Recent developments on projection-based emulators for quantum continuum states

Xilin Zhang
Facility for Rare Isotope Beams
Michigan State University

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Outline

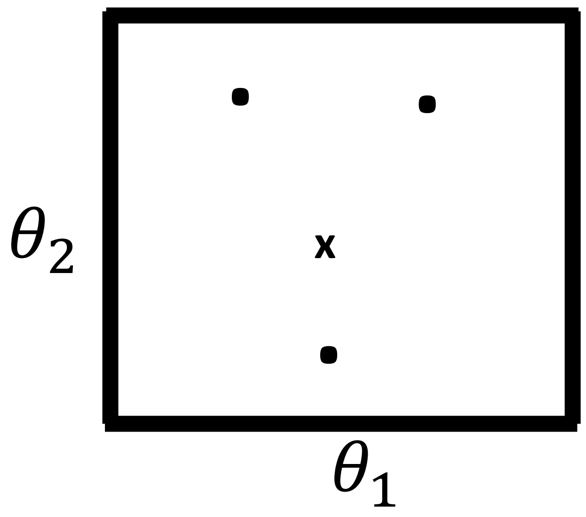
- Emulators: general discussions, applications, and eigenstate emulators
- Continuum state emulators based on real energies: two and three-body systems
- Continuum state emulations in the complex energy plane: two and three-body systems
- Summary

Emulators and their applications

Emulator (surrogate model) enables fast and accurate interpolation and extrapolation of model **outputs** in the **input** parameter space

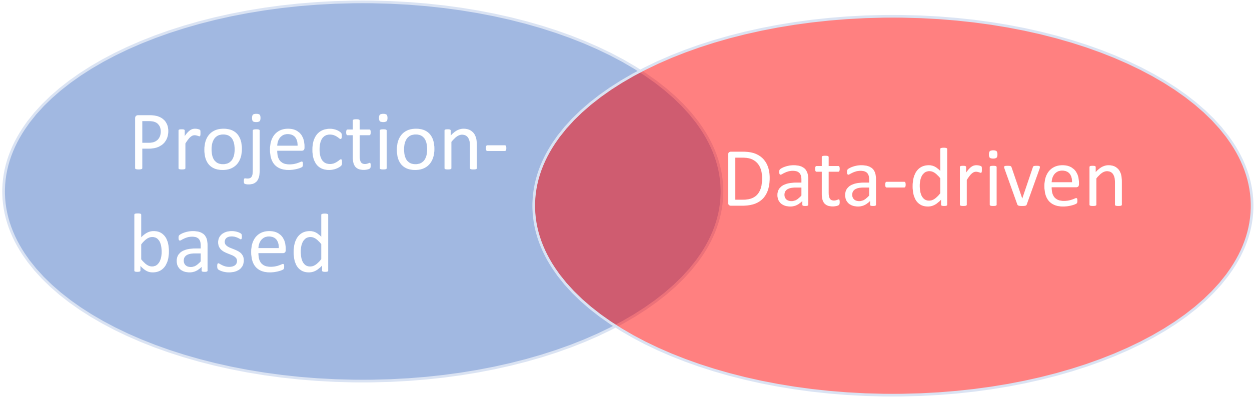
- Model calibrations and error propagation (in Bayesian statistics)
  - Chiral (e.g., three-body) interactions to exp. data (e.g., $N-d$ scattering)
  - Error propagations for many-body calculations
- New calculations
  - Extrapolations from feasible calculations→ infeasible regions
  - Calibrating macroscopic (cluster) theories against microscopic calculations: Luscher-type approach

Parameter space ($\boldsymbol{\theta}$)



Emulators

"Eigenvector continuation with subspace learning"
Dillon Frame et. al., *Phys.Rev.Lett.* 121 (2018) 3, 032501, 1711.07090

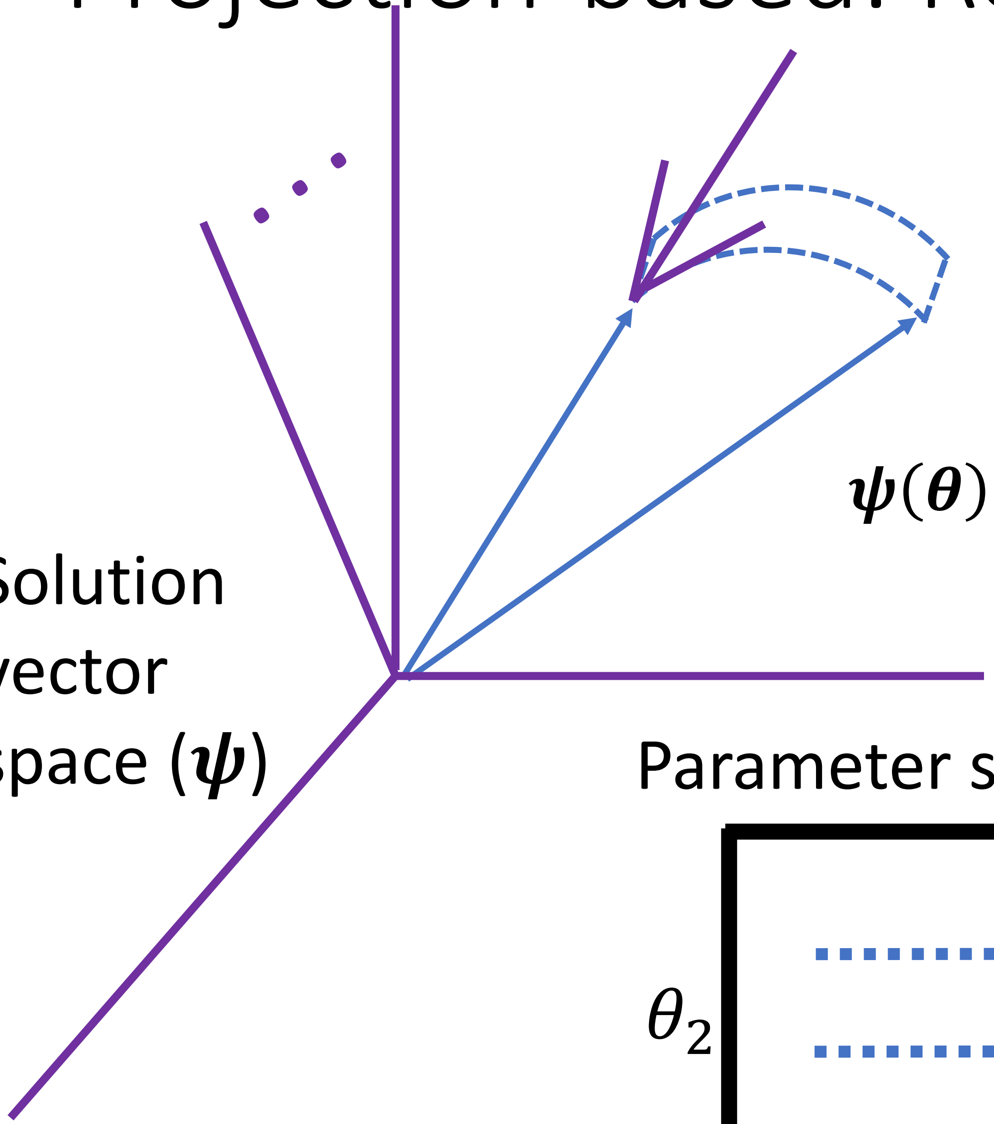


- Reduced basis method (RBM); also known as eigenvector continuation (EC) in nuclear physics
- Intrusive
- but includes more physics, requires less training data, and has better extrapolation

- Machine learning (ML): Gaussian process and neural networks
- nonintrusive
- agnostic of physics and requires more training data

"BUQEYE Guide to Projection-Based Emulators in Nuclear Physics," C. Drischler, J.A. Melendez, R.J. Furnstahl, A.J. Garcia, and XZ, 2212.04912
"Training and projecting: A reduced basis method emulator for many-body physics," Edgard Bonilla, Pablo Giuliani, Kyle Godbey, Dean Lee, *Phys.Rev.C* 106 (2022) 5, 054322, 2203.05284
"Model reduction methods for nuclear emulators, " J.A. Melendez, C. Drischler, R.J. Furnstahl, A.J. Garcia, XZ, 2203.05528

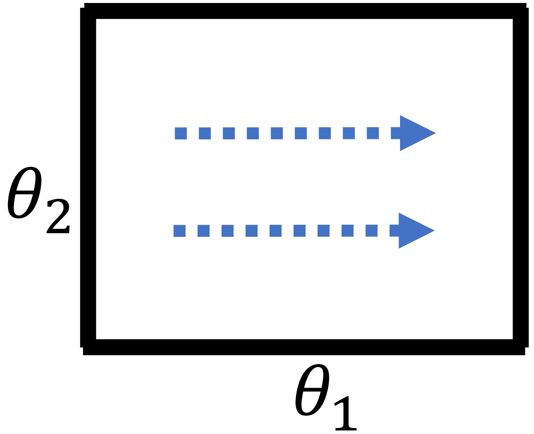
Projection-based: Reduced basis method (RBM)

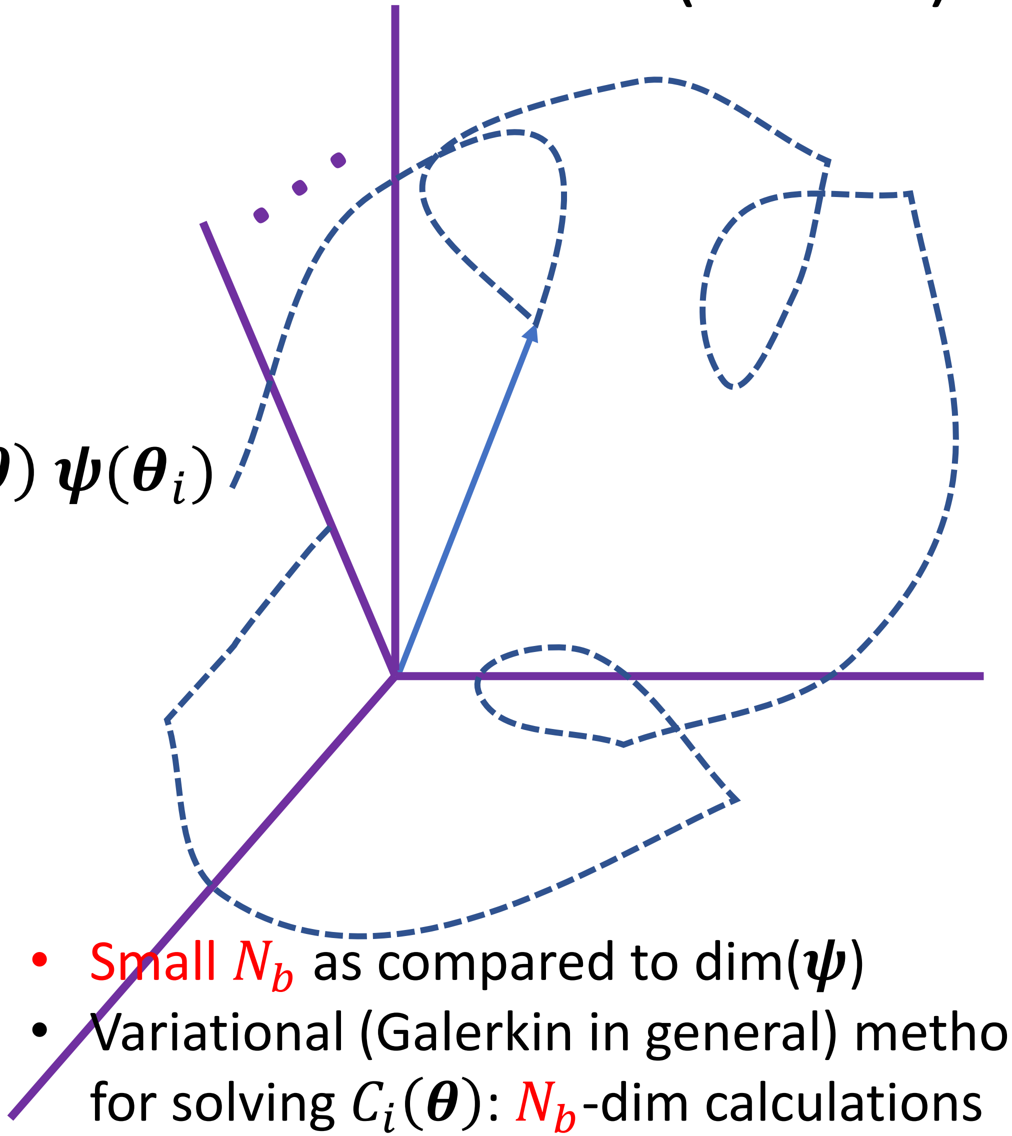


Solution vector space ($\boldsymbol{\psi}$)

$$\boldsymbol{\psi}(\boldsymbol{\theta}) = \sum_{i=1}^{N_b} C_i(\boldsymbol{\theta})\, \boldsymbol{\psi}(\boldsymbol{\theta}_i)$$

Parameter space ($\boldsymbol{\theta}$)

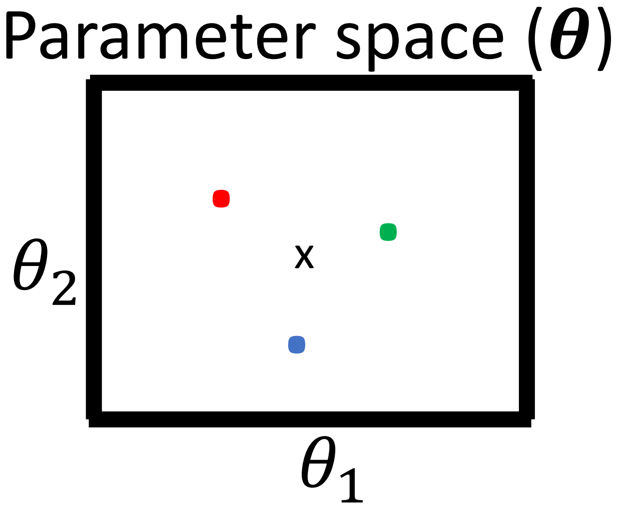


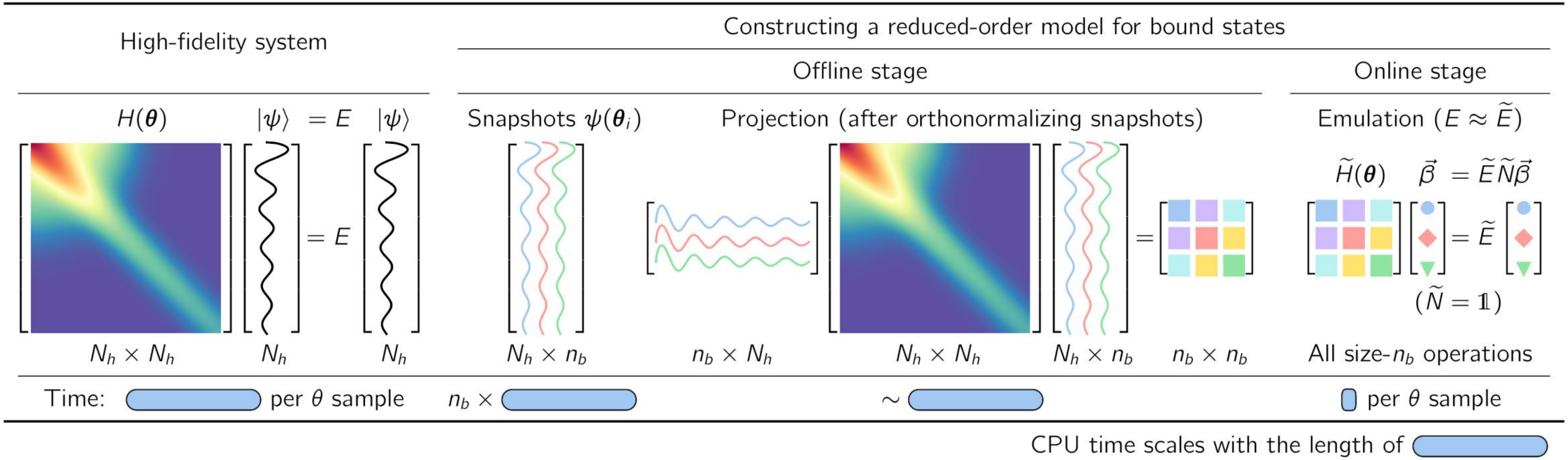


- Small N_b as compared to dim($\boldsymbol{\psi}$)
- Variational (Galerkin in general) method for solving $C_i(\boldsymbol{\theta})$: N_b-dim calculations
- Solved $\boldsymbol{\psi}$s need to be precise

RBM emulators for nuclear structure: eigen systems of *parametrized* quantum Hamiltonians $H(\boldsymbol{\theta})$

$$|\psi_t\rangle = \sum_{i=1}^{N_b} c_i |\psi_{\mathrm{gs}}(\boldsymbol{\theta}_i)\rangle$$



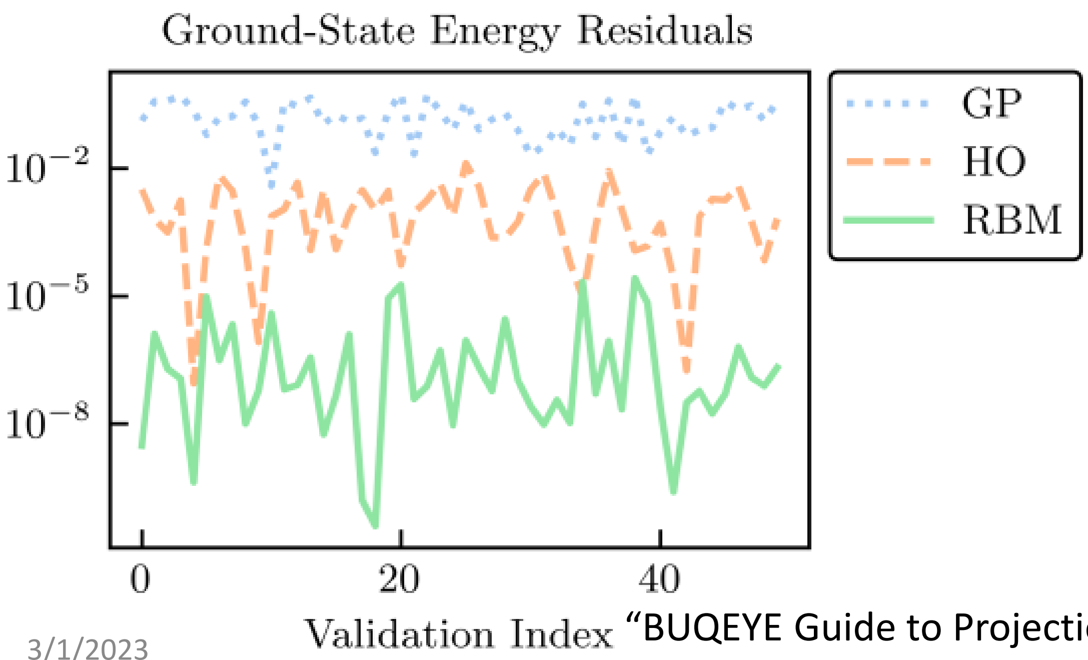


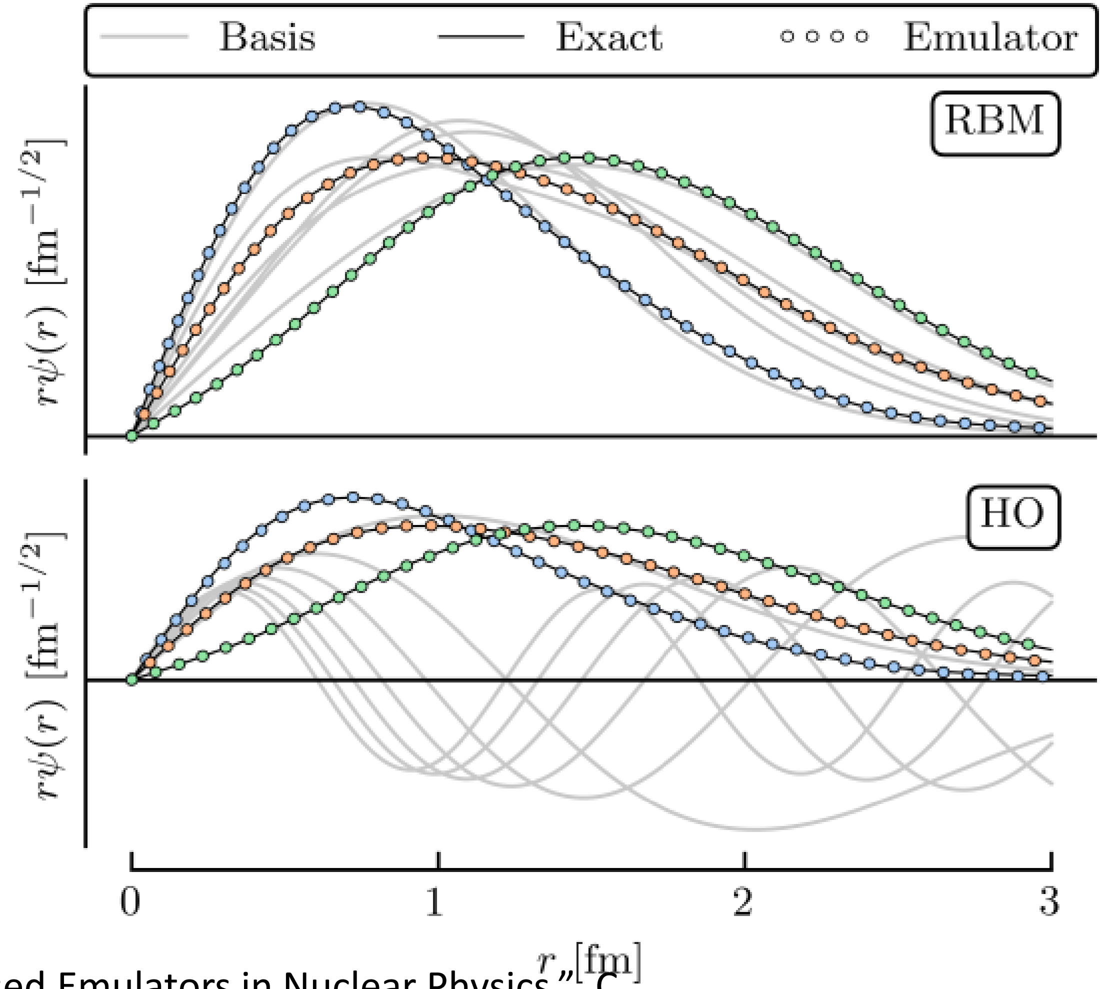
"BUQEYE Guide to Projection-Based Emulators in Nuclear Physics,"
C. Drischler, J.A. Melendez, R.J. Furnstahl, A.J. Garcia, and XZ, 2212.04912
König et. Al., (2019); Ekström et.al., (2019); Yoshida (2021, 2023); Baran et.a., (2023) Franzke et.al. (2021, 2023)

A toy-model: emulator comparisons

$$V(r;\boldsymbol{\theta}) = V_{\mathrm{HO}}(r) + \sum_{n=1}^{3} \theta_n \exp(-r^2/\sigma_n^2),$$

6 training points in 3-dim space





"BUQEYE Guide to Projection-Based Emulators in Nuclear Physics," C. Drischler, **J.A. Melendez**, R.J. Furnstahl, A.J. Garcia, and XZ, [2212.04912](2212.04912)

RBM emulators for nuclear continuum states

$$[E - H(\boldsymbol{\theta})]|\psi(\boldsymbol{\theta})\rangle = 0 \text{ for a given } E$$

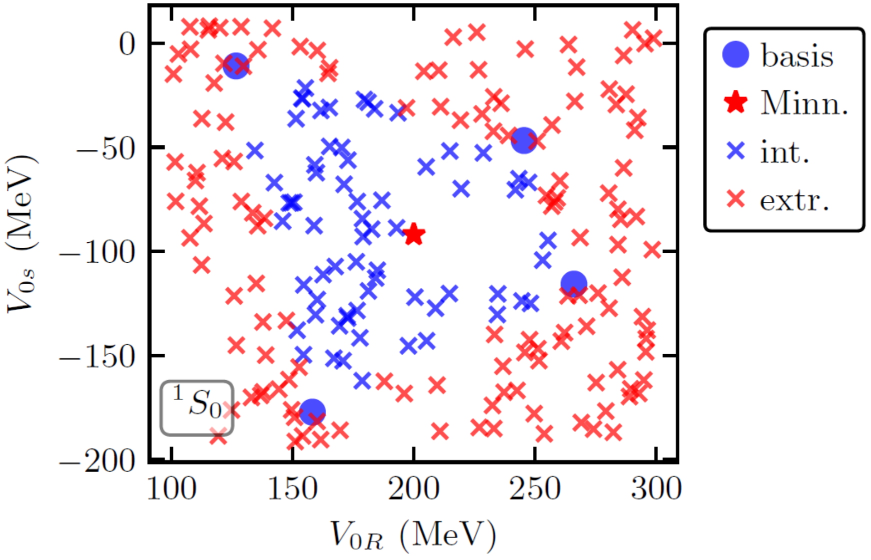
"Efficient emulators for scattering using eigenvector continuation,"R. J. Furnstahl, A. J. Garcia, P. J. Millican, and XZ, PLB **809,** 135719 (2020) [2007.03635]

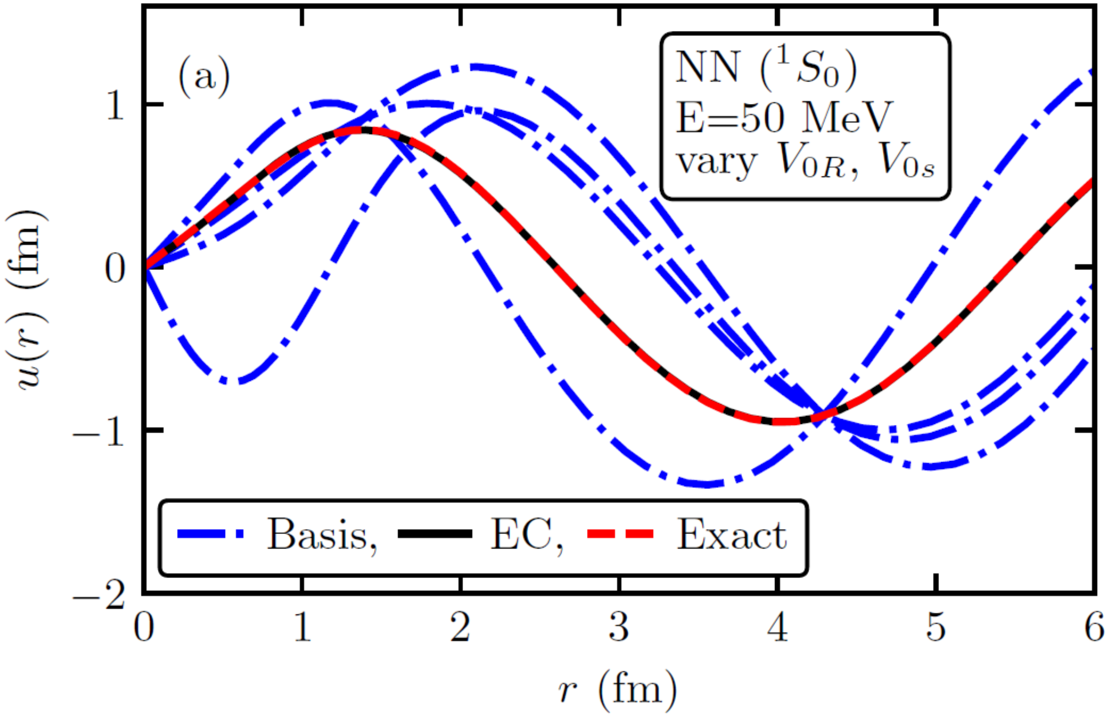
- Developed RBM emulator for two-body scatterings based on variational principle for scattering
- Systems with and without Coulomb interaction
- Complex optical potential
- General partial waves (or without pw decomp.)
- Need to deal with Kohn anomalous singularities

$$|\psi_t\rangle = \sum_{i=1}^{N_b} c_i |\psi_{\rm gs}(\boldsymbol{\theta}_i)\rangle$$

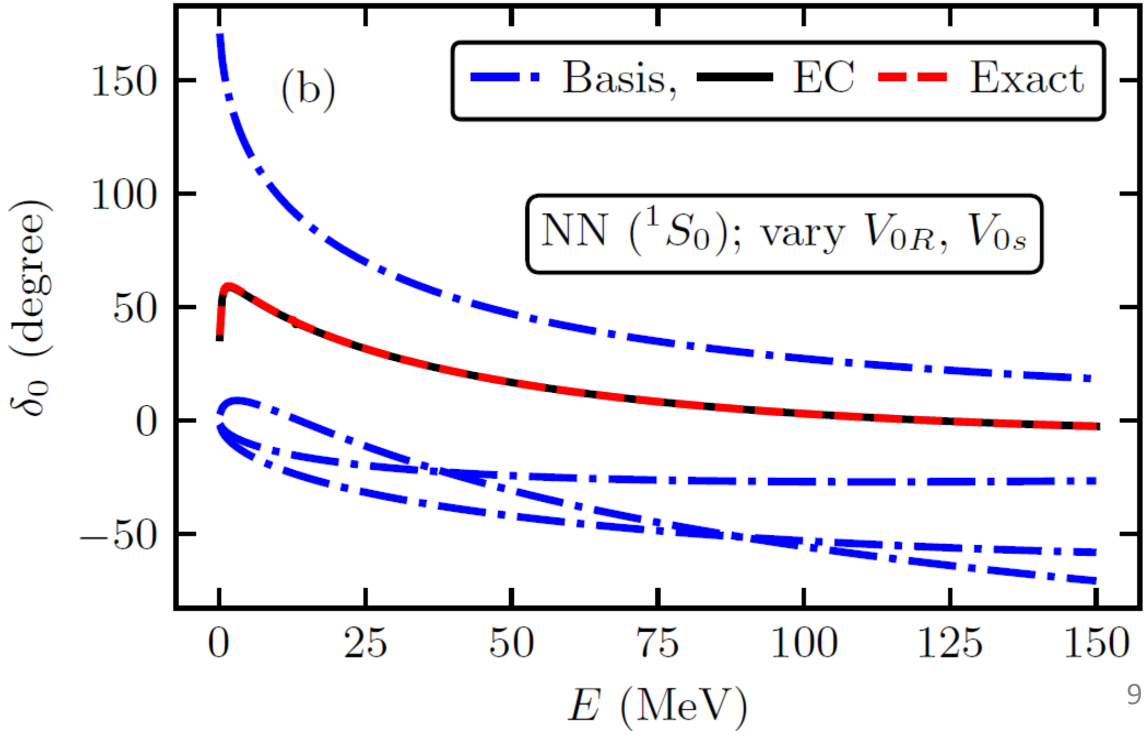
D. Bai & Z. Ren (2021); C. Drischler, et. al., (2021); J.A. Melende et.al., (2021); D. Bai (2022)…

Tests of the emulators: NN scattering



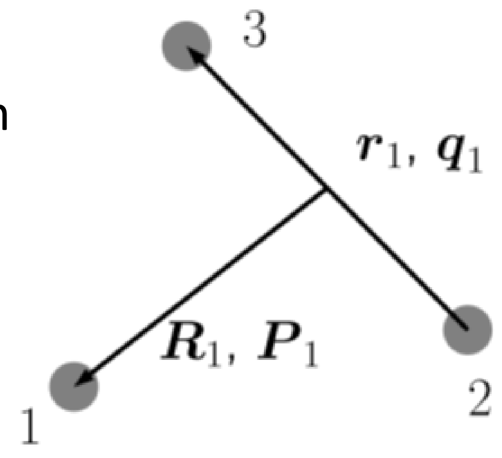


$$V_{^1S_0}(r) \equiv V_{0R}e^{-\kappa_R r^2} + V_{0s}e^{-\kappa_s r^2}$$



More complexities

“Fast emulation of quantum **three-body** scattering”, XZ and R.J. Furnstahl, Phys. Rev. C 105, 064004 (2022), 2110.04269

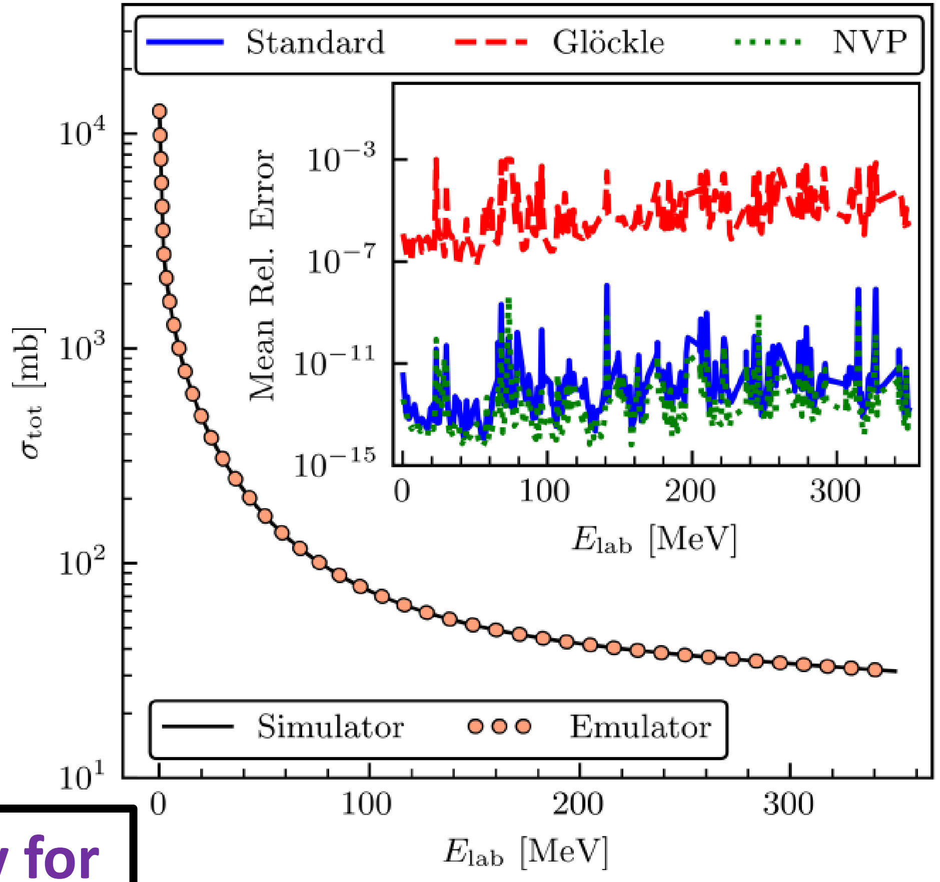


EC emulators	S relative error	Time	Memory
linear[a]	10^{-14} to 10^{-13}	ms	< MB
nonlinear-1	10^{-6} to 10^{-5}	ms	MB
nonlinear-2	10^{-4}	ms	10s MB

In contrast, the costs of full realistic calculations are 10^3s

$n-p$ coupled-channel

“Wave function-based emulation for nucleon-nucleon scattering in momentum space,” A.J. Garcia, C. Drischler, R.J. Furnstahl, J.A. Melendez, XZ (2301.05093)

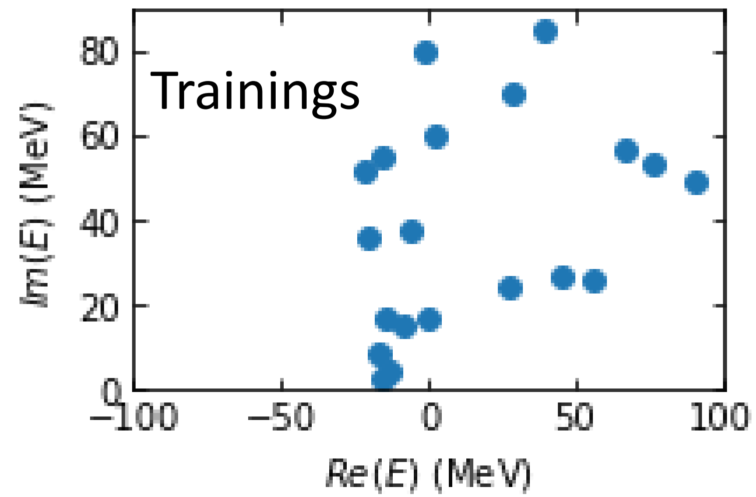


These studies require the same real energy for trainings and emulations.

Emulating continuum states in energy’s complex plane

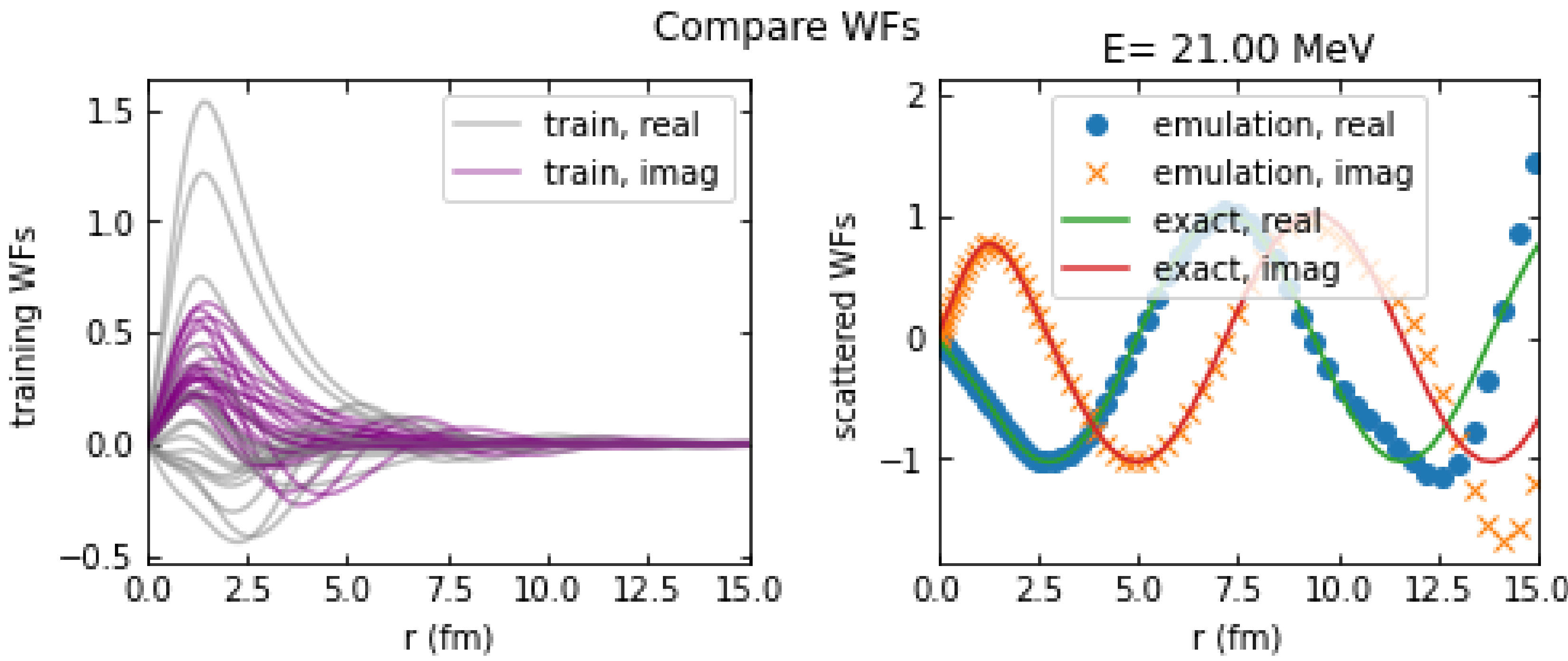
Preliminary results

Emulation in E-complex plane: two-nucleon examples



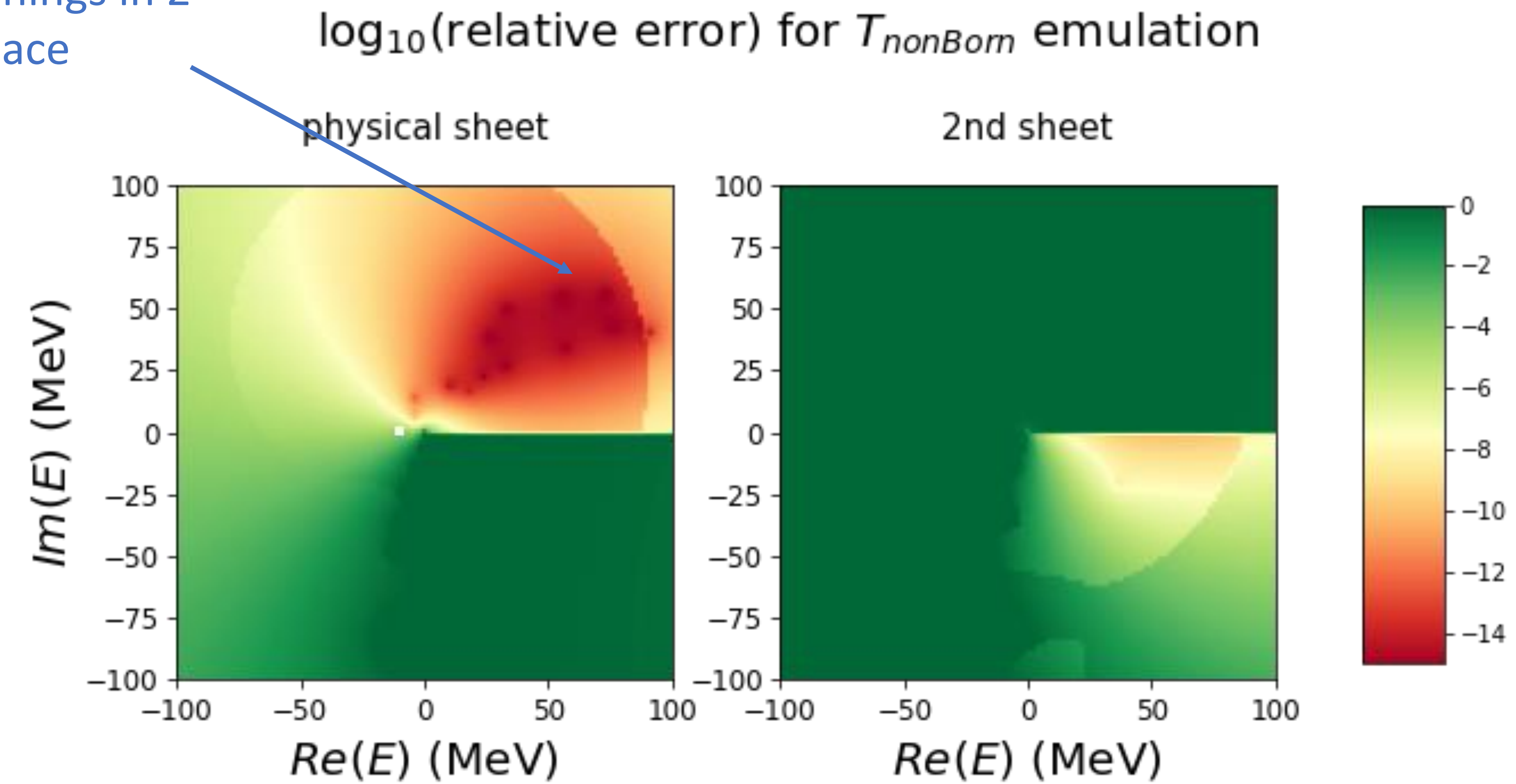
- Training (outgoing) wave functions (WFs) are localized
- Bound state methods for trainings

- Emulations → continuum states
- A new approach for computing continuum states based on structure solvers
- Also allows emulations for other parameters

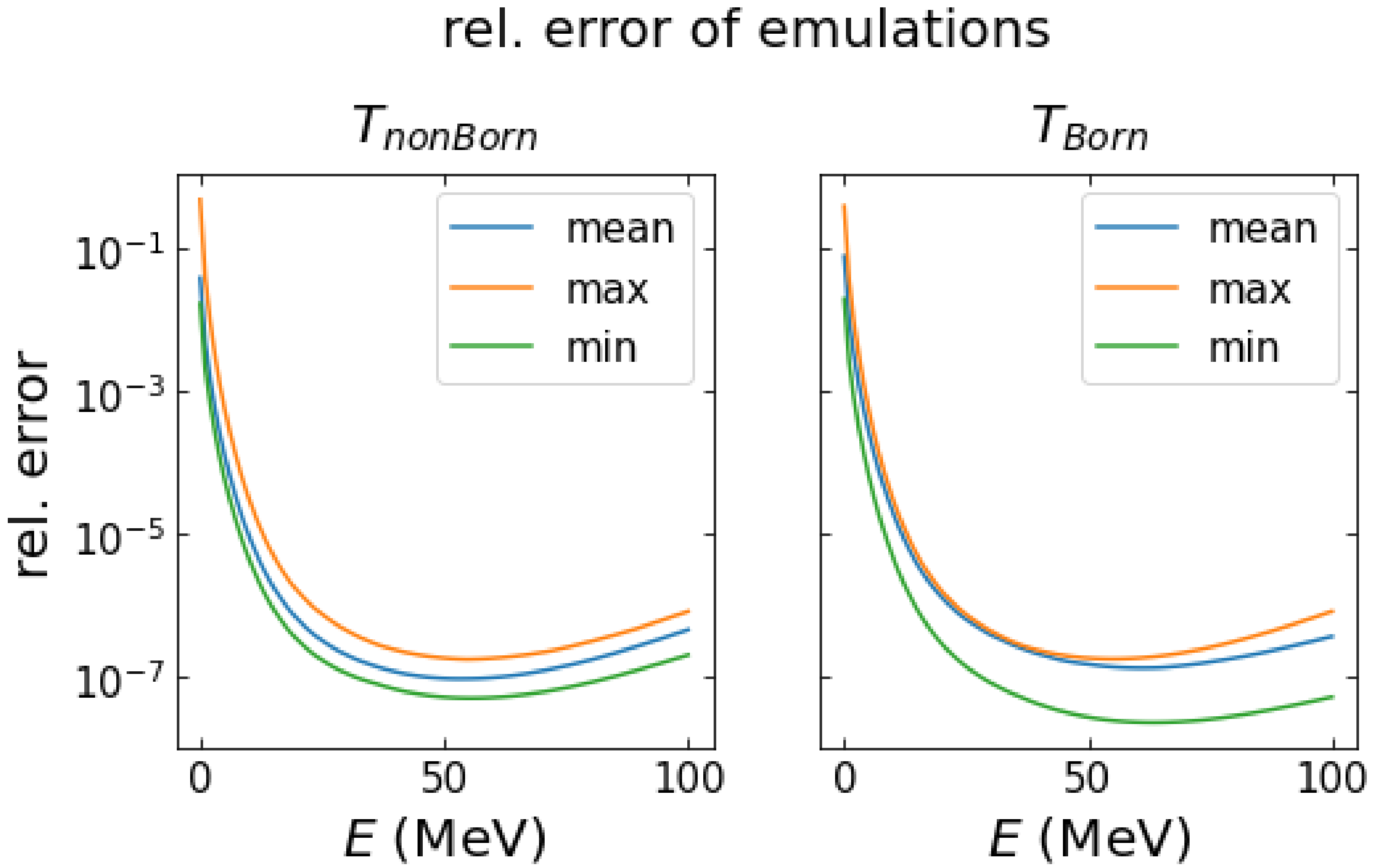


Emulation in E-complex plane: two-body in s-wave

10 Trainings in 2-dim space



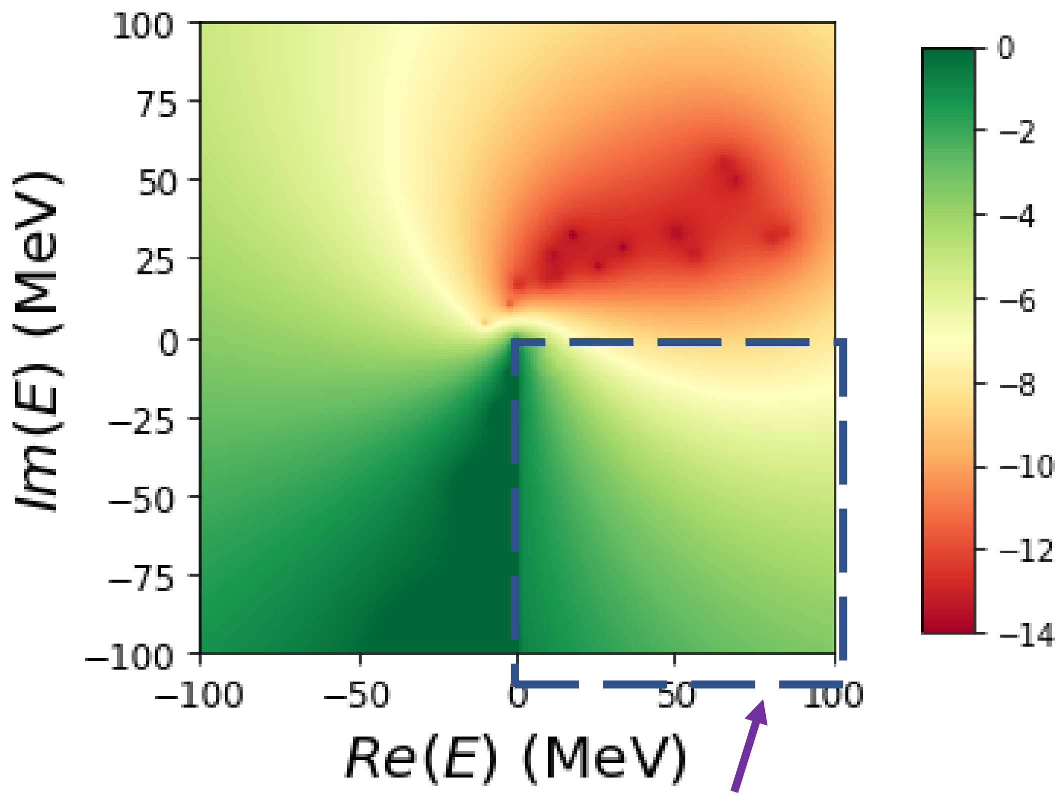
Emulation in E-complex plane: two-body in s-wave



10 training points in 4-dim space: E_{in}, $Re(E)$, $Im(E)$, potential strength

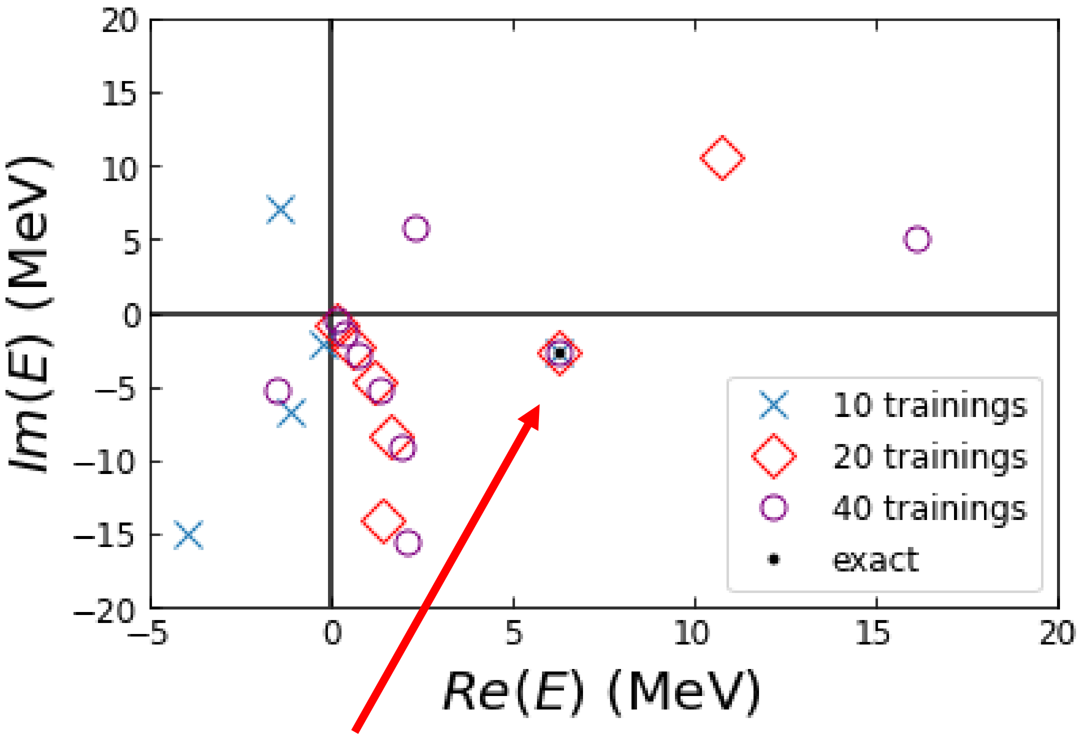
Emulation in E-complex plane: two-body in p-wave

log$_{10}$(relative error) for $T_{nonBorn}$ emulation



The 4th quadrant is on the 2nd Riemann sheet; others on the physical sheet

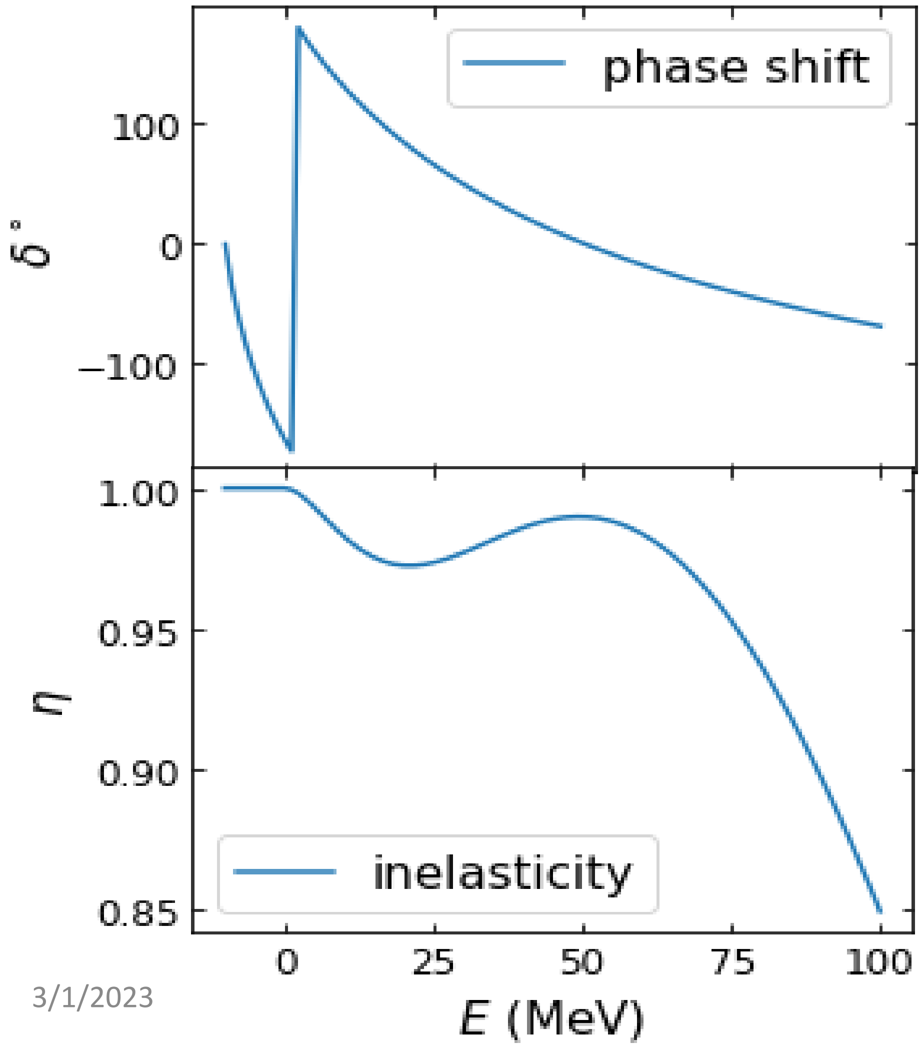
- Emulation → fast identifications of bound state and resonances
- The poles correspond to the complex eigenvalues of a complex symmetrical H (full H projected to training-solution subspace)

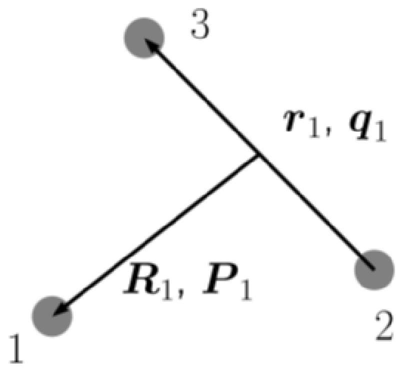


Resonance at $6.3 - 2.7i$ MeV

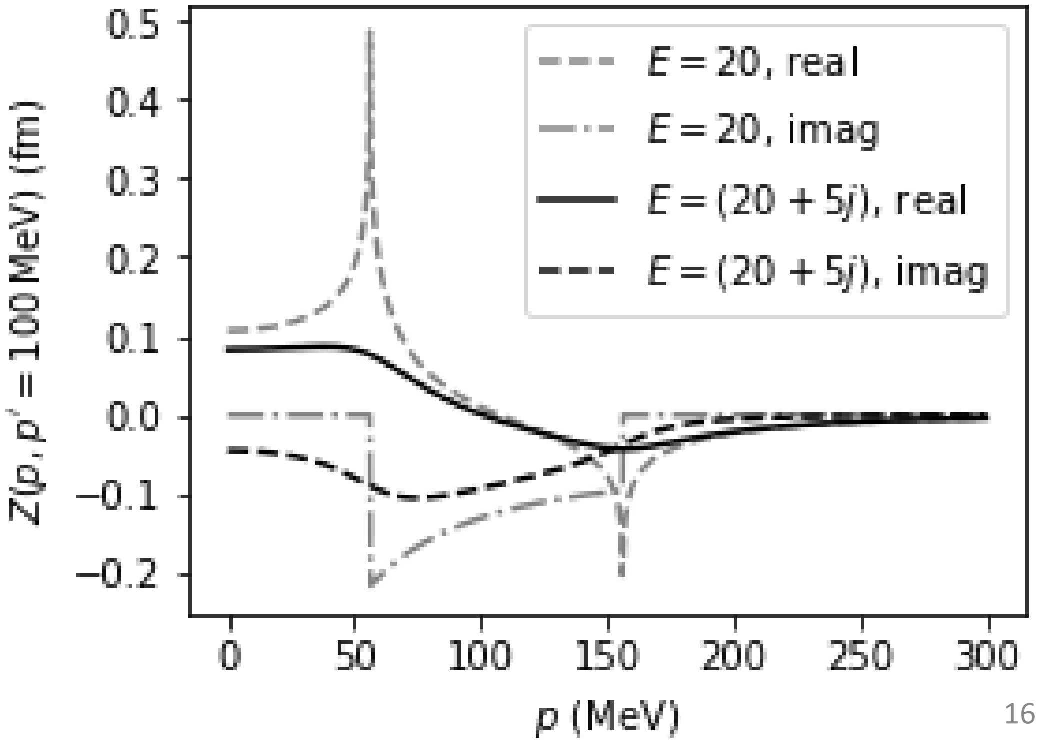
Three-boson scattering

Full calculations:



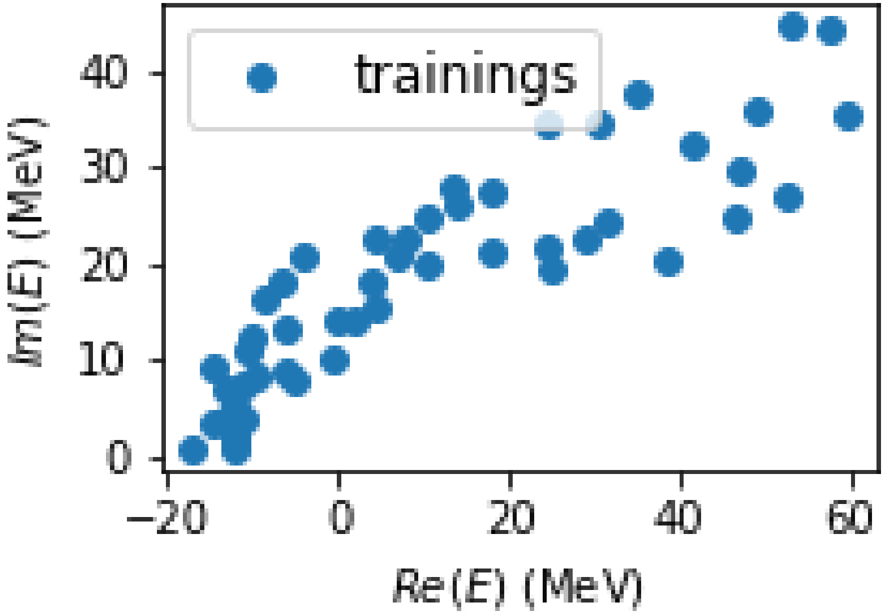


The challenge for direct continuum calculations:

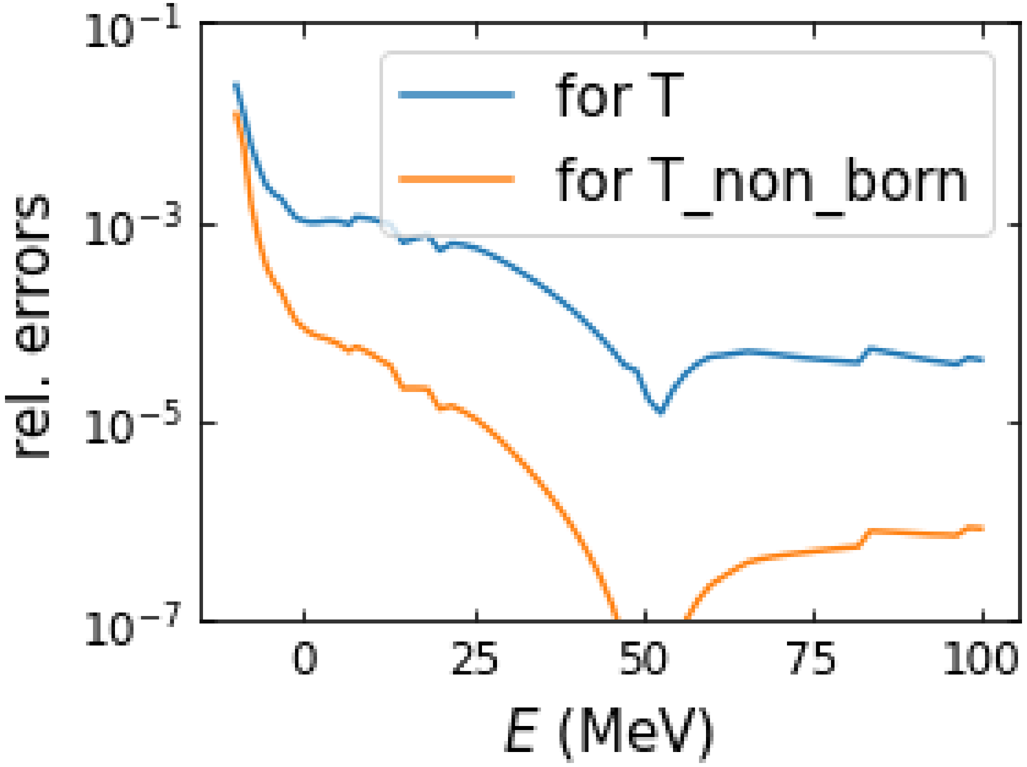


Three-boson scattering

80 training points in 3-dim space:
$E_{in}, Re(E), Im(E)$



Emulation errors



Collaborating with **Bijaya Acharya** and **Alex Gnech** (also experimenting with BIGSTICK, thanks to **Calvin Johnson**) to generalize it to many-body continuum physics

Comparisons to previous works

- Complex-E calculations have been performed before in few-body (scattering) and many-body (e.g., response function) calculations
- There are different methods for transferring the complex-E results to the real-energy region
  - extrapolation based on Pade approximations: started by Schlessinger&Schwartz 1966 (and their later works), and in nuclear physics by Kamada, Glockle, et. al. since 2003, later by Deltuva et. al.
  - Regression-based, such as in Lorentz integral transformation (Efros et. al. JPG: Nucl. Part. Phys. 34 R459, 2007, many works by Bacca et. al.)
- Complex- E emulation provides a different E-extrapolation, in addition to emulating interaction parameters

Summary

- Projection-based emulators enable efficient interpolation and extrapolation for theory outputs in the input parameter space
  - They are useful for model calibration and error propagation (in Bayesian statistics)
  - They can enable new calculations
- Real- E continuum-state emulators start progressing to realistic calculations
- Complex- E emulators provide a 2nd option; they enable continuum-state calculations based on bound-state calculation methods, efficient identification of resonances, and fast interaction parameter space exploration
- Next steps: their implementations in $N-d$ (simulation) data analysis; many-body continuum state calculations and emulations

Stay tuned!

Back up

Emulators for calibrating few-body models to simulations

INT Program on Nuclear Physics for Precision Nuclear Physics (April 19 to May 7, 2021).

8 Few-Body Emulators Based on Eigenvector Continuation
by Christian Drischler, Xilin Zhang

In this contribution we briefly recapitulate the progress made in constructing fast and accurate emulators for few-body scattering and reaction observables based on eigenvector continuation.[2] Emulators have been game changers and we envision them to play a key role in future workflows in nuclear physics and beyond. They have the potential to push the frontier of precision nuclear physics even further by enabling full Bayesian analyses of nuclear structure, scattering, and reaction observables, as well as by facilitating constraints for chiral interactions from (lattice) quantum chromodynamics (QCD). The future will show what other exciting applications are within reach.

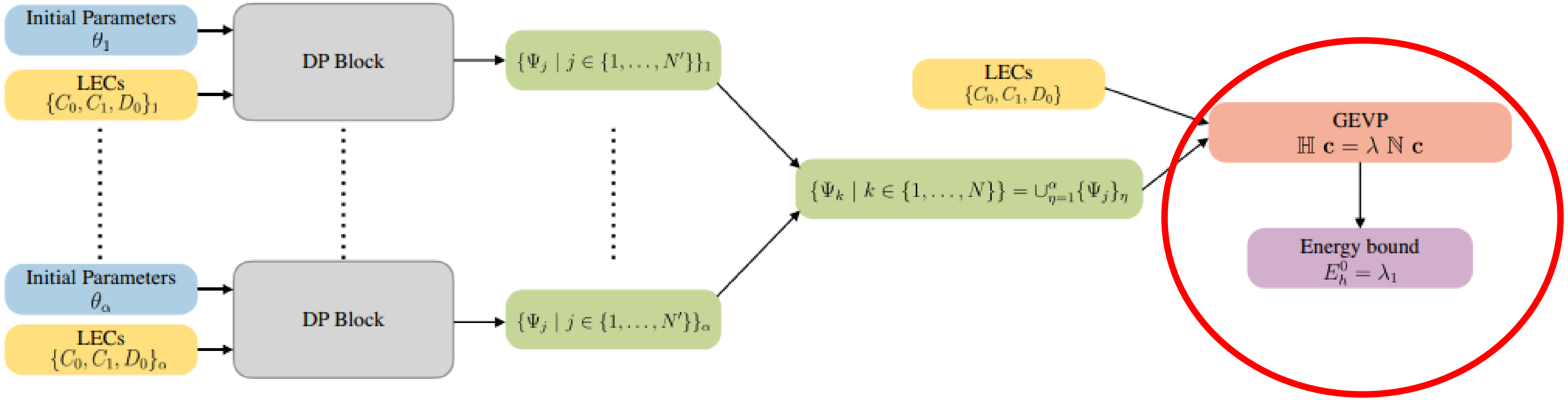
Emulators for calibrating models to simulations

PHYSICAL REVIEW D **105,** 074508 (2022)

Finite-volume pionless effective field theory for few-nucleon systems with differentiable programming

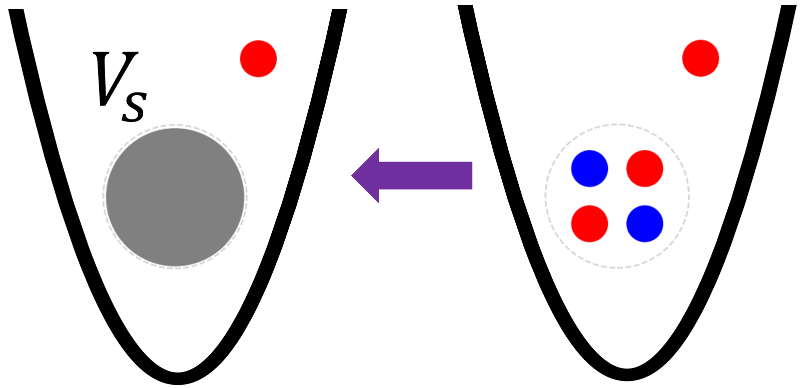
arXiv: 2202.03530

Xiangkai Sun, William Detmold, Di Luo, and Phiala E. Shanahan

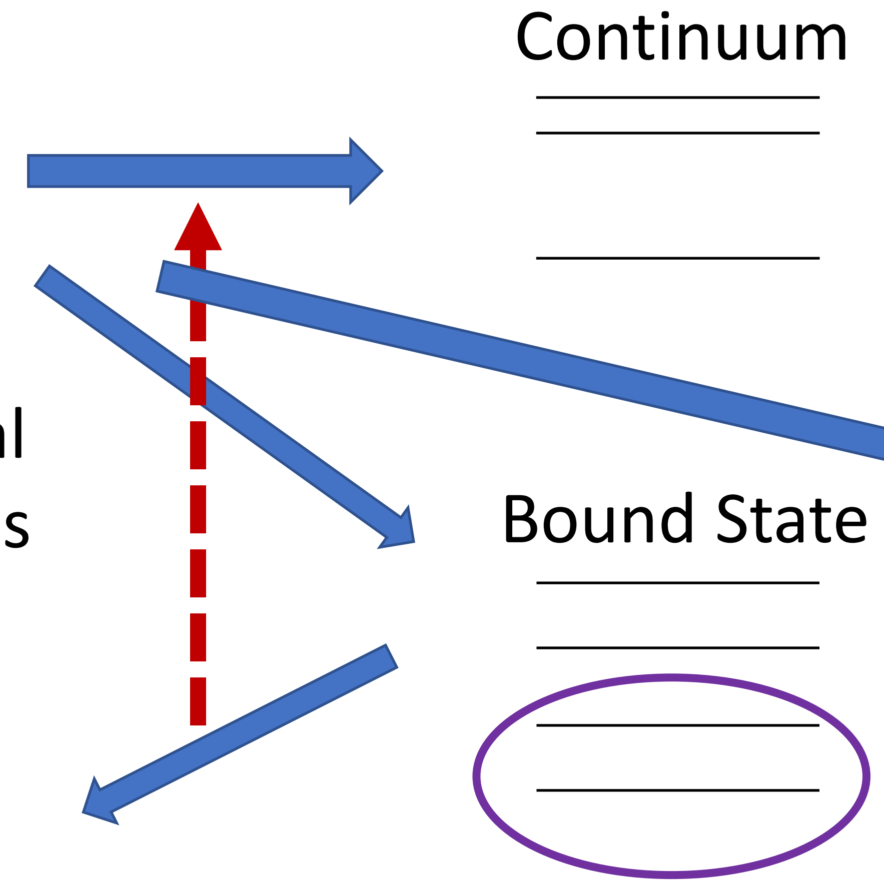


(b) Generalized eigenvalue problem (GEVP) block.

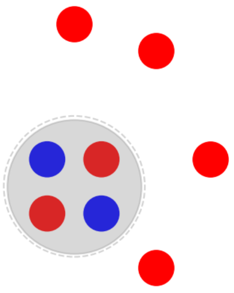
Emulators for calibrating models to simulations



Trap them in external potential within microscopic calculations



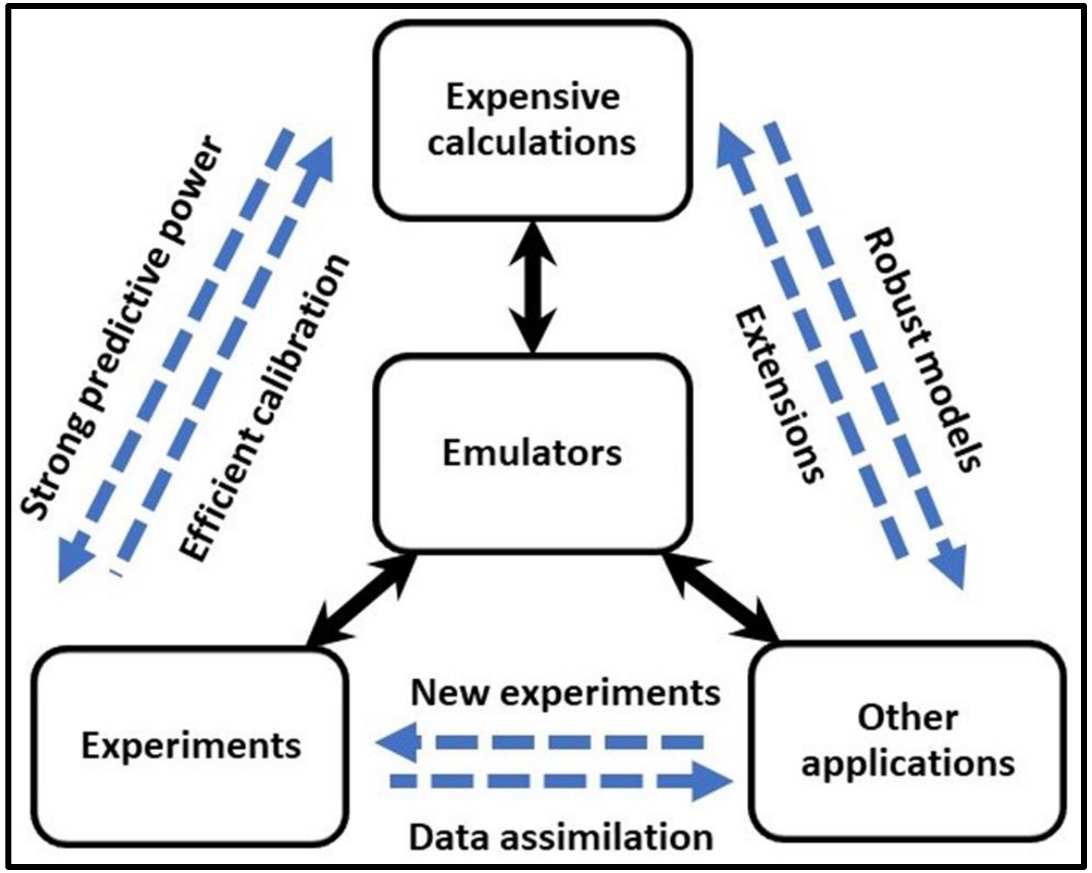
Emulators need to solve 2, 3, and 5-body systems



Constrain EFT (or model on V_s) → compute continuum states

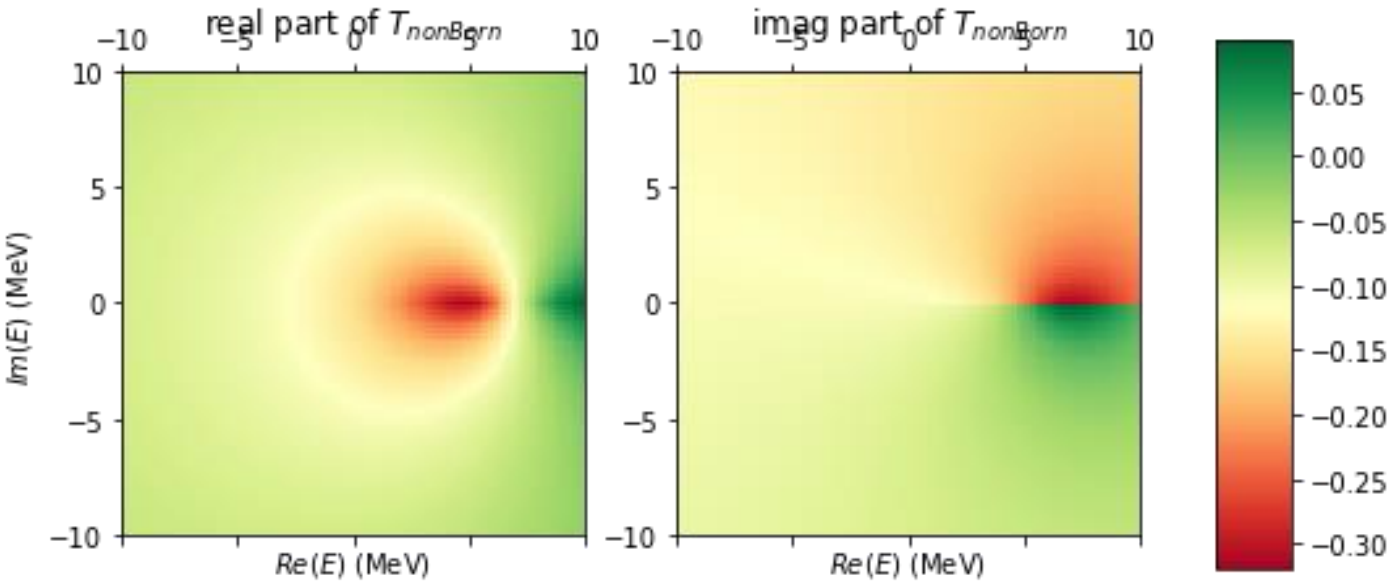
XZ, PRC 101, 051602(R) (2020) [arXiv:1905.05275]
XZ et.al., PRL 125, 112503 (2020) [2004.13575]

Back up



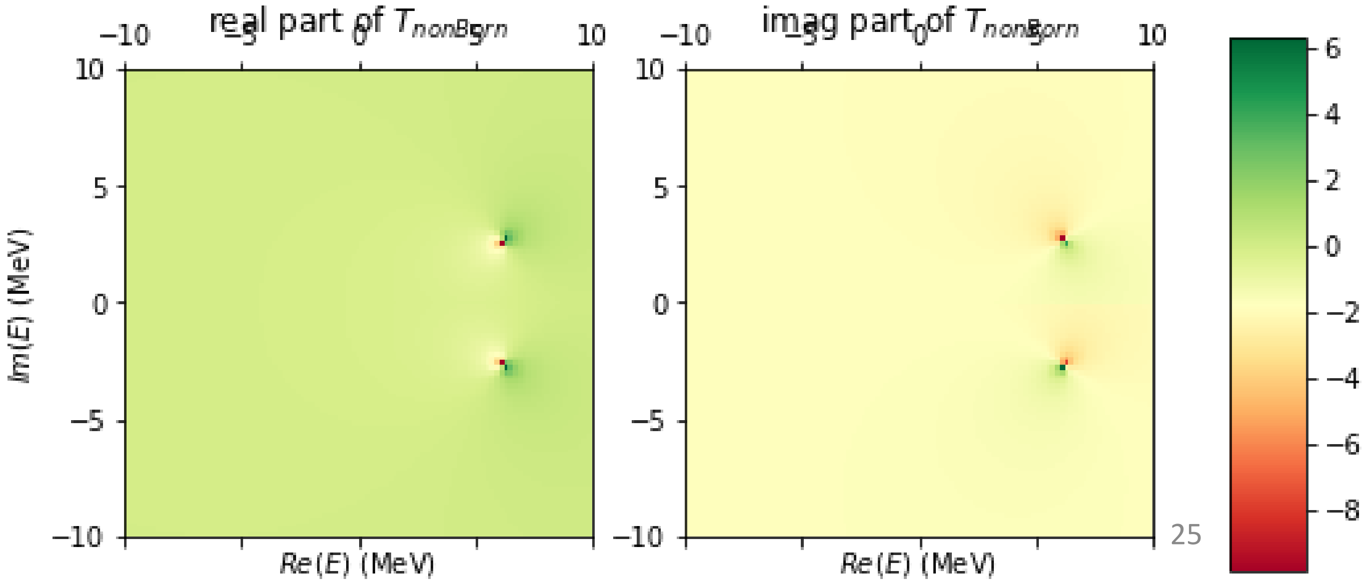
Expensive calculations
Strong predictive power
Efficient calibration
Robust models
Extensions
Emulators
Experiments
New experiments
Data assimilation
Other applications

Emulation in E-complex plane: two-body in p-wave



Physical sheet

2nd sheet



2nd sheet

Resonance at $6.3 - 2.7i$ MeV