Novel Learning Methods in Nuclear Physics

Hang Yu
Center for Computational Sciences, University of Tsukuba

1. Project Purpose

In theoretical physics, making predictions compatible with existing knowledge is always vitally important. However, in the modern computational area, there are always complicated interplays between our microscopic understandings and experimental observables. Understanding one experiment is already complicated enough, let alone making compatible calculations about multiple observables and finding out the connections between them. To achieve this target in nuclear physics, over the past years, we have witnessed the statistical effort that used a technique called history matching to find non-implausible regions. This method has grown from 30 samples to 8000 samples of microscopic interactions in several years with the help of emulators, but it is still far from available to all developments in the nuclear forces. The main obstacle is the difficulty in implementing this method. It requires good practices ranging from calculating few- and many-body observables to a complicated workflow using various statistical tools. For any new improvements on the microscopic side, we will need years of collaboration to repeat the statistical process. As a result, compatible calculations using this history-matching method are still scarce in nuclear physics.

We invented a new tool called the Multiparameter Eigenvalue Problem (MEP) emulator. Our method greatly simplifies the statistical workflow, is essentially model-driven, and can also use data-driven tools (for example, some machine learning methods). This means we can examine the process to better understand its cause and improve compatibility. Alternatively, we can choose to quickly compute connections from existing data. For the first time, we may be able to systematically answer where an ab initio theory is good and where it will fail. However, our method is still in its infancy, and we need computational resources to verify our belief.

Furthermore, our MEP emulator will apply not only to uncertainty quantification in nuclear physics. The Multiparameter Eigenvalue Problems it can solve offer many new opportunities in nuclear physics, such as muti-fidelity study and basis truncation analysis. These are two potential developments we are currently looking at.

2. Results

The initial paper about this method has been accepted by PRL.

To overcome the computational cost of repeated many-body calculations, the nuclear physics community has increasingly turned to **emulators**—fast, approximate surrogates for the exact quantum mechanical solver. First-generation emulators, such as Eigenvector Continuation (EC) and Parametric Matrix Models (PMM), have shown great promise. EC, for instance, projects the Hamiltonian onto a small subspace spanned by the exact wavefunctions at a few training points, allowing for extremely fast variational interpolation.

However, these methods still fundamentally operate within the "parameter-to-observable" paradigm. They speed up the forward calculation, but they do not solve the inverse problem itself; one must still perform the Bayesian parameter estimation.

Our group has proposed a conceptual shift: the **Multiparameter Eigenvalue Problem (MEP) emulator**. This framework establishes a direct link from "observables to observables".[1] Instead of using noisy data to fix parameters, the MEP emulator learns the

intrinsic correlations (or the "physical manifold") between different physical measurements. By treating a measurable quantity (like the binding energy of a nucleus) as an input feature, the method allows us to predict unknown observables (such as an excited state energy or a reaction cross-section) directly from available data.
This approach effectively cuts out the "middleman" of LEC calibration. In our preliminary work on the exotic nucleus **Oxygen-28** , we demonstrated that the MEP emulator could efficiently generate probability distributions for predictions, offering a rigorous way to quantify uncertainty without the prohibitive computational cost and additional assumptions of traditional parameter fitting.[1] The critical next step, and a primary objective of this MCRP proposal, is to perform a systematic study of the numerical stability and domain of validity of this new emulator to ensure it can be reliably applied across the nuclear chart.

A new application in the reaction theory has been established, and we are finalizing our manuscript.

We are also already expanding the validity of our inverse problem emulator to a new territory. With our interest in the **nuclear reaction theory** in the astrophysical environment, we find that a similar inverse problem is usually solved to compute reactions from an ab-initio perspective. In our ongoingwork, we extend the MEP method to address this bottleneck. By training the emulator to map *ab initio* observables (derived from Chiral EFT interactions) directly to scattering phase shifts, we bypass the computationally prohibitive costs associated with determining the effective interactions. We have successfully validated this framework using alpha-alpha and neutron-alpha scattering as a benchmark. Our method is model-independent, functioning seamlessly across distinct numerical methods, including both Harmonic Oscillator (NCSM and MCSM) and Lattice (NLEFT) formulations. This work enables rigorous *ab initio* predictions for scattering observables, providing a new pathway for reaction theory.

3. Roles of the MCRP and its significance
MCRP provided the essential computational foundations for both lines of research presented here. The large-scale many-body calculations required to train and validate the MEP emulator—spanning realistic nuclear systems from light nuclei to medium-mass isotopes such as Oxygen-28—would not have been feasible without access to the Pegasus, Miyabi-G, and Miyabi-C supercomputing resources allocated through MCRP. Without this support, our emulator would have remained confined to simple toy models and could not have been benchmarked against realistic nuclear interactions. The availability of these HPC resources has been decisive in establishing the numerical stability of the MEP framework and in enabling its extension to nuclear reaction theory, directly accelerating the acceptance of our PRL paper and the preparation of the ongoing reaction-theory manuscript.

4. Future plan
Foundational work:
We plan to develop the data-driven component of the MEP emulator further by incorporating constrained optimization techniques. Specifically, we will impose physically motivated constraints into the learning procedure, improving both the robustness of predictions and their physical interpretability. This will also allow us to systematically quantify the domain of validity of the emulator across the nuclear chart, addressing one of the central open questions identified in our PRL paper.

Exploratory work:
We plan to connect our ab initio reaction framework to observed astrophysical elemental abundances by computing the rates of successive alpha-capture reactions (alpha chains) in stellar fusion environments. These reactions are central to nucleosynthesis in helium-burning stars, and current theoretical predictions carry large uncertainties. By applying the MEP-based reaction emulator, we aim to provide more reliable rate estimates that can be directly compared with observed abundance patterns, offering a new ab initio pathway to nuclear astrophysics.

5. Publications and conference presentations

(1) Journal papers

- Jacobi Coordinates on Hyper-tori and Geometric Factors in the Volume Dependencies
  Hang Yu
  2025-11
  Submitted to Physical Review C.
  e-Print: 2511.06726 [nucl-th]

- Quantifying alpha clustering in the ground states of 16-O and 20-Ne
  E. Harris, M. Barbui, J. Bishop, G. Chubarian, Sebastian Konig, E. Koshchiy, K.D. Launey, Dean Lee, Zifeng Luo, Yuan-Zhuo Ma, Ulf-G. Meissner, C.E. Parker, Zhengxue Ren, M. Roosa, A. Saastamoinen, G.H. Sargsyan, D.P. Scriven, Shihang Shen, A. Volya, **Hang Yu**, G.V. Rogachev
  2025-07
  Submitted to PRL
  e-Print: 2507.17059 [nucl-ex]

- An Efficient Learning Method to Connect Observables
  Hang Yu and Takayuki Miyagi
  2025-03
  Accepted by PRL, DOI:10.1103/33q9-76qp
  e-Print: 2503.01684 [nucl-th]

(2) Presentations

- An Efficient Learning Method to Connect Observable and the Continuum, H. Yu, DRHBc 2026 workshop, Kitakyushu, Japan (April 2026) **Contributed talk**

- An Efficient Learning Method to Connect Observable, H. Yu, Frontier Nuclear Physics Symposium Related to HIAF, Huizhou, China (April 2026) **Invited talk**

- An Efficient Learning Method to Connect Observables, H. Yu, RIBF Users Meeting 2026 (March 2026) **Poster**

- An Efficient Learning Method to Connect Observables, H. Yu, Workshop on Nuclear Cluster Physics 2025 Huizhou, China (November 2025) **Contributed talk**

- A general Method for ab initio Nuclear Reaction, H. Yu, Workshop on Three-Nucleon Interactions and Nuclear Dynamics, Bochum, Germany (December 2025) **Contributed talk**

- An Efficient Learning Method to Connect Observable, H. Yu, Frontiers in NLEFT, Beihang, Beijing, China,(April 2025) **Invited talk**

(3) Others

- A General Volume Dependence Prescription from Projection-Based Inversion

Hang Yu, Serdar Elhatisari, Sebastian Koenig, Dean Lee, Yuanzhuo Ma and Takayuki Miyagi
Finalizing Manuscript. Plan to submit to PRL

Supercomputer	Use	Allocated resources*		
		Initial resources	Transferred resources**	Purchased resources
Pegasus	Yes	3600	0	0
Miyabi-G	Yes	16200	0	0
Miyabi-C	Yes	5760	0	0
	*in units of node-hour product ** If the budget transfer was performed, fill in here, such as “+ 2000” and “− 1000”.			