Overview of Emulators for Nuclear Physics

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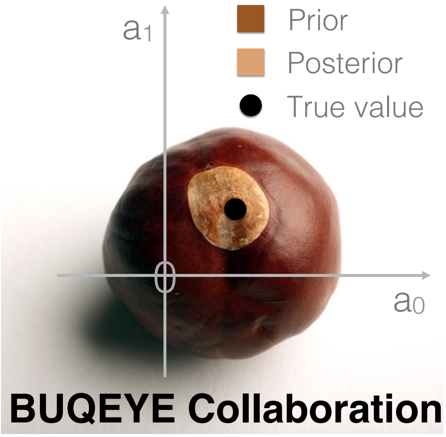
ISNET-9, May 2023

The Ohio State University



https://buqeye.github.io/

Python notebooks here!

LENPIC

https://www.lenpic.org/

NUCLEI

Nuclear Computational Low-Energy Initiative

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

BAND

Bayesian Analysis of Nuclear Dynamics

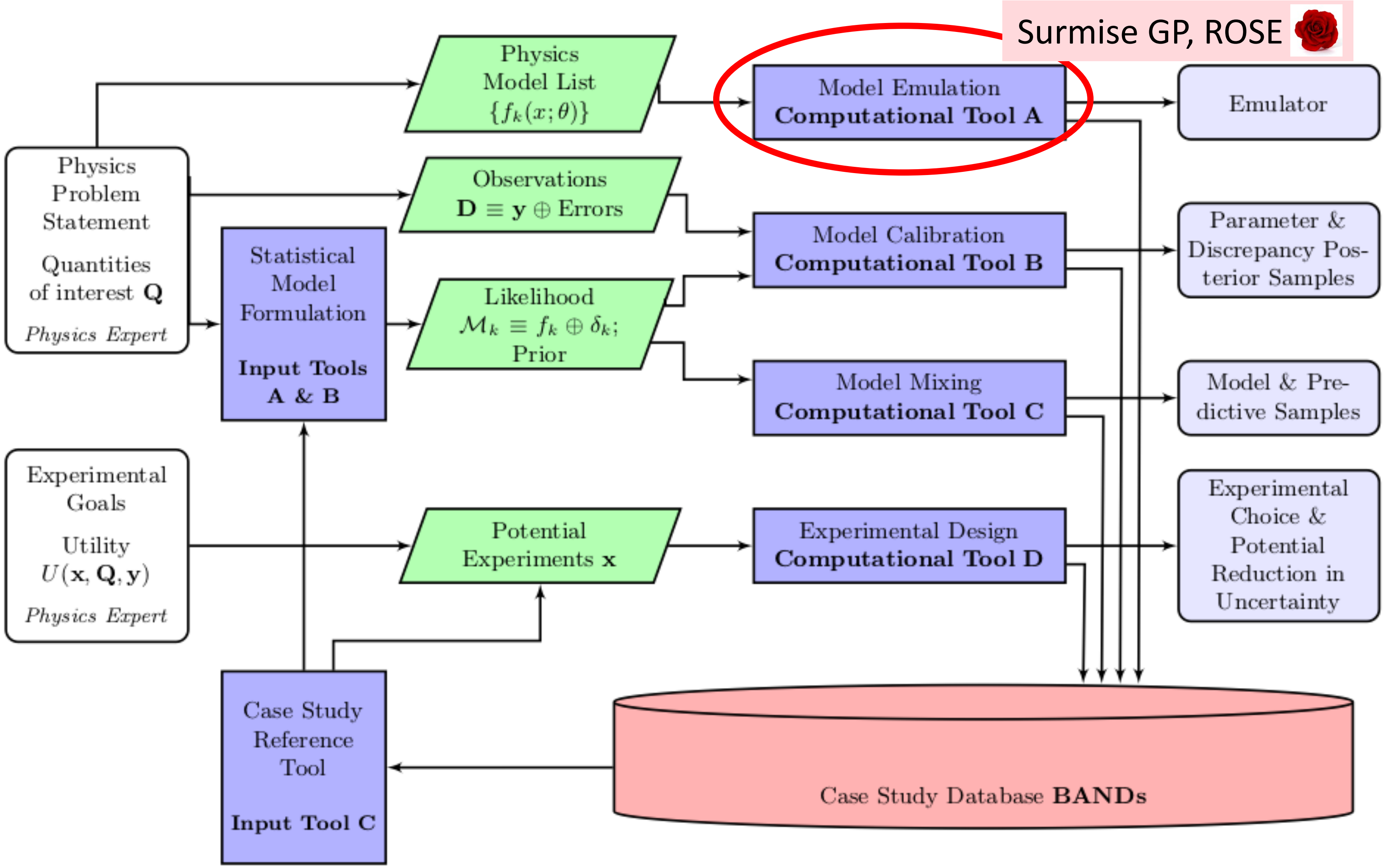
https://bandframework.github.io/

U.S. DEPARTMENT OF ENERGY

NSF

BAND (Bayesian Analysis of Nuclear Dynamics)

Goal: *Facilitate principled Uncertainty Quantification in Nuclear Physics*



An NSF CSSI Framework (started 7/2020)

Look to https://bandframework.github.io/ for papers, talks, and software!

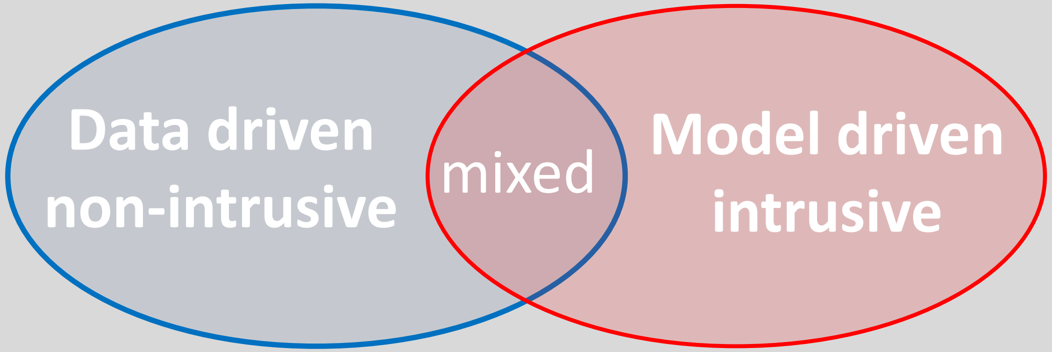
Model reduction methods → build nuclear emulators

Need: to vary parameters for design, control, optimization, UQ.

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

Solution: reduced-order model (ROM) → emulator (fast & accurate™).

General classification of ROMs



Data driven: interpolate output of high-fidelity model w/o understanding → *non-intrusive*

Examples: Gaussian processes; dynamic mode decomposition; artificial neural network, also hybrid ML

Model driven: derive reduced-order equations from high-fidelity equations → *intrusive*

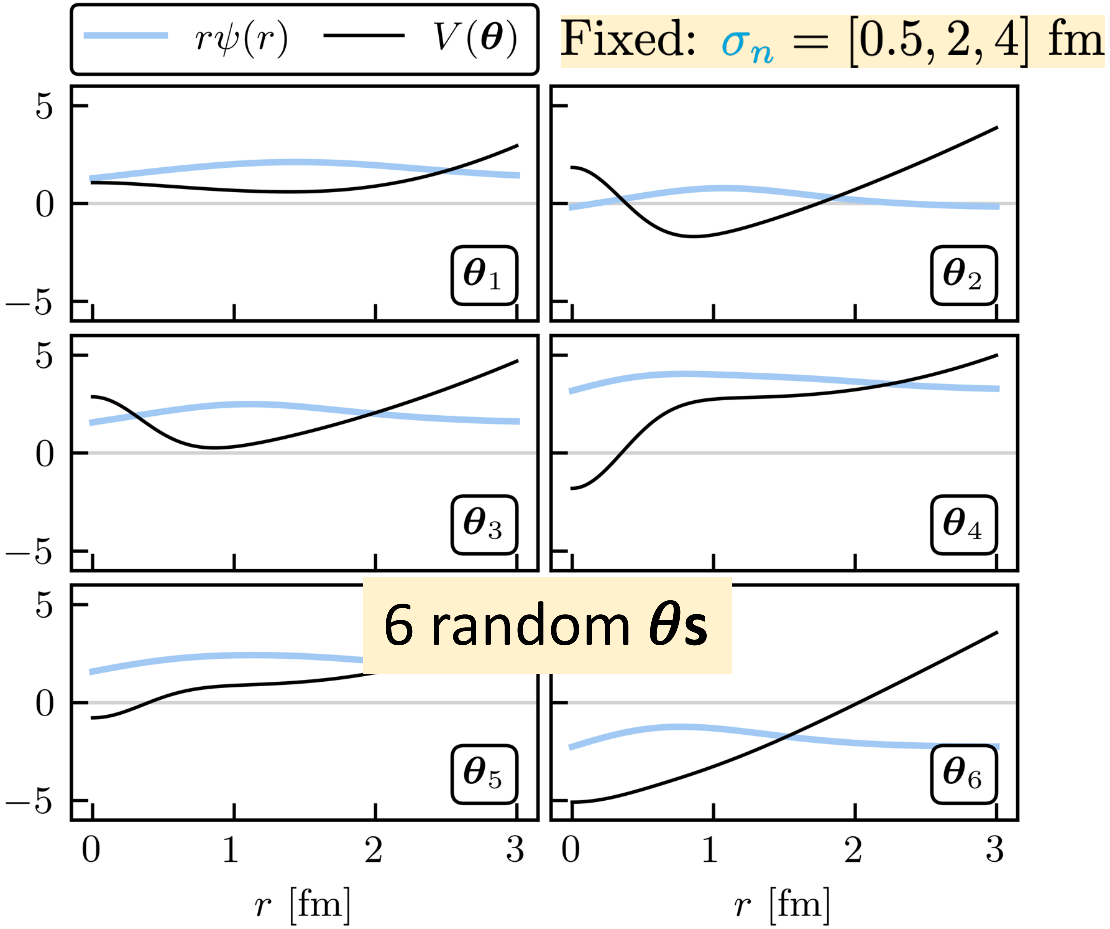
Features: physics-based, respects underlying structure → can extrapolate; often uses projection

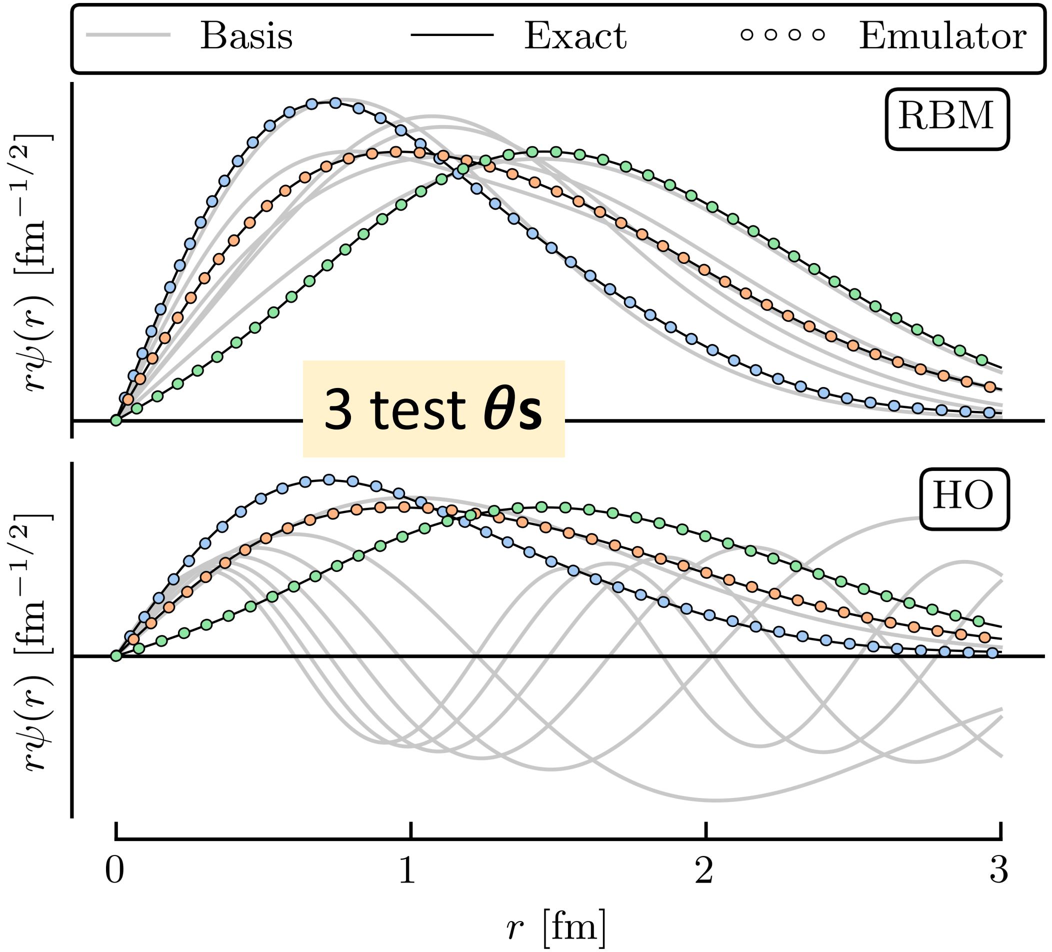
See Melendez et al., 2022 for many references from the wide ROM literature; various types of emulators already successful in NP (e.g., refs. in Drischler et al., 2022)

Illustrative example: anharmonic oscillator [Try your own!]

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

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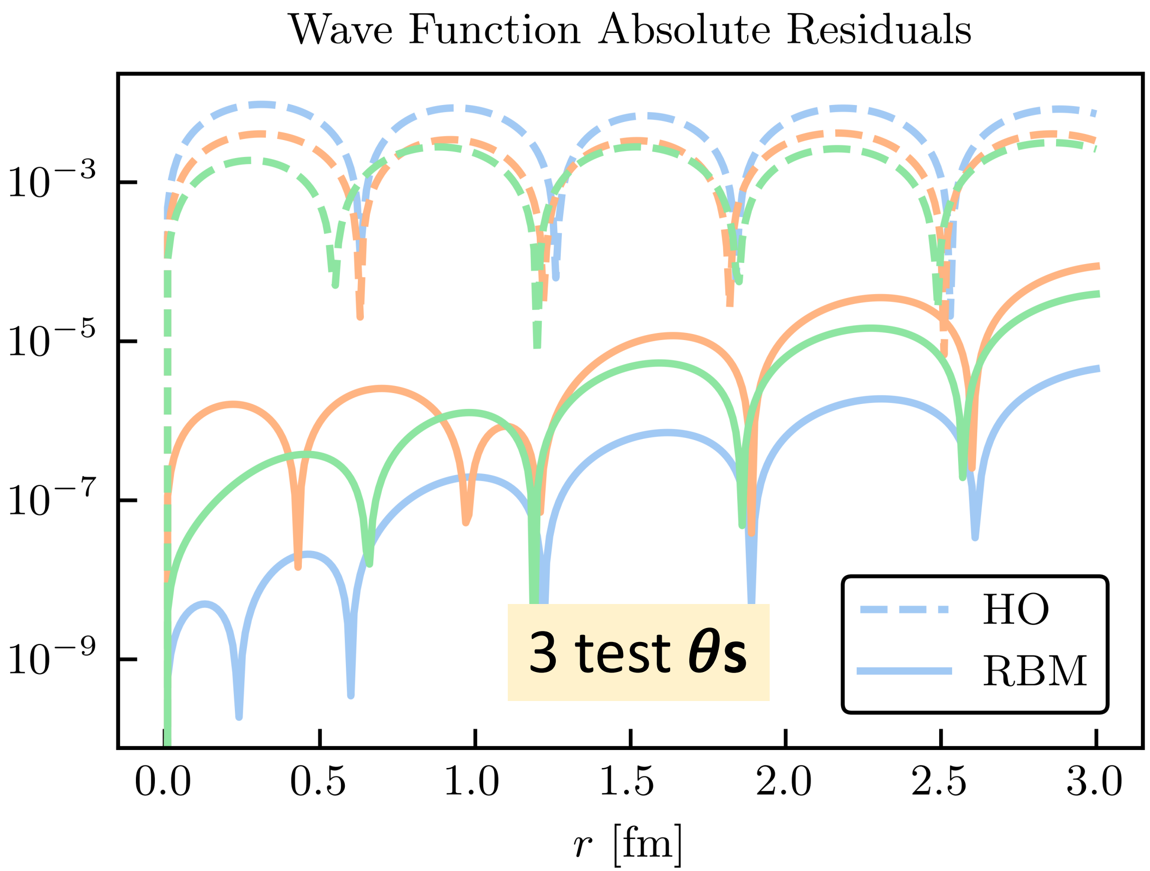

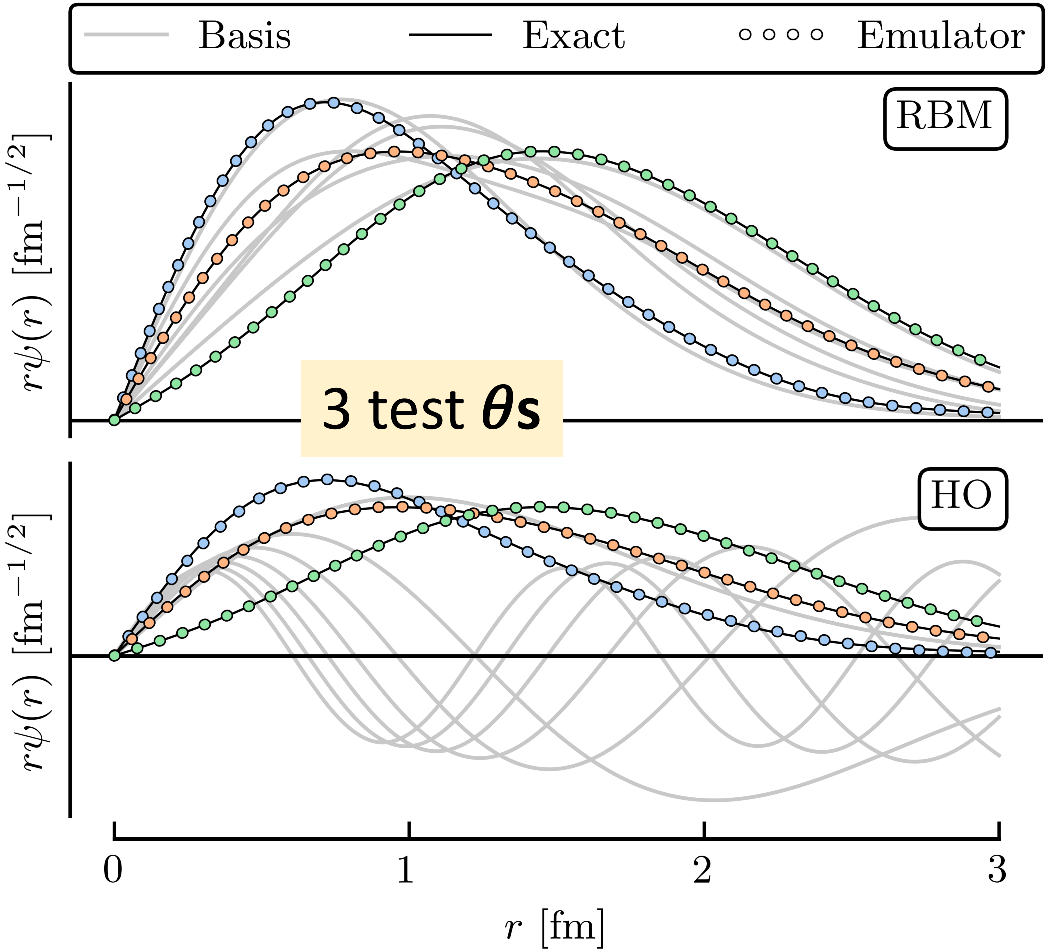

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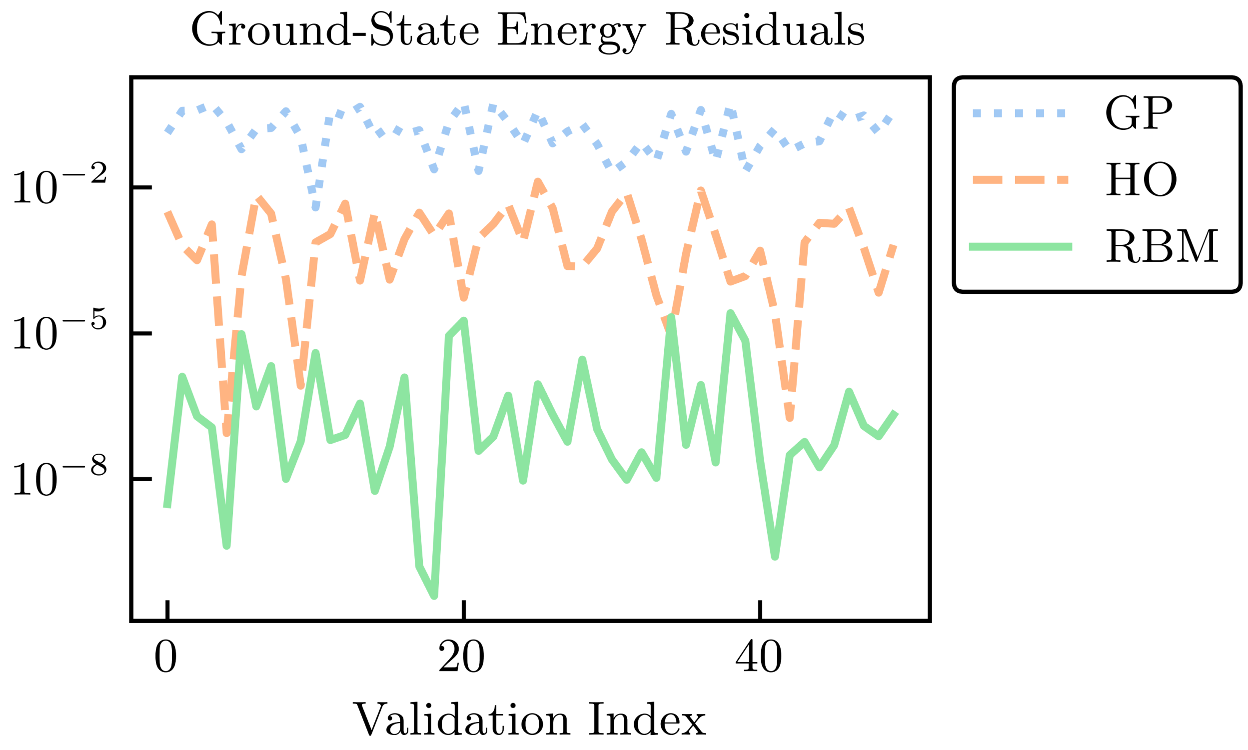
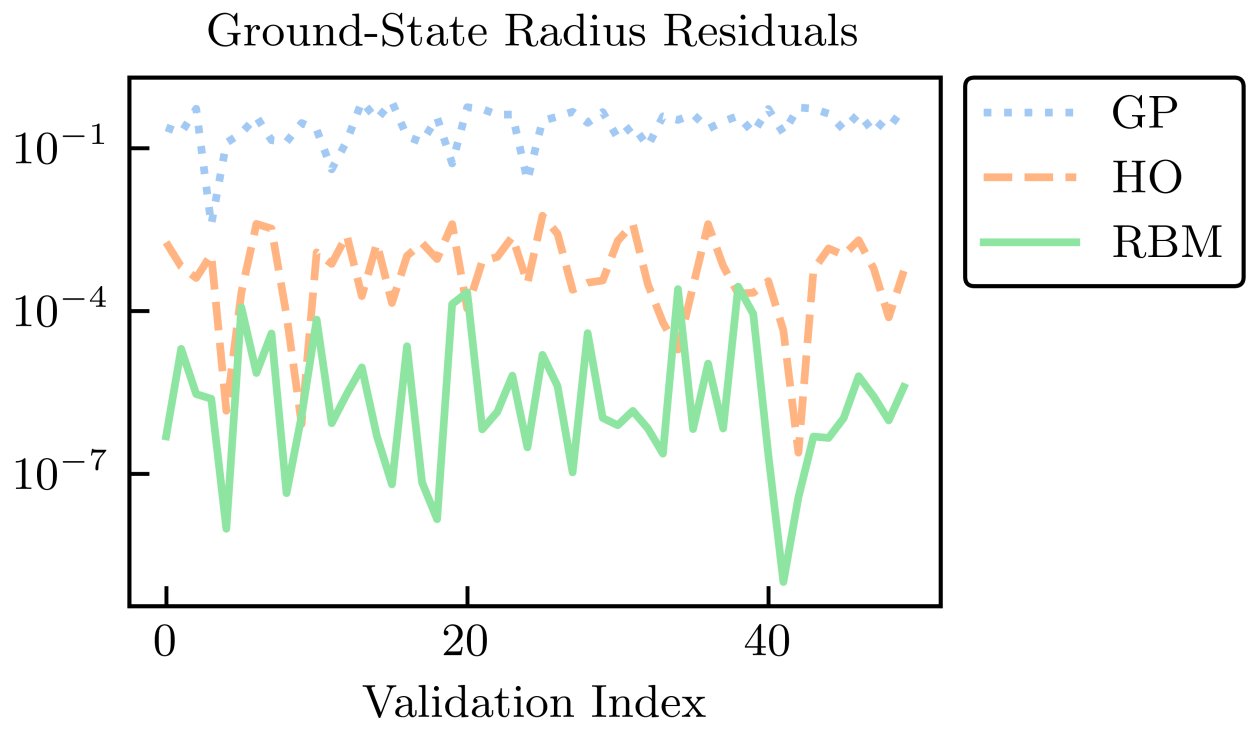
Fixed: $\sigma_n = [0.5, 2, 4]$ fm

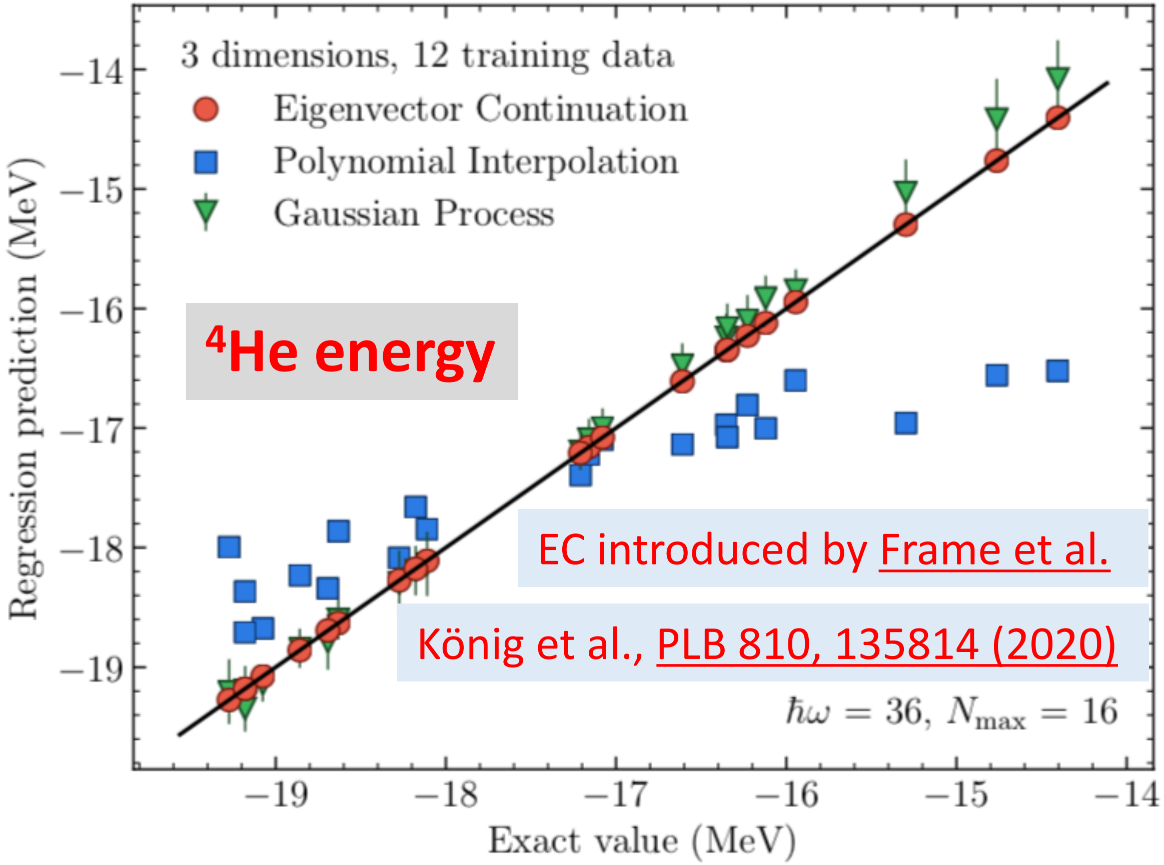


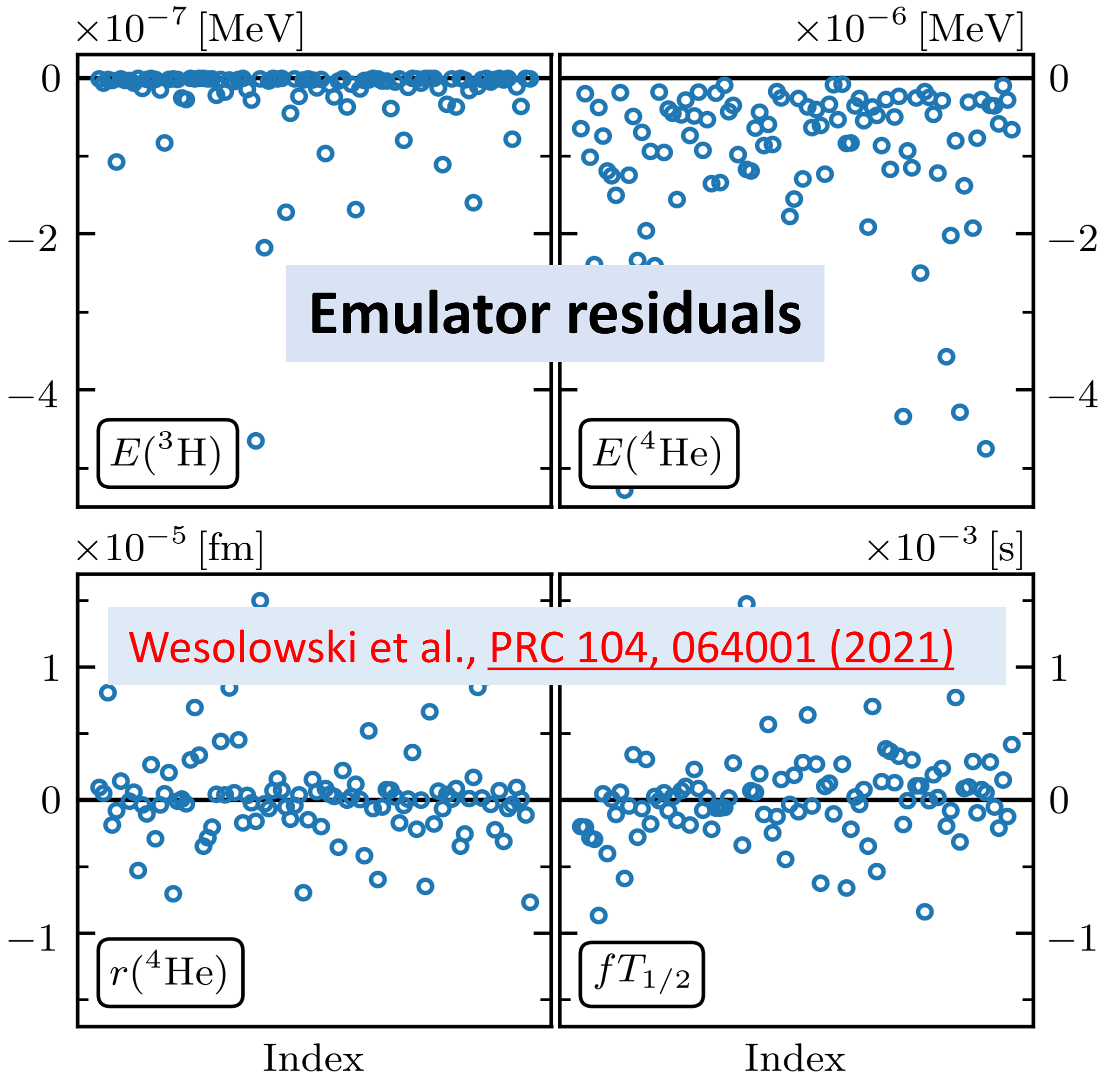


Summary: GP doesn't use the structure of the high-fidelity system to its advantage; HO emulator knows the problem to be solved is an eigenvalue problem; RBM (aka EC) training data are curves rather than scalars, takes advantage of system structure.

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 and accurate!





Emulator doesn't require specialized calculations!

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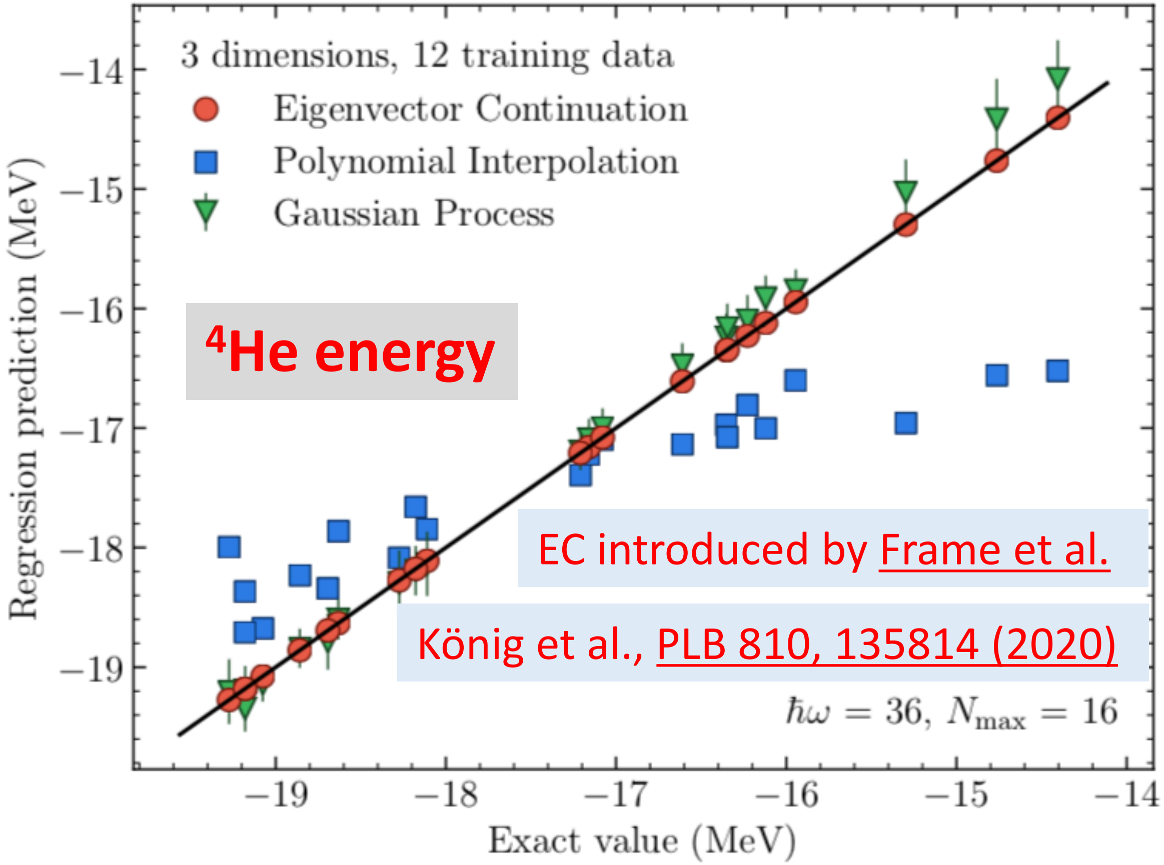
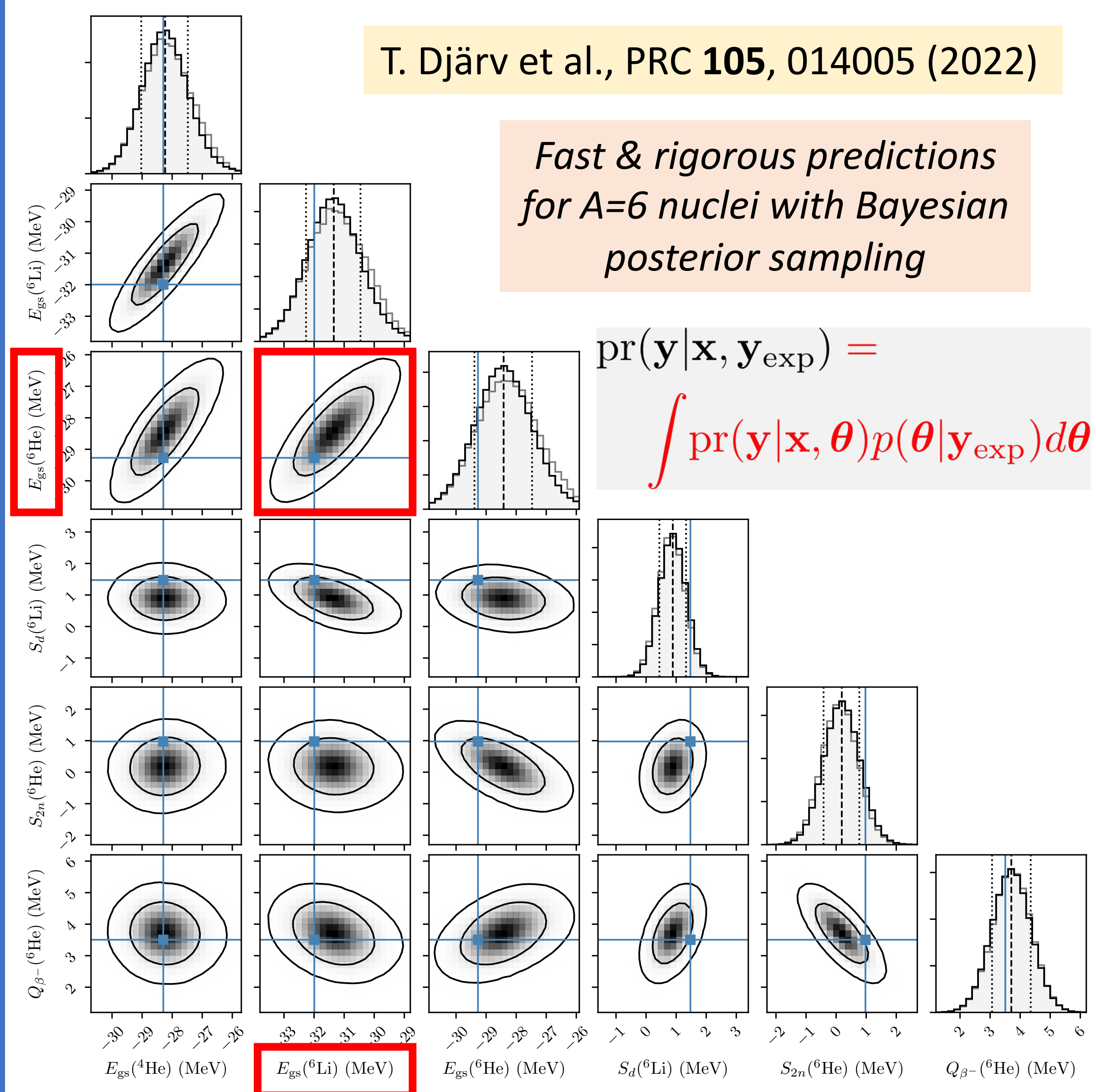


^{4}He energy

EC introduced by Frame et al.

König et al., PLB 810, 135814 (2020)



T. Djärv et al., PRC **105**, 014005 (2022)

Fast & rigorous predictions for A=6 nuclei with Bayesian posterior sampling

$$\mathrm{pr}(\mathbf{y}|\mathbf{x},\mathbf{y}_{\mathrm{exp}}) = \int \mathrm{pr}(\mathbf{y}|\mathbf{x},\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{y}_{\mathrm{exp}})d\boldsymbol{\theta}$$

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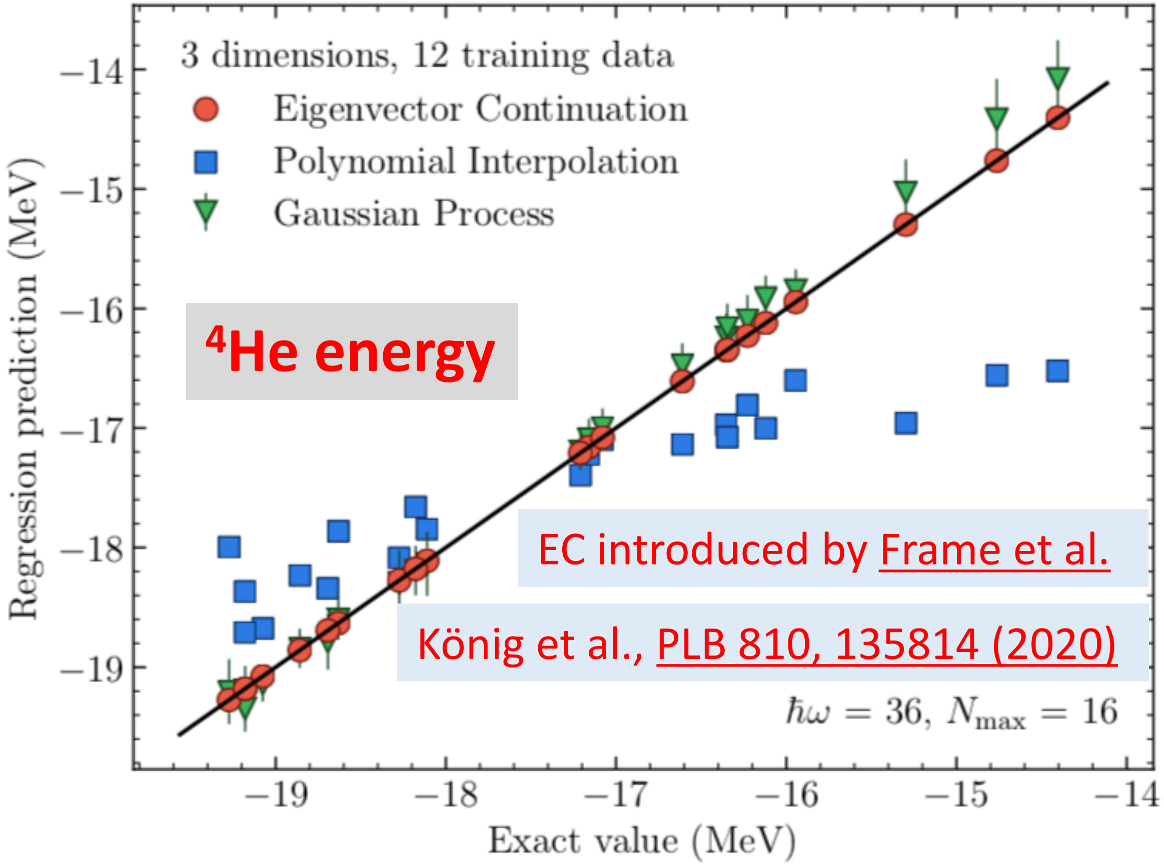

^{4}He energy

EC introduced by Frame et al.

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Already applied to many observables:

- Ground-state properties (energies, radii)
- Transition matrix elements
- Excited states
- Resonances

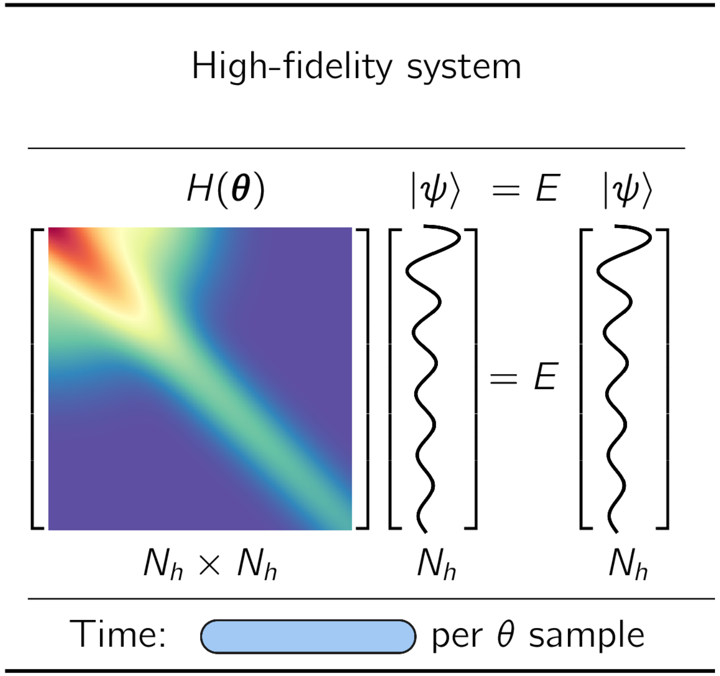
Adapted to special situations and methods

- Pairing
- Coupled cluster approach; MBPT
- Systems in a finite box
- Subspace diagonalization on quantum computers

Extended to non-eigenvalue problems

- Reactions and scattering

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)
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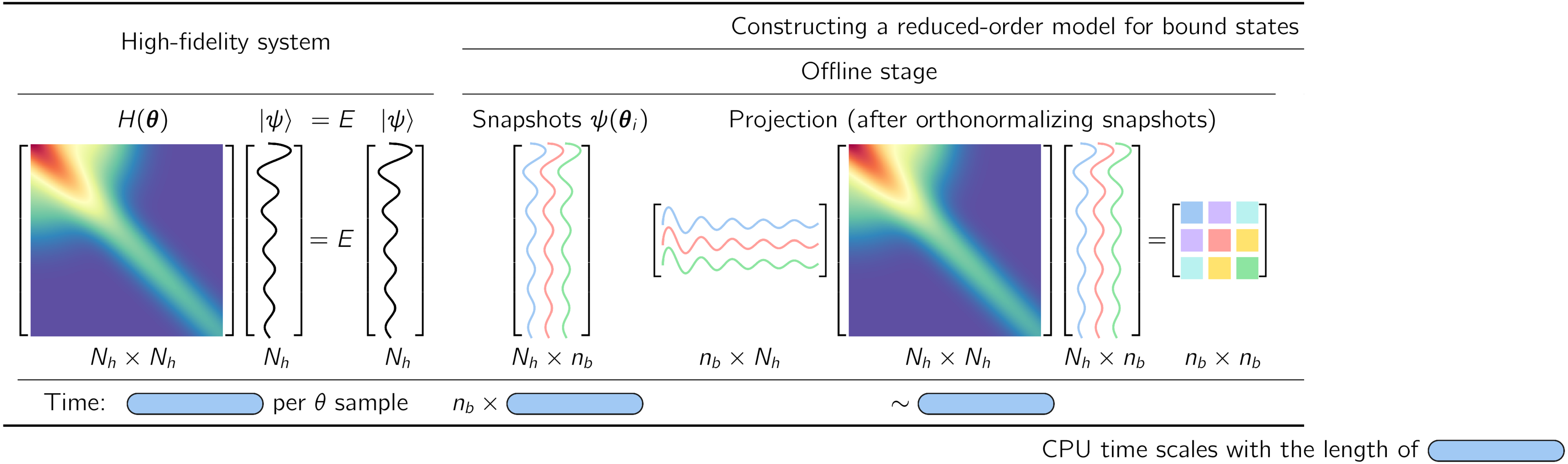

- Offline stage (pre-calculate):
  - Construct basis using snapshots from high-fidelity system (simulator)
  - Project high-fidelity system to small-space using snapshots

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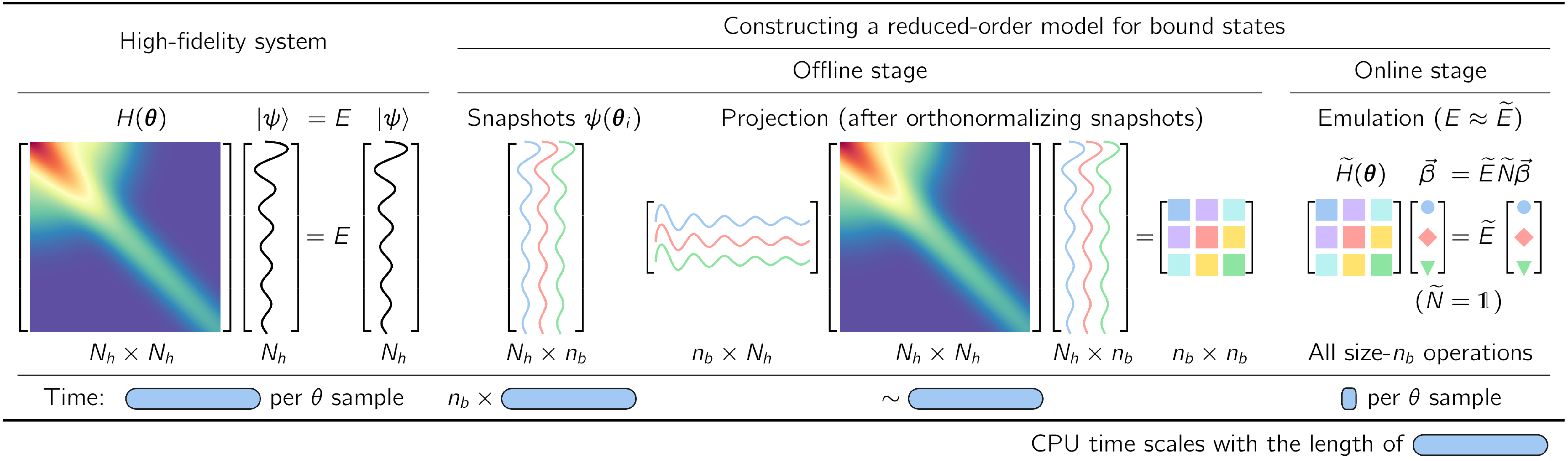

- Offline stage (pre-calculate size N_h):
  - Construct basis using snapshots from high-fidelity system (simulator)
  - Project high-fidelity system to small-space using snapshots
- Online stage (emulation size n_b only):
  - Make many predictions fast & accurately (e.g., for Bayesian analysis)

- *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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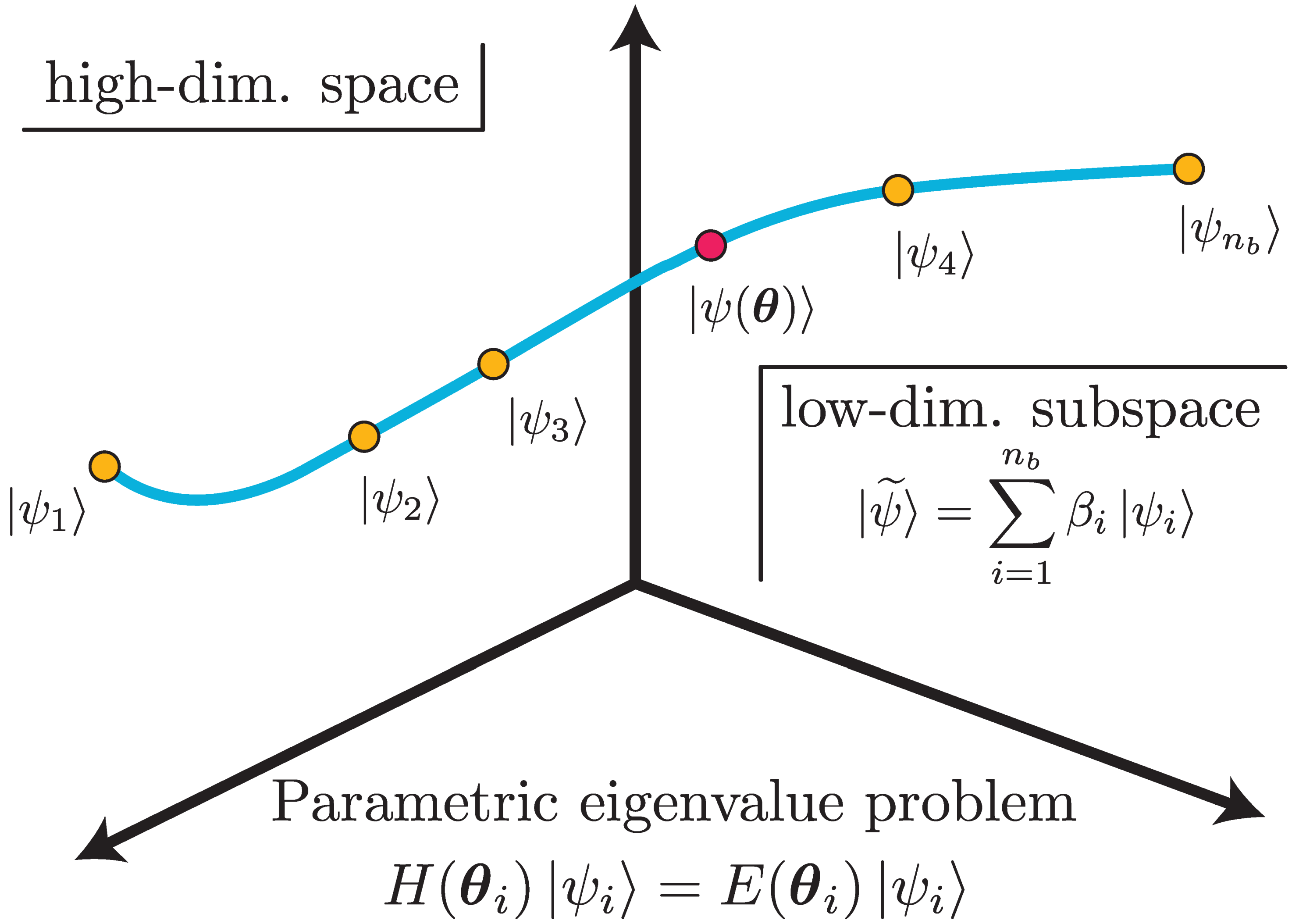
Schematic picture of projection-based emulators



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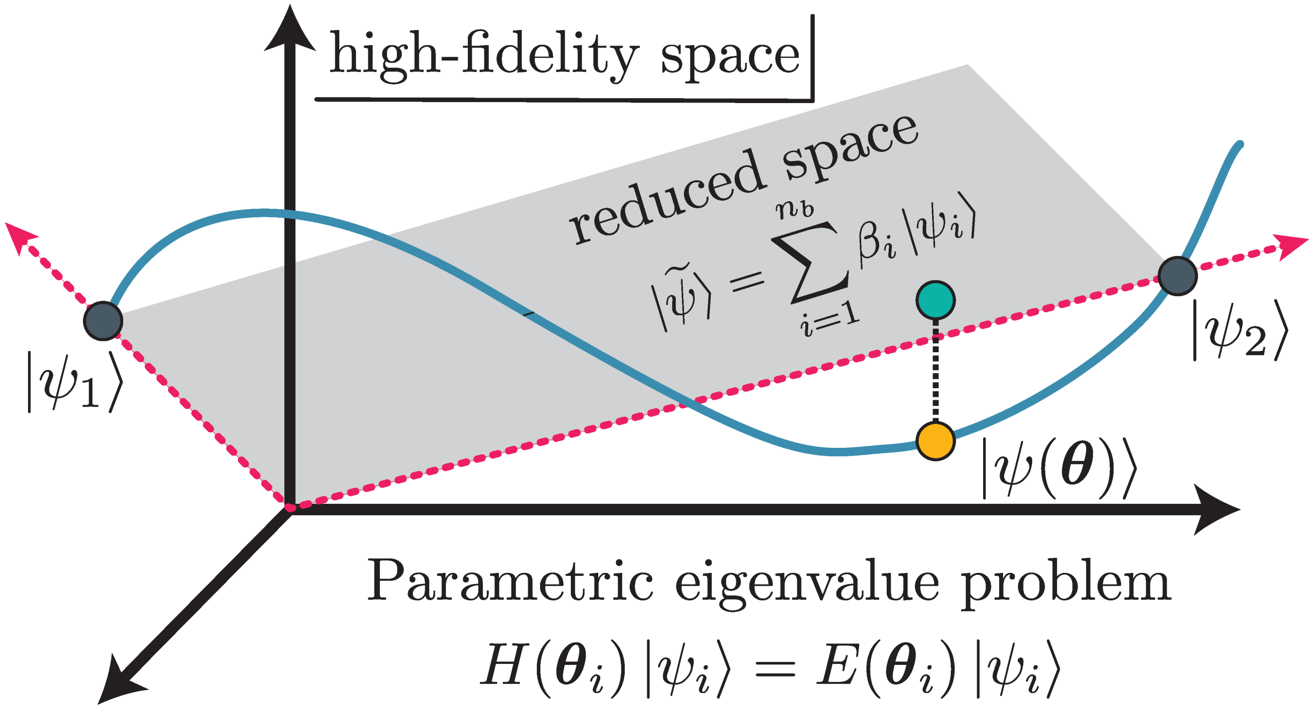


Parametric eigenvalue problem

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

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

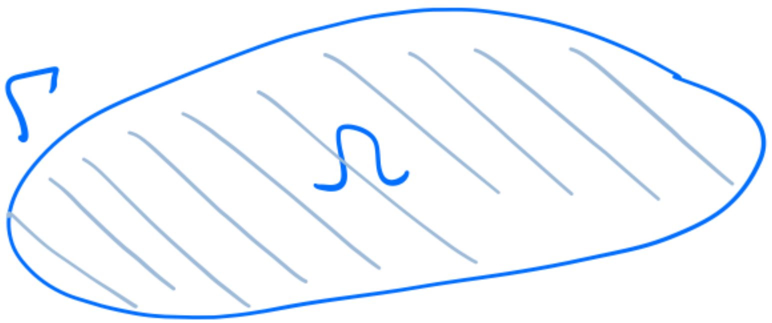
Variational vs. Galerkin for differential equations

Projection-based emulator for solution ψ to

$$D(\psi;\boldsymbol{\theta}) = 0 \text{ in } \Omega;\ \ B(\psi;\boldsymbol{\theta}) = 0 \text{ on } \Gamma$$

where D and B are operators. Example:

$$[-\nabla^2\psi = g(\boldsymbol{\theta})]_\Omega \qquad [\tfrac{\partial\psi}{\partial n} = f(\boldsymbol{\theta})]_\Gamma$$



If affine g(**θ**), f(**θ**) → calculate high-fidelity offline.
If nonlinear or nonaffine → hyper-reduction, etc.

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

Variational → stationary functional

$$S[\psi] = \int_\Omega d\Omega\, F[\psi] + \int_\Gamma d\Gamma\, G[\psi]$$

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

Solve linear algebra problem for $\vec{\beta}_*$:

$$\delta S = A\vec{\beta}_* + \vec{b} = 0$$

Galerkin projection → use weak form

$$\int_\Omega d\Omega\, \zeta\, D(\psi) + \int_\Gamma d\Gamma\, \bar{\zeta}\, B(\psi) = 0$$

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

Test bases: $|\zeta\rangle = \sum_{i=1}^{n_b} \delta\beta_i |\zeta_i\rangle,\ \ |\zeta\rangle \to |\bar{\zeta}\rangle$

$$\Rightarrow \delta\beta_i \Big[\int_\Omega d\Omega\, \zeta_i\, D(\widetilde{\psi}) + \int_\Gamma d\Gamma\, \bar{\zeta}_i\, B(\widetilde{\psi})\Big] = 0$$

Variational vs. Galerkin emulators via concrete example

E.g., Poisson equation with Neumann BCs → $[-\nabla^2\psi = g(\boldsymbol{\theta})]_\Omega$ with $[\frac{\partial\psi}{\partial n} = f(\boldsymbol{\theta})]_\Gamma$

Emulator → $\psi(\boldsymbol{\theta}) \approx \widetilde{\psi}(\boldsymbol{\theta}) = \sum_{i=1}^{n_b}(\vec{\beta}_*)_i\psi_i = X\vec{\beta}_*, \quad X \equiv [\psi_1\ \psi_2\ \cdots\ \psi_{n_b}]$ find optimal $\vec{\beta}_*$ online

Variational (Ritz)

$$S[\psi] = \int_\Omega d\Omega\,(\tfrac{1}{2}\nabla\psi\cdot\nabla\psi - g\psi) - \int_\Gamma d\Gamma\, f\psi$$

$$\Longrightarrow \delta S = \int_\Omega d\Omega\,\delta\psi(-\nabla^2\psi - g) + \int_\Gamma d\Gamma\,\delta\psi\Big(\frac{\partial\psi}{\partial n} - f\Big)$$

So δS = 0 gives the Poisson eq. and BCs. Emulate $\psi(\boldsymbol{\theta})$:

$$S[\widetilde{\psi}] \to \delta S[\widetilde{\psi}] = \sum_{i=1}^{n_b}\frac{\partial S}{\partial\beta_i}\delta\beta_i = 0$$ → n_b equations for $\vec{\beta}_*$

If linear (as here) → $\widetilde{A}\vec{\beta}_* = \vec{g} + \vec{f}, \quad \widetilde{A}_{ij} = \int_\Omega \nabla\psi_i\cdot\nabla\psi_j,$
$g_i = \int_\Omega g(\boldsymbol{\theta})\psi_i, \quad f_i = \int_\Gamma f(\boldsymbol{\theta})\psi_i$

If affine g(**θ**), f(**θ**) → calculate high-fidelity offline.

Ritz-Galerkin

Weak formulation with *test function* ζ

$$\int_\Omega d\Omega\,\zeta(-\nabla^2\psi - g) + \int_\Gamma d\Gamma\,\zeta\Big(\frac{\partial\psi}{\partial n} - f\Big) = 0$$

$$\Longrightarrow \int_\Omega d\Omega\,(\nabla\zeta\cdot\nabla\psi - g\zeta) - \int_\Gamma d\Gamma\, f\zeta = 0$$

Assert holds for $\psi \to \widetilde{\psi} = X\vec{\beta}$ and $\zeta = \sum_{i=1}^{n_b}\delta\beta_i\psi_i$

$$\delta\beta_i\Big[\int_\Omega d\Omega\,(\underbrace{\nabla\psi_i\cdot\nabla\psi_j}_{\widetilde{A}_{ij}}\beta_j - \underbrace{g\psi_i}_{g_i}) - \int_\Gamma d\Gamma\,\underbrace{f\psi_i}_{f_i}\Big] = 0$$

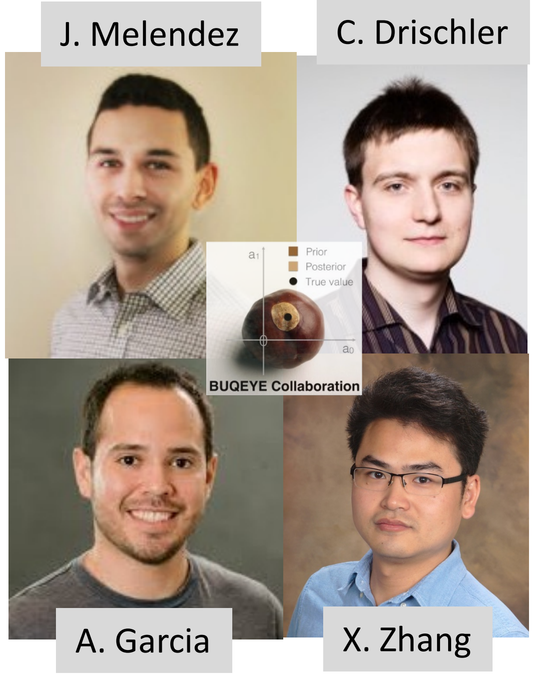
→ same result as variational, but Galerkin is more general. If $\zeta_i \neq \psi_i$, then *Petrov-Galerkin*.

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



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Name	Functional for K	Strong Form	Trial Basis	Test Basis	Constrained?
Kohn (λ)	$\widetilde{K}_E + \langle\widetilde{\psi}\|H-E\|\widetilde{\psi}\rangle$	$H\|\psi\rangle = E\|\psi\rangle$	$\|\psi_i\rangle$	$\langle\psi_i\|$	Yes
Kohn (No λ)	$\langle\widetilde{\chi}\|H-E\|\widetilde{\chi}\rangle + \langle\phi\|V\|\widetilde{\chi}\rangle + \langle\phi\|H-E\|\phi\rangle + \langle\widetilde{\chi}\|V\|\phi\rangle$	$[E-H]\|\chi\rangle = V\|\phi\rangle$	$\|\chi_i\rangle$	$\langle\chi_i\|$	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

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 $(r\psi)(0) = 0,\ (r\psi)'(0) = 1$ (see later talks)

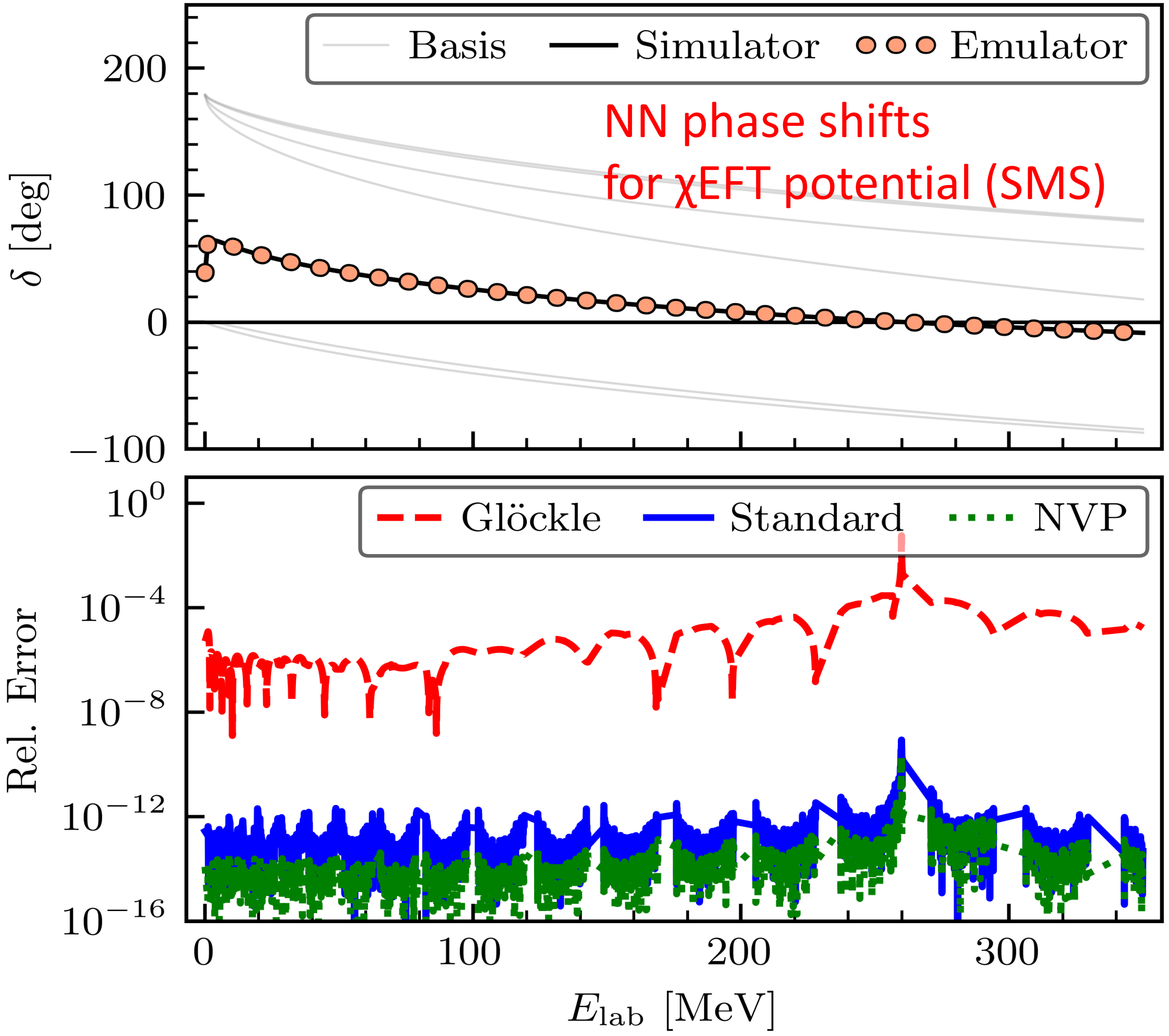
What is the best way to implement a 3-body scattering emulator?

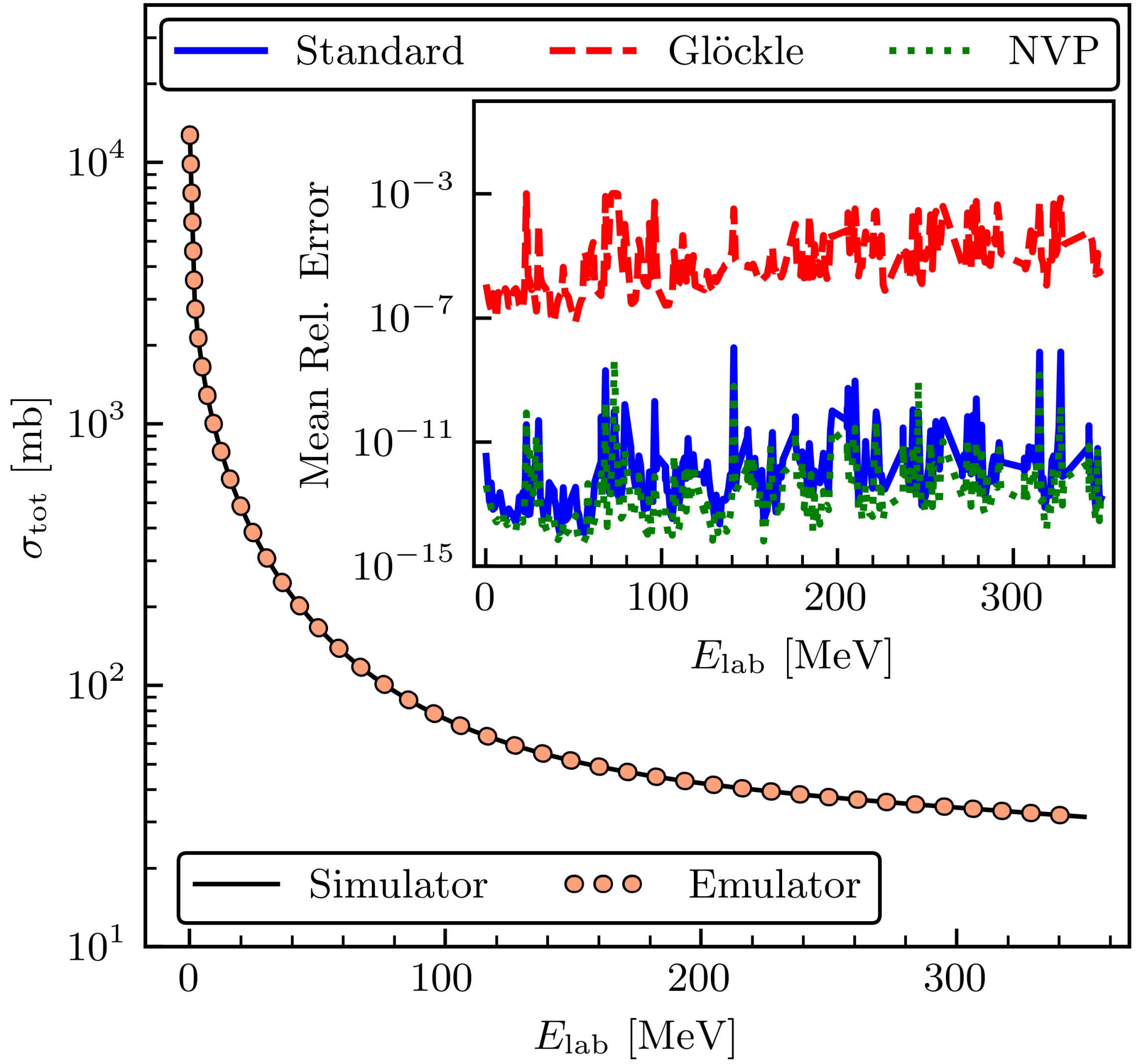
- E.g, for Bayesian χEFT LEC estimation or nuclear reactions.
- X. Zhang, rjf, PRC (2022) gave proof of principle (bosons) using KVP.

RBM emulators for NN scattering in chiral EFT (affine!)

Compare NVP to two implementations of KVP

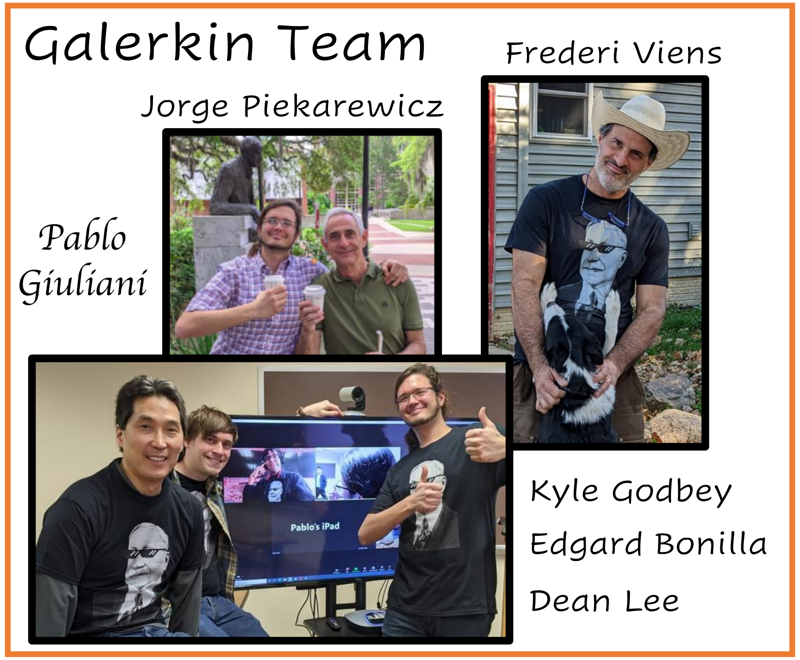
A. Garcia et al., PRC **107** (2023)

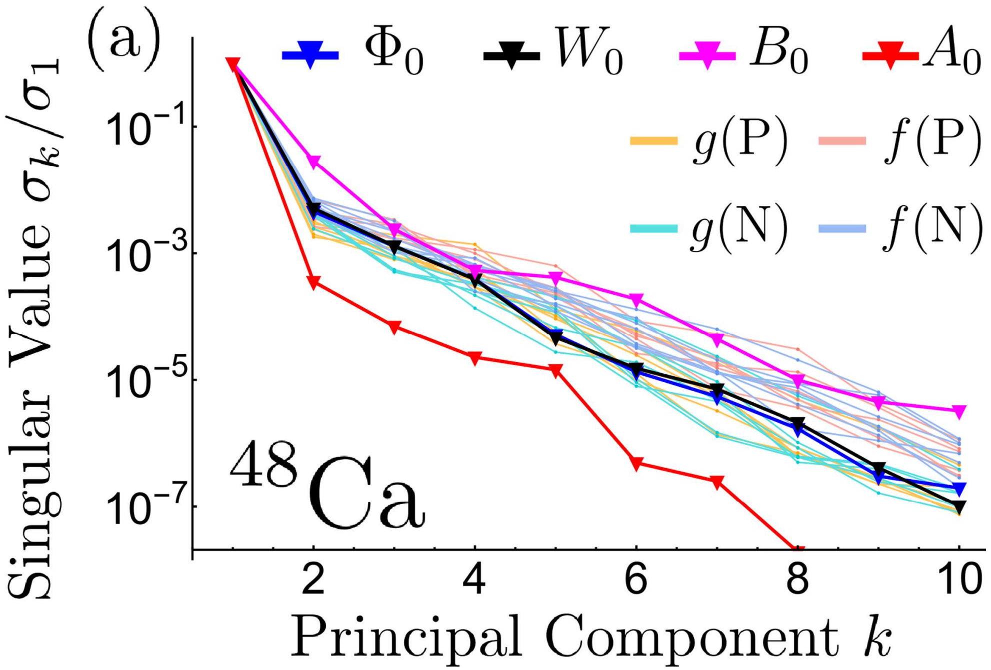


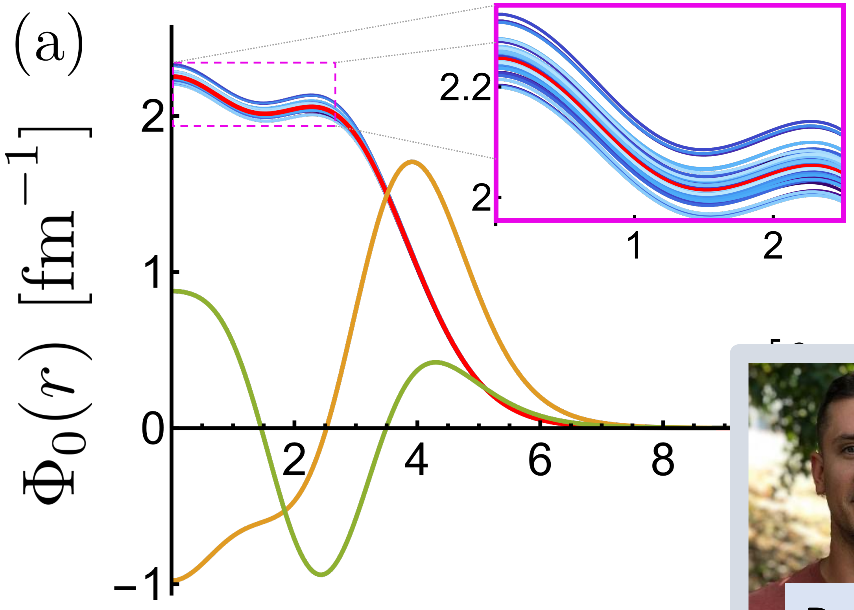


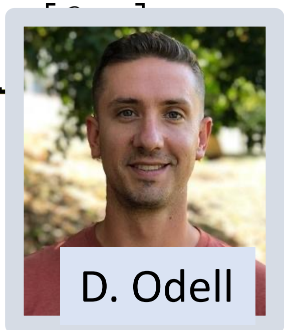
RBM emulators for EDFs and non-affine

- Energy density functionals (EDFs) present new challenges.
- P. Giuliani et al., "Bayes goes fast …" (also "Training and Projecting")
  → apply Galerkin RBM to EDFs (covariant mean field, Skyrme)
- Efficient basis to evaluate functional for many parameter sets.
- → Fast and accurate emulation, ideal for Bayesian inference!









Also today: RBM for non-linear, non-affine problems. BAND: ROSE software (e.g., for opt. potl.)

Summary of key RBM elements

Vast range of problems have been attacked with MOR in science and engineering, including heat transfer, fluid dynamics, electronic DFT, …→ coupled ode's and pde's (incl. time-dependent and nonlinear); eigenvalue problems; and more!
There's likely something out there in the MOR literature analogous to what you do!

Large speed-ups from ***offline-online*** **paradigm** if heavy compute resources are offline.
→ move size-ψ operations offline so that emulation varying **θ** online is efficient.
Key: exploit *affine* parameter dependence in operators, e.g., $H(\boldsymbol{\theta}) = \sum_n h_n(\boldsymbol{\theta}) H_n$
For non-linear systems and non-affine parameters, use *hyper-reduction* methods.

Projection-based: *(i)* choose *low-dimensional* rep. of ψ and *(ii)* write in integral form.
For *(i)*: $\tilde{\psi}(\boldsymbol{\theta}) \equiv \sum_{i=1}^{N_b} \beta_i \psi_i = X\vec{\beta}, \quad X \equiv [\psi_1\, \psi_2\, \cdots\, \psi_{N_b}]$ with *X* found offline.

Snapshot **approaches:** construct *X* from high-fidelity solutions $\psi_i = \psi(\boldsymbol{\theta}_i)$ at set $\{\boldsymbol{\theta}_i\}$.

Research avenues for emulator applications in NP (I)

- Emulator uncertainties need to be robustly quantified; this should be facilitated by the extensive literature on uncertainties in the RBM.

- What are best practices for efficient implementation of NP emulators? Can we exploit MOR software libraries from other fields, such as pyMOR?

- Galerkin and variational emulators for bound-state and scattering calculations are equivalent for properly chosen test and trial basis. But [Petrov]-Galerkin emulators are more general; applications to nonlinear problems in NP can be fruitful but face challenges, e.g., hyperreduction methods need approximations that worsen accuracy and need UQ.

- Technical aspects to explore further, e.g., greedy (or active-learning) and SVD-based algorithms for choosing training points more effectively.

Research avenues for emulator applications in NP (II)

- Further applications to reactions: long-range Coulomb interactions and optical potentials beyond two-body systems; emulators for time-dependent DFT; emulators for nuclear dynamics at much higher energy scales (JLAB/EIC).

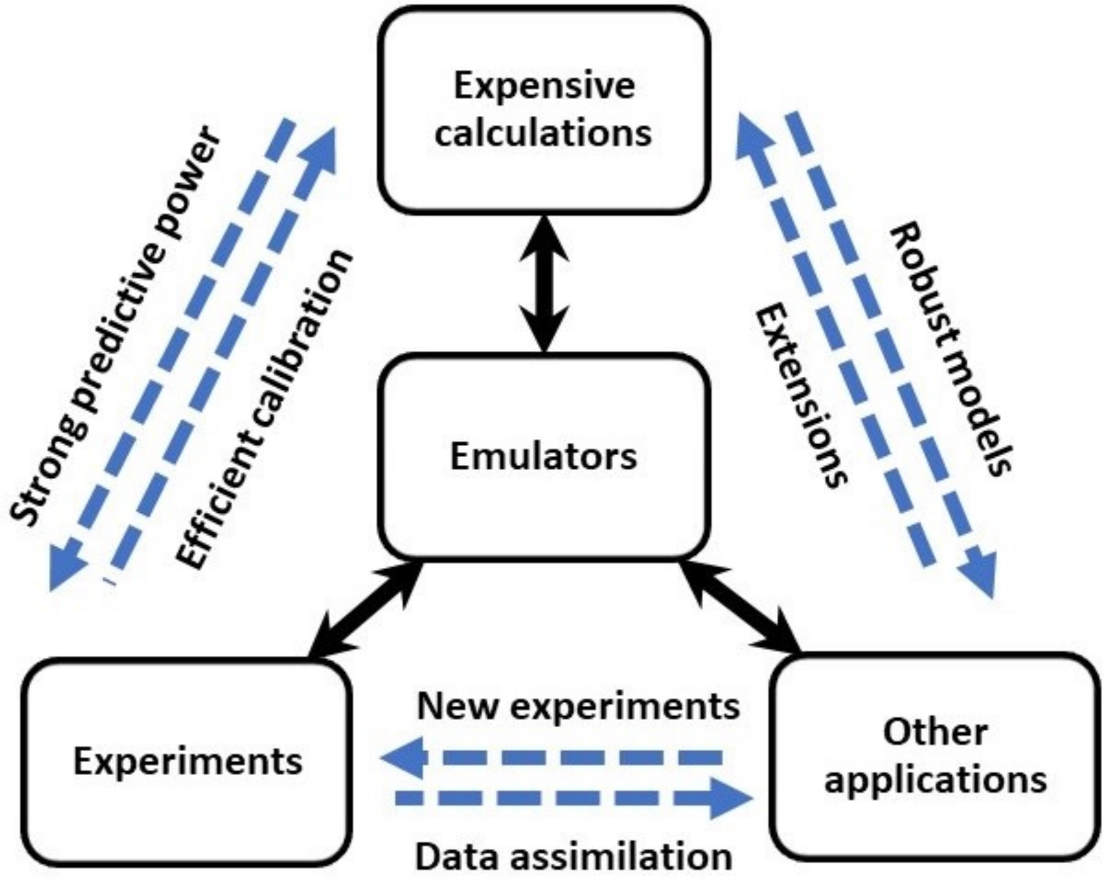
- Emulators for extrapolation far from support of training (Frame et al., 2018); emulators as resummation tool to increase convergence radius of series expansions (Demol et al., 2020); emulators to extrapolate finite-box simulations of quantum systems (Yapa and König, 2022); emulation in the complex energy plane for general quantum continuum states (Zhang, 2022).

- Exploring synergy between projection-based and machine learning methods is a new direction for MOR (e.g., POD-DL-ROM by Fresca and Manzoni, 2022).

- Can we exploit in emulator applications use of field theory and RG methods for analyzing deep neural networks (e.g., *Why is AI hard and Physics simple?* by Roberts (2021))?

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!

Thank you!

Coming attractions:

2023: Workshop on *Eigenvector continuation method in nuclear structure and reaction theory*, May 30-June 2 , at CEA, France

2023: FRIB-TA Summer School on *Practical Uncertainty Quantification and Emulator Development in Nuclear Physics*, June 26-28, at FRIB.

Jupyter and Quora *books* for nuclear applications:

Learning from Data (OSU course Physics 8820)

BUQEYE Guide to Projection-Based Emulators in Nuclear Physics

Reduced Basis Methods in Nuclear Physics

Extra slides

ANNs and GPs meet effective theories and RG

- Recent developments* merge field theory and renormalization group (RG) insights and methods to describe ANNs (e.g., *Why is AI hard and Physics simple?* by Roberts (2021)).

- Principle of *sparsity* plus effective theory approach (cf. Ising Model for counting):

$$2^{\mathcal{O}(N)} \xrightarrow[\text{locality}]{k} \mathcal{O}(N^k) \xrightarrow[\text{locality}]{\text{spatial}} \mathcal{O}(N) \xrightarrow[\text{invariance}]{\text{translational}} \mathcal{O}(1)$$

- Exploit large width limit of ANNs, in which they become GPs (via generalized central limit theorem). Finite width expansion in depth / width of network; RG flow to criticality.

- Effective [field] theory and RG approaches are natural for (nuclear) many-body theory! The perturbative approach to leading non-trivial order is like Ginzburg-Landau form.

- **Can we apply insights to emulators and forge connections with reduced basis methods?**

[*For up-to-date references, see *Structures of neural network effective theories* by Banta et al., arXiv:2305.02334.]

Lexicon for Model Order Reduction (MOR)

Term	Definition or usage
High fidelity	Highly accurate, usually for costly calculation [Full-Order Model (FOM)]
Reduced-order model	General name for an emulator resulting from applying MOR techniques.
Intrusive	Non-intrusive treats FOM as black box; intrusive requires coding.
Offline-online paradigm	Heavy compute done once (offline); cheap to vary parameters (online).
Affine	Parameter dependence factors from operators, e.g., $H(\boldsymbol{\theta}) = \sum_n h_n(\boldsymbol{\theta}) H_n$
Snapshots	High-fidelity calculations at a set of parameters and/or times.
Proper Orthogonal Decomposition (POD)	Generically the term POD is used for PCA-type reduction via SVD. In snapshot context, PCA is applied to reduce/orthogonalize snapshot basis.
Greedy algorithm	Serially find snapshot locations $\boldsymbol{\theta}_i$ at largest expected error (fast approx.).
Reduced basis methods	Or RBMs. Implement snapshot-based projection methods.
Hyper-reduction methods	Approximations to non-linearity or non-affineness (e.g., EIM).

Parametric MOR emulator workflow

Bird's eye view but still for projection-based PMOR only (i.e., not an exhaustive set!)

(1) Sampling across range of parameters θ for N_{sample} candidate snapshots → $\{\theta_i\}$

- E.g., space-filling design (like latin hypercube) or center near emulated values.
- Want $N_b \leq N_{sample}$ snapshots; locate wisely based on basis construction method.

(2) Generating a basis *X* from the snapshots to create. Multiple options, including:

- *Proper Orthogonal Decomposition* (POD) [cf. PCA] → extract most important basis vectors. Compute all N_{sample} snapshots $\psi(\boldsymbol{\theta}_i)$ but keep N_b based on SVD.
- *Greedy algorithm* is an iterative approach: next location $\boldsymbol{\theta}_i$ from *fast* estimated emulator error at N_{sample} values and choose value with largest expected error.
- For time-dependent case, sample also in time or frequency. Many options here!

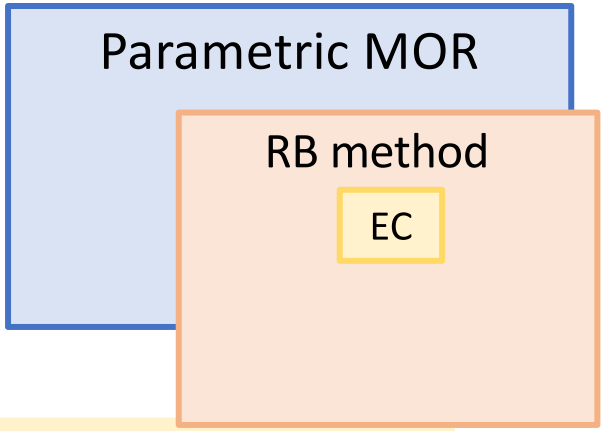
(3) Construct the reduced system. Single basis ***X*** or multiple bases across **θ**

- Linear system and affine operators → projecting to single basis works well.
- If non-linear or non-affine → *hyper-reduction* approaches: e.g., empirical interpolation method EIM or DEIM, which finds an affine (separable) expansion.

Some model reduction methods in context

Reduced Basis method (1980) widely used to emulate PDEs in reduced-order approach. Specific choices in MOR framework:

- Parameter set chosen using greedy algorithm (or POD)
- Single basis X constructed from snapshots
- RB model built from global basis projection



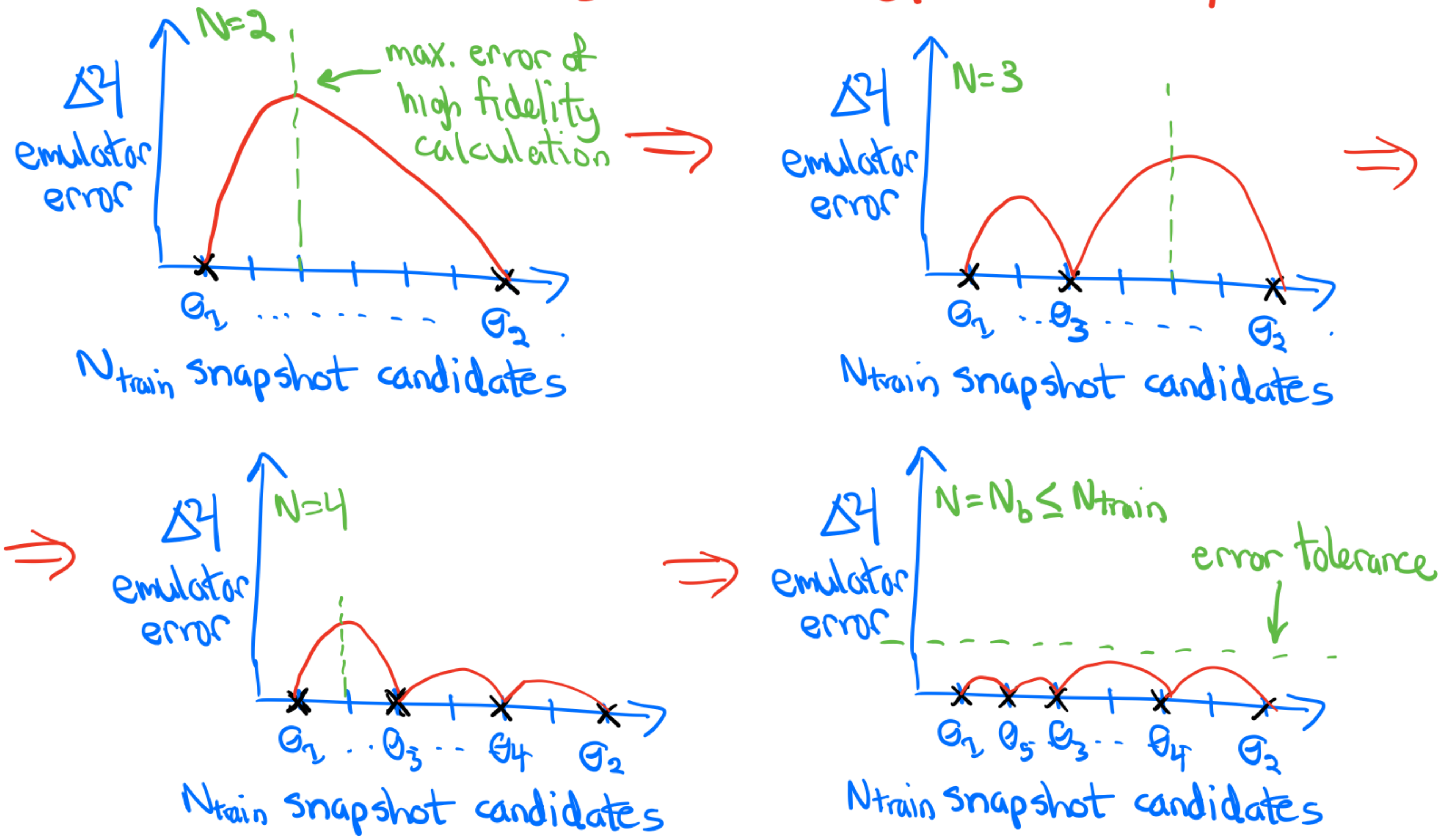
Eigenvector continuation (EC) is a particular implementation of the RB method
→ parametric reduced-order model for an eigenvalue problem (lots of prior art)

- Global basis constructed with snapshot-based POD approach
- "Active learning" by Sarkar and Lee adds greedy sampling algorithm for next $\boldsymbol{\theta}_i$

Summary: general features of *good* reduced-order emulators

- System dependent → works best when QOI lies in low-D manifold and operations on ψ can be avoided during online phase
- Relative smoothness of parameter dependence
- Affine parameter dependence (or effective hyper-reduction or other approach)

CARTOONS FOR GREEDY ALGORITHM



Stop once desired error tolerance reached (or given # steps)

Empirical interpolation method for nonaffine/nonlinear

Key: avoid costly order ψ (i.e., FOM) evaluations → approximation strategy.

- Some cases: use low-order terms of a Taylor series expansion.
- More general: selective sampling of nonlinear terms with interpolation.
- Includes empirical interpolation method (EIM) and discrete variant DEIM.

EIM basics [adapted from Hesthaven (2016)]

- Ingredients are (Q is an integer):
  - Q interpolation points $\mathbf{x}_1, \ldots, \mathbf{x}_Q$
  - Q parameter points $\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_Q$ ($\boldsymbol{\theta} \equiv \boldsymbol{\mu}$)
  - Q basis functions $h_1, \ldots h_Q$
- The function g is nonaffine in $\mathbf{x}$ and $\boldsymbol{\theta}$
- Interpolation is $I_Q[g_{\boldsymbol{\theta}}](x) = \sum_{q=1}^{Q} c_q(\boldsymbol{\theta}) h_q(x)$ where $I_Q[g_{\boldsymbol{\theta}}](x_j) = g_{\boldsymbol{\theta}}(x_j) \quad j = 1, \ldots, Q$ is found by solving
  $$\sum_{q=1}^{Q} c_q(\boldsymbol{\theta}) h_j(x_j) = g_{\boldsymbol{\theta}}(x_j) \quad j = 1, \ldots, Q$$
- The h_j are found as linear combinations of snapshots $g_{\theta 1}, \ldots, g_{\theta Q}$ (see box at right).

Algorithm: Empirical Interpolation Method

Input: A family of functions $g_\mu : \Omega \to \mathbb{R}$, parametrized by a parameter $\mu \in \mathbb{P}_{\mathrm{EIM}}$ and a target error tolerance $\mathtt{tol}$.

Output: A set of Q basis functions $\{h_q\}_{q=1}^{Q}$ and interpolation points $\{x_q\}_{q=1}^{Q}$.

Set $q = 1$. Do while $\mathtt{err} < \mathtt{tol}$:

1. Pick the sample point
$$\mu_q = \arg\sup_{\mu \in \mathbb{P}_{\mathrm{EIM}}} \left\| g_\mu - \mathrm{I}_{q-1}[g_\mu] \right\|_{\mathcal{X}_\Omega},$$
and the corresponding interpolation point
$$x_q = \arg\sup_{x \in \Omega} \left| g_{\mu_q}(x) - \mathrm{I}_{q-1}[g_{\mu_q}](x) \right|. \tag{5.5}$$
2. Define the next basis function as the scaled error function
$$h_q = \frac{g_{\mu_q} - \mathrm{I}_{q-1}[g_{\mu_q}]}{g_{\mu_q}(x_q) - \mathrm{I}_{q-1}[g_{\mu_q}](x_q)}. \tag{5.6}$$
3. Define the error
$$\mathtt{err} = \left\| \mathtt{err}_p \right\|_{L^\infty(\mathbb{P}_{\mathrm{EIM}})} \quad \text{with} \quad \mathtt{err}_p(\mu) = \left\| g_\mu - \mathrm{I}_{q-1}[g_\mu] \right\|_{\mathcal{X}_\Omega},$$
and set $q := q + 1$.

Eigenvector continuation (EC) for scattering

$$\widehat{H}(\boldsymbol{\theta}) = \widehat{T} + \widehat{V}(\boldsymbol{\theta}) = \widehat{T} + \sum_a \theta^{(a)}\mathcal{O}^{(a)} \text{ with LECs } \boldsymbol{\theta} = \{\theta^{(a)}\}$$

Affine dependence (here chiral)

K matrix: $k_\ell(E) = \tan\delta_\ell(E)$ [cf. $s_\ell(E) = e^{2i\delta_\ell(E)}$] Take $\ell = 0$ here, $p \equiv \sqrt{2\mu E}$

Kohn: $\delta\left[\frac{[k_0(E)]_{\rm trial}}{p} - \frac{2\mu}{\hbar^2}\langle\psi_{\rm trial}|\widehat{H}(\boldsymbol{\theta}) - E|\psi_{\rm trial}\rangle\right] = 0$ with $|\psi_{\rm trial}\rangle \xrightarrow[r\to\infty]{} \frac{1}{p}\sin(pr) + \frac{k_0(E)}{p}\cos(pr)$

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Could be chiral EFT or AV18 or …

K matrix: $k_\ell(E) = \tan\delta_\ell(E) \quad [\text{cf. } s_\ell(E) = e^{2i\delta_\ell(E)}] \quad \text{Take } \ell = 0 \text{ here, } p \equiv \sqrt{2\mu E}$

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EC: $|\psi_{\text{trial}}\rangle = \sum_{i=1}^{N} c_i |\psi_E(\boldsymbol{\theta}_i)\rangle \implies c_i = \sum_j (\Delta\widetilde{U})^{-1}_{ij}([k_0/p]_j - \lambda) \text{ and } \lambda = \frac{\sum_{ij}(\Delta\widetilde{U})^{-1}_{ij}([k_0/p]_j - 1)}{\sum_{ij}(\Delta\widetilde{U})^{-1}_{ij}}$

$$\text{with } \Delta\widetilde{U}_{ij}(E) \equiv \frac{2\mu}{\hbar^2}\langle\psi_E(\boldsymbol{\theta}_i)|2\widehat{V}(\boldsymbol{\theta}) - \widehat{V}(\boldsymbol{\theta}_i) - \widehat{V}(\boldsymbol{\theta}_j)|\psi_E(\boldsymbol{\theta}_j)\rangle$$

← Coulomb cancels!

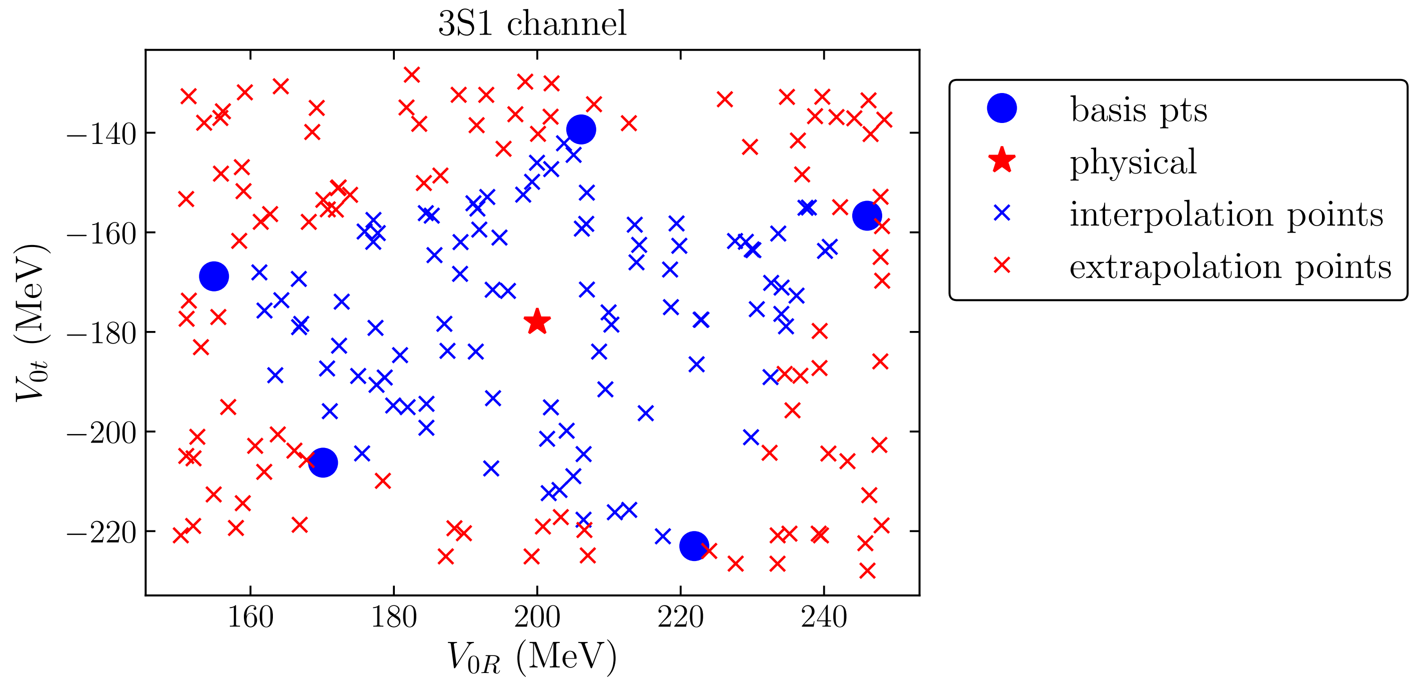
- Stationary functional for *$k_l(E)$* but not an upper (or lower bound) → still works!
- Use nugget regularization to deal with ill-conditioning and/or mix boundary conditions
- EC works for local or non-local potentials, r-space or k-space, complex potentials, 3-body
- More recent: also works for complex *E* and extrapolating in *E* *(Xilin Zhang)*

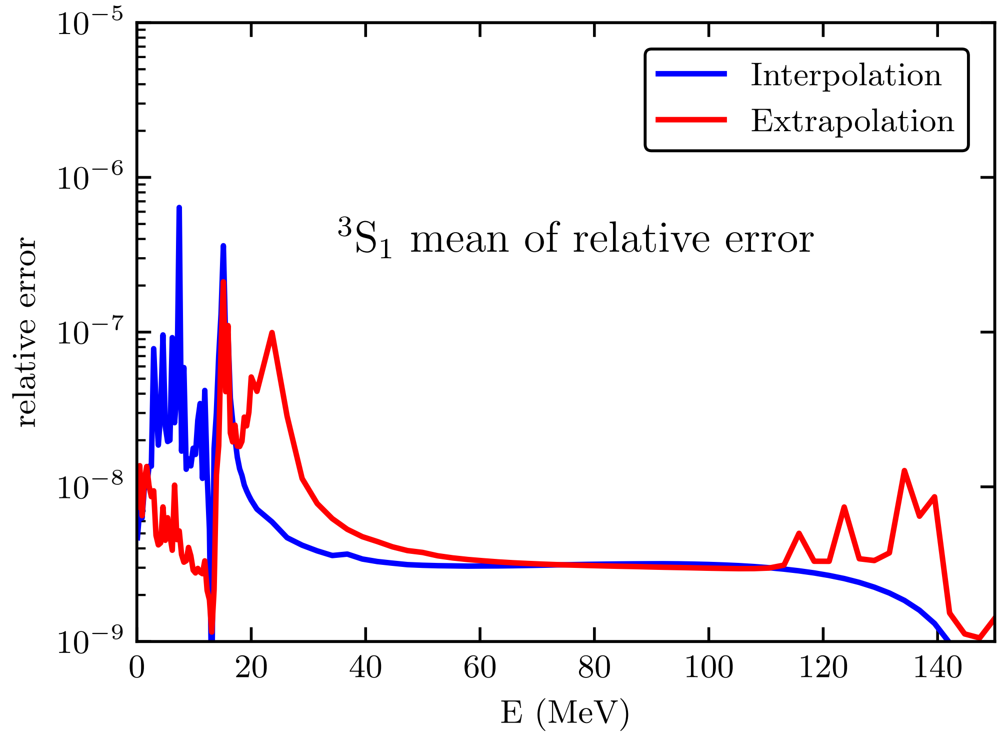
Testing eigenvector continuation (EC) for scattering

Many different model problems tested: square well, + Coulomb, Yamaguchi potential, …
→ one example: Minnesota potential in $^3S_1$ channel (other plots available with notebooks)

$$V_{^3\mathrm{S}_1}(r) = V_{0R}\, e^{-\kappa_R r^2} + V_{0t}\, e^{-\kappa_t r^2} \;\text{ with }\; \kappa_R = 1.487\,\mathrm{fm}^{-2} \kappa_t = 0.639\,\mathrm{fm}^{-2}\;\text{ (fixed)}$$

$$\boldsymbol{\theta} = \{V_{0R}, V_{0t}\} \underset{\text{“physical”}}{\longrightarrow} \{200\,\mathrm{MeV}, -178\,\mathrm{MeV}\}$$





Better: choose basis points by “greedy algorithm”

Emulating the Lippmann-Schwinger (LS) equation

LS equation:

Sets of parameters:

K-matrix formulation:

$$K(\vec{a}) = V(\vec{a}) + V(\vec{a})\, G_0(E_q)\, K(\vec{a}) \rightarrow \{\vec{a}_i\} \rightarrow K_\ell(E_q) = -\tan\delta_\ell(E_q)$$

$$E_q = q^2/2\mu$$

Newton variational principle (NVP):

$$\tilde{K}(\vec{\beta}) = \sum_{i=1}^{n_t} \beta_i K_i \longrightarrow \mathcal{K}[\tilde{K}] = V + VG_0\tilde{K} + \tilde{K}G_0V - \tilde{K}G_0\tilde{K} + \tilde{K}G_0VG_0\tilde{K}$$

$$\mathcal{K}[K_{\text{exact}} + \delta K] = K_{\text{exact}} + (\delta K)^2$$

Implementation:

$$\langle\phi'|\mathcal{K}(\vec{a},\vec{\beta})|\phi\rangle = \langle\phi'|V(\vec{a})|\phi\rangle + \vec{\beta}^T\vec{m}(\vec{a}) - \frac{1}{2}\vec{\beta}^T M(\vec{a})\vec{\beta}$$

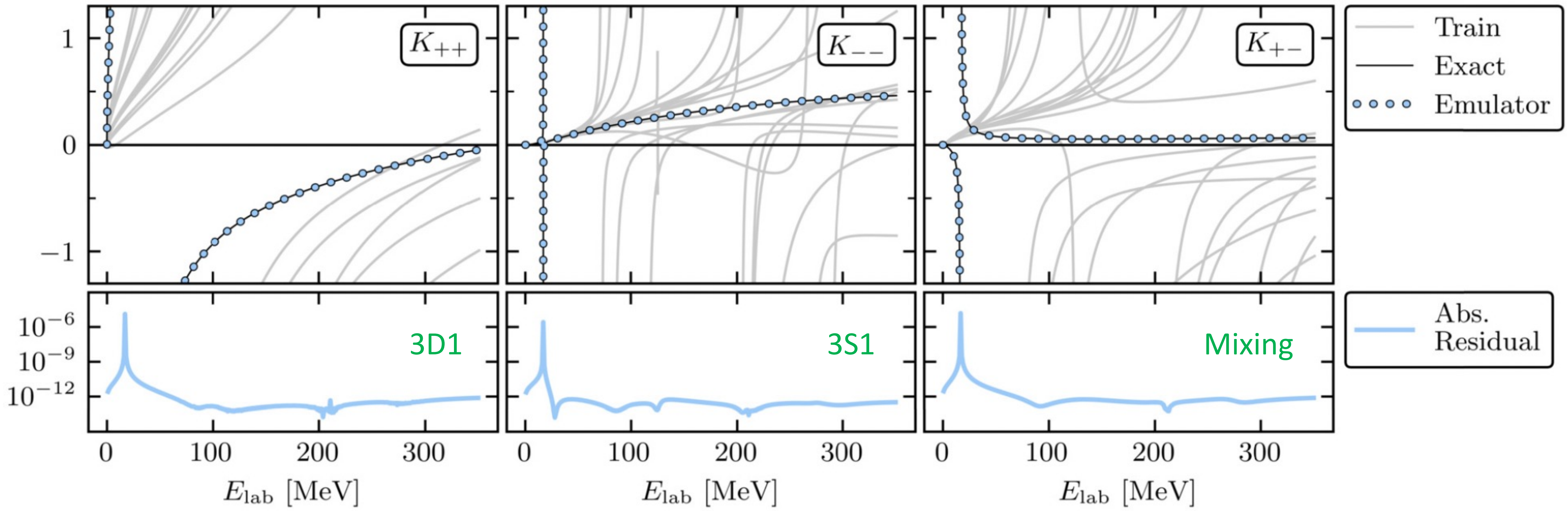
$$\frac{d\mathcal{K}}{d\vec{\beta}} = 0 \rightarrow \langle\phi'|\mathcal{K}(\vec{a},\vec{\beta})|\phi\rangle \approx \langle\phi'|V(\vec{a})|\phi\rangle + \frac{1}{2}\vec{m}^T M^{-1}(\vec{a})\,\vec{m}$$

J. A. Melendez et al., Phys. Lett. B 821, 136608 (2021)

NVP emulation: SMS chiral potential

- Emulation of 3S1-3D1 coupled channel
- Basis size of 12 at $\mathrm{N^4LO+}$

Dealing with anomalies/singularities: C. Drischler et al., arXiv: 2108.08269 (2021)



J. A. Melendez et al., Phys. Lett. B 821, 136608 (2021)