Projection-based emulators for quantum continuum states: type-I with real energies

Xilin Zhang (FRIB)

U.S. DEPARTMENT OF ENERGY | Office of Science

Theory Alliance
FACILITY FOR RARE ISOTOPE BEAMS

Objectives

- Continuum state computations are generally expensive, if possible at all. The large costs restrict or even preclude many calculations of interest, including employing the full continuum models in analyzing measurements, such as nucleon-deuteron and deuteron-nucleus scatterings.
- To solve this long-standing bottleneck problem, we have developed projection-based emulators for three-body scattering in a proof of principle study [1]. They work for a given real energy at a time and offer fast interpolation and extrapolation in the Hamiltonian parameter space.

EC emulators	S relative error	Time	Memory
linear[a]	10^{-14} to 10^{-13}	ms	$<$ MB
nonlinear-1	10^{-6} to 10^{-5}	ms	MB
nonlinear-2	10^{-4}	ms	10s MB

Table I: the performance of the three-body emulators in [1]. S is the particle-dimer scattering phase shifts.

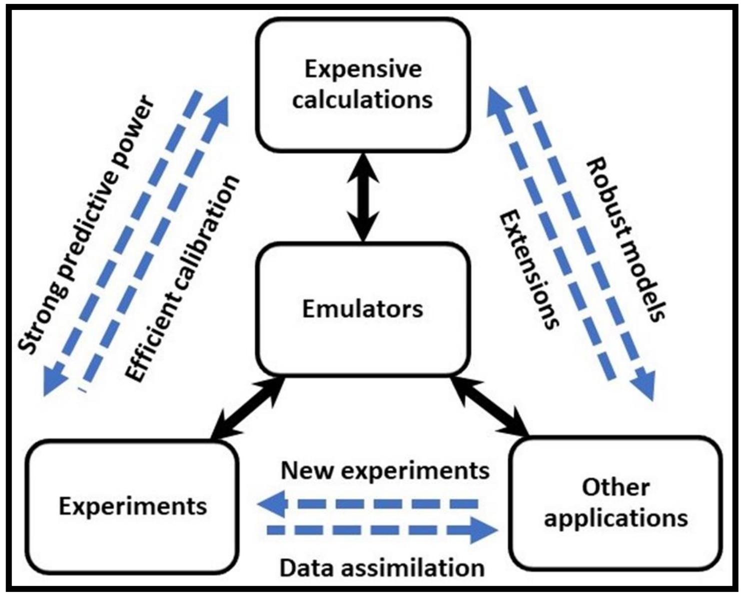

Fig. I: potential impact of emulators on general research workflow via creating new connections between different research groups [1].

Impact

- The study in [1] demonstrates the high accuracy of the projection-based emulators in the interpolations and extrapolations and the negligible computing costs for running emulators, as shown in Table I.
- The work provides a clear road map for developing the same type of emulators for nucleon-deuteron and deuteron-nucleus scatterings. The former scattering is needed for calibrating chiral interactions, the basic inputs for ab initio calculations. The latter is one main experimental tool for studying rare isotopes at FRIB.
- With these three-body emulators, physicists can perform model calibrations and error propagations with full theories in the Bayesian statistics framework. As the result, the theory content can be fully and rigorously extracted from experimental measurements.
- The emulators, as the interfaces for the large computations, allow the potential users to access these calculations and complex models with minimum costs, and thus bring the large calculations and complex models closer to the users, as shown in Fig. 1.

Accomplishments

[1] X. Zhang and R. J. Furnstahl, Phys.Rev.C 105 (2022) 6, 064004