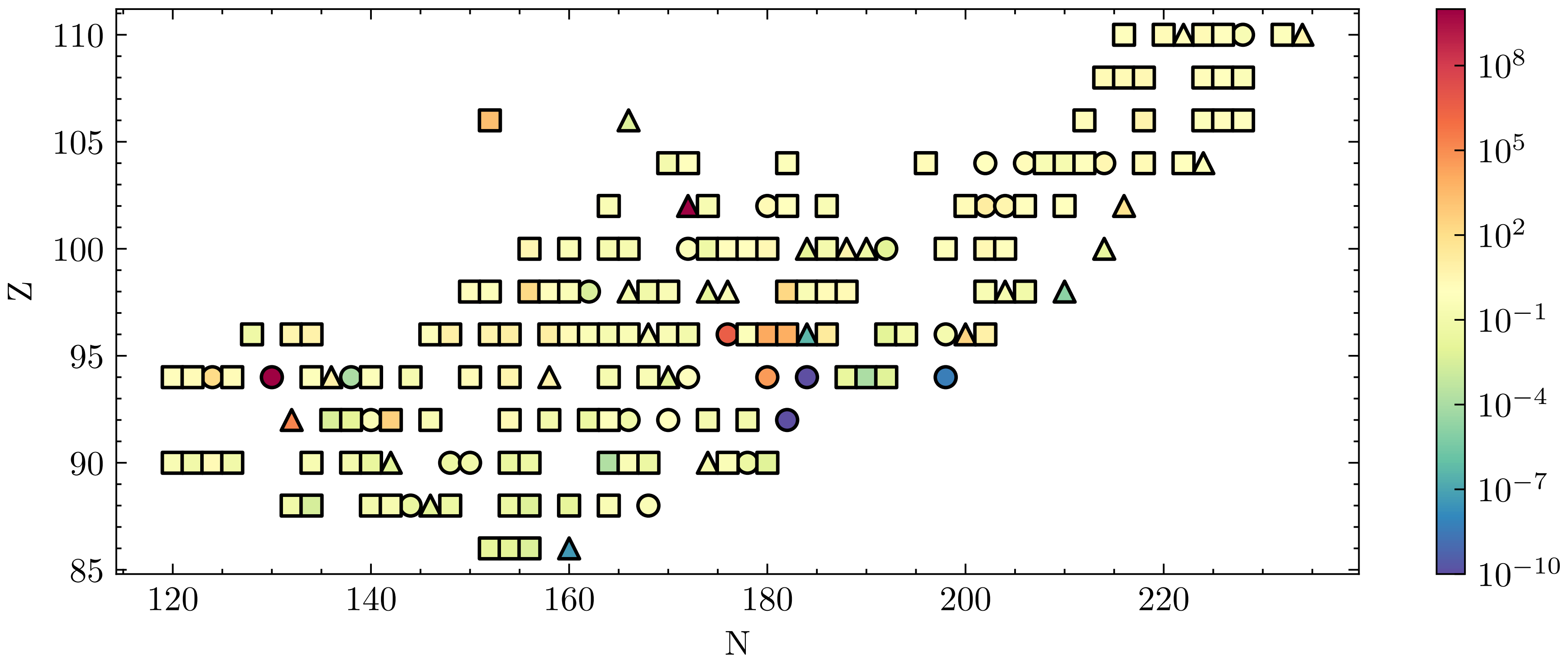
D. Lay et al., Phys. Rev. C 109, 044305 (2024)



Different datasets used for NN training, combining, and validation.



(a): the reference PES for ^{280}Cm in MeV. (b): the difference between the reference and reconstructed PESs. The energy range $0.5 \leq V^{\mathrm{DFT}} \leq 12$ MeV is shaded in gray in panel (b).



The ratio of the lifetime predicted by the NN emulator to the lifetime predicted by the DFT PES. Lifetimes are computed using NEB on the surface. The lifetimes are typically within the same order of magnitude, indicating that the NN is able to accurately reproduce the parts of the PES relevant to (spontaneous) fission.

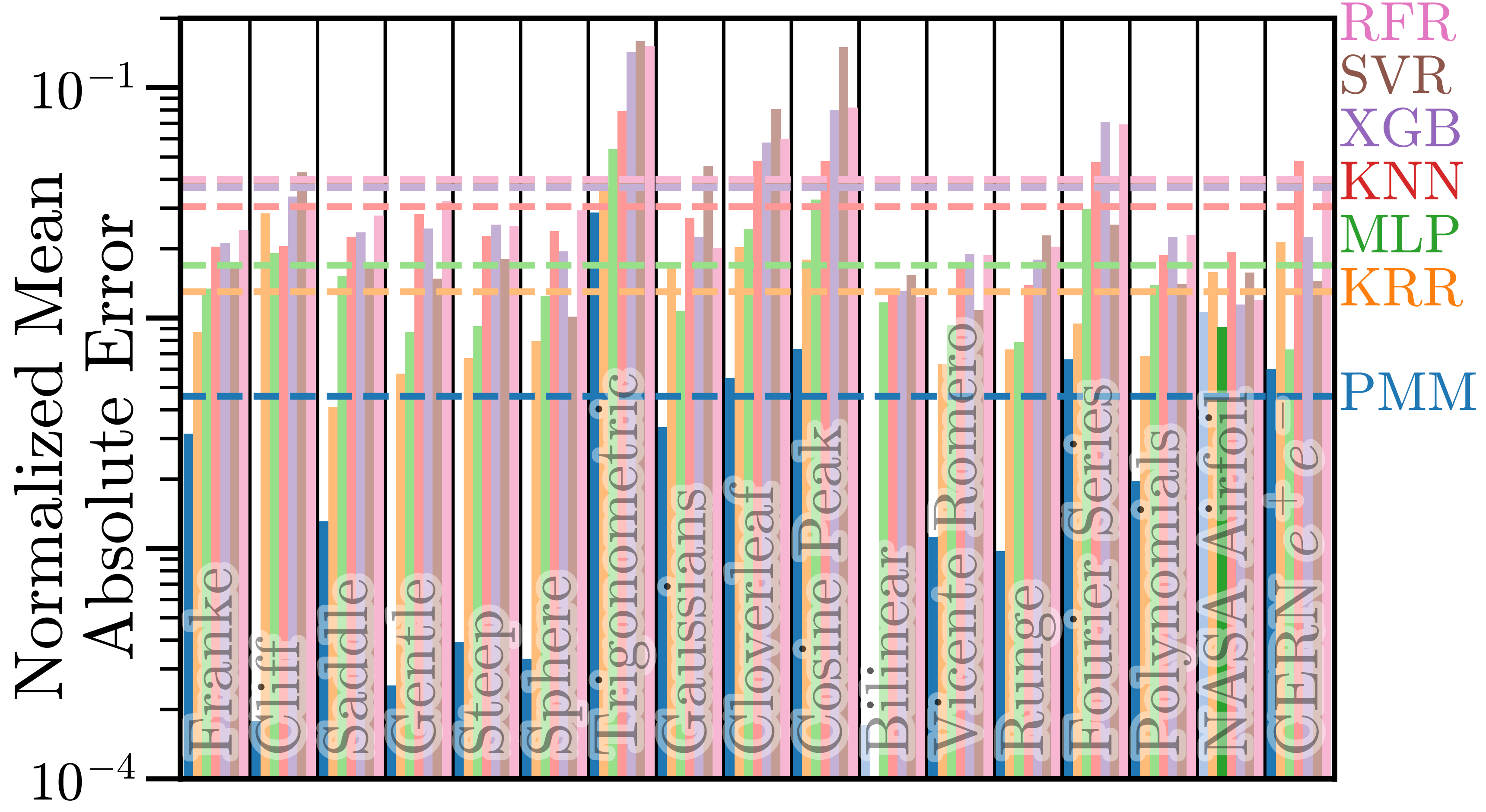
Parametric matrix model (PMM)

Patrick Cook

Danny Jammooa

Patrick Cook, Danny Jammooa, Morten Hjorth-Jensen, Daniel Lee, Dean Lee, arXiv:2401.11694

Multivariable function interpolation



Parametric Matrix Model (PMM), Kernel Ridge Regression (KRR), Multilayer Perceptron (MLP), k-Nearest Neighbors (KNN), Extreme Gradient Boosting (XGB), Support Vector Regression (SVR), and Random Forest Regression (RFR)

Heisenberg spin chain

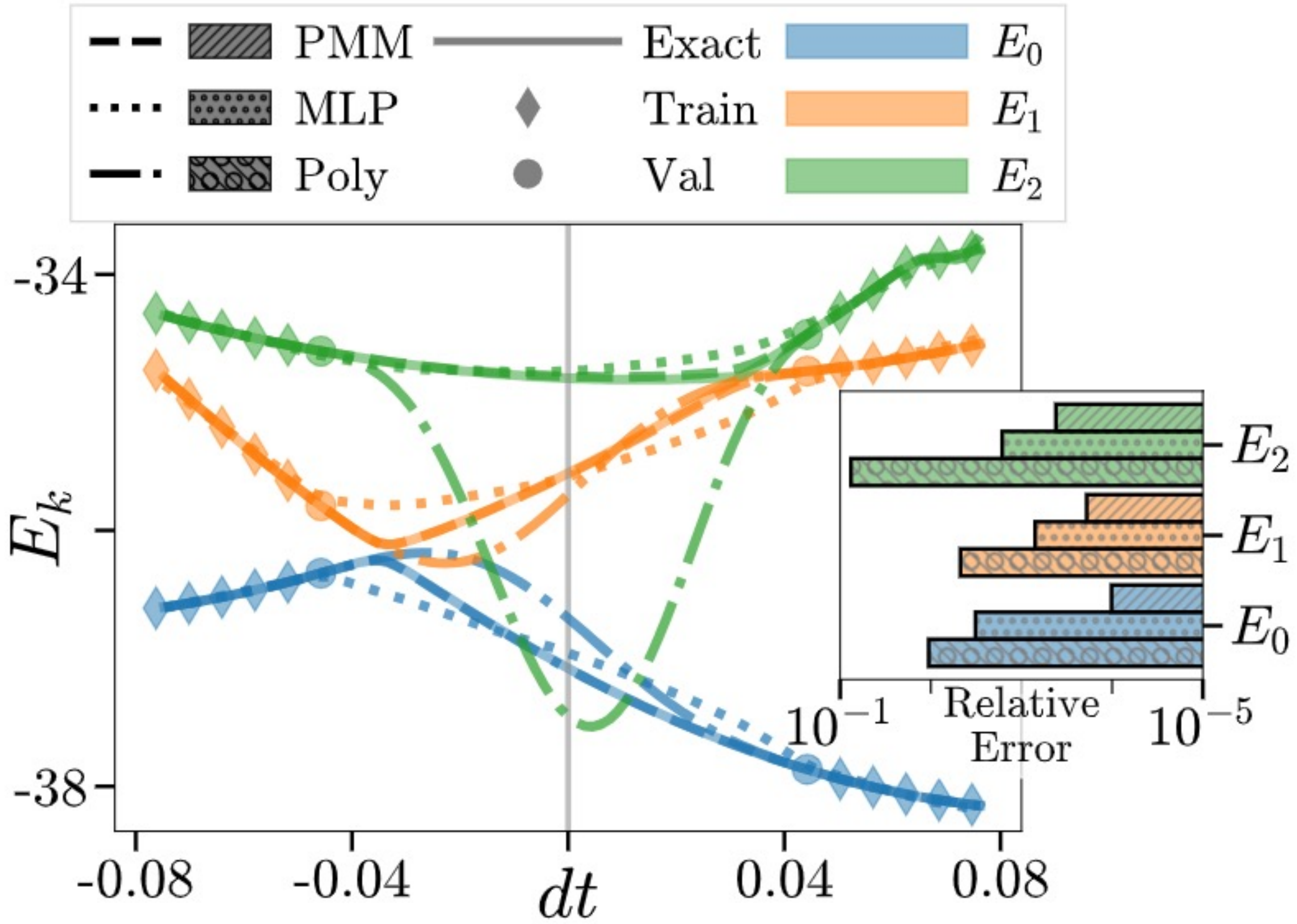
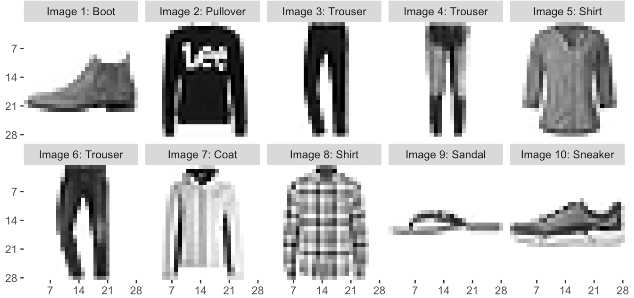


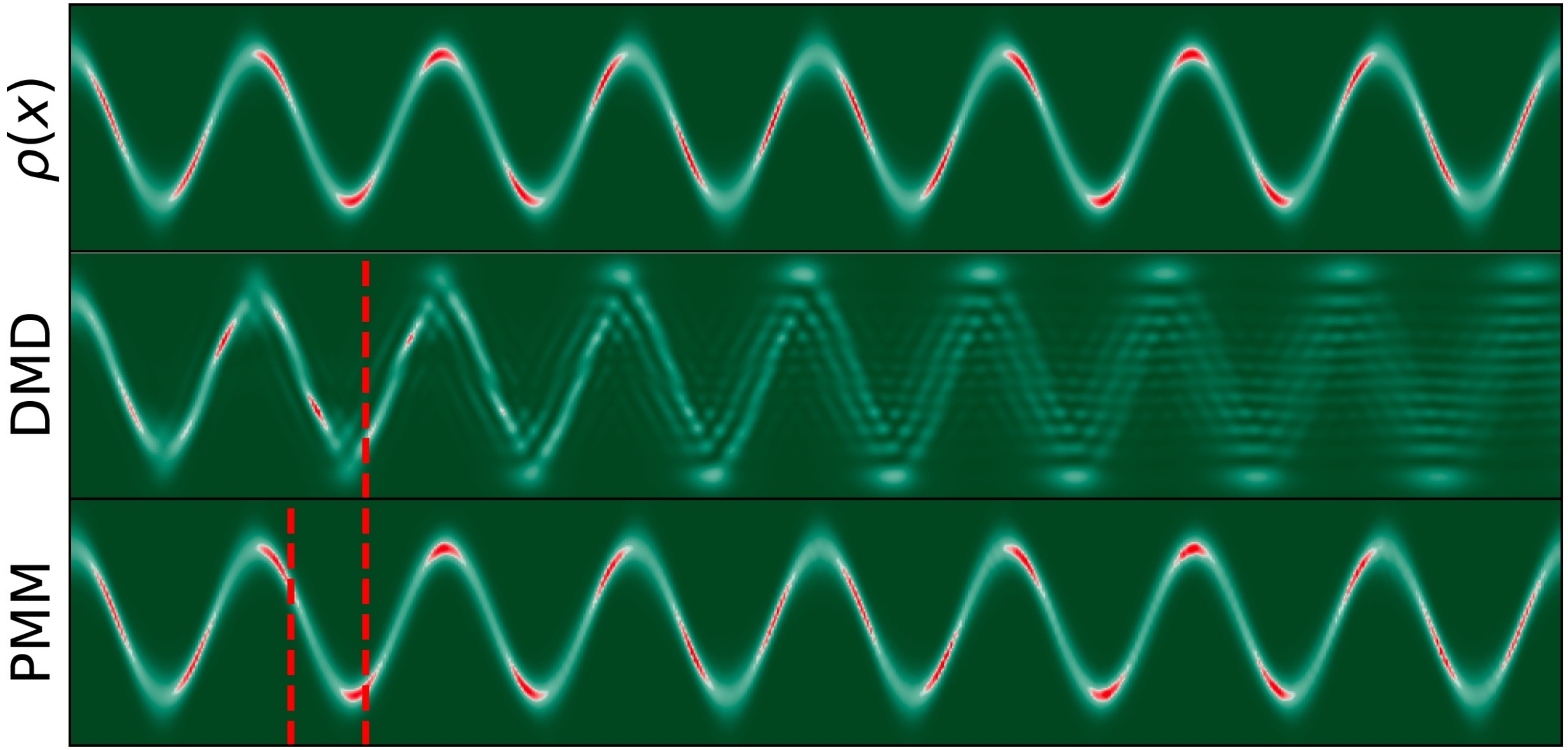
Image recognition



Dataset	Model	Accuracy	Trainable `float`
MNIST Digits[53]	PMM†	97.38	4990
	DNN-2[54]	96.5	5500
	DNN-3[54]	97.0	80 598
	DNN-5[54]	97.2	175 180
	GECCO[55]	98.04	19 000
	CTM-250[56]	98.82	31 750
	CTM-8000[56]	99.33	527 250
	Efficient-CapsNet[57]	99.84	161 824
Fashion MNIST[58]	PMM†	88.58	16 744
	GECCO[55]	88.09	19 000
	CTM-250[56]	88.25	31 750
	CTM-8000[56]	91.18	527 250
	MLP†[59]	91.63	2.9×10^6
	VGG8B(2x)[59]	95.45	28×10^6
	Fine-Tuning DARTS[60]	96.91	3.2×10^6
EMNIST Balanced[61]	PMM†	81.57	13 792
	OPIUM†[61]	78.02	8.32×10^6
	HM2-BP[62]	85.57	6.7×10^5
	CNN[63]	79.61	21 840
	CNN (Spinal FC)[63]	82.77	13 820
	CNN (Spinal FC)[63]	83.21	16 050

Gross-Pitaevskii equation

$$i\frac{\partial \Psi}{\partial t} = -\frac{1}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi + g|\Psi|^2\Psi$$




May 9-10, 2024, at FRIB