Fast and accurate emulators for scattering and nuclear matter

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Nuclear Hamiltonians for Advancing Nuclear Physics and Beyond

INT-26-1 workshop | May 12, 2026

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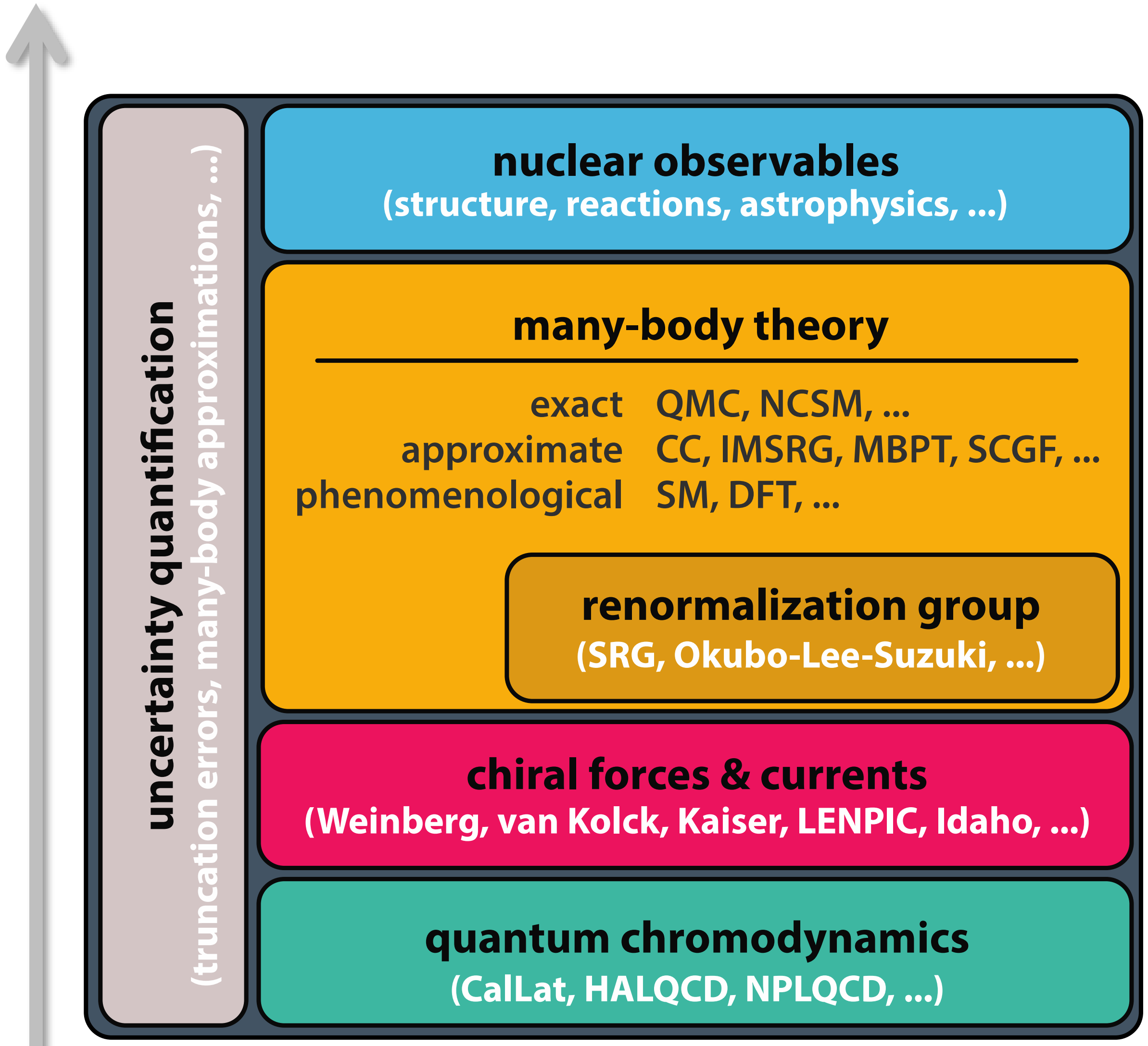
STREAMLINE
SmarT Reduction and Emulation Applying Machine Learning In Nuclear Environments

Ohio University Campus

Outline:

- **2B and 3B scattering emulators**
  - Reduced Basis Method
  - Emulator training and error estimation
  - Bayesian calibration of chiral interactions to scattering data
- **PMM-IMSRG emulator**
  - Nuclear equation of state (EOS)
  - Parametric and emulator uncertainties

Ab initio workflow (idealized)



CD & Bogner, Few Body Syst. **62**, 109
e.g., Essick, Tews, Landry, Reddy, Holz, PRC **102**, 055803

Example: nuclear equation of state (EOS)

Energy per particle, pressure, or sound speed

$$\frac{E}{A}(n, \delta, T)$$

baryon density *n*
neutron excess *δ*
temperature *T*

computational framework

solves the (many-body) Schrödinger equation requires a nuclear potential as input

chiral effective field theory

provides microscopic interactions consistent with the symmetries of *low-energy* QCD

theory of strong interactions

QCD is nonperturbative at the low energies relevant for nuclear physics (cf. pQCD & LQCD)

CD, Haxton, McElvain, Mereghetti *et al.*, PPNP **121**, 103888

Motivation: mining scattering data

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

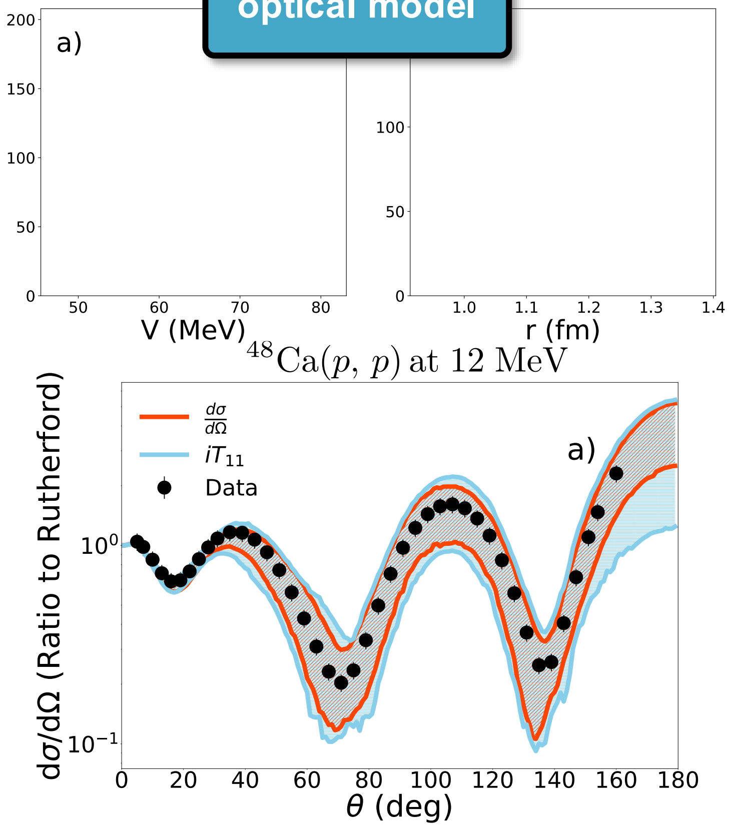
see, *e.g.*, Yang, Ekström *et al.*, arXiv:2109.13303
Furnstahl, Hammer, Schwenk, Few Body Syst. **62**, 72

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

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

BUQEYE
Chalmers
ISNET

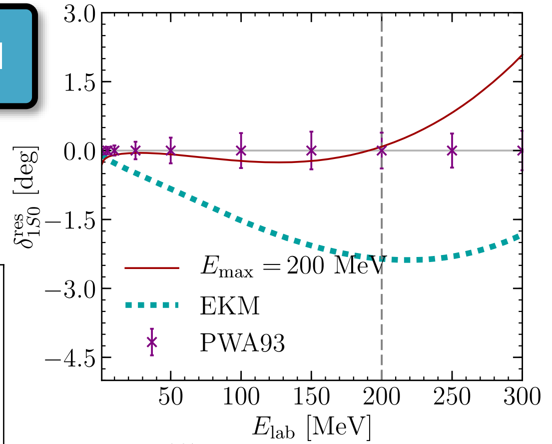
optical model

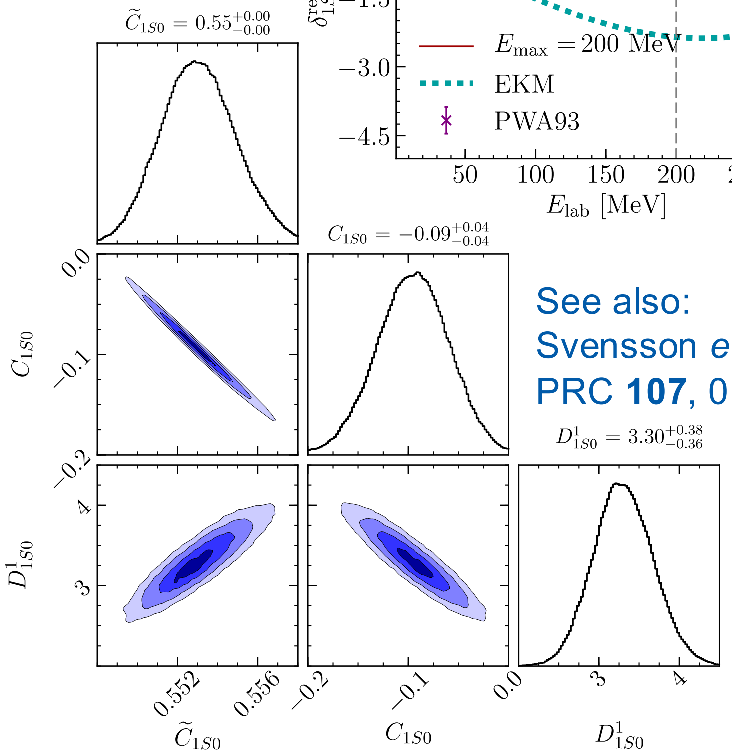


Catacora-Rios, King *et al.*, PRC **104**, 064611

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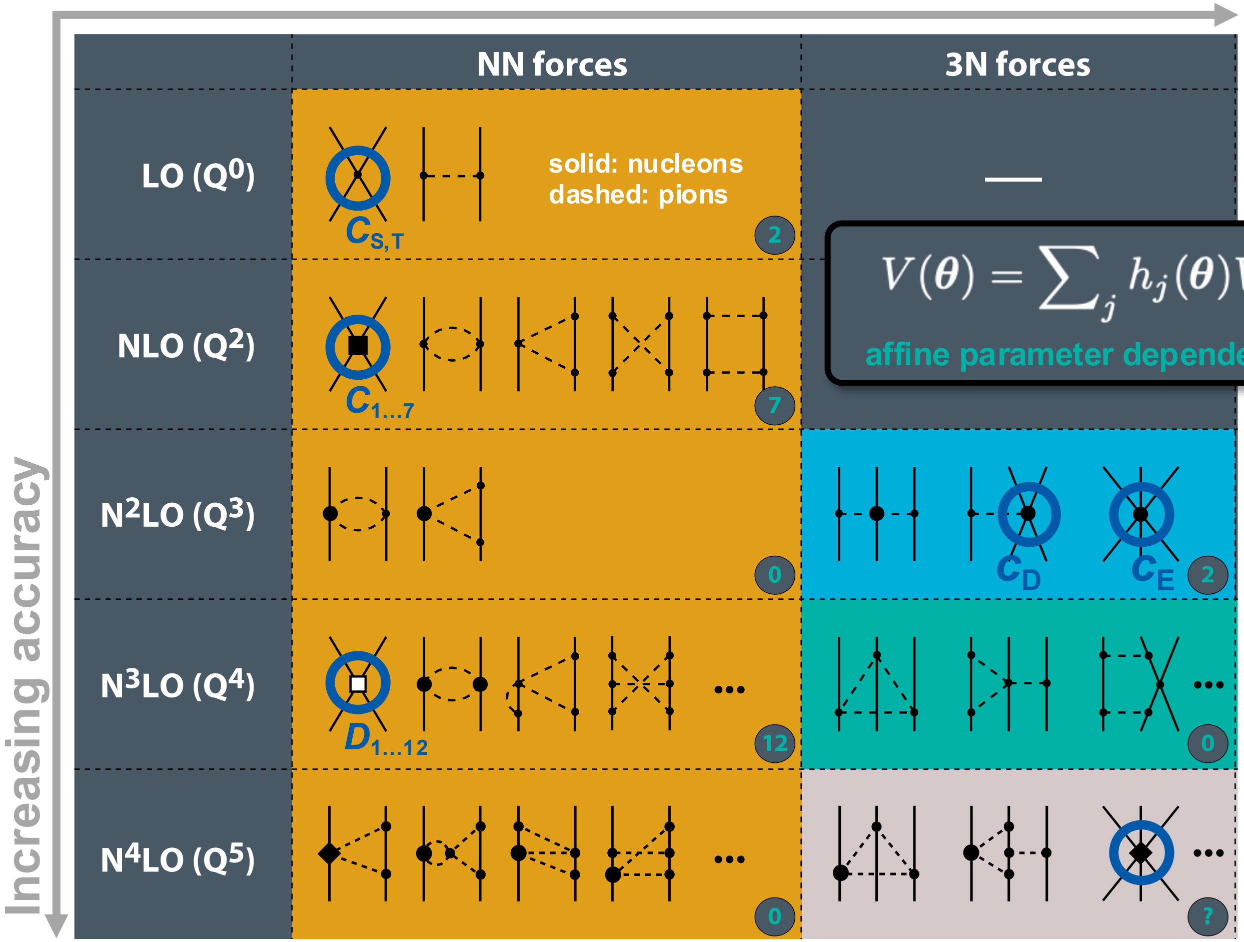
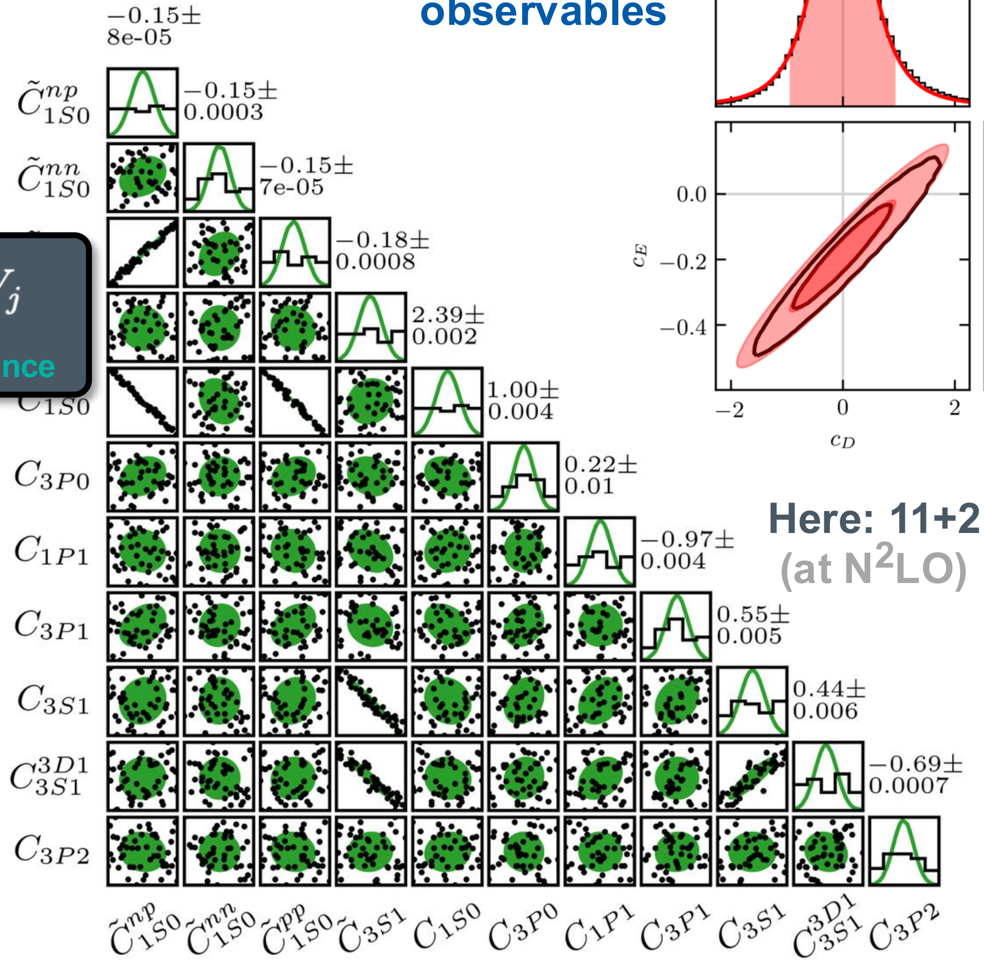
Systematic **EFT expansion of nuclear interactions**, with *many* parameters to be determined (**distribution functions**!)

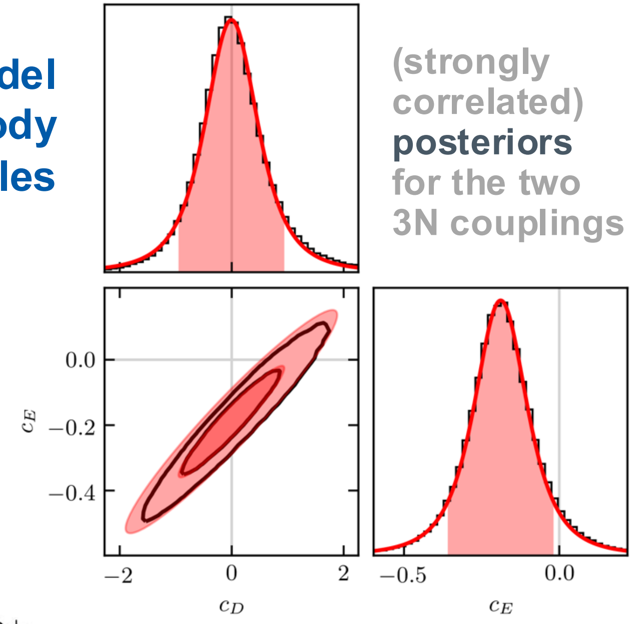


$$V(\boldsymbol{\theta}) = \sum_j h_j(\boldsymbol{\theta}) V_j$$

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 N²LO)

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

Reduced Order Models (ROMs)

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

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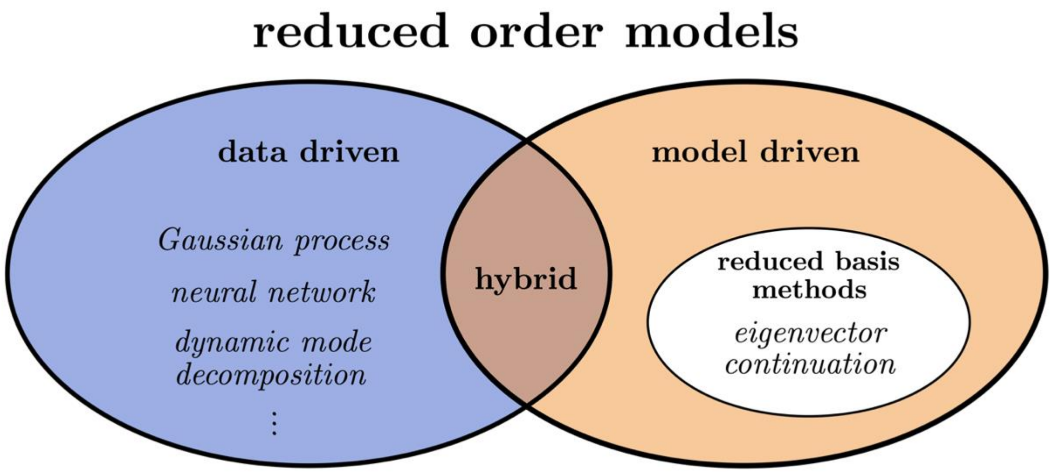
Data-driven:
interpolate output of **full-order model (FOM)** calculations (non-intrusive)



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 calculations for UQ and extrapolation

RBM for eigenvalue problems coined **Eigenvector Continuation (EC) in nuclear physics**

Frame *et al.*, PRL **121**, 032501 (2017)

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

Mini-apps: no expert knowledge or access to closed-source code required

Many RBM scattering emulators available!

Codes (Jupyter notebooks) publicly available!

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… and many more, including ROSE developed by the BAND collaboration

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

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)**

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)**

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)**

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

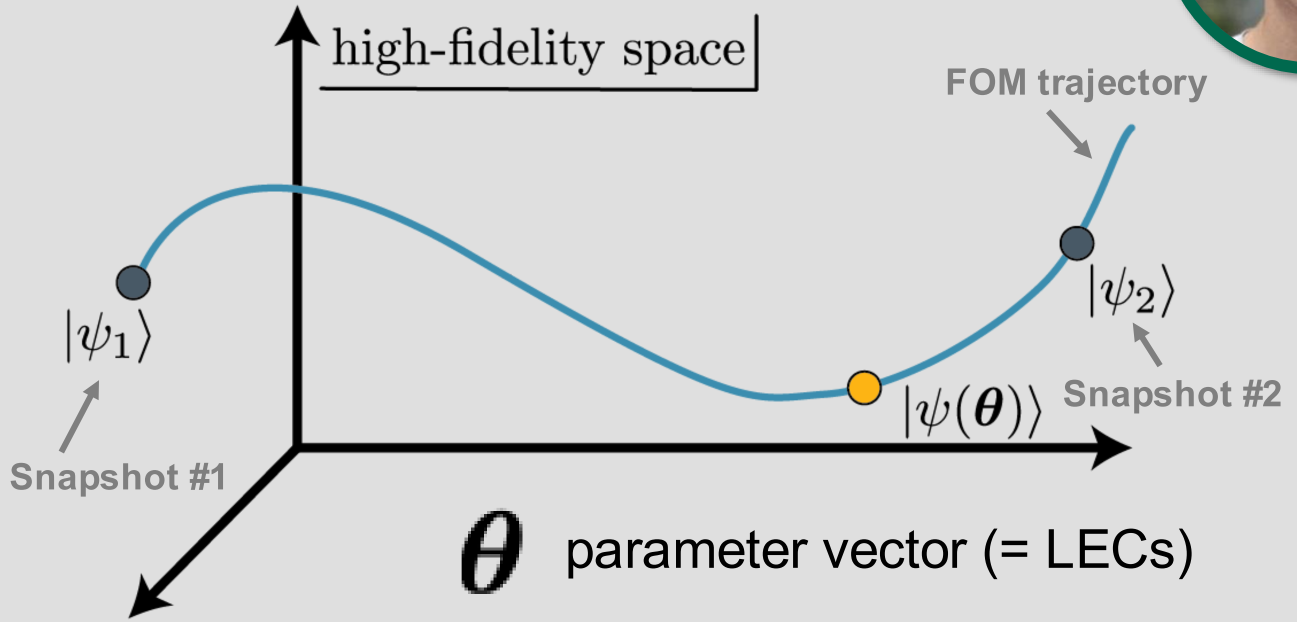
Highlight: introduces snapshot-based trial wave functions for ROMs

progress

See also: CD, Melendez, Garcia, Furnstahl, and Zhang, Front. Phys. **10**, 92931 | CD & Zhang's contribution to Few Body Syst. **63**, 67

Emulator basis construction

Maldonado, CD, Furnstahl *et al.*, PRC **112**, 024002



RBMs construct low-dimensional approximations of the full order model's solution space using a set of high-fidelity calculations, called snapshots.

Emulator basis construction

Maldonado, CD, Furnstahl *et al.*, PRC **112**, 024002

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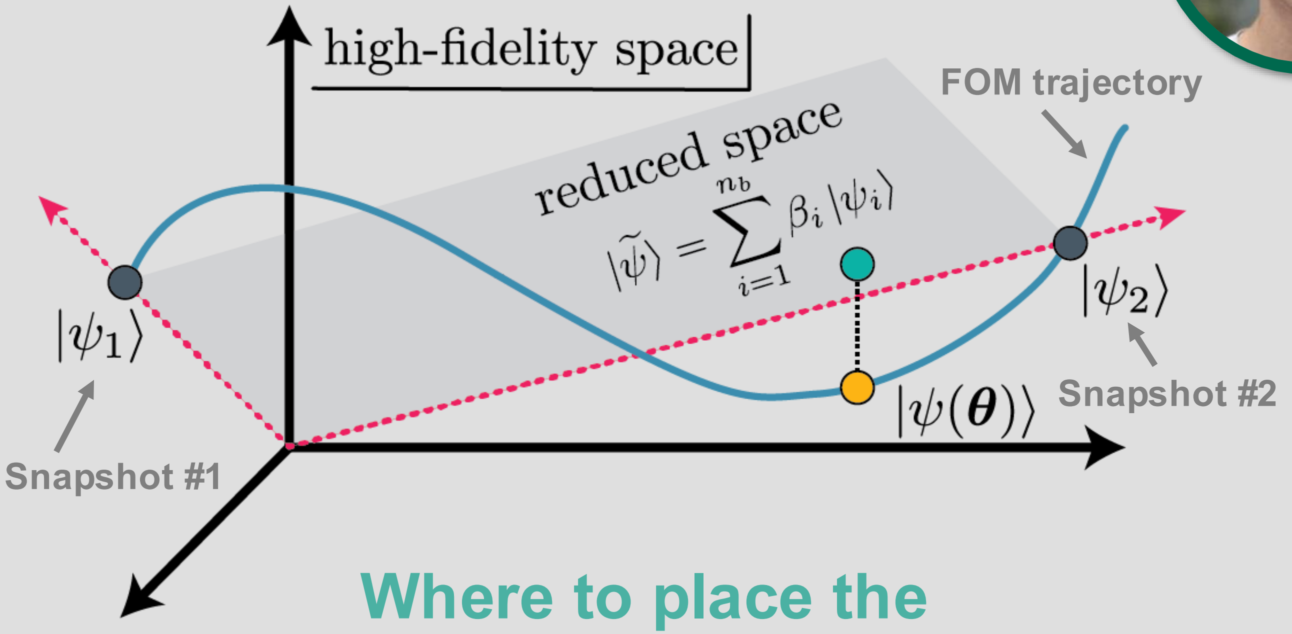
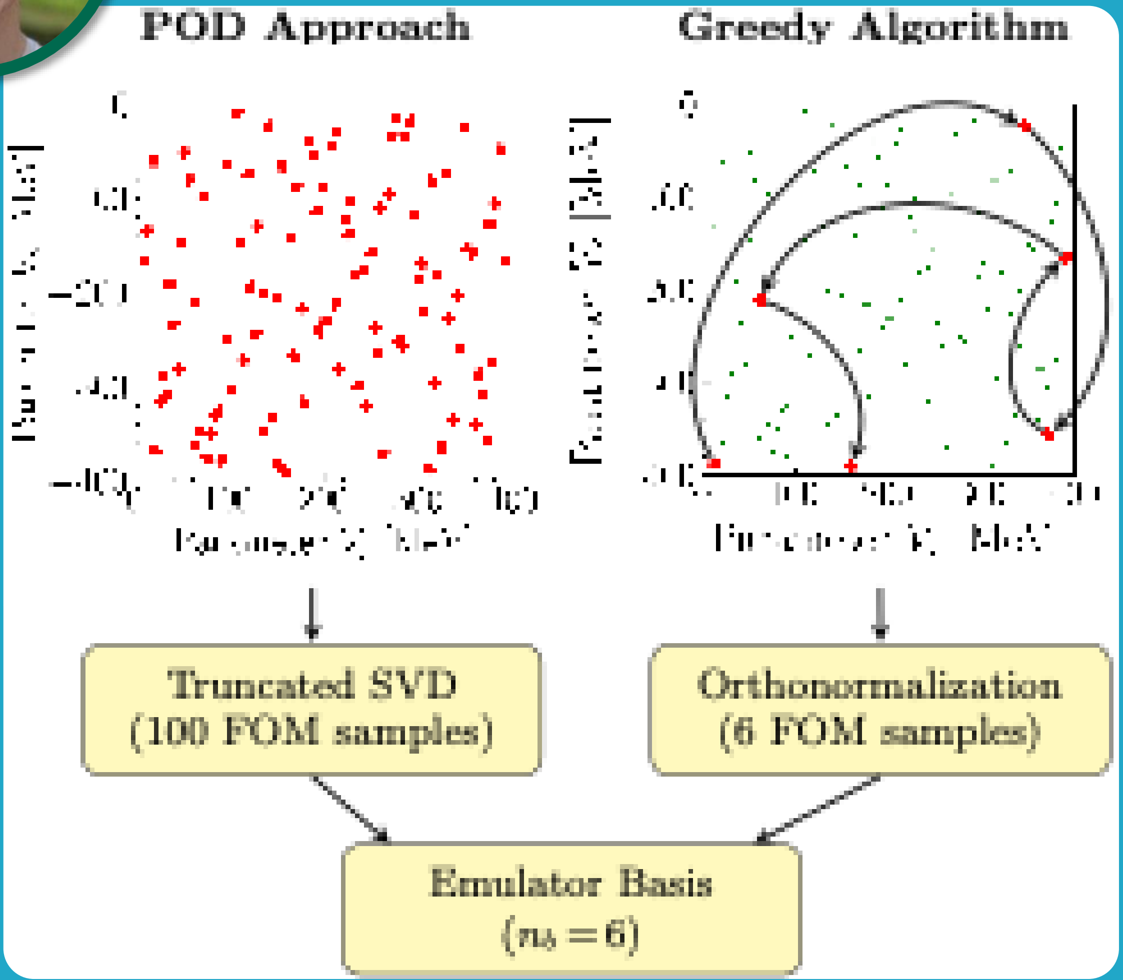


Where to place the emulator's *snapshots*?

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



Greedy method: (1) uses far *fewer* FOM solutions for training, (2) estimates emulator errors, (3) *iteratively* adds snapshots where the emulator error is largest

Greedy Algorithm in Action

start with 2 randomly placed *initial* snapshots

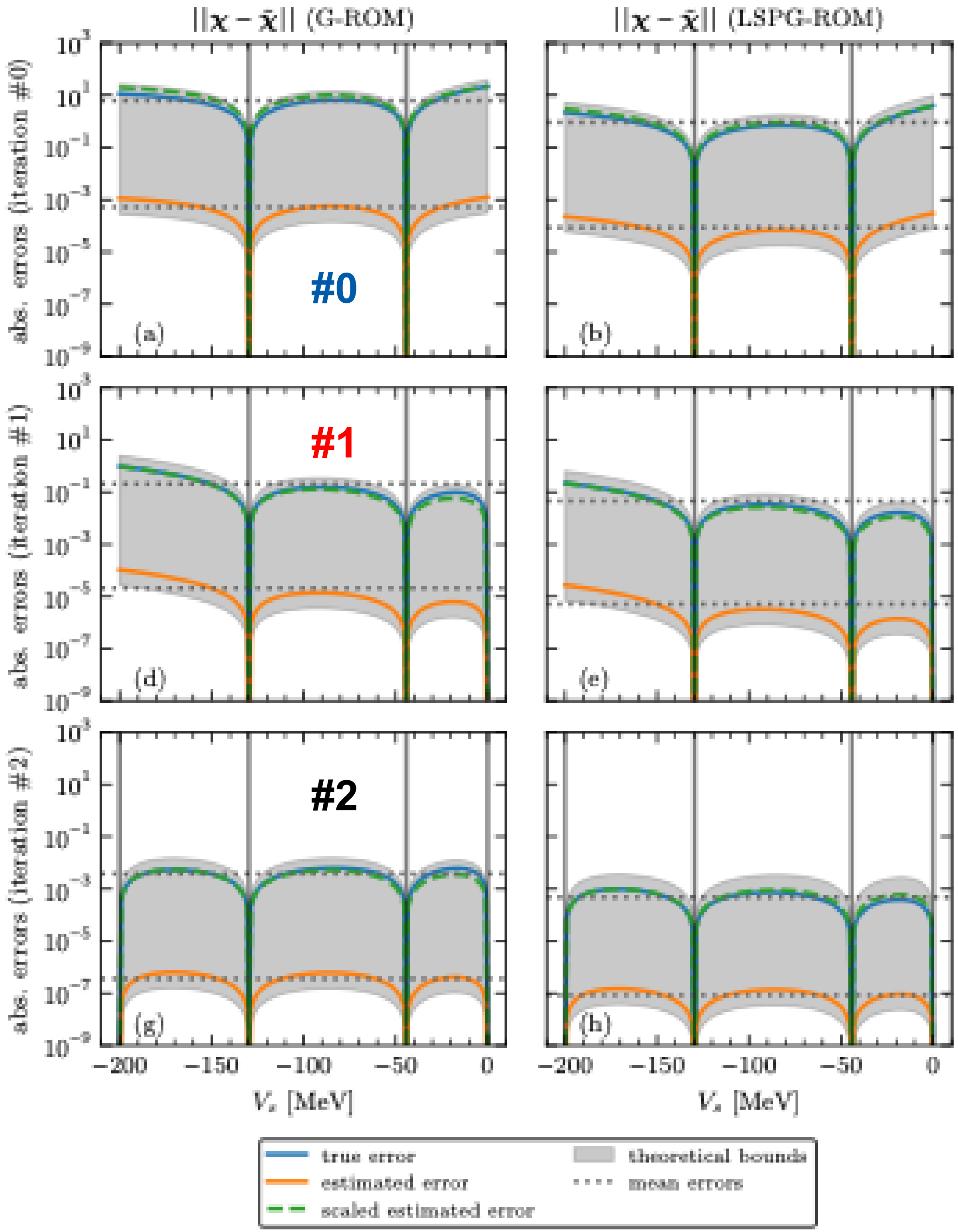
Estimate the emulator error across the parameter space

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**



Emulator basis construction

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PRC **112**, 024002

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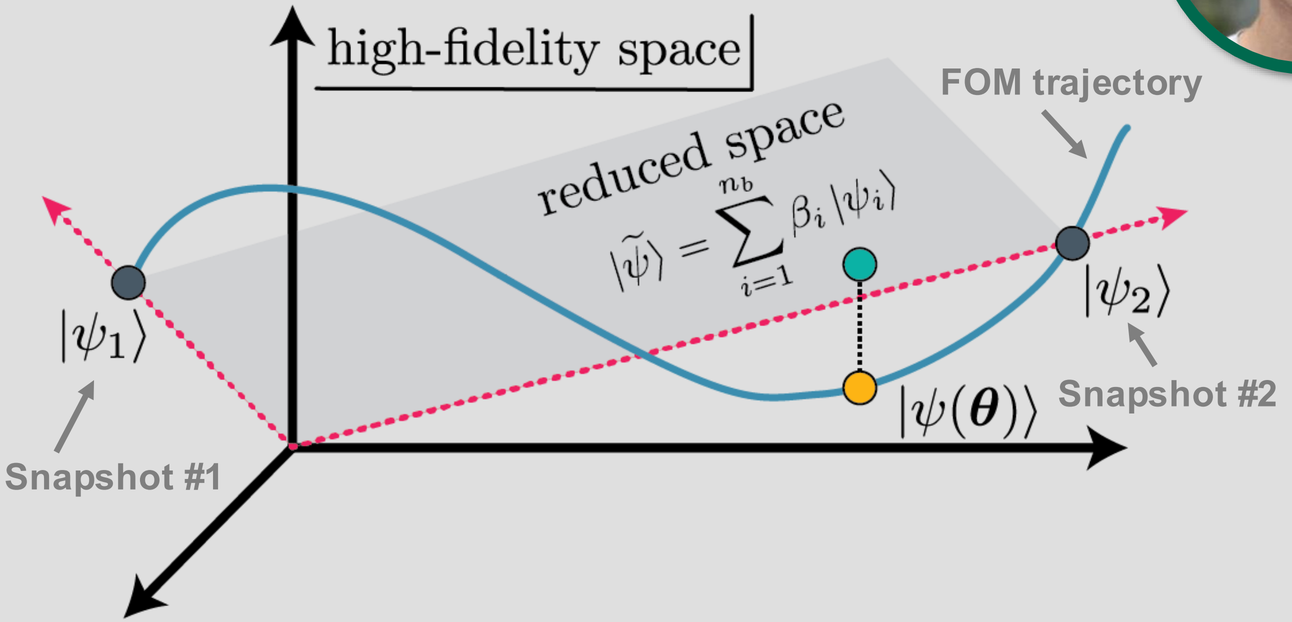


$$A(\vec{\theta})\vec{x}(\vec{\theta}) = \vec{b}(\vec{\theta})$$

Scattering solver (abstract):

Schrödinger equation (cs) or
Lippmann-Schwinger equation (ms)

Affine decompositions from potential carry over:

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

Galerkin (G) ROM

Reduction:

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

Snapshot matrix

Projection:

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

Least-Squares Petrov-Galerkin (LSPG) ROM

Reduction:
Projection:

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

$$Y = \left[A_1 X \quad \cdots \quad A_{n_\theta} X \quad b_1 \quad \cdots \quad b_{n_\theta}\right]$$

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 (*not* necessarily *proportional* to each)

Fast & accurate error estimation in the *reduced* space

Residual vector in the full-order space

$$\vec{r}(\vec{\theta}) \equiv Y^\dagger R(\vec{\theta}) = Y^\dagger A(\vec{\theta}) X \vec{\beta}(\vec{\theta}) - Y^\dagger \vec{b}(\vec{\theta})$$

Residual vector in the (*semi-)reduced* space

We showed that $\varepsilon = \left|\vec{r}(\vec{\theta})\right| \equiv \left|\vec{R}(\vec{\theta})\right|$

Theoretical error bounds

Extremal singular values

$$\sigma_{\min}(A)\,|\tilde{x} - x|_2 \leqslant \varepsilon \leqslant \sigma_{\max}(A)\,|\tilde{x} - x|_2$$

Future: estimate the extremal singular values using the Successive Constraint Method (SCM) and use *upper bound* as conservative error

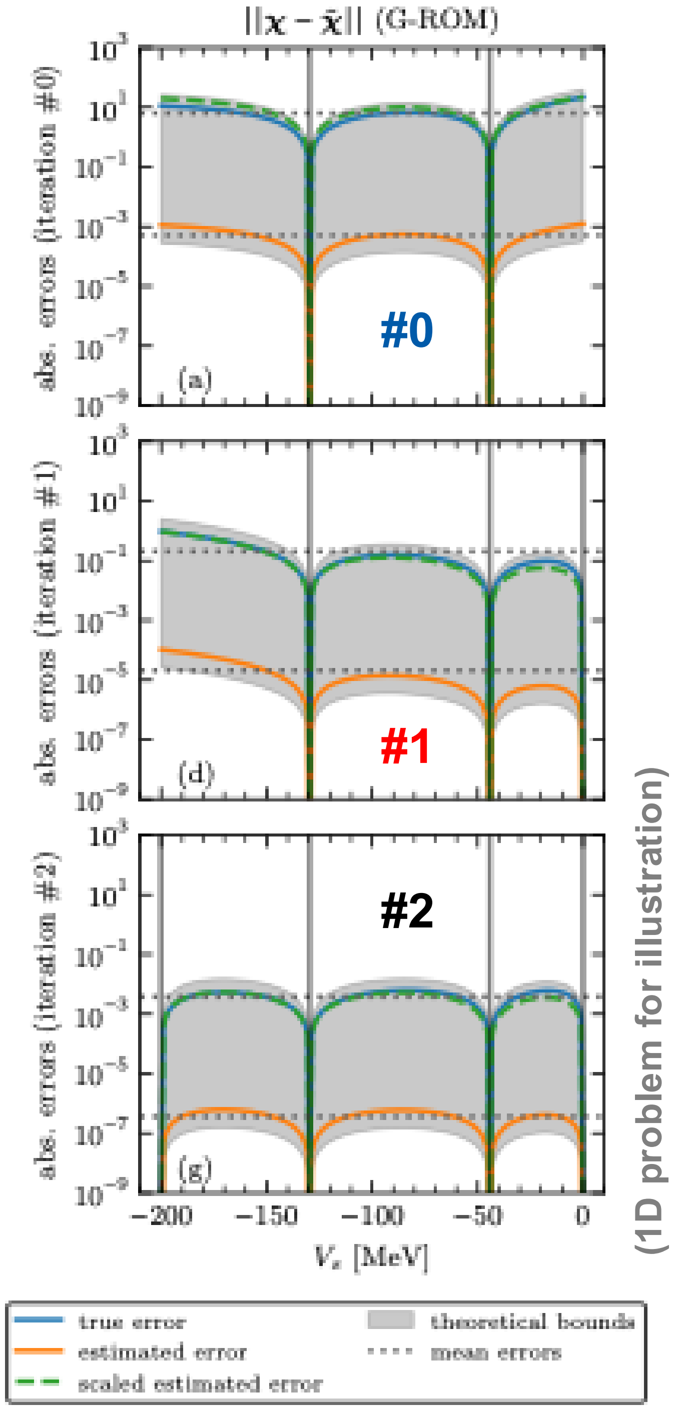
start with 2 randomly placed initial snapshots

Estimate the emulator error across the parameter space

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

Iterate until the *requested* accuracy is obtained

Greedy iteration increasing accuracy



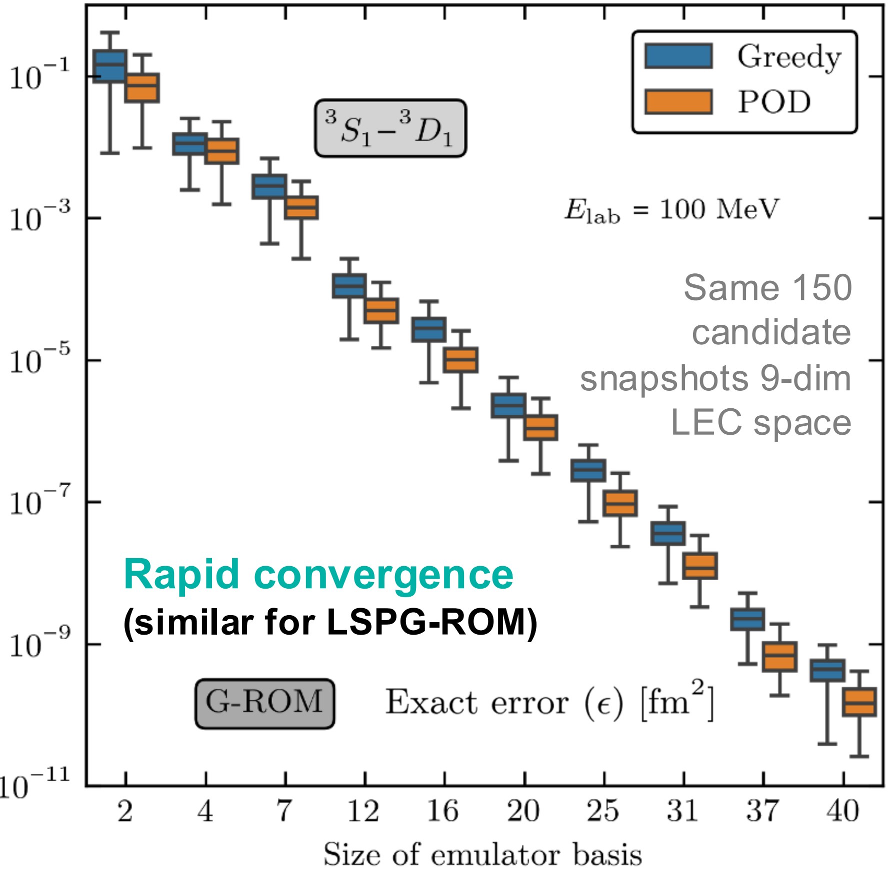
Emulating the T-matrix equation

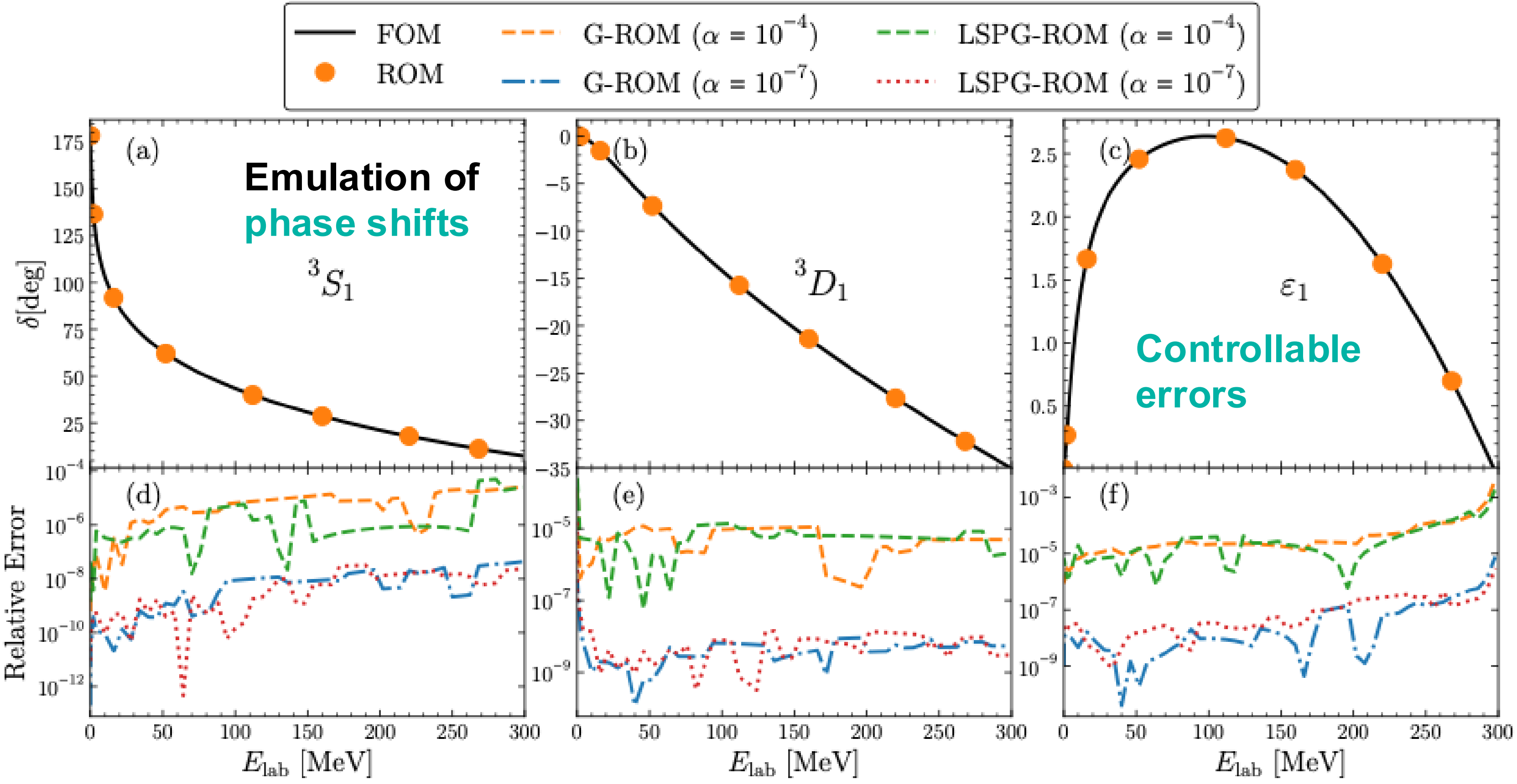
Giri, Kim, CD, Elster, and Furnstahl,
PRC **113**, 044001

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

Lippmann-Schwinger equation [momentum space]

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

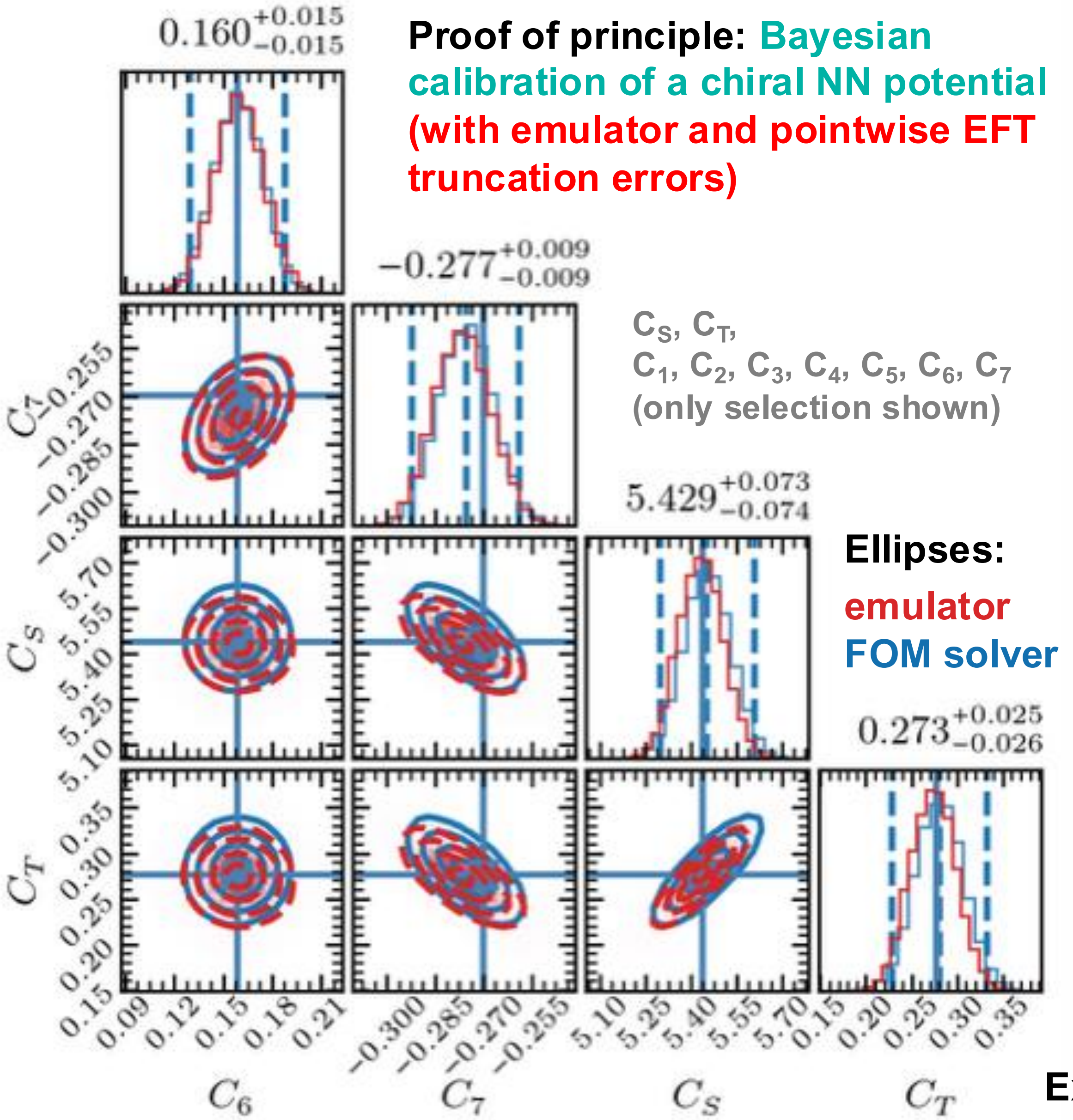




Emulation of *total* cross sections

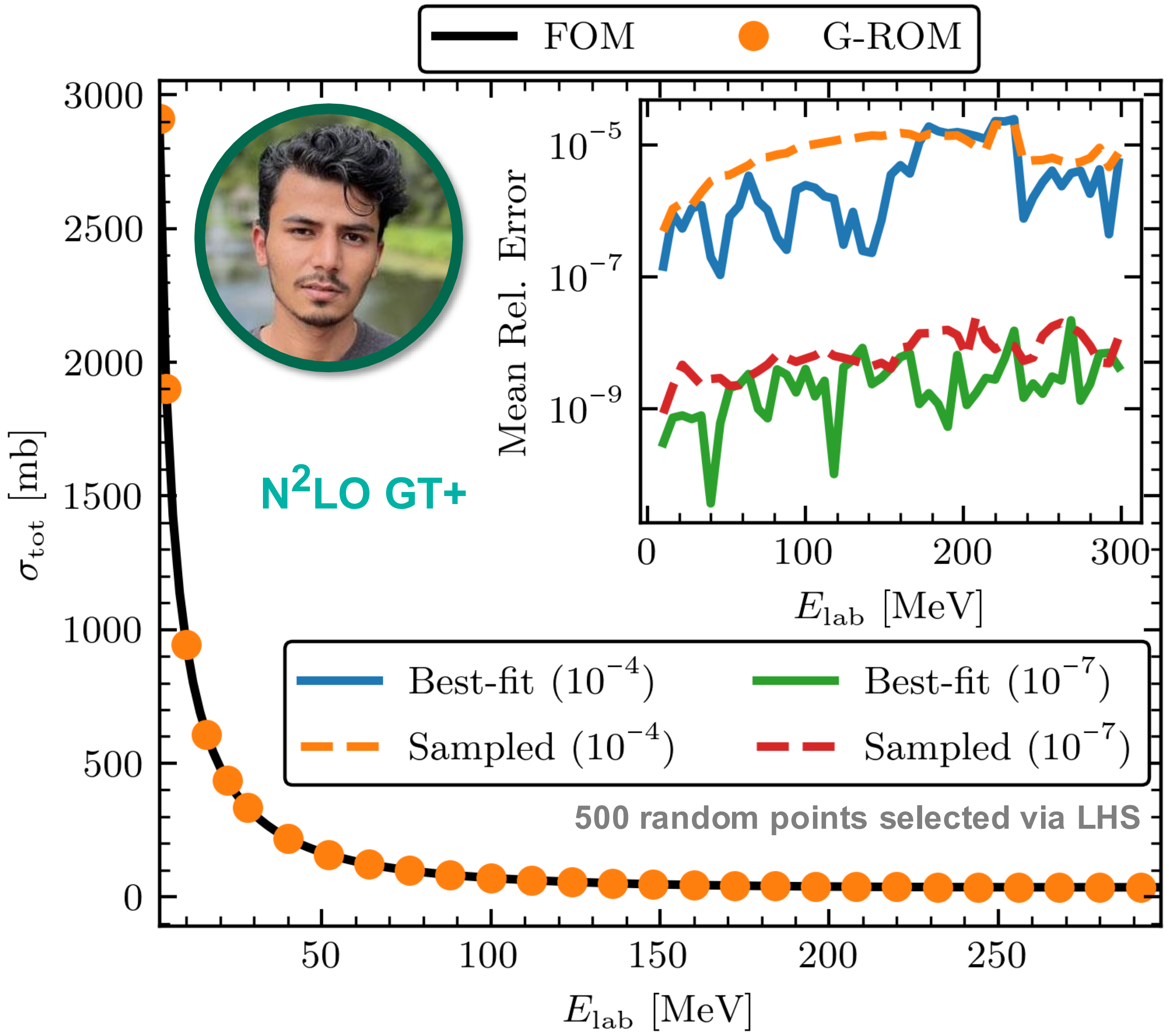
Giri, Kim, CD, Elster, and Furnstahl,
PRC **113**, 044001

Proof of principle: Bayesian calibration of a chiral NN potential (with emulator and pointwise EFT truncation errors)



C_S, C_T,
C_1, C_2, C_3, C_4, C_5, C_6, C_7
(only selection shown)

Ellipses:
emulator
FOM solver



Extension to other scattering observables and potentials in progress

Computational speedups

Giri, Kim, CD, Elster, and Furnstahl,
PRC **113**, 044001

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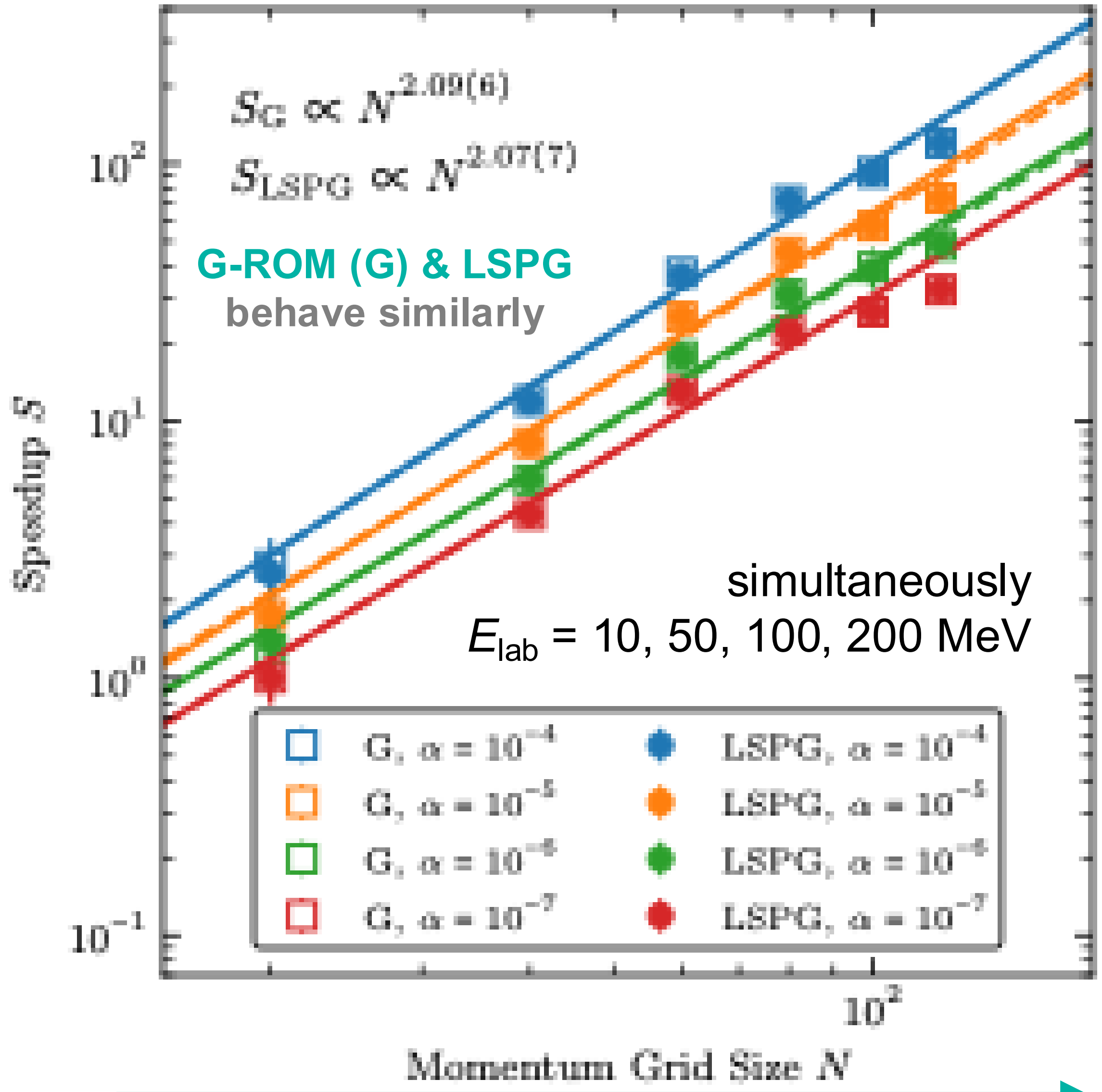
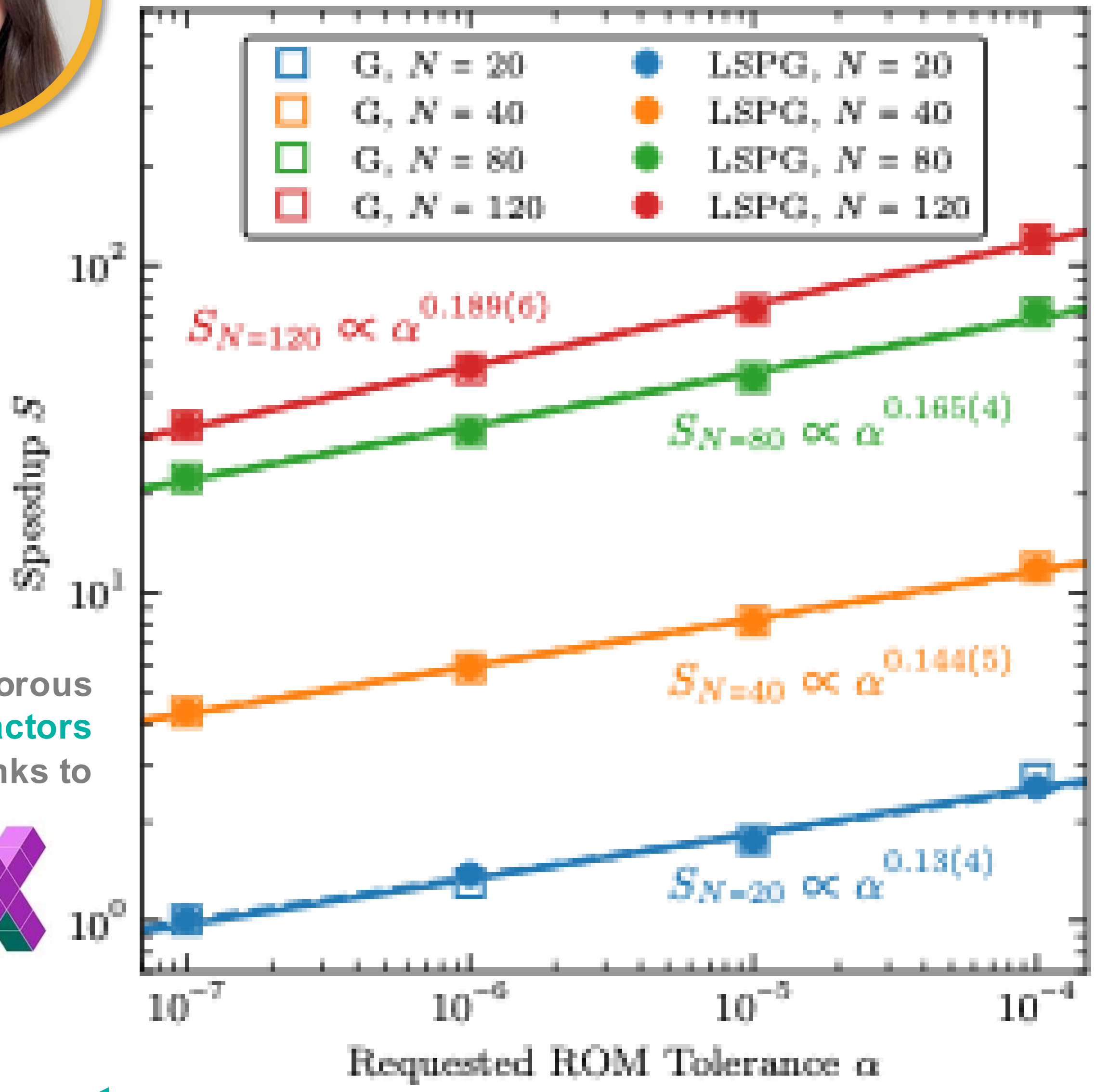


More accurate FOM

More rigorous
speed-up factors
thanks to



More accurate ROM (more snapshots needed)

N-d scattering emulator

Gnech, Zhang, CD, Furnstahl, Grassi,
Kievsky, Marcucci, and Viviani,
arXiv:2511.01844 & 2511.10420

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Emulate three-body scattering with greedy snapshot selection

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

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

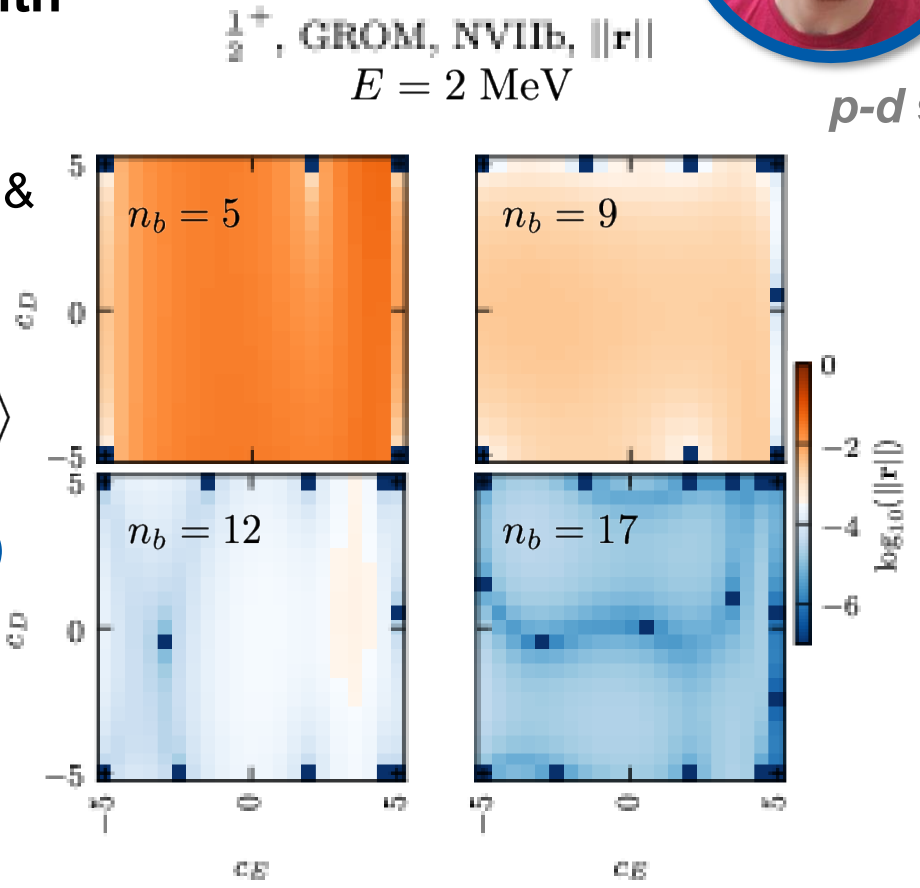
ROM: **G-ROM (G) or LSPG-ROM (LS)**

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

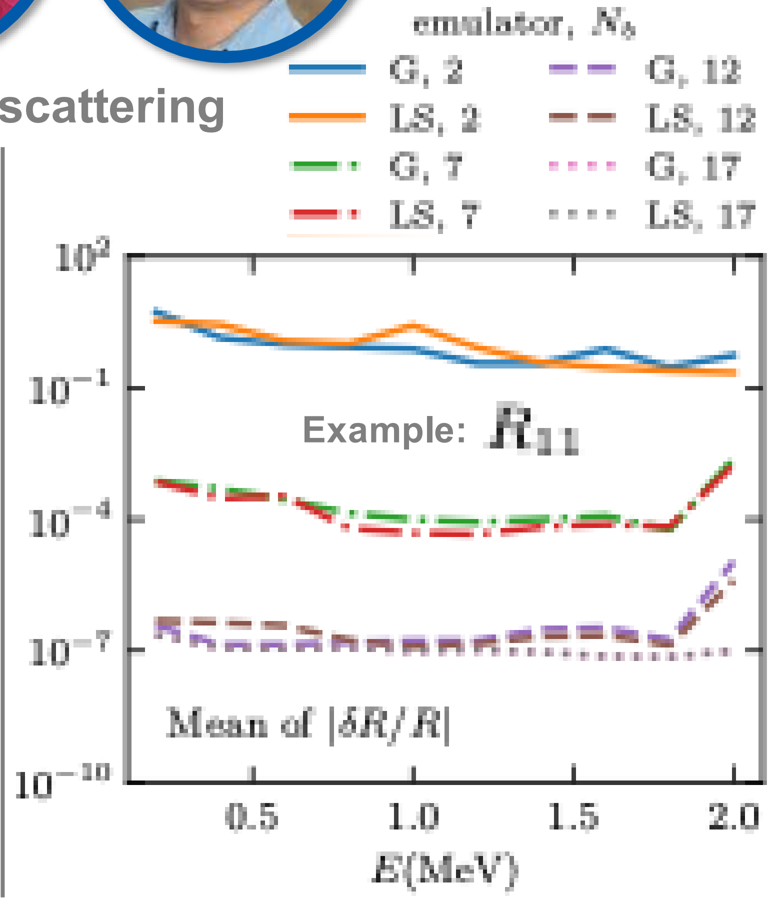
- fixed N^{3}LO NN potential (Norfolk)
- N^{2}LO **3N interactions (c_D, c_E)**

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

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



p-d scattering



Greedy algorithm: systematic reduction of emulator errors

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

Ab initio workflow (idealized)

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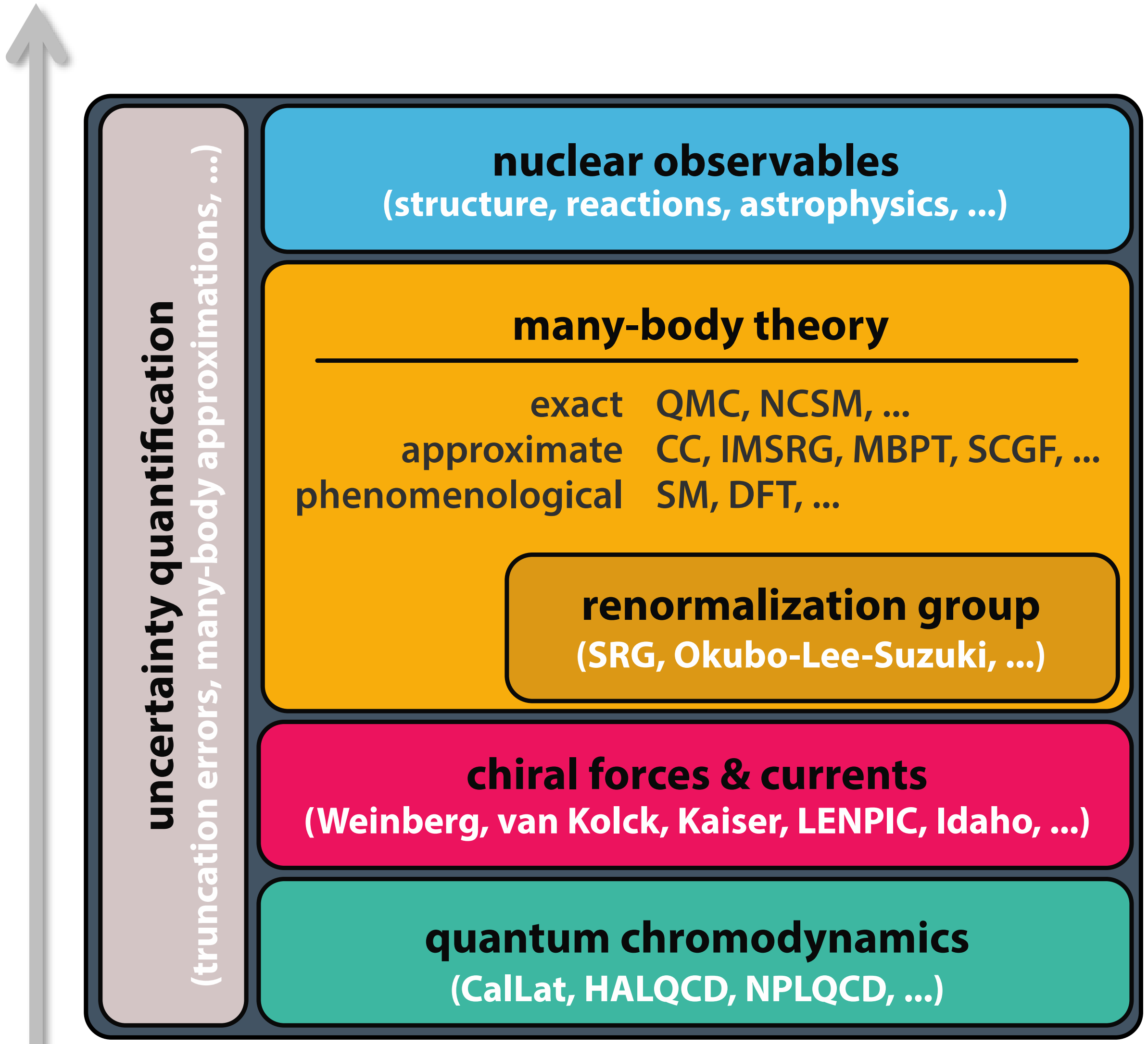

CD & Bogner, Few Body Syst. **62**, 109
e.g., Essick, Tews, Landry, Reddy, Holz, PRC **102**, 055803

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CD, Haxton, McElvain, Mereghetti *et al.*, PPNP **121**, 103888

In-Medium Similarity Renormalization Group

In collaboration with:
Kang Yu and Scott Bogner

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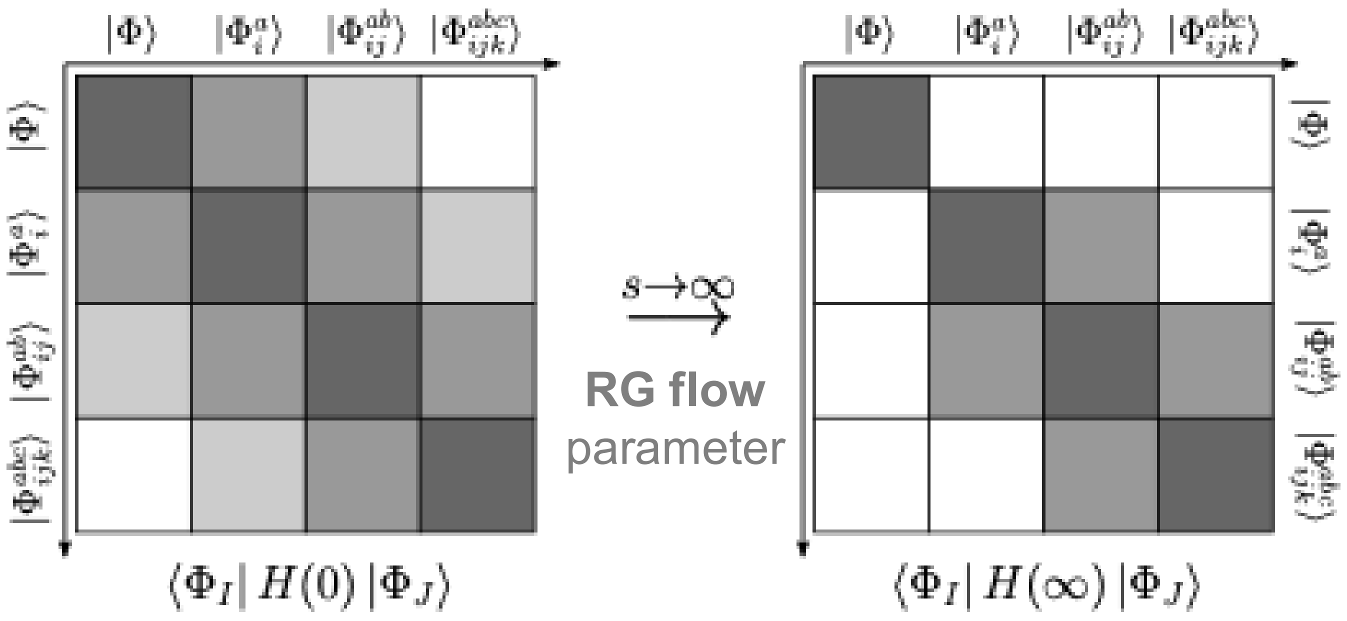
IMSRG in a nutshell:

- **non-perturbative method**
- uses a **continuous unitary transformation** to **decouple a reference state** from excited states
- Applicable to local and nonlocal forces

$$H(s) = U^\dagger(s) H U(s)$$



Our setup:

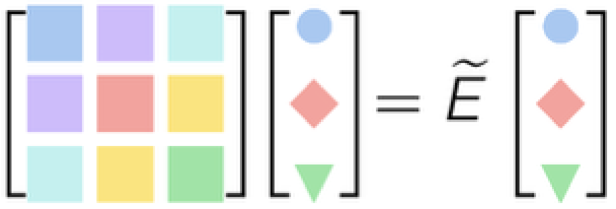
- Truncated at normal-ordered 2-body level
- **Nucleons in a cubic box**
  - **66 neutrons (and 66 protons)**
  - Isospin asymmetric systems possible
- single particle basis, with periodic boundary conditions

Directions of future calculations:
finite-temperature EOS, momentum distributions, static structure factors

Parametric matrix models (PMM) for nuclear EOS

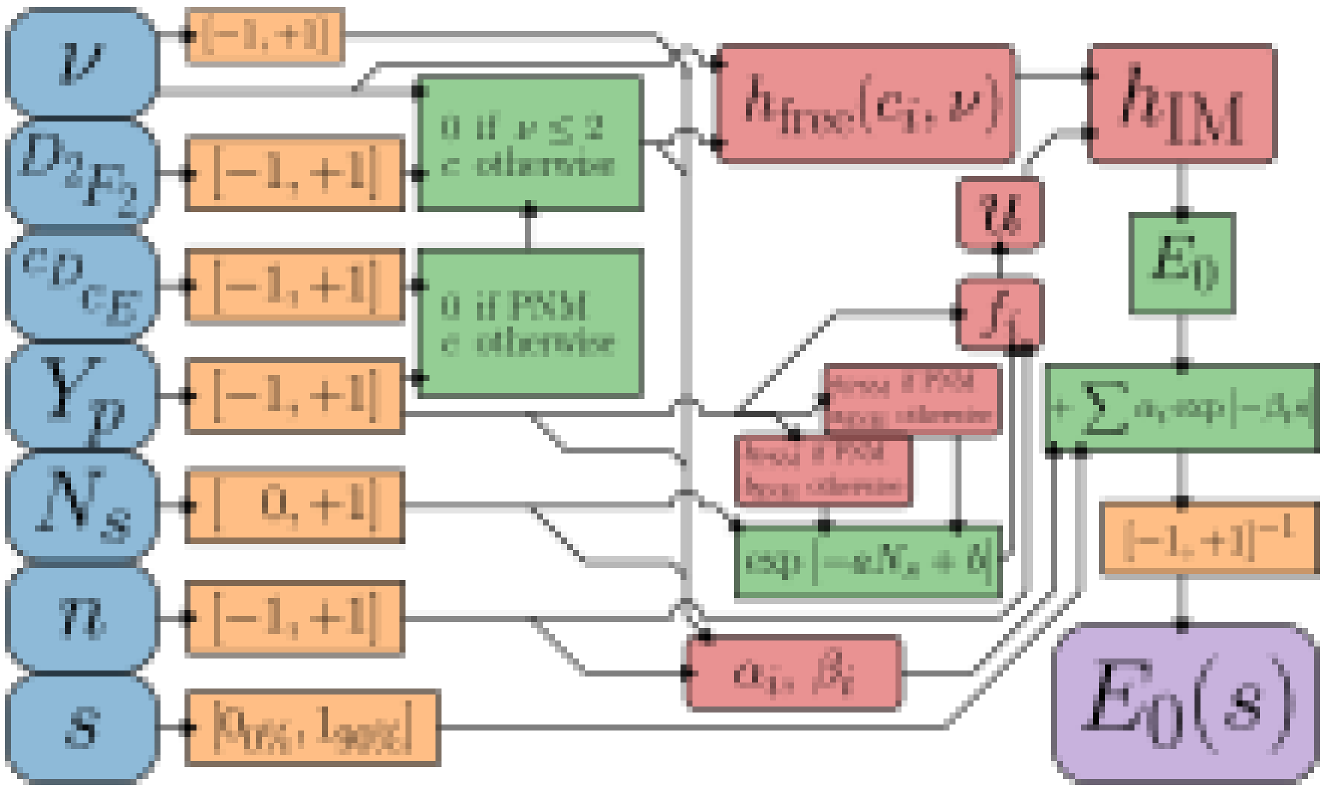
Cirigliano, Dawid, Dekens, and Reddy, PRL **135**, 022501

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



Basic idea:
RBM *without* (explicitly) known snapshot basis that is *learned* by EOS calculations and physics guidance

Model inputs



Model output(s)

Controlled extrapolation of not (fully) converged IMSRG calculation
Systematic propagation of LEC uncertainties to the EOS

PMM-IMSRG emulator for EOS

In collaboration with:
Patrick Cook, Kang Yu,
and Scott Bogner

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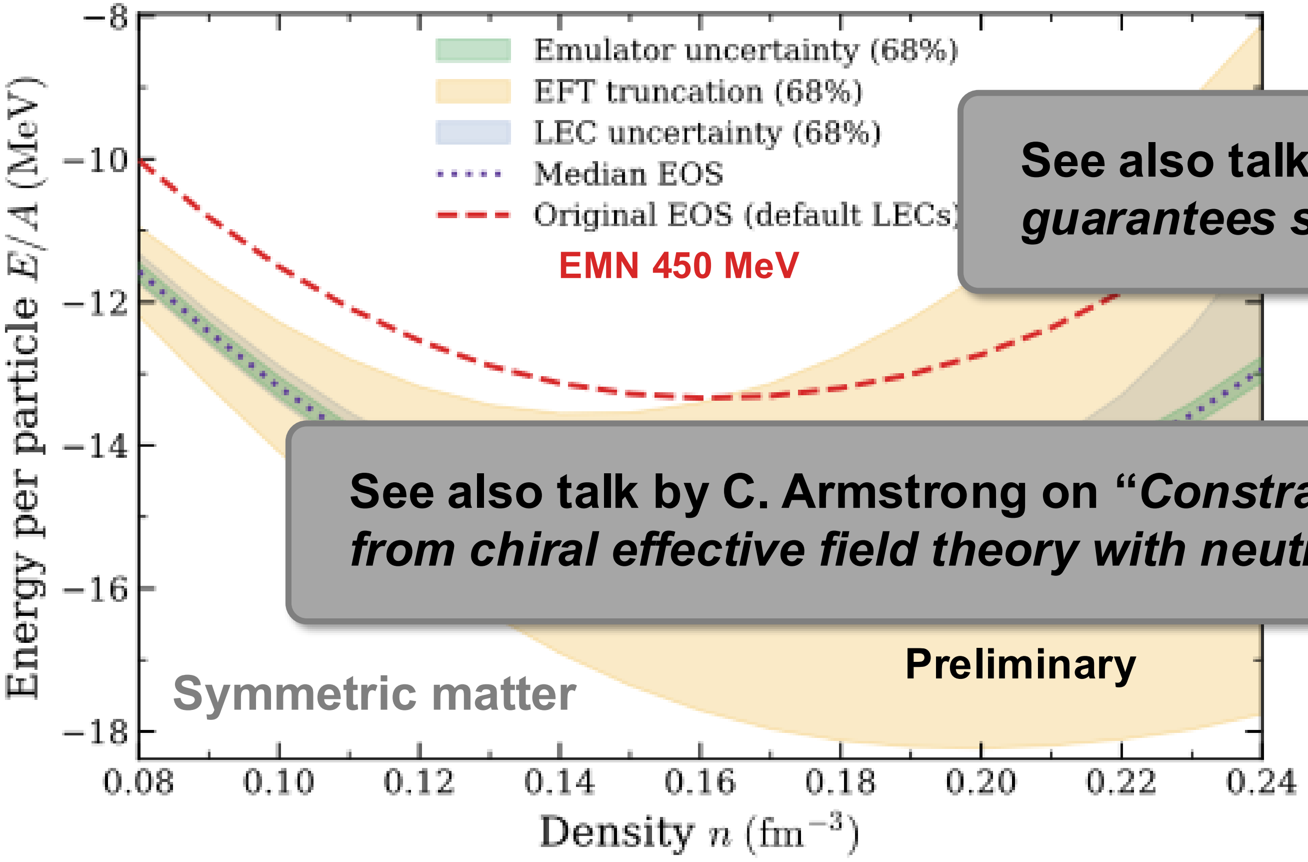
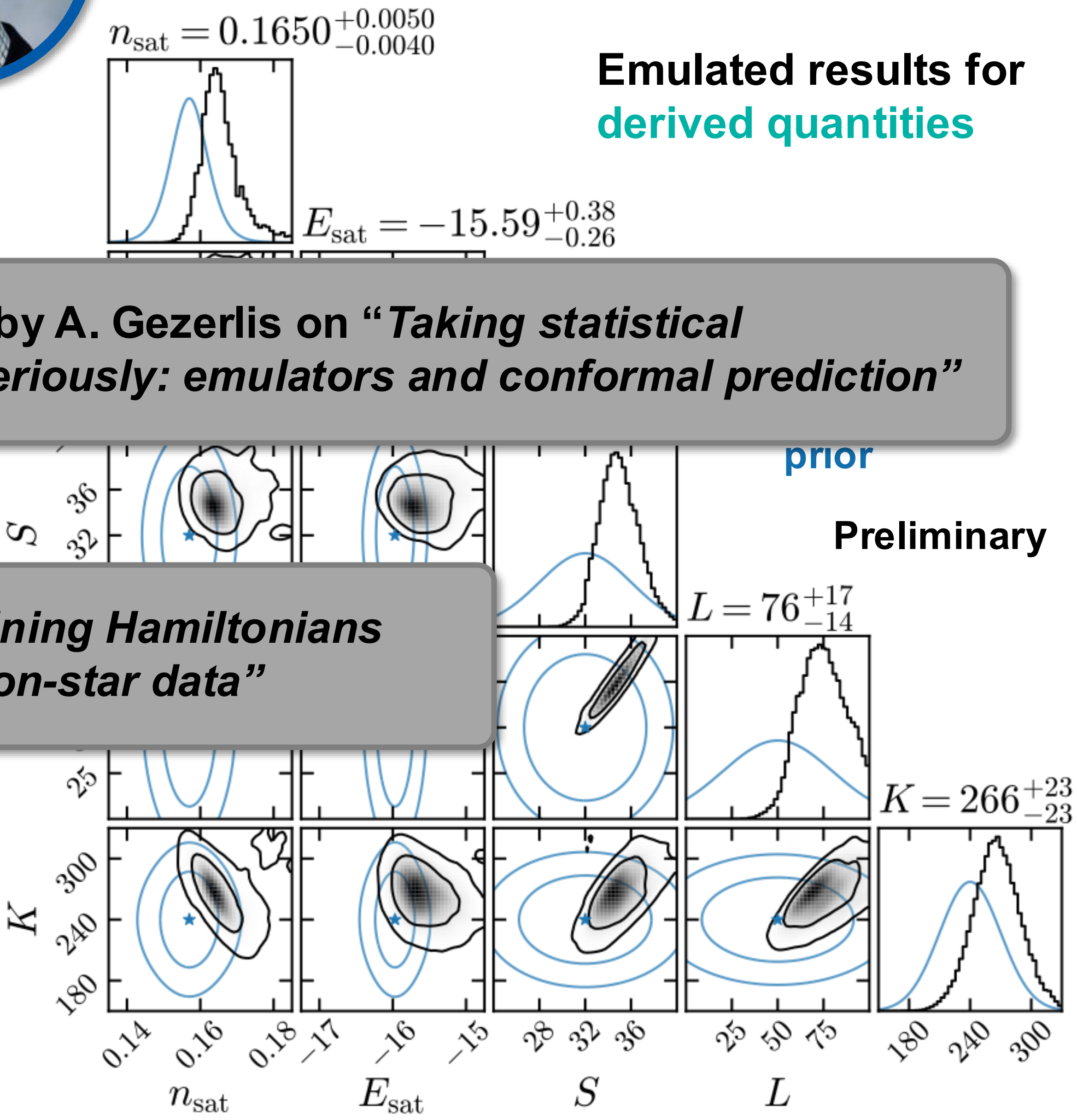
See also:
Cook *et al.*, Nature Comm. **16**, 5929 (2025)
Armstrong *et al.*, PRL **135**, 142501



Emulated results for derived quantities



See also talk by A. Gezerlis on "*Taking statistical guarantees seriously: emulators and conformal prediction*"

See also talk by C. Armstrong on "*Constraining Hamiltonians from chiral effective field theory with neutron-star data*"

Emulator errors estimated via conformal prediction

Speedup factors: >3000

Preliminary results

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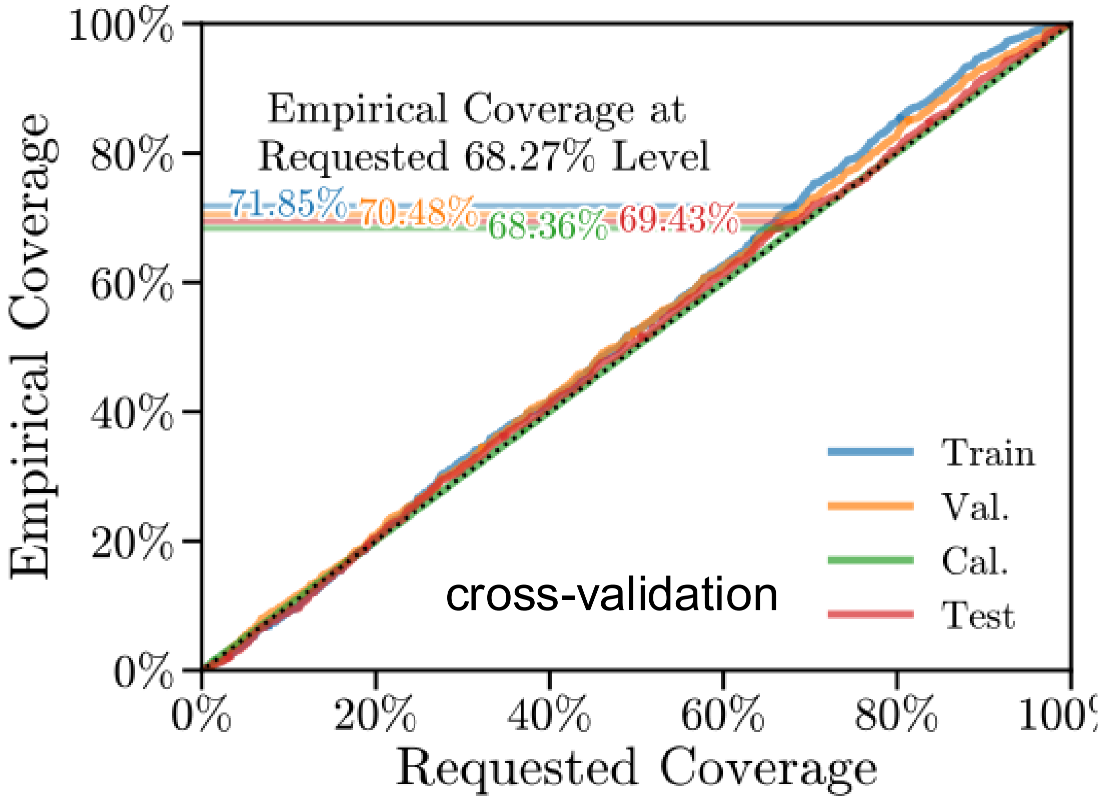
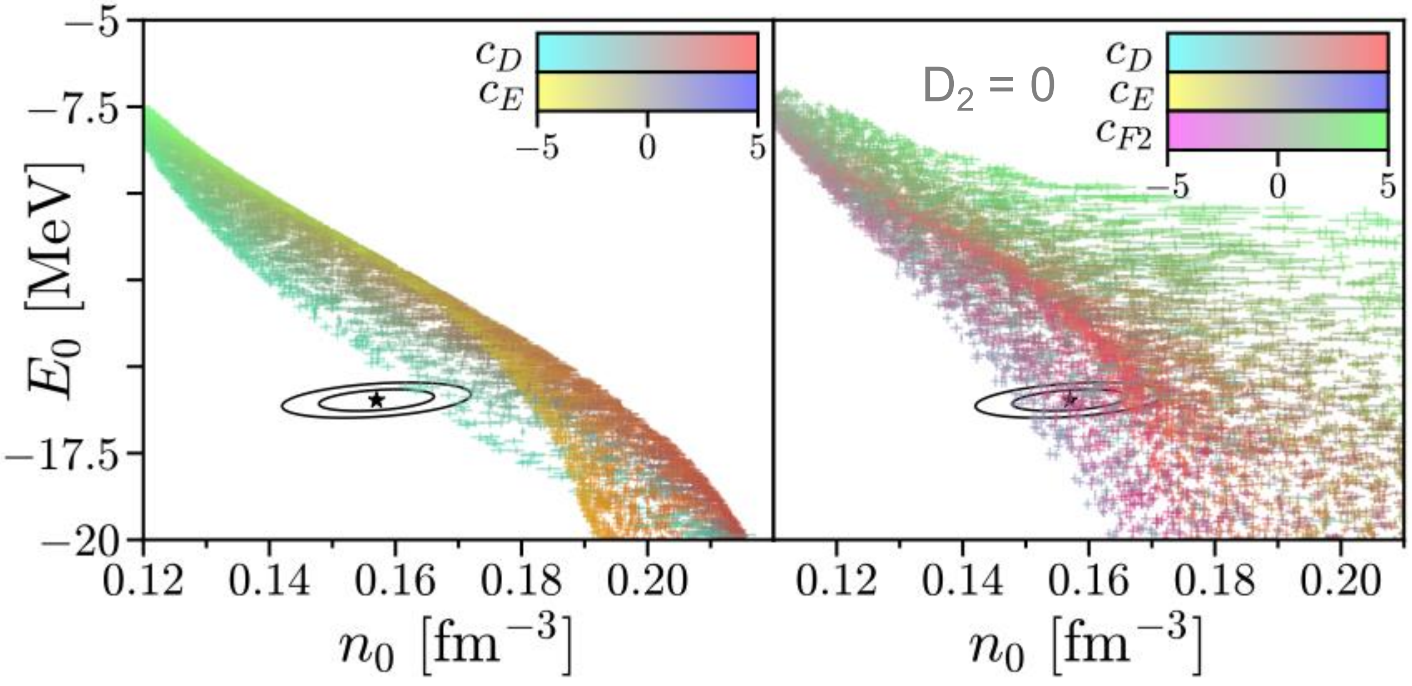




For >20% levels on the **Test Data**, the maximum:

- **over-coverage** is < 2.5%
- **under-coverage** is < 0.35%

All degrees of freedom varied (LECs, density, etc.)

Do the quark-mass-dependent 3N forces (D_2/F_2) help improve the saturation properties of NN+3N forces?

If so, what are the consequences for finite nuclei?

Cirigliano, Dawid, Dekens, and Reddy, PRL **135**, 022501
Vernik, Hebeler, and Schwenk, arXiv:2512.20454

Take-away points

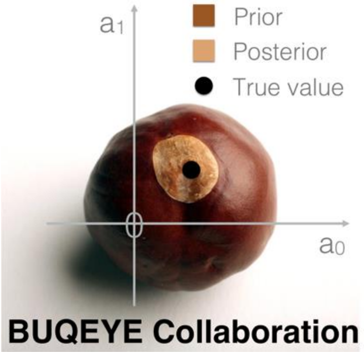
Source codes are (or will be made) publicly available!

1. **Emulators are *game changers* for principled UQ (and more!) in nuclear physics. This talk: RBM and PMM emulators**

2. **Active learning ("greedy") approach to snapshot selection** allows for the construction of fast & accurate emulators for **two- and three-body scattering: with estimation and propagation of emulator errors**

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 emulators are available. Which ones are the most efficient and/or reliable in practice?**



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

Food for thought and discussion

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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- and three-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 can we learn from the low-rank structure of chiral forces? How can we exploit that feature?

What are the best practices for deploying ROMs efficiently? What can we learn from MOR software libraries?

Can we construct improved ROMs via Petrov-Galerkin projection? These are more *general* than 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?

Low-rank updates of the T-matrix

Needs:
Applicable to LSE-like equations
Low-rank updates of the potential (nonlocal?)

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Exact emulation of few-body systems at low cost

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$$\mathbb{T} = \mathbb{V} + \mathbb{V}\mathbb{G}\mathbb{T}$$

Pion exchanges

Contacts

$$\mathbb{V} = \mathbb{V}_0 + \underbrace{\sum_i c_i \mathbb{V}_i}_{=\mathbb{X}\mathbb{C}\mathbb{Z}}$$

FOM solution at reference LECs

derived using the **Woodbury identity** for matrix inversion

$$\mathbb{T} = \mathbb{T}_0 + \tilde{\mathbb{X}}\tilde{\mathbb{C}}\tilde{\mathbb{Z}}, \qquad \text{where}$$

$$\tilde{\mathbb{C}} \equiv \left[\mathbb{1}_r - \mathbb{C}\mathbb{Z}\mathbb{G}(\mathbb{T}_0\mathbb{G} + \mathbb{1}_n)\mathbb{X}\right]^{-1}\mathbb{C},$$

$$\tilde{\mathbb{X}} \equiv (\mathbb{T}_0\mathbb{G} + \mathbb{1}_n)\mathbb{X} \quad \text{and} \quad \tilde{\mathbb{Z}} \equiv \mathbb{Z}(\mathbb{1}_n + \mathbb{G}\mathbb{T}_0).$$

$^1S_0$ **contact interactions** — **regulator**

$$\left(c_1u_1 + c_2u_2(p'^2 + p^2) + c_3u_3p'^2p^2\right)e^{-(p'^2+p^2)/\Lambda^2} \equiv \begin{pmatrix} e^{-p'^2/\Lambda^2} & p'^2e^{-p'^2/\Lambda^2} \end{pmatrix} \begin{pmatrix} c_1u_1 & c_2u_2 \\ c_2u_2 & c_3u_3 \end{pmatrix} \begin{pmatrix} e^{-p^2/\Lambda^2} \\ p^2e^{-p^2/\Lambda^2} \end{pmatrix}$$