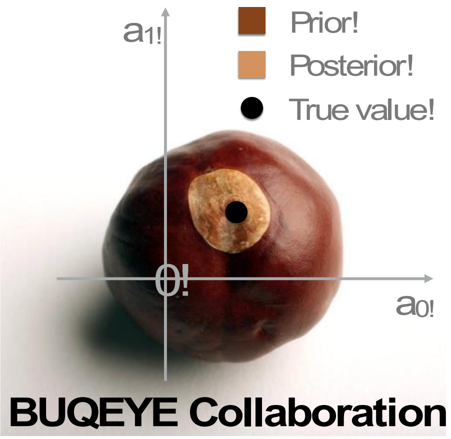
Meeting nuclear challenges with RBM emulators

RBM = Reduced basis method

Dick Furnstahl

ISNET-11, ECT*, November 2025



https://buqeye.github.io/

The Ohio State University

LENPIC

https://www.lenpic.org/

NUCLEI

Nuclear Computational Low-Energy Initiative

https://nuclei.mps.ohio-state.edu/

U.S. Department of Energy

STREAMLINE 2

Argonne National Laboratory

Oak Ridge National Laboratory

Fermilab

FRIB

BAND

Bayesian Analysis of Nuclear Dynamics

https://bandframework.github.io/

NSF

Outline

- Overview: RBM emulators for challenges in nuclear physics
- More effective RBMs and offline training: 2N and 3N scattering
- Non-affine models: optical potentials
- Complex energies: extracting and emulating continuum physics
- Summary and outlook

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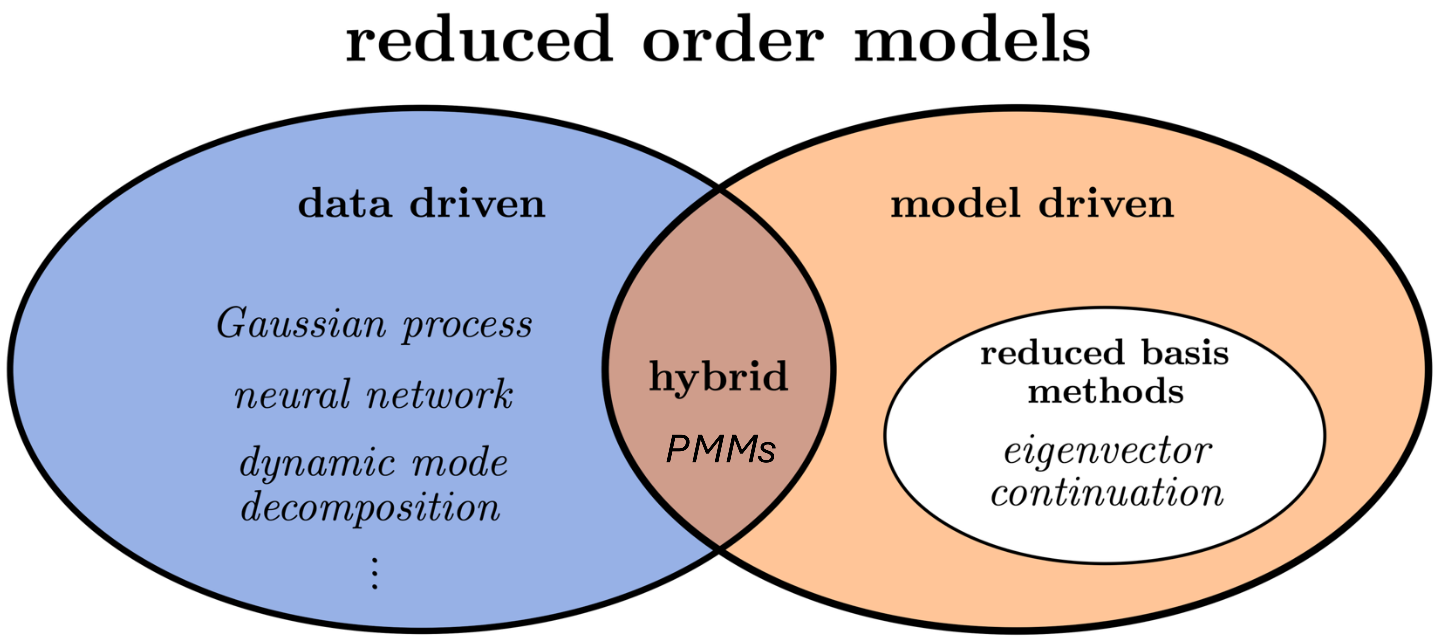
Universe of model reduction methods

UQ need: to vary parameters for calibration, sensitivity analyses, …

Exploit: much information in high-fidelity models is superfluous.

Solution: reduced-order models → emulators (fast & accurate™).



Data driven: interpolate output of high-fidelity model w/o understanding

Examples: Gaussian processes; artificial neural networks; dynamic mode decomposition; …

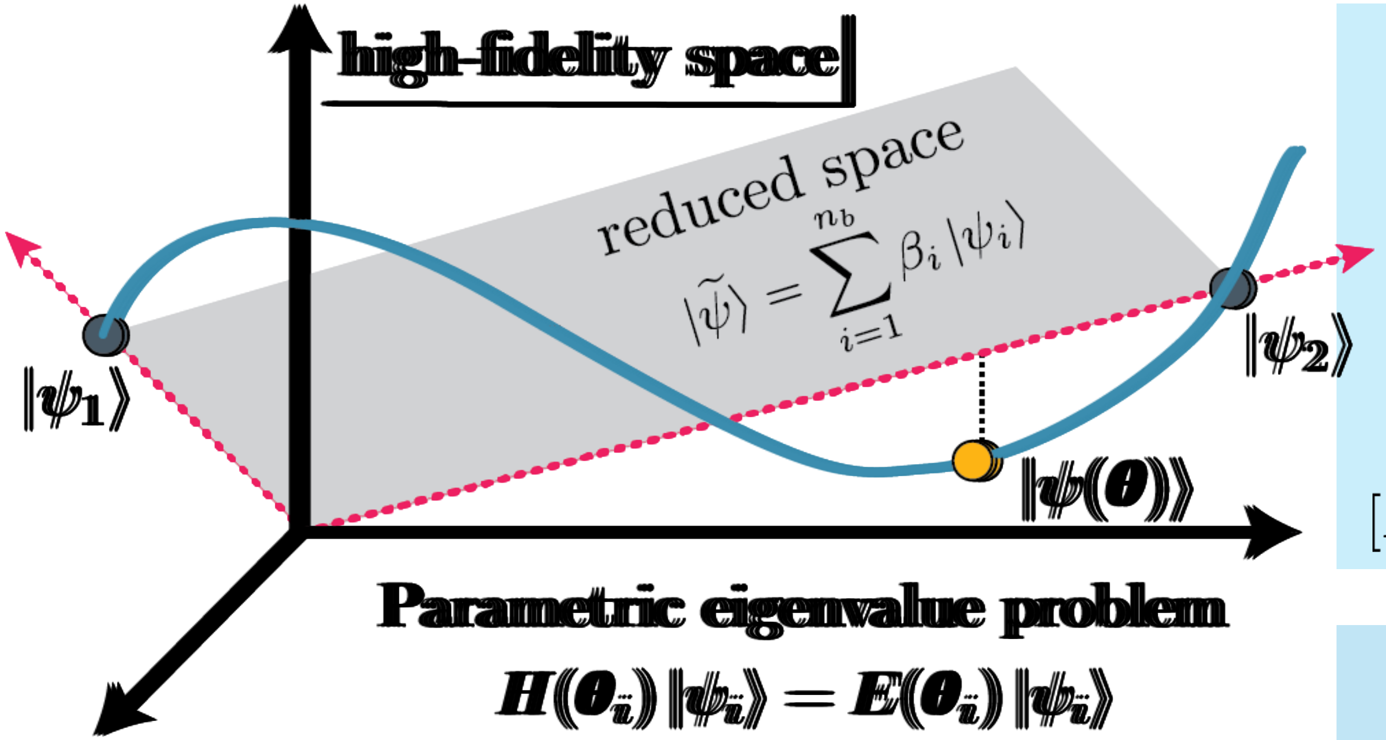
Model driven: derive reduced-order equations from high-fidelity equations

Features: physics-based, respects underlying structure → can extrapolate; often uses projection

Hybrid: learn from data but physics-informed. E.g., Parametric Matrix Models (PMMs).

Here: developments with Reduced Basis Models (RBMs)

Schematic picture of projection-based emulators



- High-fidelity trajectory is in blue.
- Two high-fidelity snapshots ($\boldsymbol{\theta}_1$, $\boldsymbol{\theta}_2$)
- They span the ROM subspace (grey)
- Subspace projection shown for $|\psi(\boldsymbol{\theta})\rangle$

Variational → stationary functional

$$\mathcal{E}[\psi] = \langle\psi|H(\boldsymbol{\theta})|\psi\rangle - E(\boldsymbol{\theta})\big(\langle\psi|\psi\rangle - 1\big)$$

Use trial $|\widetilde{\psi}\rangle = \sum_{i=1}^{n_b} \beta_i|\psi_i\rangle$ and $\langle\delta\widetilde{\psi}|$

Solve generalized eigenvalue problem:

$$\widetilde{H}(\boldsymbol{\theta})\vec{\beta}(\boldsymbol{\theta}) = \widetilde{E}(\boldsymbol{\theta})\widetilde{N}\vec{\beta}(\boldsymbol{\theta})$$

$$[\widetilde{H}(\boldsymbol{\theta})]_{ij} = \langle\psi_i|H(\boldsymbol{\theta})|\psi_j\rangle,\ [\widetilde{N}(\boldsymbol{\theta})]_{ij} = \langle\psi_i|\psi_j\rangle$$

Galerkin projection → use weak form

$$\langle\zeta|H(\boldsymbol{\theta}) - E(\boldsymbol{\theta})|\psi\rangle = 0,\ \forall\langle\zeta|$$

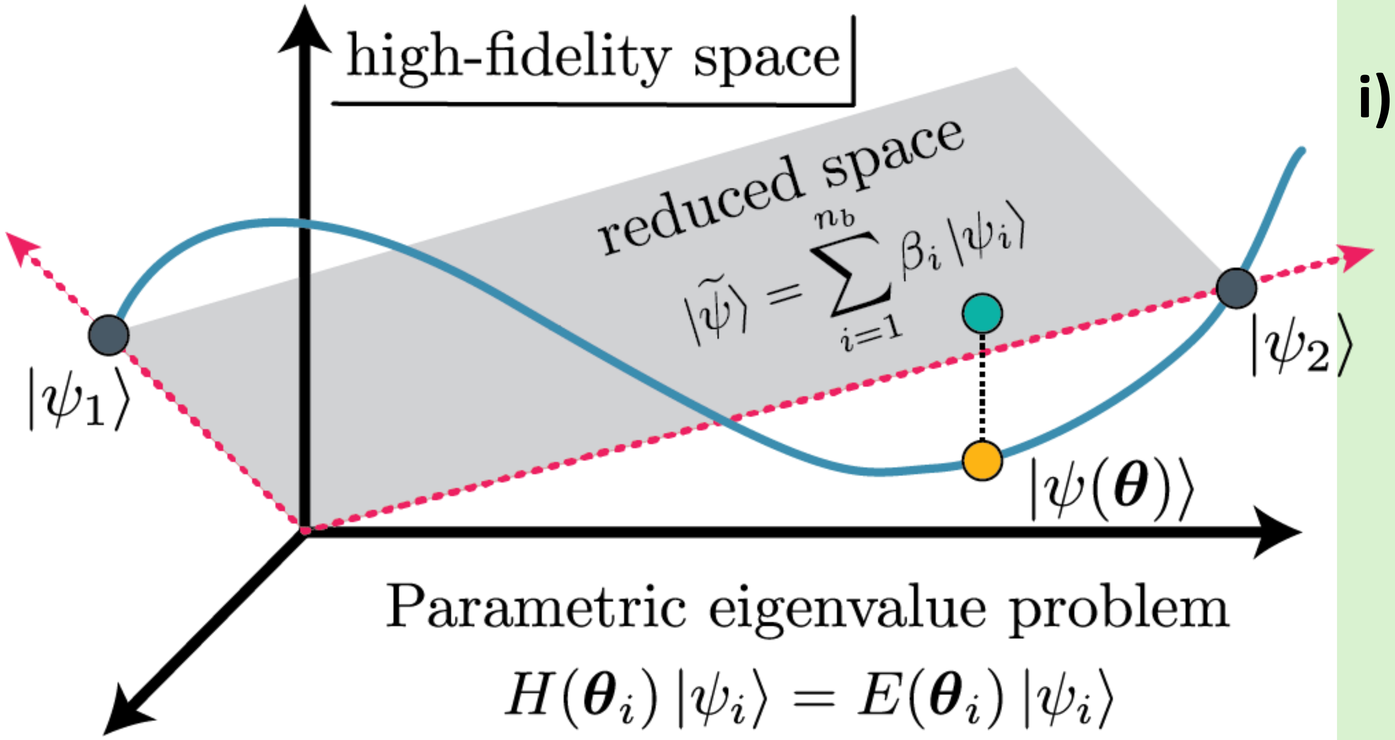
Reduce dimension: $|\psi\rangle \to |\widetilde{\psi}\rangle = \sum_{i=1}^{n_b} \beta_i|\psi_i\rangle$

Limit orthogonality: $\langle\zeta_i|H(\boldsymbol{\theta}) - \widetilde{E}(\boldsymbol{\theta})|\widetilde{\psi}\rangle = 0$

Choose $\langle\zeta_i| = \langle\psi_i|$ (Ritz) ≡ variational

More general: $\langle\zeta_i| \neq \langle\psi_i|$ (Petrov-Galerkin)

Schematic picture of projection-based emulators



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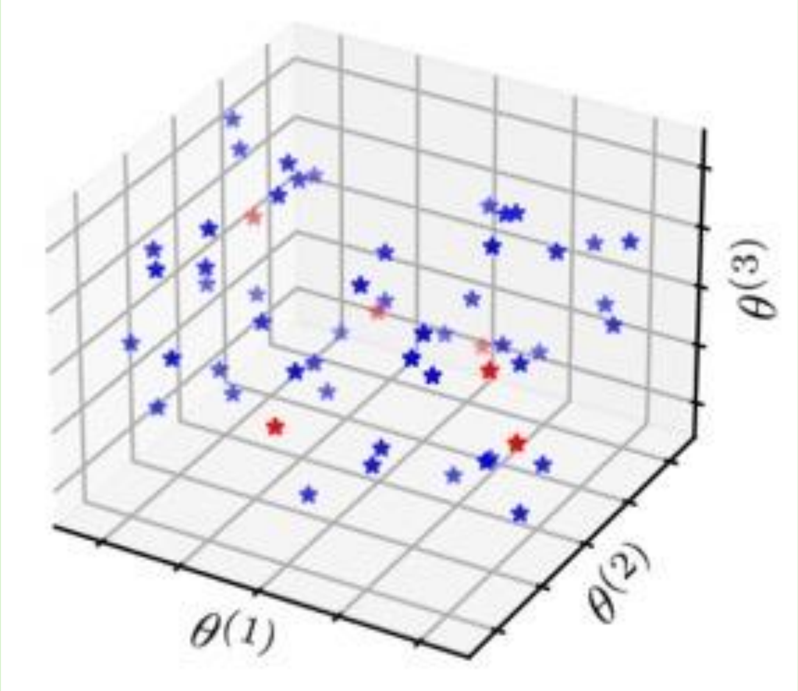
How to choose the snapshot basis?

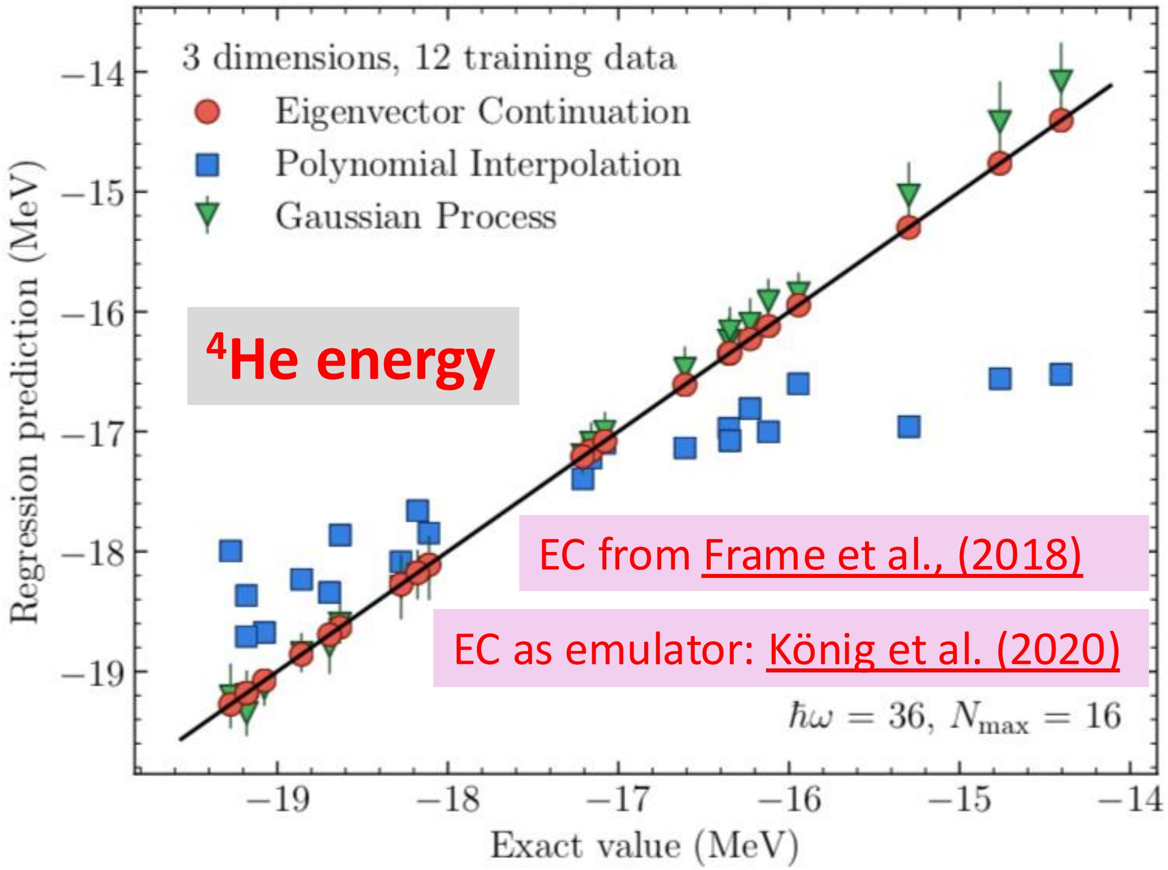
i) **Space-filling sampling** (e.g., LHC) then singular value decomposition (POD)



ii) **Develop error estimator and *greedy algorithm*** [E. Bonilla et al. (2022); A. Sarkar et al. (2022)]

Snapshot RBM emulators for nuclear observables

Ground-state eigenvectors from a selection of parameter sets is an extremely effective variational basis for other parameter sets.
Characteristics: fast & accurate! Scales!



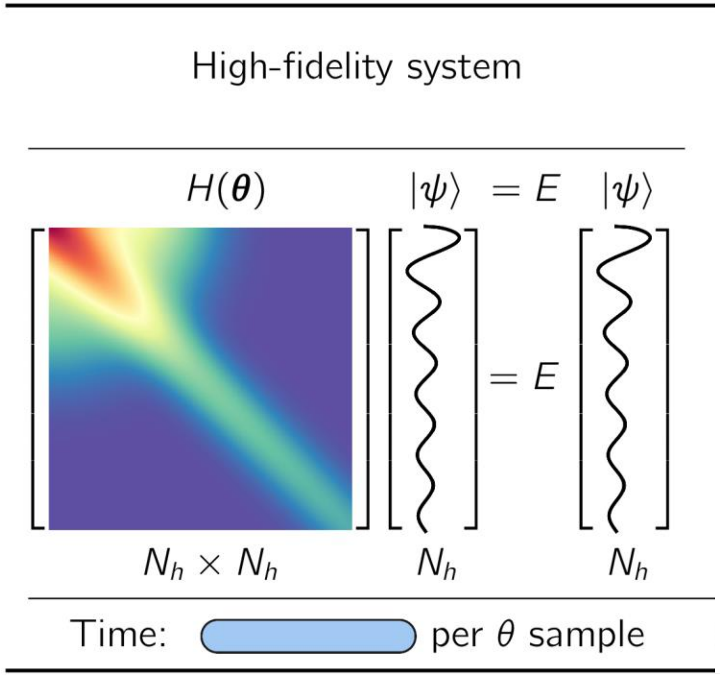
Applied to many different observables:
- Ground-state properties (energies, radii)
- Transition matrix elements
- Excited states
- Resonances

Adapted to special situations and methods
- Pairing; shell model
- Coupled cluster approach; MBPT
- Systems in a finite box
- Subspace diag. on quantum computers

Extended to non-eigenvalue problems
- Reactions and scattering; fission
- Quantum spin system phase diagrams

See Duguet et al., RMP (2024) **for more details and refs.**

Constructing a reduced-basis model (aka emulator)



CPU time scales with the length of

- J. A. Melendez et al., J. Phys. G 49, 102001 (2022)
- E. Bonilla, P. Giuliani et al., Phys. Rev. C 106, 054322 (2022)
- P. Giuliani, K. Godbey et al., Front. Phys. 10, 1212 (2022)
- C. Drischler et al., Quarto + Front. Phys. 10, 1365 (2022)

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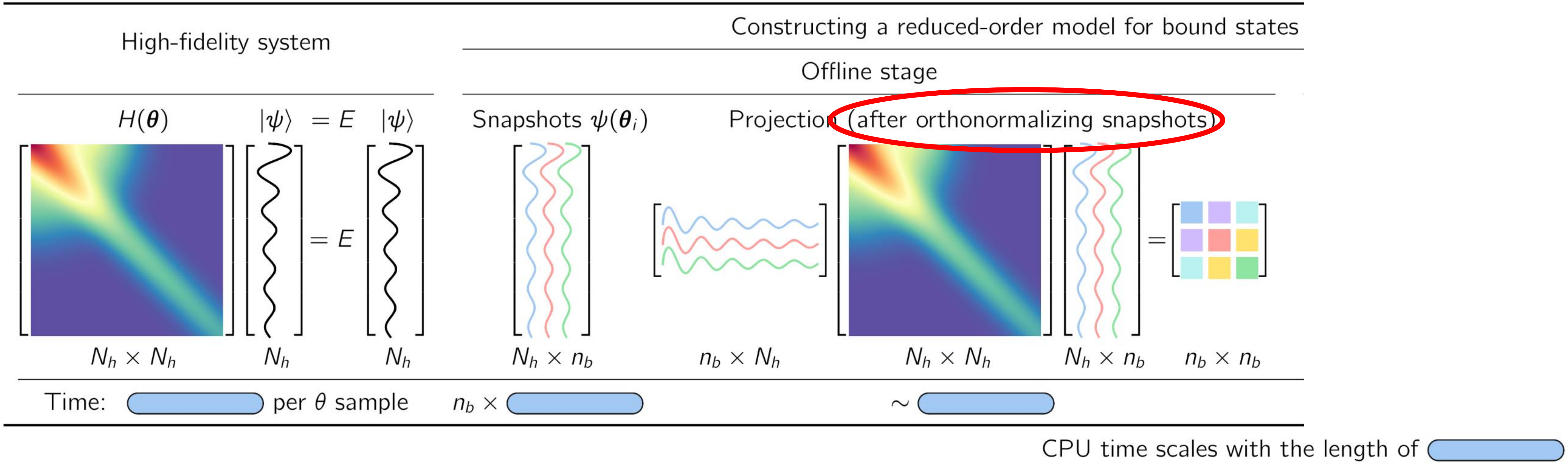

- Offline stage (pre-calculations of size N_h):
  - Construct basis using snapshots from high-fidelity system (simulator)
  - Project high-fidelity system to small-space using snapshots

- *J. A. Melendez et al., J. Phys. G 49, 102001 (2022)*
- *E. Bonilla, P. Giuliani et al., Phys. Rev. C 106, 054322 (2022)*
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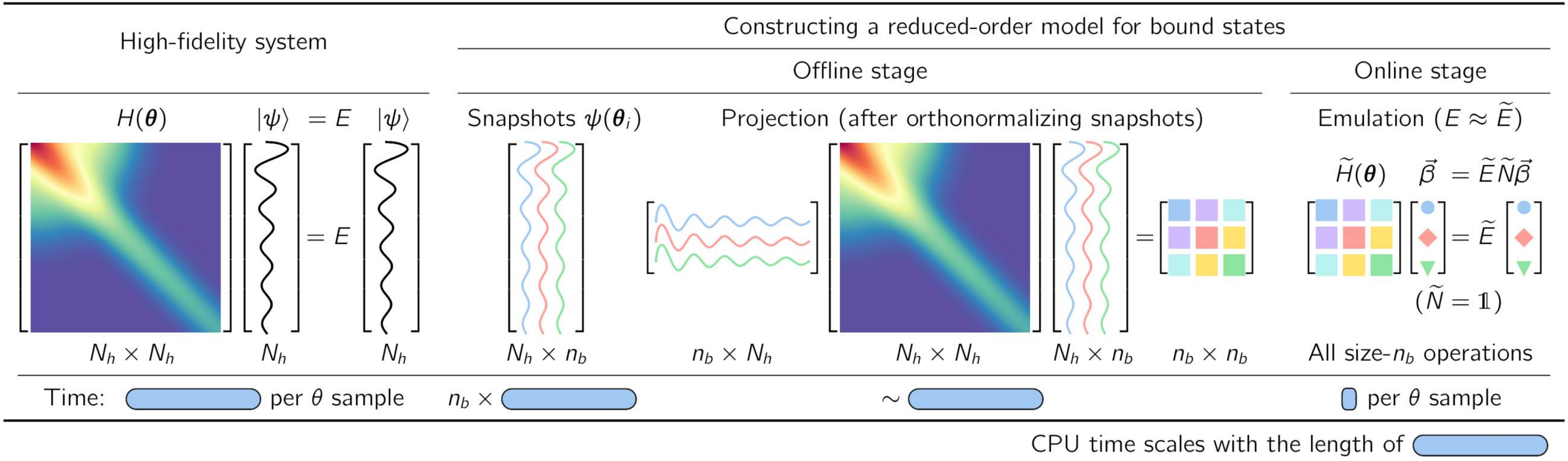

- For speed: only size-n_b operations in online stage → affine structure

$$H(\boldsymbol{\theta}) = H_0 + \sum_n \theta_n H_n$$

← affine in θ_n

What if non-affine?
We'll do that later!

$$\Rightarrow \langle\psi_i|H(\boldsymbol{\theta})|\psi_j\rangle = \langle\psi_i|H_0|\psi_j\rangle + \sum_n \boldsymbol{\theta}_n \langle\psi_i|H_n|\psi_j\rangle \longleftarrow n_b \times n_b \text{ matrices}$$

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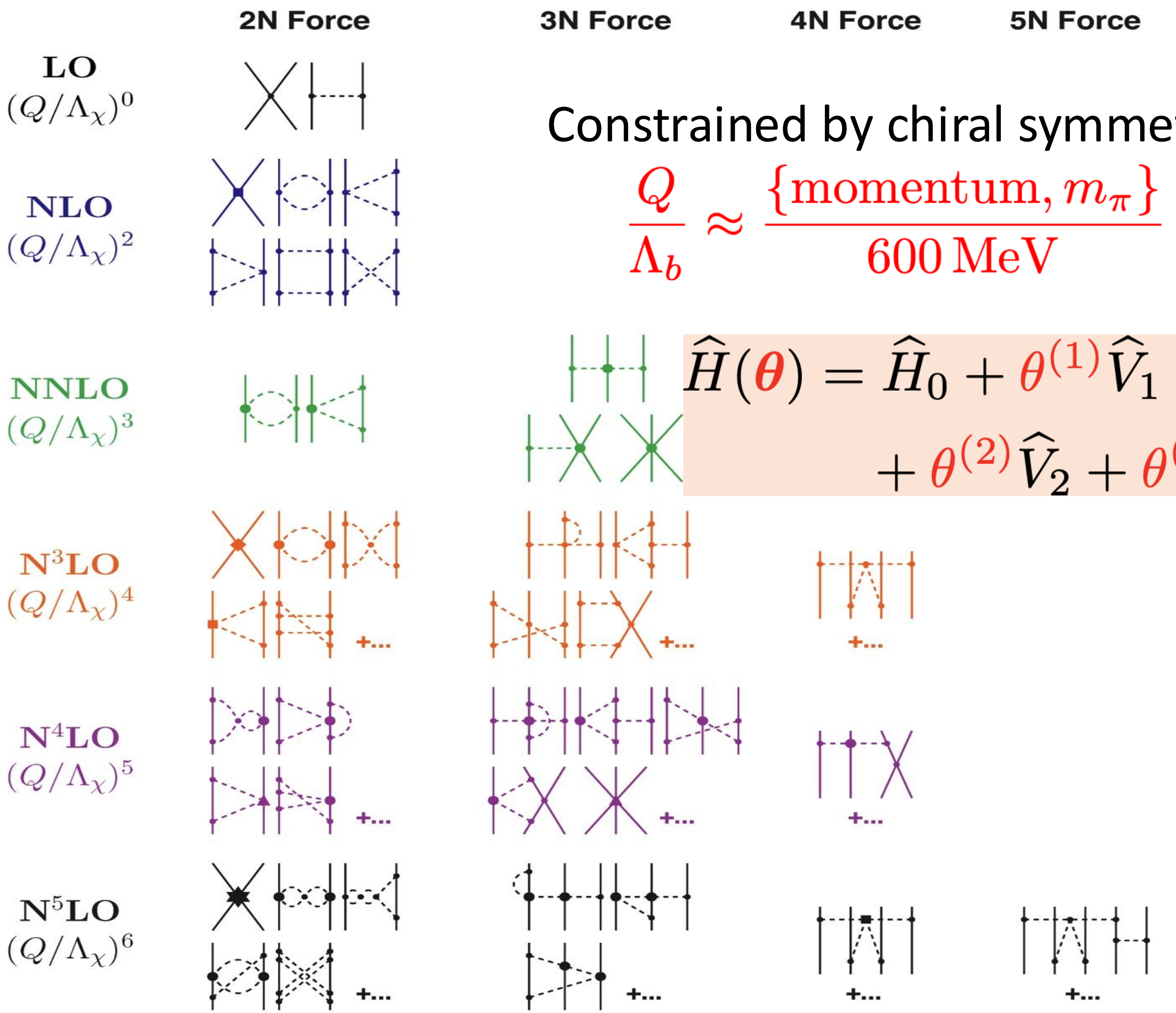
Challenges of χEFT for nuclear many-body theory

- Tremendous progress in *ab initio* calculations with multiple many-body methods
- Precision calculations need uncertainty quantification but calculations are expensive
- Largest uncertainties from Hamiltonian (2N + 3N forces)
- Systematic EFT expansion but many parameters to determine → not best fits but *distributions*



Constrained by chiral symmetry

$$\frac{Q}{\Lambda_b} \approx \frac{\{\mathrm{momentum}, m_\pi\}}{600\ \mathrm{MeV}}$$

$$\widehat{H}(\boldsymbol{\theta}) = \widehat{H}_0 + \theta^{(1)}\widehat{V}_1 + \theta^{(2)}\widehat{V}_2 + \theta^{(3)}\widehat{V}_3 + \cdots$$

Reduced order models: (Petrov-)Galerkin projections

Full-Order Model: *inhomogeneous* RSE

scattered wavefunction

$$\frac{d^2\chi(r)}{dr^2} = -\left(p^2 - 2\mu V(r) - \frac{l(l+1)}{r^2}\right)\chi(r) + 2\mu V(r)\phi(r)$$

free wavefunction

$$\frac{d^2y}{dx^2} = f(x,y), \quad \text{with} \quad y(a) = y_0 \quad \text{and} \quad y(a) = y_0'$$

special second-order ODE

High-Fidelity Solver: here, Numerov's method (iterative)

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12}(f_{n+1} + 10f_n + f_{n-1}) + \mathcal{O}(h^6)\,.$$

The generated sequence has to be matched to an asymptotic limit parametrization

Other methods include RK and leapfrog methods

Obtain matrix form of ODE solver

$$A(\vec{\theta})\vec{x}(\vec{\theta}) = \vec{b}(\vec{\theta})$$

In the case of Matrix Numerov: lower triangular, low-bandwidth matrix

Already FAST!

Affine decompositions from potential carry over:

$$A(\vec{\theta}) = \sum_i^{n_\theta} A_i\theta_i\,; \quad b(\vec{\theta}) = \sum_i^{n_\theta} b_i\theta_i$$

Galerkin (G) ROM

Reduction:

$$\vec{x}(\vec{\theta}) \approx \sum_{i=1}^{n_b} \beta_i(\vec{\theta})\vec{x}(\vec{\theta}_i) \equiv \mathbf{X}\vec{\beta}(\vec{\theta})$$

Snapshot matrix

Projection:

$$\underbrace{\left[X^\dagger A(\vec{\theta})X\right]}_{\text{Reduced matrix}}\vec{\beta}(\vec{\theta}) = X^\dagger b(\vec{\theta})$$

Least-Squares Petrov-Galerkin (LSPG) ROM

Reduction: Projection:

$$\left[Y^\dagger A(\theta)X\right]\vec{\beta} = Y^\dagger\vec{b}(\theta)$$

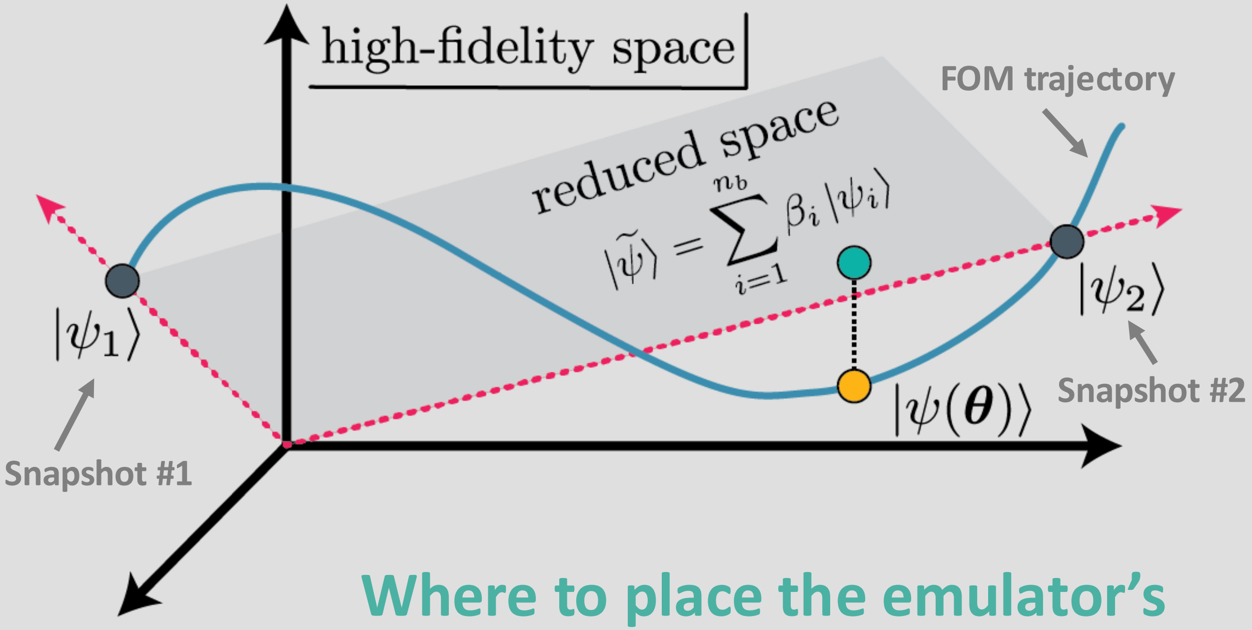
$$Y = \begin{bmatrix} A_1X & \cdots & A_{n_\theta}X & b_1 & \cdots & b_{n_\theta}\end{bmatrix}$$

Construct $YY^\dagger$ as *orthogonal* projector onto residuals

$$R(\vec{\beta}) = A(\vec{\theta})X\vec{\beta} - \vec{b}(\vec{\theta})$$

Emulator basis construction

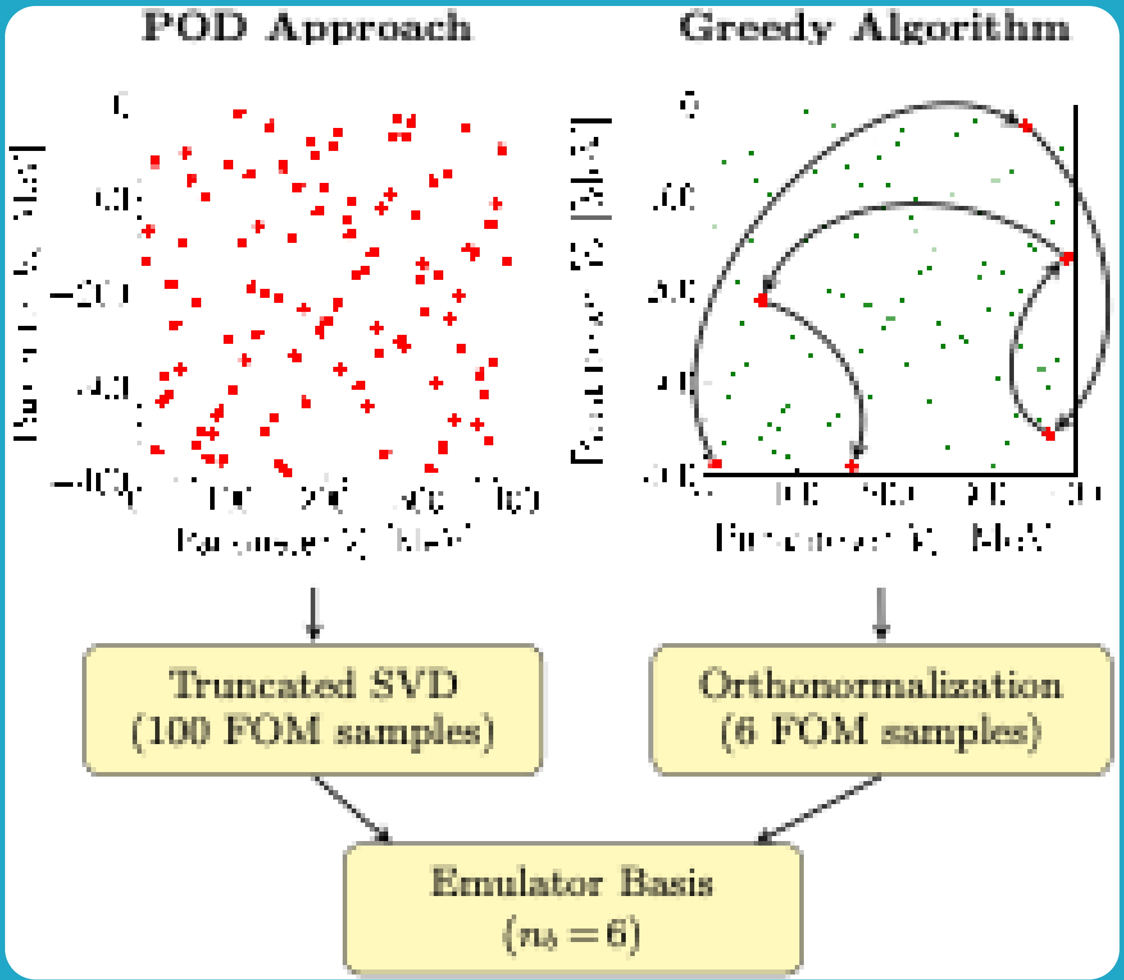
Maldonado, Drischler, rjf, Mlinarić.,
arXiv:2504.06092 (PRC 2025)



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***

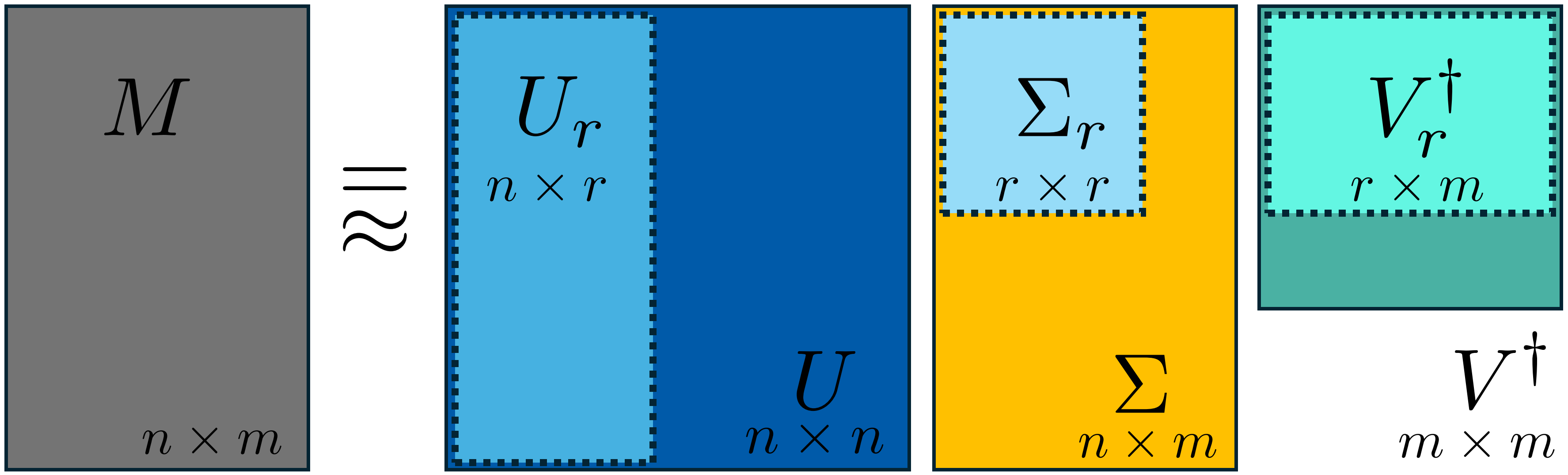
See also: Sarkar & Lee, PRR **4**, 023214 ; Bonilla *et al.*, PRC **106**, 054322



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

Proper Orthogonal Decomposition (POD)

POD is based on a (truncated) Singular Value Decomposition (SVD) of the snapshot basis:
See also Principal Component Analysis (PCA)



***U* and *V* are unitary matrices (*e.g.*, $UU^\dagger = U^\dagger U = 1\!\!|$) containing the singular vectors**

Σ is a diagonal matrix with decreasing, nonnegative diagonal entries (singular values)

Truncating singular vectors corresponding to the *r* smallest singular values results in the best possible rank-*r* approximation (in Frobenius norm) to the original *M* **(low-rank approximation)**

Greedy Algorithm in Action (preview)

start with 2 randomly placed initial snapshots

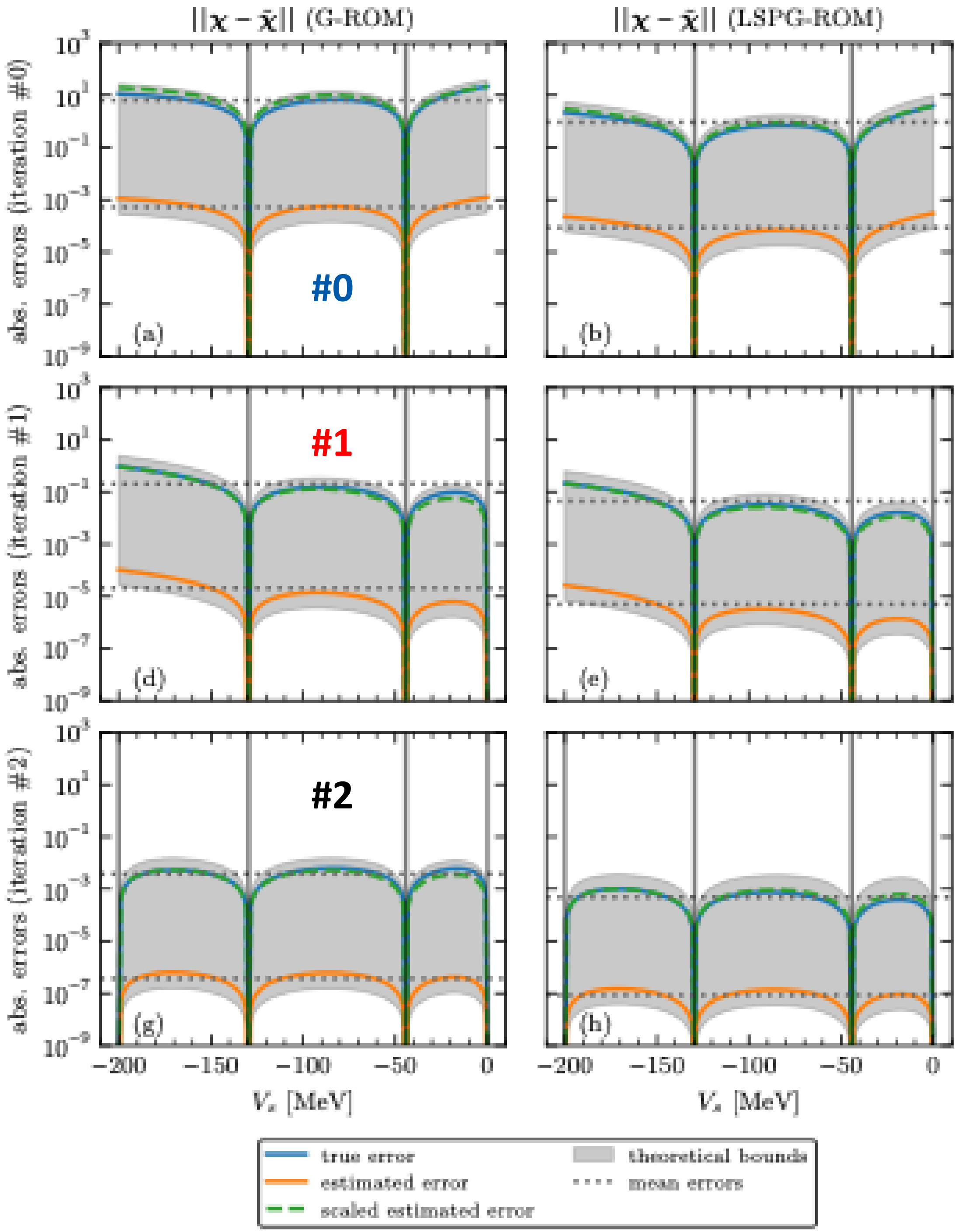
Estimate the emulator error across the parameter space

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

Iterate until the *requested* accuracy is obtained

Greedy Iteration
increasing accuracy

(1D problem for illustration)



Maldonado, Drischler, rjf, Mlinarić., arXiv:2504.06092 (PRC 2025)

Emulator error estimation for *greedy* algorithm

Error estimates: residual as a *proxy* for exact error

$$|\tilde{x} - x| \longrightarrow |R(\vec{\beta})| = |A(\vec{\theta})X\vec{\beta} - \vec{b}(\vec{\theta})|$$

exact error

(*approximatively proportional* to each other)

Fast & accurate error estimation in the *reduced* space

Theoretical error bounds

$$\frac{|R(\vec{\beta})|}{\sigma_{\max}(A)} \leqslant |\tilde{x} - x|_2 \leqslant \frac{|R(\vec{\beta})|}{\sigma_{\min}(A)}$$

Also derived: similar error bounds for phase shifts

Opportunities/challenges:

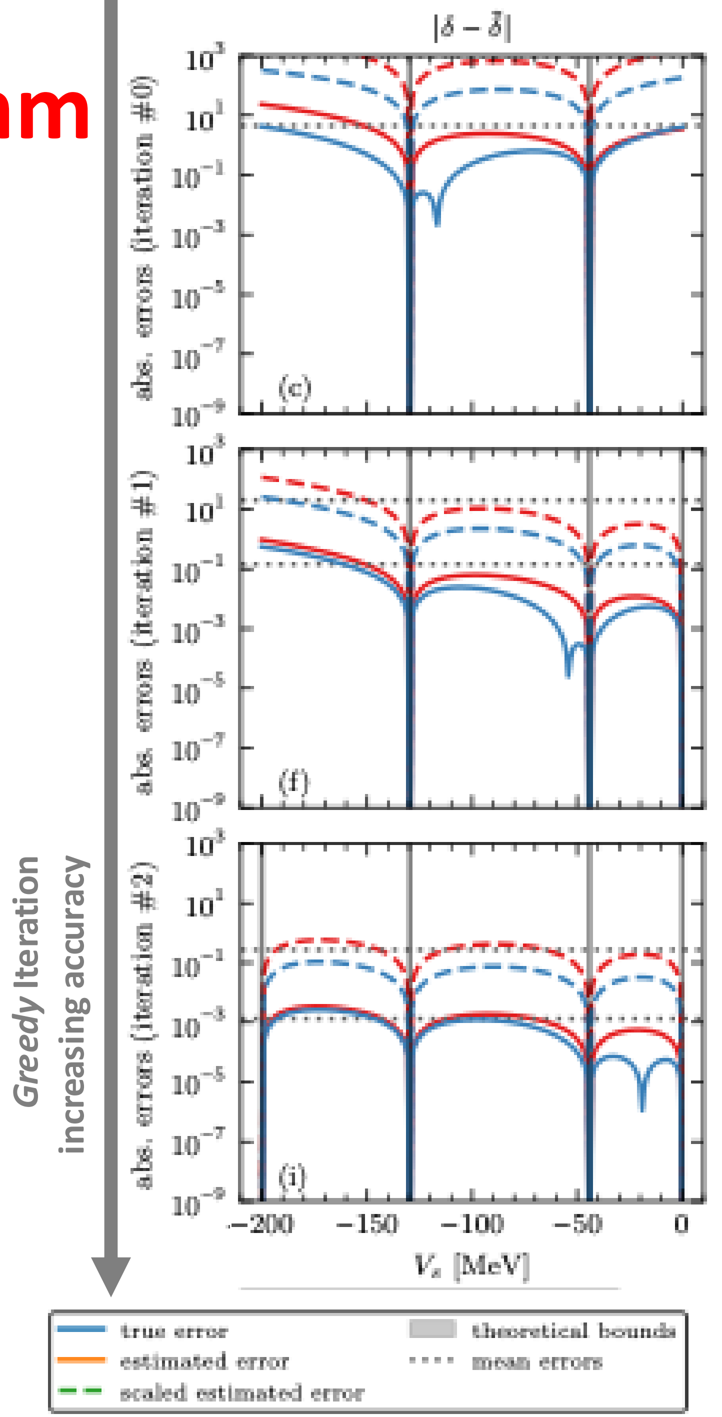
- **estimate the extremal singular values** using the Successive Constraint Method (SCM)
- use the *upper bound* as a conservative error estimate

start with 2 randomly placed initial snapshots

Estimate the emulator error across the parameter space

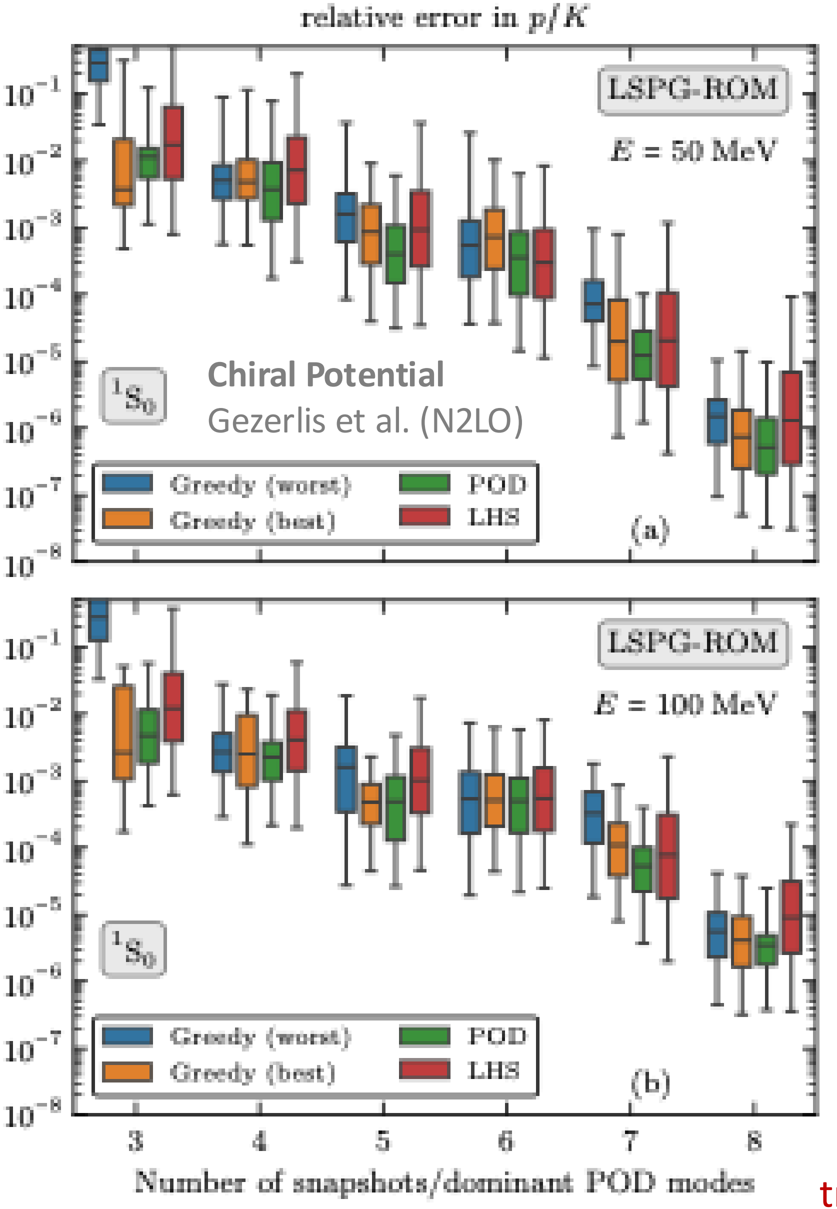
Place the next snapshot(s) at the location(s) of maximum estimated error

Iterate until the *requested* accuracy is obtained



POD vs greedy algorithm

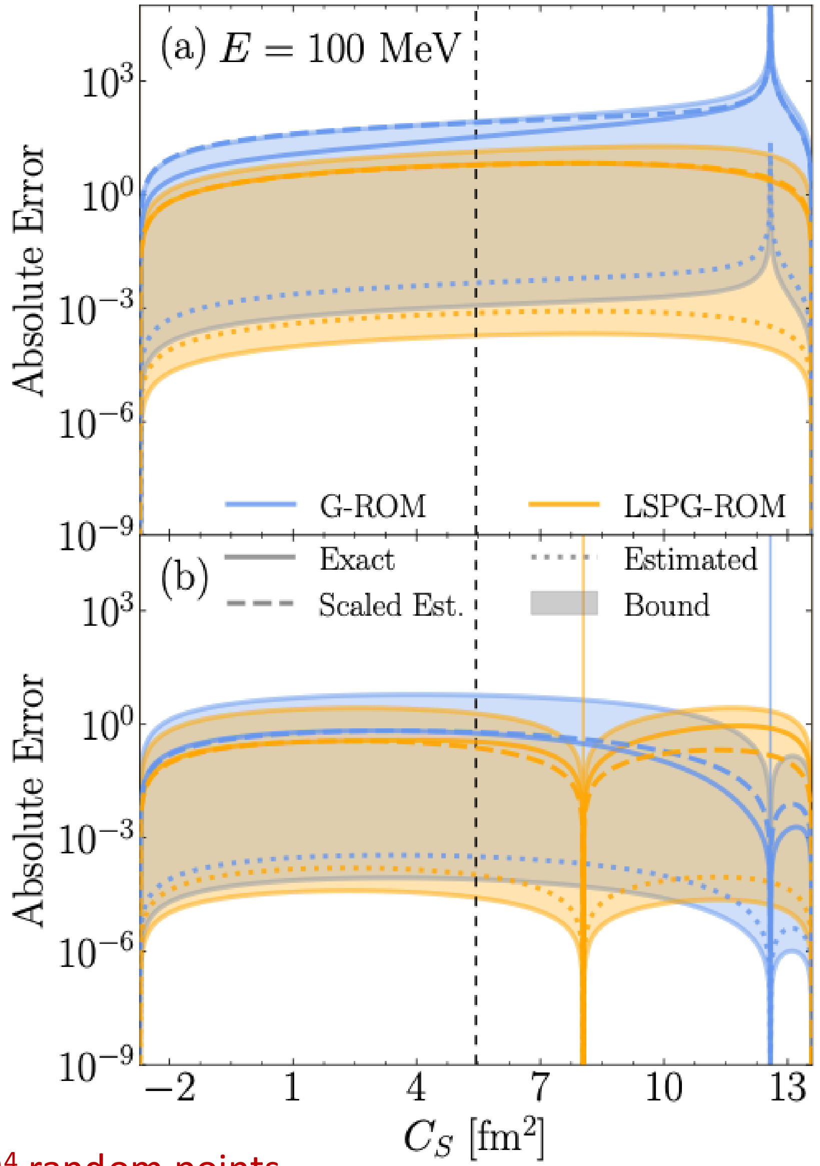
Maldonado, Drischler, rjf *et al.*, arXiv:2504.06092 (PRC 2025)



POD obtains high *accuracy* as it has access to the most information. **But: expensive!**

Greedy emulator:

- **similar accuracy** throughout but using far *fewer* high-fidelity calculations. **Much less expensive!**
- identifies & remedies poor choices of the initial snapshot bases
- Finds and **removes spurious singularities** known as Kohn anomalies (LSPG-ROM is free of such anomalies)



training set: 200 random points, validation set: 10^4 random points

Extension to coupled channels & momentum space

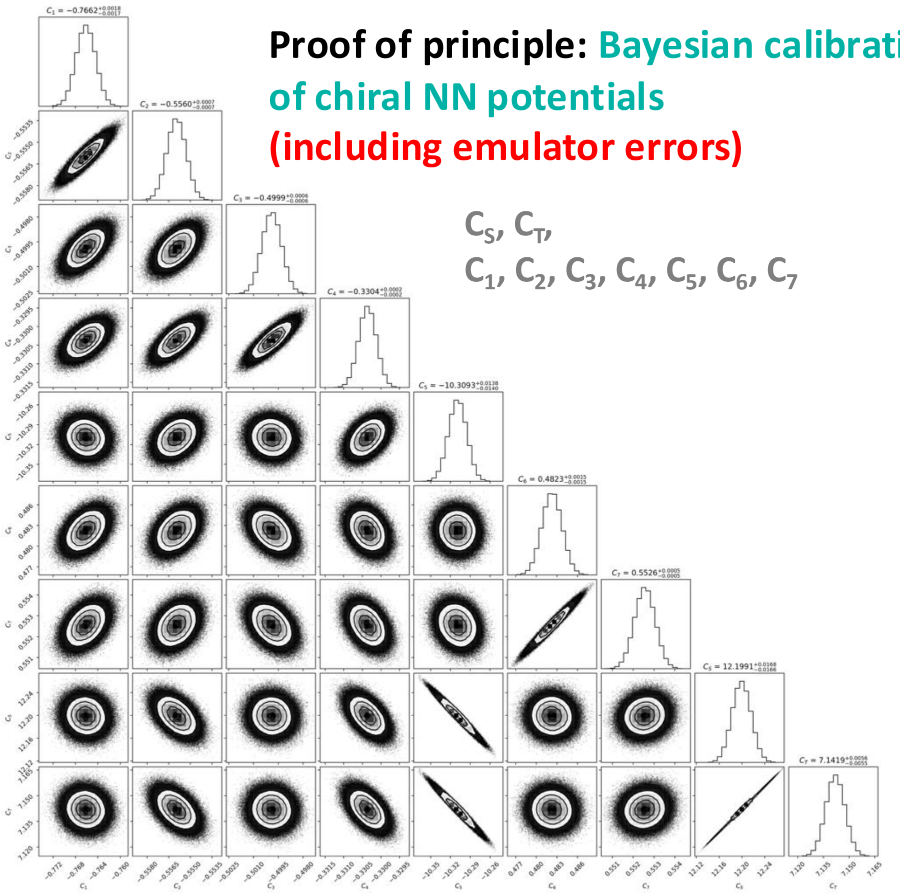
Giri, Kim, Drischler, Elster, rjf *et al.*, in prep.

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

Lippmann-Schwinger (integral) equation

gives access to a wide range of modern chiral potentials

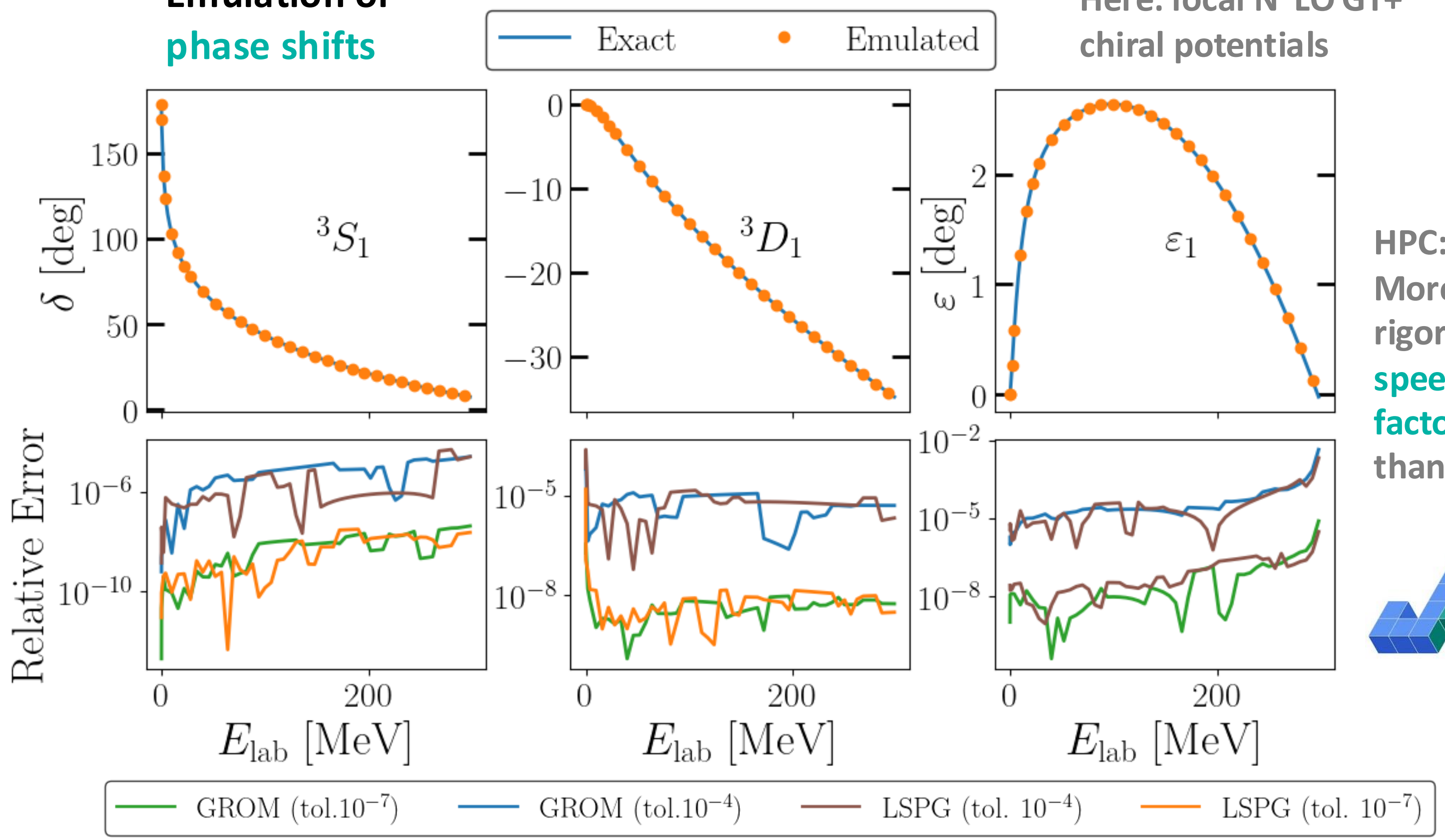
As before, the greedy algorithm exhibits a fast convergence pattern.



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 phase shifts



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

HPC: More rigorous speed-up factors thanks to

Extension to coupled channels & momentum space

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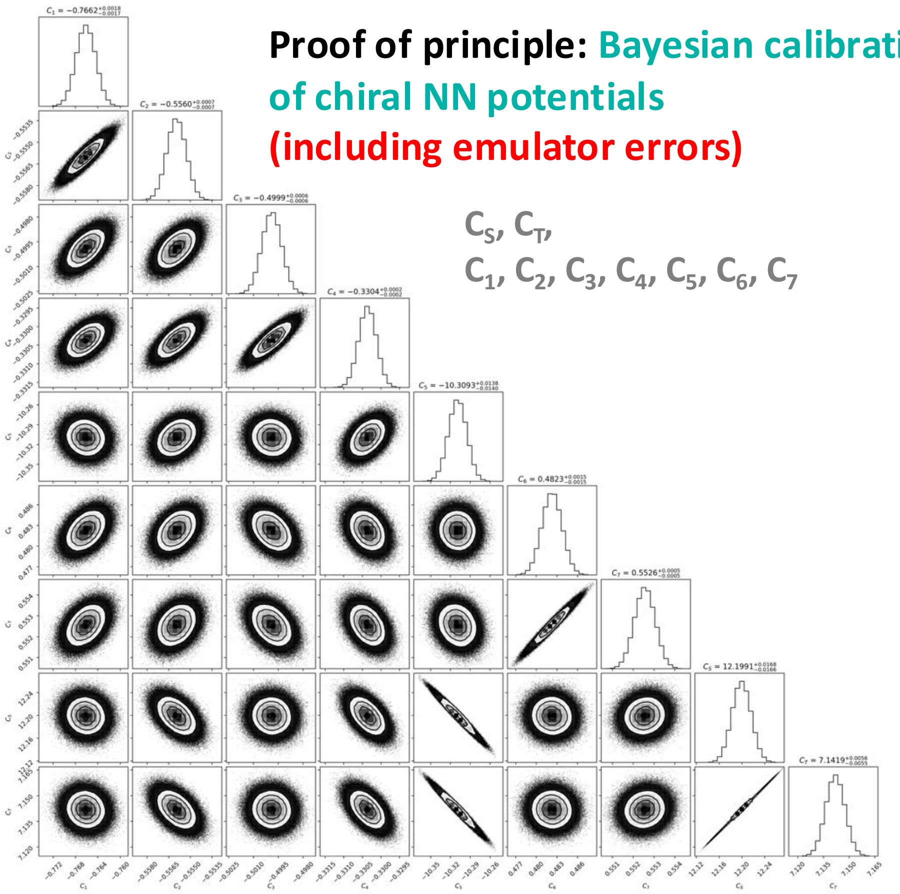

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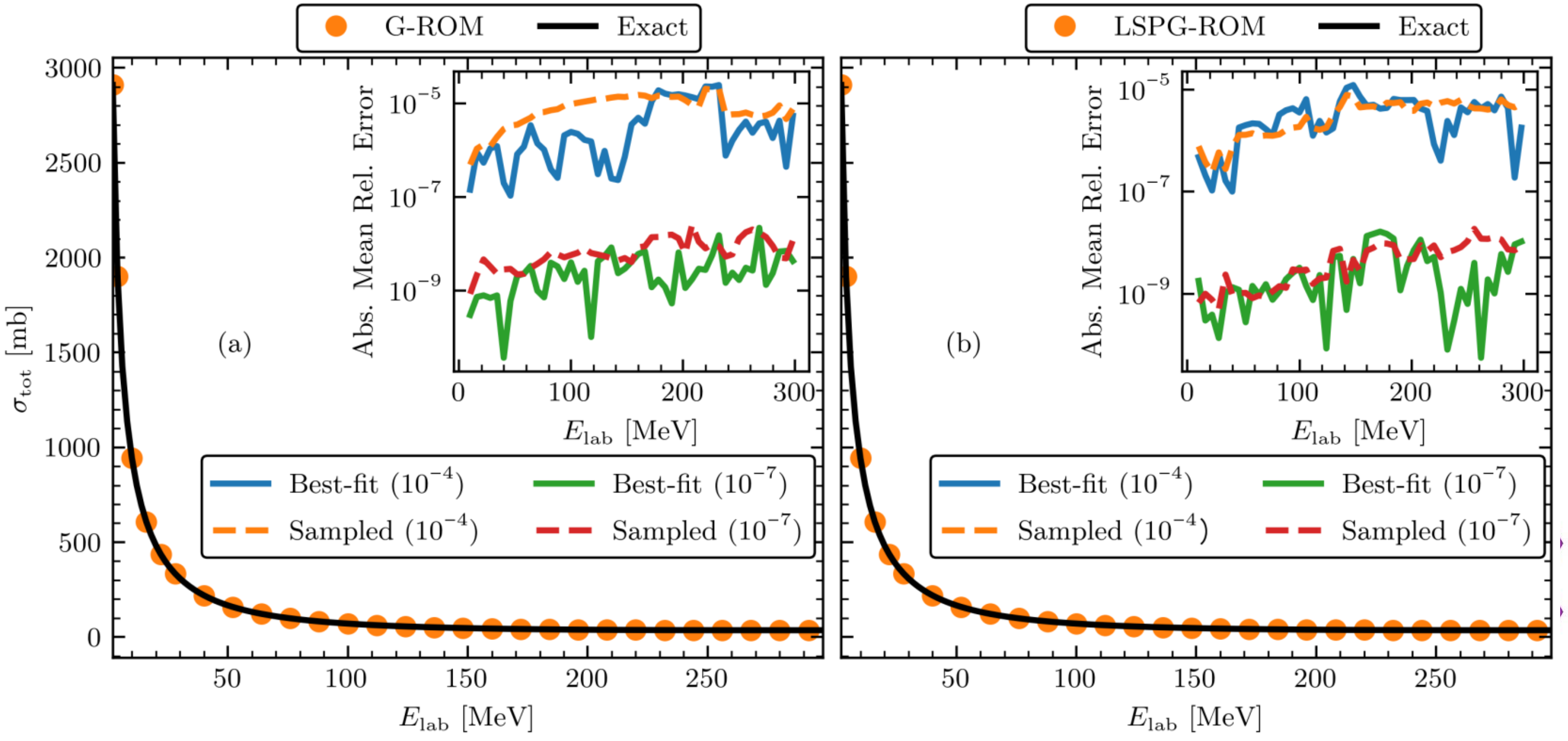
Emulation of total cross sections



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

N-d scattering emulator

Gnech, Zhang, Drischler, rjf, Grassi,
Kievsky, Marcucci, and Viviani,
arXiv:2511.01844, *arXiv:2511.10420*

Emulate **three-body scattering with greedy snapshot selection**

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

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

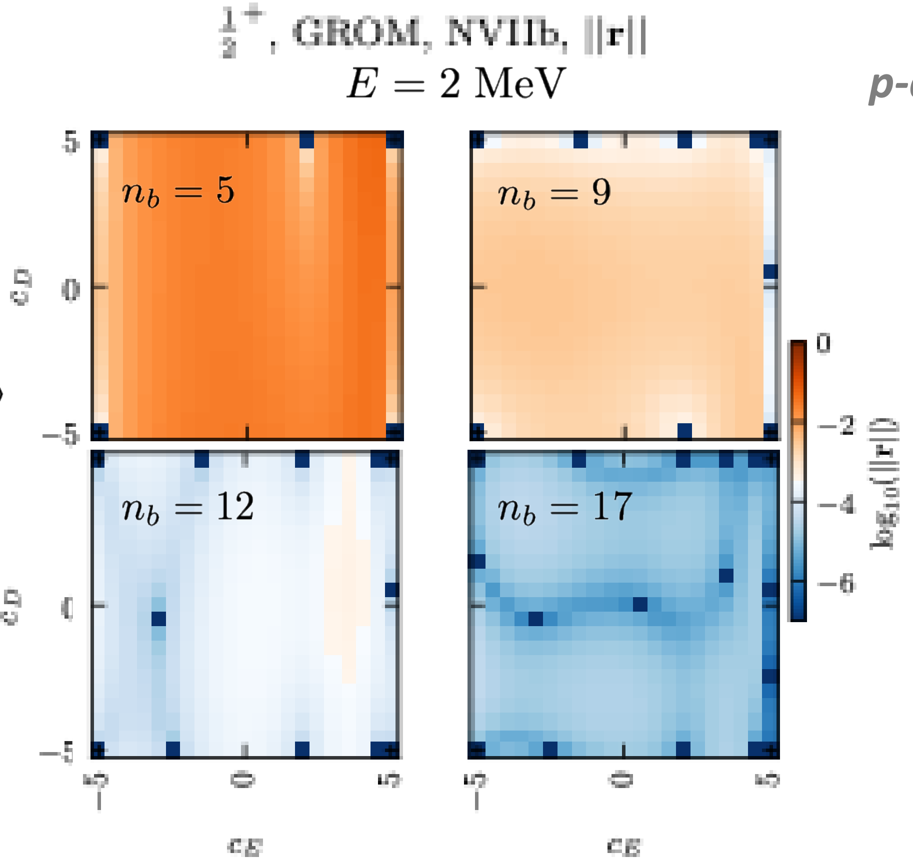
ROM: **G-ROM (G) or LSPG-ROM (LS)**

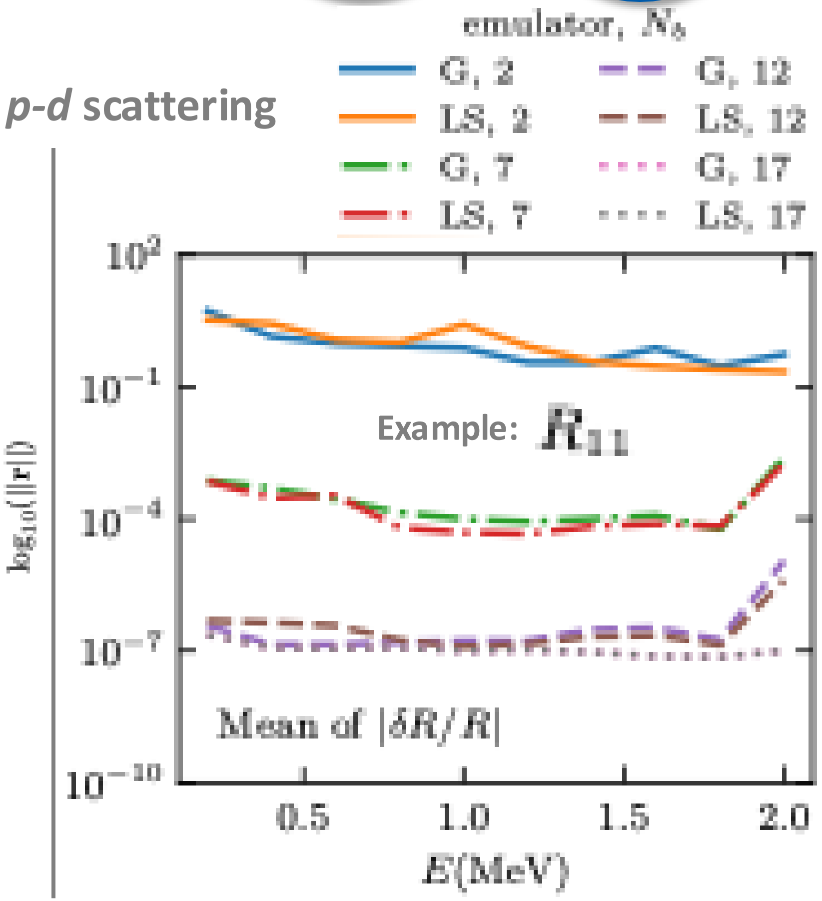
So far: ***N-d* scattering *below* the deuteron break-up threshold** with

- 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 $\quad a = \{L, S\}$



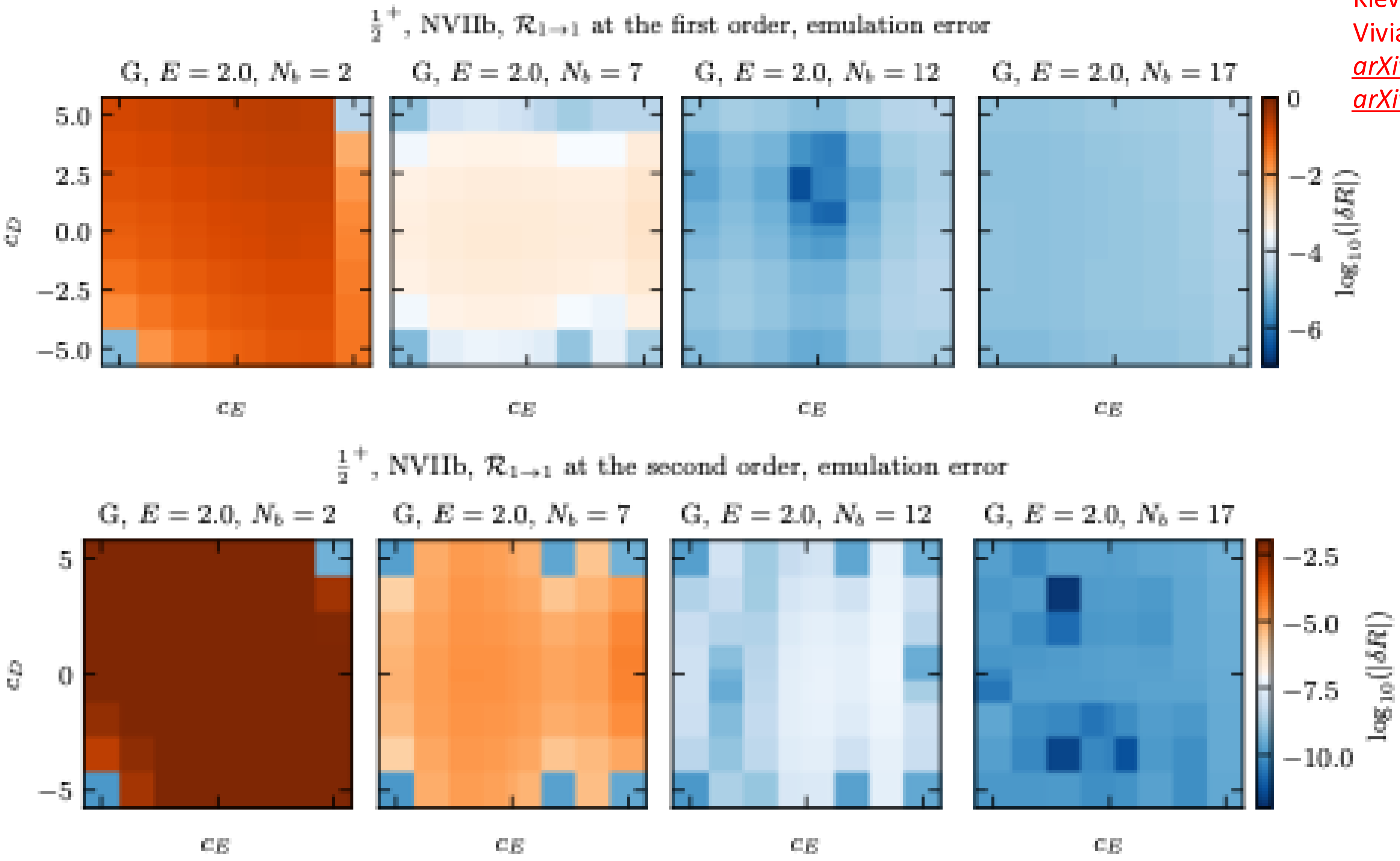


Greedy algorithm: systematic reduction of emulator errors

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

Emulation errors at first and second order

Gnech, Zhang, Drischler, rjf, Grassi, Kievsky, Marcucci, and Viviani, arXiv:2511.01844, arXiv:2511.10420



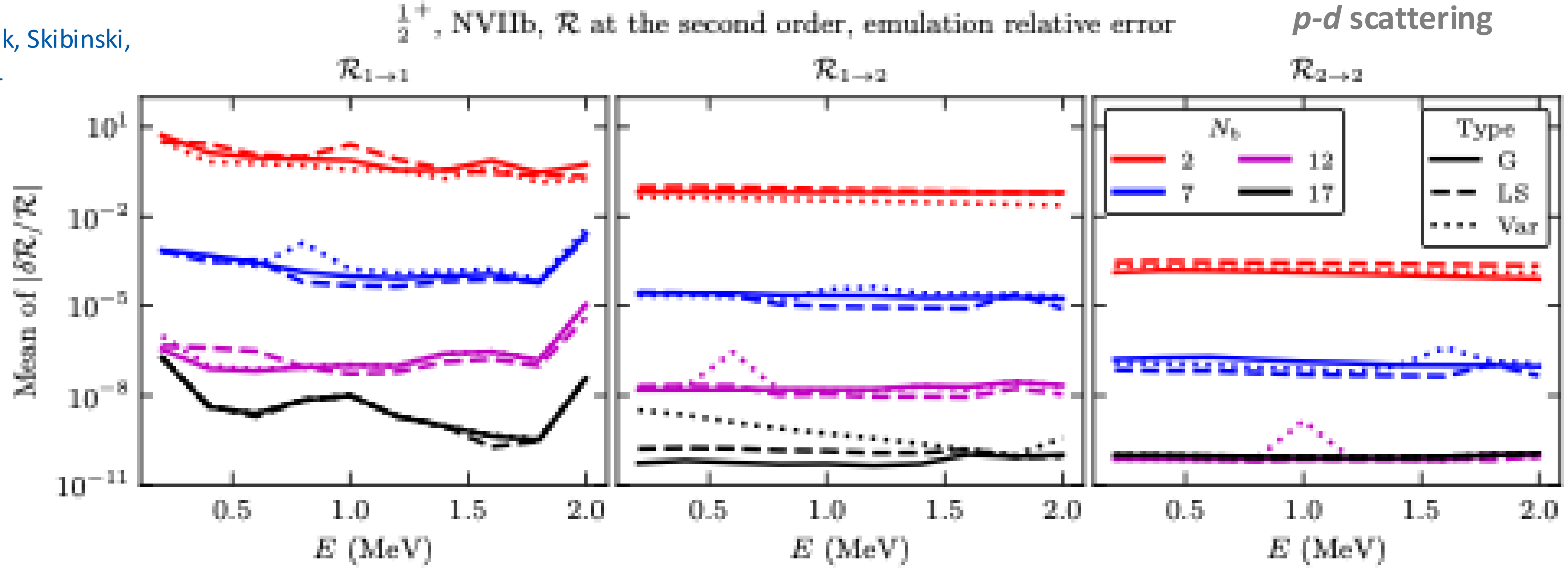
G-ROM results; similar from LSPG-ROM. Second order gives significant error reduction.

Summary points

Gnech, Zhang, Drischler, rjf, Grassi, Kievsky, Marcucci, and Viviani, arXiv:2511.01844, arXiv:2511.10420

See also:
Witala, Golak, Skibinski, EPJA **57**, 241

p-d scattering



Systematic reduction of the emulator error with increasing number of snapshots (as expected)

G-ROM and LSPG-ROM behave similarly

R_{11} is much larger than the other two components

½⁻ is less sensitive to 3N forces (= smaller residuals)

Opportunities/challenges:

- Emulation of all NN+3N LECs and up to higher *E*
- Computation of scattering observables; requires emulation across partial waves (and energy)
- Implementation in Bayesian parameter estimation
- Application to four-body scattering?

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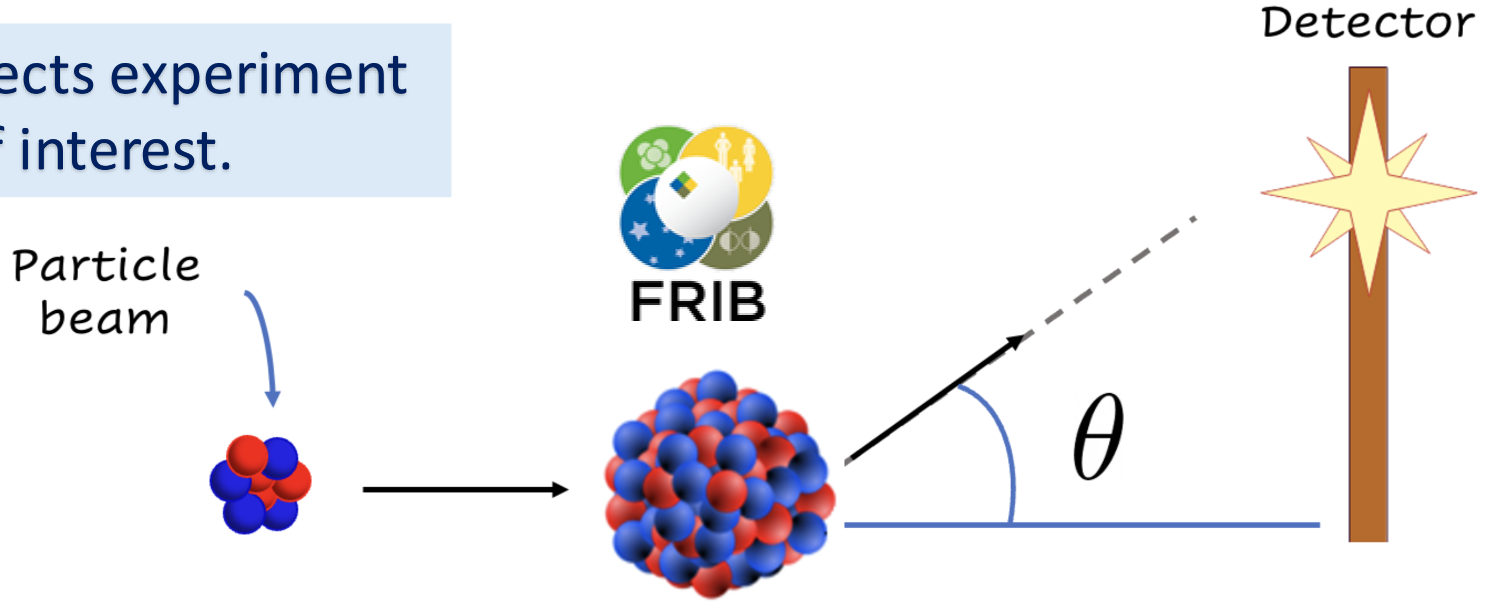
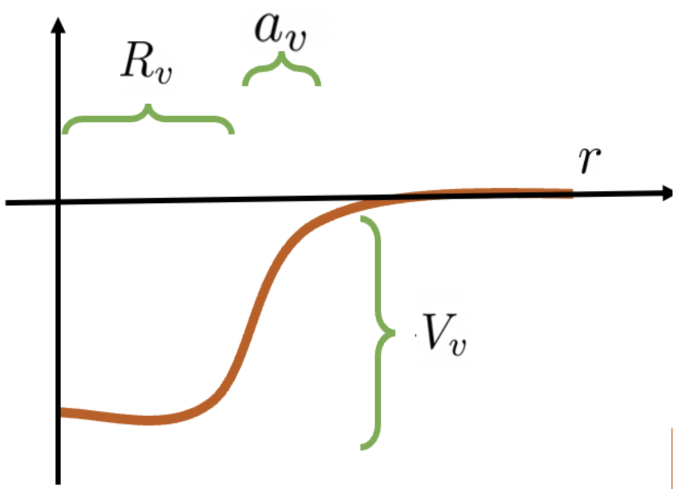
Optical potential motivation

Reaction theory connects experiment to quantities of interest.



(Optical Potentials)



$$U(r,\boldsymbol{\theta}) = -V_v\left[1+e^{(r-R_v)/a_v}\right]^{-1} + \ldots$$

**Effective interaction parameters.

Thanks to Manuel Catacora-Rios and Pablo Giuliani for graphics

BAND Bayesian Analysis of Nuclear Dynamics

RBM emulators for non-affine scattering problems

Nuclear **ROSE** in BAND Framework (free software!).
Reduced **O**rder **S**cattering **E**mulator can handle local, complex, non-affine interactions.

Strategy: convert non-affine to affine → hyper-reduction methods [Odell et al., PRC (2024)]
Example: calibrating phenomenological optical potential with EIM

Scattering → Galerkin projection but potential is non-affine in the parameters to fit ($\boldsymbol{\theta} = \{V_v, R_v, a_v, \ldots\}$):

$$U(r, \boldsymbol{\theta}) = -V_v \left[1 + e^{(r - R_v)/a_v}\right]^{-1} + \ldots$$

ROSE Team: Daniel Odell, Pablo Giuliani, Kyle Beyer, Manuel Catacora-Rios, Moses Chan, Edgard Bonilla, rjf, Kyle Godbey, Filomena Nunes

Problem: *U* doesn't factor into products of *r* and $\boldsymbol{\theta}$ functions, so integrals between test and basis functions have to be calculated every time → no offline-online speed-up!

RBM emulators for non-affine scattering problems

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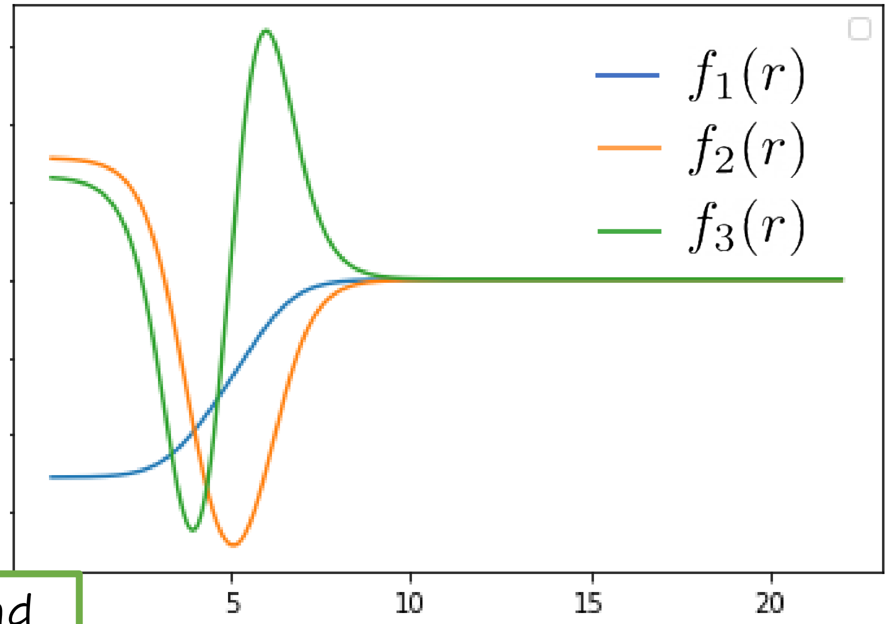
$$U(r,\boldsymbol{\theta}) = -V_v\left[1+e^{(r-R_v)/a_v}\right]^{-1} + \ldots$$

$$\implies \quad U(r,\boldsymbol{\theta}) \approx \sum_i^m b_i(\boldsymbol{\theta}) f_i(r)$$

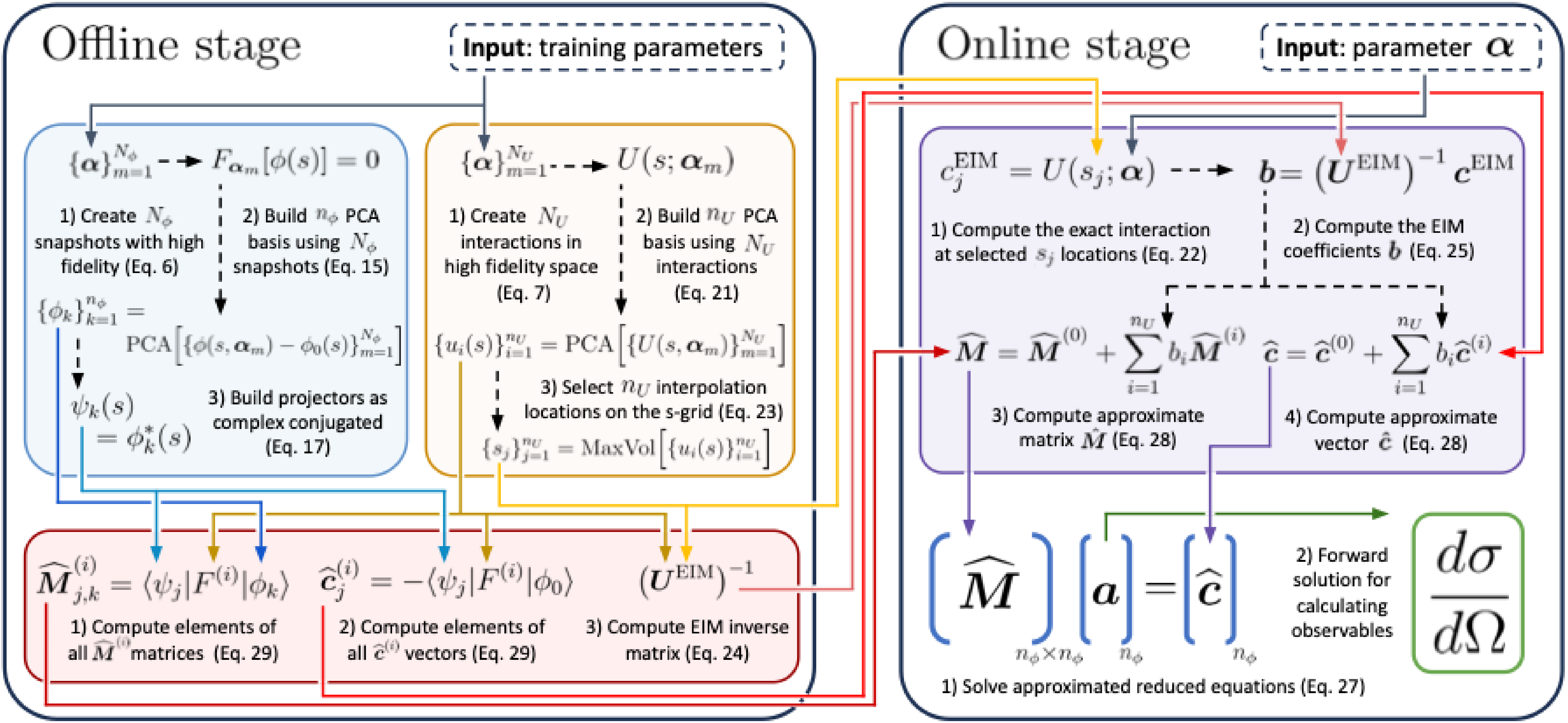
Empirical Interpolation Method: one work-around

Principal components of $U(r,\boldsymbol{\theta})$



RBM emulators for non-affine scattering problems

[Odell et al., PRC (2024)]



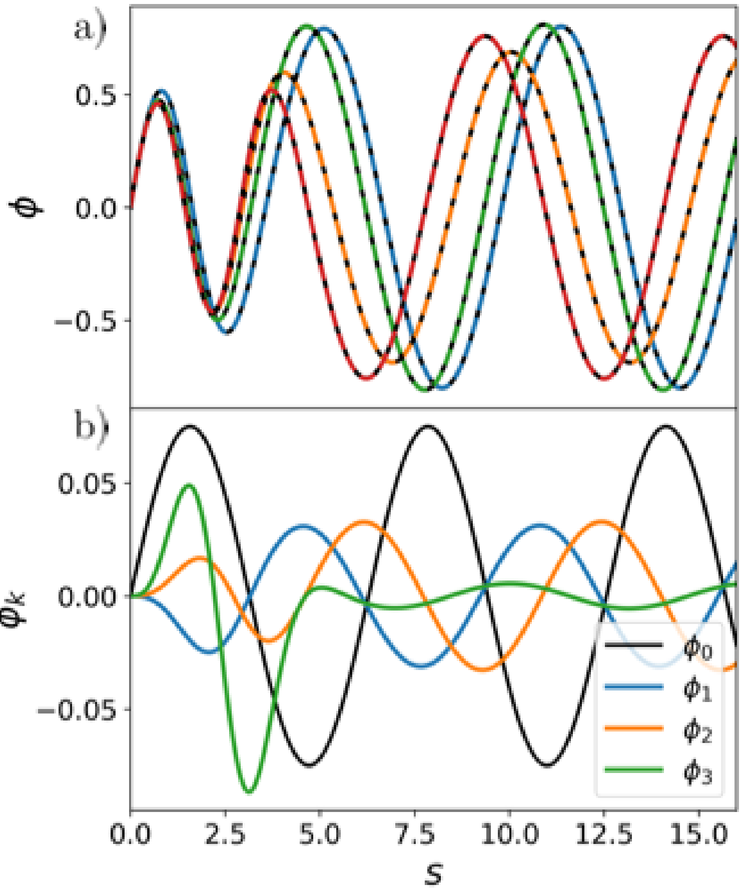
RBM emulators for non-affine scattering problems

Nuclear **ROSE** in BAND Framework (free software!).
Reduced **O**rder **S**cattering **E**mulator can handle local, complex, non-affine interactions.

[Odell et al., PRC (2024)]

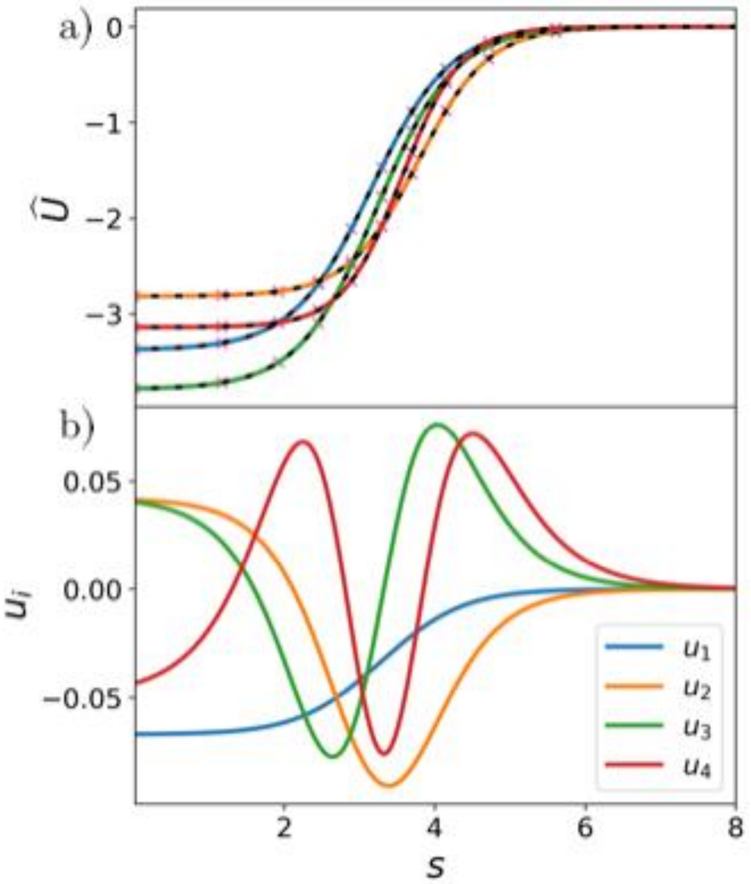
Accurate wave functions from POD (or PCA) applied to snapshots.

Leading principle components.



Accurate potentials from EIM.

Leading PCA basis components.



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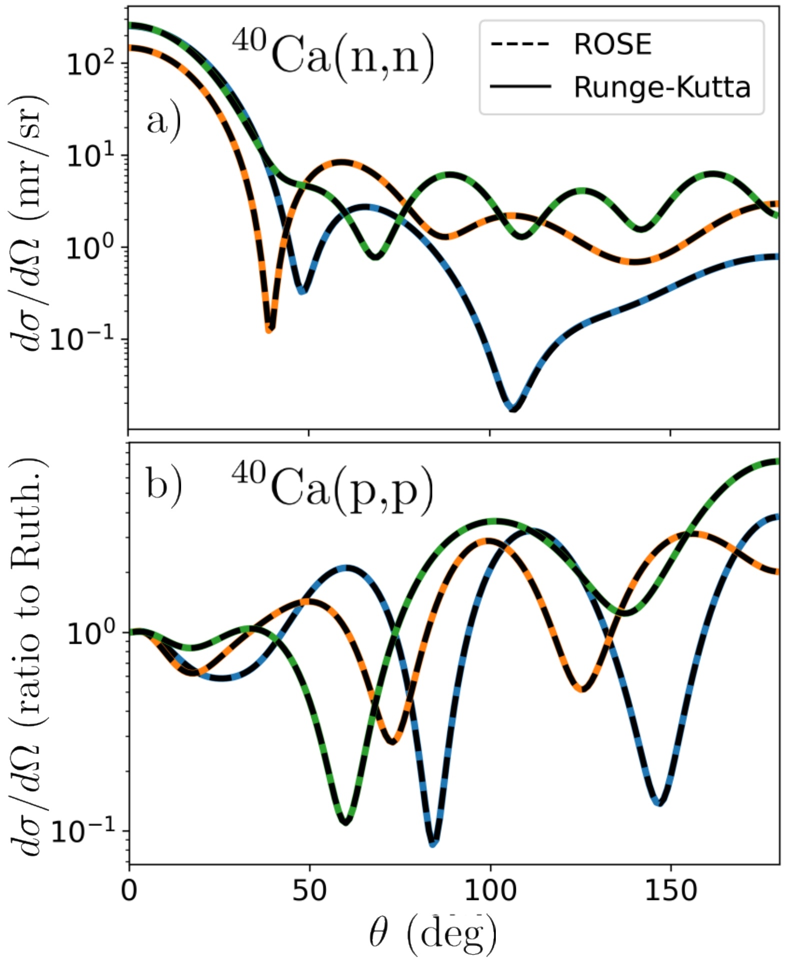
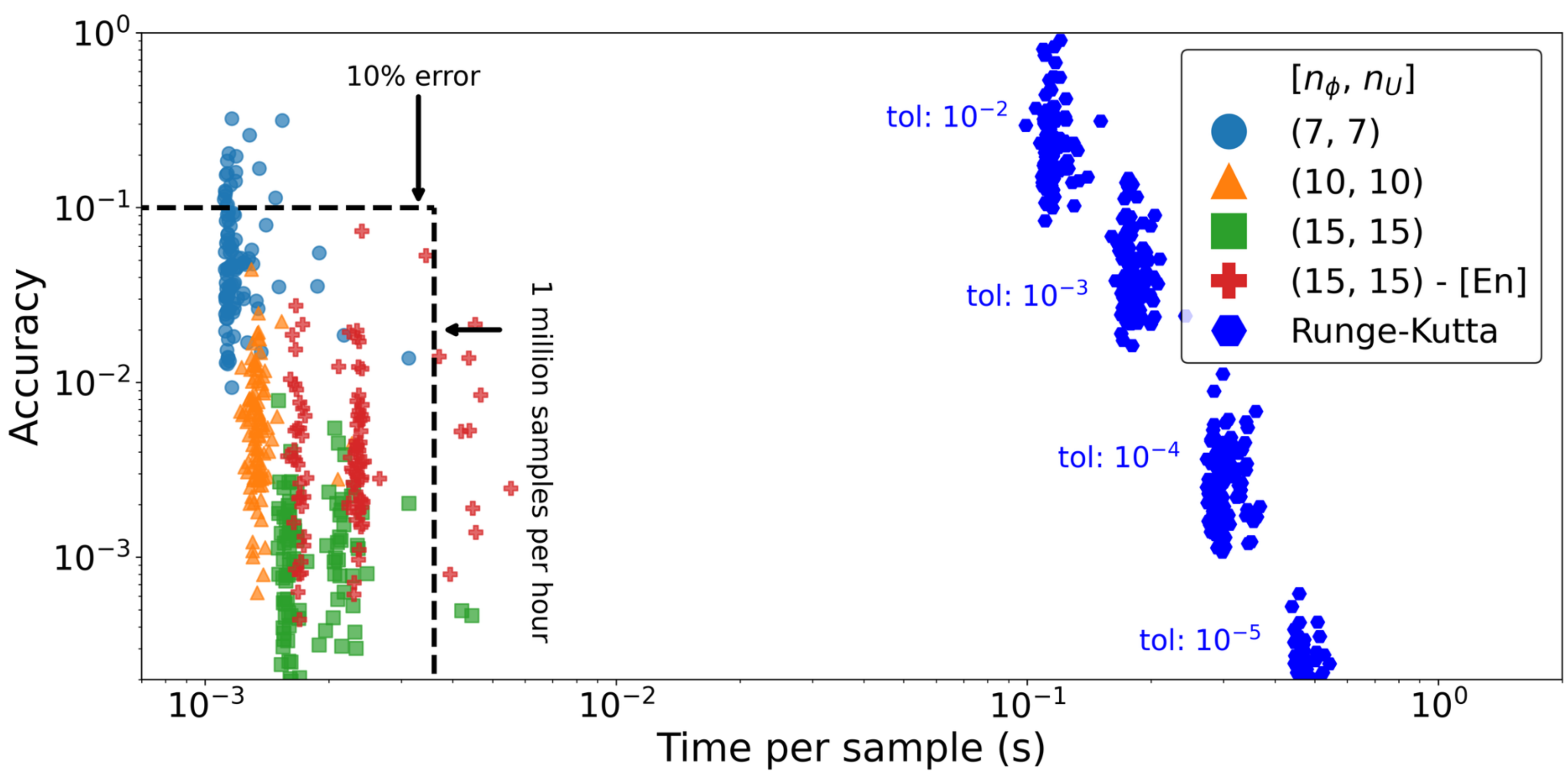


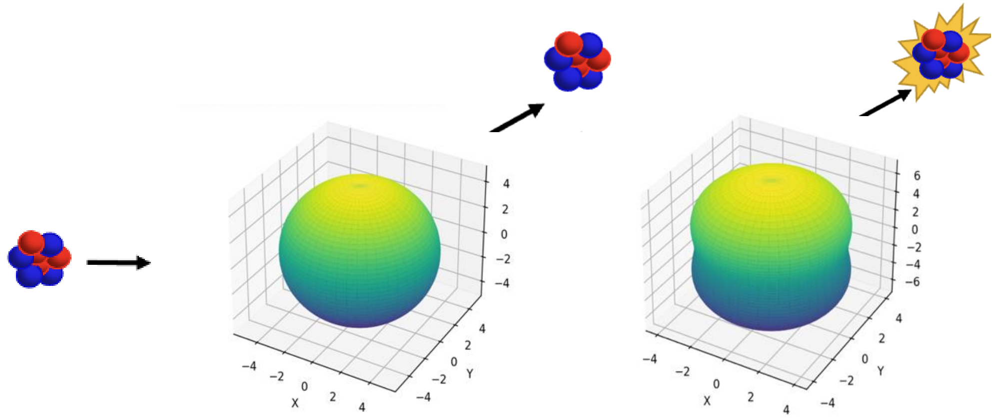
[Odell et al., PRC (2024)]



RBM emulator for coupled channels

M. Catacora-Rios et al., in prep.

Example: Inelastic scattering



$$\Psi^{\text{tot}} = a_1\phi_1(\xi)\psi_1(R) + a_2\phi_2(\xi)\psi_2(R)$$

*Elastic channel

*Inelastic channel

$$(H-E)\Psi^{\text{tot}} = 0$$

*Integrate out the ξ-dependence

$$\langle\phi_i|(H-E)\Psi^{\text{tot}}|\phi_j\rangle = 0$$

Radial equations!

Coupling term

$$[T_1 + V_1 - E_1]\psi_1 = -U_{12}\psi_2$$
$$[T_2 + V_2 - E_2]\psi_2 = -U_{21}\psi_1$$

* Single channel operator

Spherical Potentials (Woods-Saxon)

$$V_i = V(R;\alpha) + iW_s(R;\alpha) + iW_v(R;\alpha)$$

Deformed Potentials

$$U_{ij} = M_{ij}^{\lambda}V_{\lambda}(R;\alpha)$$

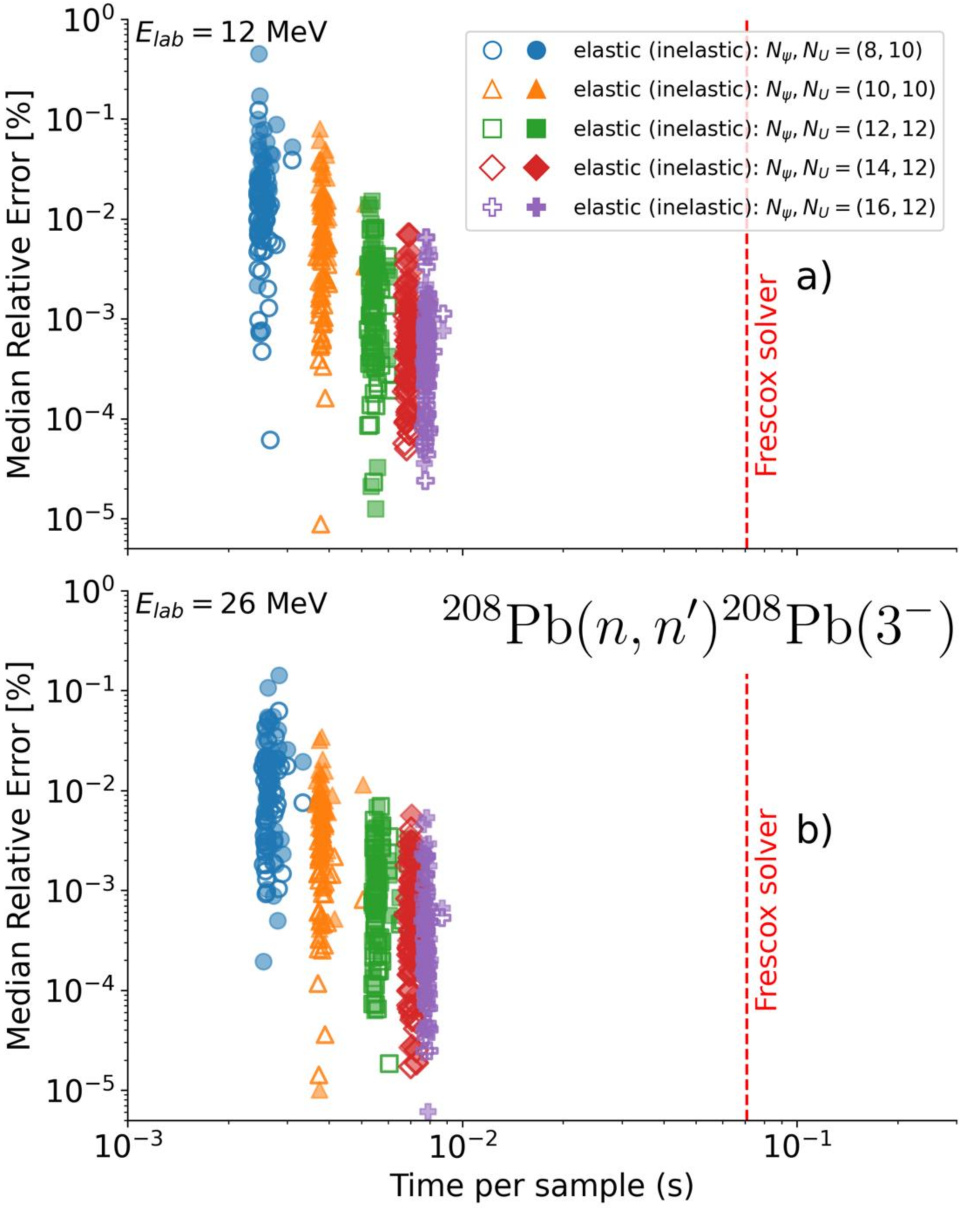
Coupling matrix elements (Angular momentum)

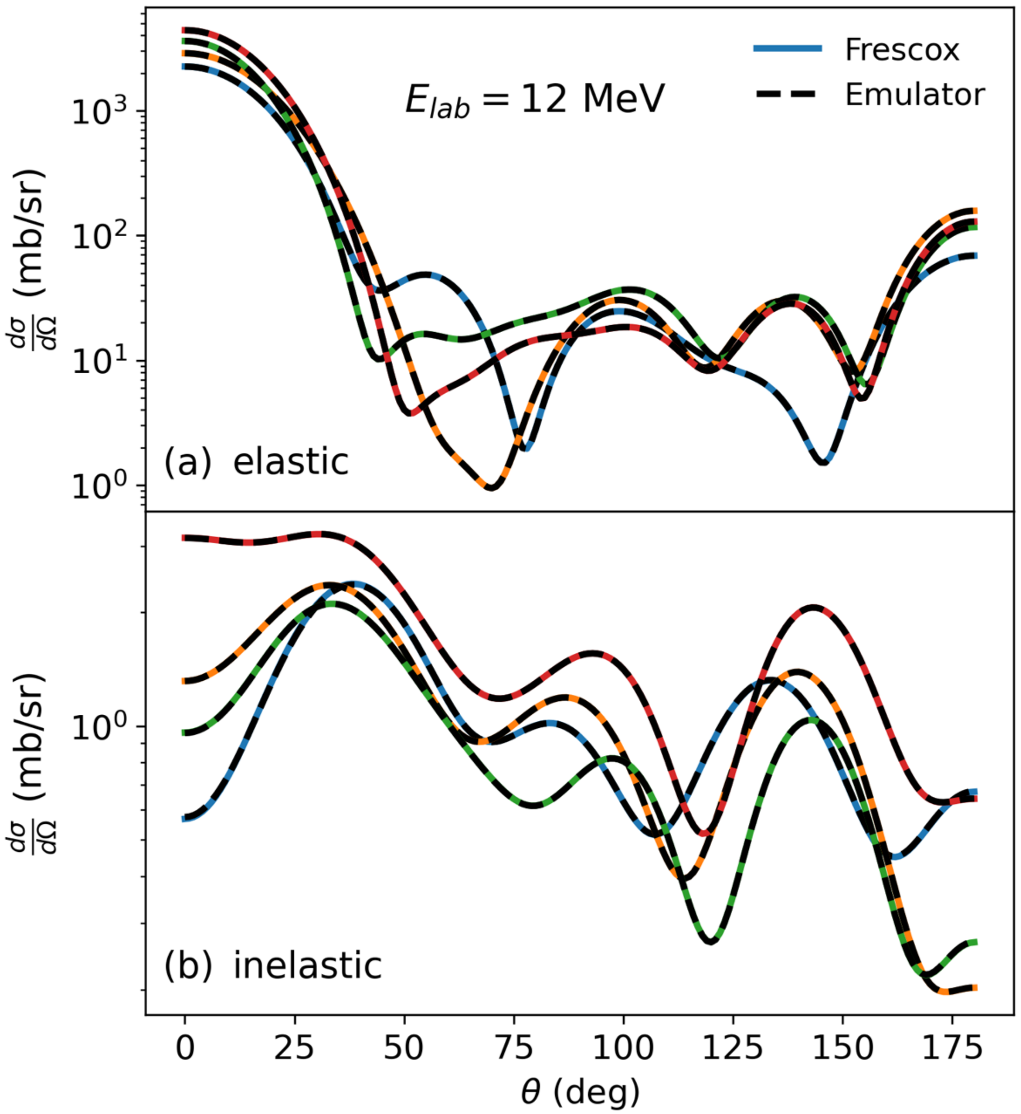
Radial and parameter dependence

Bayesian Analysis of Nuclear Dynamics

FRIB

Coupled channel emulator: Fast & Accurate





M. Catacora-Rios et al., in prep.

Outline

- Overview: RBM emulators for challenges in nuclear physics
- More effective RBMs and offline training: 2N and 3N scattering
- Non-affine models: optical potentials
- Complex energies: extracting and emulating continuum physics
- Summary and outlook

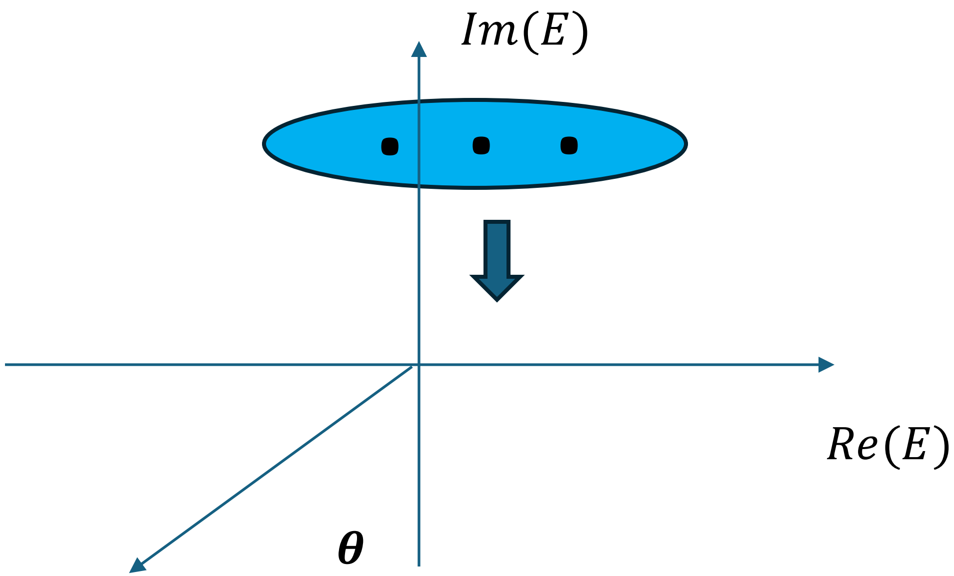
Complex-E emulator for continuum physics


X. Zhang

Challenge: sampling over many parameters when continuum physics is involved

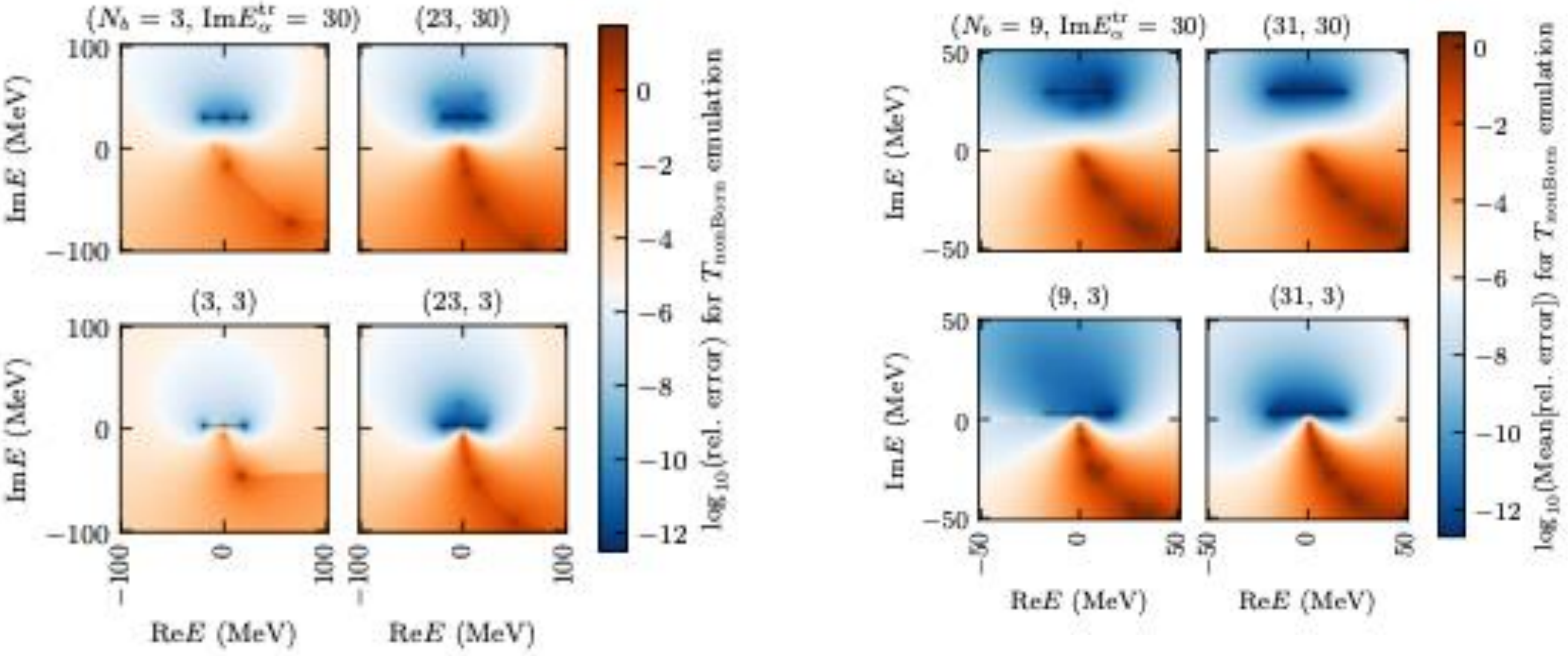
$$\mathcal{A}(E,\boldsymbol{\theta}) \equiv \left\langle \tilde{S} \middle| \frac{1}{E-H} \middle| S \right\rangle = \langle \tilde{S}|\psi\rangle$$

- Extract continuum physics from bound–state–like calculations → use complex E (Type-II methods)
- $[E - H(\boldsymbol{\theta})]|\psi(E,\boldsymbol{\theta})\rangle = |S(\boldsymbol{\theta})\rangle$ w/ complex E
  → $|\psi(E,\boldsymbol{\theta})\rangle$ is spatially localized
- $\mathcal{A}$ → response function; scattering amplitude; opt. potl.
- RBM complex-E emulator extrapolates the training results "downward" to the real axis
- H → $[H]_{n_b \times n_b}$ → spectrum
- Emulation for $\boldsymbol{\theta}$ can be done simultaneously



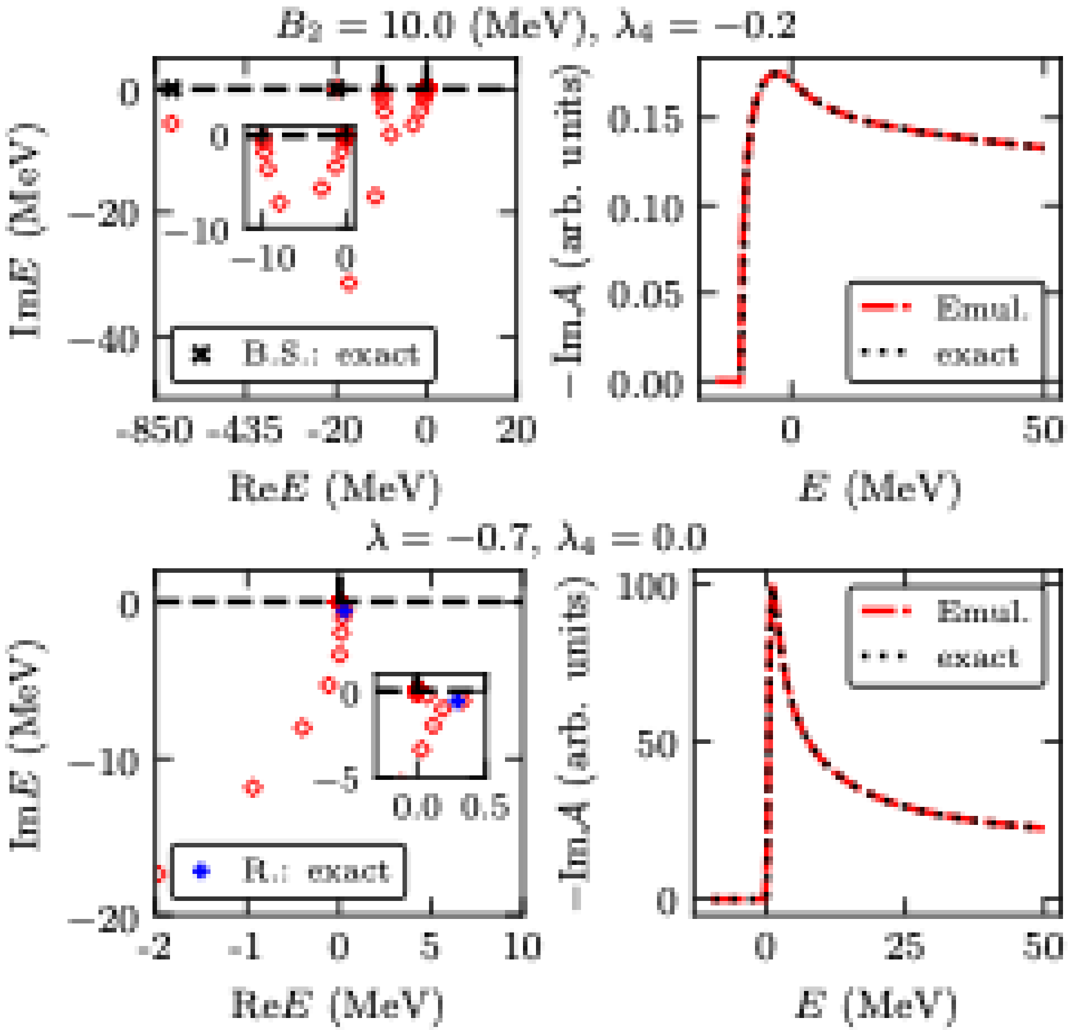
"A non-Hermitian quantum mechanics approach for extracting and emulating continuum physics based on bound-state-like calculations (: technical details)" Xilin Zhang, 2408.03309, 2411.06712 (to appear in PRL and PRC)

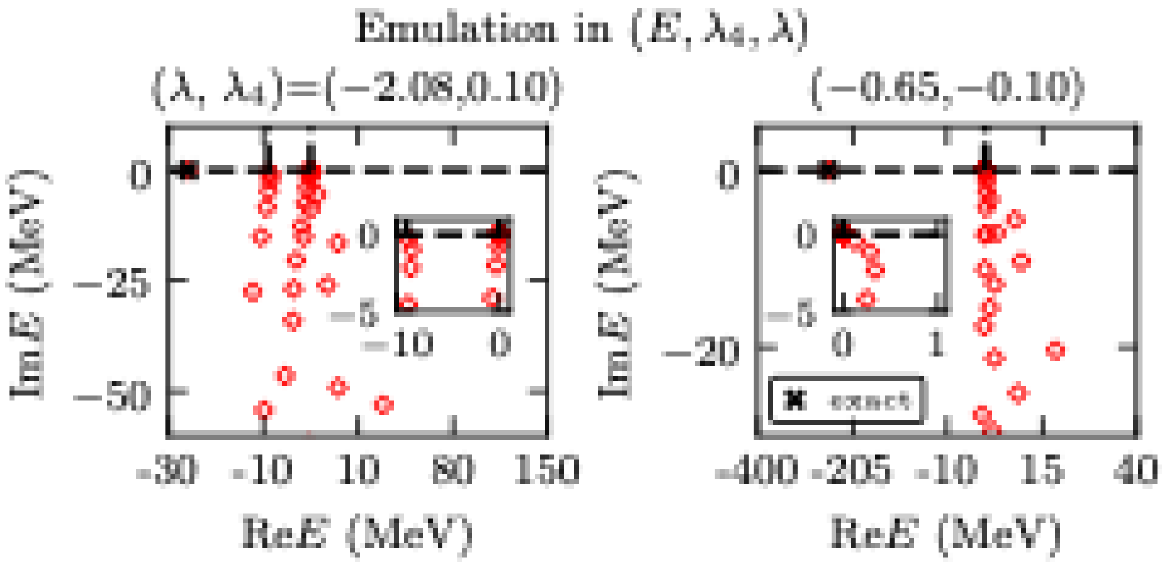
Complex-E emulator for continuum physics



Relative errors of emulated resolvent matrix element when varying basis size and training point location in the complex E plane.

Complex-E emulator for continuum physics





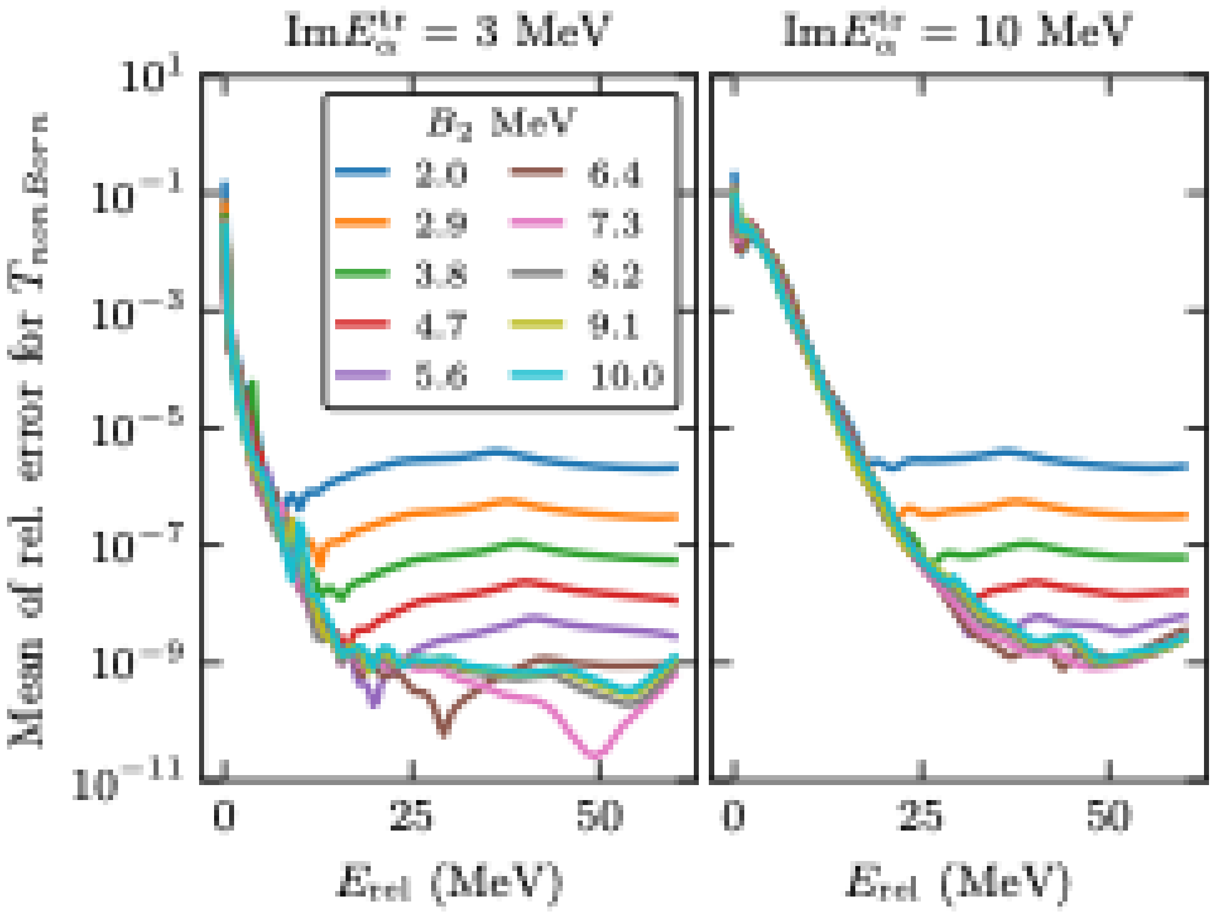
Left: Successful emulation in E at fixed $\boldsymbol{\theta}$ for three-body system of $\mathcal{A}$'s eigenvalues and –Im $\mathcal{A}$ at real energies.

Above: Successful emulation of the spectra of $\mathcal{A}$.

Complex-E emulator for continuum: scattering amplitudes

- Beyond response function extractions: compute scattering amplitudes!
- And emulate in $\boldsymbol{\theta}$!
- Figures: λ and B_2 fixed; average over λ_4's
- Related methods: "Lorentz integral transform (LIT)" and "complex energy"
- Enables $\boldsymbol{\theta}$-emulations for existing methods (and DFT linear-response calculations)

Particle-dimer scattering



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Summary of RBM emulator extensions

- Greedy algorithm / error estimates and multiple RBMs for 2N and 3N scattering
- EIM for non-affine optical potentials (including coupled channels)
- Joint emulation in complex energy E and parameters $\boldsymbol{\theta}$

Many opportunities

- Extend 3N emulators to full Bayesian calibration and UQ for chiral EFT
- Efficient Bayesian calibration for optical potentials (and beyond) → next steps?
- Many continuum applications are waiting!

Alternative to RBM?

- Parametric matrix models: impose matrix structure but learn from data

Thank you!

Jupyter and Quora books:

- Learning from Data for Physicists (Forssén, rjf, Phillips)
- BUQEYE Guide to Projection-Based Emulators in Nuclear Physics
- Reduced Basis Methods in Nuclear Physics

See Duguet et al., RMP (2024) for more on EC/RBM emulators

Extra Slides

Hybrid approach: Parametric Matrix Models (PMMs)

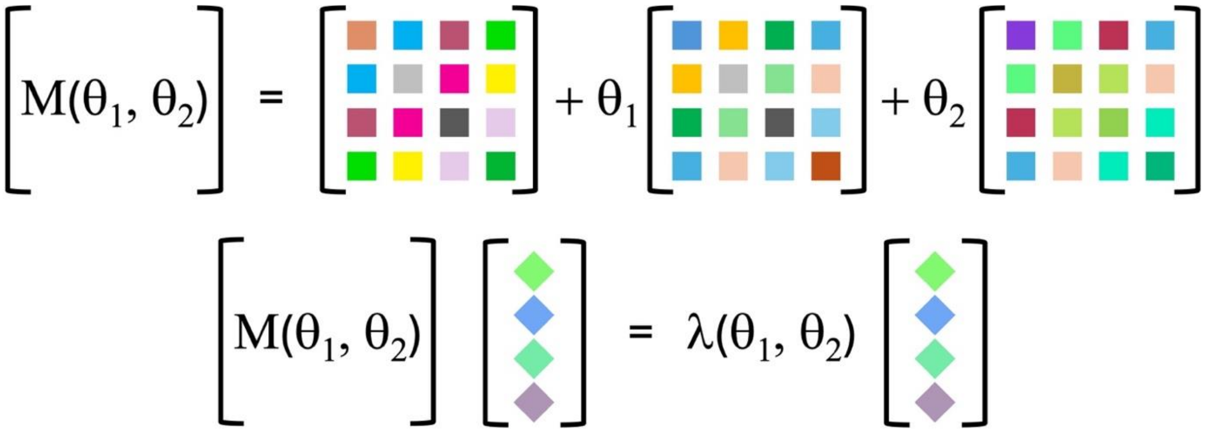
$$\widetilde{H}(\boldsymbol{\theta}) = \widetilde{H}_0 + \sum_n \boldsymbol{\theta}_n \widetilde{H}_n$$

RBM/EC: matrix elements of eigenvector snapshots → model driven

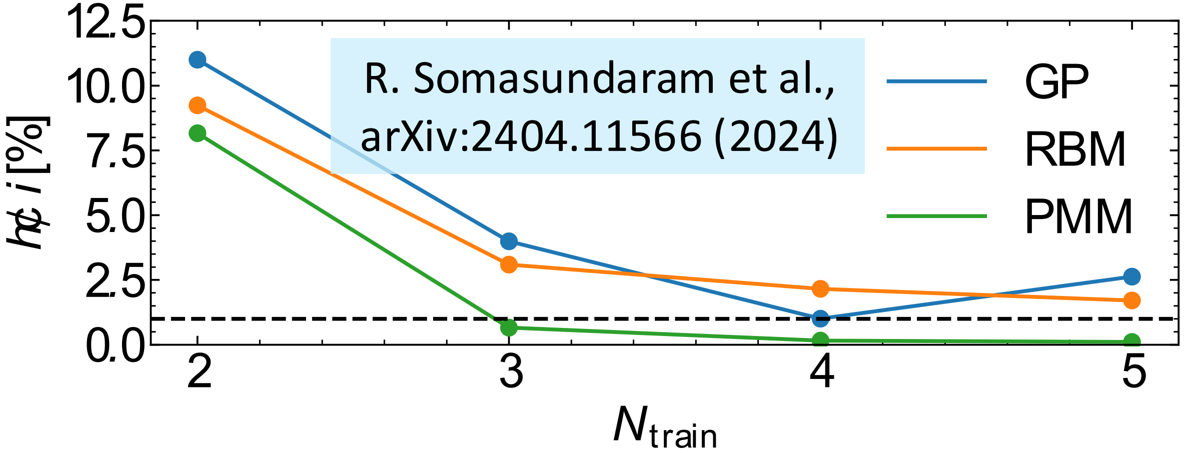
$$\widetilde{M}(\boldsymbol{\theta}) = \widetilde{M}_0 + \sum_n \boldsymbol{\theta}_n \widetilde{M}_n$$

PMM: *learn* matrix elem. from data (eigenvalues) → hybrid data driven

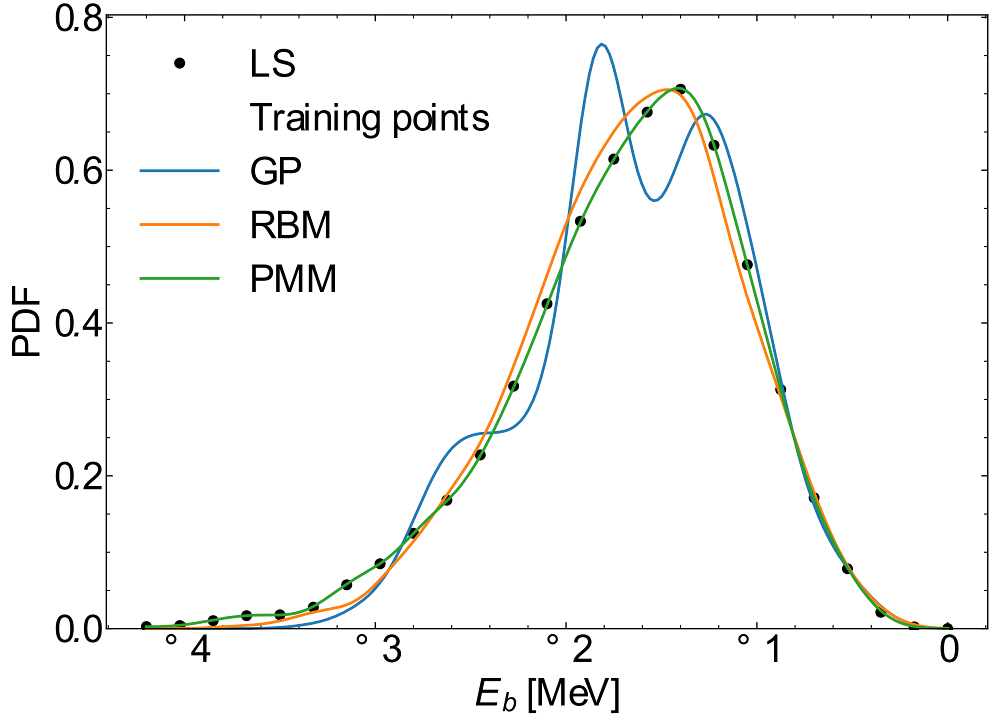
P. Cook, D. Jammooa et al., arXiv:2401.11694 (2025)



PMMs capture essential structures such as smooth analytic behavior, symmetries, and conservation laws.



Application to emulate noisy AFDMC calculations



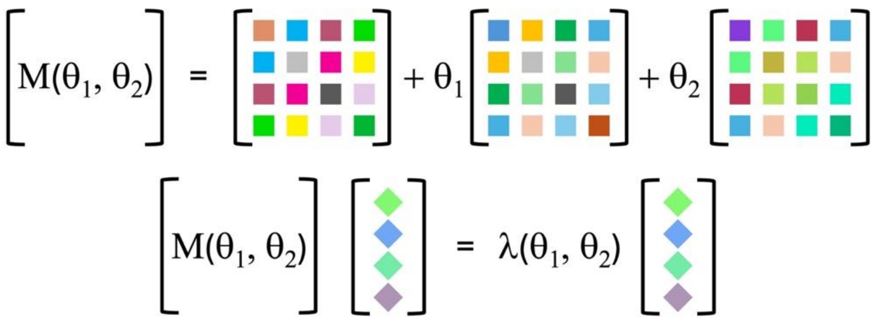
Parametric matrix models bridge physics and machine learning

Objectives

- Researchers have introduced a new class of machine learning algorithms called parametric matrix models (PMMs).
- Unlike traditional approaches that mimic neurons or optimize generic functions, PMMs are built from matrix equations that resemble the governing equations of physical systems.
- By treating inputs as parameters for the matrix elements, PMMs capture essential structures such as smooth analytic behavior, symmetries, and conservation laws.
- PMMs are universal function approximators, able to solve general machine learning tasks while retaining strong interpretability.

Impact

- Parametric matrix models represent a paradigm shift in scientific machine learning.
- By embedding physical and mathematical structure directly into their design, PMMs produce interpretable results that adhere to known constraints, unlike many “black box” neural networks.
- This makes them especially powerful for scientific discovery, where extrapolation, efficiency, and interpretability are critical.
- PMMs can outperform state-of-the-art methods in scientific computing and compete strongly on broader machine learning tasks.



Parametric matrix models emulate physical systems through matrix equations, enabling accurate and interpretable predictions with fewer parameters than conventional machine learning methods.

Accomplishments

- “Parametric Matrix Models,” Cook, Jammooa, Hjorth-Jensen, Lee, Lee, Nat. Commun. 16, 5929 (2025).
- https://frib.msu.edu/news-center/news/researchers-develop-new-machine-learning-method

RBM implementation freedom: examples from scattering

Codes (Jupyter notebooks) publicly available!

Wave-function-based emulation for nucleon-nucleon scattering in momentum space (General Kohn & Newton Variational Principle)

2023

Garcia, CD, Furnstahl, Melendez, and Zhang, Phys. Rev. C **107**, 054001

Highlight: extends snapshot-based KVP to <u>momentum space & coupled channels</u>

Toward emulating nuclear reactions using eigenvector continuation (General Kohn Variational Principle)

2021

CD, Quinonez, Giuliani, Lovell, and Nunes, Phys. Lett. B **823,** 136777

Highlight: Schwartz anomaly mitigation | proof of principle: <u>parameter estimation</u>

Fast & accurate emulation of two-body scattering observables without wave functions (Newton Variational Principle)

2021

Melendez, CD, Garcia, Furnstahl, and Zhang, Phys. Lett. B **821**, 136608

Highlight: VP without (trial) wave functions | in <u>momentum space</u> | coupled channels

Efficient emulators for scattering using eigenvector continuation (Kohn Variational Principle for the *K*-matrix)

2020

Furnstahl, Garcia, Millican, and Zhang, Phys. Lett. B **809**, 135719

Highlight: introduces <u>snapshot-based trial wave functions</u> for ROMs

progress

See also: CD, Melendez, Garcia, Furnstahl, and Zhang, Front. Phys. **10**, 92931 | see also ROSE in Odell *et al.*, PRC **109**, 044612

RBM implementation freedom: examples from scattering

Quantum mechanical two-body scattering problem can be formulated in multiple ways: Schrödinger equation in coordinate or momentum space; variational methods; …

Variational Principle		Galerkin Projection Information			
Name	Functional for K	Strong Form	Trial Basis	Test Basis	Constrained?
Kohn (λ)	$\widetilde{K}_E + \langle\widetilde{\psi}\vert H - E\vert\widetilde{\psi}\rangle$	$H\vert\psi\rangle = E\vert\psi\rangle$	$\vert\psi_i\rangle$	$\langle\psi_i\vert$	Yes
Kohn (No λ)	$\langle\widetilde{\chi}\vert H - E\vert\widetilde{\chi}\rangle + \langle\phi\vert V\vert\widetilde{\chi}\rangle + \langle\phi\vert H - E\vert\phi\rangle + \langle\widetilde{\chi}\vert V\vert\phi\rangle$	$[E-H]\vert\chi\rangle = V\vert\phi\rangle$	$\vert\chi_i\rangle$	$\langle\chi_i\vert$	No
Schwinger	$\langle\widetilde{\psi}\vert V\vert\phi\rangle + \langle\phi\vert V\vert\widetilde{\psi}\rangle - \langle\widetilde{\psi}\vert V - VG_0V\vert\widetilde{\psi}\rangle$	$\vert\psi\rangle = \vert\phi\rangle + G_0V\vert\psi\rangle$	$\vert\psi_i\rangle$	$\langle\psi_i\vert$	No
Newton	$V + VG_0\widetilde{K} + \widetilde{K}G_0V - \widetilde{K}G_0\widetilde{K} + \widetilde{K}G_0VG_0\widetilde{K}$	$K = V + VG_0K$	K_i	K_i	No

See Drischler et al., (2022) for details and references

Every variational way for scattering has a Galerkin counterpart!

Non-variational, also, e.g., "origin" emulator $(r\psi)(0) = 0,\ (r\psi)'(0) = 1$

What is the best way to implement a 3-body scattering emulator?

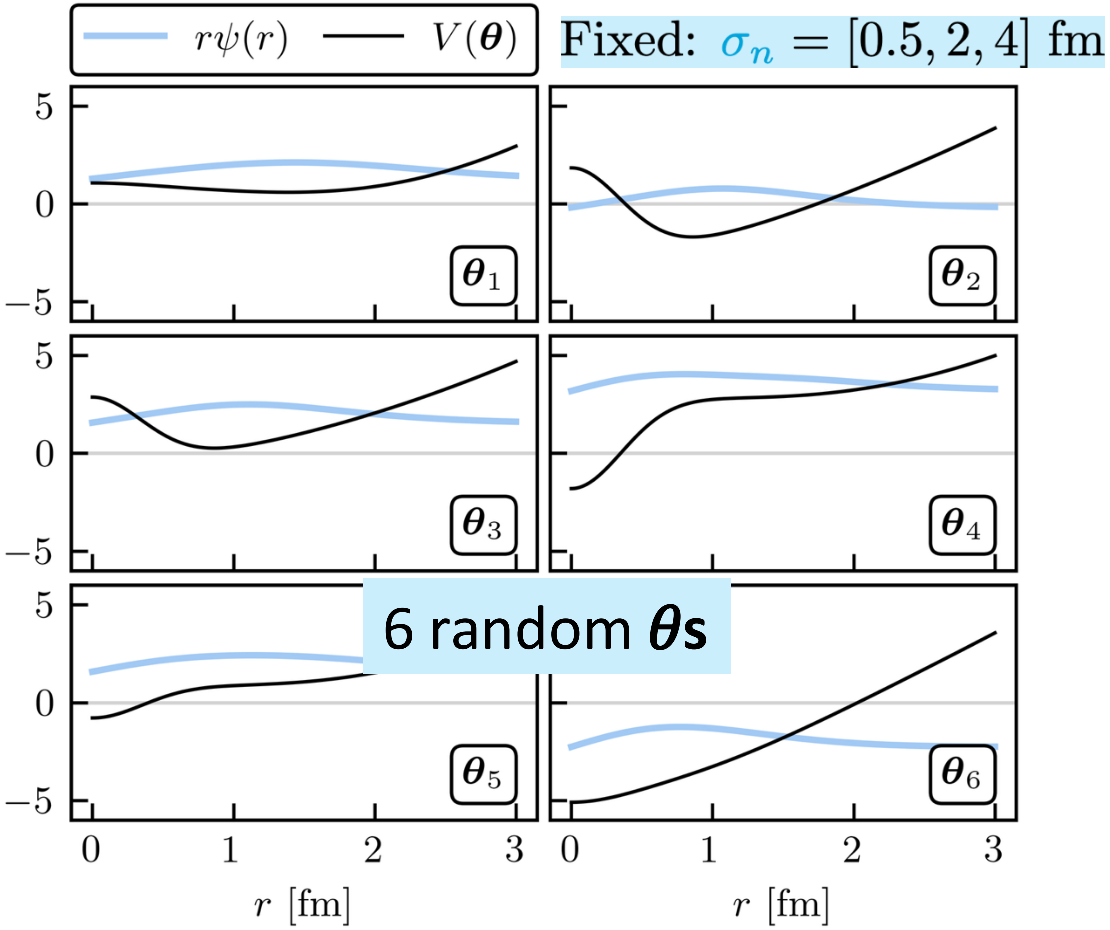
- E.g, for Bayesian χEFT LEC estimation or nuclear reactions.
- X. Zhang, rjf, PRC (2022) gave proof of principle (bosons) using KVP.

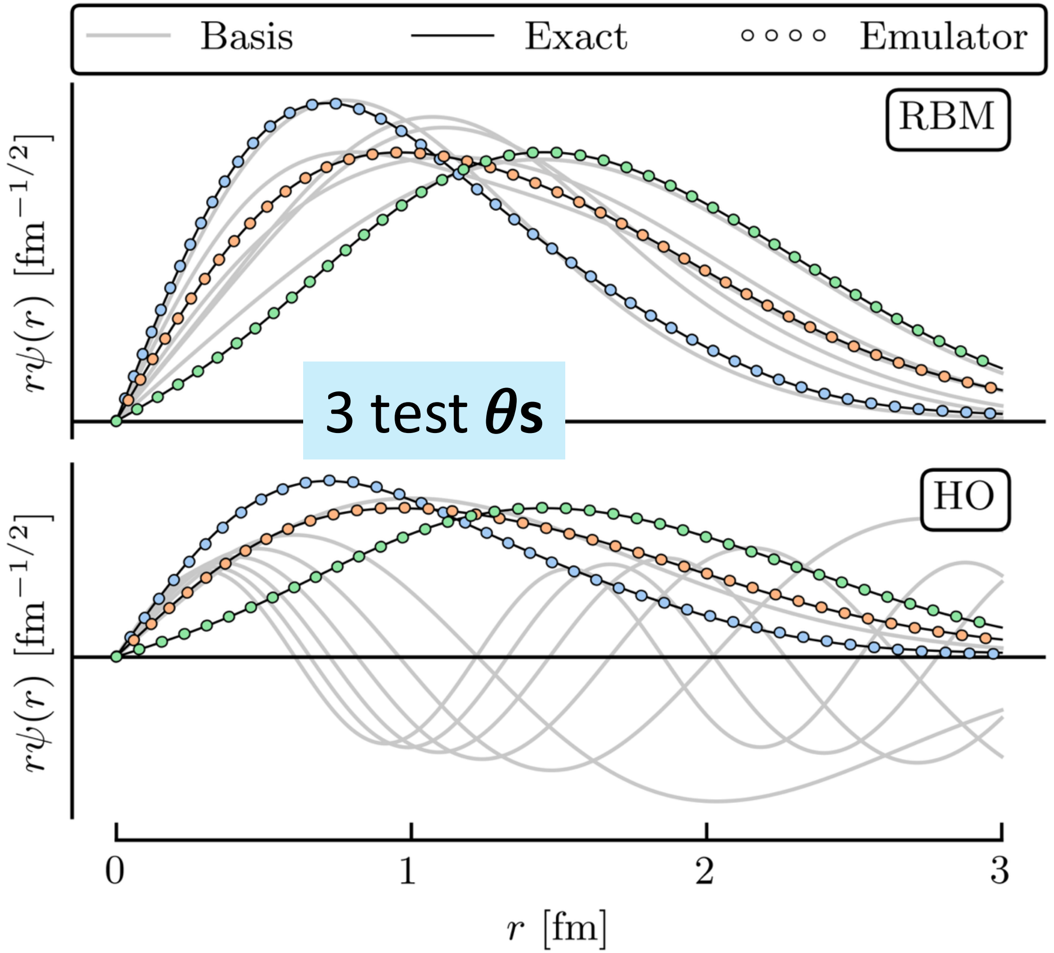
Illustrative example: anharmonic oscillator [Try your own!]

Eigenvalue problem: $H(\boldsymbol{\theta})|\psi\rangle = E|\psi\rangle$

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

← affine!





Variational emulator → diagonalize the Hamiltonian $H(\boldsymbol{\theta})$ in a *finite* basis: $\sum_{i=1}^{n_b} \beta_i \psi_i$

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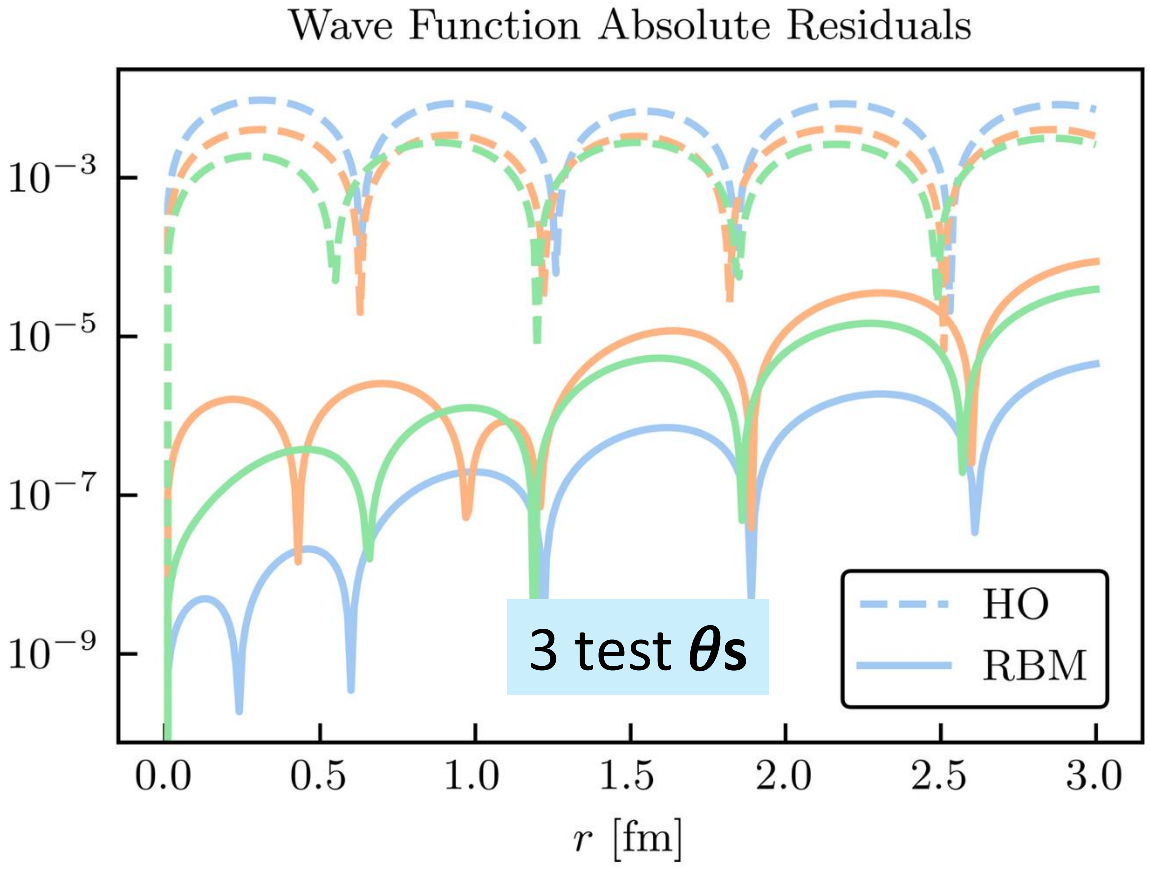
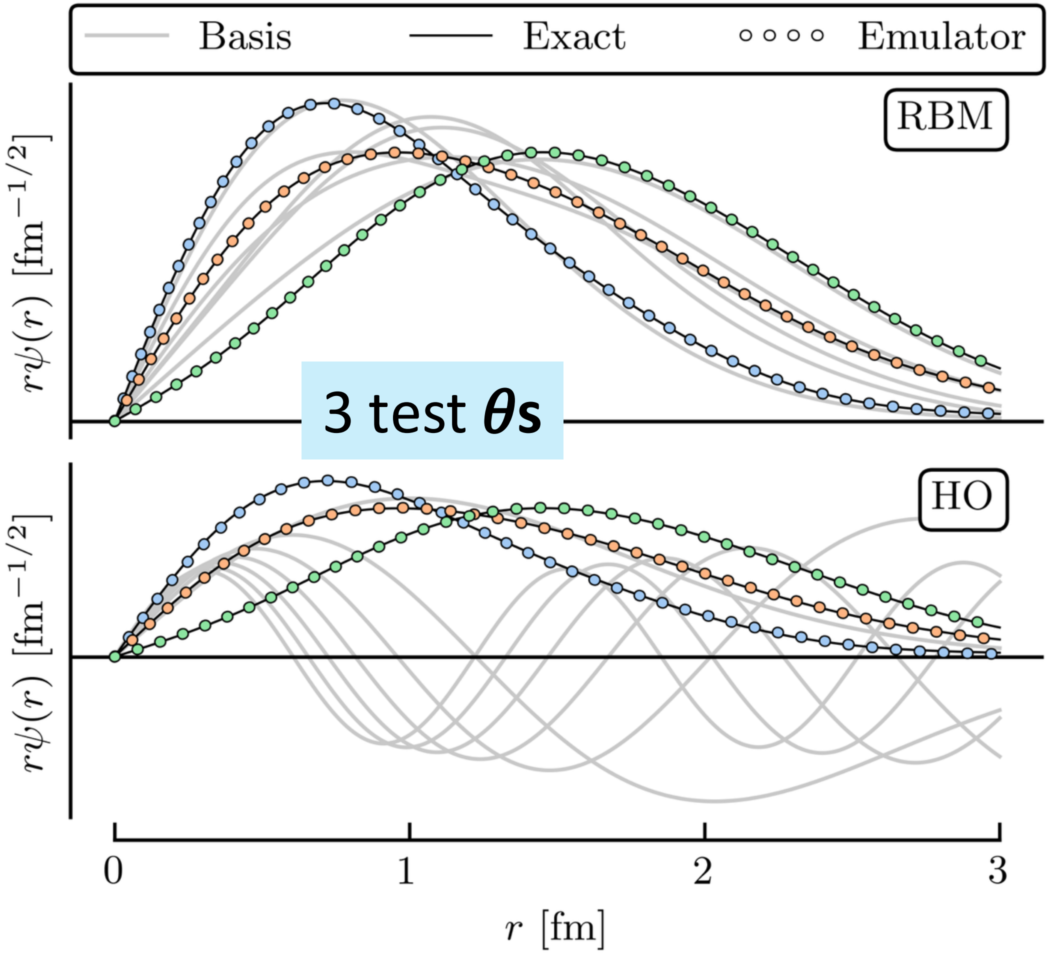
Eigenvalue problem: $H(\boldsymbol{\theta})|\psi\rangle = E|\psi\rangle$ $\quad V(r;\boldsymbol{\theta}) = V_{\mathrm{HO}}(r) + \sum_{n=1}^{3} \theta^{(n)} e^{-r^2/{\sigma_n}^2}$ ← affine!





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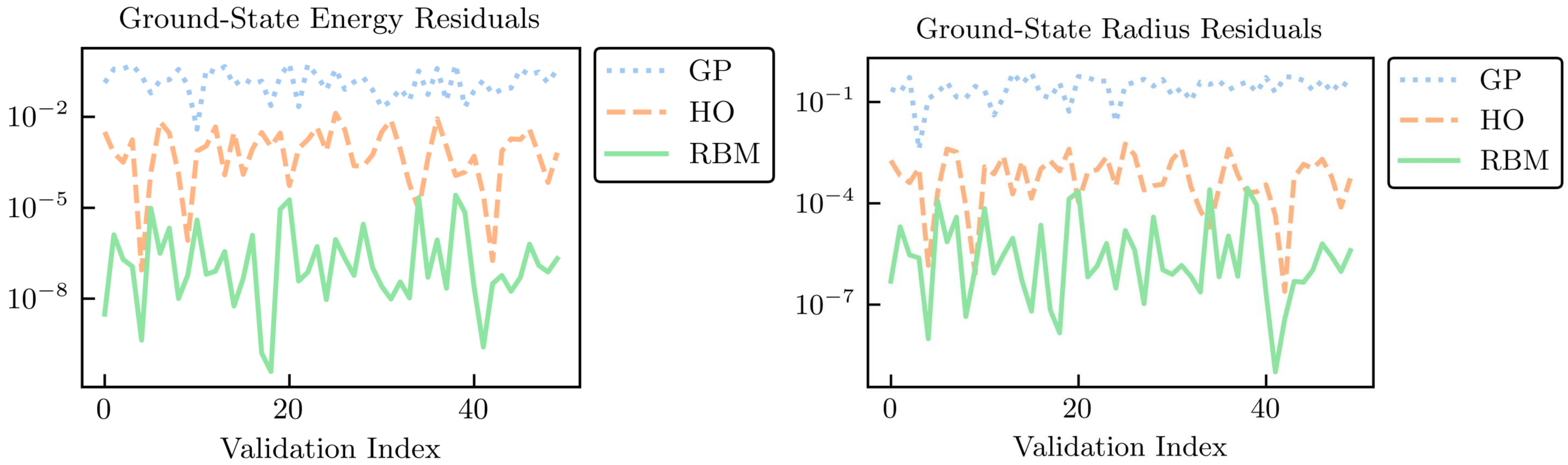
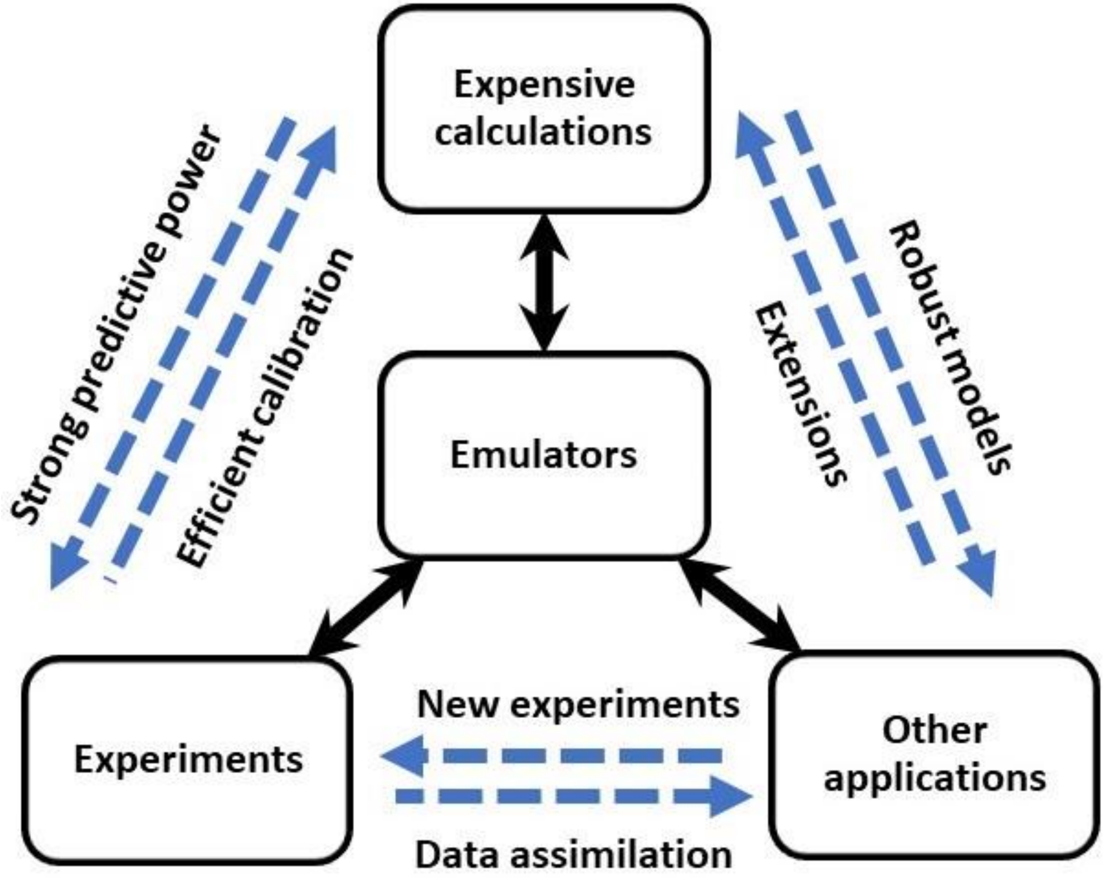
Fixed: $\sigma_n = [0.5, 2, 4]$ fm



Summary: GP doesn't use the structure of the high-fidelity system to its advantage; HO emulator knows the problem to be solved is an eigenvalue problem; RBM (aka EC) training data are curves rather than scalars, takes advantage of system structure.

Role of emulators: new workflows for NP applications

From Xilin Zhang, rjf, *Fast emulation of quantum three-body scattering*, Phys. Rev. C **105**, 064004 (2022).



How can ISNET facilitate these new workflows based on shared emulators?

If you can create fast & accurate™ emulators for observables, you can do calculations without specialized expertise and expensive resources!

CC-Emulator Workflow Chart

User inputs: $\{\alpha_k\}_{k=1}^{N_{RBM}}$ $\{\alpha_k\}_{k=1}^{N_{EIM}}$ P–T system (states, numerical details) After off-line: $\{\alpha_k\}_{k=1}^{N_{solve}}$

n_{RBM} n_{EIM}^{sph} n_{EIM}^{def} δ–strength