Emulators for nuclear physics across energy scales

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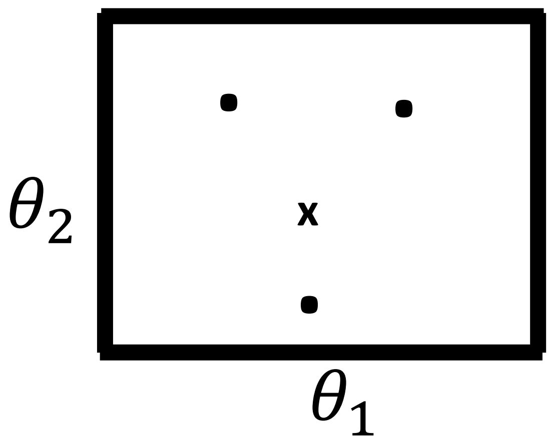
INT program (INT-23-1A):
Intersection of nuclear structure and high-energy nuclear collisions, Feb. 2023, Seattle, WA

Outline

- Two main types of emulators: projection-based and data-driven
- Data-driven emulators in heavy-ion collision physics
- Projection-based emulators in low-energy nuclear physics and hadronic physics
- Relevance for connecting nuclear structure and high-energy nuclear collisions?

Emulator (surrogate model) enables fast and accurate interpolation and extrapolation of model **outputs** in the **input** parameter space

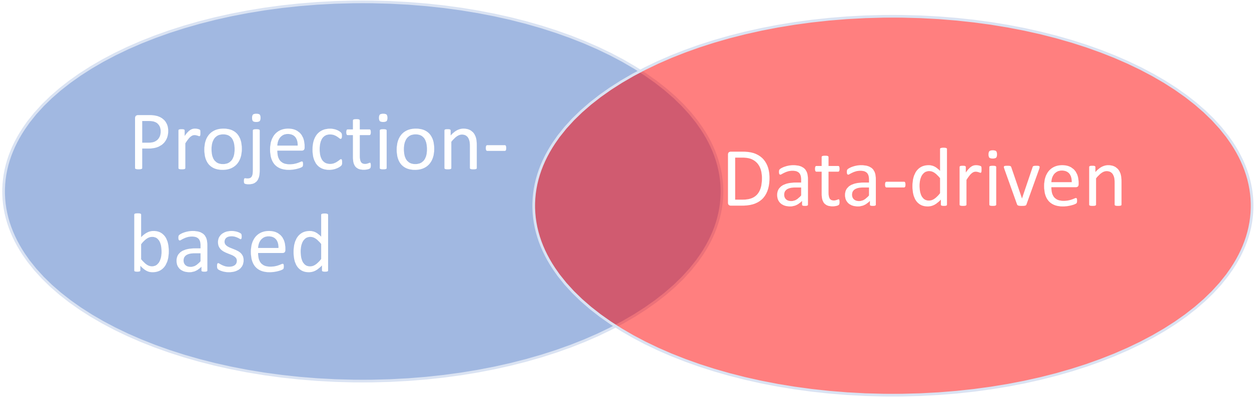
- Model calibration
- Feasible calculation→ infeasible region



Parameter space ($\boldsymbol{\theta}$)

“Eigenvector continuation with subspace learning”
Dillon Frame et. al., *Phys.Rev.Lett.* 121 (2018) 3, 032501, 1711.07090

Emulators



- Reduced basis method (RBM); also known as eigenvector continuation (EC) in nuclear physics
- Intrusive
- but includes more physics and requires less training data

- Machine learning (ML): Gaussian process and neural networks
- nonintrusive
- agnostic of physics and requires more training data

“BUQEYE Guide to Projection-Based Emulators in Nuclear Physics,” C. Drischler, J.A. Melendez, R.J. Furnstahl, A.J. Garcia, and XZ, 2212.04912
“Training and projecting: A reduced basis method emulator for many-body physics,” Edgard Bonilla, Pablo Giuliani, Kyle Godbey, Dean Lee, *Phys.Rev.C* 106 (2022) 5, 054322, 2203.05284
“Model reduction methods for nuclear emulators, ” J.A. Melendez, C. Drischler, R.J. Furnstahl, A.J. Garcia, XZ, 2203.05528

Taken from 1310.0222

Data-driven emulators in heavy-ion collision physics

Emulator: Gaussian process

PHYSICAL REVIEW C **103**, 054904 (2021)

Multisystem Bayesian constraints on the transport coefficients of QCD matter

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(JETSCAPE Collaboration)

PHYSICAL REVIEW C **104**, 024905 (2021)

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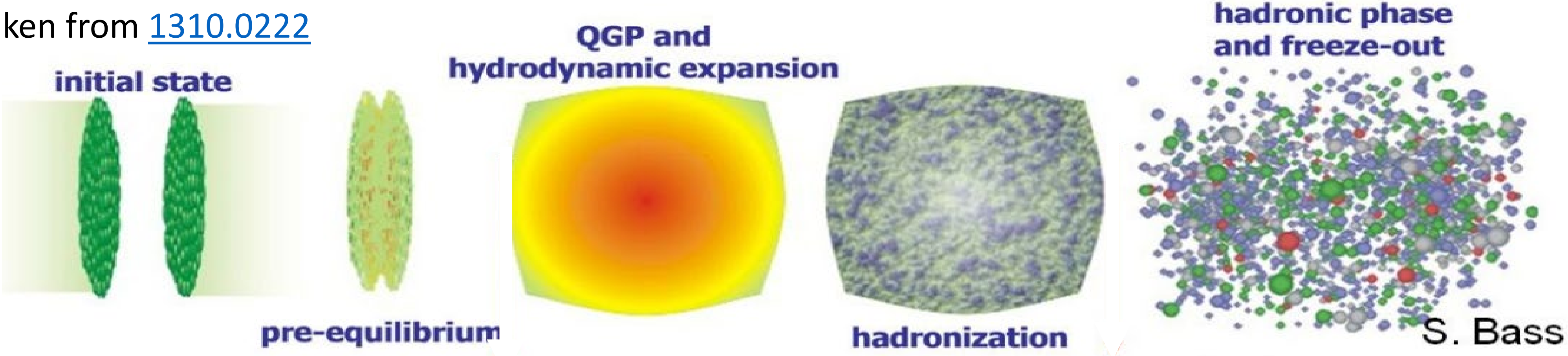

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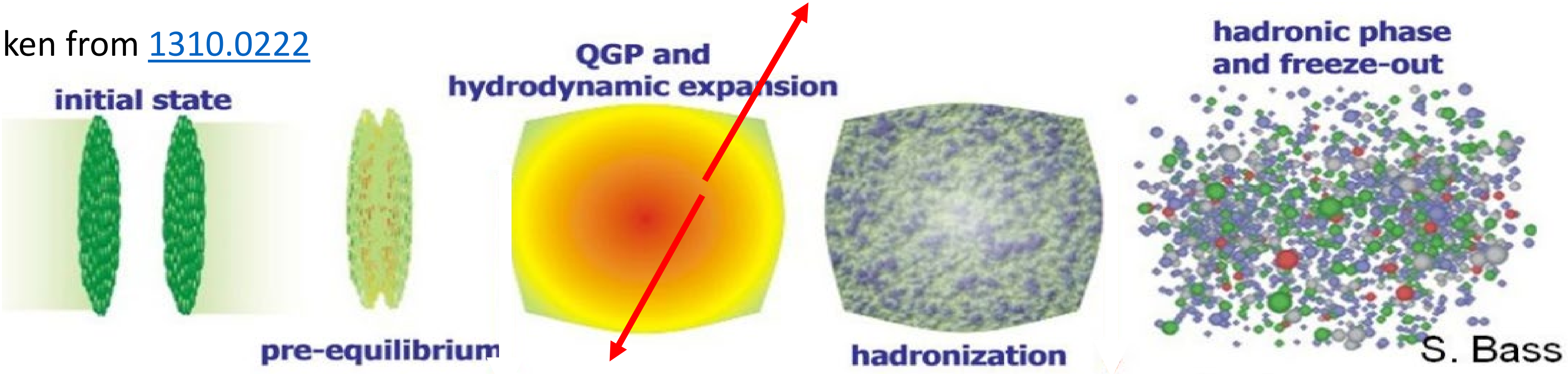

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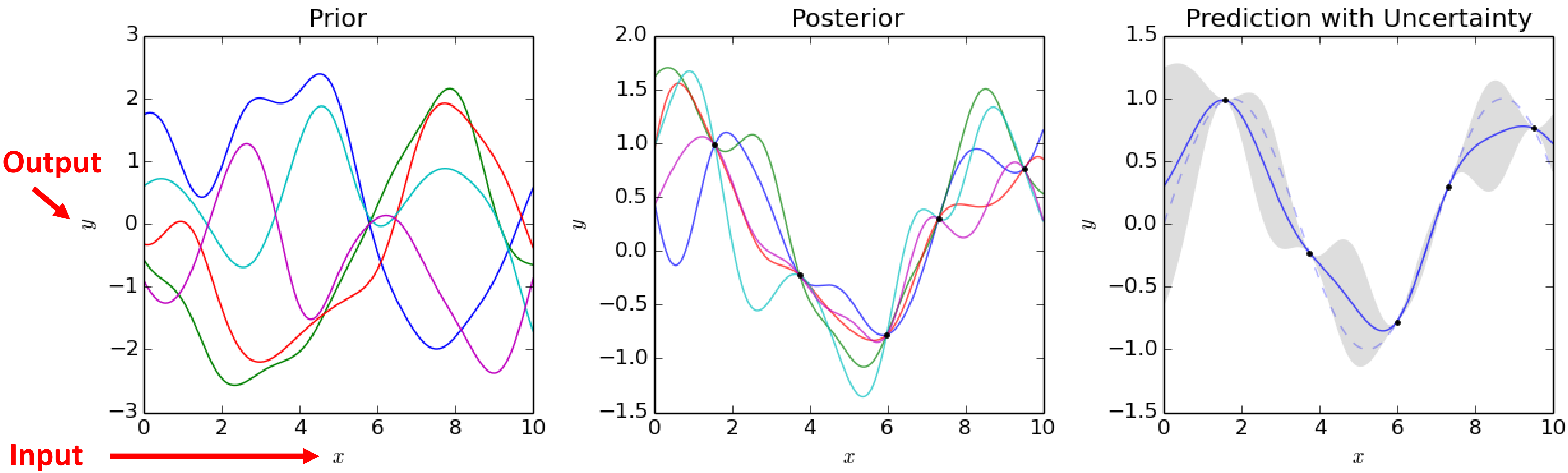
Data-driven emulators

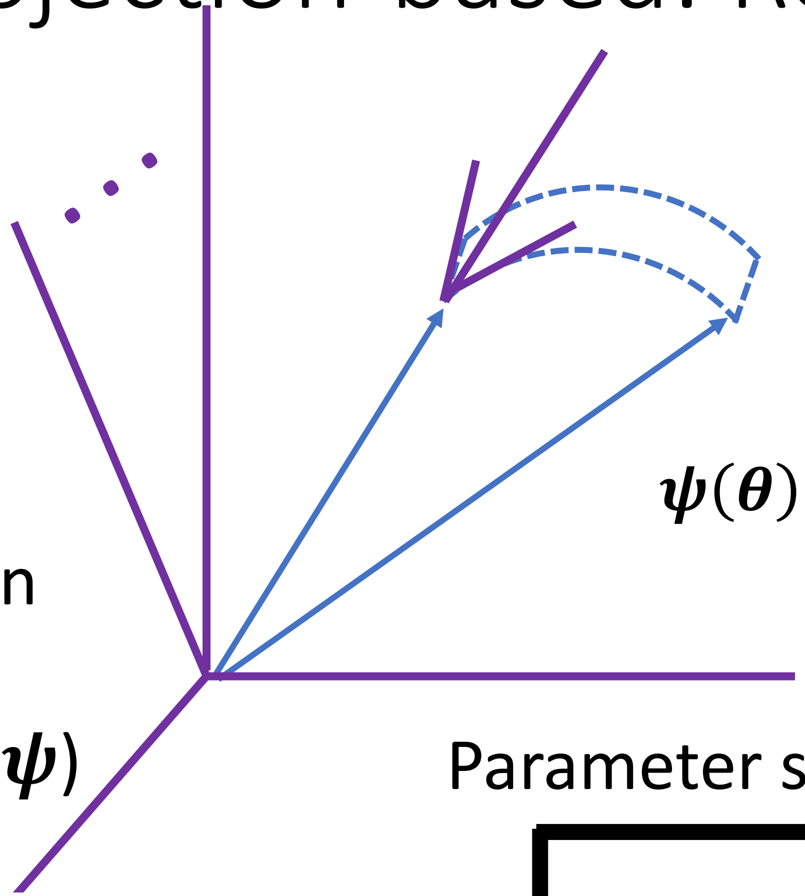
Gaussian process



Neural networks

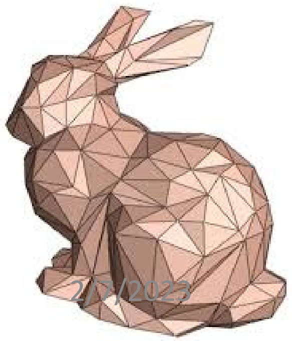
Universal functions with hyperparameters → conditioned on data
→ interpolation and extrapolation

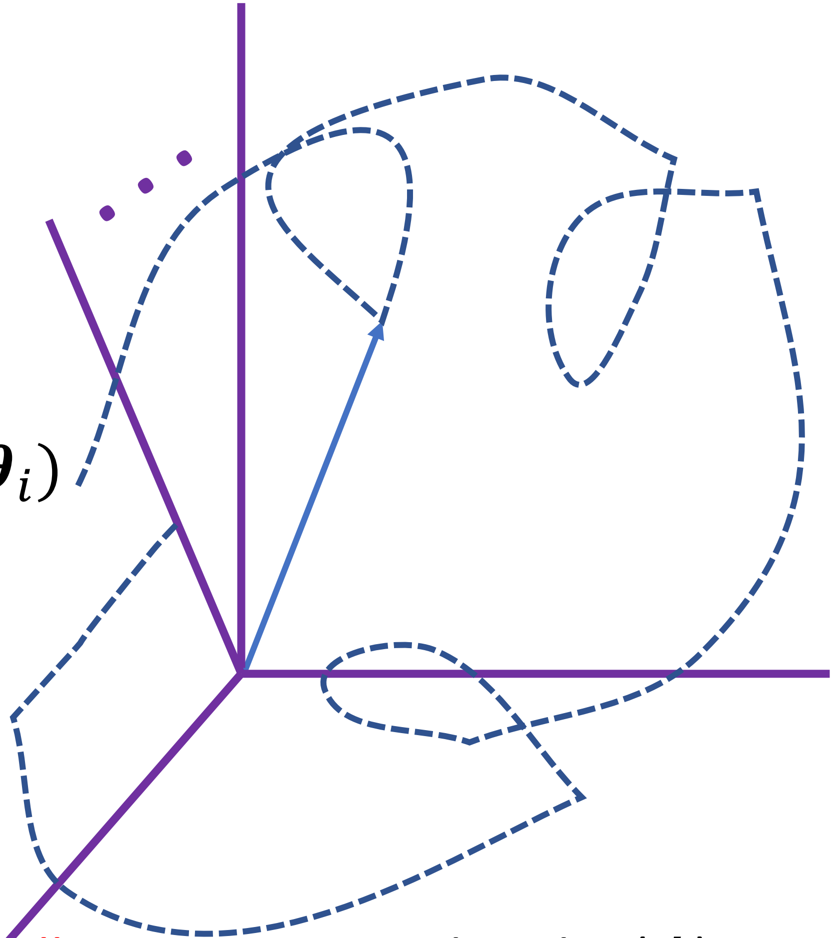
Projection-based: Reduced basis method



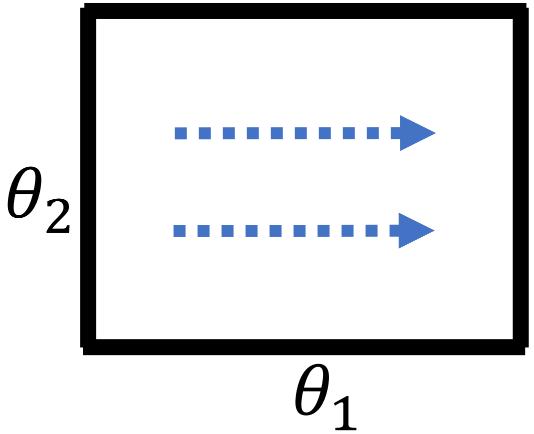
Solution vector space ($\boldsymbol{\psi}$)

$$\boldsymbol{\psi}(\boldsymbol{\theta}) = \sum_{i=1}^{N_b} C_i(\boldsymbol{\theta})\, \boldsymbol{\psi}(\boldsymbol{\theta}_i)$$





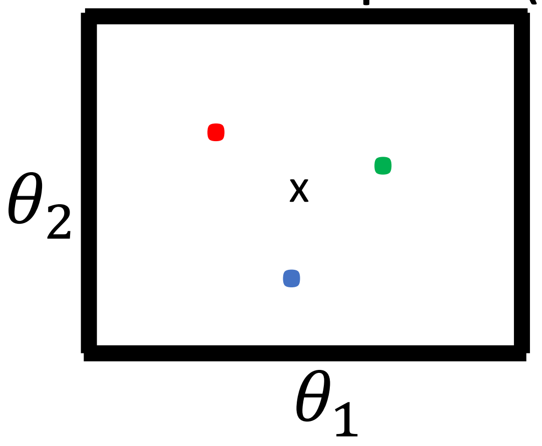
Parameter space ($\boldsymbol{\theta}$)



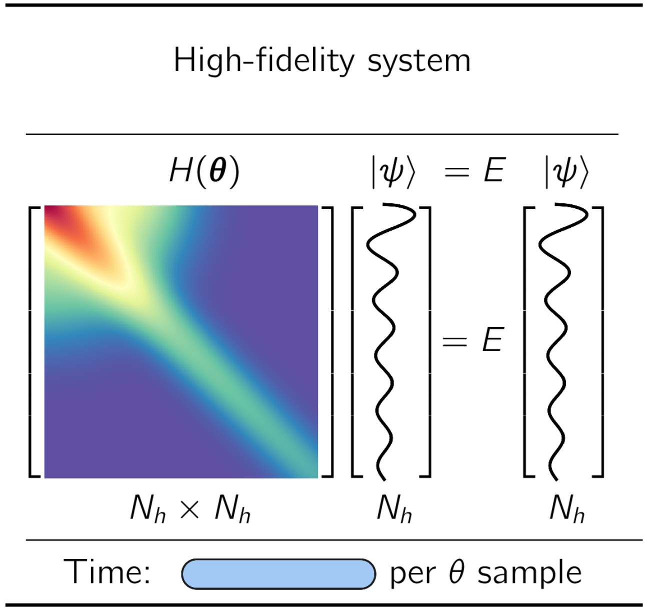
- Small N_b as compared to dim($\boldsymbol{\psi}$)
- Variational (Galerkin in general) method for solving $C_i(\boldsymbol{\theta})$: N_b-dim calculations
- Solved $\boldsymbol{\psi}$s need to be precise

RBM emulators for nuclear structure: eigen systems of *parametrized* quantum Hamiltonians $\boldsymbol{H(\theta)}$ (*large* dimensions for *many*-body systems)

Parameter space ($\boldsymbol{\theta}$)



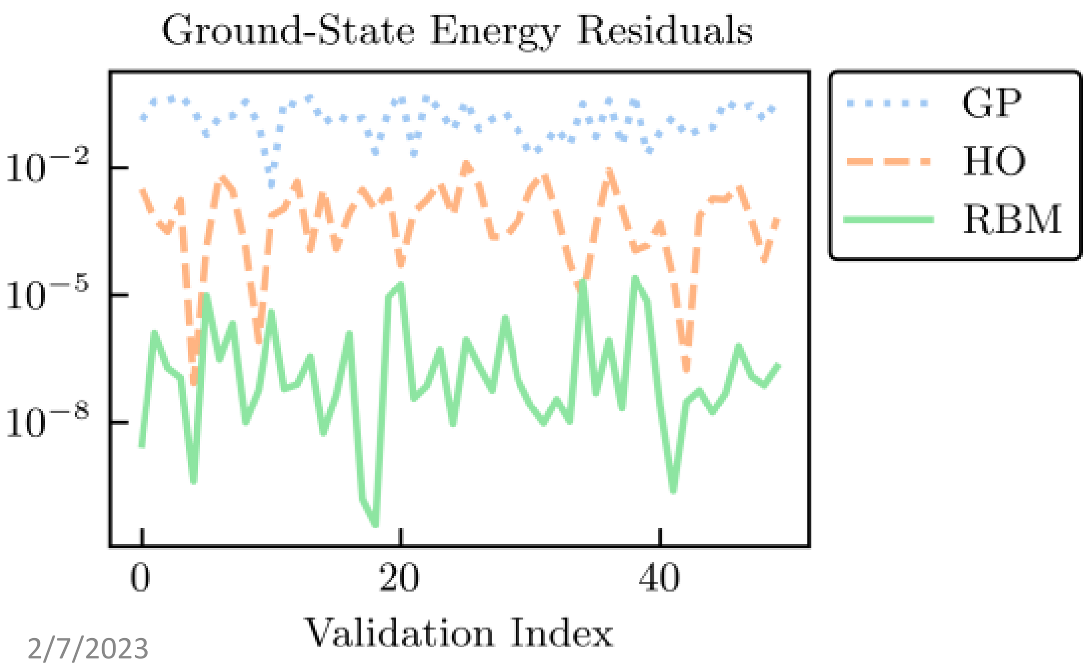
$$|\psi_t\rangle = \sum_{i=1}^{N_b} c_i |\psi_{\rm gs}(\boldsymbol{\theta}_i)\rangle$$

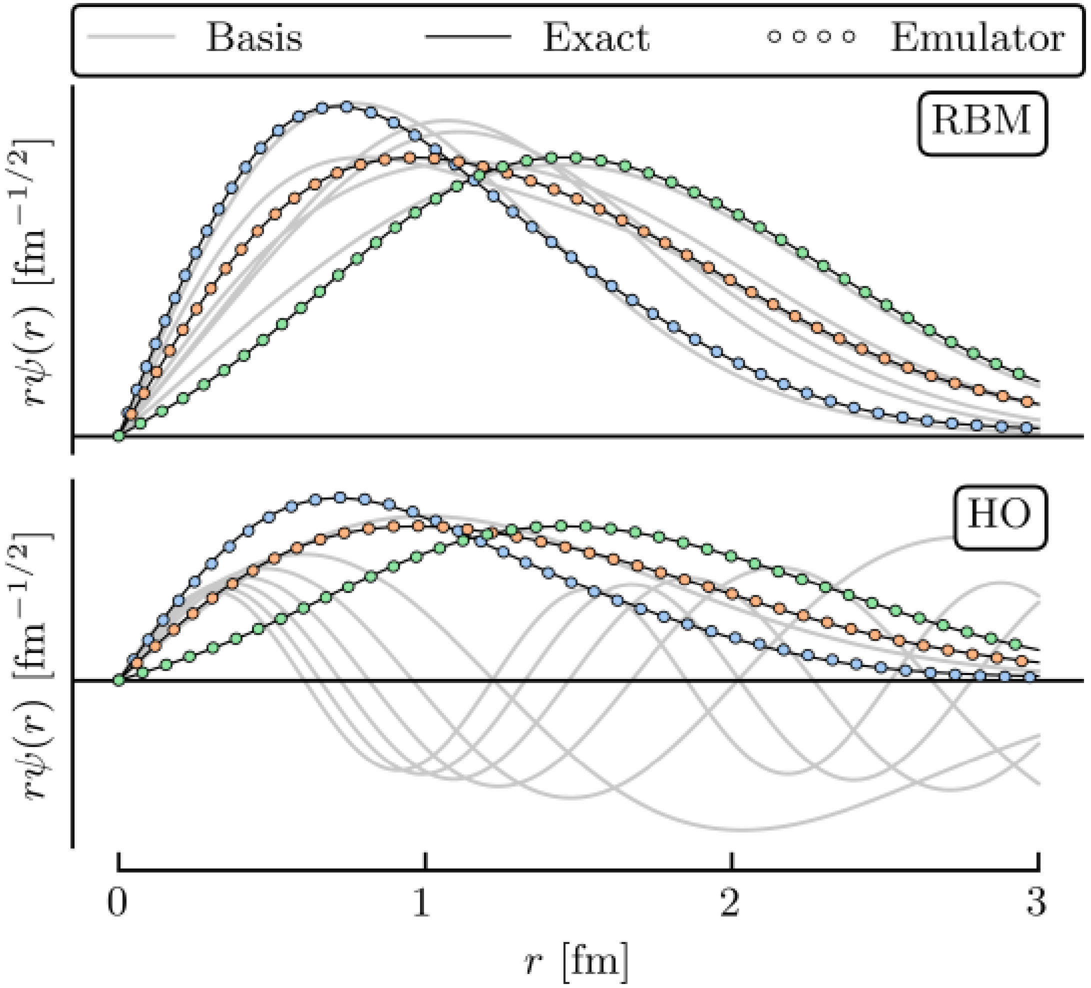


A toy-model demo

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

6 training points in 3-dim space





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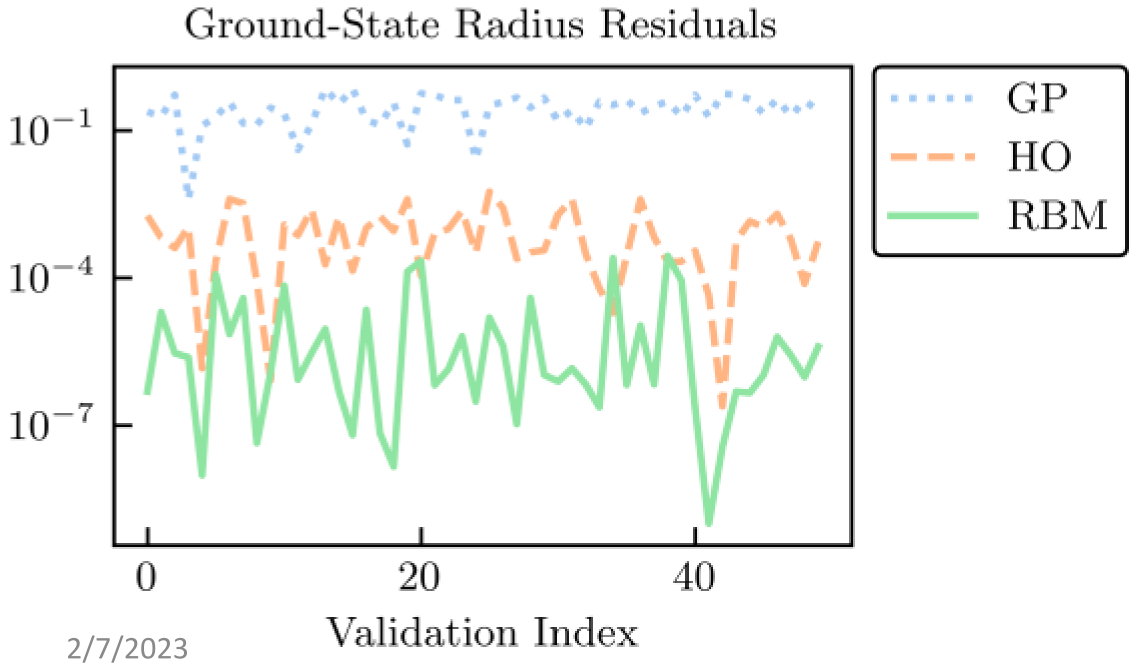
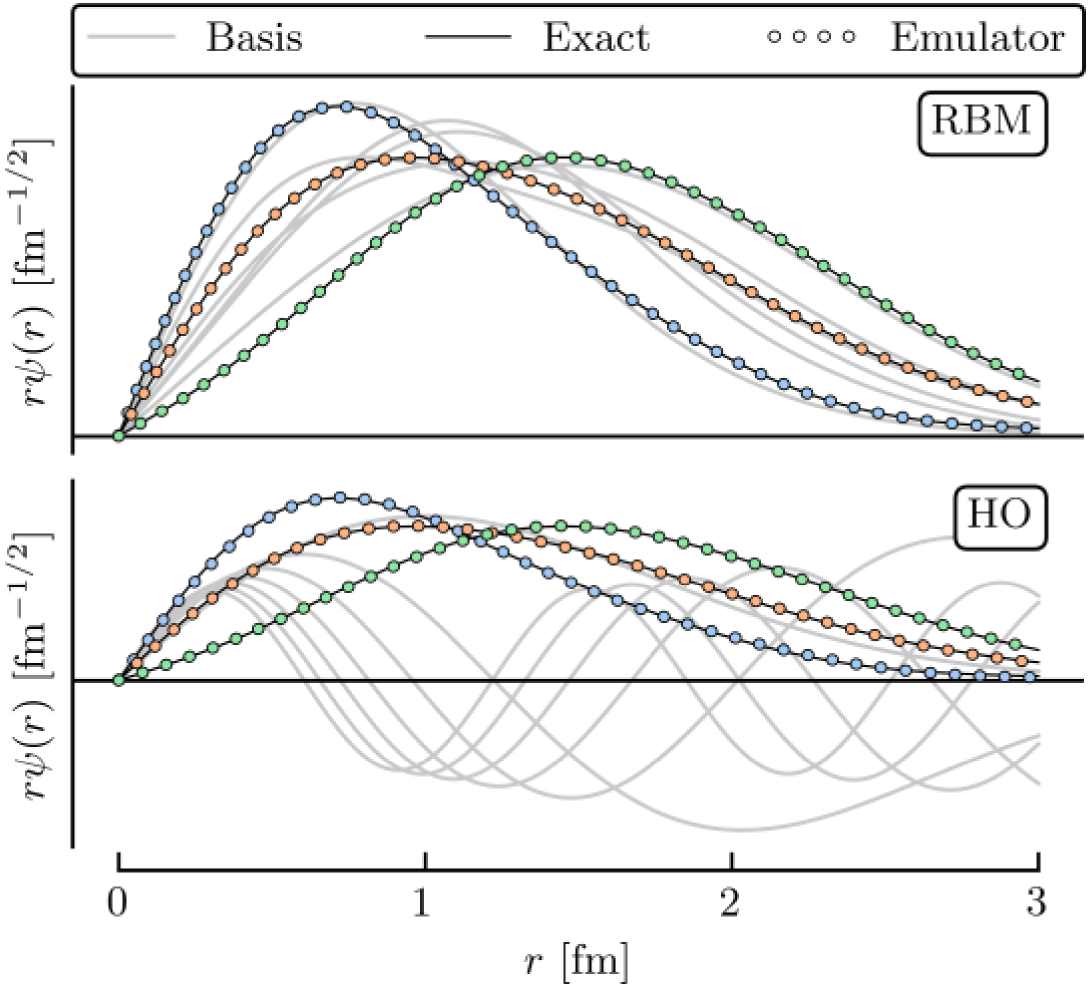
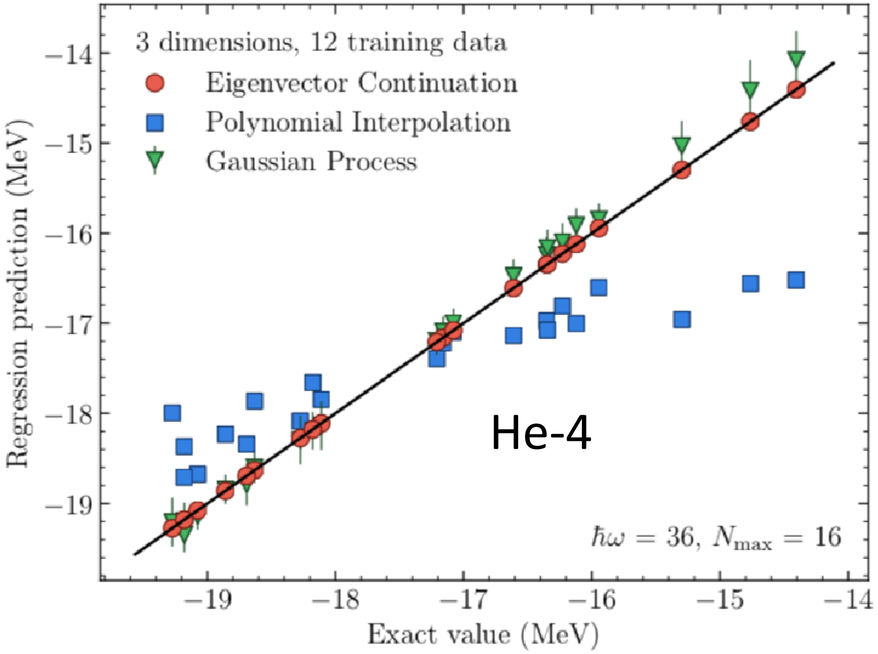




RBM emulator for ab initio nuclear structure calculations

S. König, A. Ekström, K. Hebeler, D. Lee, A. Schwenk
Eigenvector Continuation as an Efficient and Accurate Emulator for Uncertainty Quantification
Phys. Lett. B 810 (2020) 135814
arXiv:1909.08446



A. Ekström and G. Hagen
Global sensitivity analysis of bulk properties of an atomic nucleus
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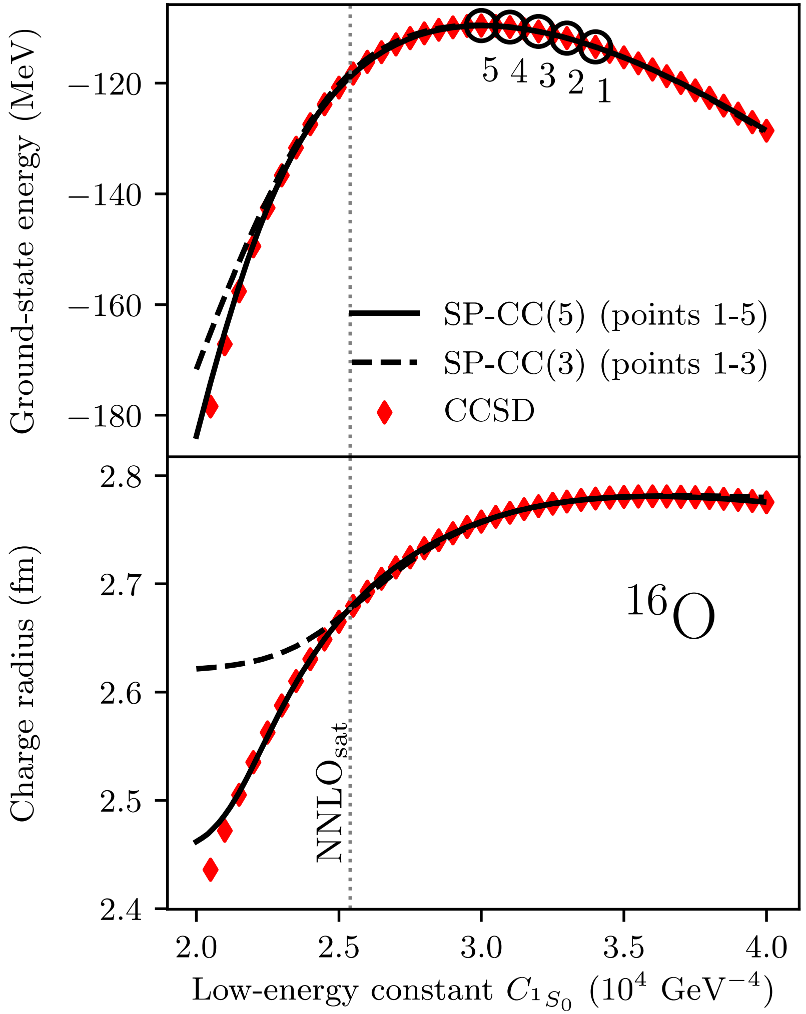

"about 1 Million sample in 16-dim space, 20 years calculation → 1 hour on a standard laptop."

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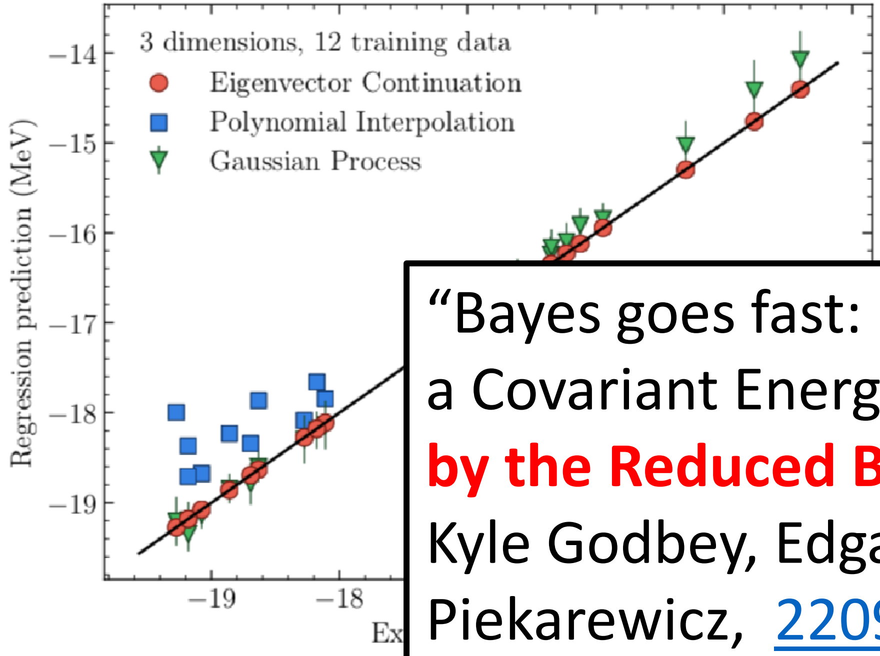

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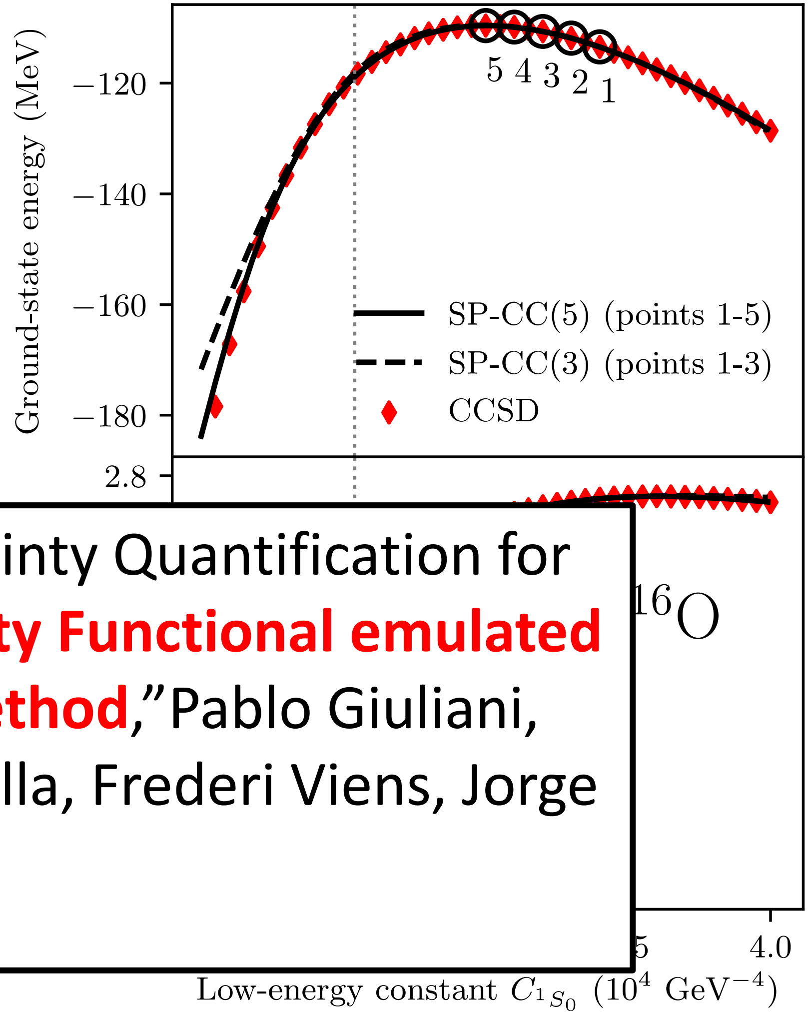


"Bayes goes fast: Uncertainty Quantification for a Covariant Energy **Density Functional emulated by the Reduced Basis Method**," Pablo Giuliani, Kyle Godbey, Edgard Bonilla, Frederi Viens, Jorge Piekarewicz, 2209.13039

"about 1 Million sample in 16-dim space, 20 years calculation → 1 hour on a standard laptop."

RBM emulators for nuclear continuum: inhomengenous linear equation (*large* dimensions for *few*-body systems)

- $[E - H(\boldsymbol{\theta})]|\psi(\boldsymbol{\theta})\rangle = 0$ for arbitrary E: for modeling nuclear scattering and reactions based on nucleon-nucleon interactions.

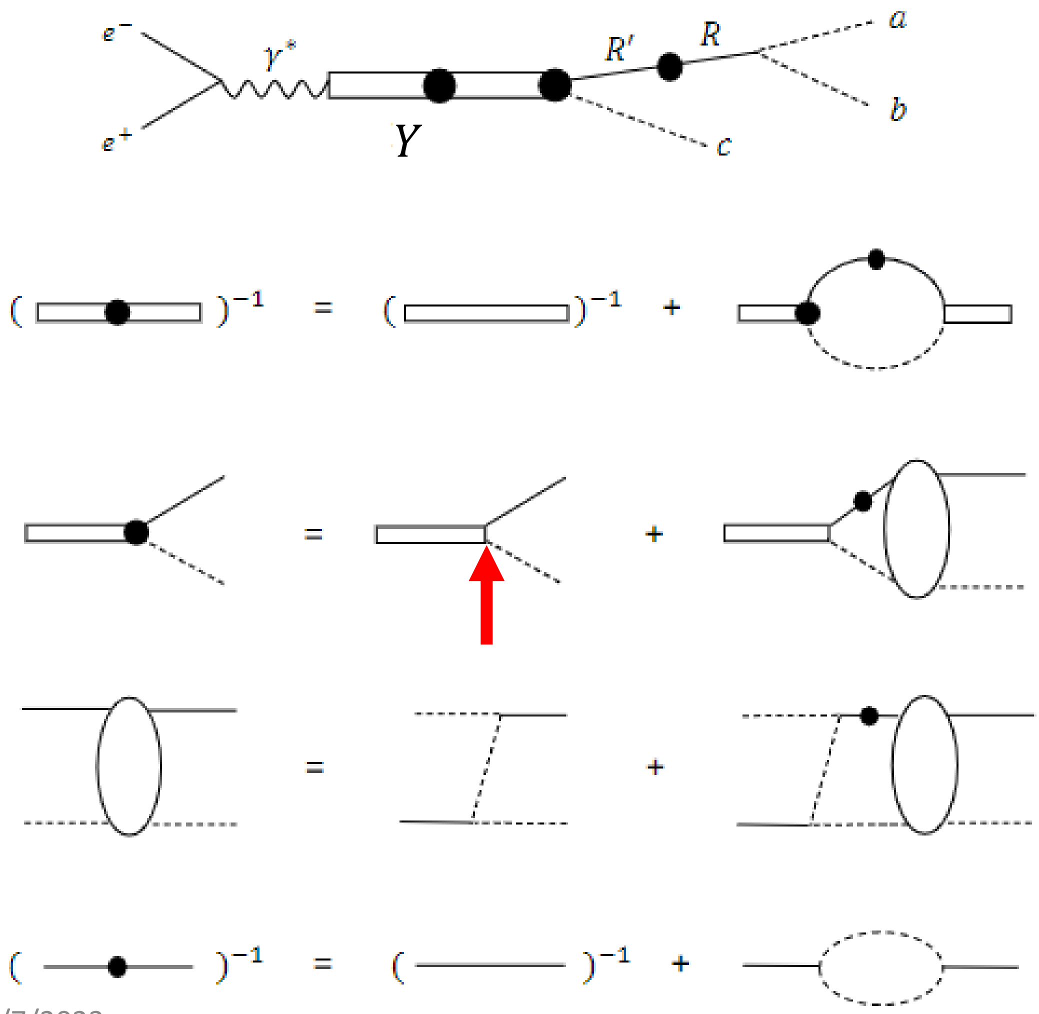
"Efficient emulators for scattering using eigenvector continuation,"R. J. Furnstahl, A. J. Garcia, P. J. Millican, and XZ, PLB **809,** 135719 (2020) [2007.03635]

Developed RBM emulator for two-body scatterings

"Fast emulation of quantum three-body scattering", XZ and R.J. Furnstahl, Phys. Rev. C 105, 064004 (2022), 2110.04269

EC emulators	S relative error	Time	Memory
linear[a]	10^{-14} to 10^{-13}	ms	$<$ MB
nonlinear-1	10^{-6} to 10^{-5}	ms	MB
nonlinear-2	10^{-4}	ms	10s MB

RBM emulators for hadronic reactions

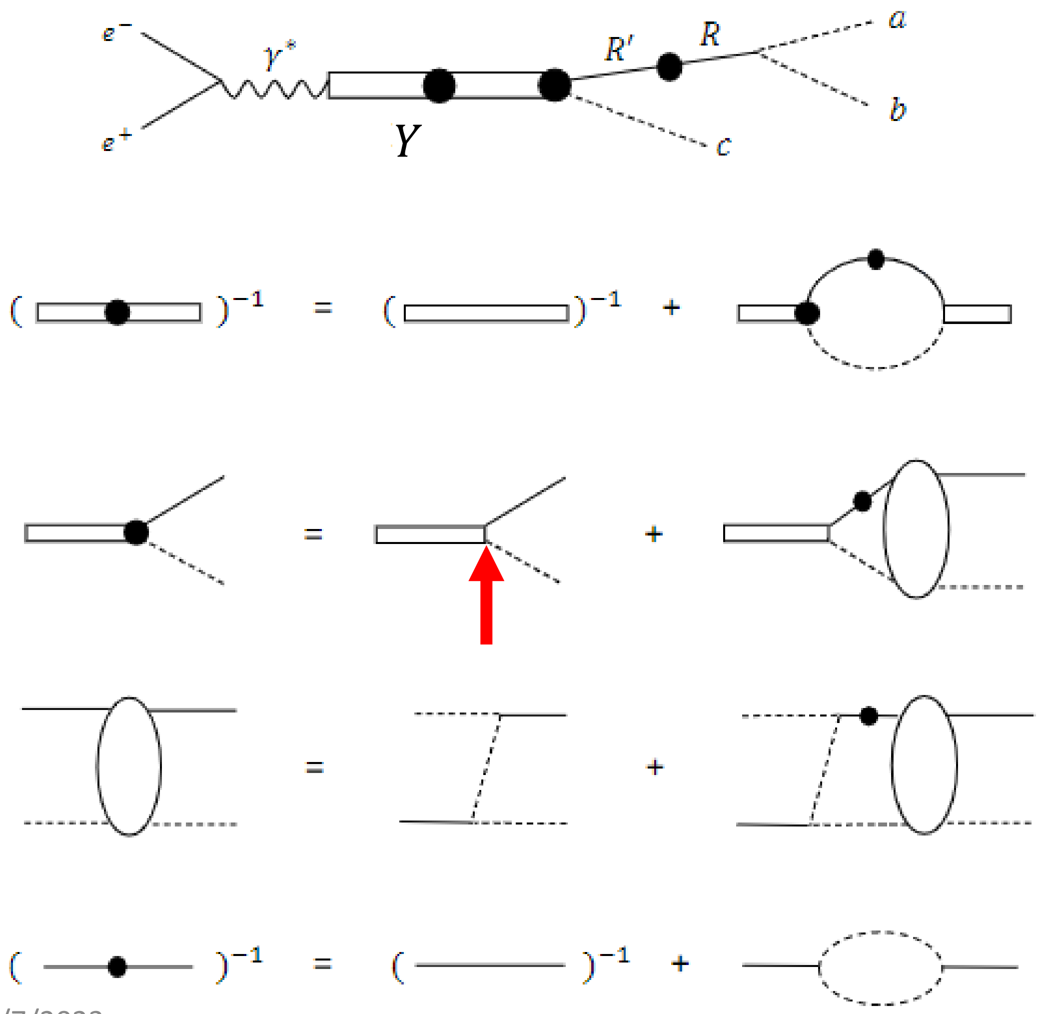


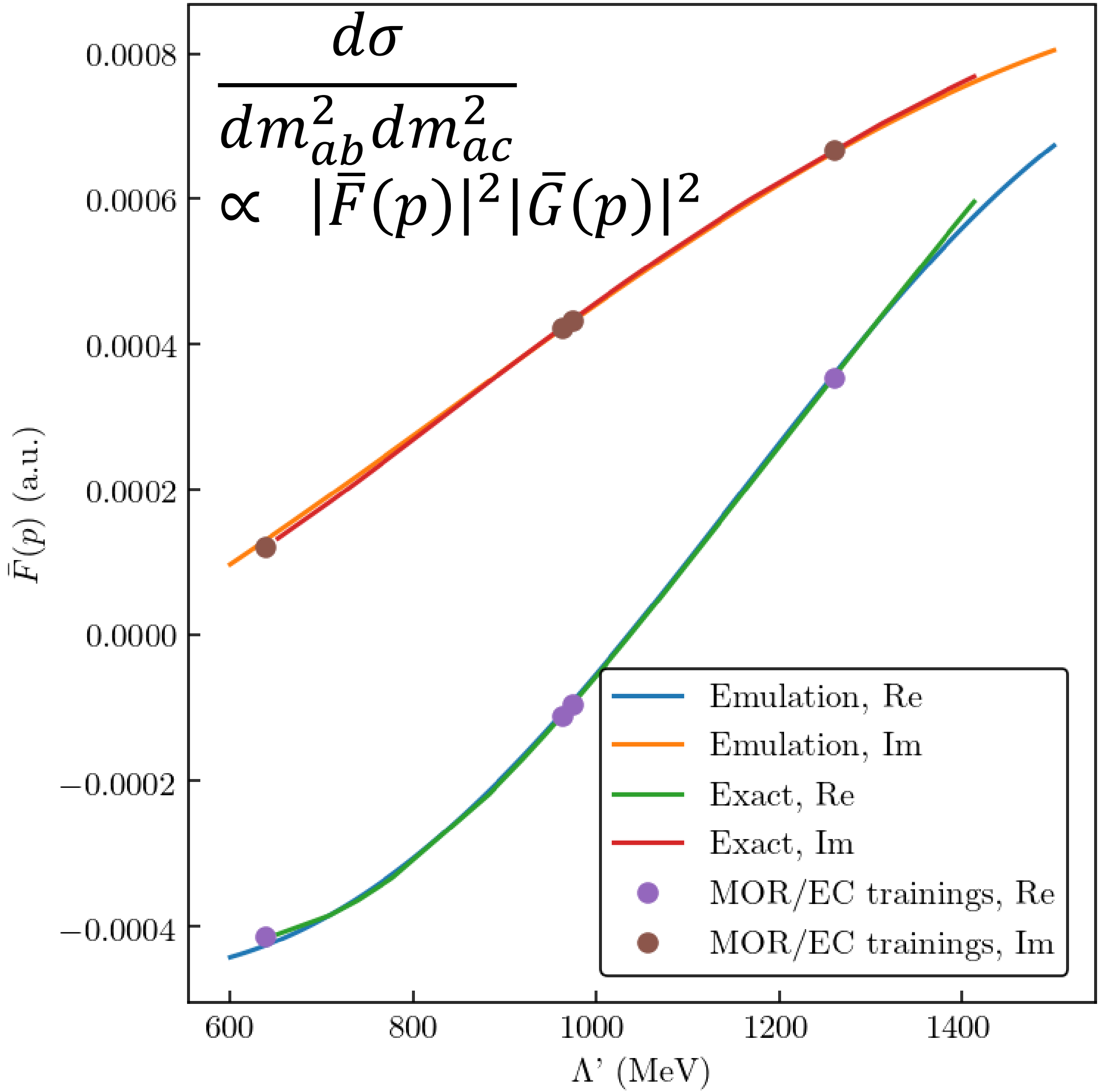
$$e^+ + e^- \rightarrow J/\psi + \pi + \pi$$

In collaboration with
Satoshi Nakamura (USTC)

- Coupled-integral equations
- 1-dim parameter space: varying Λ', the form factor for the coupling $Y \rightarrow R + c$

RBM emulators for hadronic reactions



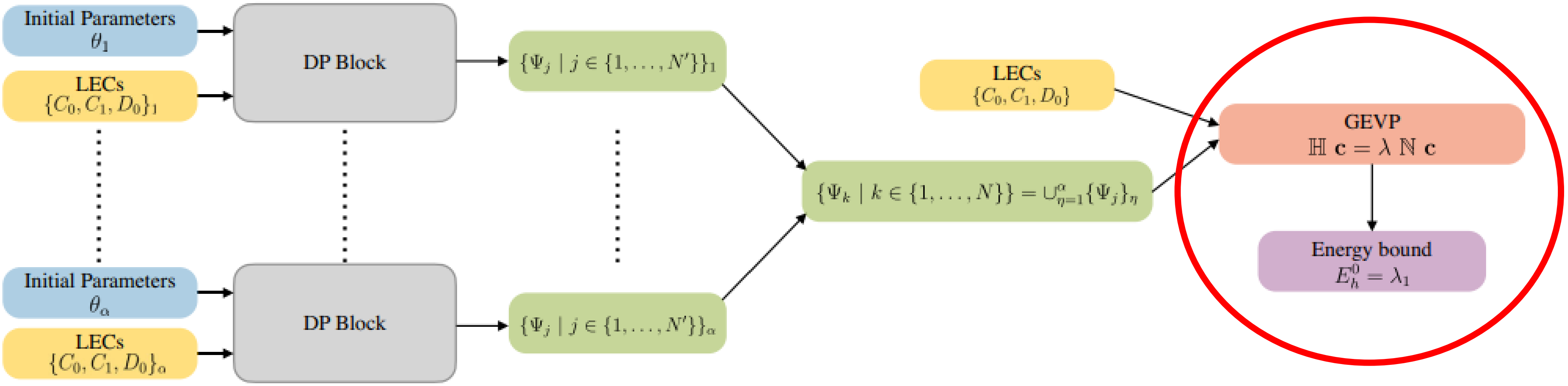


RBM emulators for calibrating model to Lattice QCD results

PHYSICAL REVIEW D **105**, 074508 (2022)

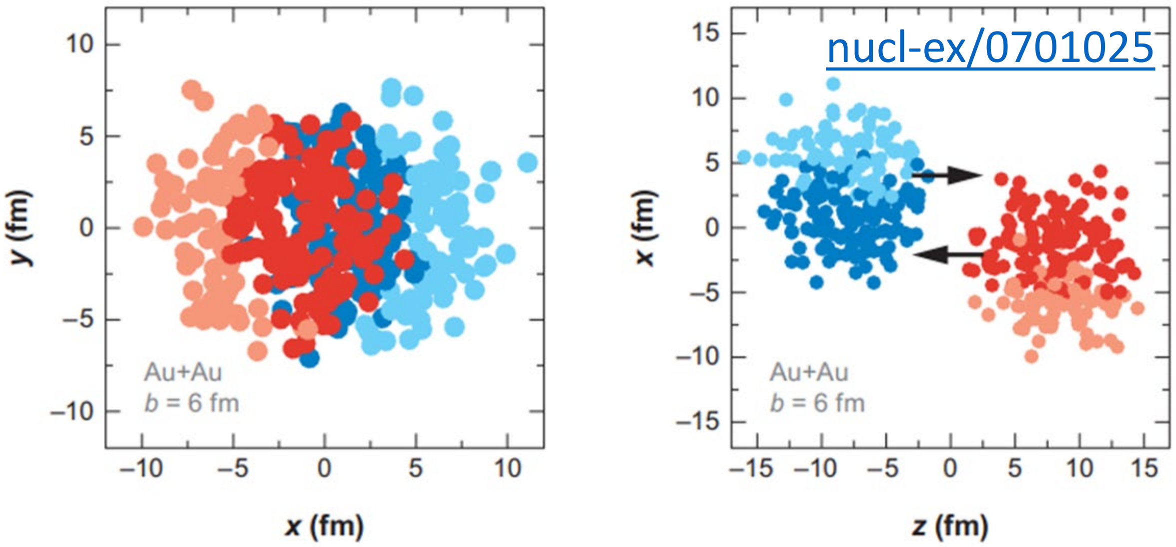
Finite-volume pionless effective field theory for few-nucleon systems with differentiable programming

Xiangkai Sun, William Detmold, Di Luo, and Phiala E. Shanahan



(b) Generalized eigenvalue problem (GEVP) block.

Emulators for connecting nuclear structure and high-energy nuclear collisions



- Data-driven emulators for dynamics after thermalizations
  - Projection-based emulators for relativistic hydrodynamic simulation?
- Projection-based emulator for nuclear wave functions
  - Can we define the nuclear-structure-input for heavy-ion simulations in terms of matrix elements of operators, so that we can be away from scheme/scale/model-dependence?
  - One-body densities in the “intrinsic” frame could be scheme-dependent.
  - Does the “deformed nucleus” picture (thinking nucleus as a deformed and rotating liquid drop) guarantee a systematic framework for multiple-particle correlations? I.e., do intrinsic shapes explain systematically all the multiple-particle correlations?

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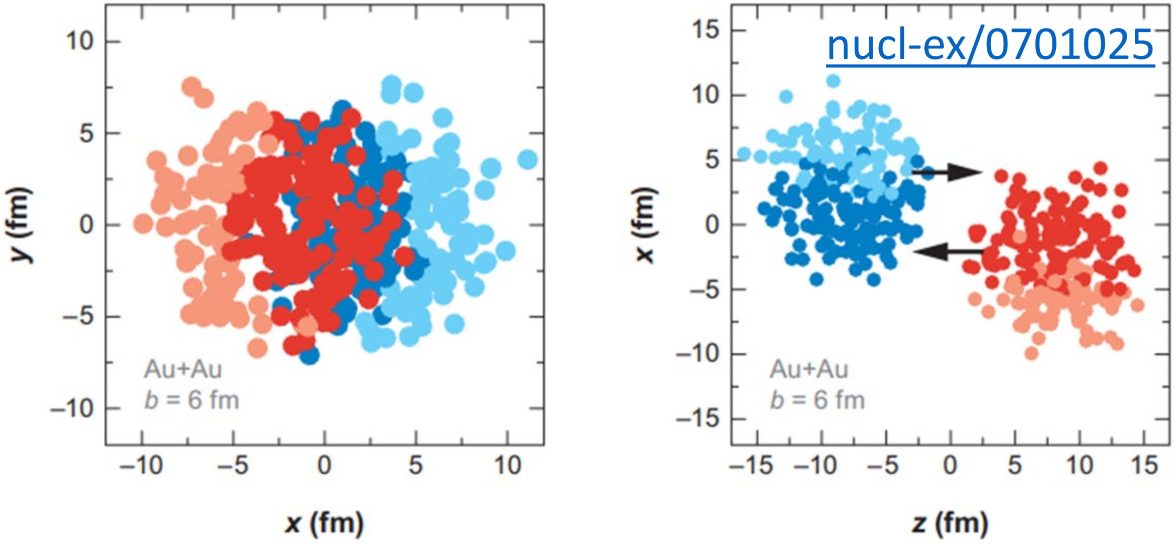

nucl-ex/0701025

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Summary

- Emulators are critical for fitting complex models
- Both projection-based and data-driven are being applied in different nuclear physics areas
- Nuclear structure emulator could be relevant for connecting nuclear structure and high-energy nuclear collisions