# Fast & accurate emulation of two-body scattering

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Eigenvector continuation & related techniques in nuclear structure & reaction theory

May 31, 2023 | Espace de Structure Nucléaire Théorique (CEA/DSM-DAM)

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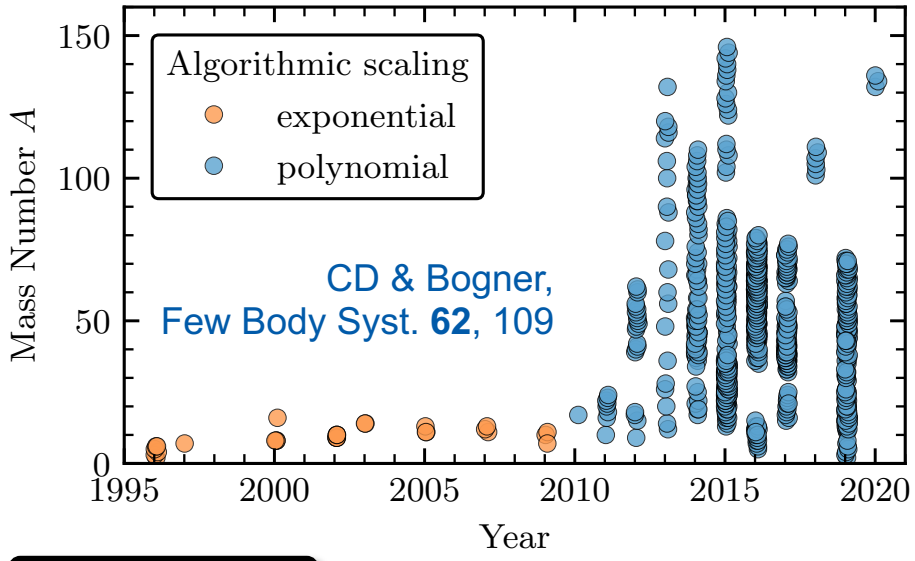
**Reduced Order Model (ROM) Classification**

## Keywords:

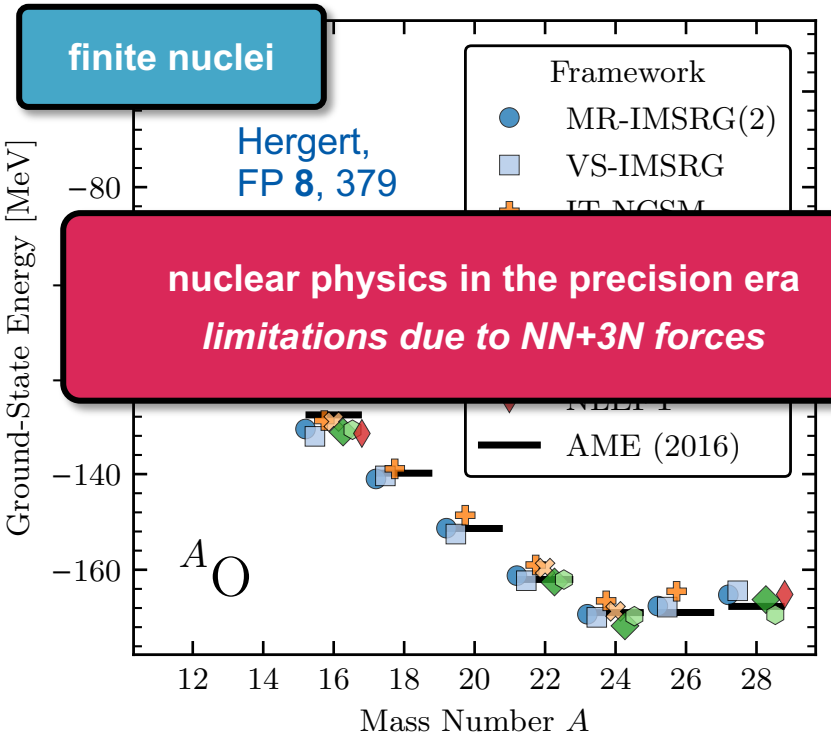
- **Parametric Model Order Reduction**
- Reduced Basis Method
- **Galerkin Projection (Methods)**
- *Offline-Online* Decomposition
- Nuclear Scattering and Reactions
- Schwartz (or Kohn) Anomalies

**Ohio University Campus**

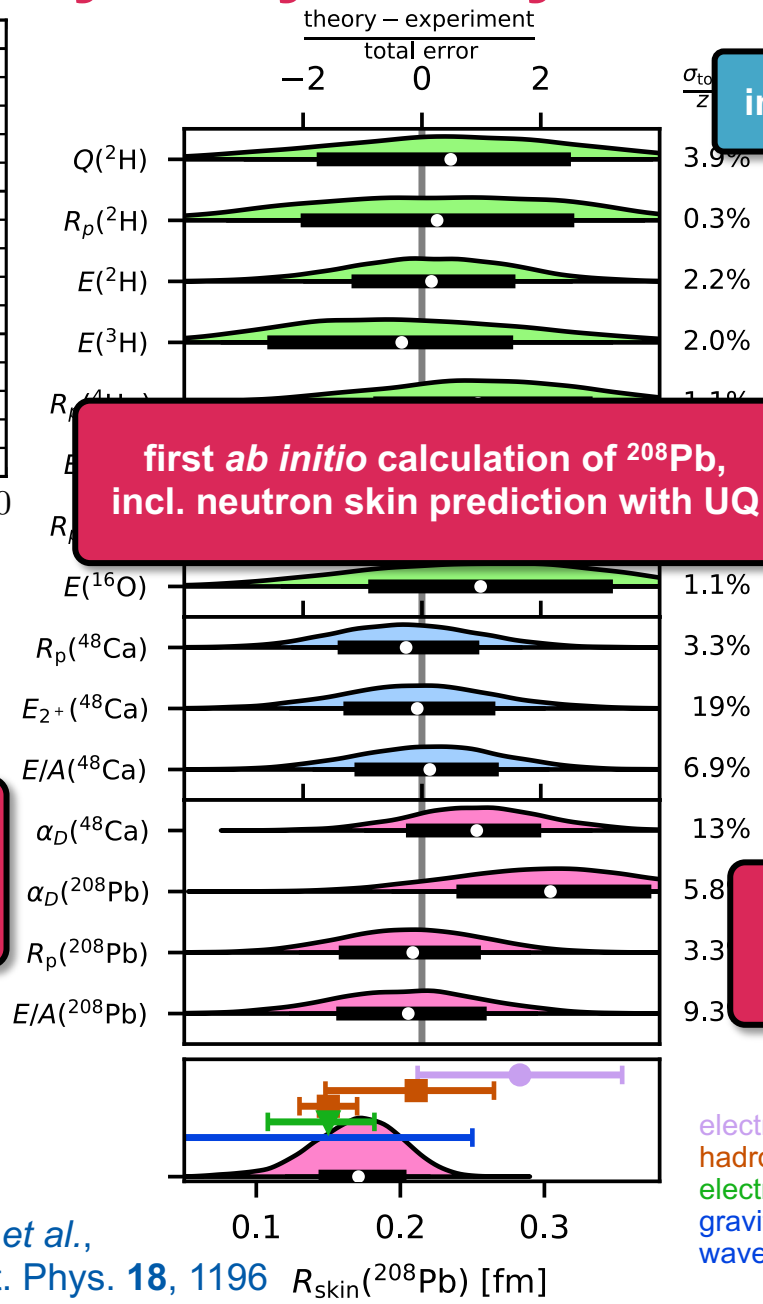
# Major process: CEFT, many-body theory, and UQ!




**finite nuclei**

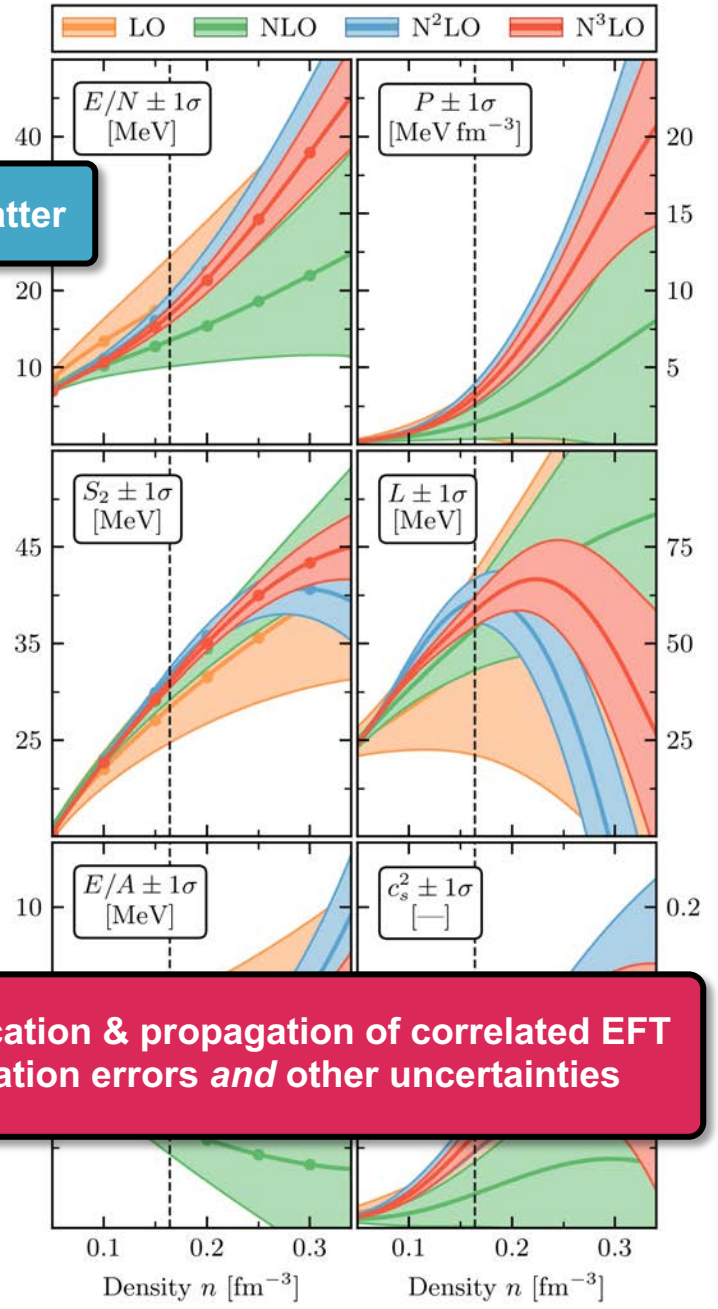



**nuclear physics in the precision era**
***limitations due to NN+3N forces***




**first *ab initio* calculation of $^{208}$Pb, incl. neutron skin prediction with UQ**

**infinite matter**




**quantification & propagation of correlated EFT truncation errors *and* other uncertainties**

electroweak
hadronic
electromagnetic
gravitational waves

CD, Furnstahl, Melendez, Phillips, PRL **125**, 202702

# Motivation: mining scattering data

See also: talks at ISNET-9 last week at WUSTL: https://physics.wustl.edu/isnet9

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**Scattering experiments yield invaluable data** for testing, validating, and improving chiral EFT (as well as reaction theory)

**Competing formulations of chiral EFT with open questions** on issues including

- EFT power counting
- sensitivity to regulator artifacts
- Differing predictions for medium-mass to heavy nuclei

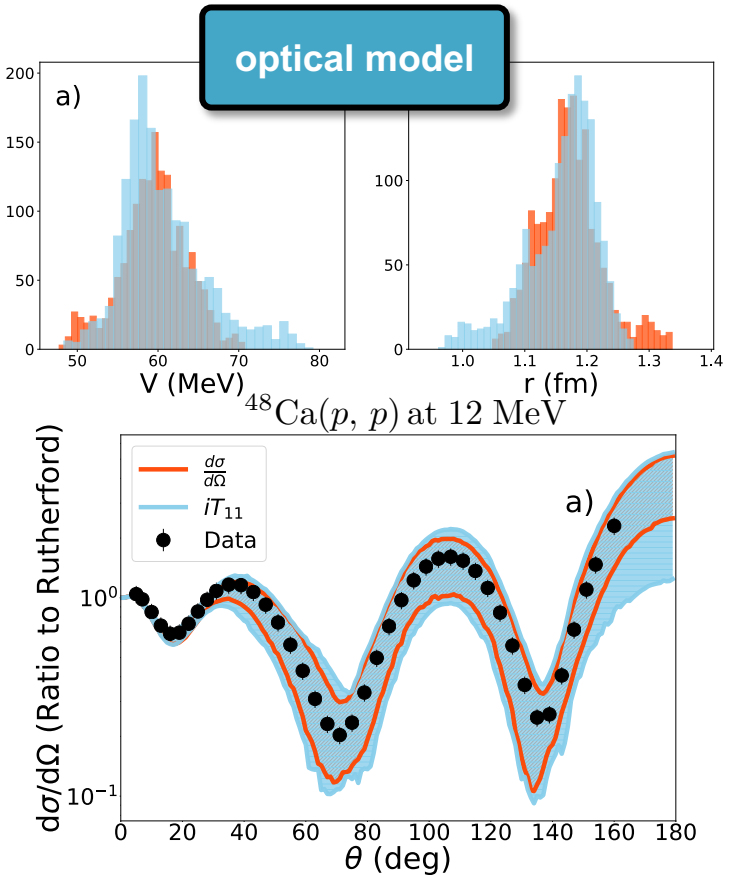
see, *e.g.*, Yang, Ekström *et al.*, arXiv:2109.13303
Furnstahl, Hammer, Schwenk, Few Body Syst. **62**, 72

**Bayesian methods** can provide important insights into the issues of these potentials:

- parameter estimation
- model comparison
- sensitivity analysis

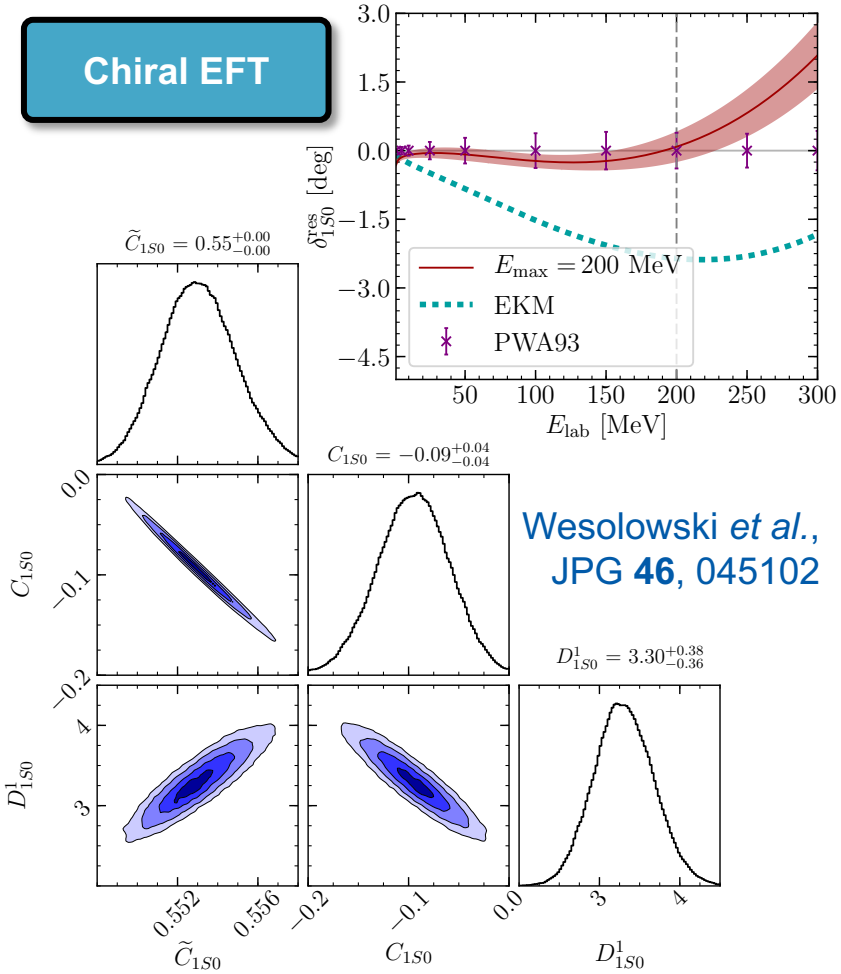
BUQEYE
Chalmers
ISNET

**optical model**




Catacora-Rios *et al.*,
PRC **104**, 064611

**Chiral EFT**




Wesolowski *et al.*,
JPG **46**, 045102

Scattering eqns. (FOM) can be solved accurately in few-body systems.
**But:** prohibitively slow for statistical analyses of $A > 2$ scattering

**Construct ROMs by removing superfluous information**

# Eigenvector Continuation vs Reduced Basis Method

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PHYSICAL REVIEW LETTERS

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Featured in Physics

## Eigenvector Continuation with Subspace Learning

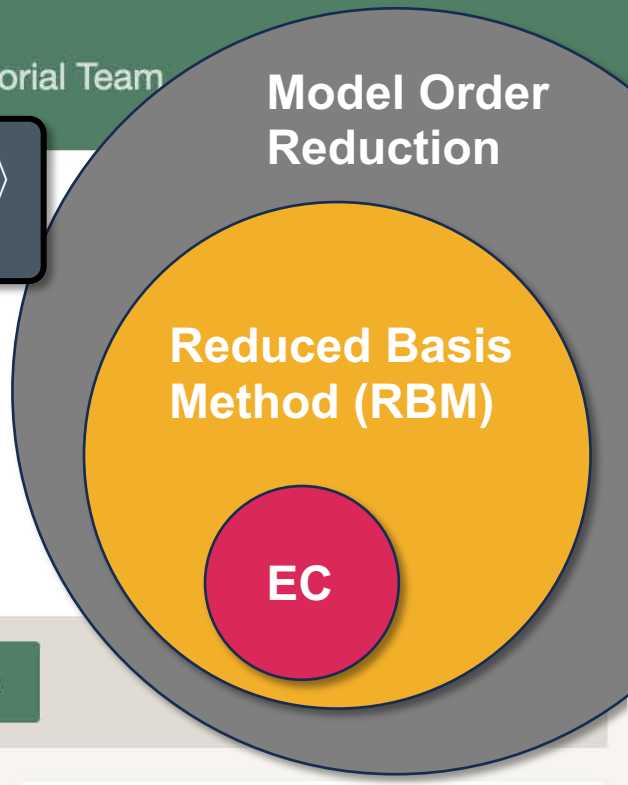
Dillon Frame, Rongzheng He, Ilse Ipsen, Daniel Lee, Dean Lee, and Ermal Rrapaj
Phys. Rev. Lett. **121**, 032501 – Published 17 July 2018

Physics See Synopsis: Making Quantum Computations Behave

Article | References | Citing Articles (59) | Supplemental Material | PDF | HTML | Export Citation

$$H(\boldsymbol{\theta})\,|\psi(\boldsymbol{\theta})\rangle = E(\boldsymbol{\theta})\,|\psi(\boldsymbol{\theta})\rangle$$

Schrödinger Equation




**EC has been a *game changer***
**for applying Bayesian methods in NP**

! Eigenvector continuation (EC) is a **specific implementation of the RBM** (which has been known for decades) for emulating parametric eigenvalue (and scattering) problems

» **Exciting opportunities to learn from the PMOR community,** including language, algorithms, software, workflows error analysis, and many more

Literature Guide: Melendez, CD, Garcia, Furnstahl, and Zhang, J. Phys. G **49**, 102001

# Open-Source MOR software libraries

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TABLE I. A sampling of recent MOR software libraries; see Ref. [13, Sec. 13.3] for an extensive listing.

| Library | Language | Website | Remark |
|---|---|---|---|
| pyMOR[a] [86] | Python | pymor.org | focuses on RBMs for parameterized PDEs; integrates with external PDE solvers |
| libROM | C++ | librom.net | library for efficient MOR techniques and physics-constrained data-driven methods; includes POD, DMD, projection-based ROM, hyper-reduction, greedy algorithm |
| MORLAB [87] | MATLAB | mpi-magdeburg.mpg.de/projects/morlab | MOR of dynamical systems based on the solution of matrix equations using spectral projection methods |
| modred [88] | Python | modred.readthedocs.io | library for computing modal decompositions and ROMs, including POD, DMD, and Petrov-Galerkin projection |
| pyROM [89] | Python | github.com/CurtinIC/pyROM | framework that employs Python visualisation tools; includes POD and DMD |
| pressio [90] | C++ | pressio.github.io | minimally-intrusive interface for MOR routines, including Galerkin projections |

[a] See also the website of the Model Reduction for Parametrized Systems (MoRePaS) collaboration: morepas.org.

# Road Map: RBMs for emulating scattering observables

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**0** **A few remarks on projection-based ROMs (mainly for bound states)**

Melendez, CD, Garcia, Furnstahl, and Zhang, J. Phys. G **49**, 102001
CD, Melendez, Garcia, Furnstahl, and Zhang, Front. Phys. **10**, 92931

**1** **(General) Kohn Variational Principle:** ***Toward emulating nuclear reactions using eigenvector continuation*** **(with wave functions)**

CD, Quinonez, Giuliani, Lovell, and Nunes, Phys. Lett. B **823,** 136777
extends: Furnstahl, Garcia, Millican, and Zhang, Phys. Lett. B **809**, 135719

**2** **Newton Variational Principle**: ***Fast & accurate emulation of two-body scattering observables without wave functions***

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

**See also Xilin Zhang's talk:**
*Further developments on emulators for quantum continuum states*

**3** ***Wave-function-based emulation for nucleon-nucleon scattering in momentum space (Kohn vs Newton VP)***

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

See also: CD & Zhang's contribution to Few Body Syst. **63**, 67

# Pedagogical Introduction

https://kylegodbey.github.io/nuclear-rbm/
Bonilla, Giuliani *et al.*, PRC **106**, 054322

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frontiers (pedagogical review article)

## BUQEYE Guide to Projection-Based Emulators in Nuclear Physics

Front. Phys. **10**, 92931 (open access)

C. Drischler,[1,2,*] J. A. Melendez,[3] R. J. Furnstahl,[3] A. J. Garcia,[3] and Xilin Zhang[2]

**ABSTRACT**

The BUQEYE collaboration (Bayesian Uncertainty Quantification: Errors in Your EFT) presents a pedagogical introduction to projection-based, reduced-order emulators for applications in low-energy nuclear physics. The term *emulator* refers here to a fast surrogate model capable of reliably approximating high-fidelity models. As the general tools employed by these emulators are not yet well-known in the nuclear physics community, we discuss variational and Galerkin projection methods, emphasize the benefits of offline-online decompositions, and explore how these concepts lead to emulators for bound and scattering systems that enable fast & accurate calculations using many different model parameter sets. We also point to future extensions and applications of these emulators for nuclear physics, guided by the mature field of model (order) reduction. All examples discussed here and more are available as interactive, open-source Python code so that practitioners can readily adapt projection-based emulators for their own work.

**Keywords: emulators, reduced-order models, model order reduction, nuclear scattering, uncertainty quantification, effective field theory, variational principles, Galerkin projection**

Pedagogical & interactive Jupyter notebooks online!

see also our Literature Guide Melendez, CD *et al.*, J. Phys. G **49**, 102001

**Discusses:**

eigen-emulators

(variational vs Galerkin) Model Reduction

scattering emulators

open questions future directions

Companion website with lots of pedagogical material: https://github.com/buqeye/frontiers-emulator-review

# Constructing ROMs: Variational & Galerkin Projection

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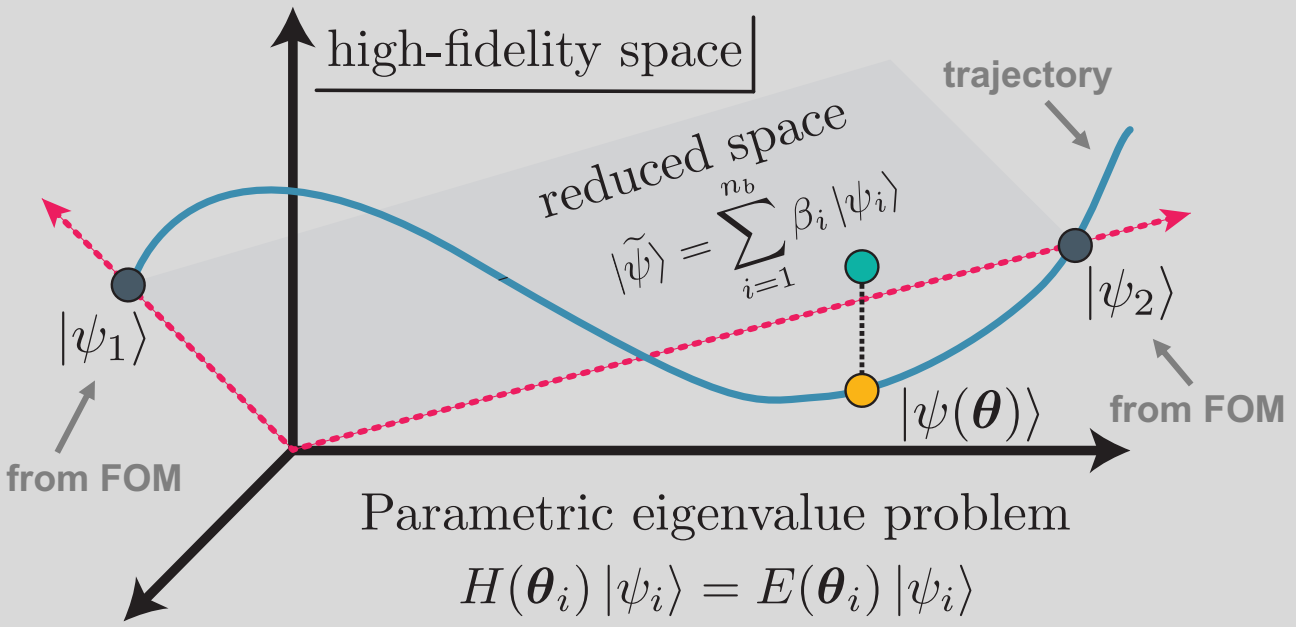


Parametric eigenvalue problem

$$H(\boldsymbol{\theta}_i)\,|\psi_i\rangle = E(\boldsymbol{\theta}_i)\,|\psi_i\rangle$$

Results in very effective trial wave functions!

## Galerkin Projection

**Consider weak form:**

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

**Reduce:** $|\psi\rangle \rightarrow \left|\tilde{\psi}\right\rangle = \sum_{i=1}^{n_b} \beta_i\,|\psi_i\rangle \equiv \mathbf{X}\boldsymbol{\beta}$

**Choose $n_b$ test functions** $\langle\zeta_i| = \langle\psi_i|$ **:**

$$\langle\zeta_i|\,H(\boldsymbol{\theta}) - \tilde{E}(\boldsymbol{\theta})\,|\tilde{\Psi}\rangle = 0 \quad \forall i$$

**Other choices possible ➜ Petrov-Galerkin ROM**

## Variational Approach

**Functional:**

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

**Trial wave function:** $\left|\tilde{\psi}\right\rangle = \sum_{i=1}^{n_b} \beta_i\,|\psi_i\rangle \equiv \mathbf{X}\boldsymbol{\beta}$

**Find stationary point of the functional**

## Reduced Order Model

$$\tilde{H}(\boldsymbol{\theta})\boldsymbol{\beta} = \tilde{E}(\boldsymbol{\theta})\tilde{N}\boldsymbol{\beta}$$ generalized eigenvalue problem

$$\tilde{H}(\boldsymbol{\theta}) = \boldsymbol{X}^\dagger H(\boldsymbol{\theta})\boldsymbol{X}$$ projected Hamiltonian

$$\tilde{N} = \boldsymbol{X}^\dagger\boldsymbol{X}$$ norm matrix

$$\boldsymbol{X} = [\psi_1\ \psi_2\ \ldots\ \psi_{n_b}]$$ snapshots

# Illustrative example: anharmonic oscillator

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

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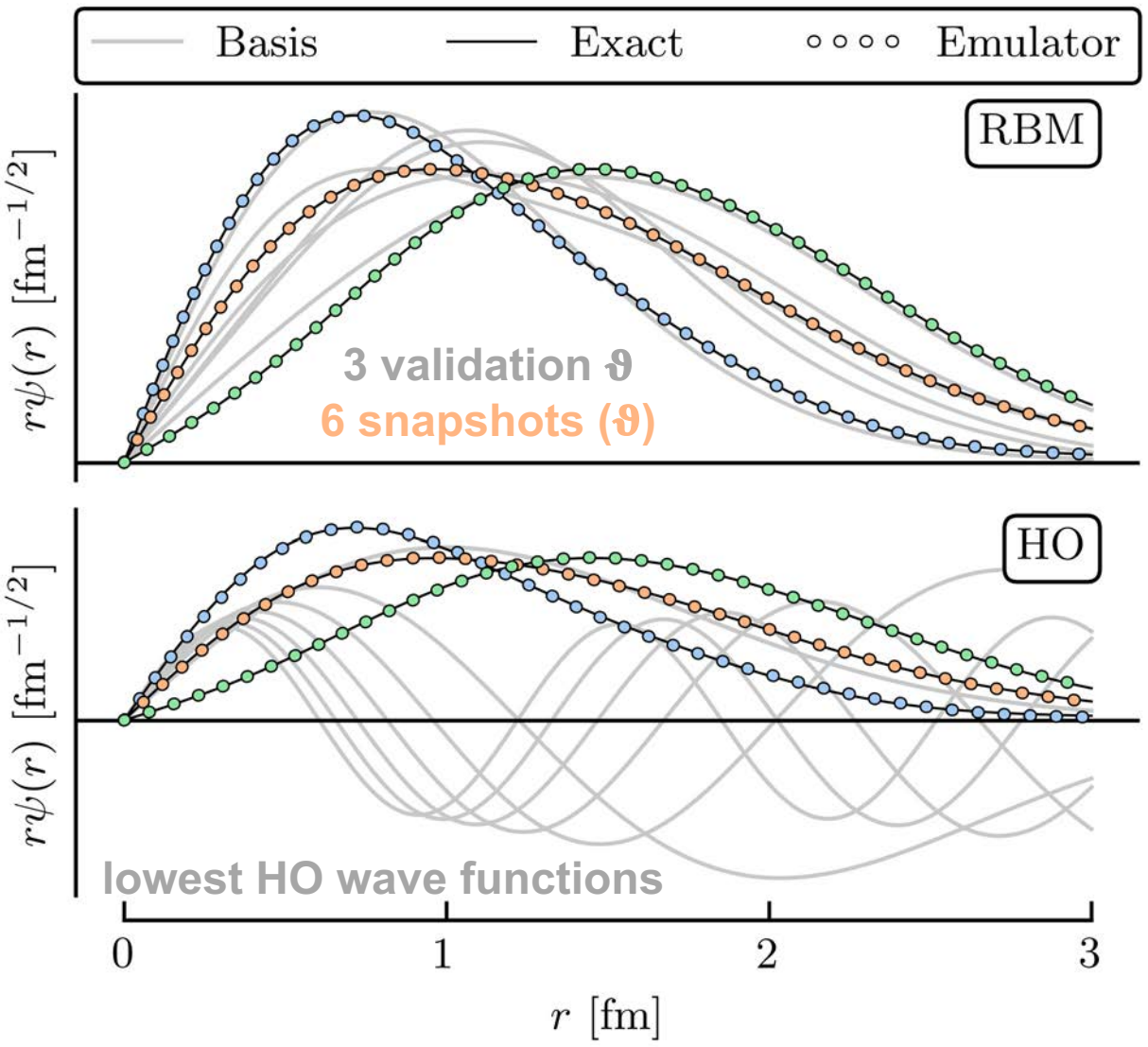
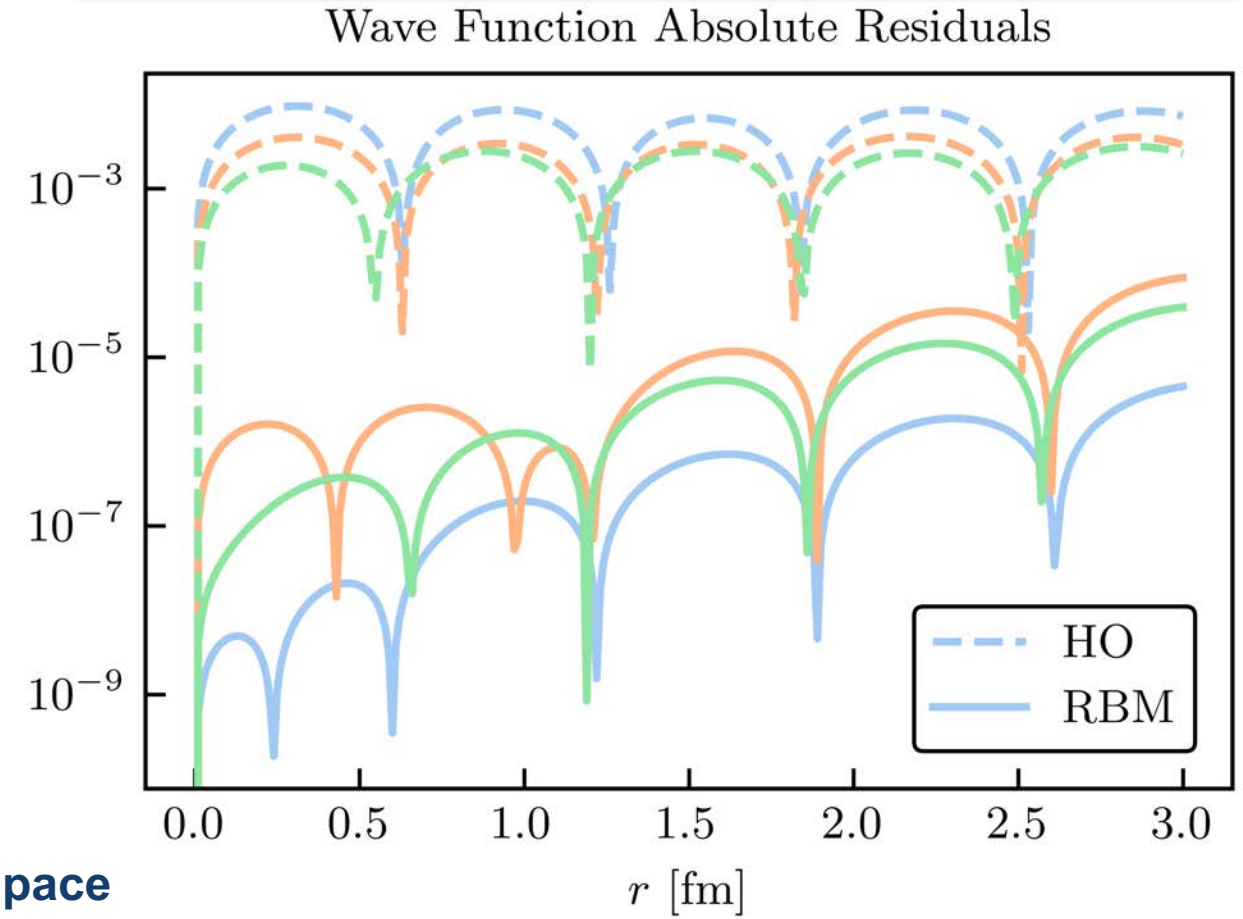



$$V(r,\boldsymbol{\theta}) = V_{\text{HO}} + \sum_{n=1}^{3} \boldsymbol{\theta}^{(n)} e^{-r^2/\sigma_n^2}$$

$\sigma_n = [0.5, 2, 4]$ fm (affine)




**Results obtained via diagonalization in the reduced space**

# Illustrative example: anharmonic oscillator

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

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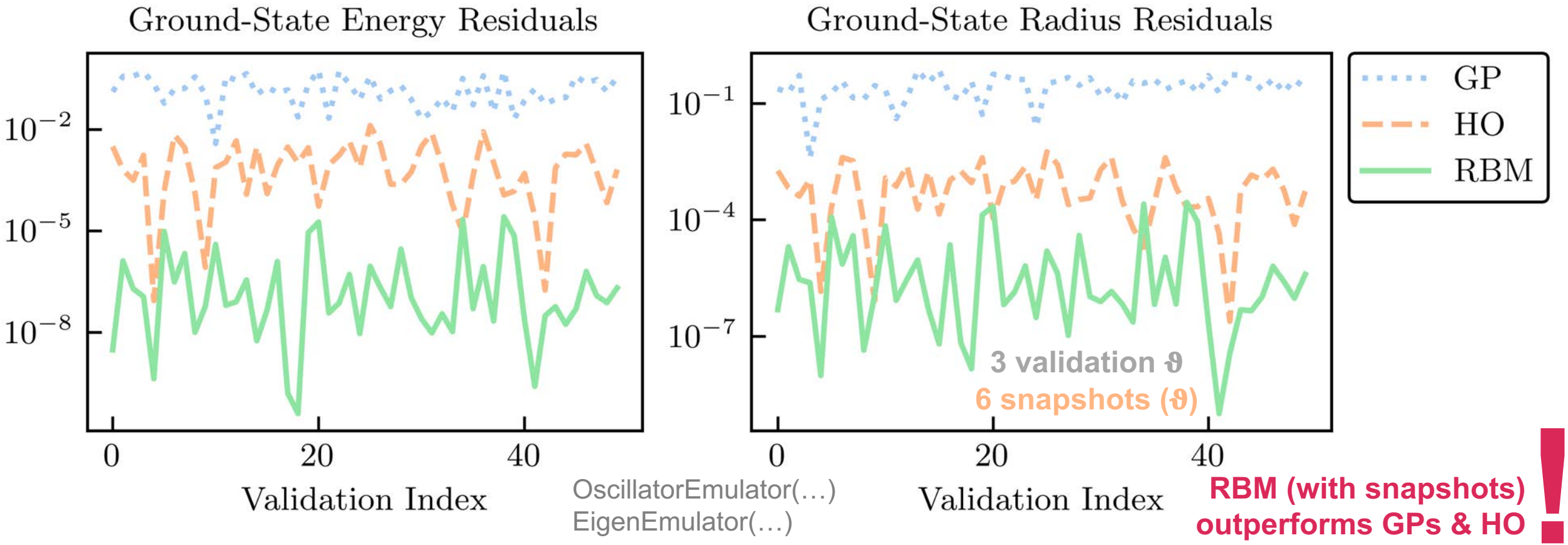
**RBM combines the ideas from the other emulators:**

- ✓ Uses **snapshot (wave) functions** rather than scalar (energies) for training (no nodes)
- ✓ Knows about the **underlying eigenvalue problem**

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

$\sigma_n = [0.5, 2, 4]$ fm (affine)




OscillatorEmulator(…)
EigenEmulator(…)

**RBM (with snapshots) outperforms GPs & HO**

# Constructing Galerkin-ROMs

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

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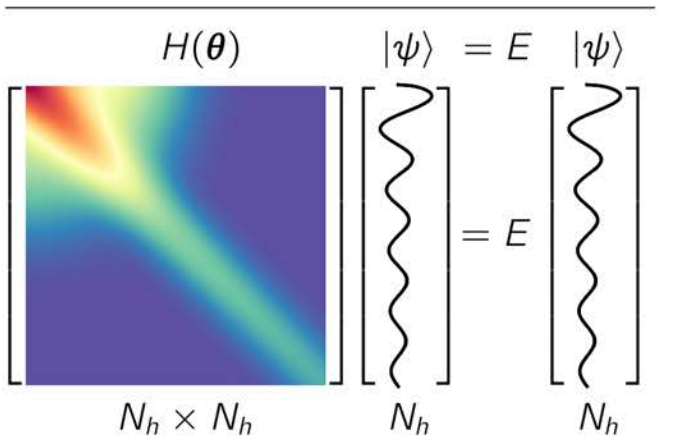
High-fidelity system




Time: ⬭ per $\theta$ sample

Construct **(snapshot-based) ROMs** by systematically removing *superfluous* information in high-fidelity models

CPU time scales with the length of ⬭

**Offline-online decomposition:**

**Perform all demanding operations *once* upfront** (which is crucial for achieving high speed-ups)

Is *straightforward* for operators with an **affine parameter dependence**

use **hyper-reduction methods** to handle non-linear systems and/or non-affine parameters

**Offline stage (size-$N_h$ operations):**

- Solve high-fidelity system and construct snapshot basis
- Project high-fidelity system to reduced space

**Online stage (size-$n_b$ operations only):**

- fast & accurate model predictions (*e.g.*, for MC sampling)

# Constructing Galerkin-ROMs

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

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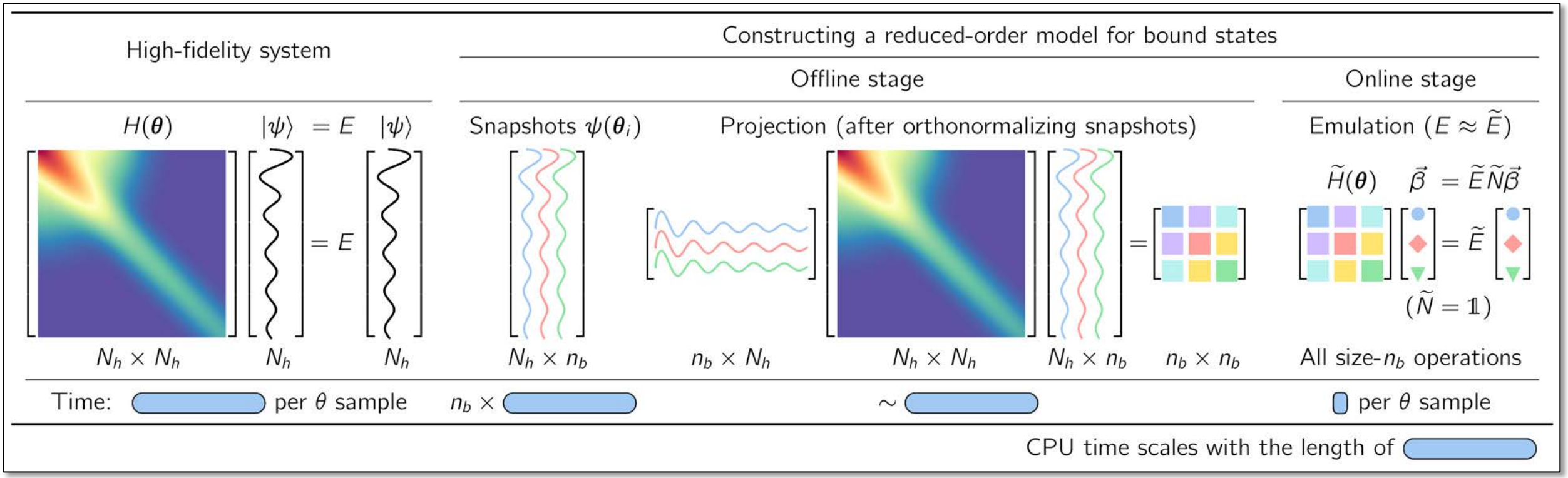


**Offline-online decomposition:**

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# Affine Parameter Dependence | Snapshot basis

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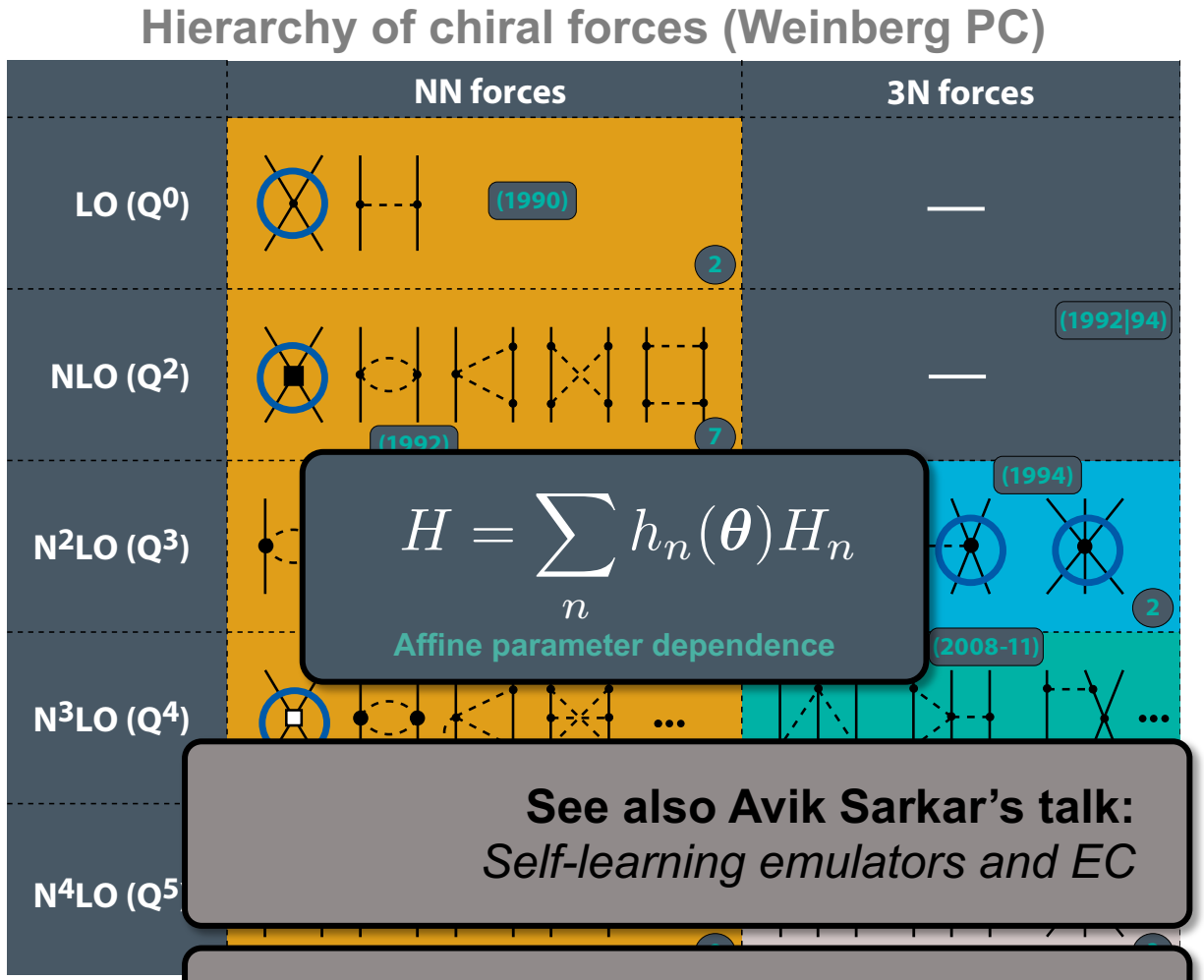


## How to choose the snapshot basis?

**Multiple approaches and their hybrids possible. For instance:**

- obtain space-filling snapshots using **Latin hypercube** sampling (for small $\vartheta$ spaces)
- choose the snapshots near the to-be-emulated parameter ranges (ideally interpolation)
- Proper Orthogonal Decomposition (POD)
- **Greedy algorithms** and other active-learning methods to reduce the emulator's error iteratively

*e.g.*, see Sarkar & Lee, PRR **4**, 023214

**The POD can be used to diagnose and (further) optimize the snapshot basis.**

# Proper Orthogonal Decomposition (POD)

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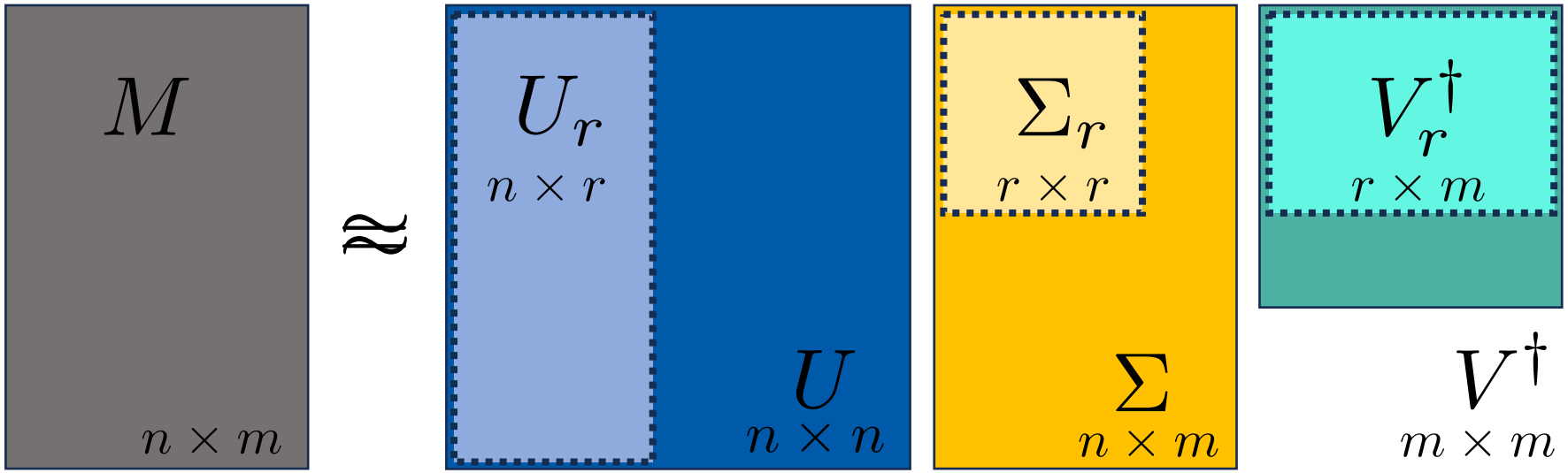
**POD is based on a (truncated) Singular Value Decomposition (SVD) of the snapshot basis:**
See also Principal Component Analysis (PCA)




***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)**

# Road Map: RBMs for scattering observables

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**0** **A few remarks on projection-based emulators in general**

Melendez, CD, Garcia, Furnstahl, and Zhang, J. Phys. G **49**, 102001
CD, Melendez, Garcia, Furnstahl, and Zhang, Front. Phys. **10**, 92931

**1** **(General) Kohn Variational Principle: *Toward emulating nuclear reactions using eigenvector continuation* (with wave functions)**

CD, Quinonez, Giuliani, Lovell, and Nunes, Phys. Lett. B **823,** 136777
extends: Furnstahl, Garcia, Millican, and Zhang, Phys. Lett. B **809**, 135719

**2** **Newton Variational Principle: *Fast & accurate emulation of two-body scattering observables without wave functions***

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

**See also Xilin Zhang's talk:**
*Further developments on emulators for quantum continuum states*

**3** ***Wave-function-based emulation for nucleon-nucleon scattering in momentum space***

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

See also: CD & Zhang's contribution to Few Body Syst. **63**, 67

# Kohn Variational Principle with RBM

Furnstahl, Garcia, Millican, Zhang,
PLB **809**, 10135719

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**1**

$$\beta\left[|\psi_{\rm trial}\rangle\right] = \frac{K_\ell}{p} - 2\mu\,\langle\psi_{\rm trial}\,|\,H(\boldsymbol{\theta}) - E\,|\,\psi_{\rm trial}\rangle \qquad p = \sqrt{2\mu E}$$

**2** ***stationary*** **approximation to exact $K_l$ matrix [accurate up to $O(\delta u^2)$]**

$$u^{\rm trial}_{\ell,E}(r) \sim \frac{1}{p}\sin(\eta_\ell) + \frac{K_\ell}{p}\cos(\eta_\ell) \qquad \eta_\ell = kr - \frac{\pi}{2}\ell \qquad H(\boldsymbol{\theta}) = T + V(\boldsymbol{\theta})$$

**3**

**Training: solve RSE *exactly* for a set $\{\boldsymbol{\theta}_i\}_{i=1}^{N_b}$ and construct the trial wave function:** $|\psi_{\rm trial}\rangle = \sum_{i=1}^{N_b} c_i\,|\psi_E(\boldsymbol{\theta}_i)\rangle$

**4**

**5**

**Given *H*(*θ*), the *stationary point* is obtained by simple linear algebra:** $\delta\beta[\psi_{\rm trial}] = 0 \quad \text{s.t.} \quad \sum_{i=1}^{N_b} c_i = 1$

$$c_i = \sum_j (\Delta\widetilde{U})^{-1}_{ij}\left(\frac{K^{(j)}_\ell(E)}{p} - \lambda\right) \qquad \lambda = \frac{-1 + \sum_{ij}(\Delta\widetilde{U})^{-1}_{ij}\frac{K^{(j)}_\ell(E)}{p}}{\sum_{ij}(\Delta\widetilde{U})^{-1}_{ij}}$$

**with matrix** $\Delta\tilde{U}_{ij} = 2\mu\,\langle\psi_E(\boldsymbol{\theta}_i)\,|\,2V(\boldsymbol{\theta}) - V(\boldsymbol{\theta}_i) - V(\boldsymbol{\theta}_j)\,|\,\psi_E(\boldsymbol{\theta}_j)\rangle$

**6**

**Approximate $K_l$ = tan $\delta_l$:** $[K_\ell(E)]_{\rm exact} \approx \sum_i c_i K^{(i)}_\ell(E) - \frac{p}{2}\sum_{ij} c_i \Delta\widetilde{U}_{ij} c_j$

**emulate** ↓

↑ **validate**




for *R* matrix theory, see Bai & Ren, PRC **103**, 014612

# Wave functions and phase shifts

Furnstahl, Garcia, Millican, Zhang,
PLB **809**, 10135719

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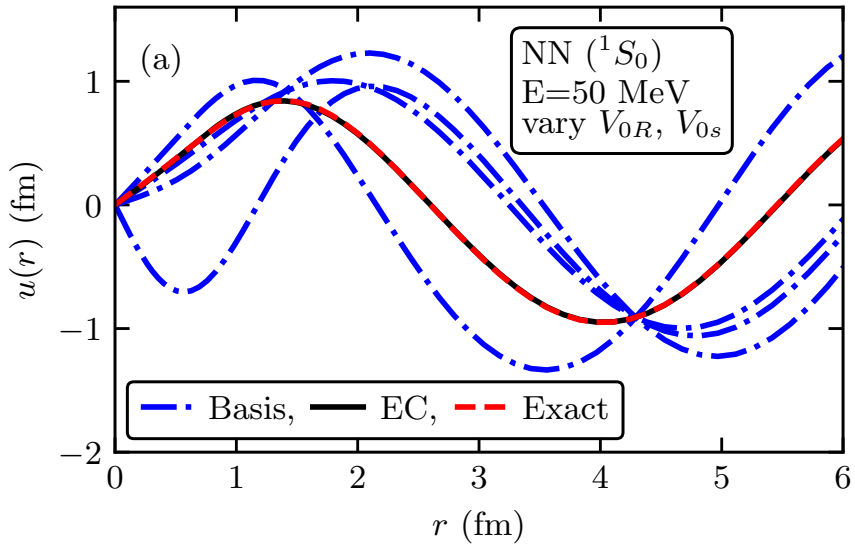
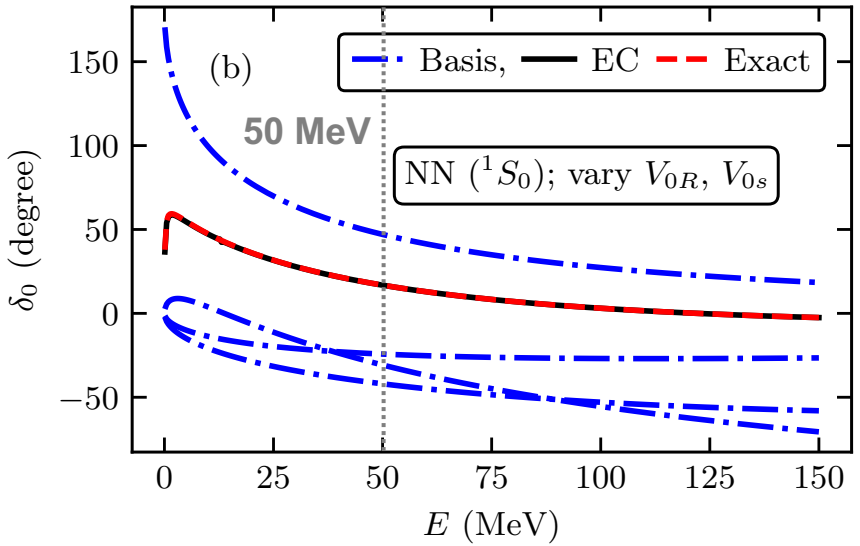
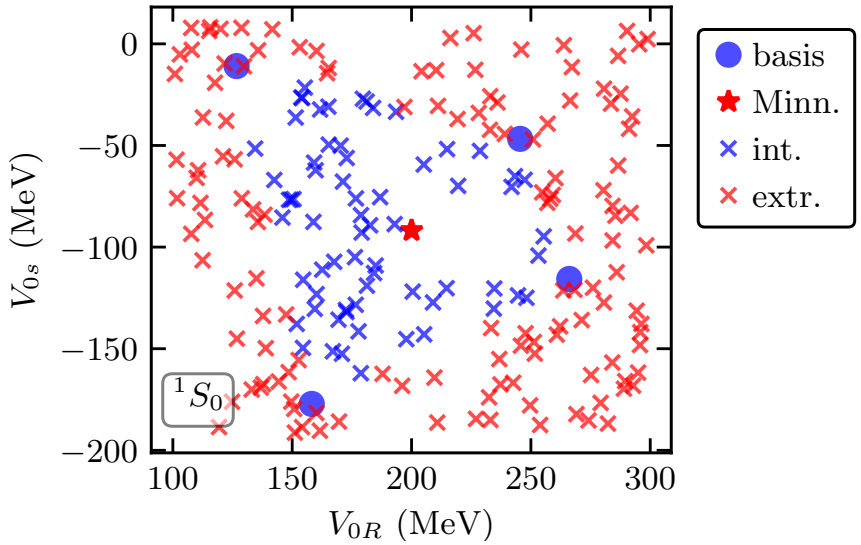



**Minnesota potential**

$$V(r) = V_{0R} e^{-\kappa_R r^2} + V_{0s} e^{-\kappa_s r^2}$$

**Training set**: 4 Hamiltonians with different ($V_{0R}$, $V_{0s}$ ● ) and fixed ($\kappa_R$, $\kappa_s$)




Emulated wavefunctions and phase shifts **reproduce well the exact results** at the *physical point* (★)

## Also studied:

- local & nonlocal potentials
- incl. optical potentials
- higher partial waves

# Small residuals

Furnstahl, Garcia, Millican, Zhang,
PLB **809**, 10135719

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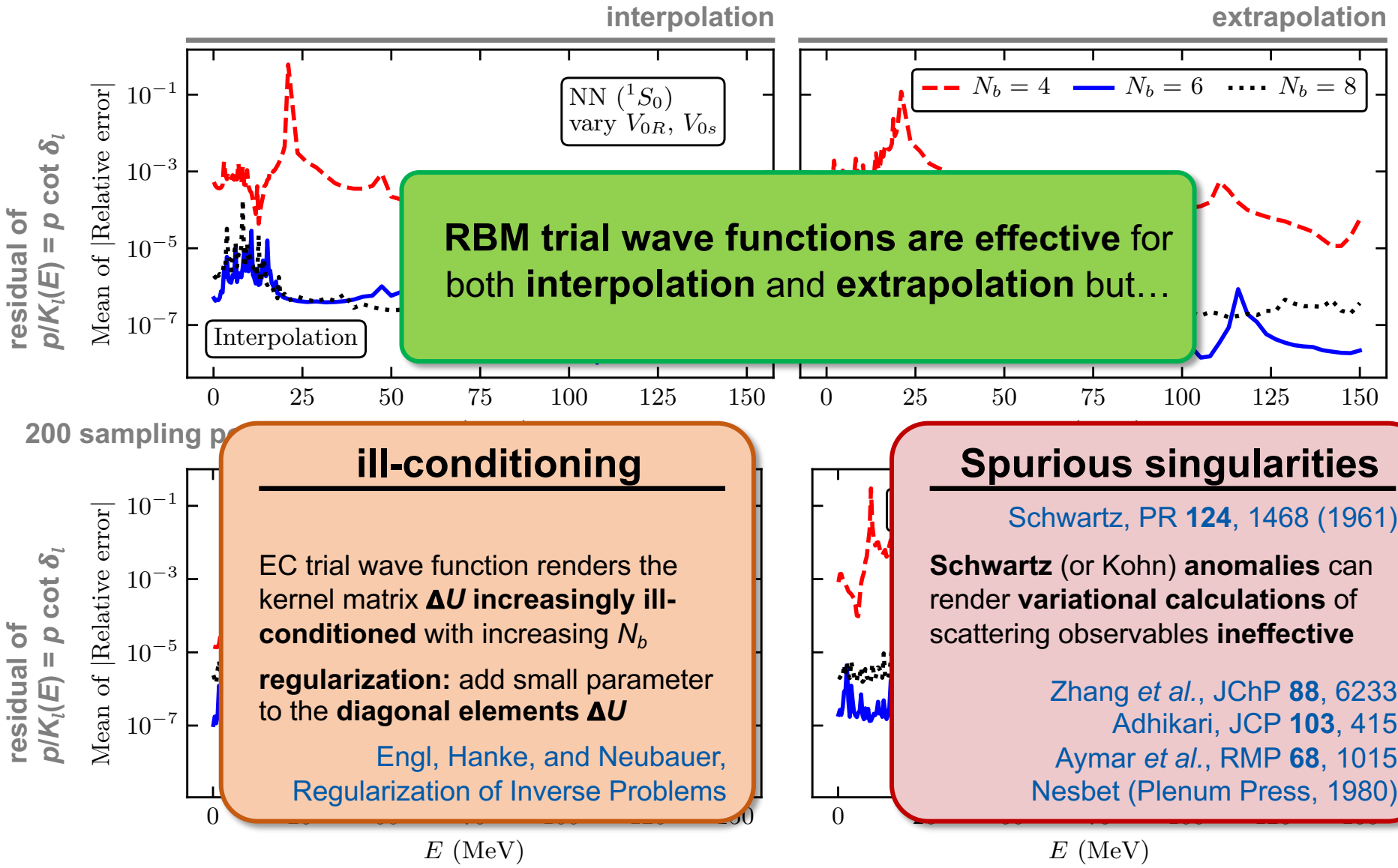


**RBM trial wave functions are effective** for both **interpolation** and **extrapolation** but…

## ill-conditioning

EC trial wave function renders the kernel matrix **Δ*U* increasingly ill-conditioned** with increasing $N_b$

**regularization:** add small parameter to the **diagonal elements Δ*U***

Engl, Hanke, and Neubauer, Regularization of Inverse Problems

## Spurious singularities

Schwartz, PR **124**, 1468 (1961)

**Schwartz** (or Kohn) **anomalies** can render **variational calculations** of scattering observables **ineffective**

Zhang *et al.*, JChP **88**, 6233
Adhikari, JCP **103**, 415
Aymar *et al.*, RMP **68**, 1015
Nesbet (Plenum Press, 1980)

# General Kohn variational principle

Lucchese, PRA **40**, 112

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$$\beta_u\left[|\psi_{\rm trial}\rangle\right] = \frac{L_\ell}{p} - \frac{2\mu}{\det u}\langle\psi_{\rm trial}\,|\,H(\boldsymbol{\theta}) - E\,|\,\psi_{\rm trial}\rangle$$

***stationary*** **approximation to exact $L_l$ matrix [accurate up to $O(\delta u^2)$]**

$$u^{\rm trial}_{\ell,E}(r) \sim \frac{1}{p}\phi^{(0)}_\ell(r) + \frac{L_\ell}{p}\,\phi^{(1)}_\ell(r) \qquad \phi^{(0)}_\ell(r) \sim u_{00}\sin(\eta_\ell) + u_{01}\cos(\eta_\ell) \qquad \phi^{(1)}_\ell(r) \sim u_{10}\sin(\eta_\ell) + u_{11}\cos(\eta_\ell) \qquad \eta_\ell = kr - \frac{\pi}{2}\ell$$

**Training:** solve RSE ***exactly*** for a set $\{\boldsymbol{\theta}_i\}_{i=1}^{N_b}$ and constr

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

**Given** obtain

$$c_i =$$

$$\delta[\eta$$

$$c_i = 1$$

$$\lambda = \frac{-1 + \sum_{ij}(\Delta U)_{ij}\,L^{(0)}_\ell(E)}{\sum_{ij}(\Delta\widetilde{U})^{-1}_{ij}}$$

with matrix $\Delta U_{ij} = \frac{}{\det u}\langle\psi_E(\boldsymbol{\theta}_i)\,|\,2V(\boldsymbol{\theta}) - V(\boldsymbol{\theta}_i) - V(\boldsymbol{\theta}_j)\,|\,\psi_E(\boldsymbol{\theta}_j)\rangle$

$$L = K \;\text{ for }\; u = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$$

$$L = S \;\text{ for }\; u = \begin{bmatrix}i & -1\\ i & 1\end{bmatrix}$$

$$L = T \;\text{ for }\; u = \begin{bmatrix}1 & 0\\ i & 1\end{bmatrix}$$

**… any *nonsingular* matrix**

$$K = \frac{u_{01} + u_{11}L}{u_{00} + u_{10}L}$$

**Approximate $L_l$:** $\quad [L_\ell(E)]_{\rm exact} \approx \sum_i c_i L^{(i)}_\ell(E) - \frac{1}{2}\sum_{ij} c_i \Delta\widetilde{U}_{ij} c_j$

emulate

validate

for applications to N-d scattering, see:

Viviani, Kievsky, and Rosati, FBS **30**, 3

Kievsky, NPA **624**, 125

Kievsky, Viviani, and Rosati, NPA **577**, 511

# Schwartz anomalies

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

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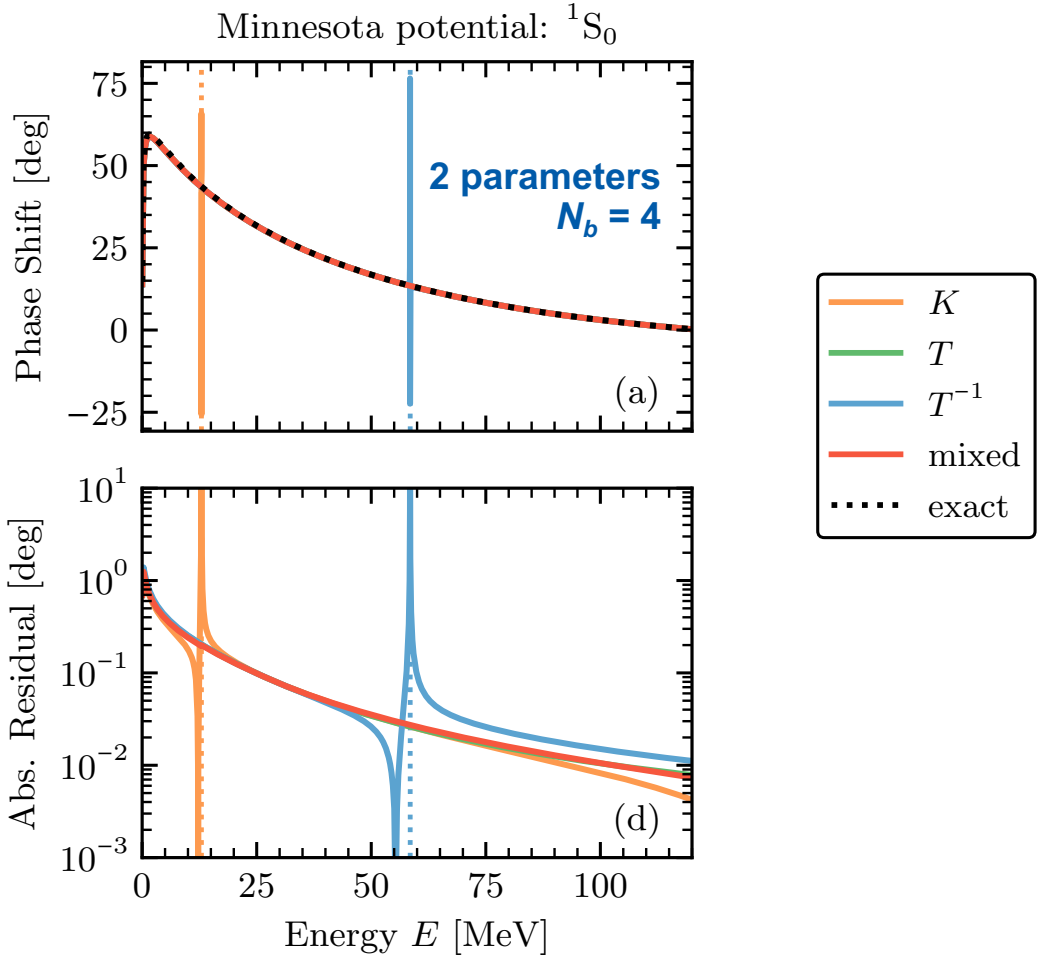


**Minnesota potential**

$$V(r) = V_{0R} e^{-\kappa_R r^2} + V_{0s} e^{-\kappa_s r^2}$$

**Spurious singularities** occur when there is no (unique) stationary approximation due to the functional; *i.e.*,

$$\det \Delta\widetilde{\mathbf{U}}^{(\mathbf{u})} = 0$$
$$\sum_{ij} (\Delta\widetilde{\mathbf{U}}^{(\mathbf{u})})^{-1}_{ij} = 0$$

**No guarantee:** all KVPs are prone to Schwartz anomalies, and we found anomalies for all potentials studied

**Advantage:** for complex KVPs and/or optical potentials both, the real *and* imaginary part, need to cross zero

see also: Lucchese, Phys. Rev. A **40**, 112
Schwartz, Phys. Rev. **124**, 1468
Nesbet, *Variational methods in electron-atom scattering theory*

# Schwartz anomalies

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

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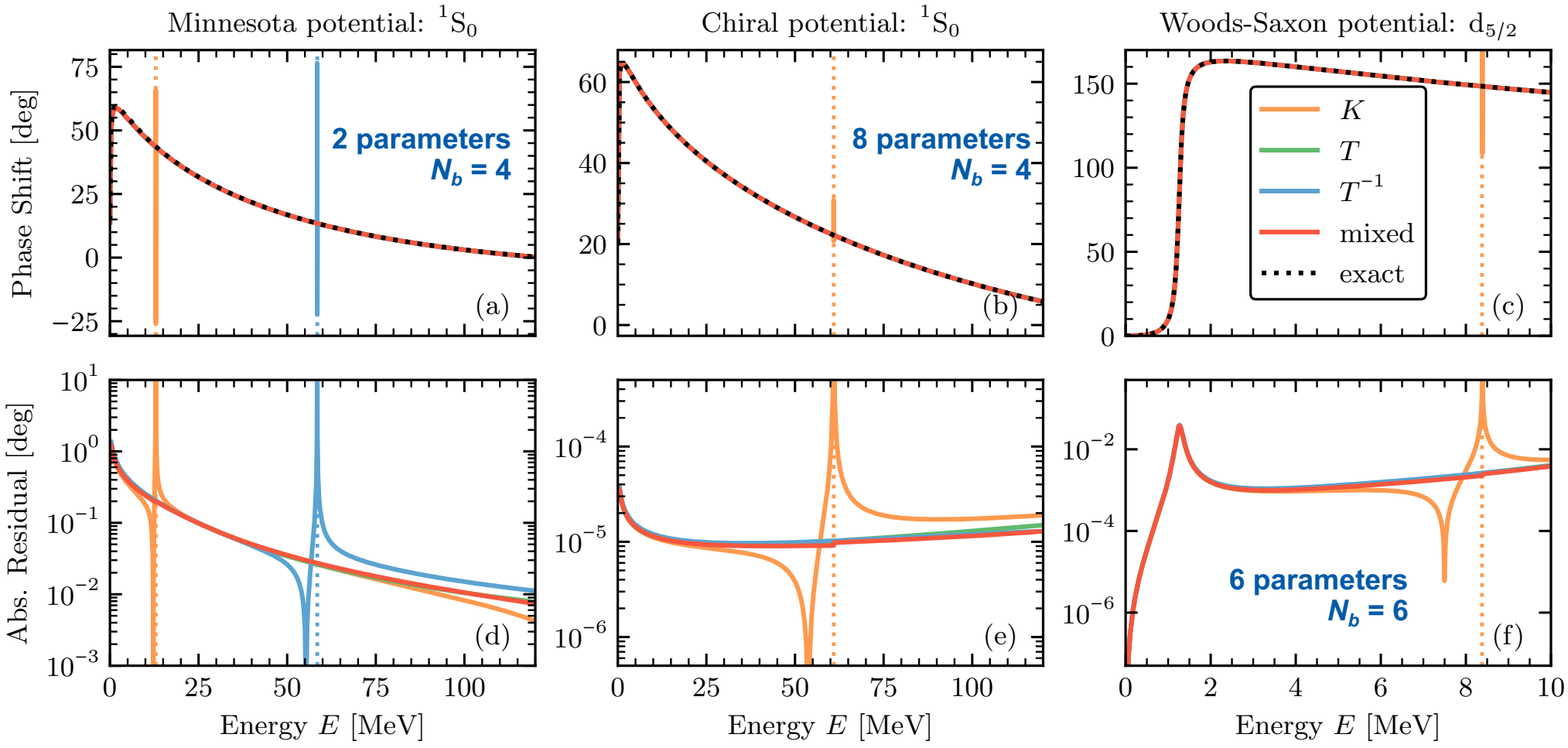
## realistic real potentials




**NN** scattering

**n+$^{10}$Be** scattering

# Anomaly detection and removal

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

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**Basic idea:** emulate a variety of matrices associated with different boundary conditions and **check for consistency**

$$\Delta^{(L)}(L_1, L_2) = \frac{L(L_1)}{L(L_2)} - 1$$

relative error

Viviani, Kievsky, and Rosati, FBS **30**, 3
Kievsky, Viviani, and Rosati, NPA **577**, 511

**Filter out all inconsistent pairs** $\{L_i, L_j\}_{ij}$ and **average over ("mix") the remaining pairs** with weight $\Delta^{(L)}(L_i, L_j)$

**Vary the size of the training set** to shift the Schwartz anomalies and repeat

general case (via Möbius transform)

$$L'(L) \equiv \mathcal{L}^{-1}_{\mathbf{u}'}\left(K(L)\right) = \frac{-u'_{01} + u'_{00}K(L)}{u'_{11} - u'_{10}K(L)}$$

**How can Kohn anomalies be detected and removed** ?

| Using: | $\delta$ | $L_1 =$ **K** | $L_2 =$ **T** | **S** |
|---|---|---|---|---|
| $\chi(R) =$ | $e^{\imath\delta}[F\cos\delta + G\sin\delta]$ | $\frac{1}{1-\imath\mathbf{K}}[F + \mathbf{K}G]$ | $F + \mathbf{T}H^+$ | $\frac{1}{2}[H^- - \mathbf{S}H^+]$ |
| $\delta =$ | $\delta$ | $\arctan\mathbf{K}$ | $\arctan\frac{\mathbf{T}}{1+\imath\mathbf{T}}$ | $\frac{1}{2\imath}\ln\mathbf{S}$ |
| $\mathbf{K} =$ | $\tan\delta$ | $\mathbf{K}$ | $\frac{\mathbf{T}}{1+\imath\mathbf{T}}$ | $\imath\frac{1-\mathbf{S}}{1+\mathbf{S}}$ |
| $\mathbf{T} =$ | $e^{\imath\delta}\sin\delta$ | $\frac{\mathbf{K}}{1-\imath\mathbf{K}}$ | $\mathbf{T}$ | $\frac{1}{2}(1-\mathbf{S})$ |
| $\mathbf{S} =$ | $e^{2\imath\delta}$ | $\frac{1+\imath\mathbf{K}}{1-\imath\mathbf{K}}$ | $1+2\imath\mathbf{T}$ | $\mathbf{S}$ |
| $V = 0$ | $\delta = 0$ | $\mathbf{K} = 0$ | $\mathbf{T} = 0$ | $\mathbf{S} = 1$ |
| $V$ real | $\delta$ real | $\mathbf{K}$ real | $\lvert 1+2\imath\mathbf{T}\rvert = 1$ | $\lvert\mathbf{S}\rvert = 1$ |

Thompson & Nunes, Cambridge University Press (2009)

# Anomaly detection and removal

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

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**But: not all KVPs are complementary.**
We derived **a simple analytic condition to identify redundant KVPs.**

**Redundant (canonical) pairs:**

$(S, T)$

$(K^{-1}, T^{-1})$

$(S, S^{-1})$*

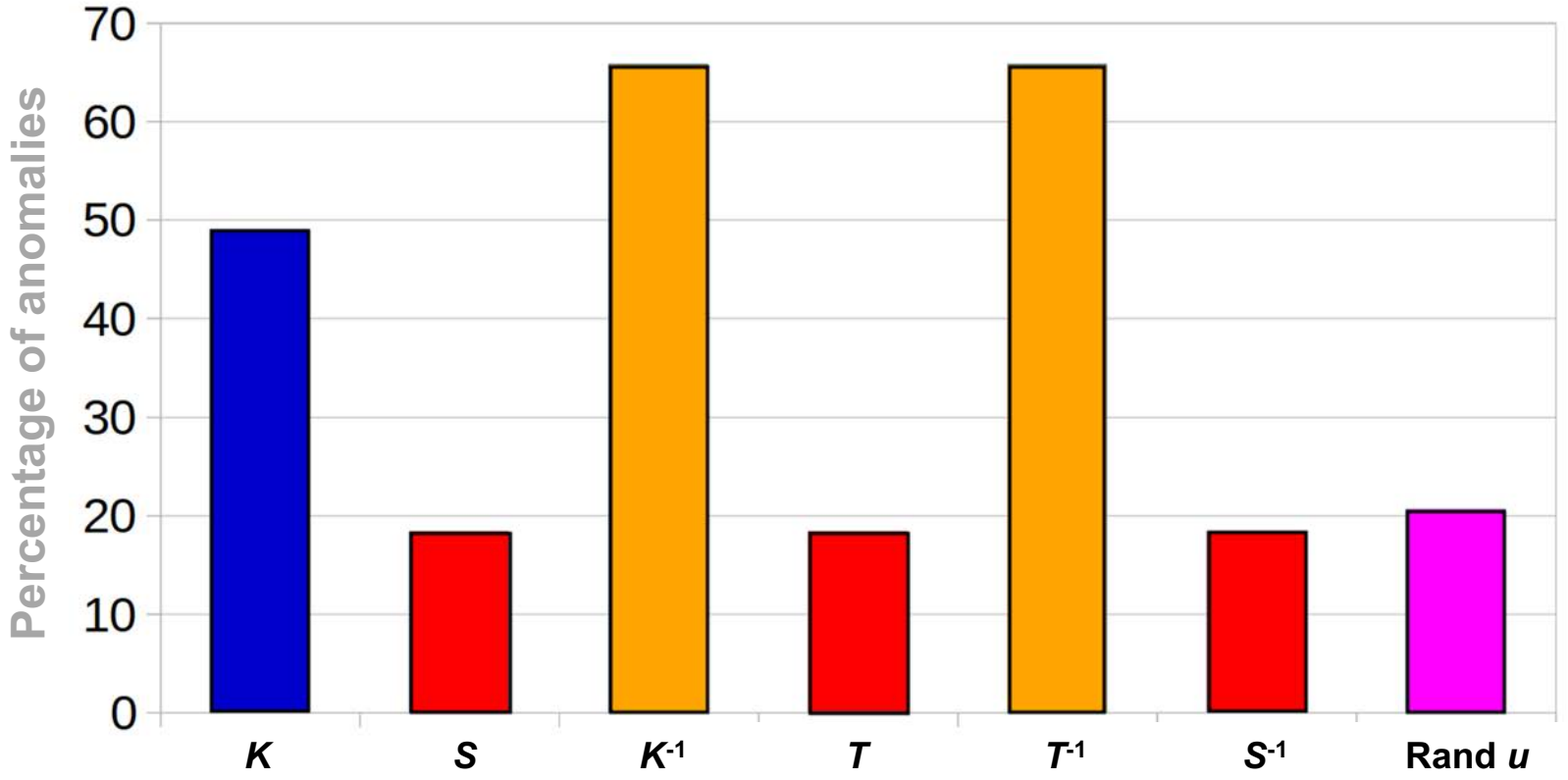
**generalized *S*- & *T*-matrix KVP**

***complex conjugated if *V* is real**

**We showed analytically that KVPs are redundant if the *cross-kernel matrix* is singular:**

$$\mathbf{c} = \begin{pmatrix} u_{11} & u'_{11} \\ -u_{10} & -u'_{10} \end{pmatrix}$$

**How can Kohn anomalies be detected and removed ?**




*L* = 0 | *A* = 40 | *E* = 5-20 MeV
Woods-Saxon potential
5 training points

5 random matrices covering a wide range in |det(*u*)|
sample size: 500

# Numerical noise due to ill-conditioning

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

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## Condition number increases
### with increasing number of training points

!

$$c_i = \sum_j (\Delta\tilde{U})^{-1}_{ij} \left( L^{(j)}_\ell(E) - \lambda \right) \quad \lambda = \frac{-1 + \sum_{ij} (\Delta\tilde{U})^{-1}_{ij} L^{(j)}_\ell(E)}{\sum_{ij} (\Delta\tilde{U})^{-1}_{ij}}$$

**Methods to control the noise in matrix inversions include:**

- nugget regularization
- Moore-Penrose inverse
- **Tikhonov regularization**

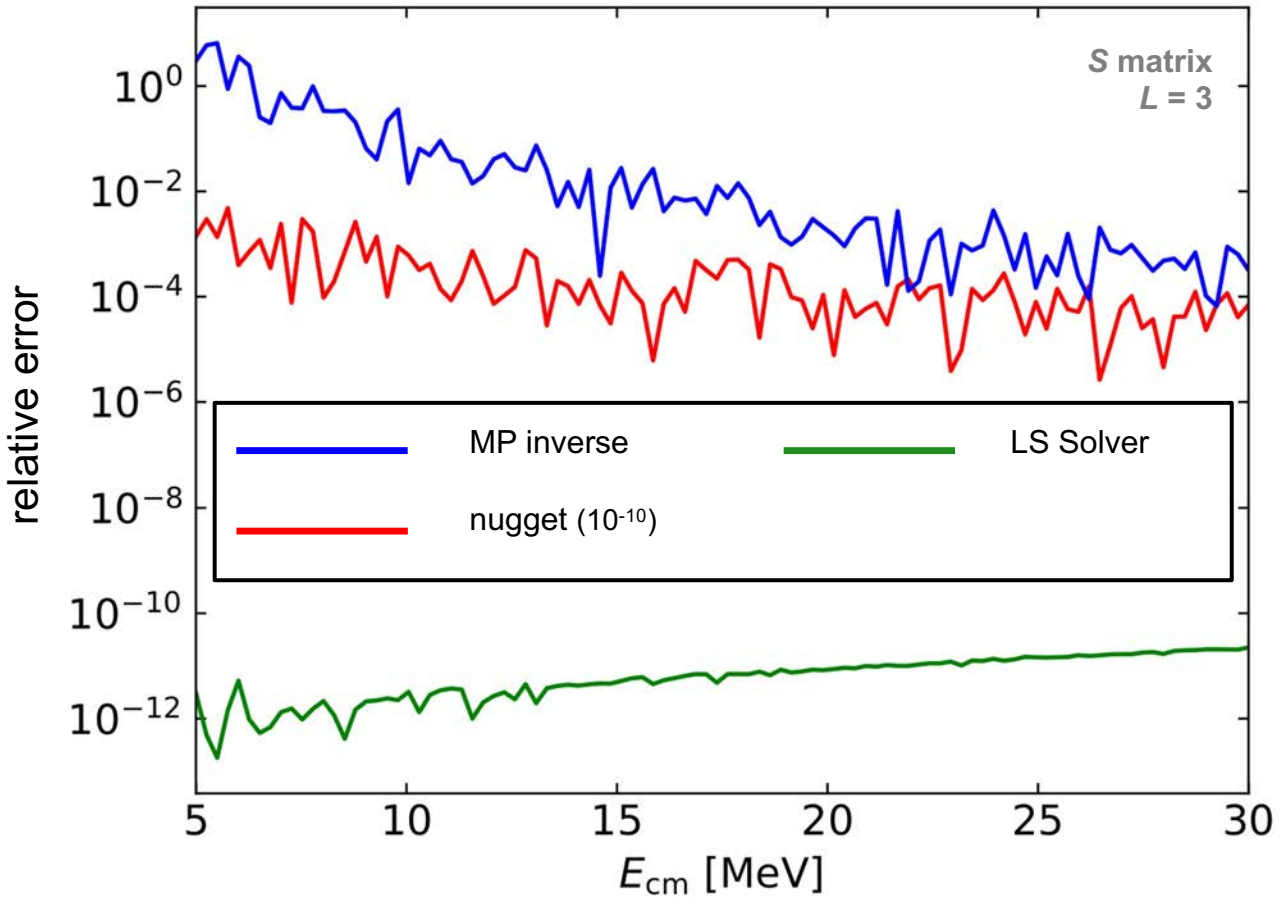
**Golden Rule of numerical linear algebra:**
Don't compute a matrix inverse unless you must.

**Simple yet robust:** find *stationary point* numerically (*e.g.*, using an LS solver)

$$\begin{pmatrix} \Delta\tilde{U} & 1 \\ \mathbf{1}^T & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{c} \\ \lambda \end{pmatrix} = \begin{pmatrix} \boldsymbol{L} \\ 1 \end{pmatrix}$$

**inverse-free, if possible**

(Most methods will apply some sort of regularization)



# Emulated differential cross sections

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

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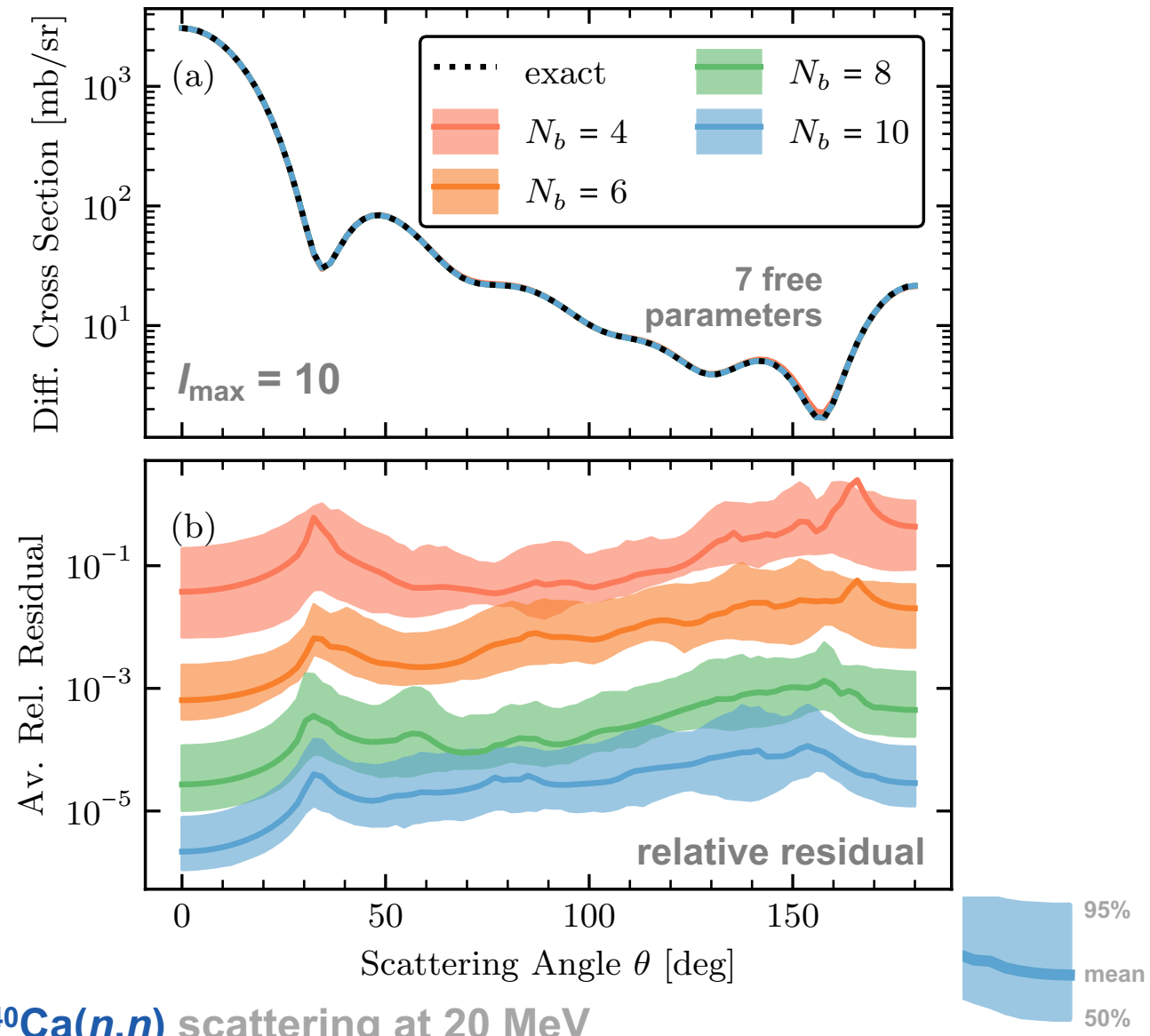


**$^{40}$Ca($n$,$n$) scattering at 20 MeV**

**Realistic optical potential**

$$V(r) = -V_v\, f_{\rm WS}(r; R_v, a_v) - iW_v\, f_{\rm WS}(r; R_w, a_w)$$

**(Woods-Saxon form)**

**Training set**: **$N_b$ random points** within a ±20% interval centered around the Koning–Delaroche values to probe a **realistic region of the parameter space**

**Sample again 500 random points:** resulting bands are spanned by the *median* and *95% limit* of the residuals

**For $N_b$ > 6,** the emulator **residuals do not exceed the experimental uncertainty**, typically ≈10%

# UQ with an optical model

CD, Quinonez, Guiliani, Lovell, and Nunes, PLB **823**, 136777

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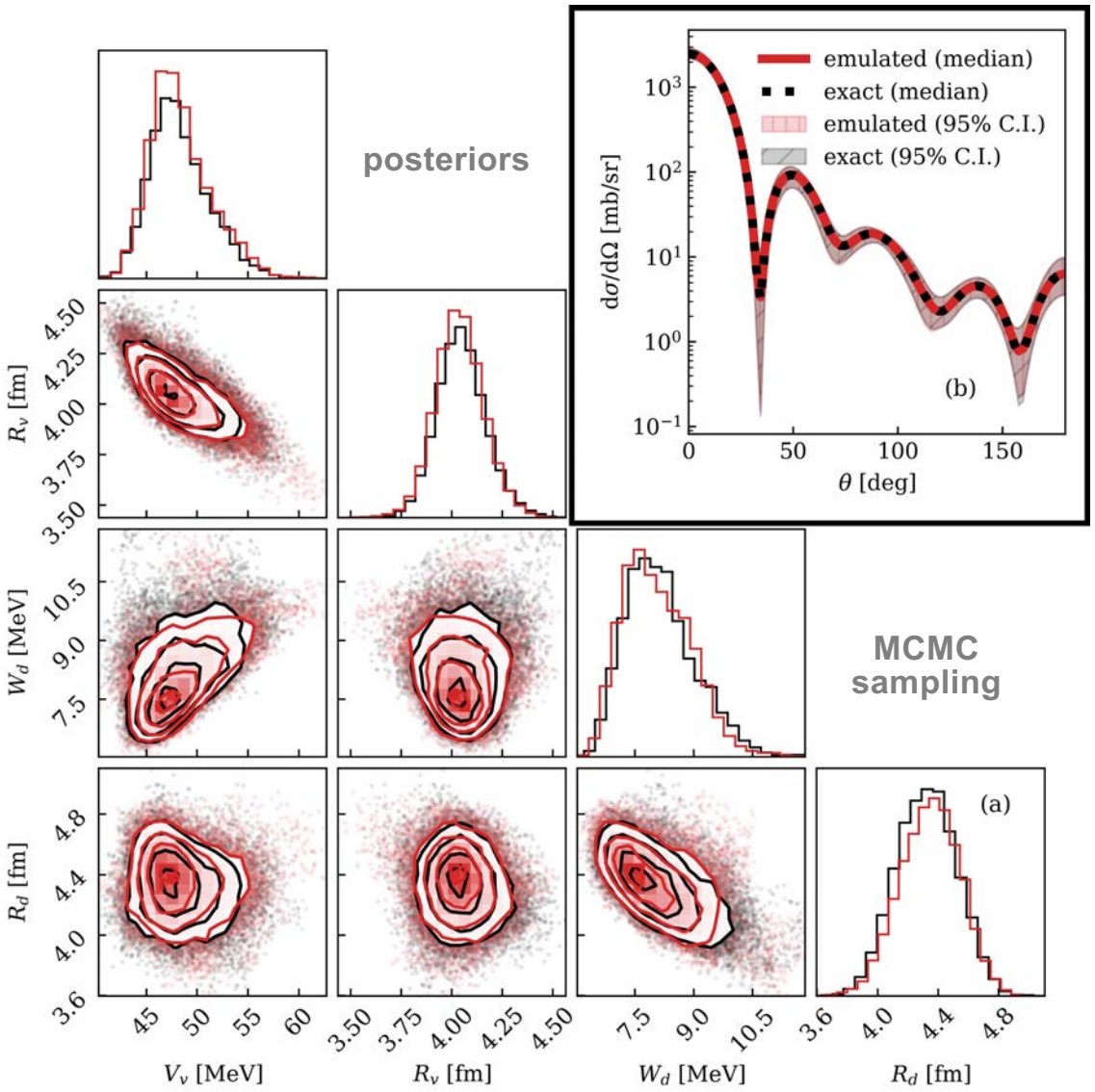


$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left| \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta)(S_l - 1) \right|^2$$

**Koning–Delaroche (optical) potential**

Train emulators across partial-wave channels up to $l$ = 10, with $N_b$ = 8

**Proof of principle:** fast & accurate emulation of scattering observables for parameter estimation (using mock data)

**excellent agreement** between emulator (**red**) and exact scattering solution (**black**)

Mixed approach obtains **anomaly-free results** without adapting the training set

**Goal:** improving next-generation optical models & chiral interactions in the FRIB era

**Kohn Variational Principle** $^{40}$Ca($n$,$n$) scattering at 20 MeV

# Road Map: RBMs for scattering observables

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**0** **A few remarks on projection-based emulators (mainly for bound states)**

Melendez, CD, Garcia, Furnstahl, and Zhang, J. Phys. G **49**, 102001
CD, Melendez, Garcia, Furnstahl, and Zhang, Front. Phys. **10**, 92931

**1** **(General) Kohn Variational Principle: *Toward emulating nuclear reactions using eigenvector continuation* (with wave functions)**

CD, Quinonez, Giuliani, Lovell, and Nunes, Phys. Lett. B **823,** 136777
extends: Furnstahl, Garcia, Millican, and Zhang, Phys. Lett. B **809**, 135719

**2** **Newton Variational Principle: *Fast & accurate emulation of two-body scattering observables without wave functions***

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

**See also Xilin Zhang's talk:**
*Further developments on emulators for quantum continuum states*

**3** ***Wave-function-based emulation for nucleon-nucleon scattering in momentum space***

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

See also: CD & Zhang's contribution to Few Body Syst. **63**, 67

# Newton variational principle

R. G. Newton, *scattering theory of waves and particles*

Melendez, CD, Garcia, Furnstahl, and Zhang, PLB **821**, 136608

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$$\mathcal{K}[\widetilde{K}] = V + VG_0\widetilde{K} + \widetilde{K}G_0V - \widetilde{K}G_0\widetilde{K} + \widetilde{K}G_0VG_0\widetilde{K},$$

**with the free-space Green's function $G_0$( $E_q = q^2/(2\mu)$ )**

***stationary*** **approximation to exact *K* (or *T*) matrix [accurate up to $O(\delta K^2)$]** 1

**Training: solve LSE *exactly* for a set $\{\boldsymbol{\theta}_i\}_{i=1}^{N_b}$ and construct the trial *K* (or *T*) matrix:** 2

$$\widetilde{K}(\vec{\beta}) = \sum_{i=1}^{N_b} \beta_i K_i$$

**Given $H(\boldsymbol{\theta})$, the *stationary point* is obtained by simple linear algebra:** 3

$$\frac{\mathrm{d}\mathcal{K}}{\mathrm{d}\vec{\beta}}\Big|_{\vec{\beta}_\star} = 0 \qquad M\vec{\beta}_\star(\boldsymbol{\theta}) = \vec{m}$$

**with matrices** 4

$$m_i(\boldsymbol{\theta}) = \langle\phi'|\left[K_iG_0V(\boldsymbol{\theta}) + V(\boldsymbol{\theta})G_0K_i\right]|\phi\rangle$$

$$M_{ij}(\boldsymbol{\theta}) = \langle\phi'|\left[K_iG_0K_j - K_iG_0V(\boldsymbol{\theta})G_0K_j + K_jG_0K_i - K_jG_0V(\boldsymbol{\theta})G_0K_i\right]|\phi\rangle$$

**Approximate *K*:** 5

$$\langle\phi'|K|\phi\rangle \approx \langle\phi'|\mathcal{K}_\star|\phi\rangle = \langle\phi'|V|\phi\rangle + \frac{1}{2}\vec{m}^{\intercal}M^{-1}\vec{m}.$$

emulate

validate

# Emulating phase shifts

Melendez, CD, Garcia, Furnstahl, and Zhang, PLB **821**, 136608

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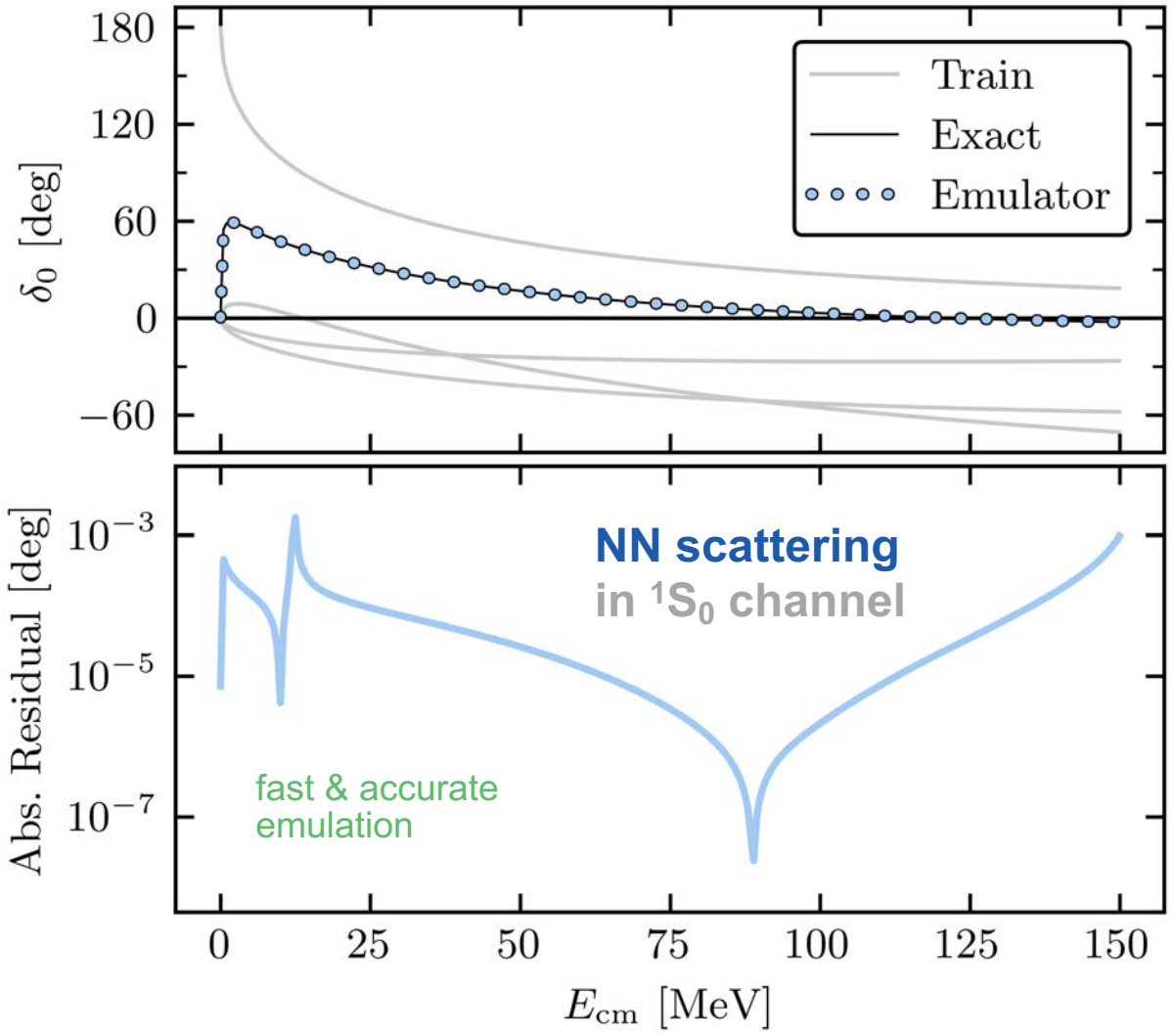
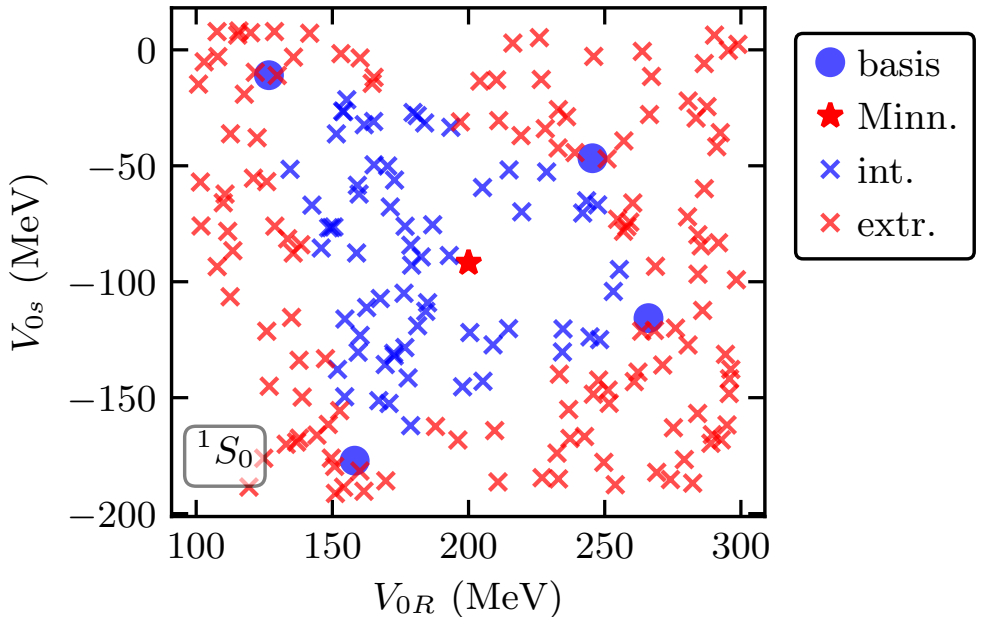



**Newton Variational Principle**

**Minnesota potential**

$$V(r) = V_{0R} e^{-\kappa_R r^2} + V_{0s} e^{-\kappa_s r^2}$$

**Training set**: 4 Hamiltonians with different ($V_{0R}$, $V_{0s}$ ● ) and fixed ($\kappa_R$, $\kappa_s$)




**More accurate than equivalent KVP calculation:** KVP residuals: $O(10^{-3})$

# Using the emulator for extrapolation

Melendez, CD, Garcia, Furnstahl, and Zhang, PLB **821**, 136608

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**Minnesota potential**

$$V(r) = V_{0R}e^{-\kappa_R r^2} + V_{0s}e^{-\kappa_s r^2}$$

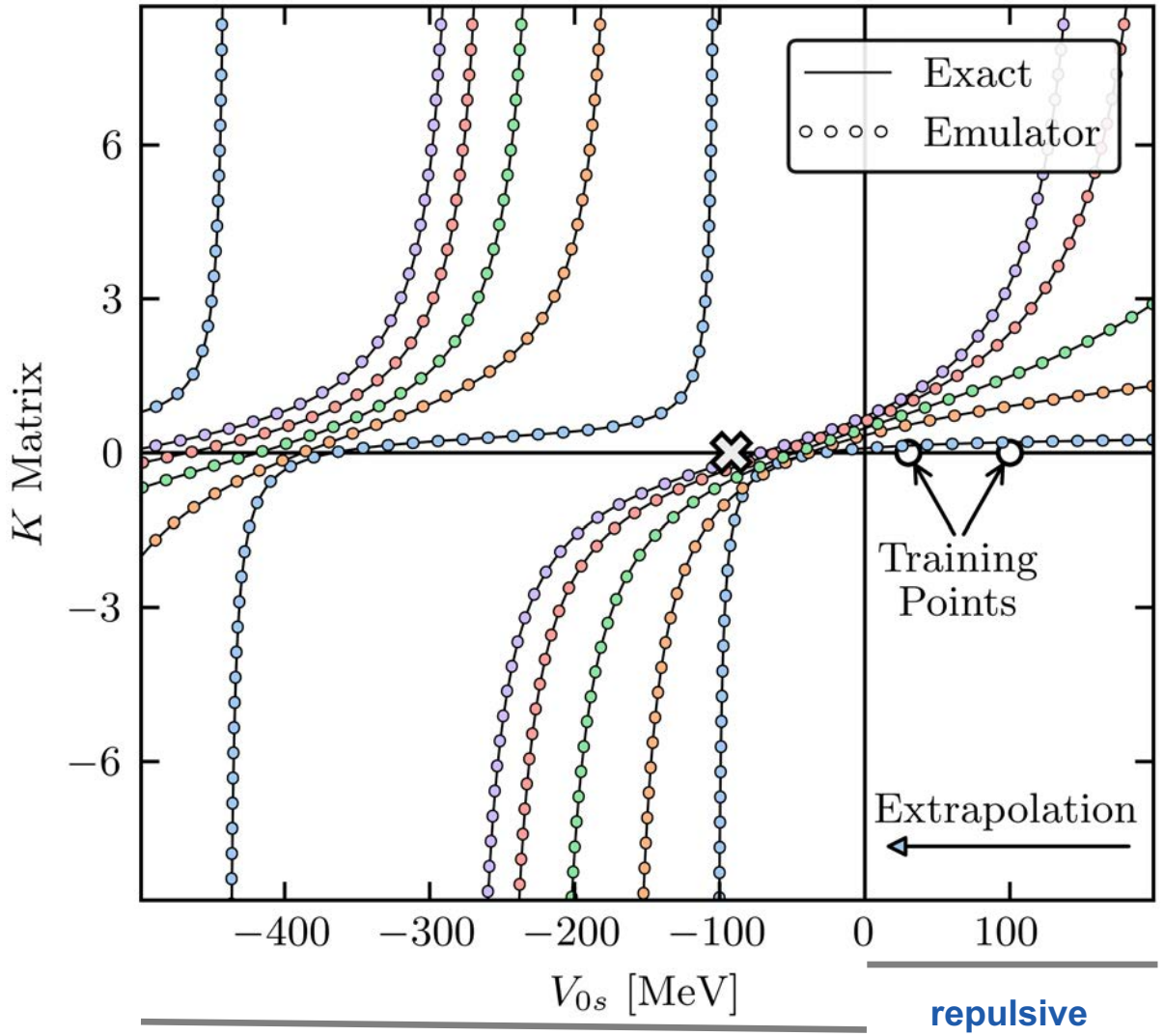
emulator as a **robust tool for extrapolations** (even from the repulsive to attractive regime)

**Training set**: two parameter sets with different $V_{0s} > 0$ (purely repulsive) and ($V_{0R}$, $\kappa_R$, $\kappa_s$) fixed at the physical point

Colors correspond to different c.m. energies in the range 1–70 MeV.

**Remarkable extrapolation** far from the support of data and **across singularities in the $K$ and $K^{-1}$ matrix**

on-shell $^1S_0$ $K$ matrix




**Newton Variational Principle**

# Adding the Coulomb potential

Melendez, CD, Garcia, Furnstahl, and Zhang, PLB **821**, 136608

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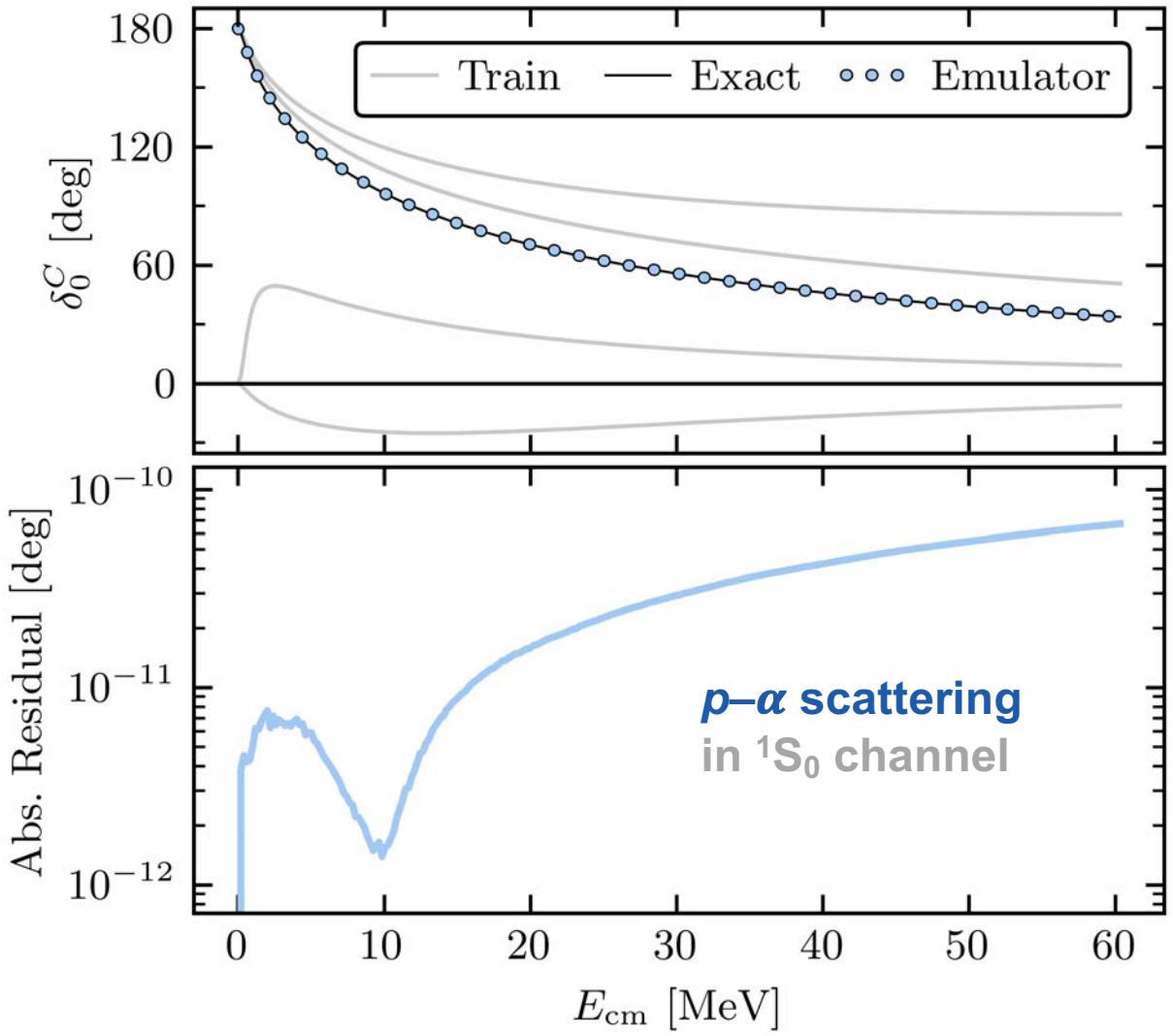


**Newton Variational Principle**

nonlocal potential

$$V_\ell(r,r') = V^{(0)}_{p\alpha,\ell} r'^\ell r^\ell e^{-\beta_\ell(r+r')}$$

**Long range potentials:** problematic for any LS equation (whether an emulator is used)

**Vincent-Phatak method:** cut off the Coulomb potential at a finite radius and then restore this physics using a matching procedure

**Training set**: 4 Hamiltonians with different *linear* parameters $V_{p\alpha}$ and *nonlinear* $\beta_0$ fixed at the physical point.

**Residuals are negligible** in this range

# Coupled channel scattering

Melendez, CD, Garcia, Furnstahl, and Zhang, PLB **821**, 136608

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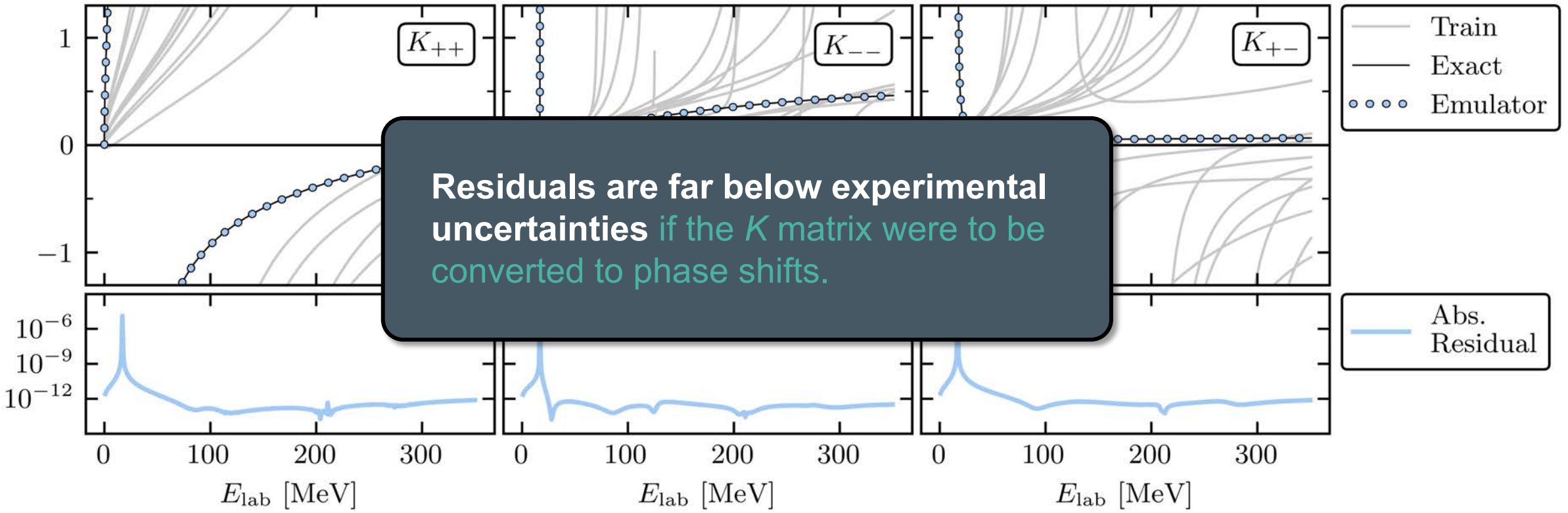
## Straightforwardly extended to coupled channel scattering

**$^3S_1$–$^3D_1$ channel with**
**6 free parameters (LECs)**




**Residuals are far below experimental uncertainties** if the *K* matrix were to be converted to phase shifts.

**SMS chiral NN potential at N$^4$LO+** with momentum cutoff Λ = 450 MeV

Reinert, Krebs, and Epelbaum, EPJ A **54**, 86

**12 training points** randomly chosen in the range [-5, +5] in the units used in the potential

**Newton Variational Principle**

# Emulating total cross sections

Melendez, CD, Garcia, Furnstahl, and Zhang, PLB **821**, 136608

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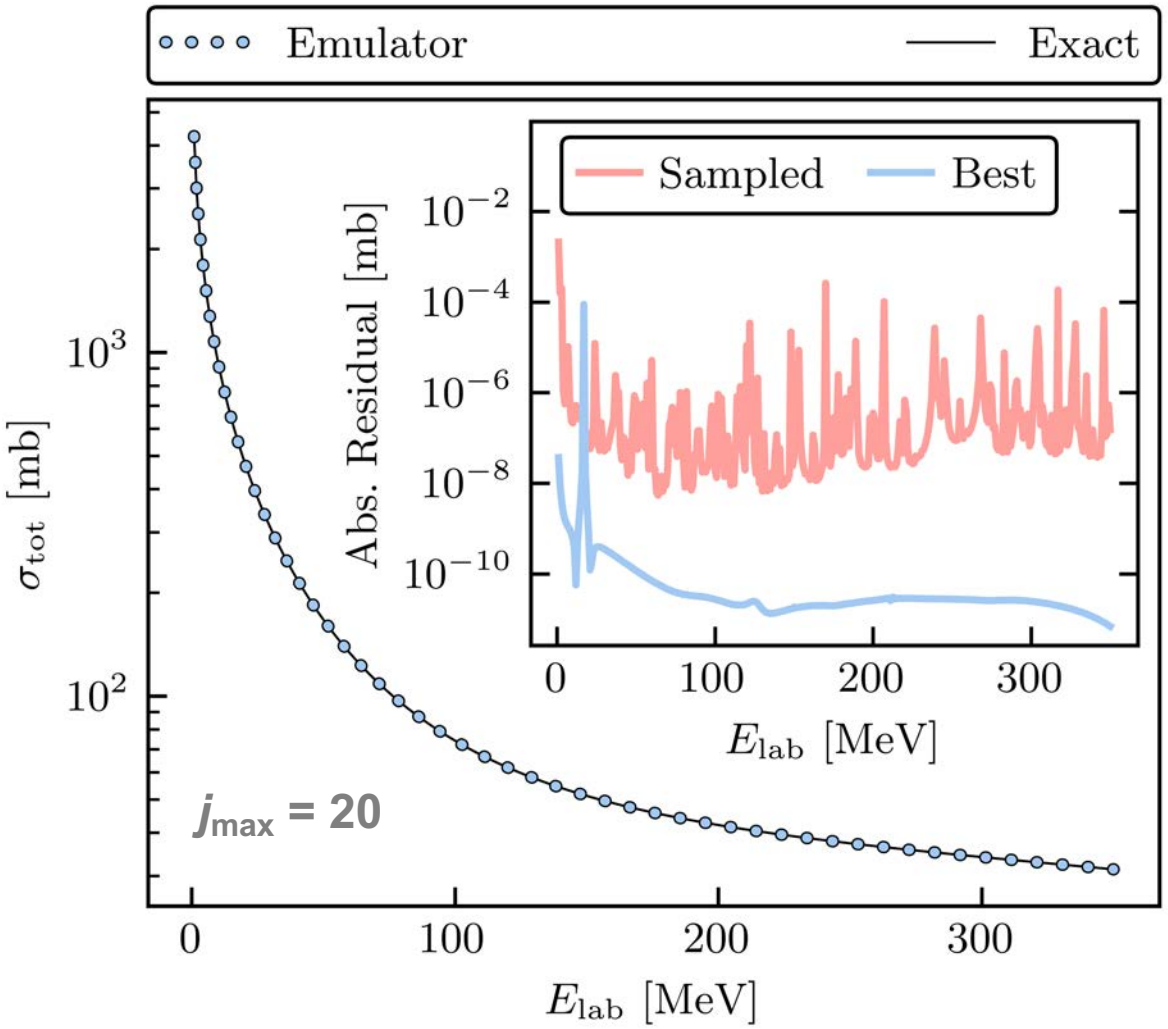
**SMS chiral NN potential at N$^4$LO+** with momentum cutoff $\Lambda$ = 450 MeV




**Newton Variational Principle**

$$\sigma_{\rm tot}(q) = -\frac{\pi}{2q^2}\sum_{j=0}^{j_{\rm max}}(2j+1)\,{\rm Re}\{{\rm Tr}[S_j(q)-\mathbb{1}]\}$$

**Train emulators across partial-wave channels up to *j* = 4** (while the remaining channels are fixed)

**26 free parameters (LECs)** varied

**Residuals are vanishingly small** compared to the **cross section** and its experimental uncertainty

Randomly **sample 500 values: extrapolation of ±10 [unit]** beyond the range of the training data

**>300x**

faster than the exact calculation

# Emulating gradients

Melendez, CD, Garcia, Furnstahl, and Zhang, PLB **821**, 136608

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**Minnesota potential**

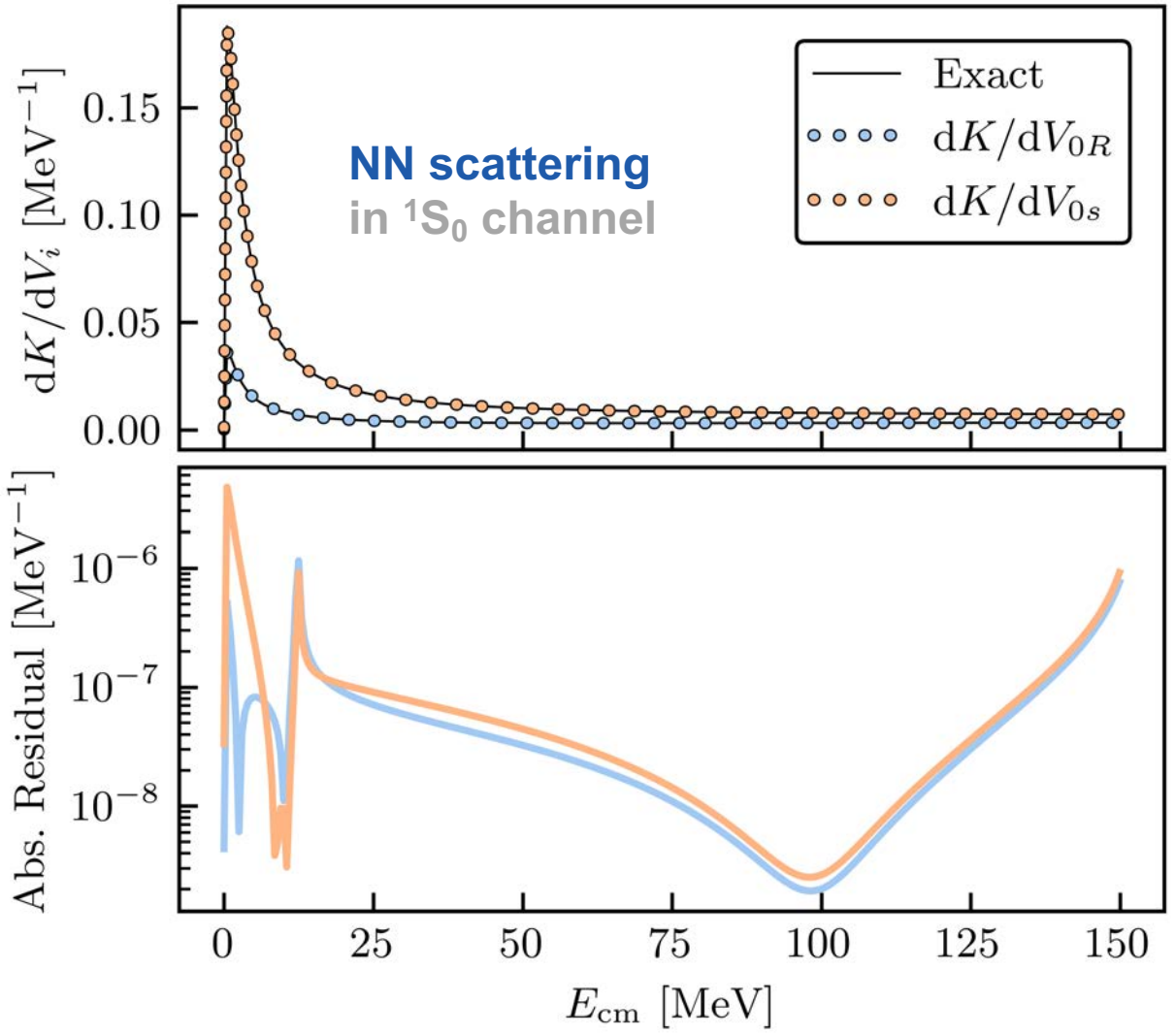
$$V(r) = V_{0R} e^{-\kappa_R r^2} + V_{0s} e^{-\kappa_s r^2}$$

**Gradients w.r.t. the input parameters** are useful for various optimization and Monte Carlo sampling algorithms.

**Proof of principle:**

We find that **emulated gradients**

- have **negligible residuals** at the physical point and
- can be incorporated in optimizers with **little computational overhead**




**Newton Variational Principle**

# Road Map: RBMs for scattering observables

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

See also: CD & Zhang's contribution to Few Body Syst. **63**, 67

# Kohn vs Newton Variational Principle

Garcia , CD, Furnstahl, Melendez, and Zhang, PRC **107**, 054001

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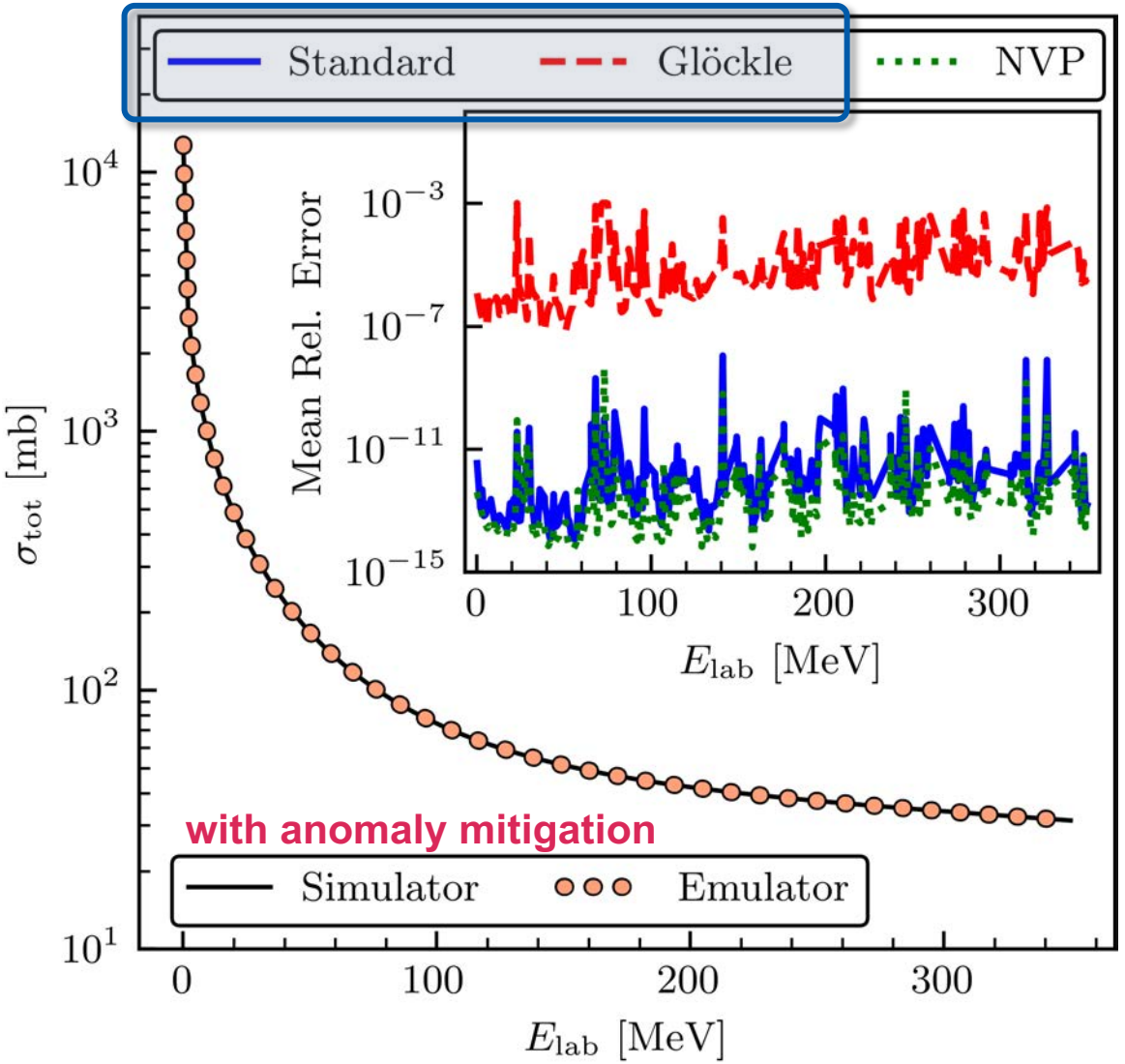
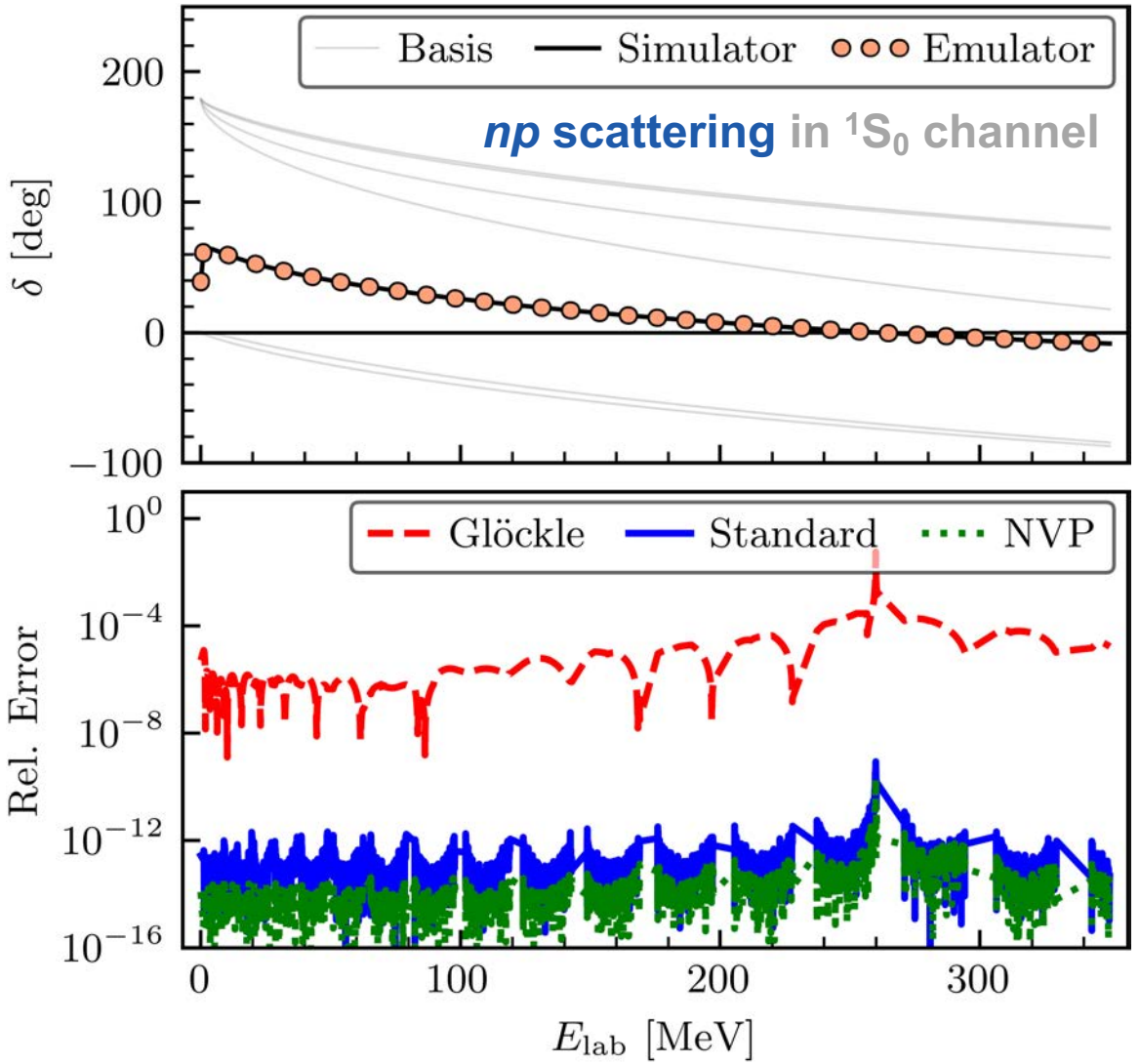
**two implementations of the KVP**




**SMS chiral NN potential at N$^4$LO+** with momentum cutoff $\Lambda$ = 450 MeV Reinert, Krebs, and Epelbaum, EPJ A **54**, 86

# Complementary approaches

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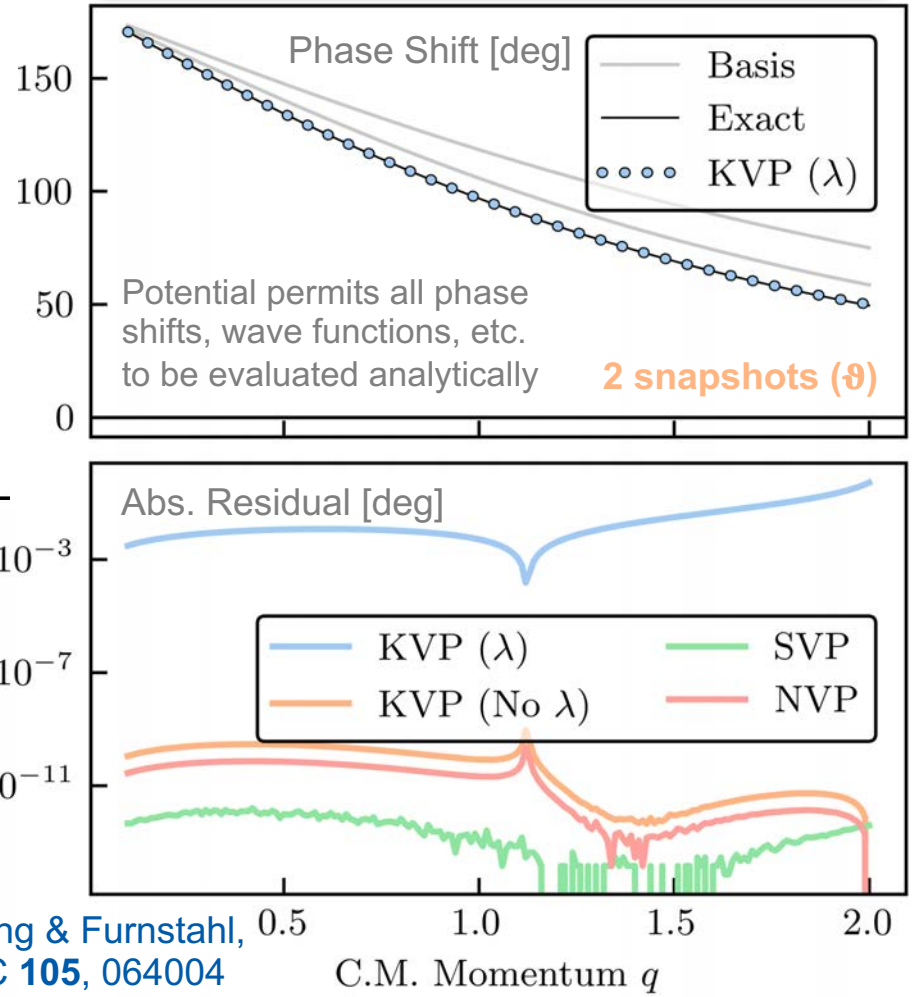
| Variational Principle | | Galerkin Projection Information | | | |
|---|---|---|---|---|---|
| Name | Functional for $K$ | Strong Form | Trial Basis | Test Basis | Constrained? |
| Kohn ($\lambda$) | $\widetilde{K}_E + \langle\widetilde{\psi}\|H-E\|\widetilde{\psi}\rangle$ | $H\|\psi\rangle = E\|\psi\rangle$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

Yamaguchi potential

$$V_\ell = \sum_{ij}^{n=2} |v_i^\ell\rangle\, \Lambda_{ij}\, \langle v_j^\ell|$$




These variational emulators have G-ROM counterparts. But there are also **non-variational, *e.g.*, "origin" ROMs** with $(r\psi)(0) = 0,\ (r\psi)'(0) = 1$

**Complementary approaches to construct (two-body) ROMs:**
coordinate vs momentum space; variational vs Galerkin methods; …

**How do we construct *reliable* three-body scattering ROMs?**

Zhang & Furnstahl, PRC **105**, 064004

# Questions! Answers?

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**How large are emulator errors? When are they non-negligible? Are simple implementations of ROMs *good enough* for NP?**

- convergence analyses are needed (for inter- and extrapolation)
- Understand their limitations and investigate potential improvements

**How can we construct efficient greedy algorithms? POD-based and hybrid methods should be further investigated.**

**How can we leverage ROMs' remarkable extrapolation capabilities? For continuous *and* discrete problems?**

## G-ROMs for two-body scattering

various implementations available (BUQEYE website)
approximate but highly accurate and inexpensive
offline-online decompositions important
hyper-reduction methods for non-affine/-linear problems

**What are the best practices for implementing ROMs efficiently? What can we learn from MOR software libraries like pyMOR or libROM?**

**Can we construct improved ROMs via Petrov-Galerkin projection? These ROMs are more general than G-ROMs (and variational ROMs).**

**What are the limits of hyper-reduction methods (in terms of accuracy and speed) applied to non-linear problems in NP?**

**How can we leverage ROMs as collaboration tools and open-source mini-apps accessible to non-experts?**

**Extensive MOR/RBM literature can (and should) provide guidance.**