Fast & accurate emulators for two- and three-body scattering

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Next generation *ab initio* nuclear theory

ECT* workshop | July 15, 2025

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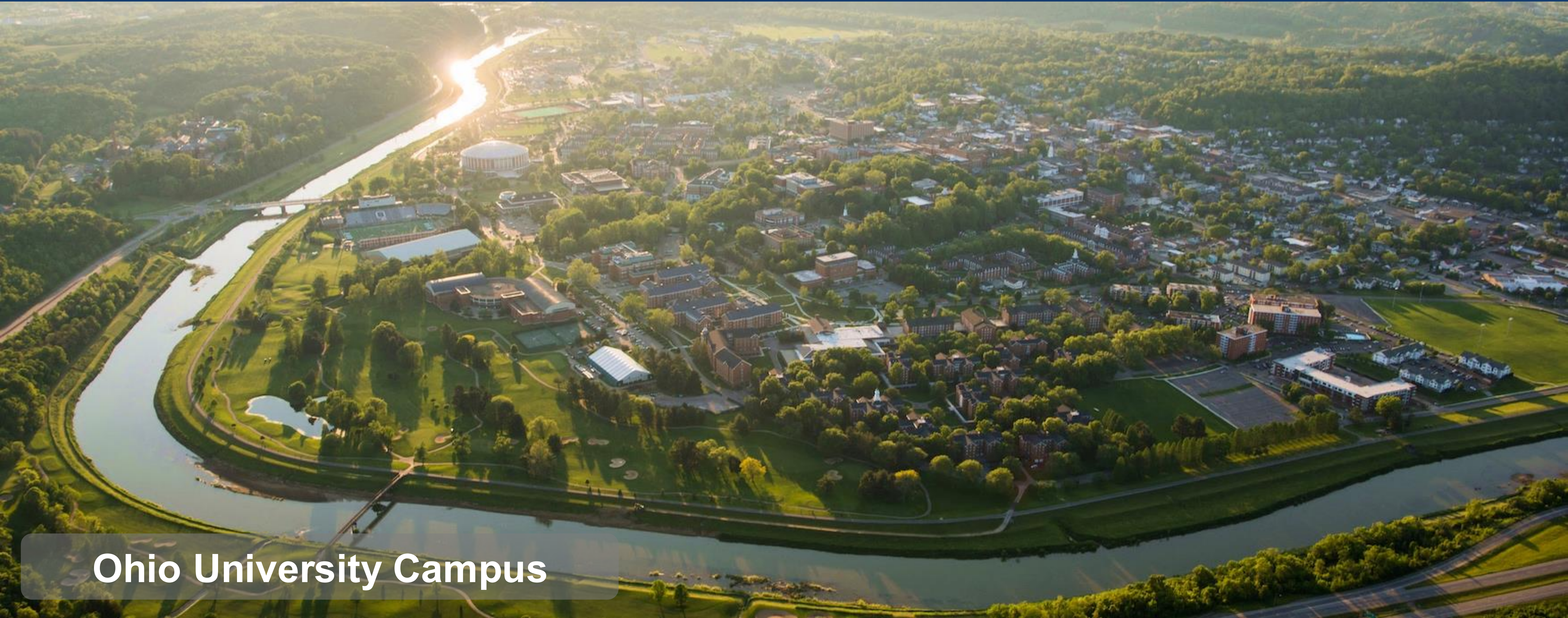

Outline

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Introduction / Motivation: **mining scattering data**

- Emulators facilitate principled UQ of (chiral) NN+3N interactions

Emulators for two-body scattering

- Prototype for Parametric MOR: methods and terminology
  - Variational calculation and **Petrov-Galerkin projections**
  - Training algorithms: POD vs **greedy algorithm (with error estimation)**
  - Efficient offline-online decomposition
  - Kohn anomalies: what they are and how to remove them
- **Applications:** scattering phase shifts and cross sections

STREAMLINE
SmarT Reduction and Emulation Applying Machine Learning In Nuclear Environments

Emulators for three-body (*N*-*d*) scattering

- **Preliminary results** below the deuteron-breakup threshold

Motivation: mining scattering data

See the talk "Experiments to explore three-nucleon forces" by Kimiko Sekiguchi

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Scattering experiments yield invaluable data for calibrating, validating, and improving chiral EFT (and optical models)

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

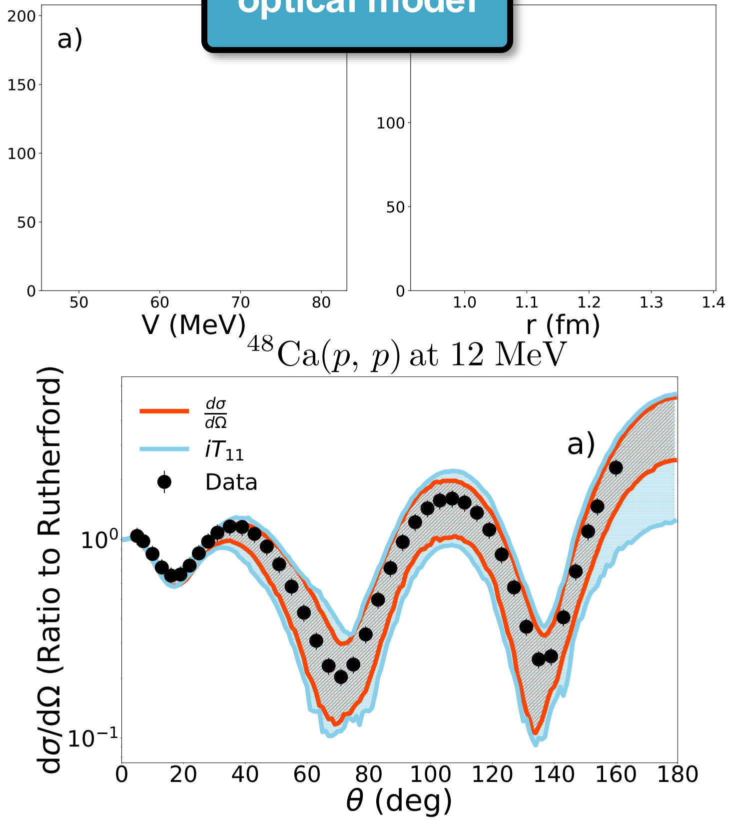
see, *e.g.*, Yang, Ekström *et al.*, arXiv:2109.13303
Furnstahl, Hammer, Schwenk, Few Body Syst. **62**, 72

Bayesian methods have become standard for principled UQ in nuclear physics:

- parameter estimation
- model comparison
- sensitivity analysis
- ...

BUQEYE
Chalmers
ISNET

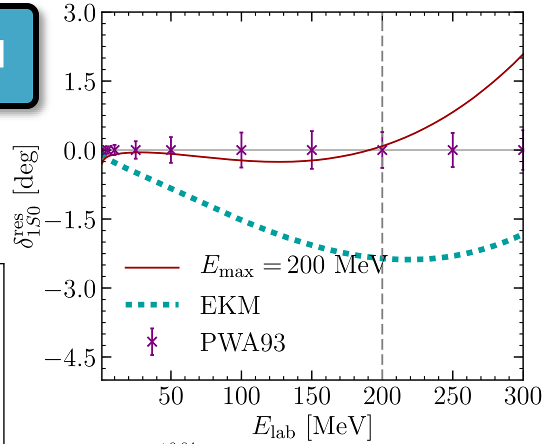
optical model

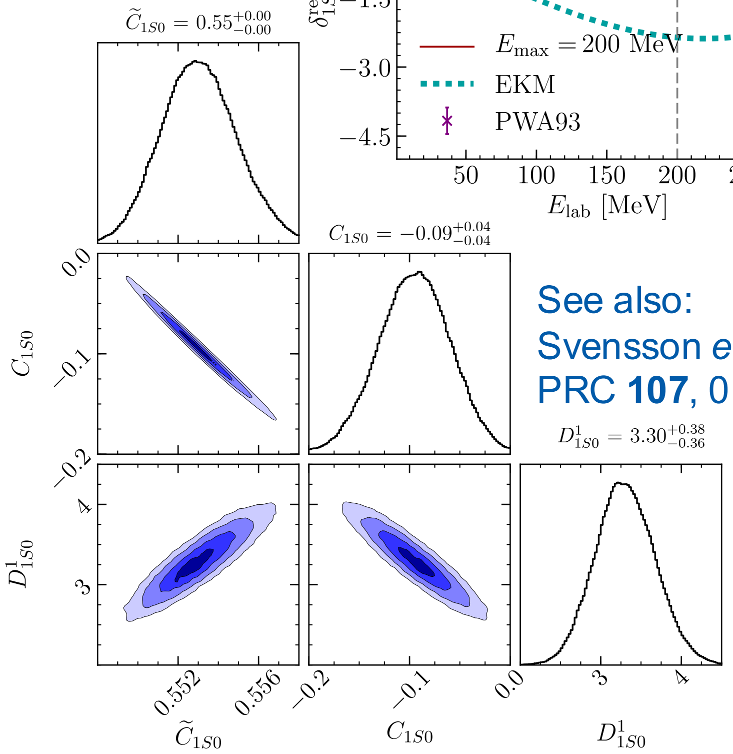


Catacora-Rios, King *et al.*, PRC **104**, 064611

chiral potential

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





See also: Svensson *et al.*, PRC **107**, 014001

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

Construct emulators by removing superfluous information

Bayesian parameter estimation

$\boldsymbol{\theta}$ parameter vector

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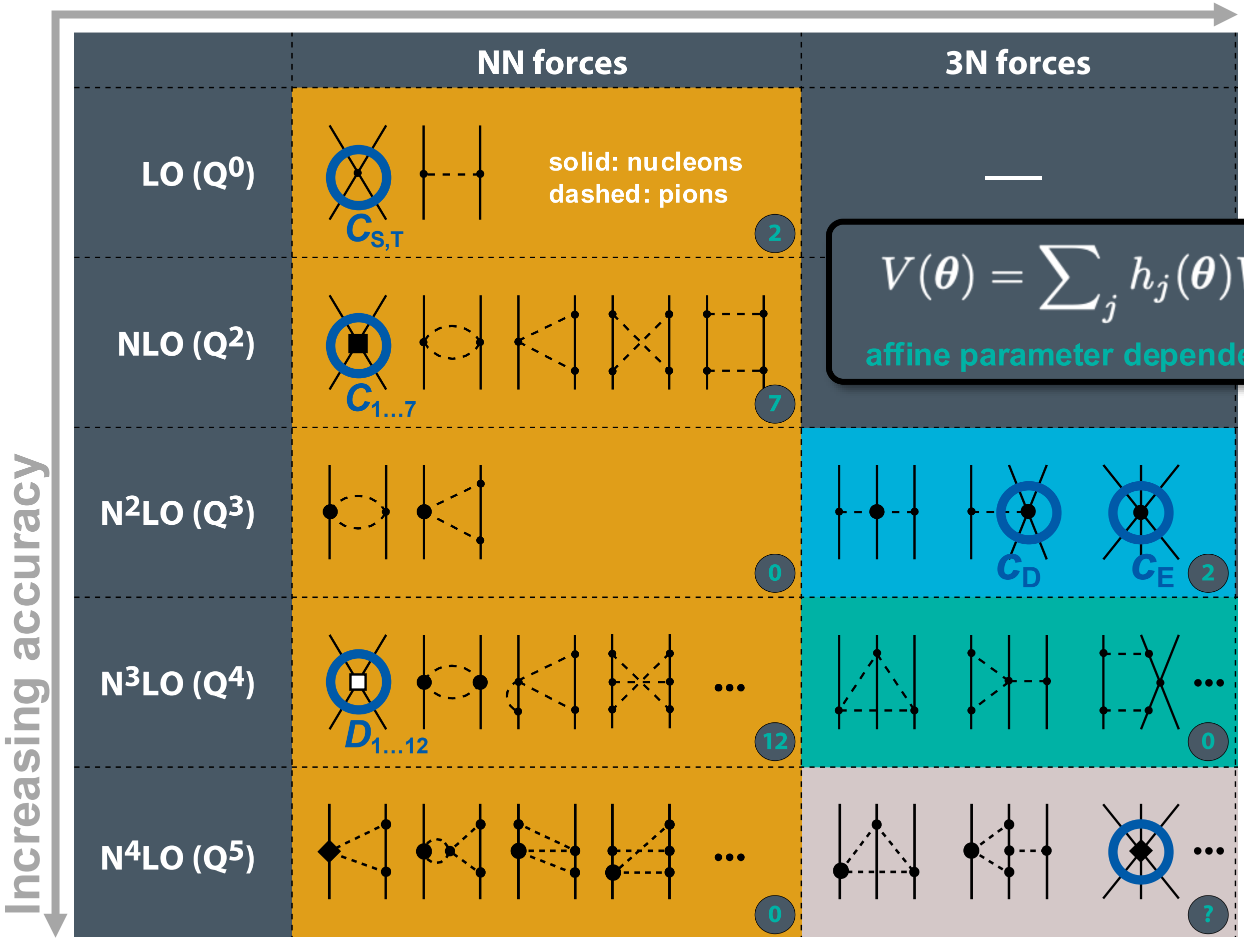
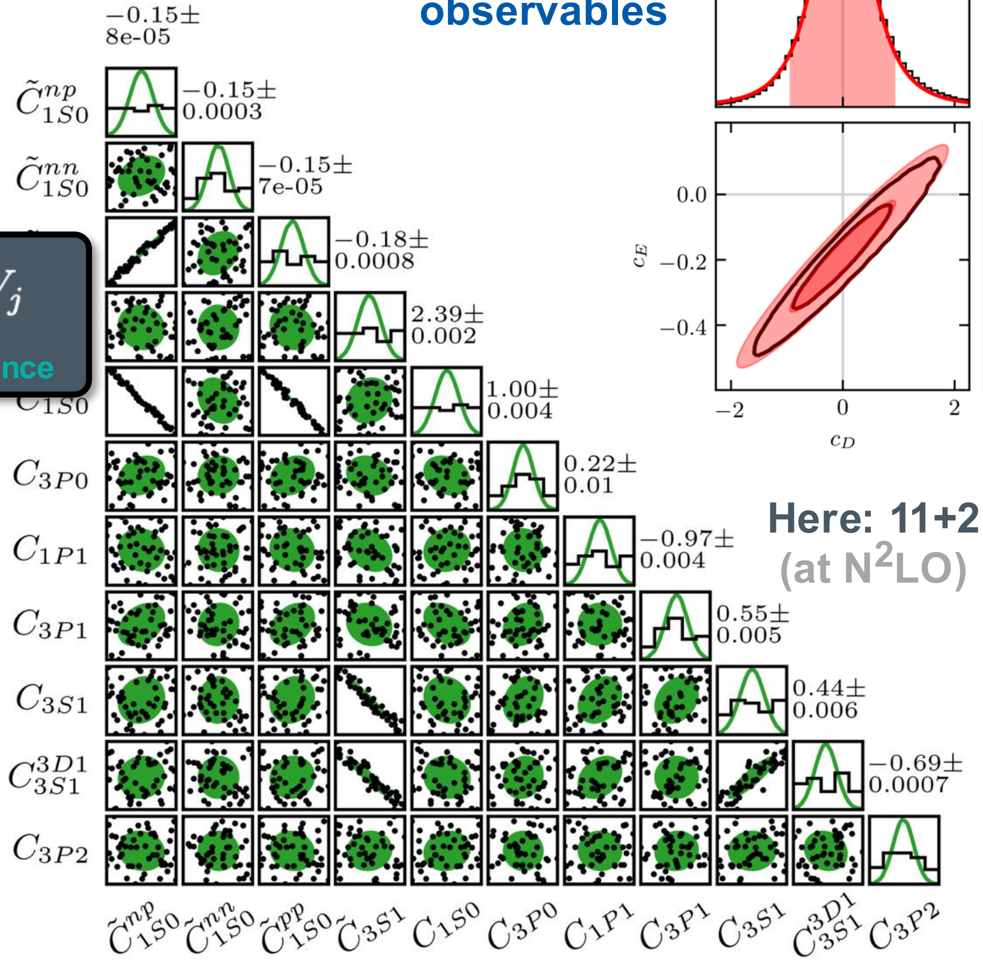
Systematic **EFT expansion of nuclear interactions**, with *many* parameters to be determined (**distribution functions**!)

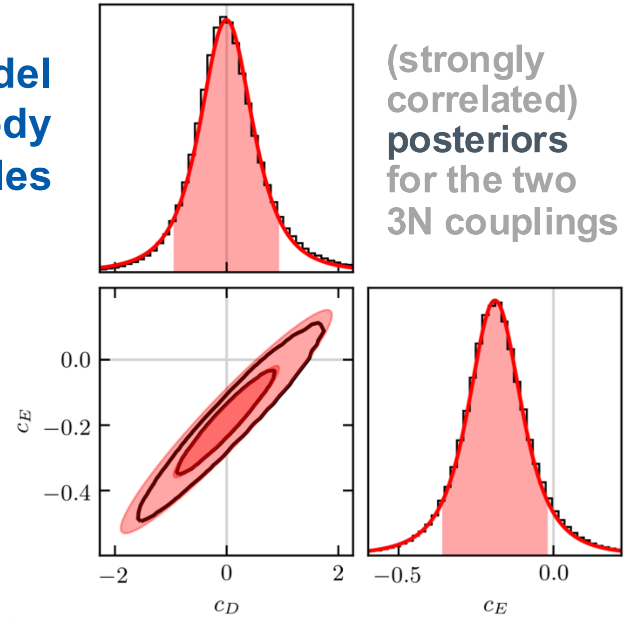


$$V(\boldsymbol{\theta}) = \sum_j h_j(\boldsymbol{\theta}) V_j$$

affine parameter dependence

Bayesian fits of model parameters to few-body observables





(strongly correlated) **posteriors** for the two 3N couplings

Here: 11+2 parameters (at N^2LO)

but typically closer to 30 parameters

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Krebs, Machleidt, Meißner, ...

Wesolowski, Svensson *et al.*, PRC **104**, 064001
Svensson, Ekström, Forssén, PRC **107**, 014001 & PRC **109**, 064003

Bayesian parameter estimation

$\boldsymbol{\theta}$ parameter vector

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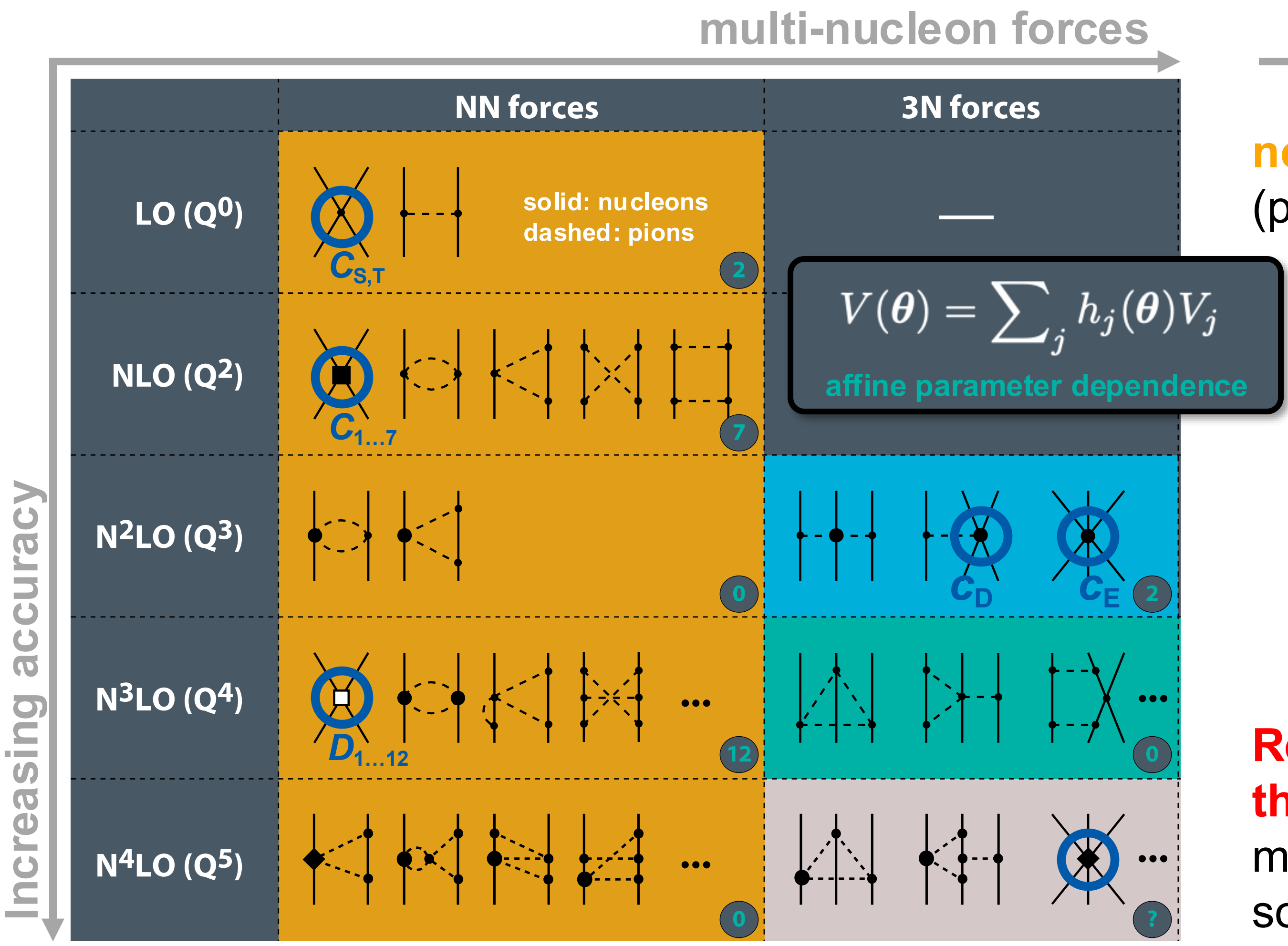
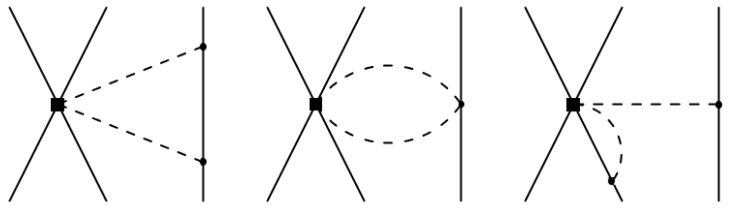
Systematic **EFT expansion of nuclear interactions**, with many parameters to be determined (**distribution functions**!)



Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Krebs, Machleidt, Meißner, ...

More on 3N forces

new loop contributions to 3N forces recently identified (promoted to N^{3}LO from N^{5}LO in WPC)



D_2, F_2, E_2

2π-exchange interactions induced by insertions of the D_2 operator

Cirigliano, Dawid, Dekens, Reddy, arXiv:2411.00097 (PRL in press)

Recent progress on deriving and implementing the 13+ 3N contact interactions at N^{4}LO, motivated by obtaining higher accuracy, solving the A_y puzzle, …

See Maria Dawid's *Rising Researchers* seminar online

Reduced Order Models (ROMs)

Many emulator applications:
many-body accelerators, nuclear properties, reactions, accelerator physics, EOS, many-body accelerators, …

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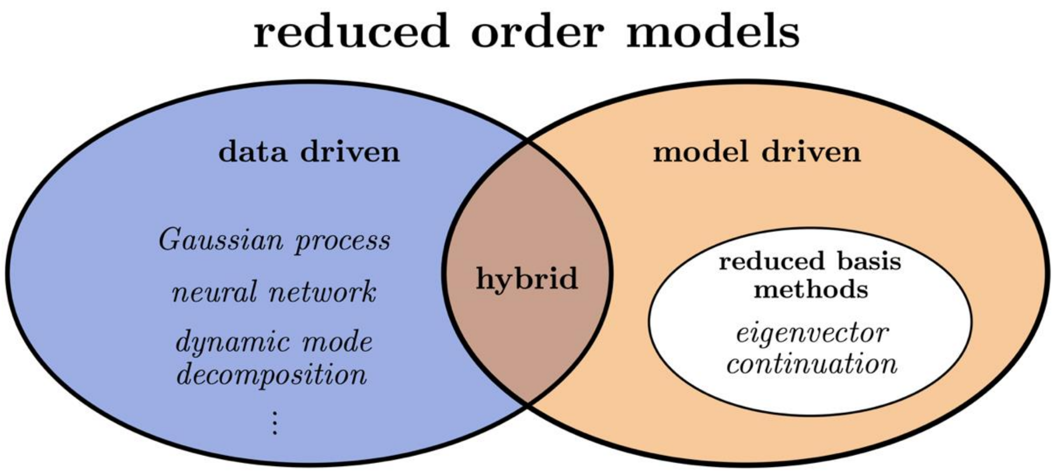
Data-driven:
interpolate output of **full-order model (FOM)** calculations (non-intrusive)



Duguet, Eström, Furnstahl, König, Lee, RMP **96**, 031002

Model-driven:
derive ROM equations from **full order model (FOM)** equations (intrusive)

often, via subspace projections; enables **extrapolation**

FOM (or high-fidelity) solver required

Hybrid: e.g., Parametric Matrix Models

ROMs are *game changers* in enabling otherwise impossible nuclear physics calculations for UQ and more

RBM for eigenvalue problems reinvented in the last few years, coined **Eigenvector Continuation (EC)** Frame *et al.*, PRL **121**, 032501 (2017)

Mini-apps: **fast & accurate model predictions without having expert knowledge and closed-source code**

Emulator (here: Petrov-Galerkin ROMs)

Low-dimensional *surrogate models* that can approximate high-fidelity model calculations with high accuracy at a small computational cost.

Recent emulator applications include:
Cook *et al.*, Nature Commun. **16**, 5929
Reed *et al.* ApJ **974** 285
Somasundaram *et al.*, PLB **866**, 139558

Constructing ROMs: Variational & Galerkin Projections

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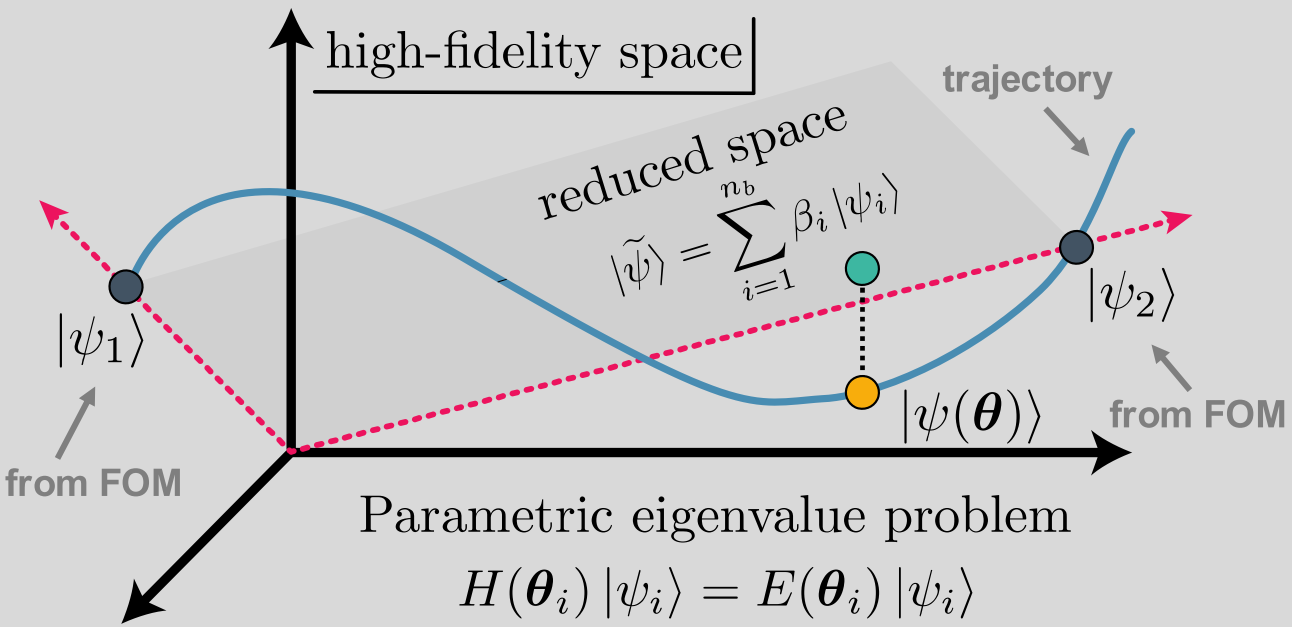

Parametric eigenvalue problem

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

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

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

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

Other choices possible → Petrov-Galerkin ROM

Variational Approach

Functional:

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

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

Find stationary point of the functional

Reduced Order Model

$\widetilde{H}(\boldsymbol{\theta})\boldsymbol{\beta} = \widetilde{E}(\boldsymbol{\theta})\widetilde{N}\boldsymbol{\beta}$	**generalized eigenvalue problem**
$\widetilde{H}(\boldsymbol{\theta}) = \boldsymbol{X}^\dagger H(\boldsymbol{\theta})\boldsymbol{X}$	**projected Hamiltonian**
$\widetilde{N} = \boldsymbol{X}^\dagger\boldsymbol{X}$	**norm matrix**
$\boldsymbol{X} = [\psi_1\ \psi_2\ \ldots\ \psi_{n_b}]$	**snapshots**

Emulator basis construction

Maldonado, CD, Furnstahl *et al.*,
arXiv:2504.06092 (PRC in press)

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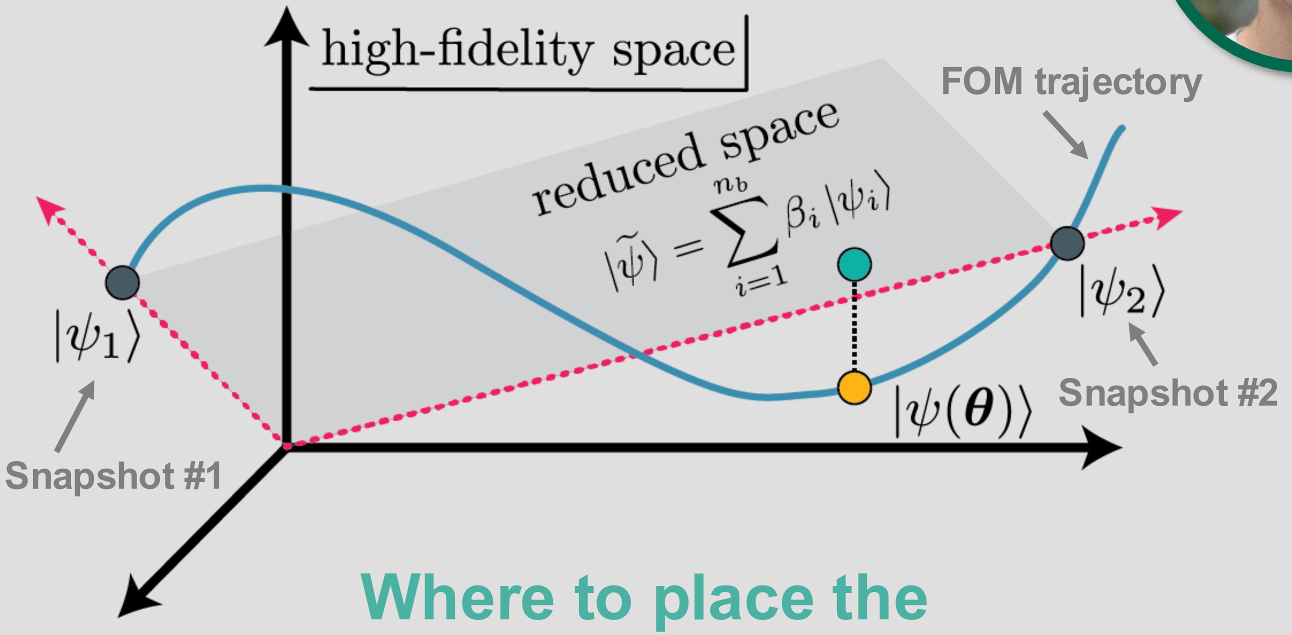
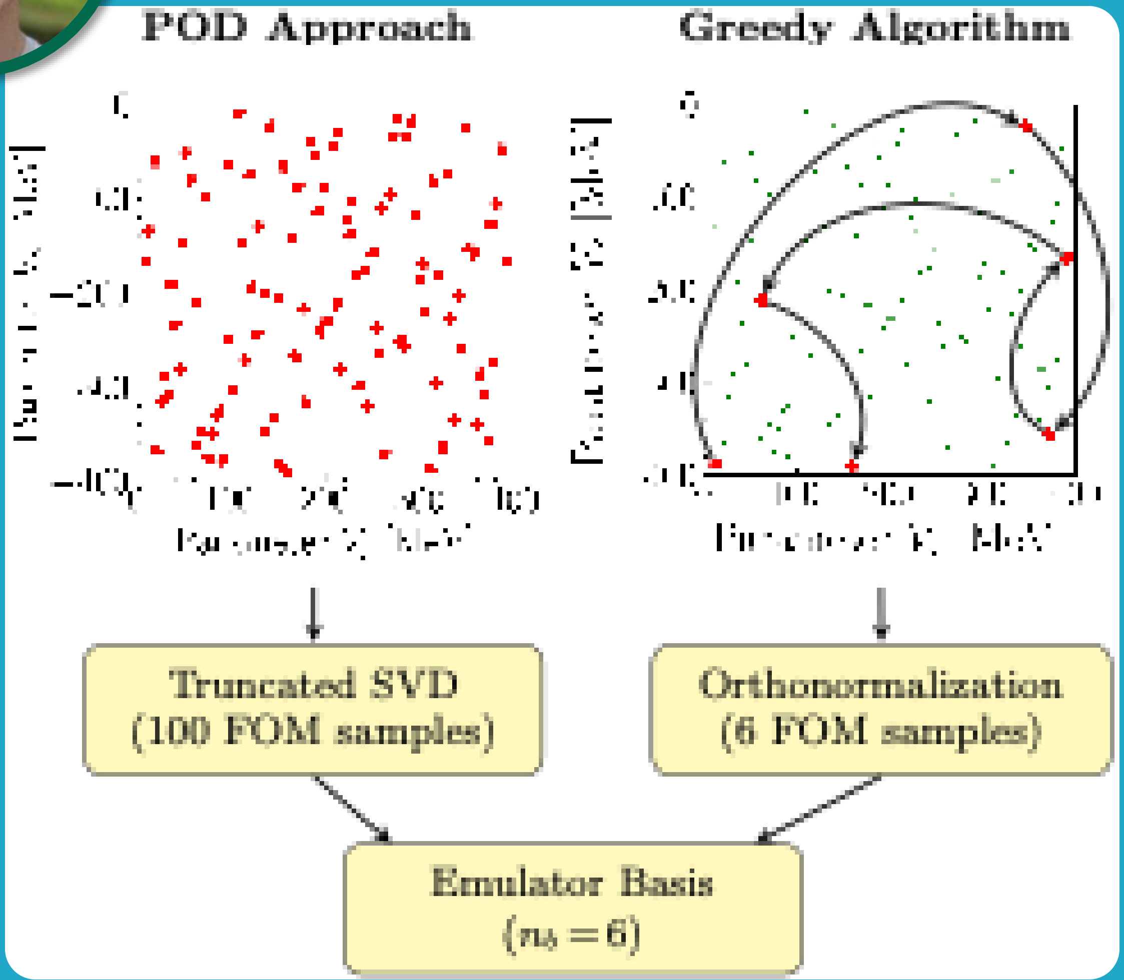


Where to place the emulator's *snapshots*?

1. **Space-filling sampling** combined with a **Proper Orthogonal Decomposition (POD)**
2. **Active learning** approach based on **error estimation** and a ***greedy algorithm***

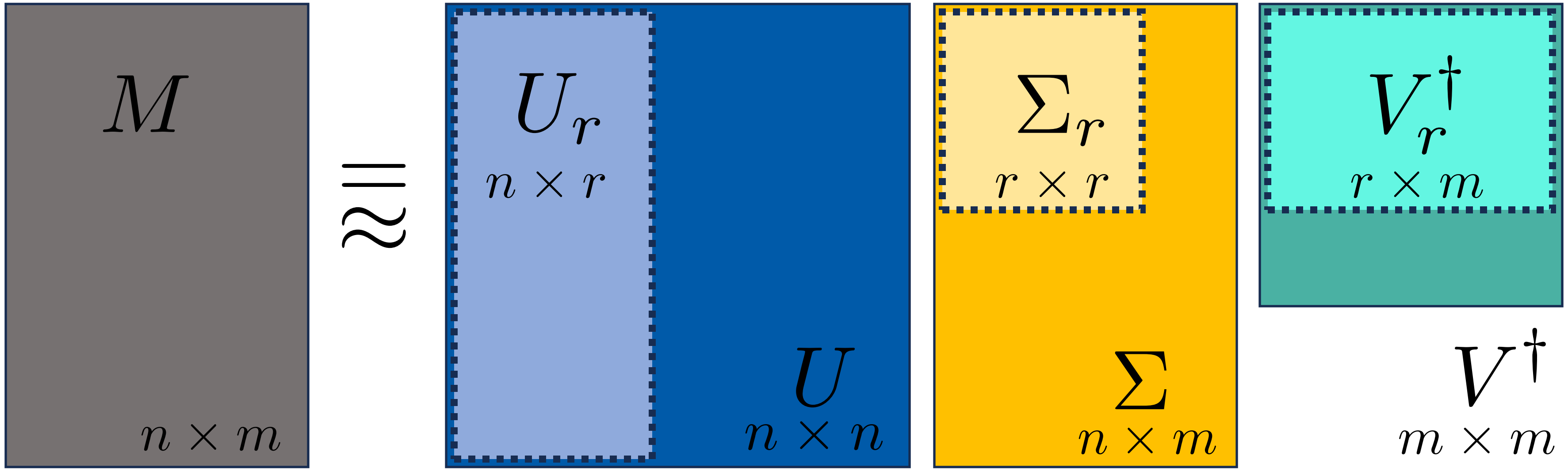
See also: Sarkar & Lee, PRR **4**, 023214 ; Bonilla *et al.*, PRC **106**, 054322



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.*, $UU^\dagger = U^\dagger U = \mathbb{1}$) 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

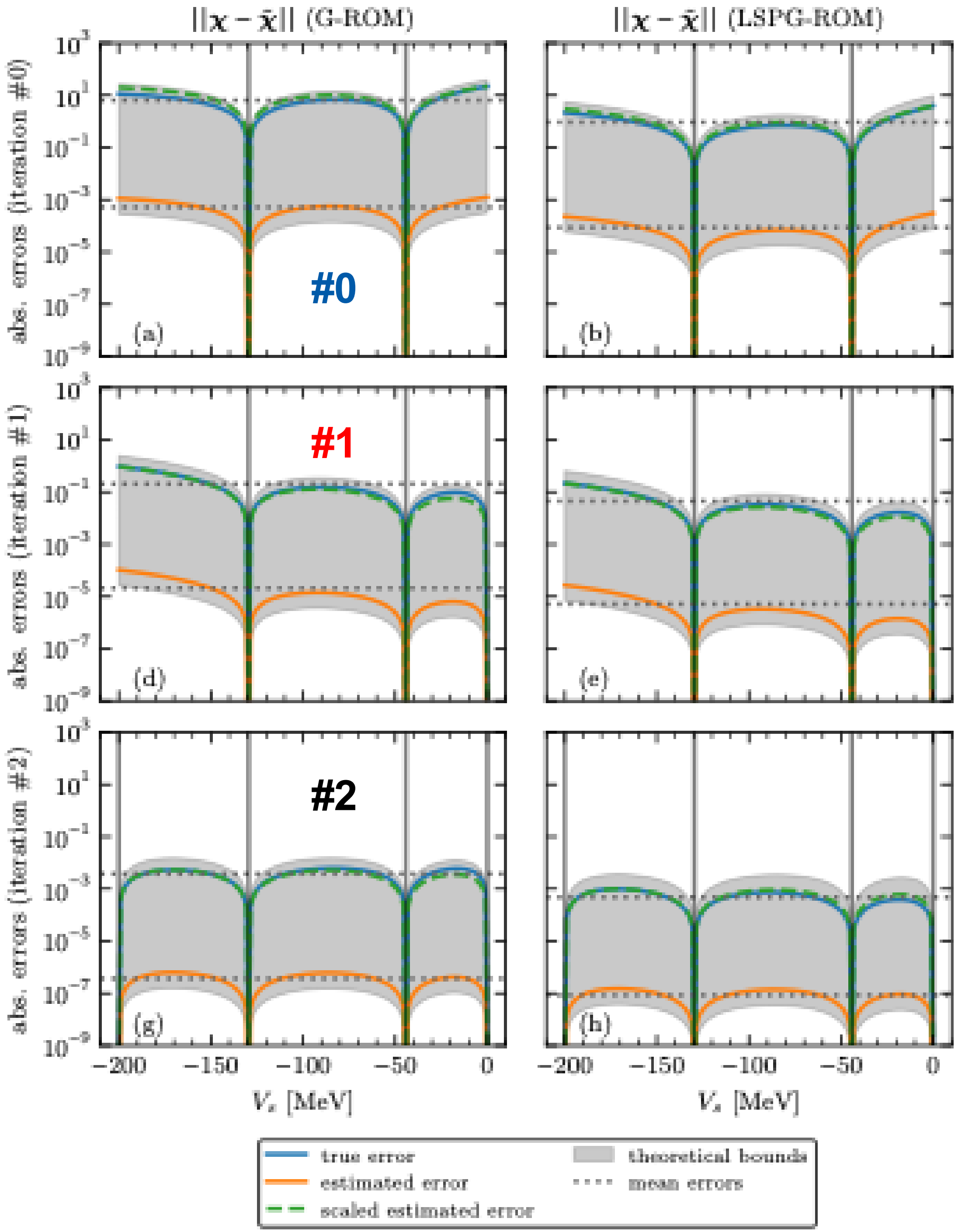
Estimate the emulator error across the parameter space

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

Iterate until the *requested* accuracy is obtained

(1D problem for illustration)

Greedy **Iteration increasing accuracy**



Reduced order models: (Petrov-)Galerkin projections

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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

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

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:

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

Reduced matrix

Least-Squares Petrov-Galerkin (LSPG) ROM

Reduction:
Projection:

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

$$Y = \left[A_1X \quad \cdots \quad A_{n_\theta}X \quad b_1 \quad \cdots \quad b_{n_\theta}\right]$$

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

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

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:

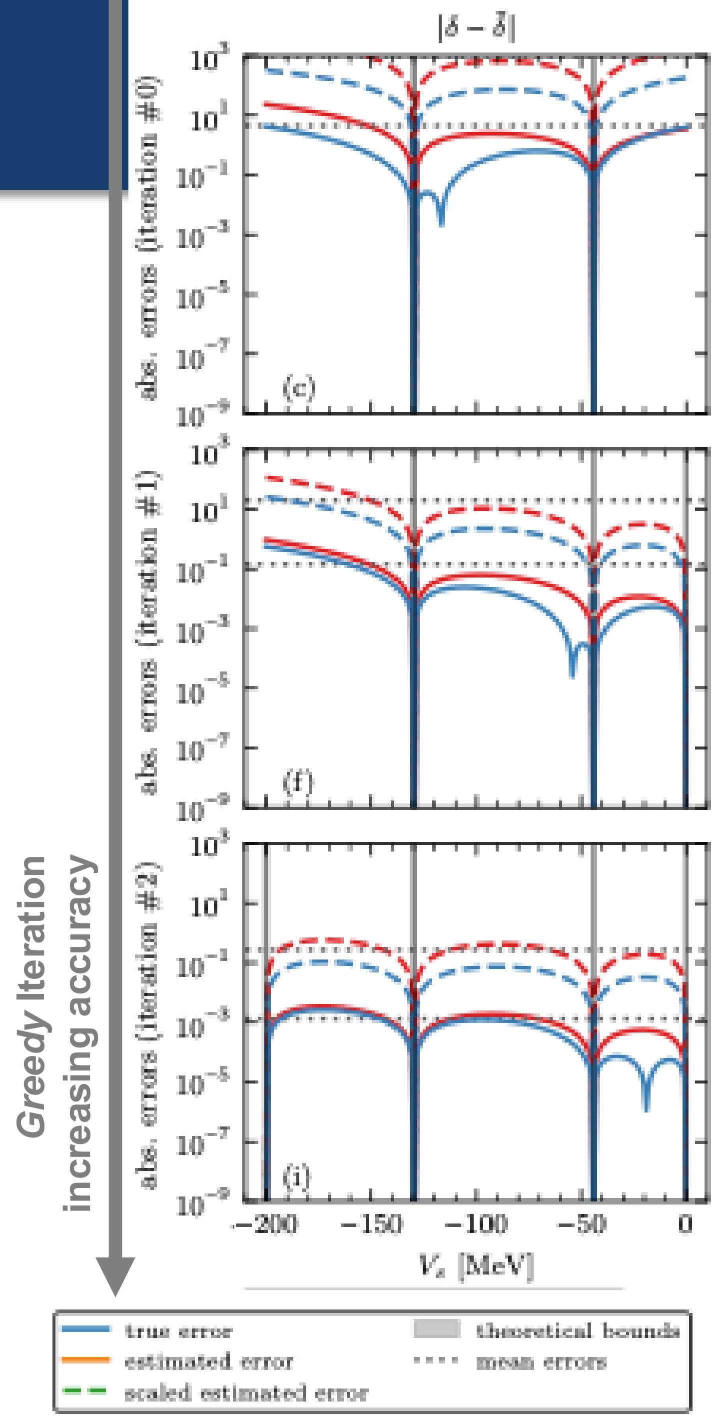
- **estimate the extremal singular values** using the Successive Constraint Method (SCM)
- use the *upper bound* as a conservative error estimate

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, CD, Furnstahl *et al.*,
arXiv:2504.06092 (PRC in press)

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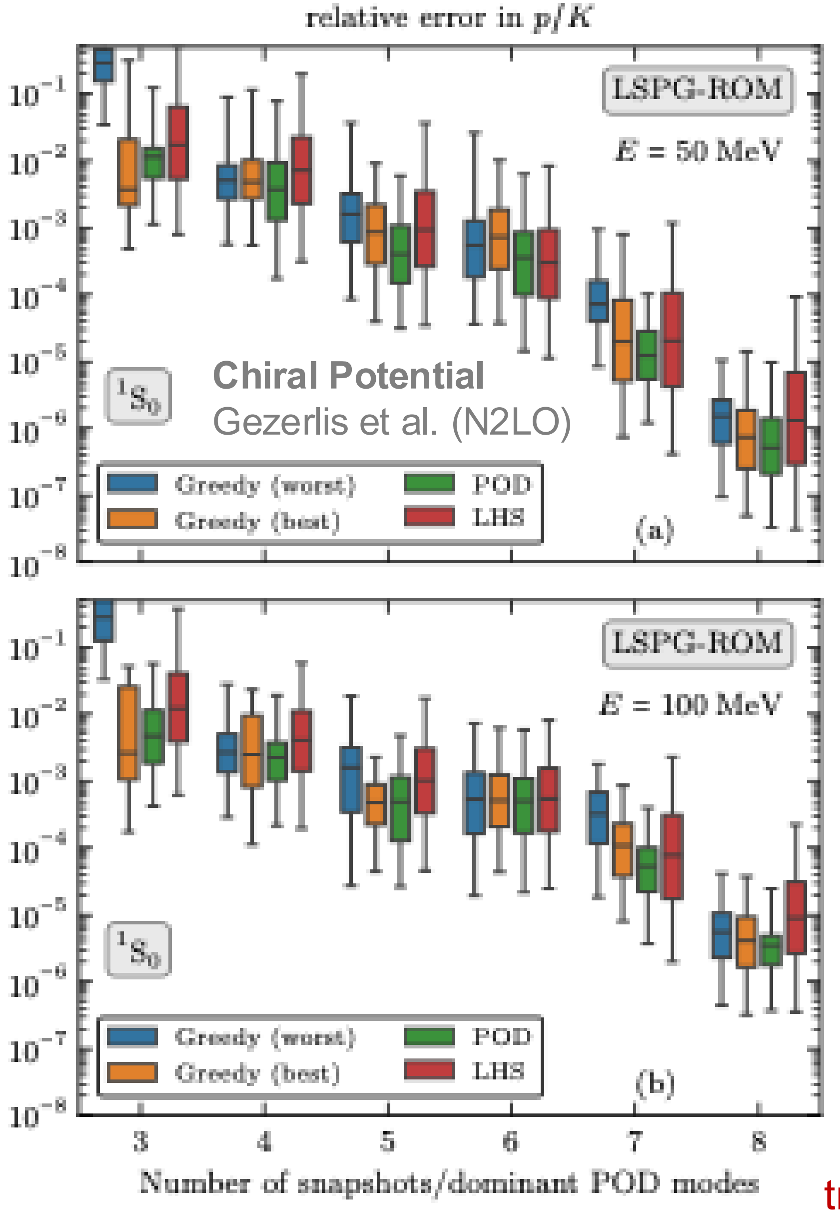
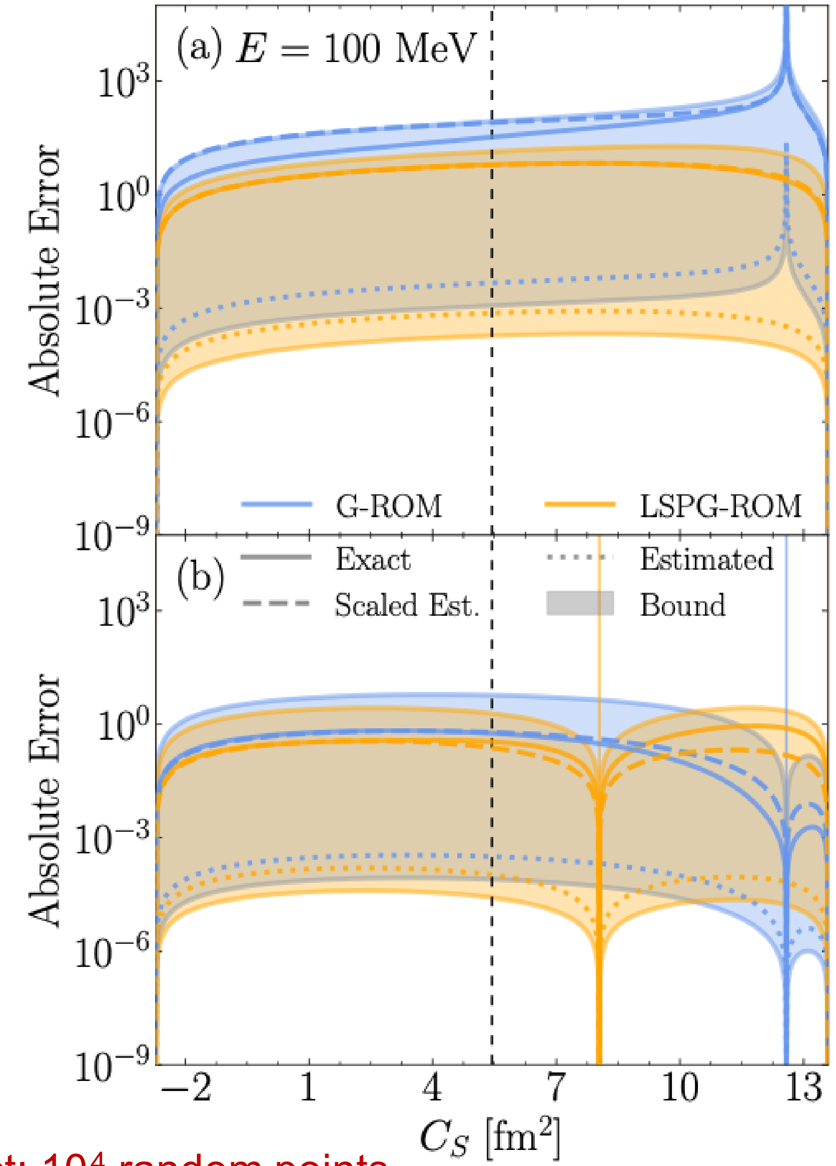


POD obtains high *accuracy* as it has access to the most information. **But: expensive!**

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)



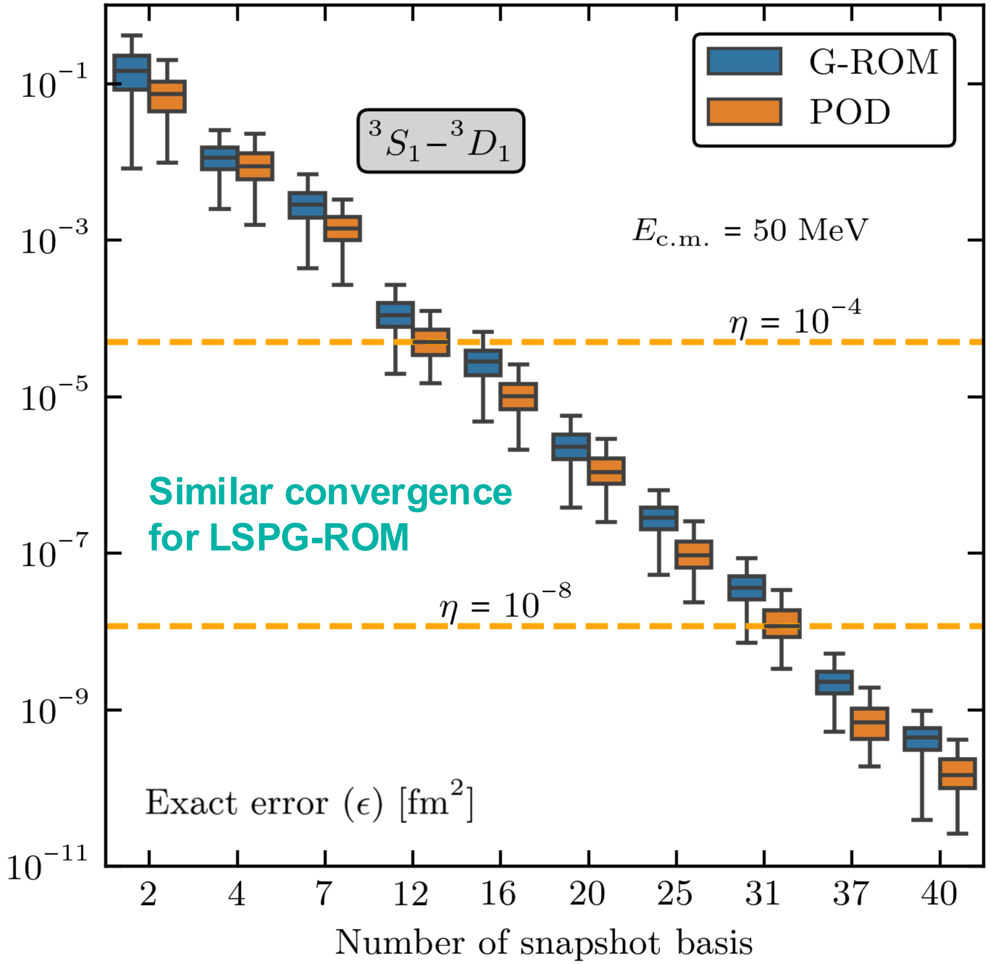
training set: 200 random points, validation set: 10^4 random points

Work in progress

Giri, Kim, CD, Elster, Furnstahl *et al.*, in prep.

$$T^{j}_{\ell\ell'}(k,k';E) = V^{j}_{\ell\ell'}(k,k') + \sum_{\ell''} \lim_{\varepsilon\to 0} \int_0^\infty dk''\, k''^2 \frac{V^{j}_{\ell\ell''}(k,k'')T^{j}_{\ell''\ell'}(k'',k';E)}{E - E'' + i\varepsilon}$$

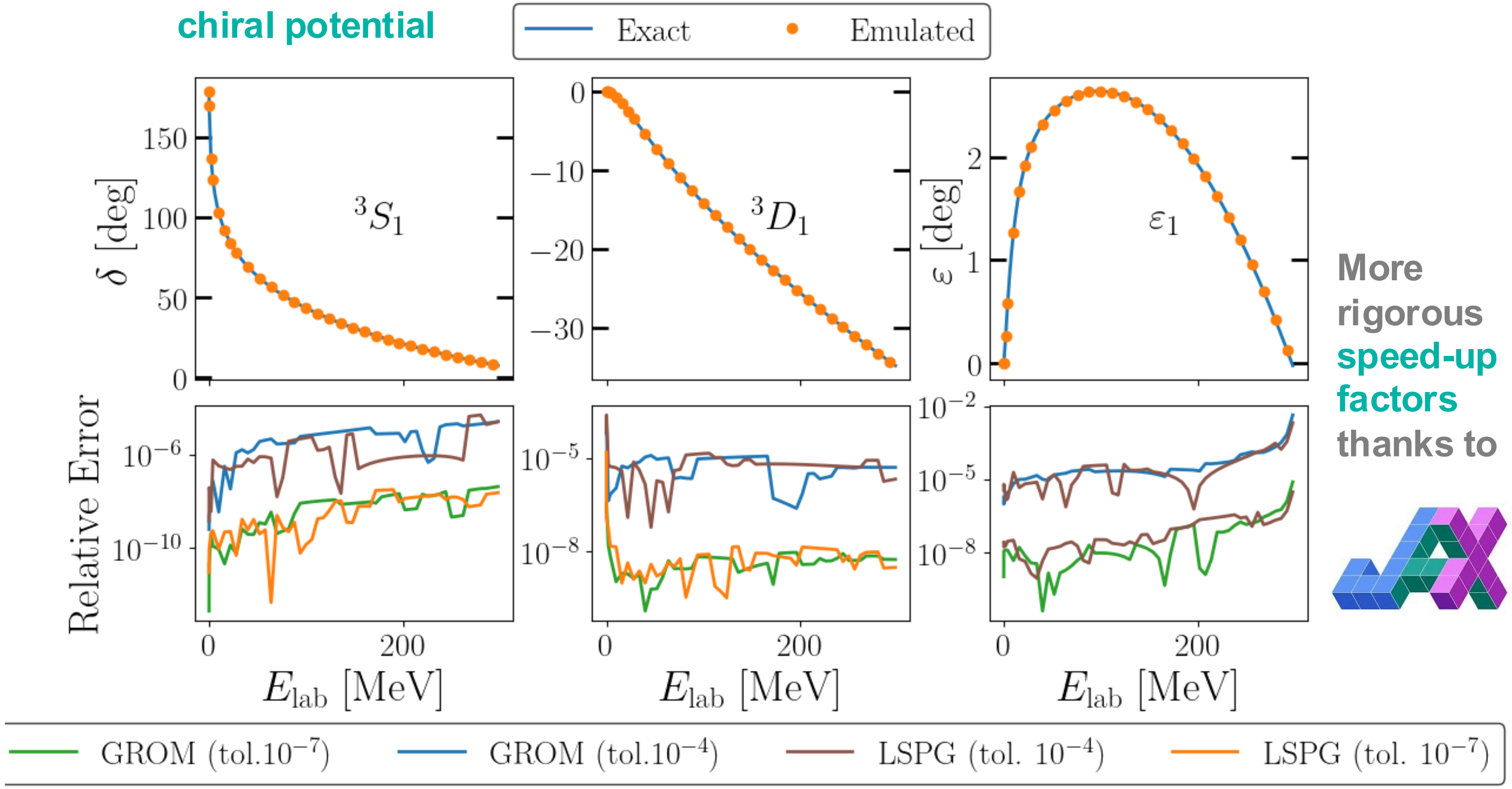
Lippmann-Schwinger (integral) equation



Similar convergence for LSPG-ROM

Extension to coupled channels & momentum space in progress (via scattering *T*-matrix equation)

Local N^{2}LO GT+ chiral potential



More rigorous **speed-up factors** thanks to

Variational ROMs for two-body scattering

Codes (Jupyter notebooks) publicly available!

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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 momentum space & coupled channels

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: parameter estimation

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 momentum space | 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 snapshot-based trial wave functions for ROMs

progress

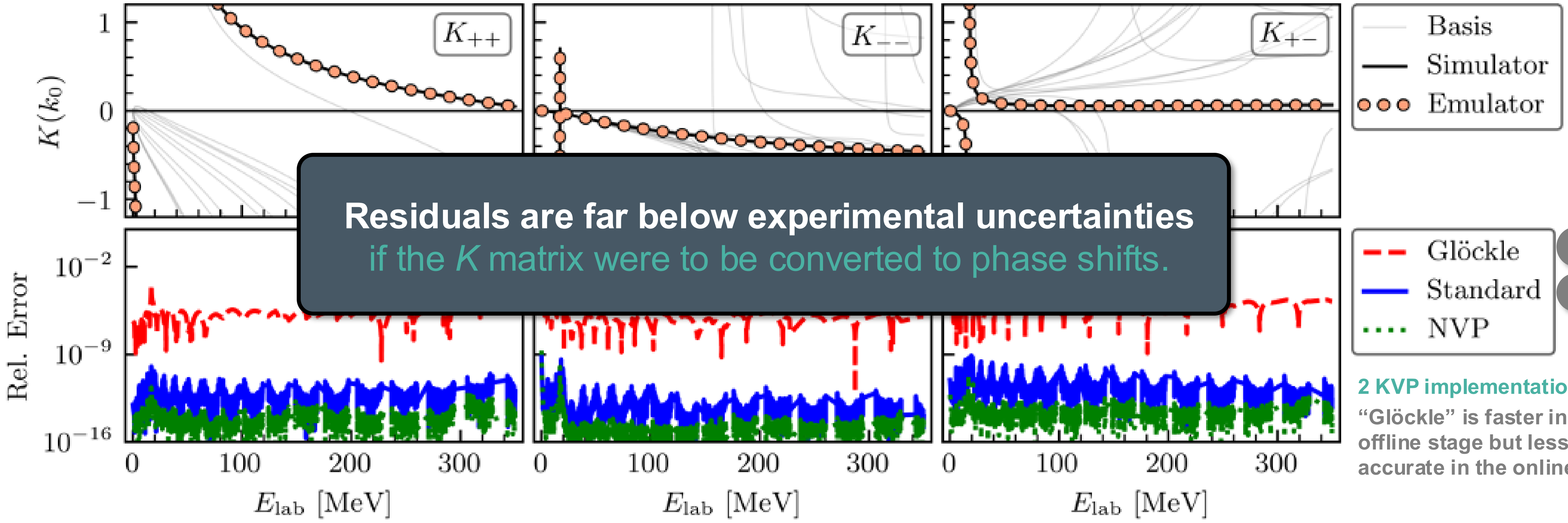
See also: CD, Melendez, Garcia, Furnstahl, and Zhang, Front. Phys. **10**, 92931 | see also ROSE in Odell *et al.*, PRC **109**, 044612

Emulating the on-shell K matrix

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

(Snapshot-based) KVP extended to
- momentum space Kohn, PR **84**, 495 (1951)
- 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.

2 KVP implementations:
"Glöckle" is faster in the offline stage but less accurate in the online stage

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 sampled in the range [-5, +5] in the units used in the potential

Kohn Variational Principle (MS)

Emulating total cross sections

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

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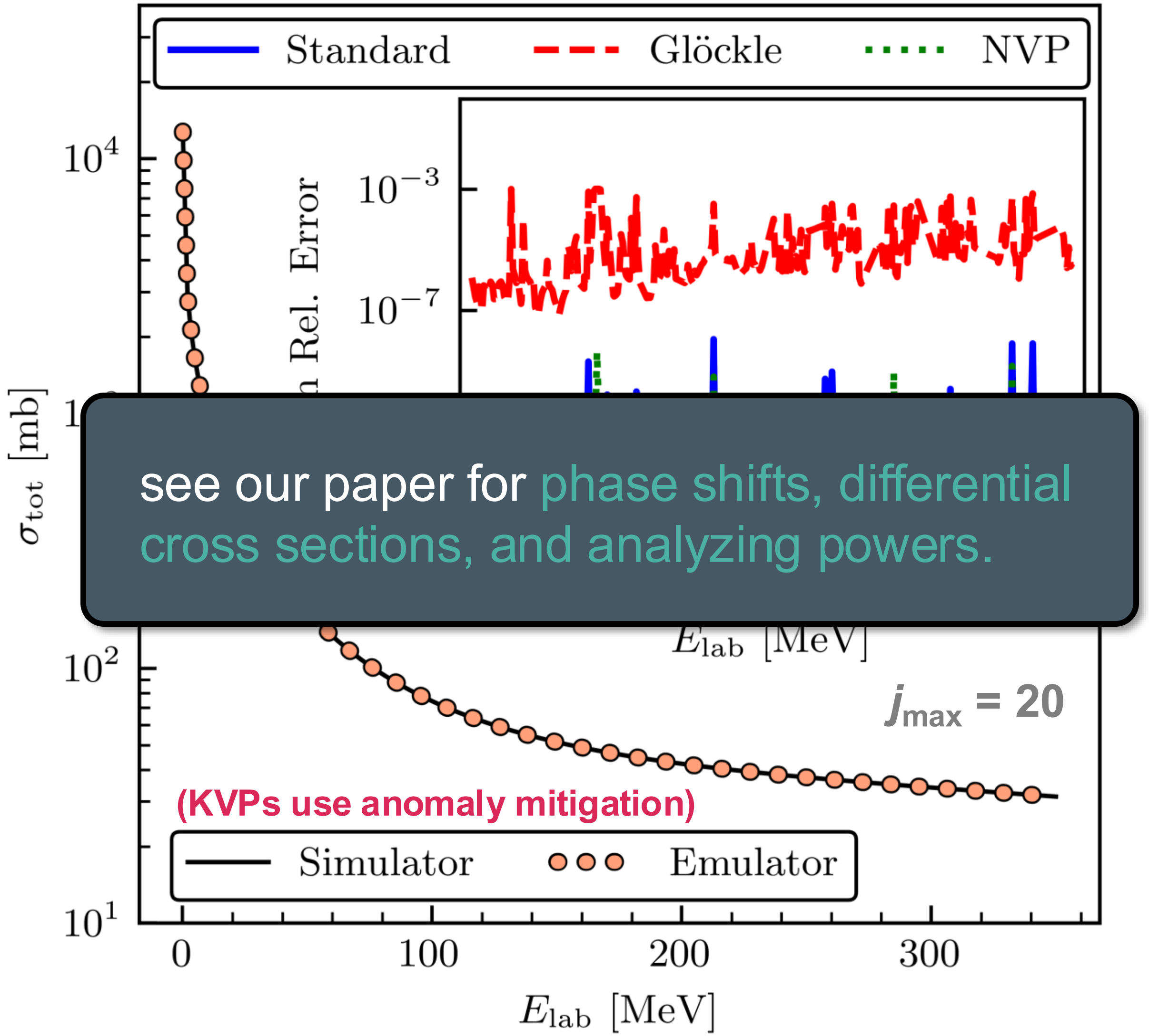
SMS chiral NN potential at N^4LO+ with momentum cutoff Λ = 450 MeV



see our paper for phase shifts, differential cross sections, and analyzing powers.

$$\sigma_{\mathrm{tot}}(k_0) = \frac{\pi}{2k_0^2}\sum_{j=0}^{j_{\max}}(2j+1)\,\mathrm{Re}\{\mathrm{Tr}[S_j(k_0) - \mathbb{1}_4]\}$$

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

25 free parameters (LECs) varied; 50 snapshots used for training

KVP (Std.) and NVP residuals are vanishingly small compared to the **cross section** and its experimental uncertainty

500 random LEC samples in the range [-5, +5] in the units used in the potential (same range as the training points)

≳300x

faster than high-fidelity calculation

(highly implementation dependent)

N-d scattering emulator

Gnech, Zhang, CD, Furnstahl, Grassi, Kievsky, Marcucci, and Viviani, in prep.

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

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

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

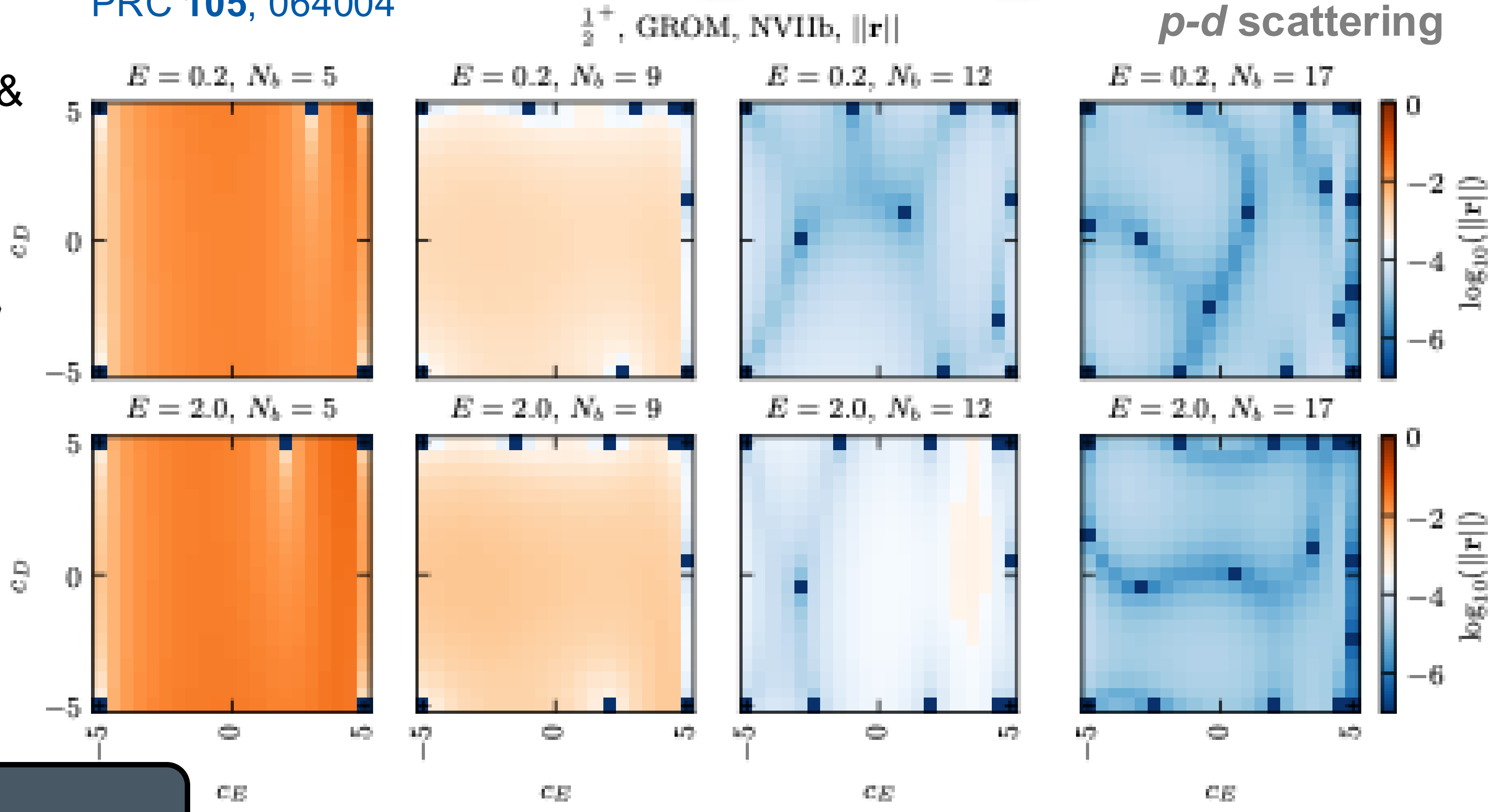
$$\mathcal{F}_{a,a'}\left[\Psi^a, \Psi^{a'}\right] \equiv \mathcal{R}_{a,a'} - \left\langle \Psi^{a'} \middle| \hat{H} - E \middle| \Psi^a \right\rangle$$

ROM: G-ROM or LSPG-ROM

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

- fixed N3LO NN potential (Norfolk)
- N^2LO **3N interactions (c_D, c_E)**

_p-d_ scattering



$$|\Psi^a\rangle = \sum_{\xi=1}^{N_A} c_\xi^a |\xi\rangle + \sum_{a'} \left(\delta_{a,a'} |\Omega_{a'}^R\rangle + \mathcal{R}_{a,a'} |\Omega_{a'}^I\rangle\right)$$

FOM trial wave function $a = \{L, S\}$

See also the review articles:
Kievsky *et al.*, J. Phys. G **35**, 063101
Marcucci *et al.*, Front. Phys. **8**

Preliminary results for emulating *R*-matrix elements across large (c_D, c_E) ranges

Proof of principle

Gnech, Zhang, CD, Furnstahl, Grassi, Kievsky, Marcucci, and Viviani, in prep.

Preliminary results

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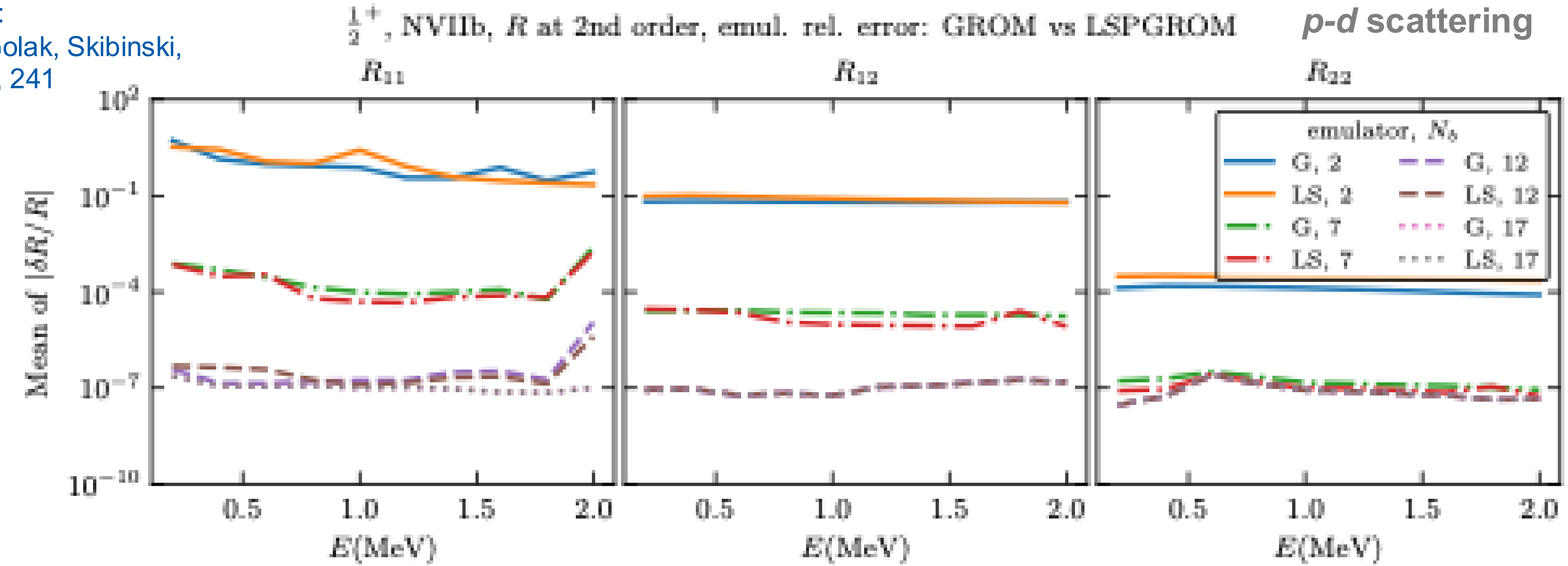
See also:
Witala, Golak, Skibinski, EPJA **57**, 241

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

$\frac{1}{2}^-$ 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?**

Take-away points

Source codes are (or will be made) publicly available!

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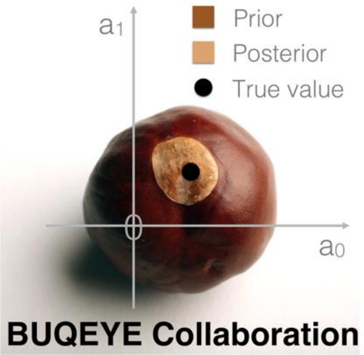
1. **Emulators are game changers for principled UQ (and more!) in nuclear physics. Much can be learned from the mature MOR field.**

2. **Active learning ("greedy") approach to snapshot selection** allows for the construction of fast & accurate emulators for **two- and three-body scattering: *N-d* scattering is a work in progress**

3. **Promising proof-of-principle emulator for three-body scattering based on the KVP, but more work is needed for applications to Bayesian parameter estimation of chiral interactions**

4. **Many options to construct scattering emulators are available. Which one(s) are the most efficient and/or reliable in practice?**

STREAMLINE
SmarT Reduction and Emulation Applying Machine Learning In Nuclear Environments



Many thanks to my collaborators: Ch. Elster, R. Furnstahl, A. Giri, A. Gnech, A. Grassi, A. Kievsky, J. Kim, J. Maldonado, L. Marcucci, P. Mlinarić, X. Zhang

Model (Order) Reduction for Nuclear Physics

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frontiers (pedagogical review article)

BUQEYE Guide to Projection-Based Emulators in Nuclear Physics

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

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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

see also Duguet et al., Rev. Mod. Phys. **96**, 031002

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