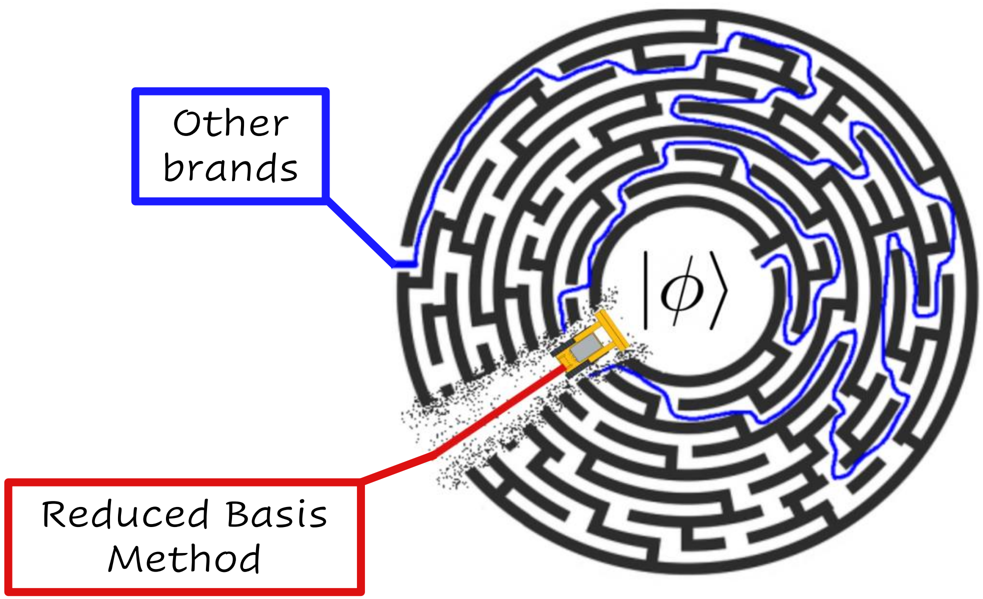
Reduced basis methods for uncertainty quantification in nuclear physics



Pablo Giuliani
giulianp@frib.msu.edu

Outline

Why → Uncertainty Quantification? ← How

The Reduced Basis Method

How it works

Problems table

Applications and Results

Takeaways

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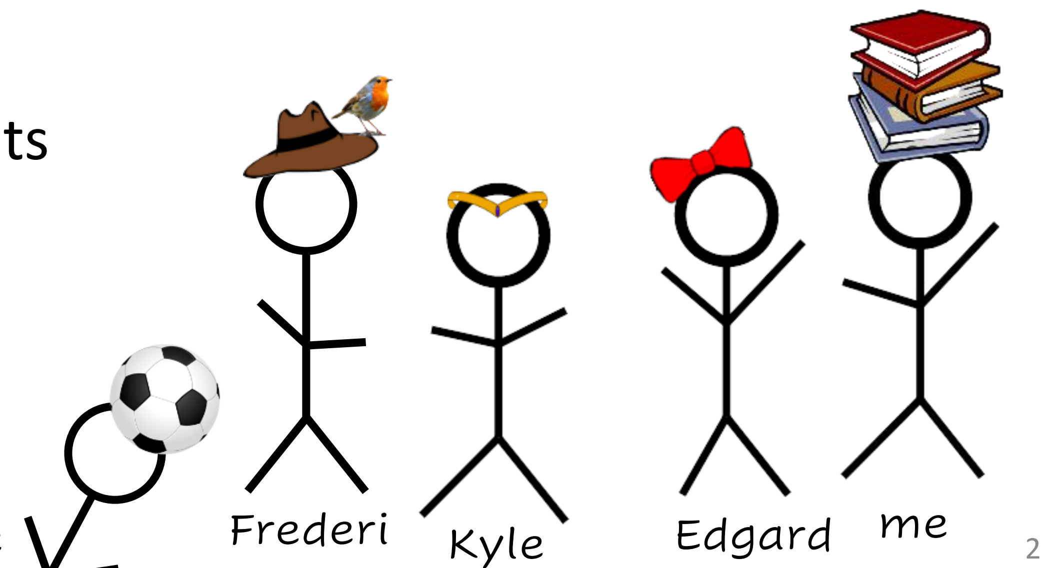

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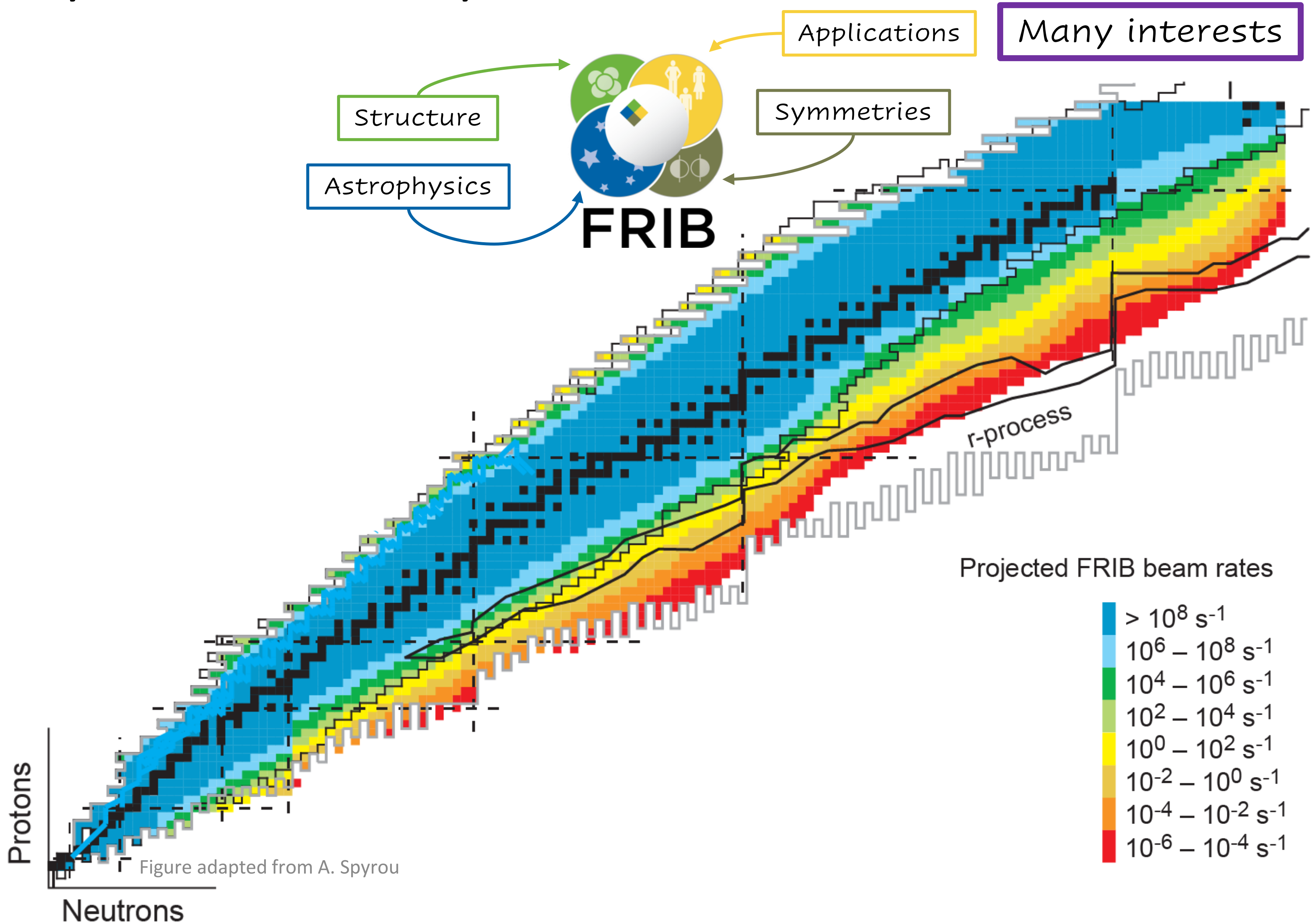


Figure adapted from A. Spyrou

Why Uncertainty Quantification?

r-process

Lifetimes (Fission) (β decay)

Masses Capture rates …

Structure

Applications

Many interests

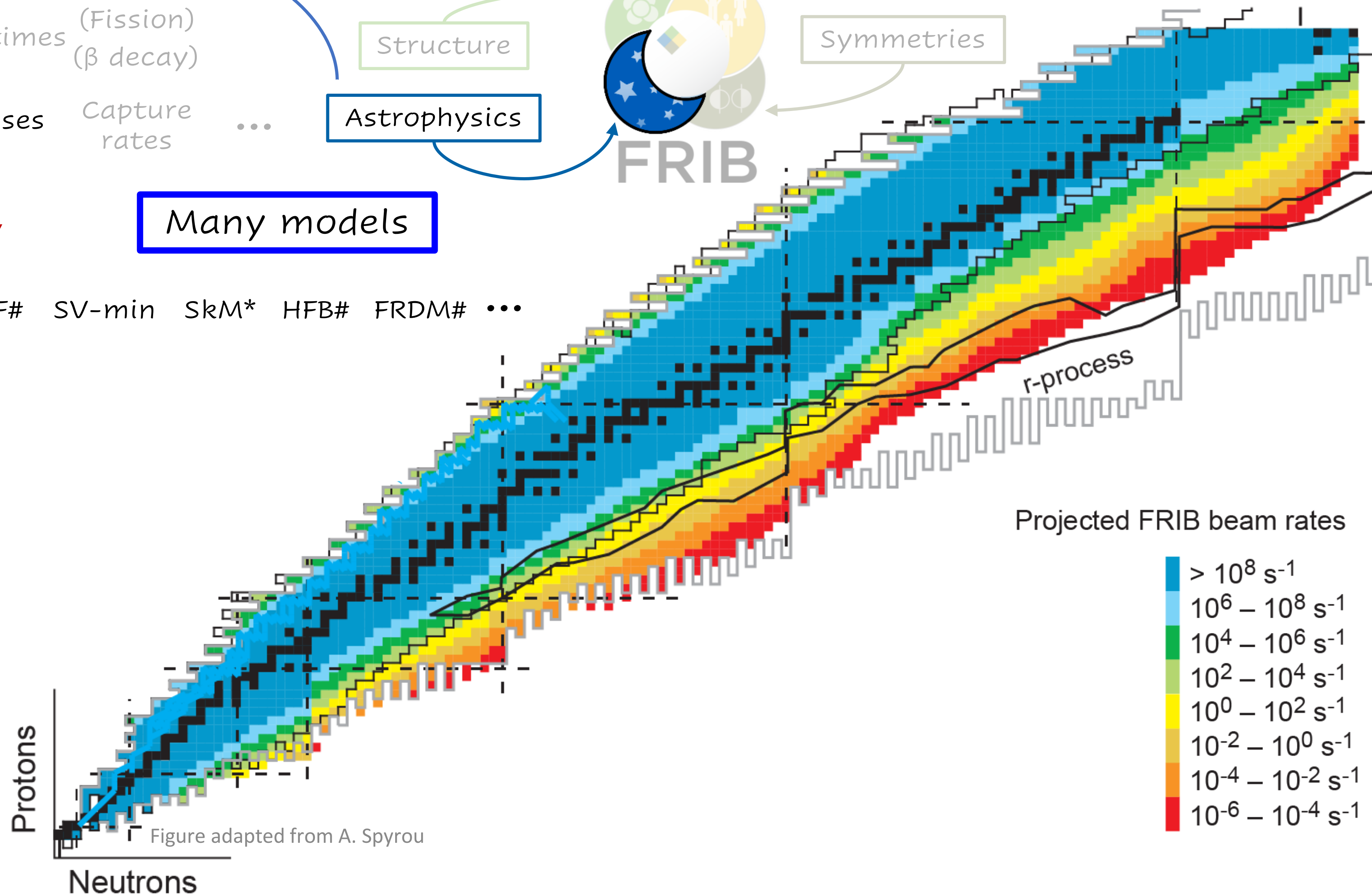
Symmetries

Astrophysics

FRIB

Many models

UNEDF# SV-min SkM* HFB# FRDM# •••



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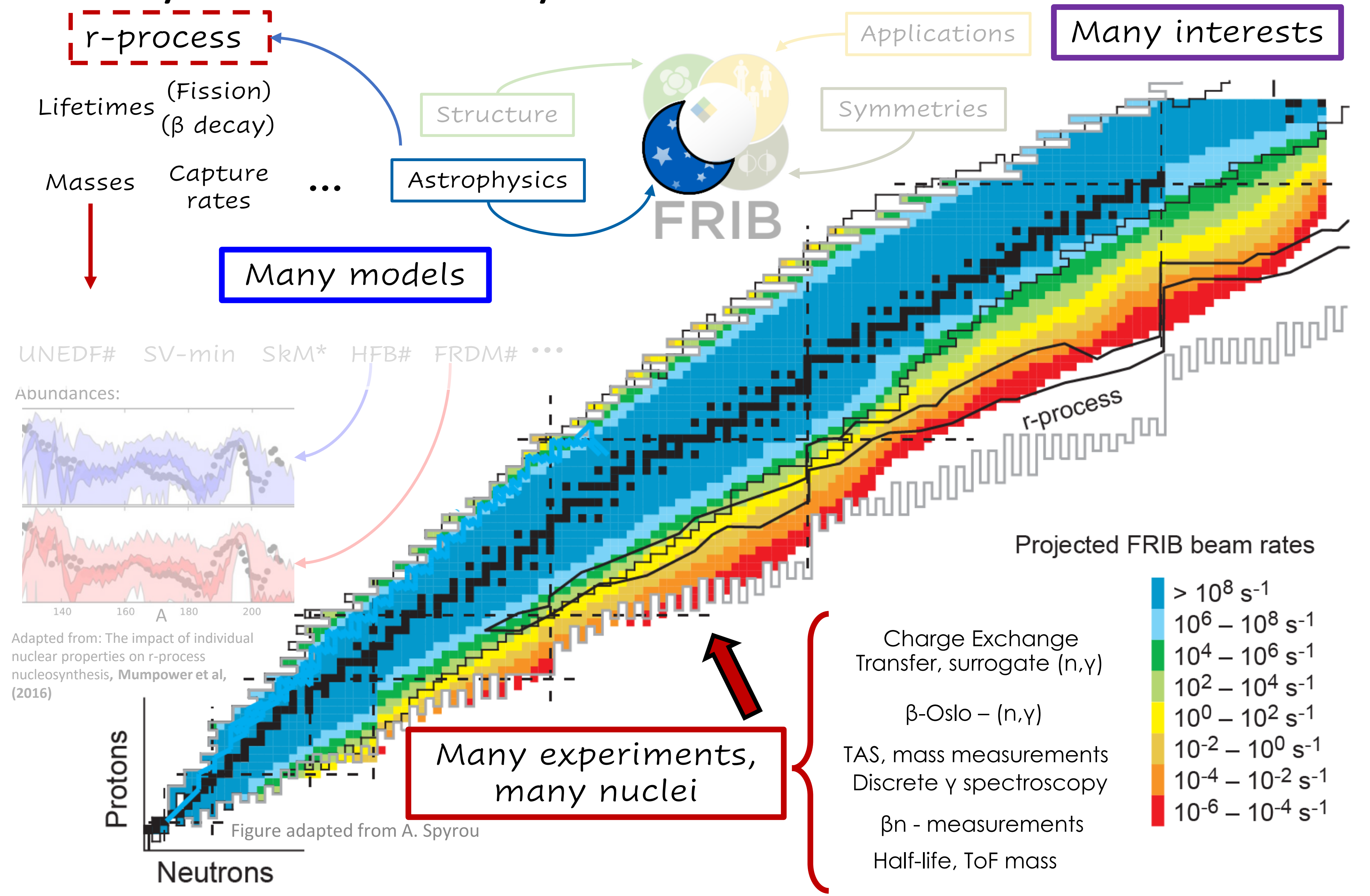

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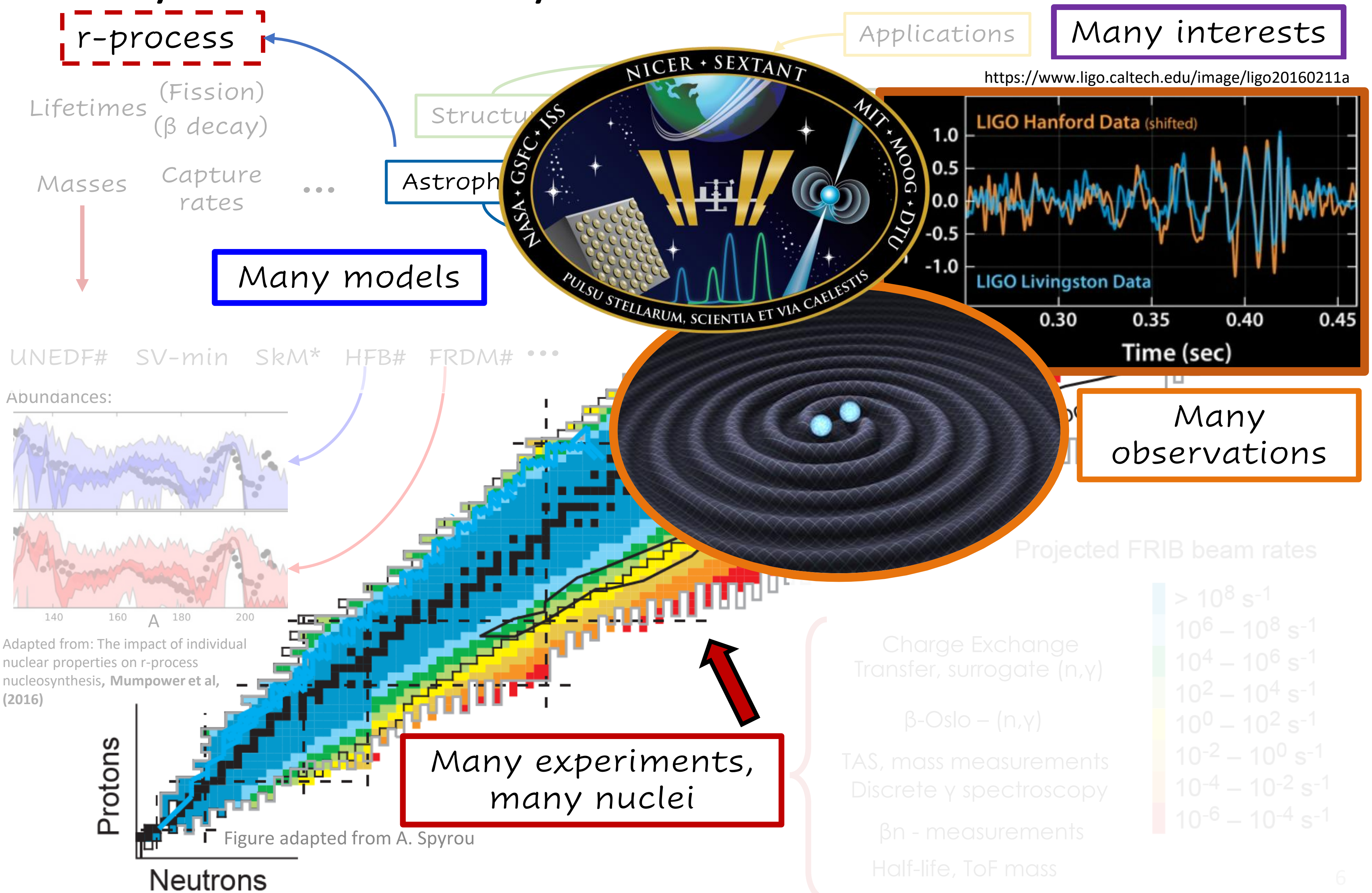

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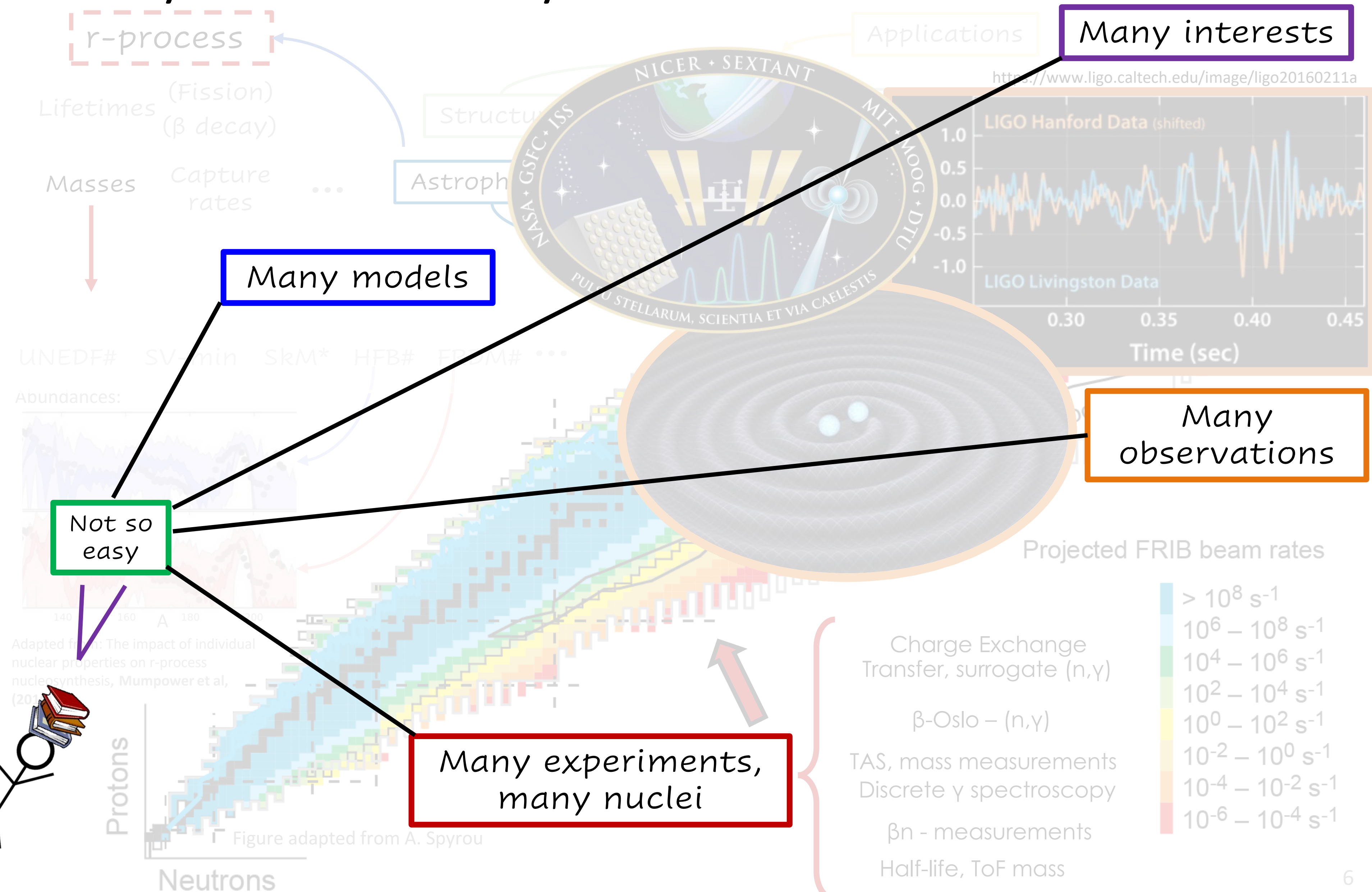

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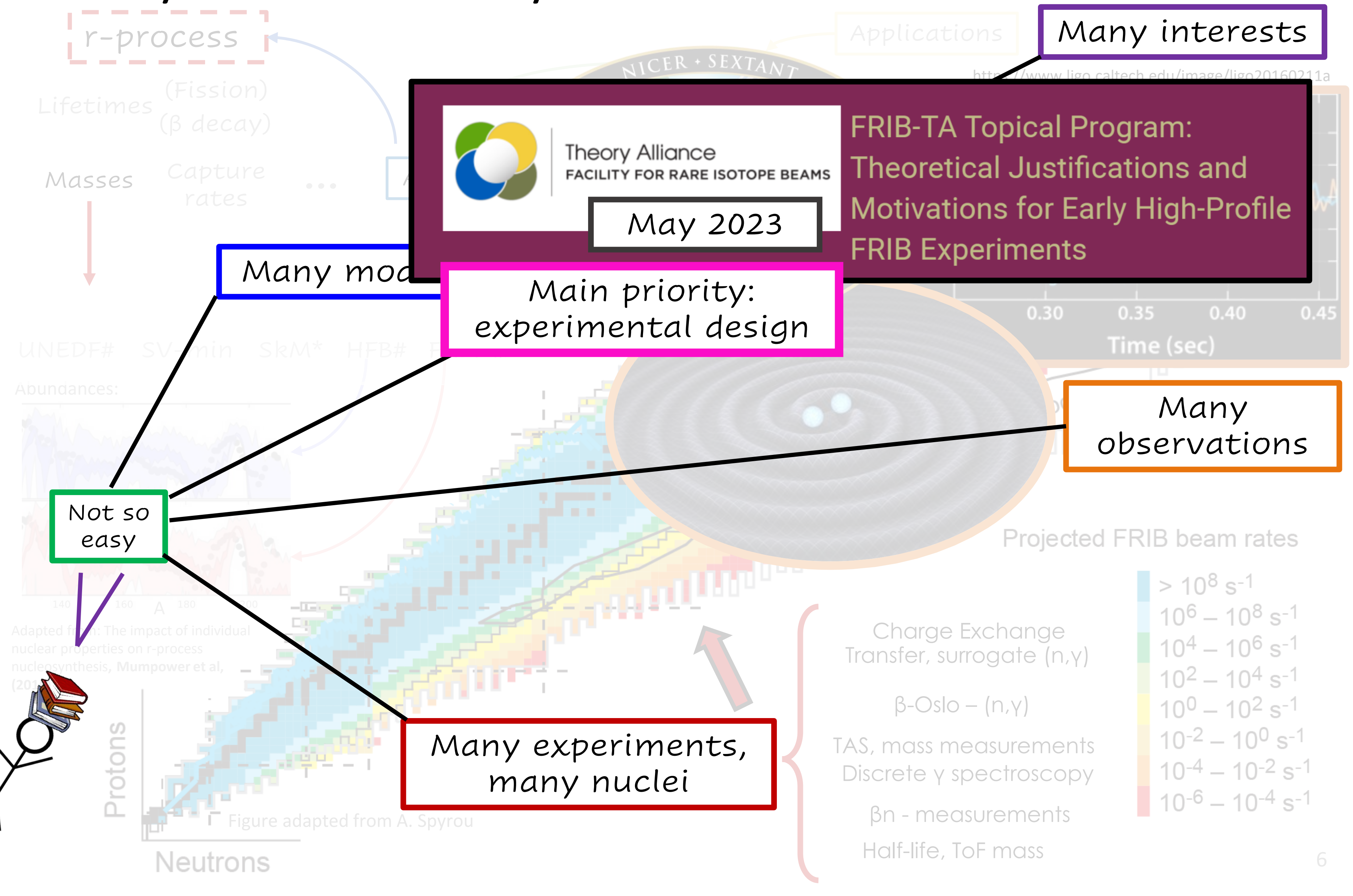

Why Uncertainty Quantification?

NSAC Long Range Plan Town Hall Meeting on Nuclear Structure, Reactions and Astrophysics

Nov 14 – 16, 2022

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Bayesian methods for extrapolations to stellar energies

Needs

Daniel Phillips

- Detailed discussion of systematic uncertainties, ideally with covariance matrices, in experimental publications; theory-experiment collaborations
- Collaboration with statisticians (e.g., through ISNET series of meetings, funding for inter-disciplinary collaboration) on forefront statistical approaches for these problems

At the intersection of low-energy nuclear physics and fundamental symmetries

Alejandro Garcia

Experiencing a revolution in our field brought by:

2. Improved theory allowing for optimizing opportunities and calculating SM expectations, including uncertainties.

Tremendous progress

in CEFT, many-body theory, UQ & HPC

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Nuclear data for astrophysics (in neutron-rich environments)

Studies examining variations in theoretical **γ-strength functions** and **nuclear level densities** show the large impact of (n,γ) rate uncertainties on astrophysical neutron capture processes (*i*-process and *r*-process)

Nicole Vassh

C. Hebborn

Enchancing the accuracy of optical potentials

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Max Brodeur, Vincenzo Cirigliano, Alejandro Garcia, **Kyle Leach**, Dan Melconian, Peter Mueller, Saori Pastore, Jaideep Singh, Ragnar Stroberg

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This is very important to us

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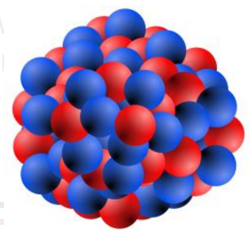

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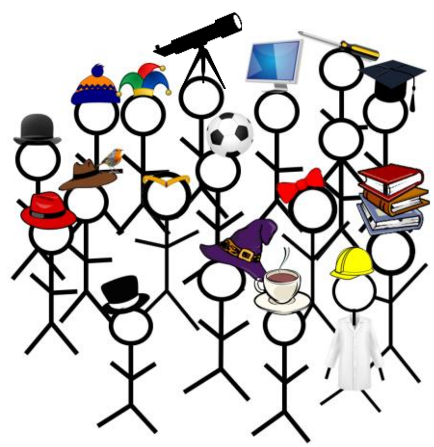

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statistics
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Work in collaboration with experts

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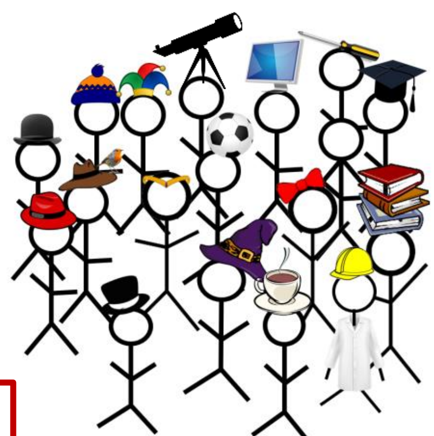

mathematics
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Communication

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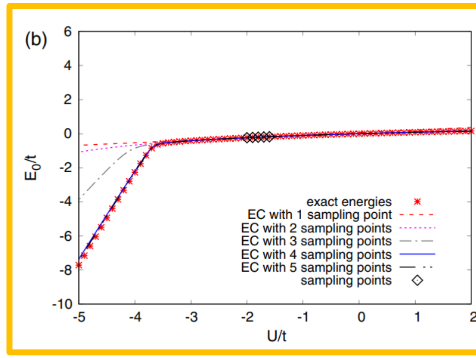
Eigenvector Continuation with Subspace Learning *(2018)*

Dillon Frame,[1,2] Rongzheng He,[1,2] Ilse Ipsen,[3] Daniel Lee,[4] Dean Lee,[1,2] and Ermal Rrapaj[5]



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"eigenvector continuation"

About 188 results (**0.08** sec)

control parameter in the Hamiltonian matrix exceeds some threshold value. In this Letter we present a new technique called eigenvector continuation that can extend the reach of these methods. The key insight is that while an eigenvector resides in a linear space with enormous dimensions, the eigenvector trajectory generated by smooth changes of the Hamiltonian matrix is well approximated by a very low-dimensional manifold. We

Communication

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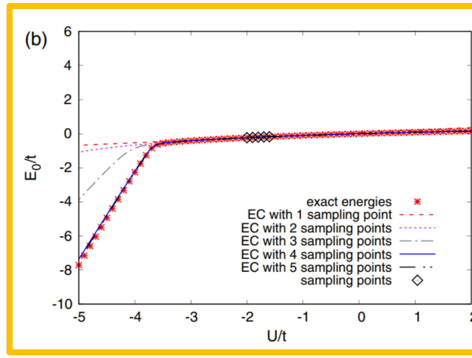

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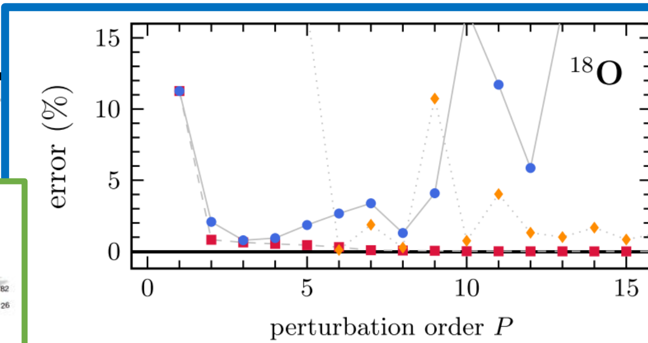
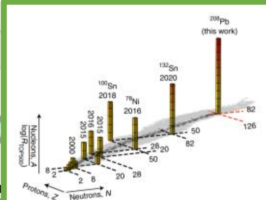


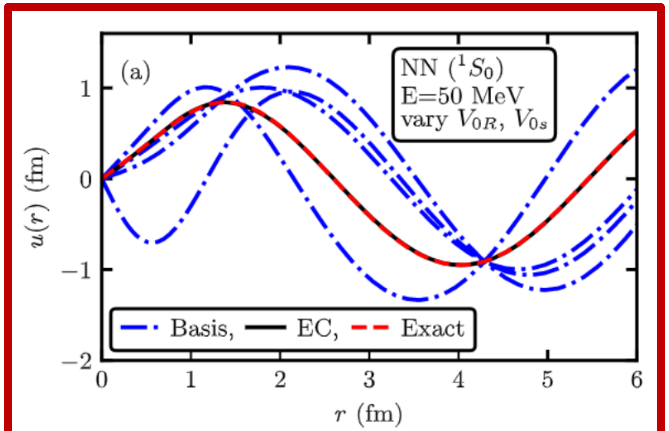


Ab initio predictions link the neutron skin of ^{208}Pb to nuclear forces (2022)

Baishan Hu[1,11], Weiguang Jiang[2,11], Takayuki Miyagi[1,3,4,11], Zhonghao Sun[5,6,11], Andreas Ekström[2], Christian Forssén[2], Gaute Hagen[1,5,6], Jason D. Holt[1,7], Thomas Papenbrock[5,6], S. Ragnar Stroberg[8,9] and Ian Vernon[10]

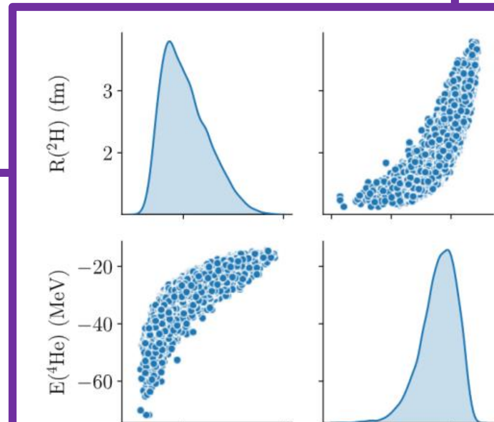
Improved many-body expansions from eigenvector continuation (2020)

P. Demol,[1] T. Duguet,[1,2] A. Ekström,[3] M. Frosini,[2] K. Hebeler,[4,5] S. König,[4,5,6] D. Lee,[7] A. Schwenk,[4,5,8] V. Somà,[2] and A. Tichai[9,8,4,5,*]



Eigenvector continuation as an efficient and accurate emulator for uncertainty quantification (2020)

S. König[a,b,c,*], A. Ekström[d], K. Hebeler[a,b], D. Lee[e], A. Schwenk[a,b,f]



Efficient emulators for scattering using eigenvector continuation

R.J. Furnstahl, A.J. Garcia, P.J. Millican, Xilin Zhang* (2020)

Communication

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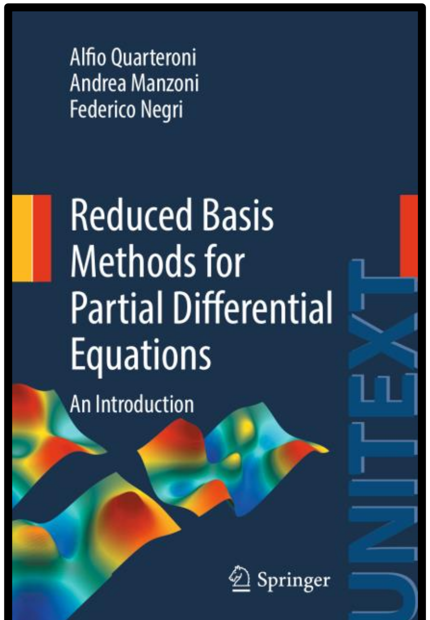

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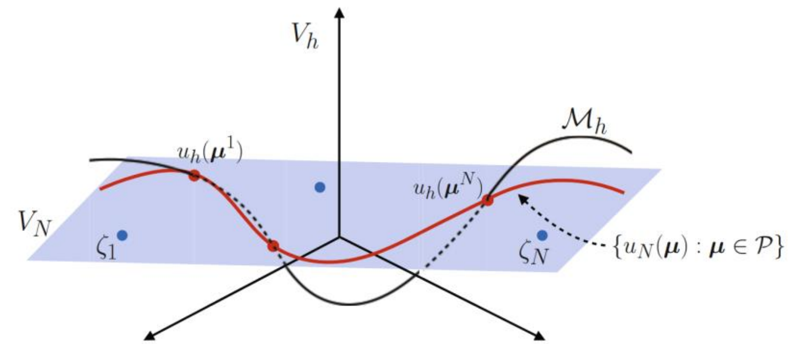

Fig. 3.1 The "snapshots" $u_h(\boldsymbol{\mu}^n), 1 \le n \le N$ on the parametric manifold $\mathscr{M}_h$, the RB space $V_N = \text{span}\{\zeta_1, \ldots, \zeta_N\}$ = ... solutions $u_N(\boldsymbol{\mu}) \in V_N$, $\boldsymbol{\mu}$ ...

we will further discuss these issues in Chap. 5. The idea behind RB methods is to generate an approximate solution to problem (3.11) belonging to a low-dimensional subspace $V_N \subset V_h$ of dimension $N \ll N_h$. The smaller N, the cheaper the reduced problem to solve. Precisely, setting a RB method entails:

1. the construction of a basis of V_N. We start from a set of high-fidelity solutions

$$\{u_h(\boldsymbol{\mu}^1), \ldots, u_h(\boldsymbol{\mu}^N)\}, \tag{3.18}$$

that we call *snapshots*, corresponding to a set of N selected parameters

$$S_N = \{\boldsymbol{\mu}^1, \ldots, \boldsymbol{\mu}^N\} \subset \mathscr{P}. \tag{3.19}$$

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Dimensionality reduction and polynomial chaos acceleration of Bayesian inference in inverse problems

Youssef M. Marzouk[a,*], Habib N. Najm[b]

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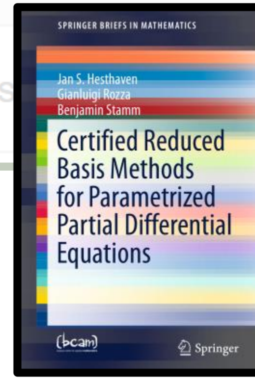
A REDUCED ORDER MODEL FOR MULTI-GROUP TIME-DEPENDENT PARAMETRIZED REACTOR SPATIAL KINETICS (2014)

Sartori, et al



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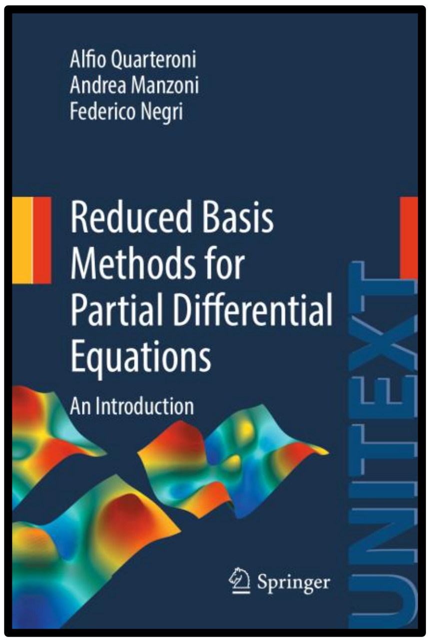

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Reduced-order modeling of time-dependent PDEs with multiple parameters in the boundary data

Max D. Gunzburger[a,*,1], Janet S. Peterson[a,1], John N. Shadid[b,2]

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An 'empirical interpolation' method: application to efficient reduced-basis discretization of partial differential equations

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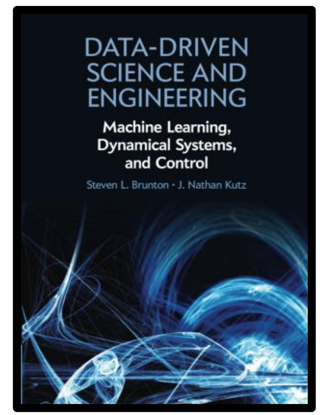

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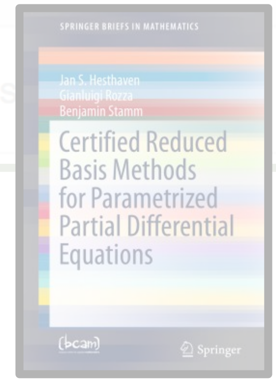

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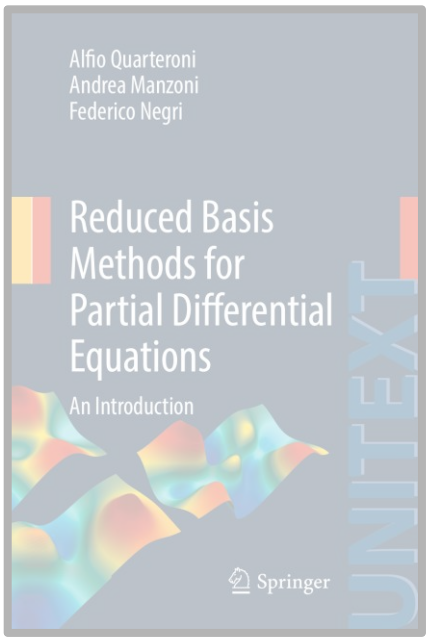

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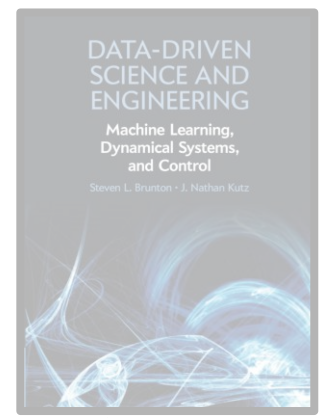

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Improved many-body expansions from eigenvector continuation (2020)

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Dimensionality reduction and polynomial chaos acceleration of Bayesian inference in inverse problems

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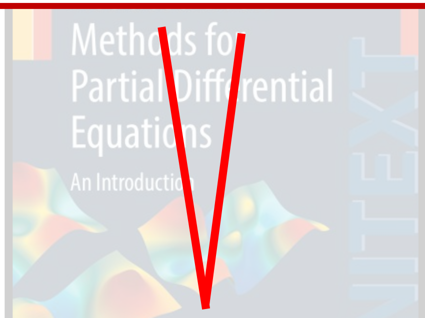
The nuclear potential that we employ is additive in the $d = 16$ LECs, i.e., we can express the Hamiltonian as $H(\mathbf{c}) = H_0 + \sum_{i=1}^{d} c_i H_i$, where H_0 includes the kinetic energy. Any Hamiltonian with more than one interaction parameter can be written in this form, where each c_i in general may be depend nonlinearly on other parameters. Furthermore, each term H_i for $i = 1, \ldots, 16$ can be projected onto the EC subspace once and then used for an arbitrary number of emulations. Each of these corresponds to a

[1] Note that because the κ parameters do not appear linearly in the Hamiltonian, one can no longer make a single set of matrix elements calculations for all of the test parameter sets. In other contexts this might be a relevant computational disadvantage.

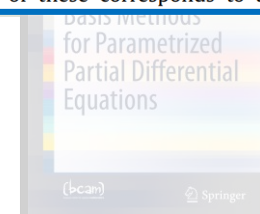
$$V_{^1S_0}(r) \equiv V_{0R} e^{-\kappa_R r^2} + V_{0s} e^{-\kappa_s r^2}$$

$$V_{^3S_1}(r) \equiv V_{0R} e^{-\kappa_R r^2} + V_{0t} e^{-\kappa_t r^2}$$



…r modeling of time-dependent PDEs …e parameters in the boundary data

…er[a,*,1], Janet S. Peterson[a,1], John N. Shadid[b,2] (2006)



(2016)

An 'empirical interpolation' method: application to efficient reduced-basis discretization of partial differential equations

Maxime Barrault[a], Yvon Maday[b], Ngoc Cuong Nguyen[c], Anthony T. Patera[d]

(2004)

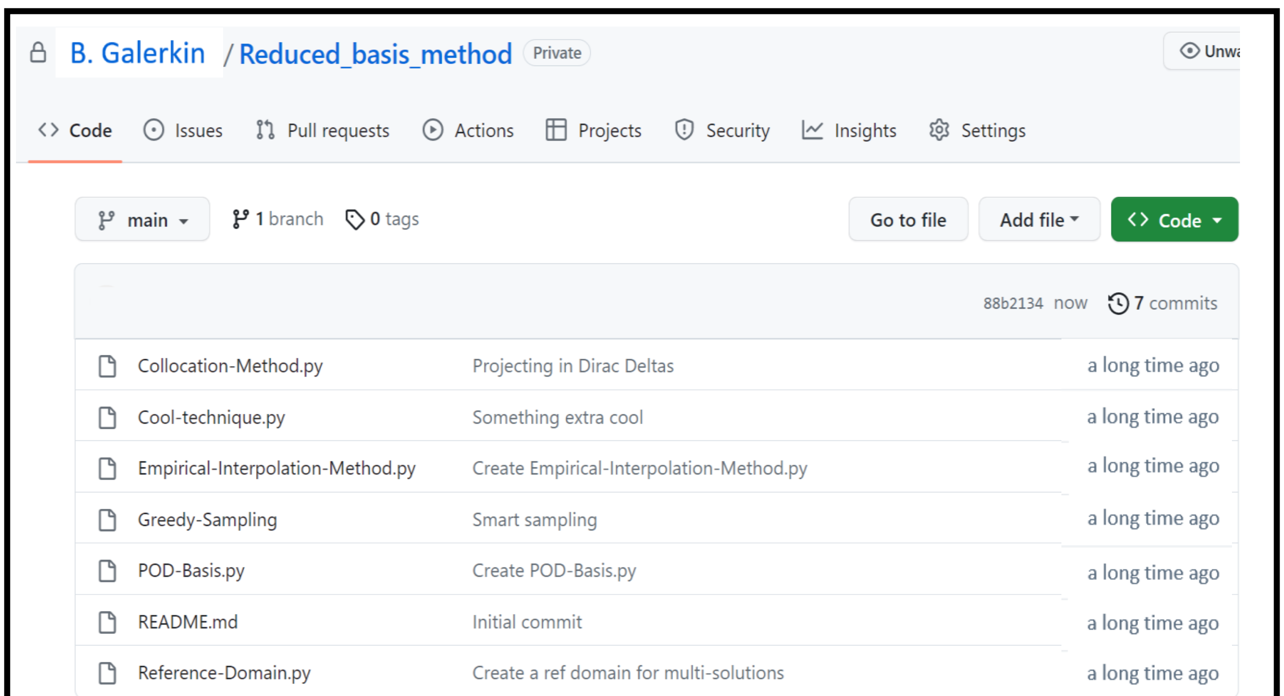
(2019)

Efficient emulators for scattering using eigenvector continuation

R.J. Furnstahl, A.J. Garcia, P.J. Millican, Xilin Zhang* (2020)

~~Why~~ Uncertainty Quantification?

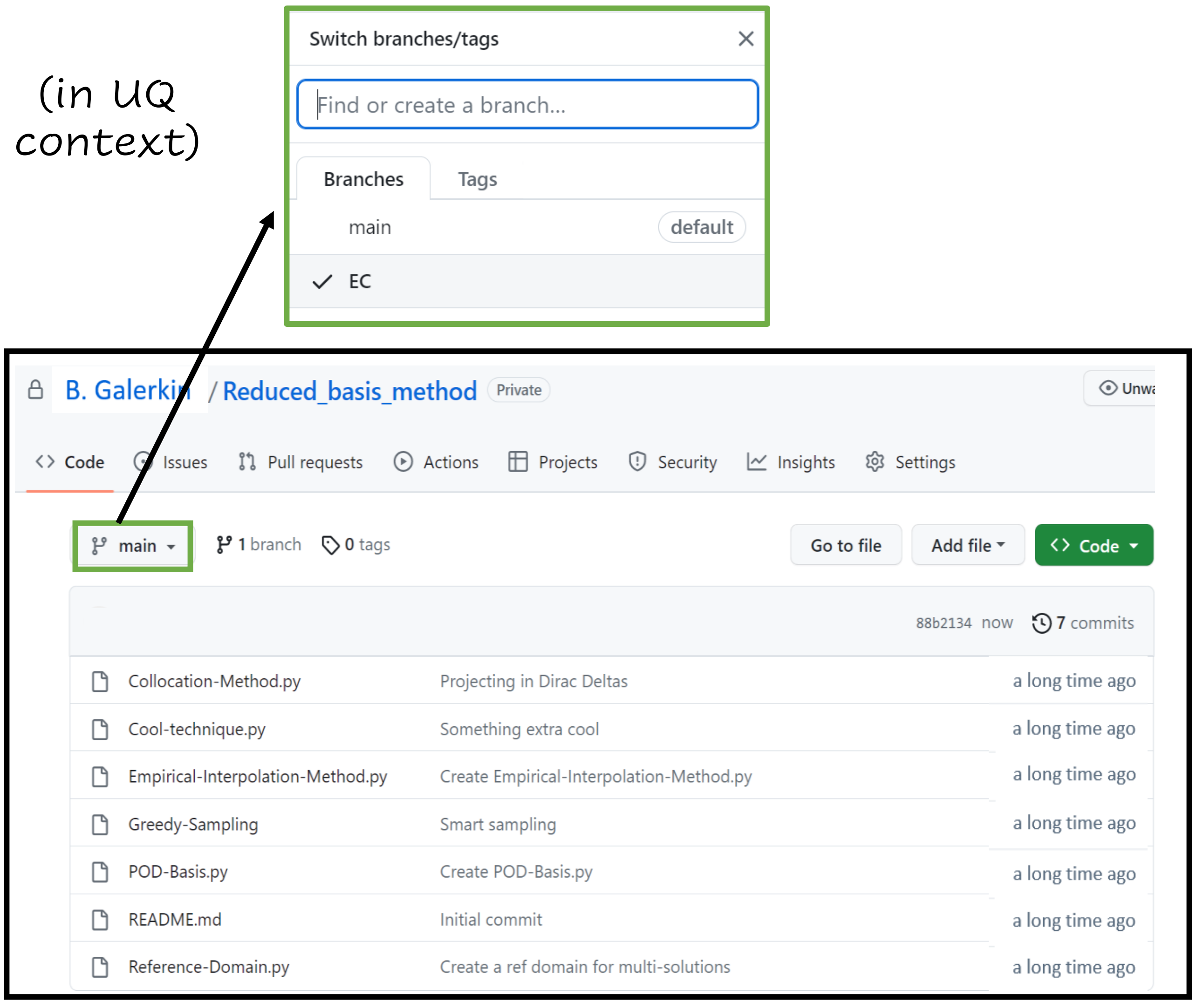
How → *Communication with experts*



~~Why~~ Uncertainty Quantification?

How → *Communication with experts*

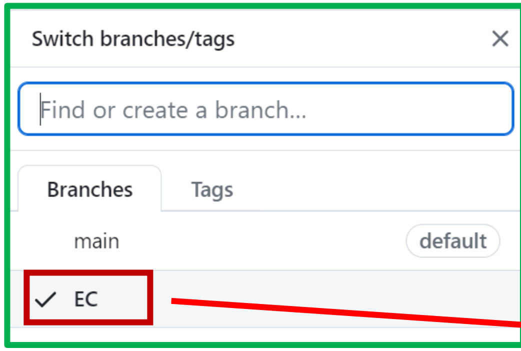
(in UQ context)

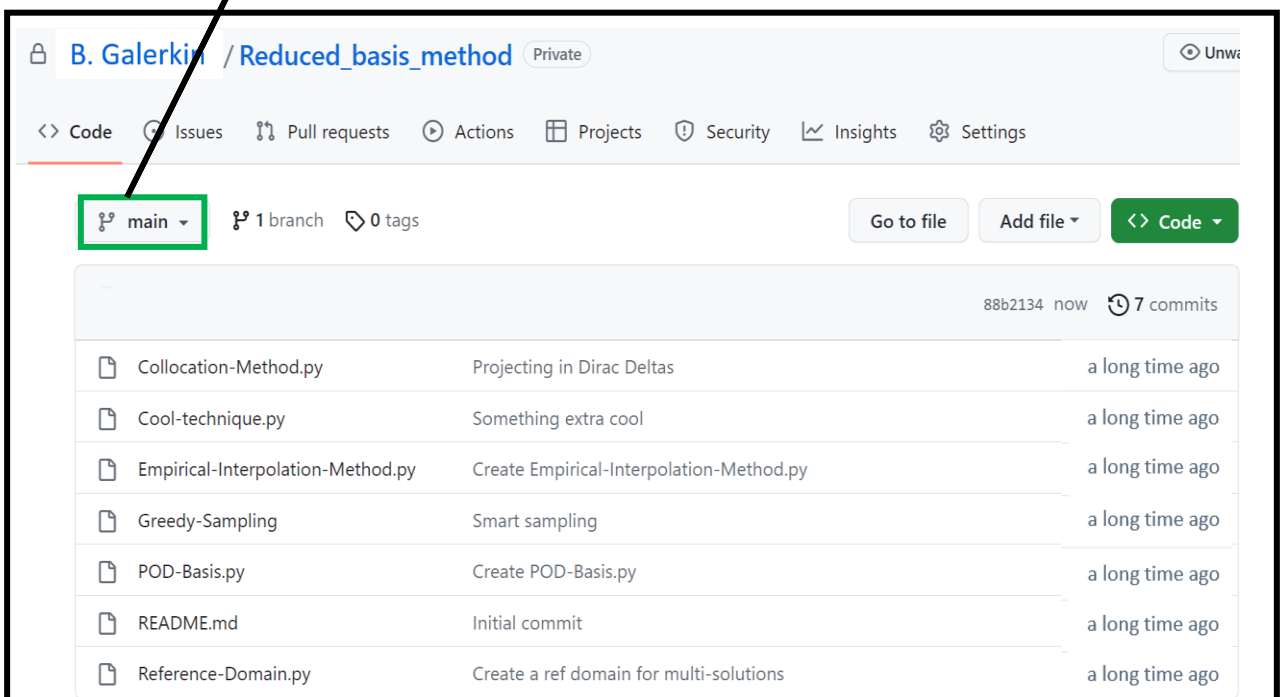


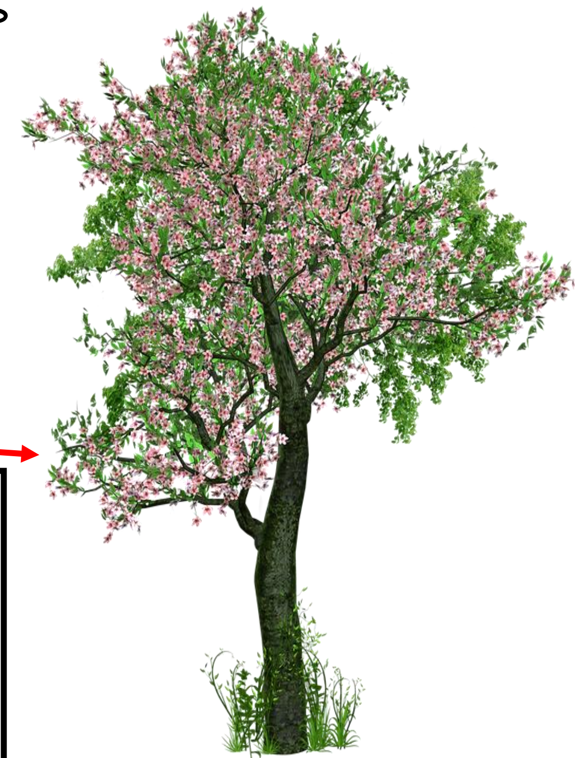
~~Why~~ Uncertainty Quantification?

How → *Communication with experts*

(in UQ context)







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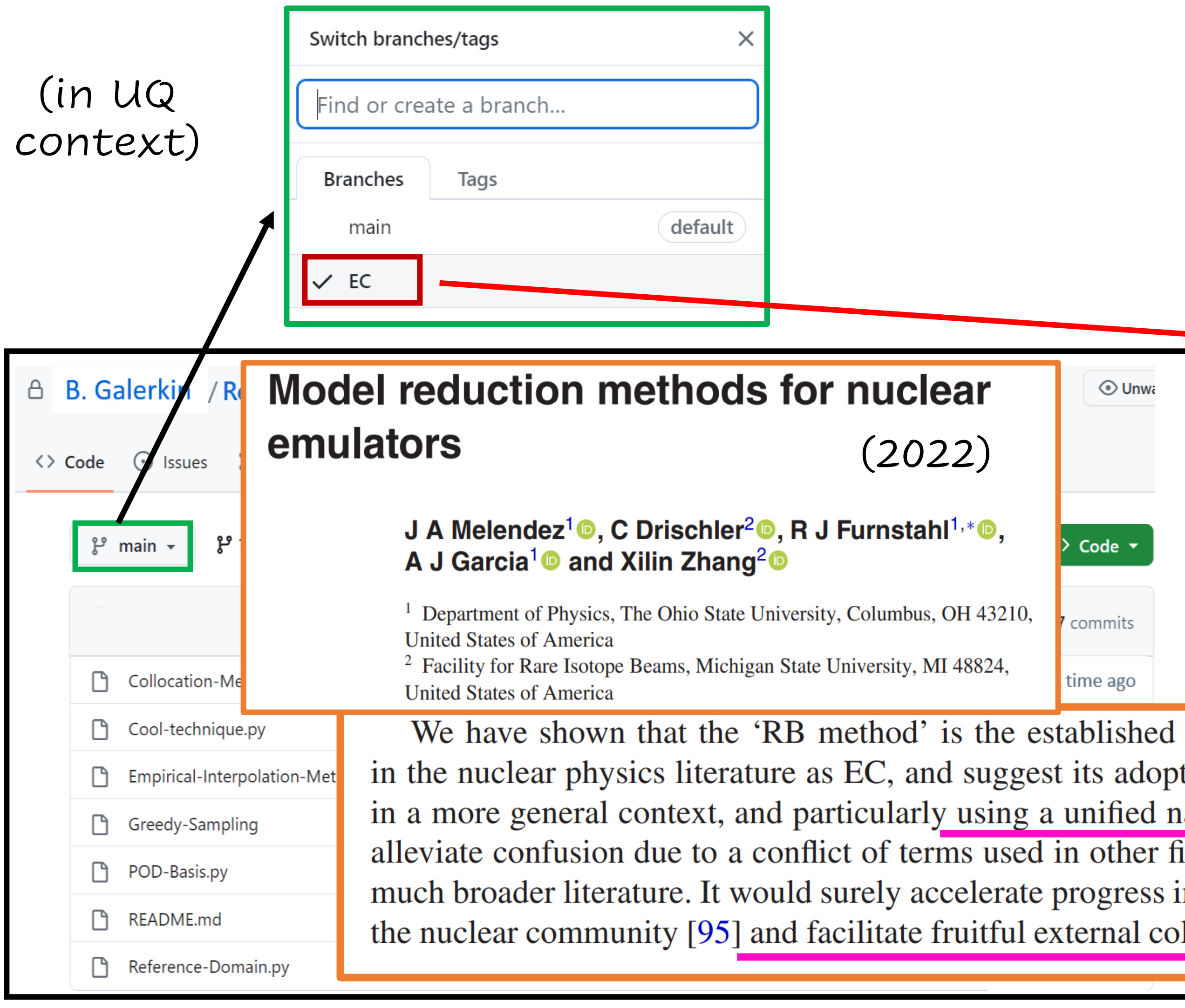
(in UQ context)



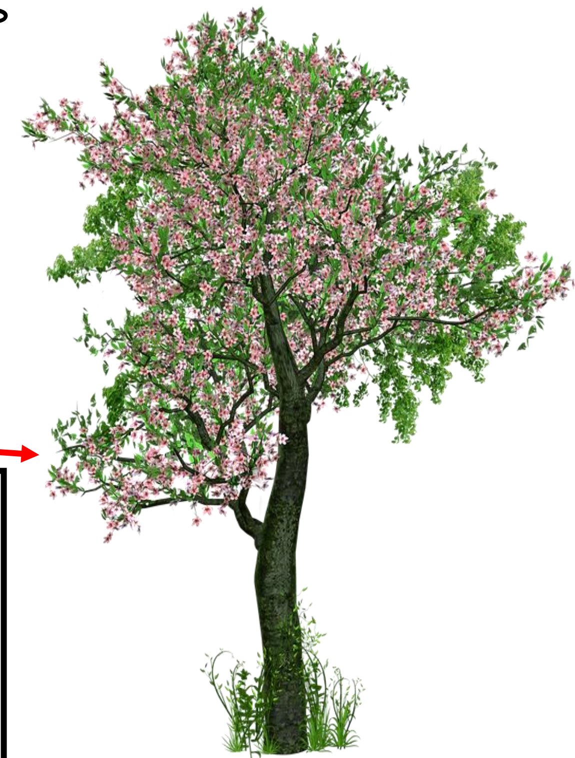
Model reduction methods for nuclear emulators *(2022)*

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

[1] Department of Physics, The Ohio State University, Columbus, OH 43210, United States of America

[2] Facility for Rare Isotope Beams, Michigan State University, MI 48824, United States of America

We have shown that the 'RB method' is the established name of the methods described in the nuclear physics literature as EC, and suggest its adoption. We believe that putting EC in a more general context, and particularly using a unified naming convention, will not only alleviate confusion due to a conflict of terms used in other fields, but will permit access to a much broader literature. It would surely accelerate progress in the application of emulators in the nuclear community [95] and facilitate fruitful external collaborations.



~~Why~~ Uncertainty Quantification?

How → Communication with experts

(in UQ context)

Training and Projecting: Extending Eigenvector Continuation through a Galerkin Method formulation

Edgard Bonilla,[1,*] Pablo Giuliani,[2,3,*] Kyle Godbey,[2] and Dean Lee[2,4]

[1] *Department of Physics, Stanford University, Stanford, CA 94305, USA*
[2] *FRIB/NSCL Laboratory, Michigan State University, East Lansing, Michigan 48824, USA*
[3] *Department of Statistics and Probability, Michigan State University, East Lansing, Michigan 48824, USA*
[4] *Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA*

(Dated: January 25, 2022)

We propose the Galerkin Continuation method (GC), which combines the insight from Eigenvector Continuation (EC), with the formulation used for Galerkin methods. We show connections between GC and some of the established results in the EC literature, and how it can be used to extend the techniques of EC for the emulation of a broad set of problems, including non-linear equations. As a first study, we apply GC to two non-linear problems: the one dimensional Gross Pitaevskii equation, and the nuclear many body via density functional theory for ^{48}Ca, the latter of which also tests the formalism in the case of coupled equations. GC is able to reproduce the exact results in both problems with a very small error, showing a performance in interpolation and extrapolation similar to the one observed in previous EC applications. We conclude this letter with insights for potential real-case applications of the proposed method, as well as future directions to explore for its improvement.

~~Why~~ Uncertainty Quantification?

This is very important to us

How → Communication with experts

(in UQ context)

Switch branches/tags

Find or create a branch...

Branches Tags

main default

✓ EC

B. Galerkin / Reduced basis method Private

Code Issues

main

Collocation-M...
Cool-techniq...
Empirical-Inte...
Greedy-Samp...
POD-Basis.py
README.md
Reference-Do...

(Jan 2022)

Training and Projecting: Extending Eigenvector Continuation through a Galerkin Method formulation

Edgard Bonilla,[1,*] Pablo Giuliani,[2,3,*] Kyle Godbey,[2] and Dean Lee[2,4]

[1] *Department of Physics, Stanford University, Stanford, CA 94305, USA*
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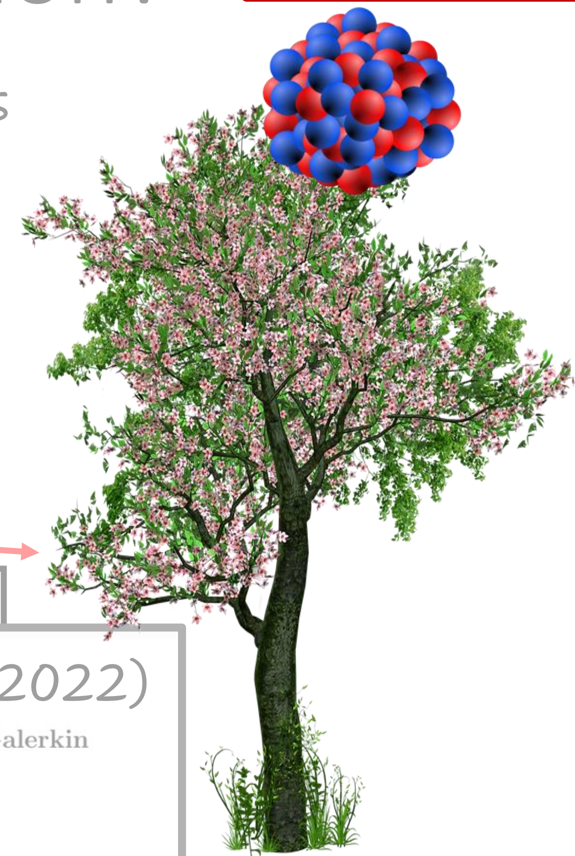


Outline

Why

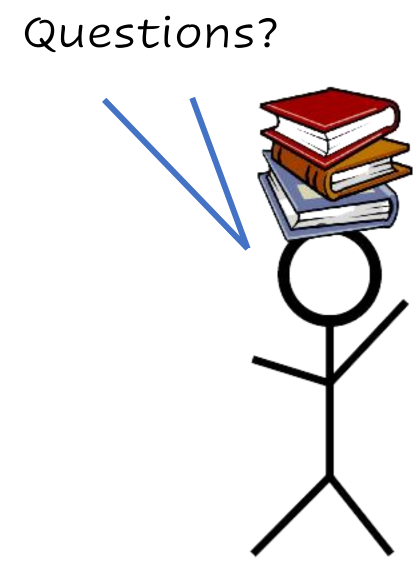
Uncertainty Quantification?

How

The Reduced Basis Method

- How it works
- Problems table
- Applications and Results

Takeaways

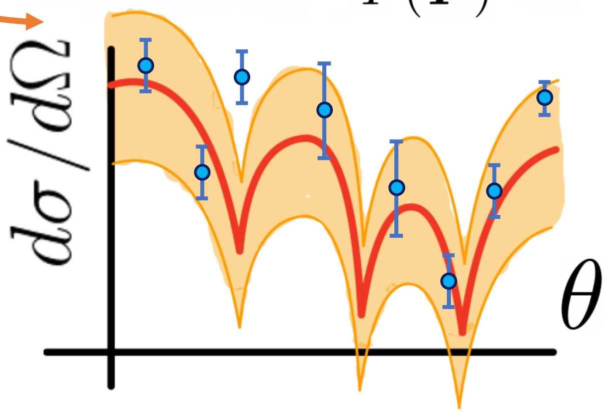


Emulators

5,000,000
parameter samples

Bayesian statistics

$$P(\alpha|\boldsymbol{Y}) = \frac{P(\boldsymbol{Y}|\alpha)P(\alpha)}{P(\boldsymbol{Y})}$$



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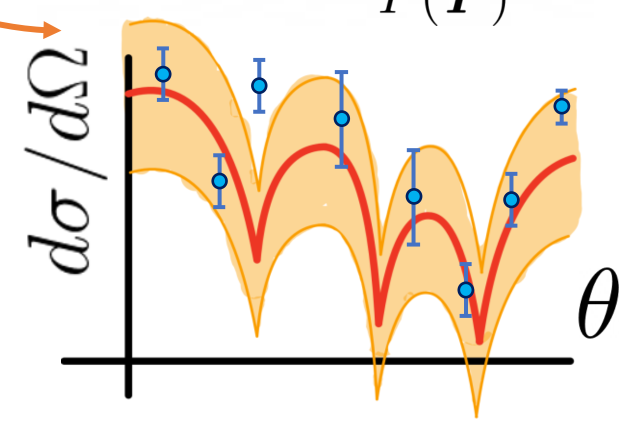
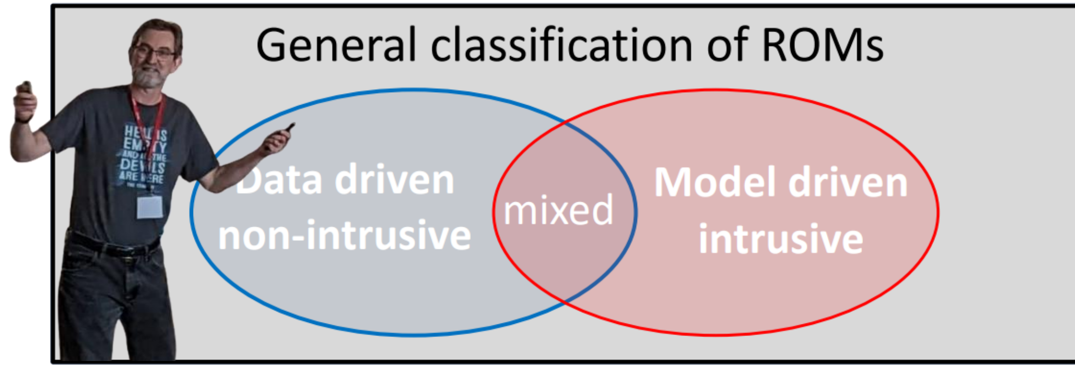


$f(\alpha, x)$ → $\hat{f}(\alpha, x)$

"Exact" "Emulated"

Emulators



Dick’s talk at ISNET

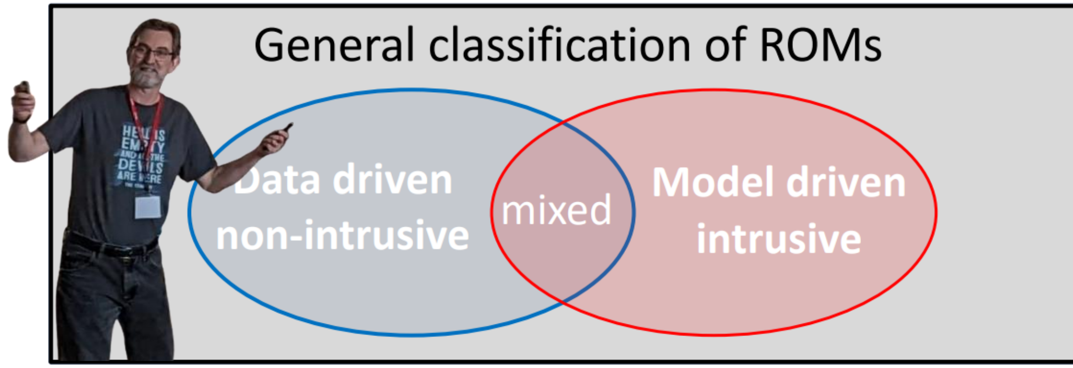
High fidelity computation → Emulator

Emulator → Gaussian Process

Emulator → Neural Networks

Emulator → Reduced Basis Method

Emulators



Dick's talk at ISNET

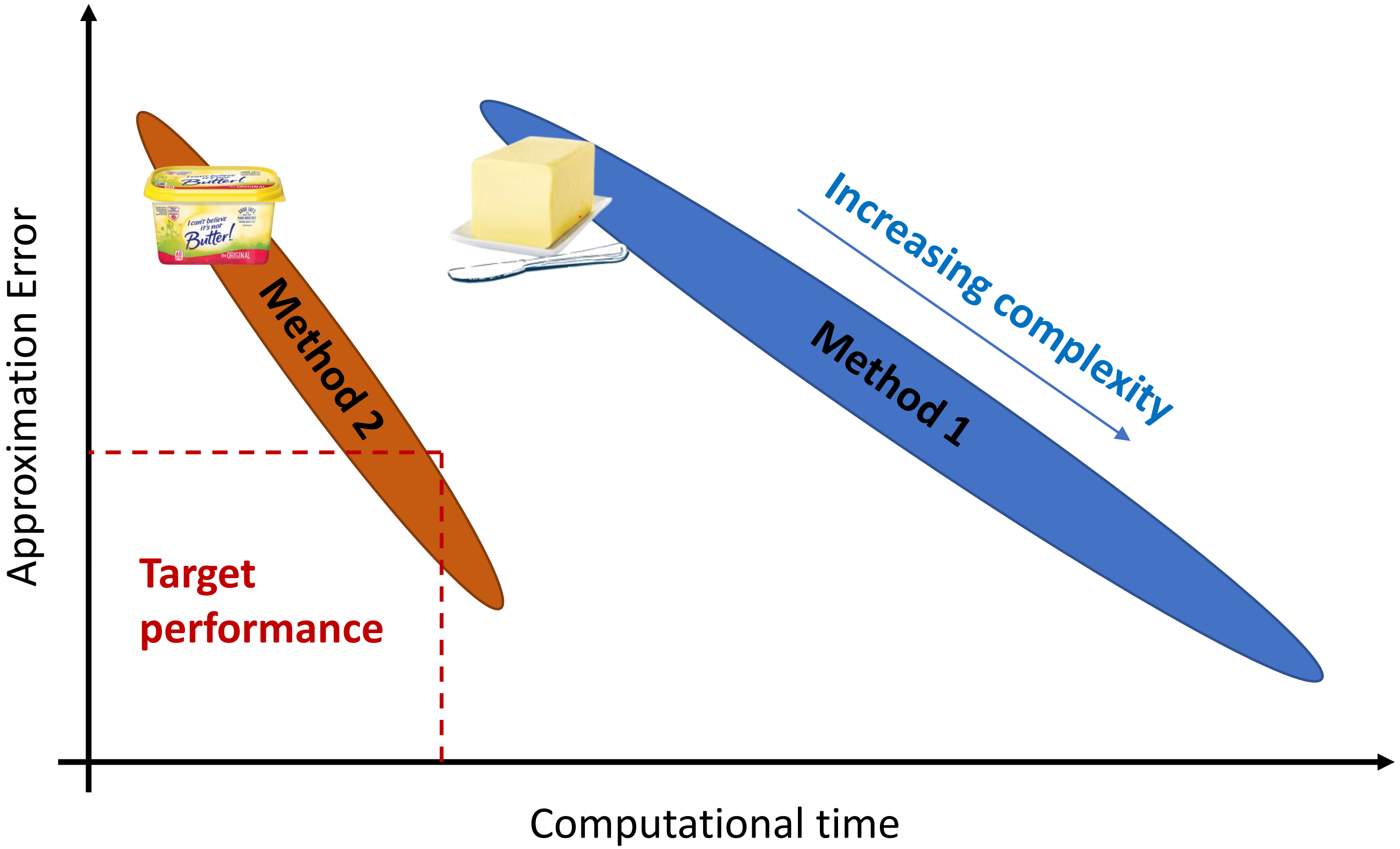
Gaussian Process

High fidelity computation → Emulator → Neural Networks

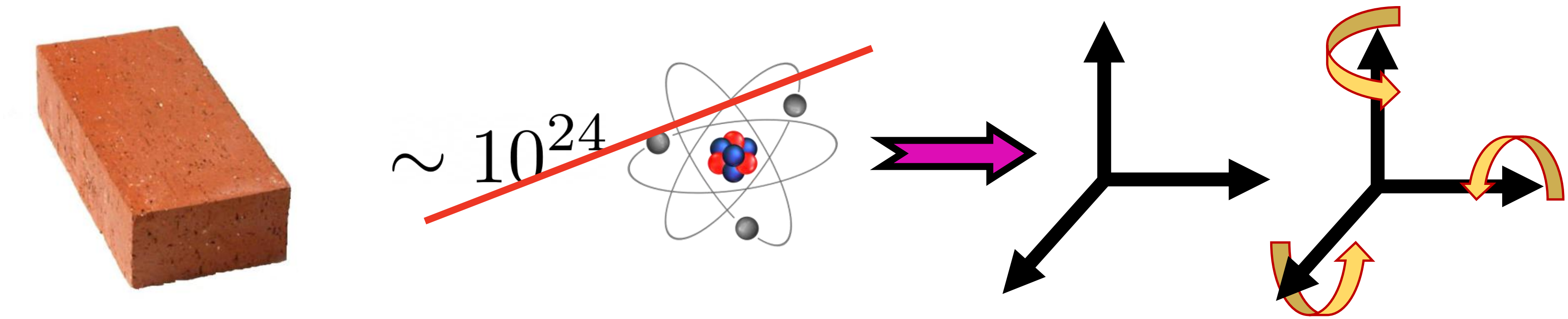
Reduced Basis Method

Reduced Order Models

Computation Accuracy vs Time

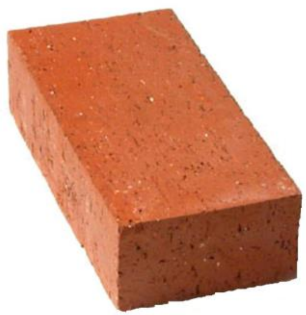


The Reduced Basis Method

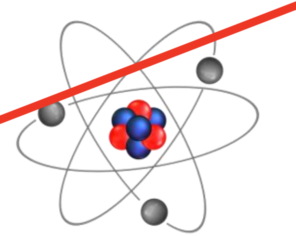


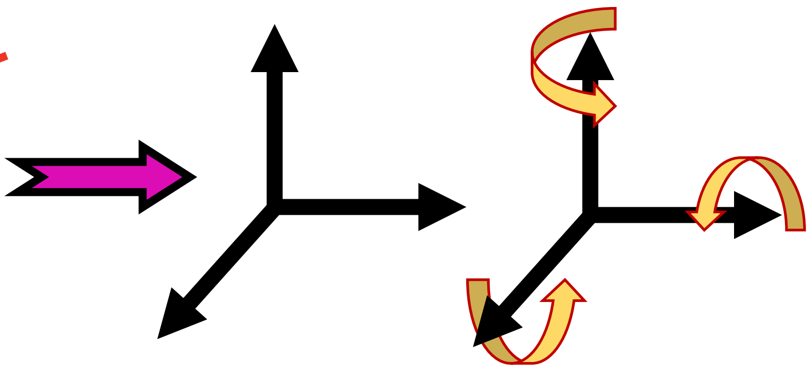
3 translations + 3 rotations

The Reduced Basis Method



$\sim 10^{24}$

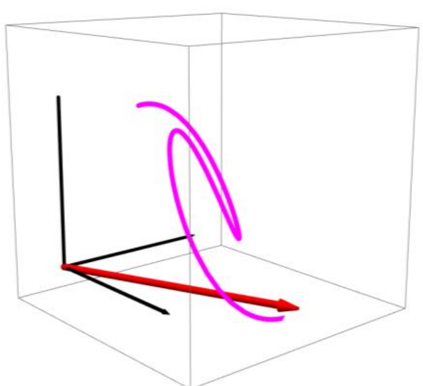


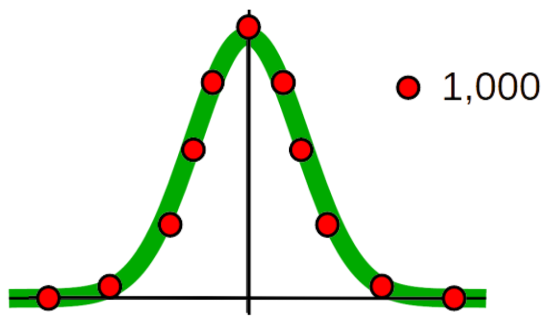


3 translations + 3 rotations

parameters

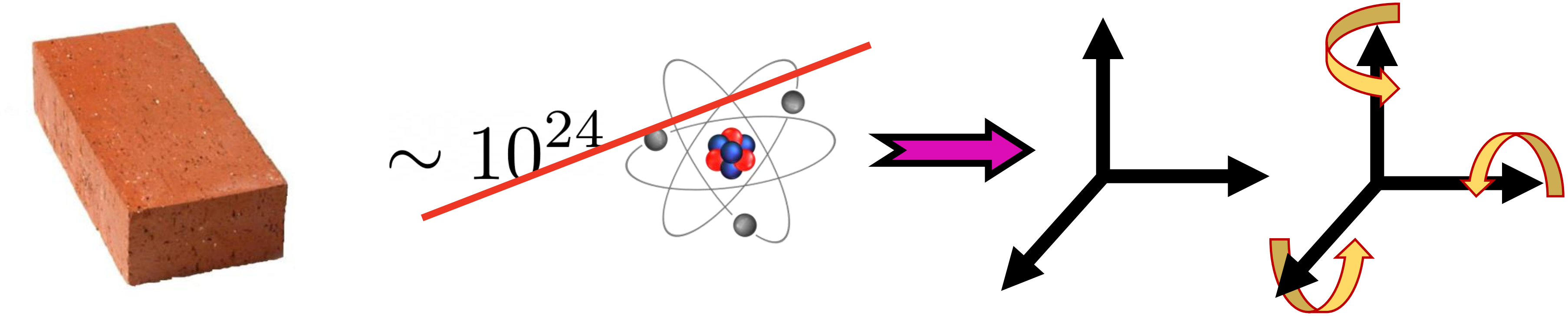
$$\mathcal{H}_\alpha \phi(x) = \lambda \phi(x)$$





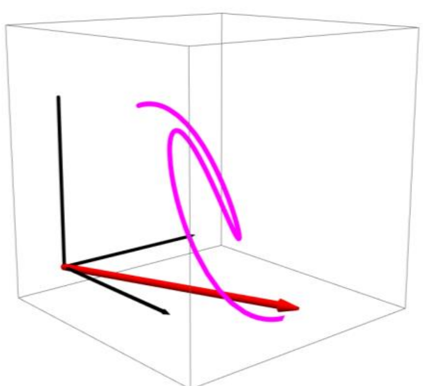
Finite element

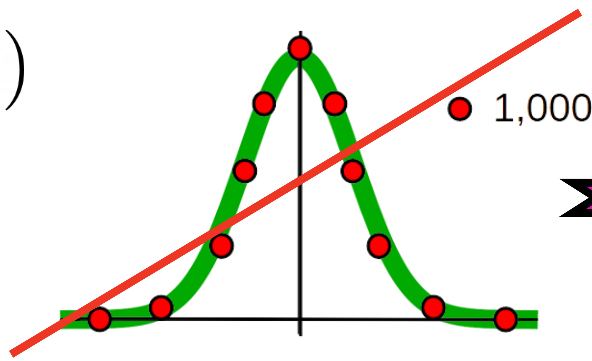
The Reduced Basis Method



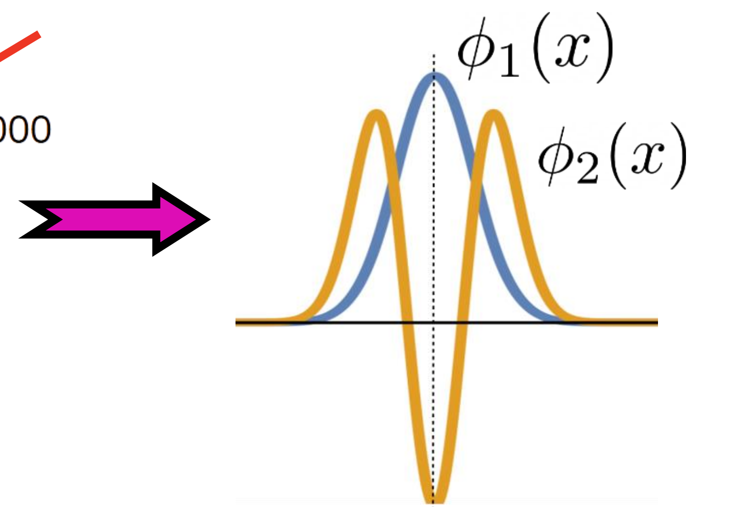
parameters

$$\mathcal{H}_\alpha \phi(x) = \lambda \phi(x)$$



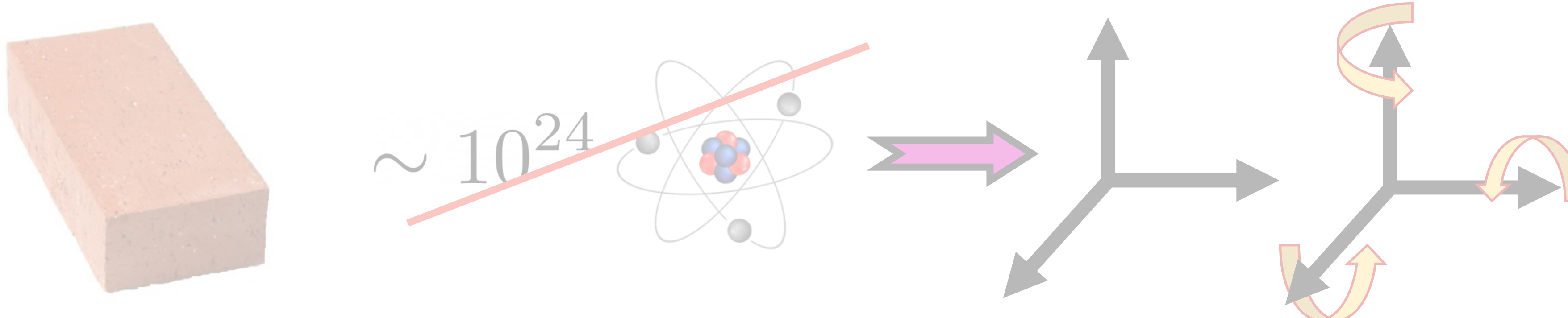


Finite element



$$\phi(x) \approx a_1\phi_1(x) + a_2\phi_2(x)$$

The Reduced Basis Method



3 translations + 3 rotations

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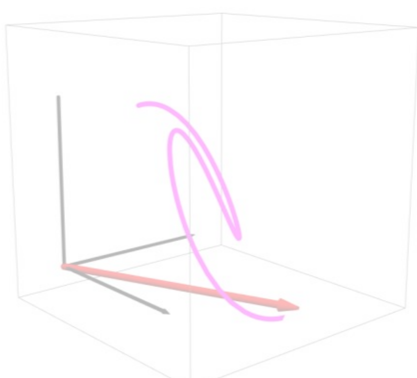

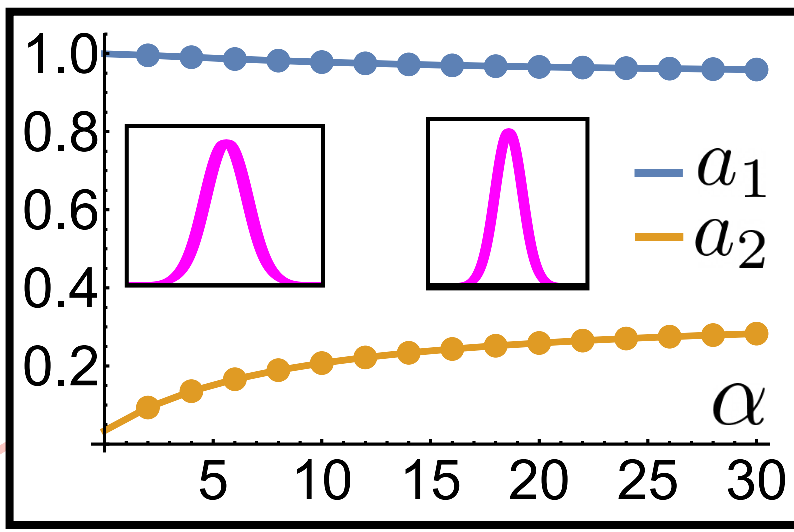

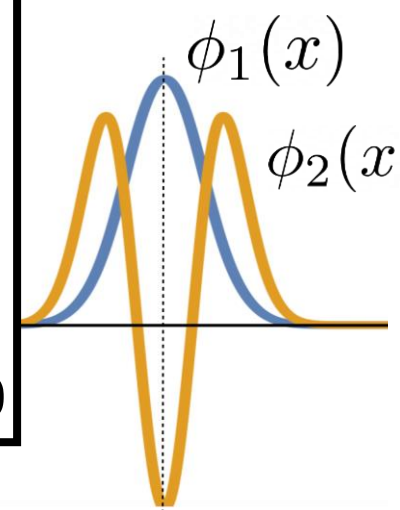

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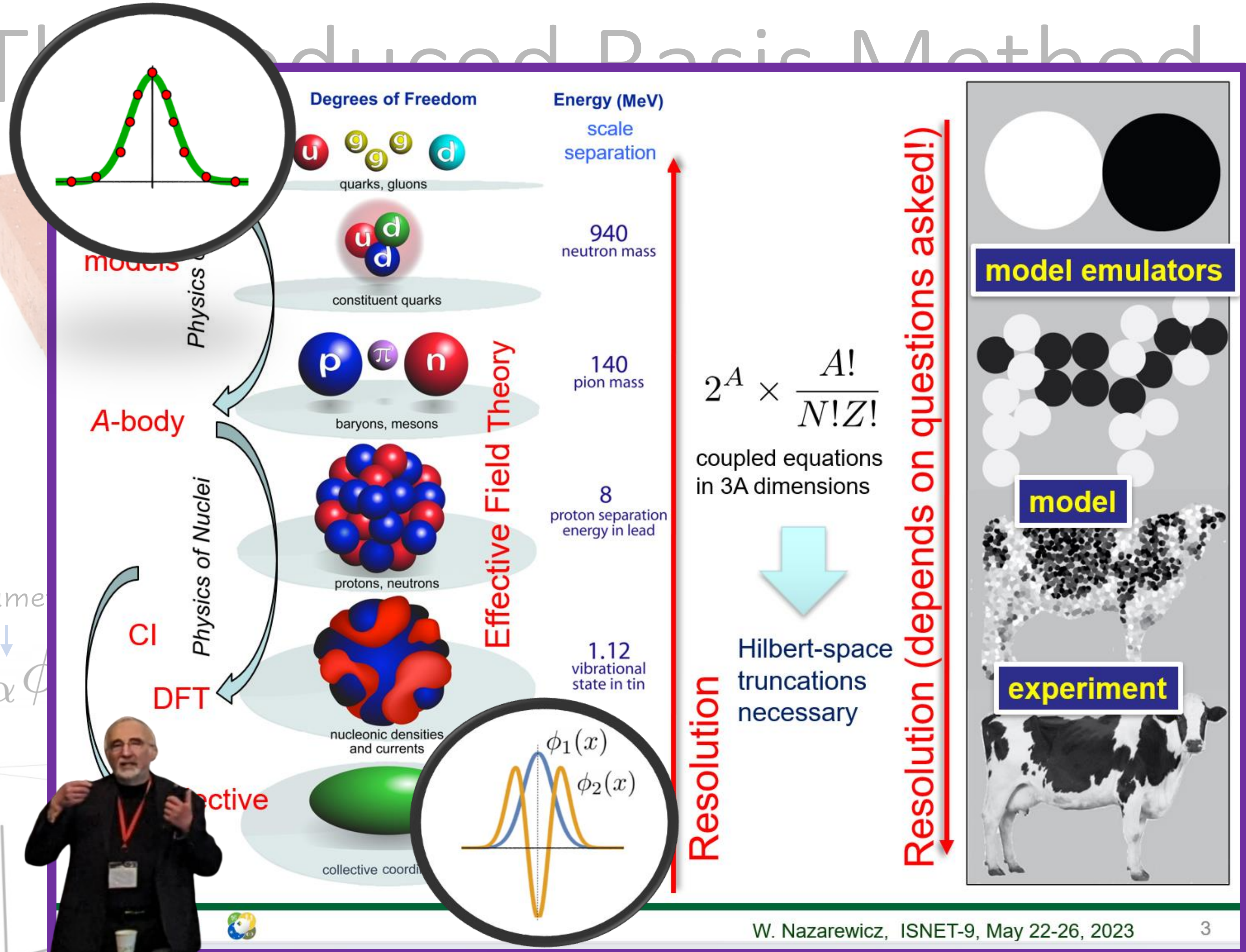
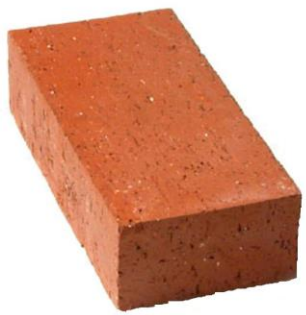


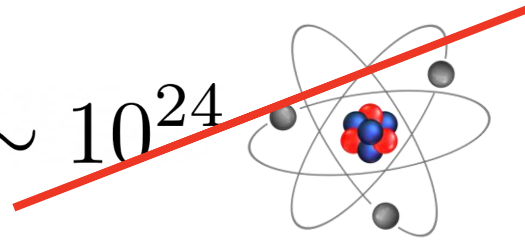
Witek's talk at ISNET

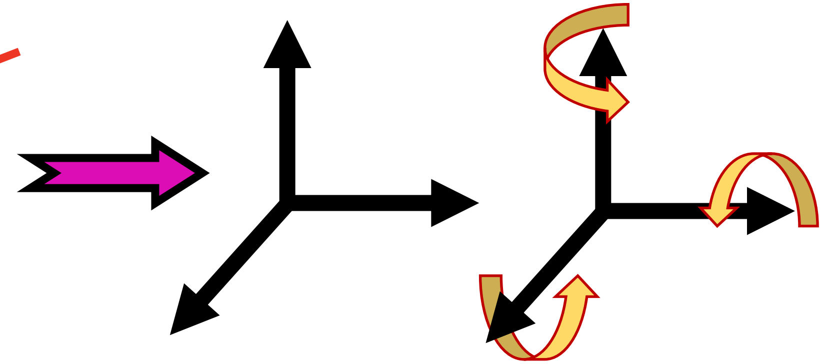
$$\phi(x) \approx a_1\phi_1(x) + a_2\phi_2(x)$$

The Reduced Basis Method

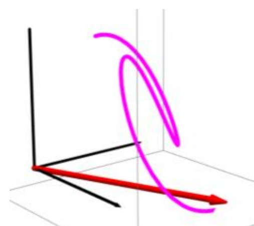


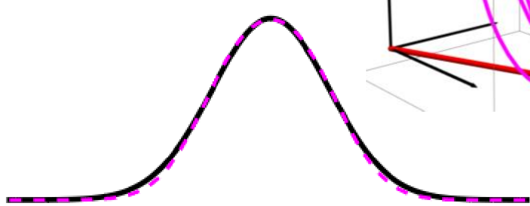
$\sim 10^{24}$

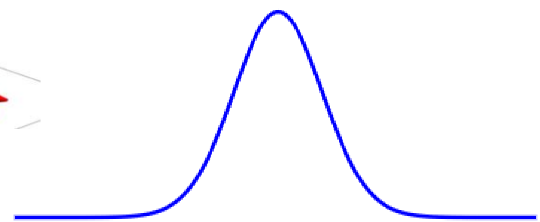




3 translations + 3 rotations





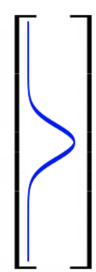


$$\phi(x) \approx a_1\phi_1(x) + a_2\phi_2(x)$$

— $\phi(x)$

- - $\hat{\phi}(x)$

a_1



a_2

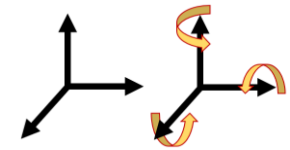
Changing the trapping strength α

The Reduced Basis Method

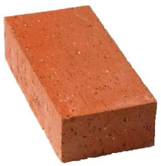
$$F_\alpha[\phi(x)] = 0$$

General differential equation

$$\left(\mathcal{H}_\alpha \phi(x) - \lambda \phi(x) = 0\right)$$



The Reduced Basis Method



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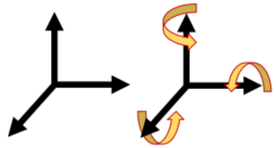
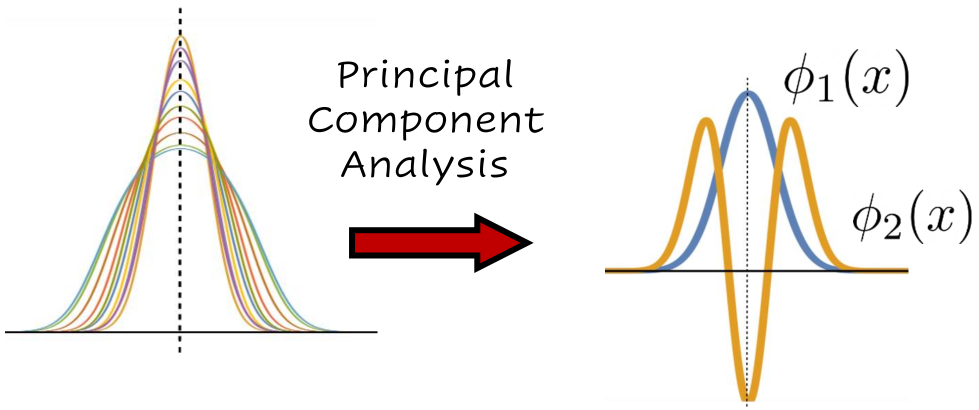
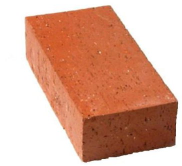


1) Choose a basis

$$\hat{\phi}(x) = \phi_0 + \sum_k^n a_k \phi_k(x)$$

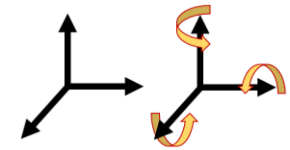


The Reduced Basis Method



$$F_\alpha[\phi(x)] = 0$$

General differential equation
$\left(\mathcal{H}_\alpha \phi(x) - \lambda \phi(x) = 0\right)$



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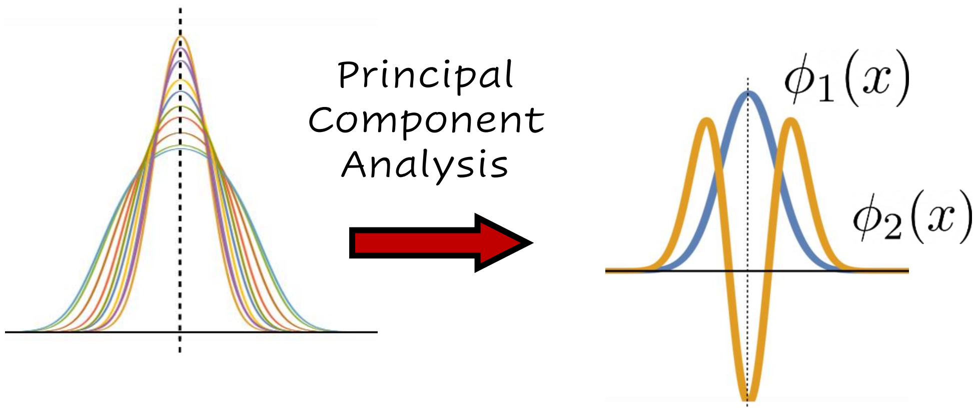


2) Project

$$j = \{1, n\} \quad \langle \psi_j | F_\alpha[\hat{\phi}(x)] \rangle = 0$$

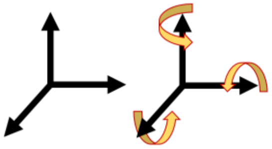
One equation per coefficient

The Reduced Basis Method

$$F_\alpha[\phi(x)] = 0$$

General differential equation

$$\left(\mathcal{H}_\alpha \phi(x) - \lambda \phi(x) = 0\right)$$



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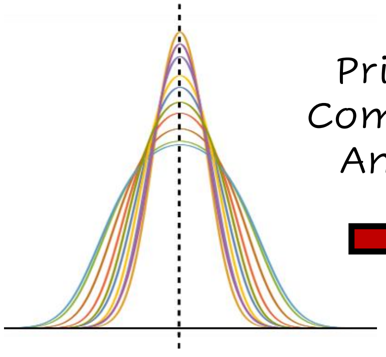
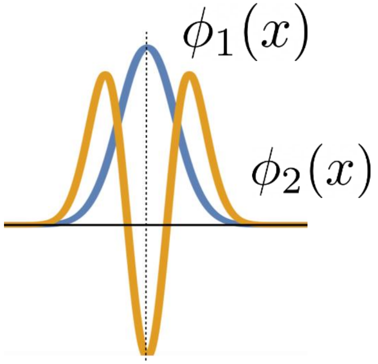


Principal Component Analysis



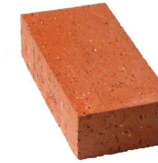
2) Project

Usually, a challenge

$$j = \{1, n\} \quad \langle \psi_j | F_\alpha[\hat{\phi}(x)] \rangle = 0$$

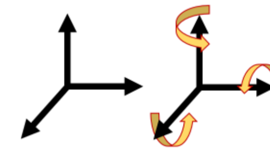
One equation per coefficient

The Reduced Basis Method



$$F_\alpha[\phi(x)] = 0$$

General differential equation
$$\left(\mathcal{H}_\alpha \phi(x) - \lambda \phi(x) = 0\right)$$



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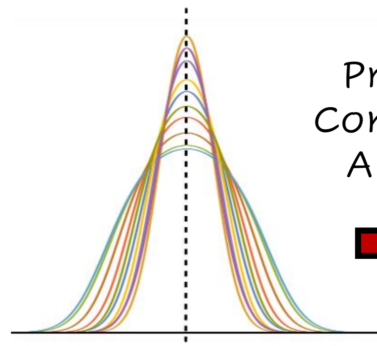
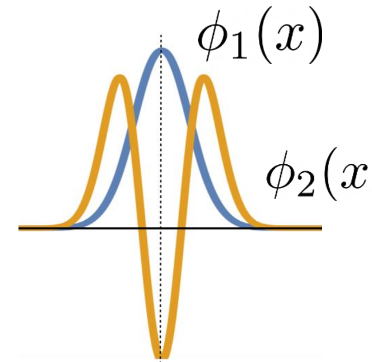


Principal Component Analysis



2) Project

Usually, a challenge

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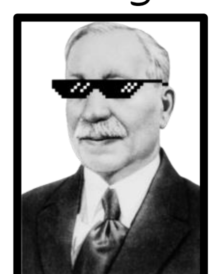
One equation per coefficient

Galerkin

Training and Projecting



https://doi.org/10.1103/PhysRevC.106.054322

https://kylegodbey.github.io/nuclear-rbm

jupyter {book}

Reduced Basis Methods in Nuclear Physics

https://www.frontiersin.org/articles/10.3389/fphy.2022.1092931/full

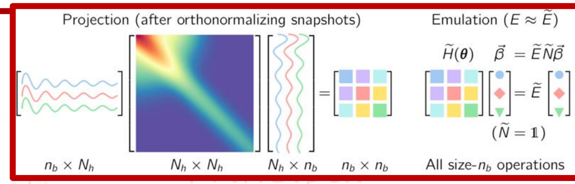
BUQEYE Guide to Projection-Based Emulators in Nuclear Physics

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

[1] *Department of Physics and Astronomy & Institute of Nuclear and Particle Physics, Ohio University, Athens, OH 45701, USA*

[2] *Facility for Rare Isotope Beams, Michigan State University, MI 4*

[3] *Department of Physics, The Ohio State University, Columbus, O*



Model reduction methods for nuclear emulators

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

[1] Department of Physics, The Ohio State University, Columbus, OH 43210, United States of America

[2] Facility for Rare Isotope Beams, Michigan State University, MI 48824, United States of America

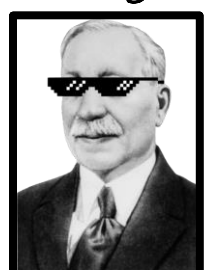
https://doi.org/10.1088/1361-6471/ac83dd

BAND

Bayesian Analysis of Nuclear Dynamics

and friends!

Training and Projecting



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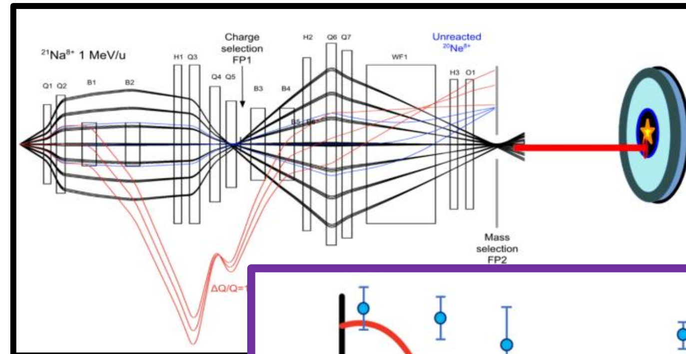
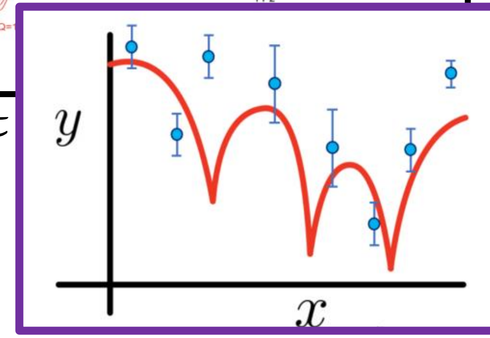


Experiment

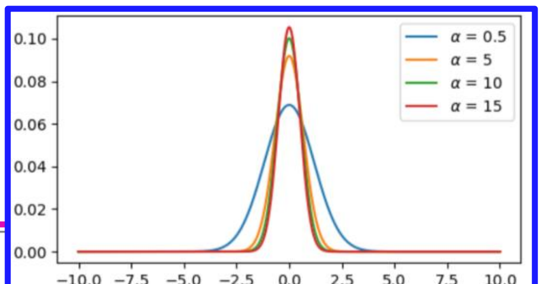


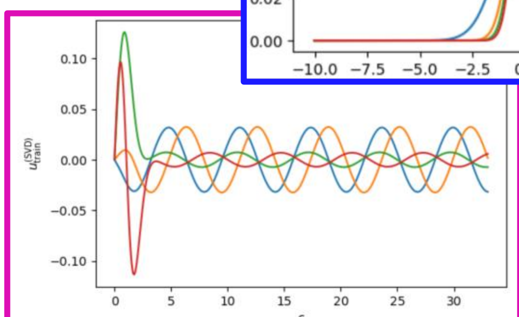
Theory

Motivation

Examples

Bound Systems





Scattering

(with Empirical Interpolation Method)

Code

```python
#We select four basis and obtain the following gorgeous functions:
nbasis = 4

fig, ax = plt.subplots(dpi=100)
fig.patch.set_facecolor('white')

for i in range(nbasis):
    ax.plot(s_mesh, U[:, i])

ax.set_xlabel(r'$s$')
ax.set_ylabel(r'$u_{\rm train}^{({\rm SVD})}$');
```

RBM Jupyter Book

Kyle Beyer

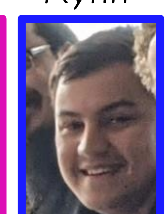
Edgard Bonilla

Kyle Godbey

Ruchi Garg

Daniel Odell

Eric Flynn



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Reduced Basis Methods in Nuclear Physics

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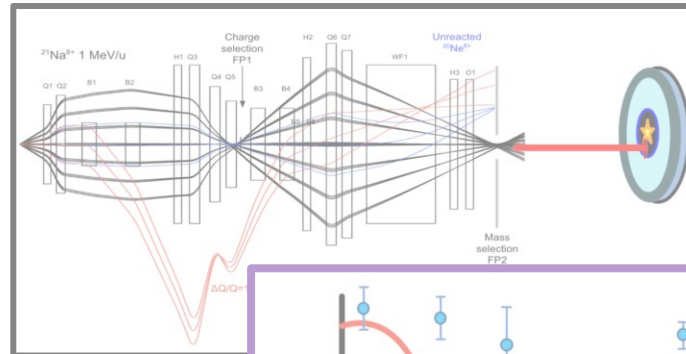

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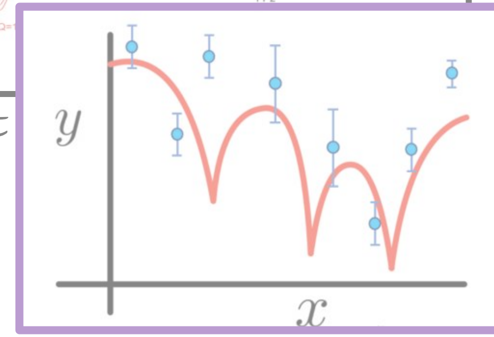

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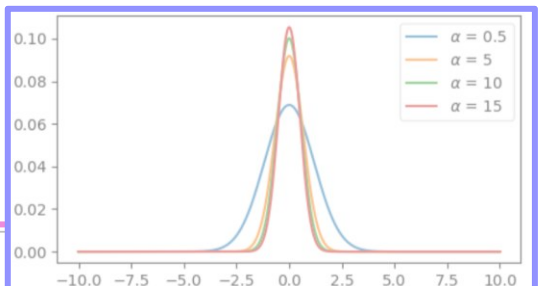
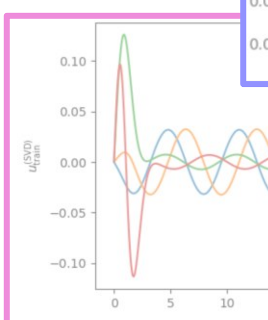
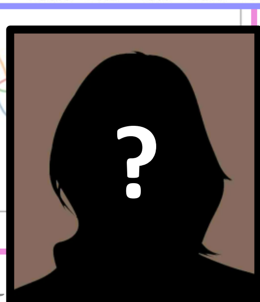
Examples

Bound Systems



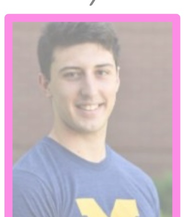


Scatt

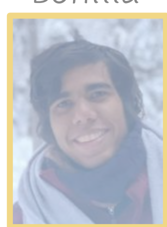


you?

Kyle Beyer

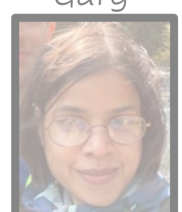


Edgard Bonilla

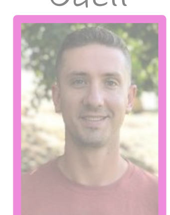


Kyle Godbey

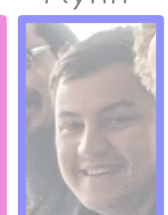
Ruchi Garg



Daniel Odell



Eric Flynn



RBM Jupyter Book

https://kylegodbey.github.io/nuclear-rbm

Problems Table

For uncertainty quantification

1) No variational principle → Galerkin projection

2) Sensitivity to training points → Proper Orthogonal Decomposition

3) Expensive high-fidelity → Greedy algorithm

4) Boundary conditions → Independent term

5) Incompatible domains → Reference domain

6) Non-affine operators → Empirical Interpolation Method / Collocation Method

7) Emulation error → Certified Error Control

Applications and Results

1 **Training and Projecting: A Reduced Basis Method Emulator for Many-Body Physics**

March 2022

Edgard Bonilla,[1,*] Pablo Giuliani,[2,3,†] Kyle Godbey,[2,‡] and Dean Lee[2,4,§]

Training and Projecting

https://doi.org/10.1103/PhysRevC.106.054322

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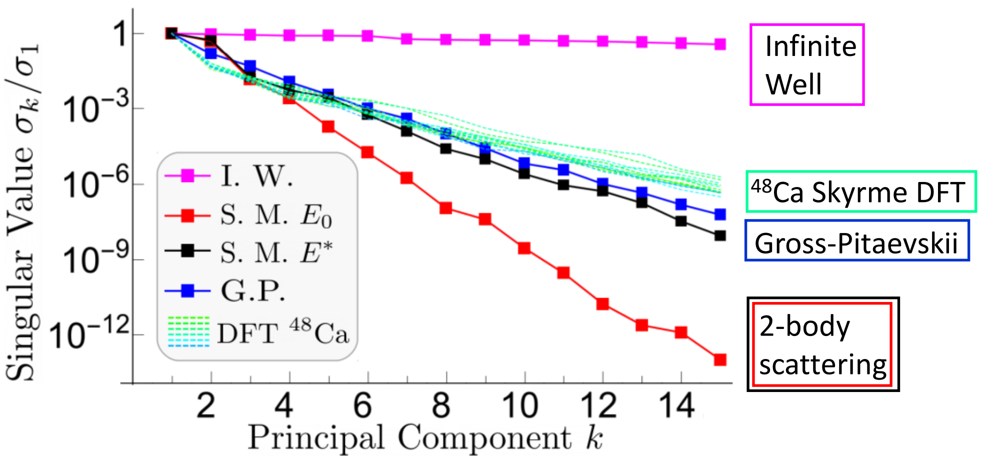

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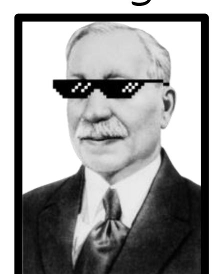

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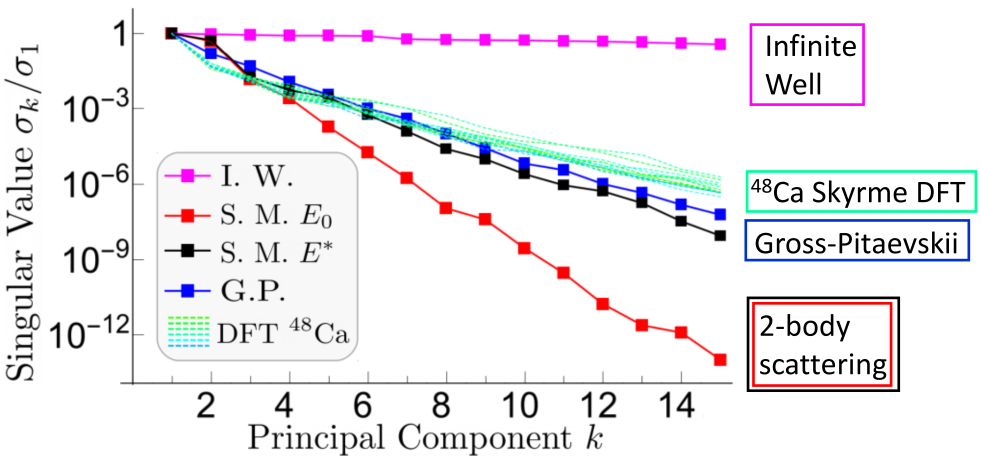
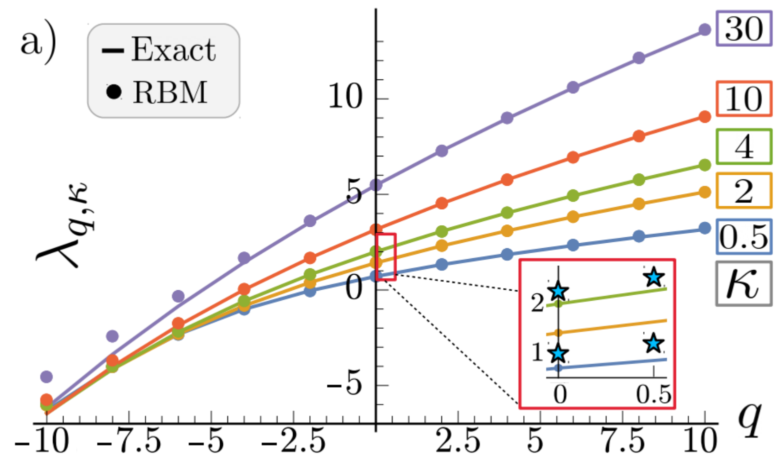


2) Very accurate



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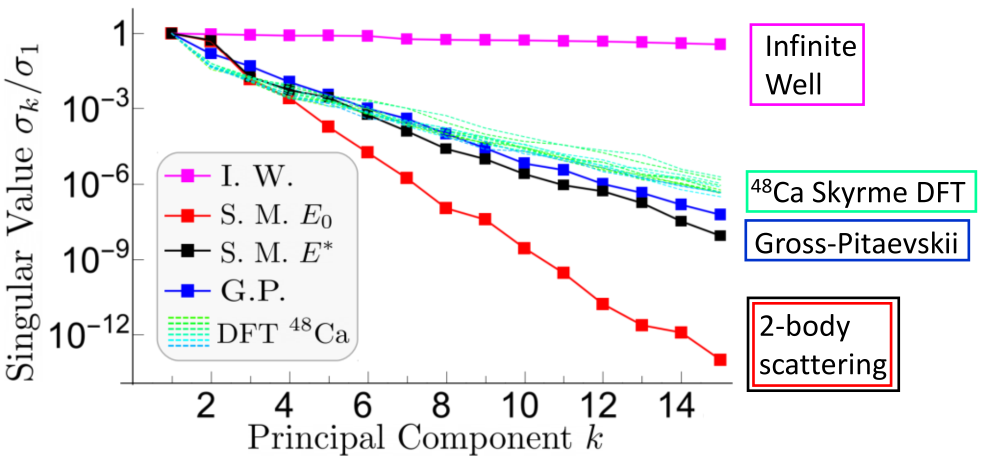

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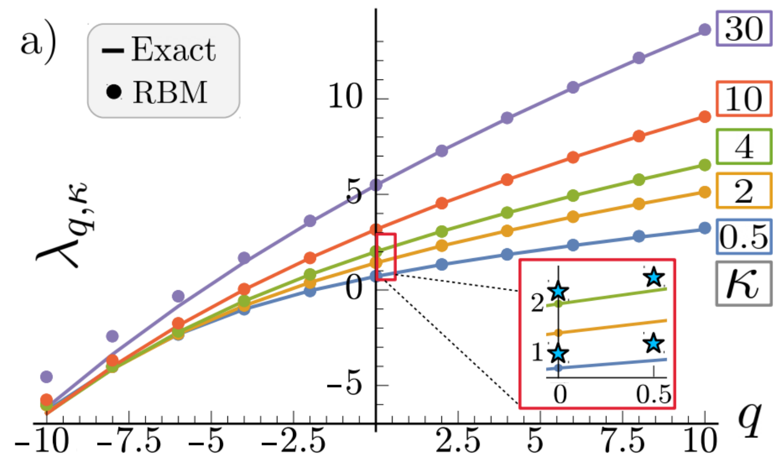
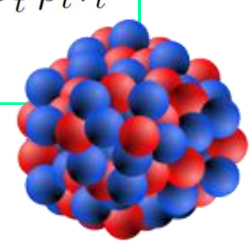


3) Very fast

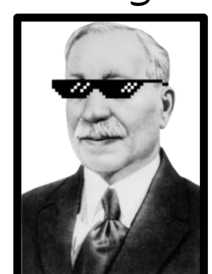
Skyrme Density Functional

$$\mathcal{H}_t(r) = C_t^{\rho}\rho_t^2 + C_t^{\rho\Delta\rho}\rho_t\Delta\rho_t + C_t^{\tau}\rho_t\tau_t + C_t^{J}\overleftrightarrow{J}_t^2 + C_t^{\rho\nabla J}\rho_t\nabla\cdot\mathbf{J}_t,$$



Mili-seconds

Training and Projecting



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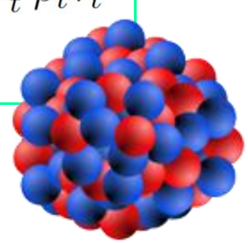

Mili-seconds

Training and Projecting

VERY non-linear

$$\rho(r)^{\alpha}$$

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2-body scattering

$$F_{q,\kappa}(\phi) = -\phi'' + \kappa x^2\phi + q|\phi|^2\phi - \lambda_{q,\kappa}\phi = 0$$

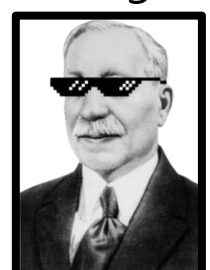
Gross-Pitaevskii

$$\hat{h}^{(i)}[\Phi]\phi^{(i)} - \lambda^{(i)}\phi^{(i)} = 0$$

Skyrme DFT

$$\langle\psi_j|F_\alpha(\hat{\phi}_\alpha)\rangle = 0, \quad \text{for all } j$$

Training and Projecting



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Skyrme DFT

Can even invert matrices

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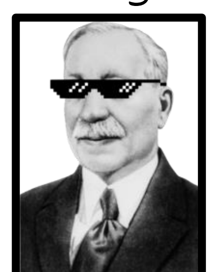
Training and Projecting



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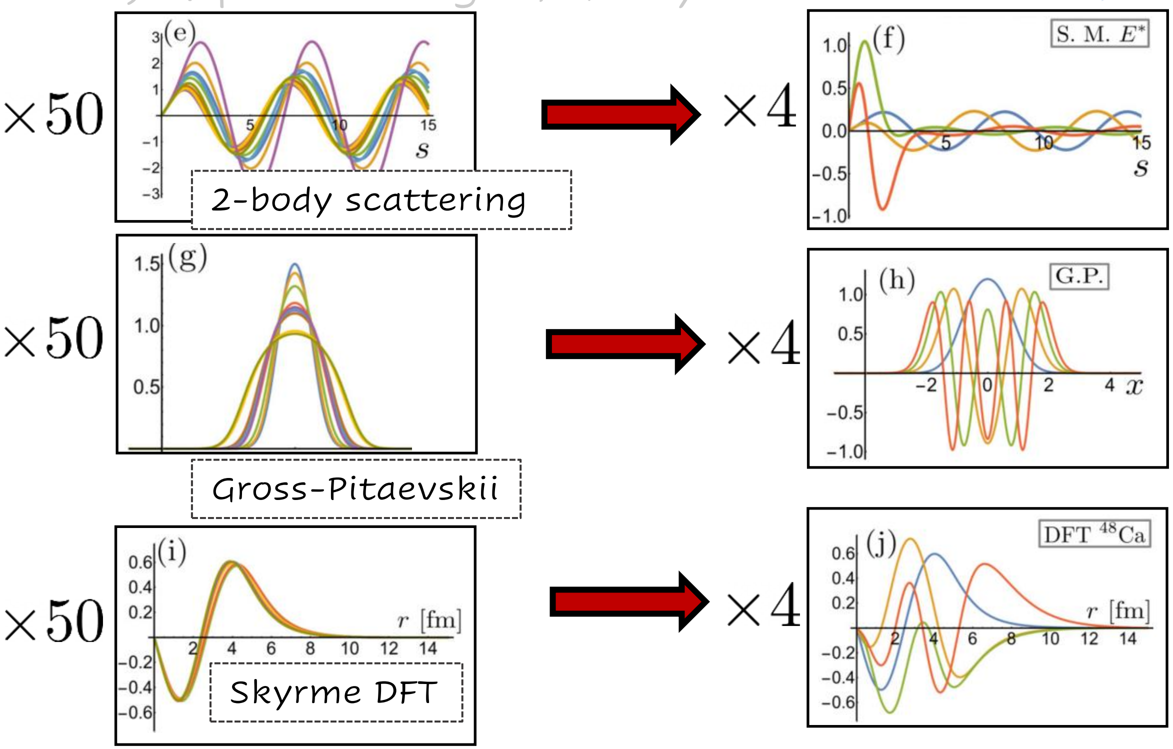
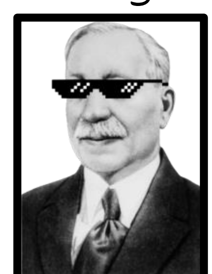


NOT snapshots

$$\hat{\phi}(x) = \phi_0 + \sum_k^n a_k \phi_k(x)$$

Training and Projecting



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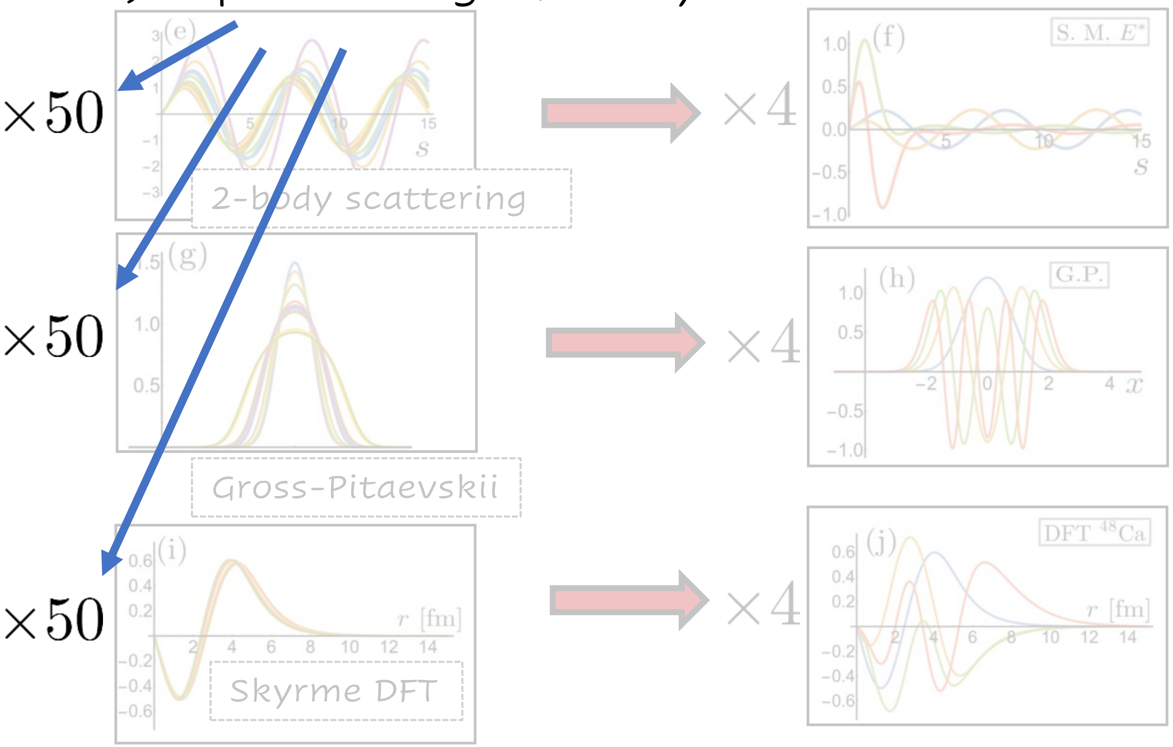

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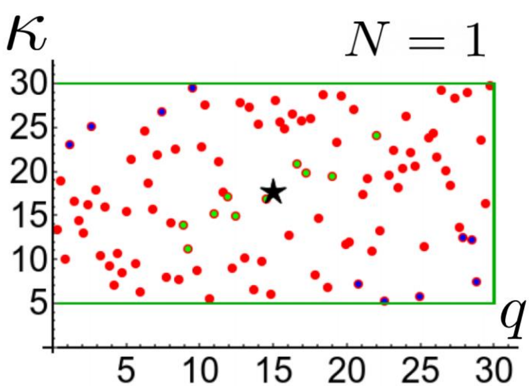

● $||F_\alpha(\phi)||^2$ Small (Nothing to learn)

● $||F_\alpha(\phi)||^2$ Big (Lots to learn)

Residual

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Training and Projecting

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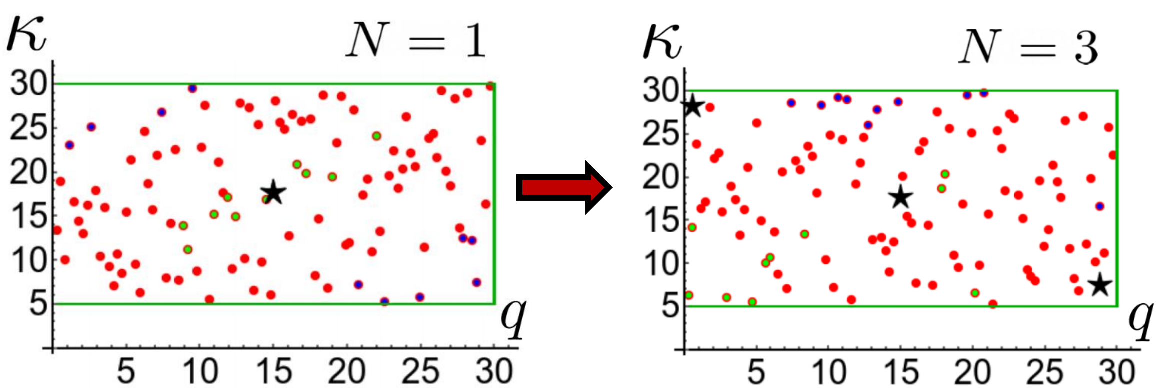

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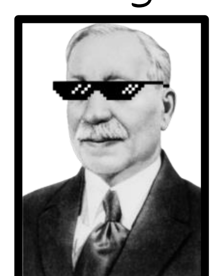
Training and Projecting



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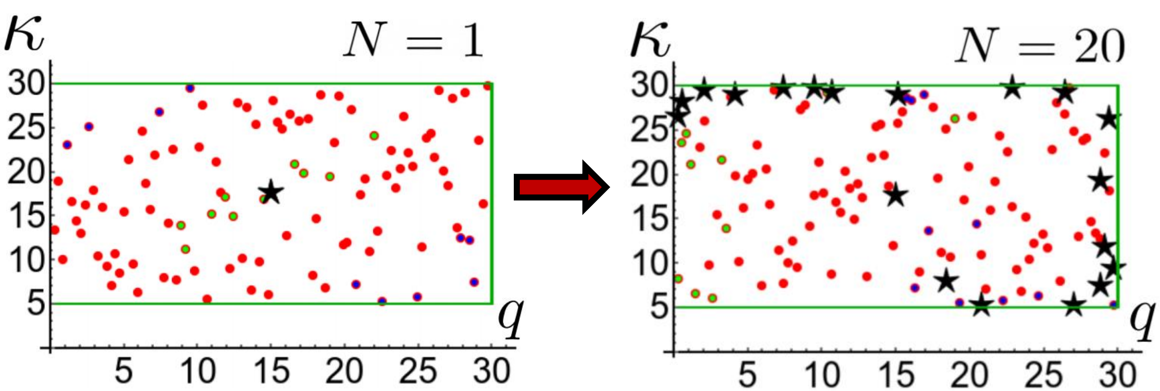

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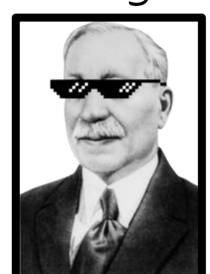
Training and Projecting



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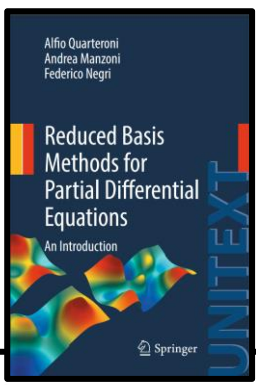

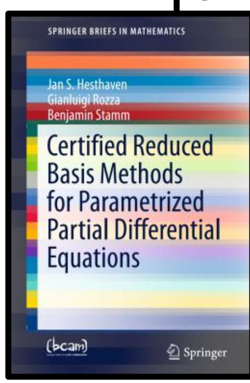

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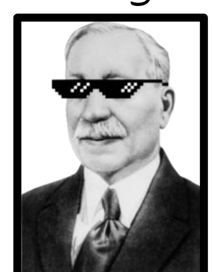

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Applications and Results

September 2022

2 **Bayes goes fast: Uncertainty Quantification for a Covariant Energy Density Functional emulated by the Reduced Basis Method**

Pablo Giuliani,[1,2,*] Kyle Godbey,[1,†] Edgard Bonilla,[3,‡] Frederi Viens,[2,4,§] and Jorge Piekarewicz[5,¶]

Bayes goes fast

https://doi.org/10.3389/fphy.2022.1054524

Applications and Results

September 2022

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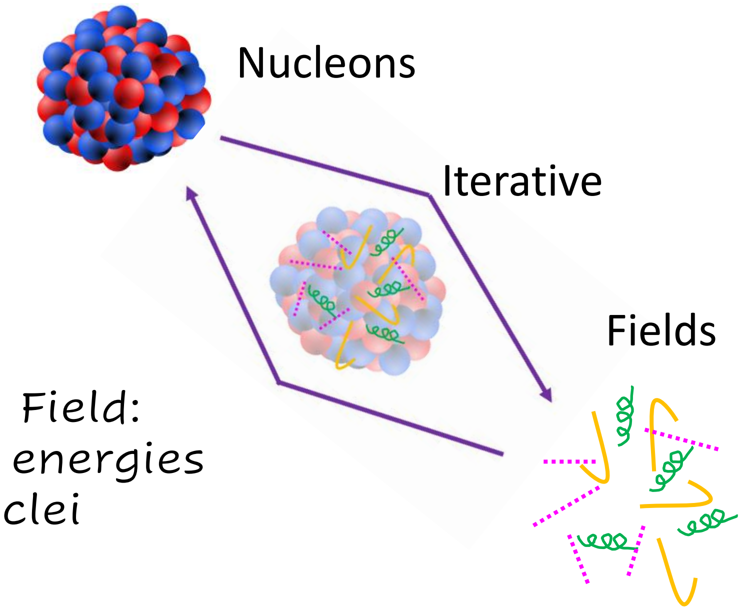


Relativistic Mean Field:
wave functions and energies
of spherical nuclei

Bayes goes fast

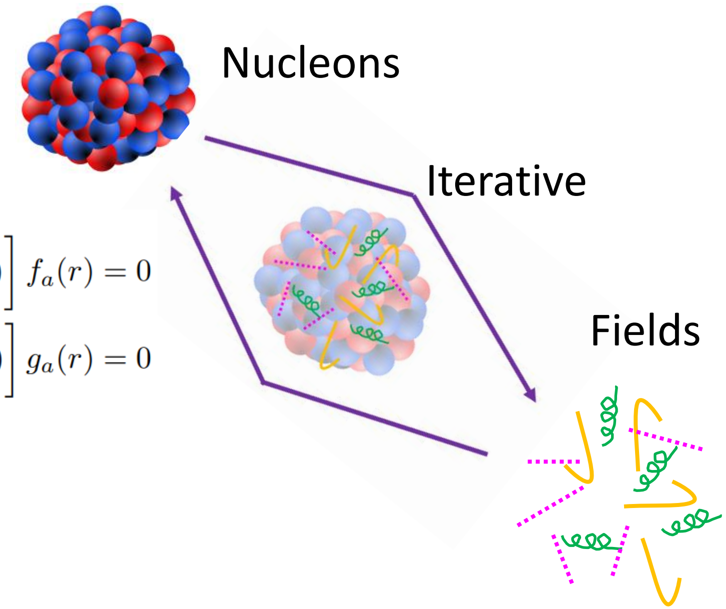
https://doi.org/10.3389/fphy.2022.1054524

Applications and Results

September 2022

2 **Bayes goes fast: Uncertainty Quantification for a Covariant Energy Density Functional emulated by the Reduced Basis Method**

Pablo Giuliani,[1,2,*] Kyle Godbey,[1,†] Edgard Bonilla,[3,‡] Frederi Viens,[2,4,§] and Jorge Piekarewicz[5,¶]



Dirac Equations

$$\left(\frac{d}{dr}+\frac{\kappa}{r}\right)g_a(r)-\left[E_a+M-\Phi_0(r)-W_0(r)\mp\frac{1}{2}B_0(r)-e\begin{Bmatrix}1\\0\end{Bmatrix}A_0(r)\right]f_a(r)=0$$

$$\left(\frac{d}{dr}-\frac{\kappa}{r}\right)f_a(r)+\left[E_a-M+\Phi_0(r)-W_0(r)\mp\frac{1}{2}B_0(r)-e\begin{Bmatrix}1\\0\end{Bmatrix}A_0(r)\right]g_a(r)=0$$

Field Equations

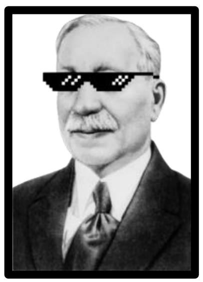
$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_{\rm s}^2\right)\Phi_0(r)-g_{\rm s}^2\left(\frac{\kappa}{2}\Phi_0^2(r)+\frac{\lambda}{6}\Phi_0^3(r)\right)=-g_{\rm s}^2\Big(\rho_{\rm s,p}(r)+\rho_{\rm s,n}(r)\Big),$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_{\rm v}^2\right)W_0(r)-g_{\rm v}^2\left(\frac{\zeta}{6}W_0^3(r)+2\Lambda_{\rm v}B_0^2(r)W_0(r)\right)=-g_{\rm v}^2\Big(\rho_{\rm v,p}(r)+\rho_{\rm v,n}(r)\Big),$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_\rho^2\right)B_0(r)-2\Lambda_{\rm v}g_\rho^2W_0^2(r)B_0(r)=-\frac{g_\rho^2}{2}\Big(\rho_{\rm v,p}(r)-\rho_{\rm v,n}(r)\Big),$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)A_0(r)=-e\rho_{\rm v,p}(r),$$

Bayes goes fast



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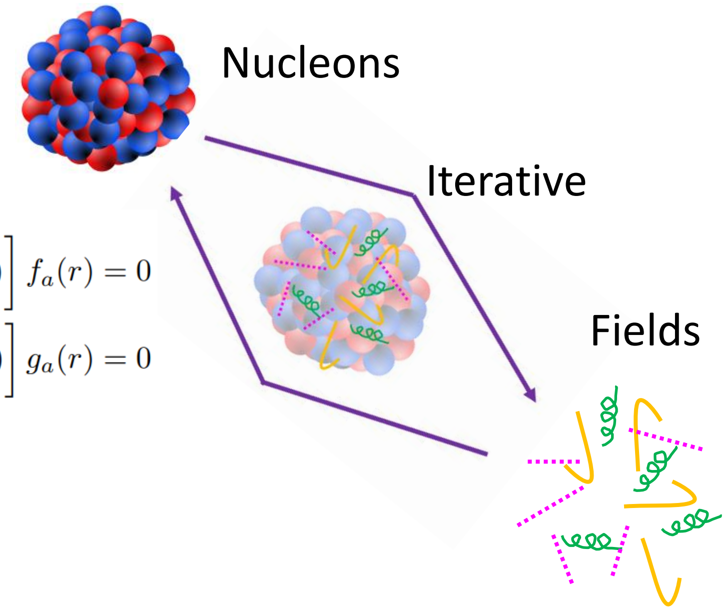

Dirac Equations

$$\left(\frac{d}{dr}+\frac{\kappa}{r}\right)g_a(r)-\left[E_a+M-\Phi_0(r)-W_0(r)\mp\frac{1}{2}B_0(r)-e\left\{\begin{matrix}1\\0\end{matrix}\right\}A_0(r)\right]f_a(r)=0$$

$$\left(\frac{d}{dr}-\frac{\kappa}{r}\right)f_a(r)+\left[E_a-M+\Phi_0(r)-W_0(r)\mp\frac{1}{2}B_0(r)-e\left\{\begin{matrix}1\\0\end{matrix}\right\}A_0(r)\right]g_a(r)=0$$

Field Equations

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_{\rm s}^2\right)\Phi_0(r)-g_{\rm s}^2\left(\frac{\kappa}{2}\Phi_0^2(r)+\frac{\lambda}{6}\Phi_0^3(r)\right)=-g_{\rm s}^2\Big(\rho_{\rm s,p}(r)+\rho_{\rm s,n}(r)\Big),$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_{\rm v}^2\right)W_0(r)-g_{\rm v}^2\left(\frac{\zeta}{6}W_0^3(r)+2\Lambda_{\rm v}B_0^2(r)W_0(r)\right)=-g_{\rm v}^2\Big(\rho_{\rm v,p}(r)+\rho_{\rm v,n}(r)\Big),$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_{\rho}^2\right)B_0(r)-2\Lambda_{\rm v}g_{\rho}^2W_0^2(r)B_0(r)=-\frac{g_{\rho}^2}{2}\Big(\rho_{\rm v,p}(r)-\rho_{\rm v,n}(r)\Big),$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)A_0(r)=-e\rho_{\rm v,p}(r),$$

Parameters α

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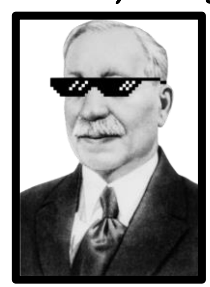

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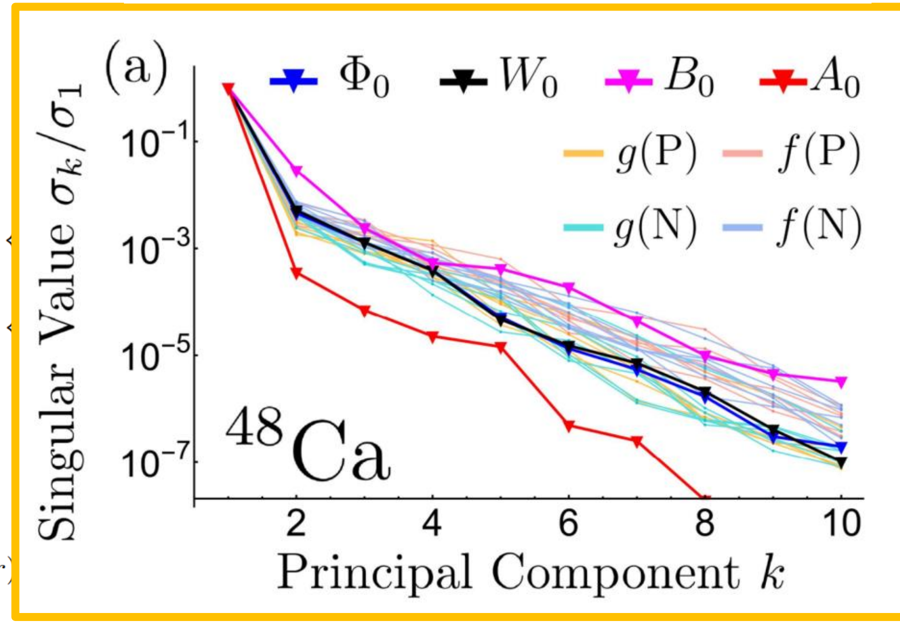
Low dimensional manifold



Dirac Equations

$$\left(\frac{d}{dr}+\frac{\kappa}{r}\right) g_a(r) - \left[E_a + M - \Phi_0(r) - W_0(r) \mp \frac{1}{2}B_0(r) - e\right.$$

$$\left(\frac{d}{dr}-\frac{\kappa}{r}\right) f_a(r) + \left[E_a - M + \Phi_0(r) - W_0(r) \mp \frac{1}{2}B_0(r) - e\right.$$

Field Equations

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_{\rm s}^2\right)\Phi_0(r) - g_{\rm s}^2\left(\frac{\kappa}{2}\Phi_0^2(r)+\frac{\lambda}{6}\Phi_0^3(r)\right) = -g_{\rm s}^2\left(\rho_{\rm s,p}(r)\right.$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_{\rm v}^2\right)W_0(r) - g_{\rm v}^2\left(\frac{\zeta}{6}W_0^3(r)+2\Lambda_{\rm v}B_0^2(r)W_0(r)\right) = -g_{\rm v}^2\left(\rho_{\rm v,p}(r)+\rho_{\rm v,n}(r)\right),$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_{\rho}^2\right)B_0(r) - 2\Lambda_{\rm v}g_\rho^2W_0^2(r)B_0(r) = -\frac{g_\rho^2}{2}\left(\rho_{\rm v,p}(r)-\rho_{\rm v,n}(r)\right),$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)A_0(r) = -e\rho_{\rm v,p}(r),$$

Parameters α

Bayes goes fast

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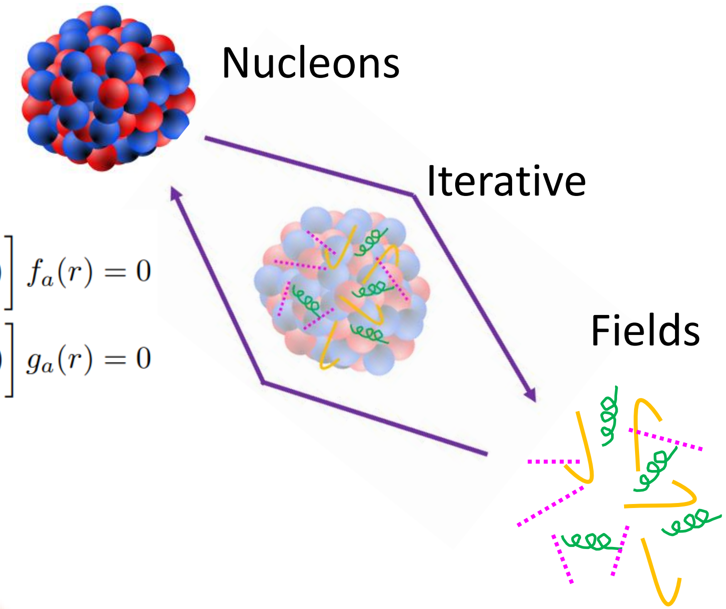

Dirac Equations

$$\left(\frac{d}{dr}+\frac{\kappa}{r}\right)g_a(r)-\left[E_a+M-\Phi_0(r)-W_0(r)\mp\frac{1}{2}B_0(r)-e\begin{Bmatrix}1\\0\end{Bmatrix}A_0(r)\right]f_a(r)=0$$

$$\left(\frac{d}{dr}-\frac{\kappa}{r}\right)f_a(r)+\left[E_a-M+\Phi_0(r)-W_0(r)\mp\frac{1}{2}B_0(r)-e\begin{Bmatrix}1\\0\end{Bmatrix}A_0(r)\right]g_a(r)=0$$

Field Equations

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_s^2\right)\Phi_0(r)-g_s^2\left(\frac{\kappa}{2}\Phi_0^2(r)+\frac{\lambda}{6}\Phi_0^3(r)\right)=-g_s^2\Big(\rho_{s,p}(r)+\rho_{s,n}(r)\Big),$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_v^2\right)W_0(r)-g_v^2\left(\frac{\zeta}{6}W_0^3(r)+2\Lambda_v B_0^2(r)W_0(r)\right)=-g_v^2\Big(\rho_{v,p}(r)+\rho_{v,n}(r)\Big),$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_\rho^2\right)B_0(r)-2\Lambda_v g_\rho^2 W_0^2(r)B_0(r)=-\frac{g_\rho^2}{2}\Big(\rho_{v,p}(r)-\rho_{v,n}(r)\Big),$$

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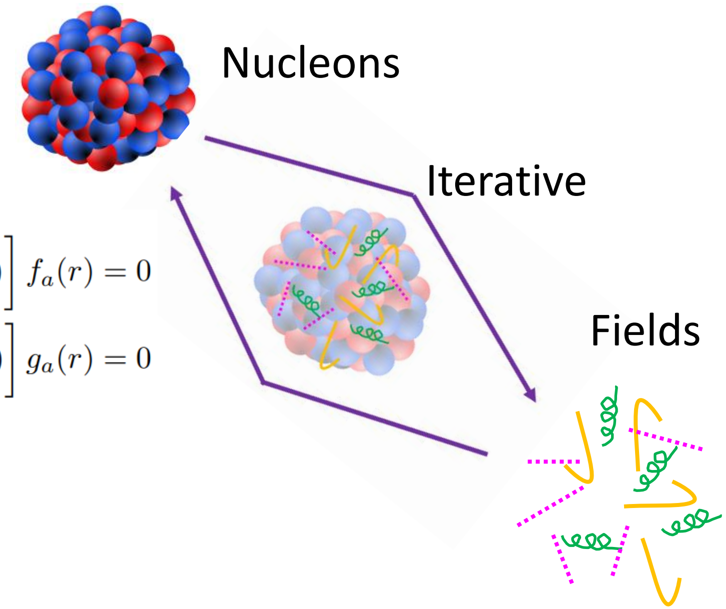

Dirac Equations

$$\langle g_{a,k}^{(j)}| \left(\frac{d}{dr}+\frac{\kappa}{r}\right) g_a(r) - \left[E_a + M - \Phi_0(r) - W_0(r) \mp \frac{1}{2}B_0(r) - e\begin{Bmatrix}1\\0\end{Bmatrix} A_0(r)\right] f_a(r) = 0$$

$$\langle f_{a,k}^{(j)}| \left(\frac{d}{dr}-\frac{\kappa}{r}\right) f_a(r) + \left[E_a - M + \Phi_0(r) - W_0(r) \mp \frac{1}{2}B_0(r) - e\begin{Bmatrix}1\\0\end{Bmatrix} A_0(r)\right] g_a(r) = 0$$

Field Equations

$$\langle \Phi_j(r)| \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_{\rm s}^2\right)\Phi_0(r) - g_{\rm s}^2\left(\frac{\kappa}{2}\Phi_0^2(r)+\frac{\lambda}{6}\Phi_0^3(r)\right) = -g_{\rm s}^2\Big(\rho_{\rm s,p}(r)+\rho_{\rm s,n}(r)\Big),$$

$$\langle W_j(r)| \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_{\rm v}^2\right)W_0(r) - g_{\rm v}^2\left(\frac{\zeta}{6}W_0^3(r)+2\Lambda_{\rm v}B_0^2(r)W_0(r)\right) = -g_{\rm v}^2\Big(\rho_{\rm v,p}(r)+\rho_{\rm v,n}(r)\Big),$$

$$\langle B_j(r)| \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_{\rho}^2\right)B_0(r) - 2\Lambda_{\rm v}g_\rho^2 W_0^2(r)B_0(r) = -\frac{g_\rho^2}{2}\Big(\rho_{\rm v,p}(r)-\rho_{\rm v,n}(r)\Big),$$

$$\langle A_j(r) \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)A_0(r) = -e\rho_{\rm v,p}(r),$$

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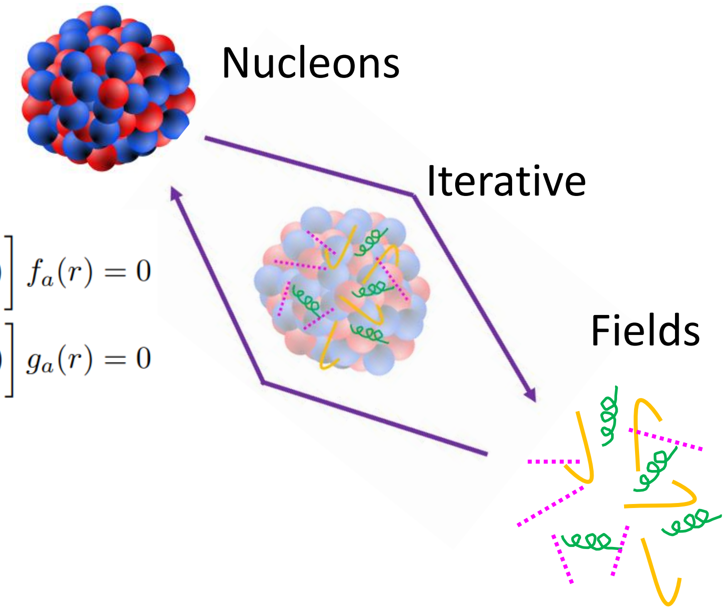


Dirac Equations

$$\langle g^{(j)}_{a,k}| \left(\frac{d}{dr}+\frac{\kappa}{r}\right) g_a(r) - \left[E_a + M - \Phi_0(r) - W_0(r) \mp \frac{1}{2}B_0(r) - e\begin{Bmatrix}1\\0\end{Bmatrix} A_0(r)\right] f_a(r) = 0$$

$$\langle f^{(j)}_{a,k}| \left(\frac{d}{dr}-\frac{\kappa}{r}\right) f_a(r) + \left[E_a - M + \Phi_0(r) - W_0(r) \mp \frac{1}{2}B_0(r) - e\begin{Bmatrix}1\\0\end{Bmatrix} A_0(r)\right] g_a(r) = 0$$

Field Equations

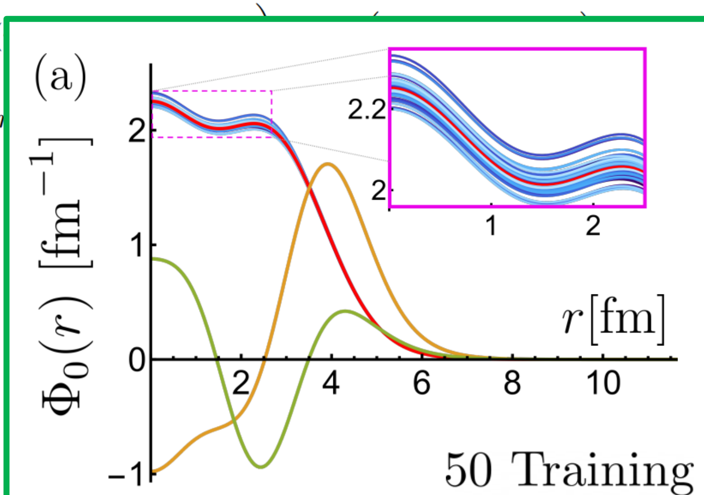
$$\langle \Phi_j(r)| \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_s^2\right)\Phi_0(r) - g_s^2\left(\frac{\kappa}{2}\Phi_0^2(r)+\frac{\lambda}{6}\Phi_0^3(r)\right) = -g_s^2\left(\rho_{s,p}(r)+\rho_{s,n}(r)\right),$$

$$\langle W_j(r)| \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_v^2\right)W_0(r) - g_v^2\left(\frac{\zeta}{6}W_0^3(\ldots$$

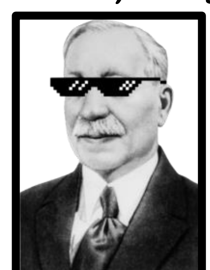
$$\langle B_j(r)| \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_\rho^2\right)B_0(r) - 2\Lambda_v g_\rho^2 W_0^2(\ldots$$

$$\langle A_j(r)| \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)A_0(r) = -e\rho_{v,p}(r),$$

$$\Phi_0(r) \approx \hat{\Phi}_0(r) = \sum_{k=1}^{n_\Phi} a_k^\Phi \; \Phi_k(r)$$



Bayes goes fast



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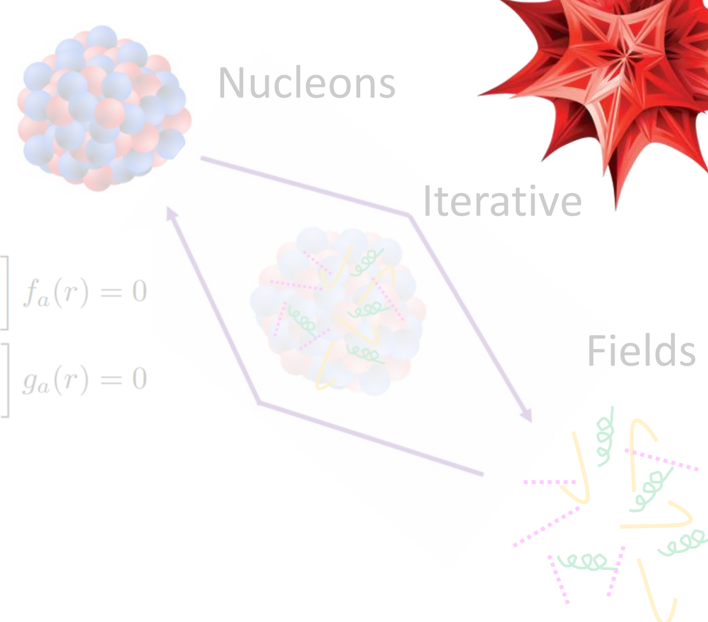
1

```
ΦEq = ((D2).Φ - ms^2*Φ + 2/r*(D1.Φ) -
   gs^2*(κ/2*Φ^2 + λ/6*Φ^3 - 2*Λs*B^2*Φ) +
   gs^2*ρs)
```



$$\langle g_{a,k}^{(j)}| \left(\frac{d}{dr}+\frac{\kappa}{r}\right) g_a(r) - \left[E_a + M - \Phi_0(r) - W_0(r) \mp \frac{1}{2}B_0(r) - e\begin{Bmatrix}1\\0\end{Bmatrix} A_0(r)\right] f_a(r) = 0$$

$$\langle f_{a,k}^{(j)}| \left(\frac{d}{dr}-\frac{\kappa}{r}\right) f_a(r) + \left[E_a - M + \Phi_0(r) - W_0(r) \mp \frac{1}{2}B_0(r) - e\begin{Bmatrix}1\\0\end{Bmatrix} A_0(r)\right] g_a(r) = 0$$

Field Equations

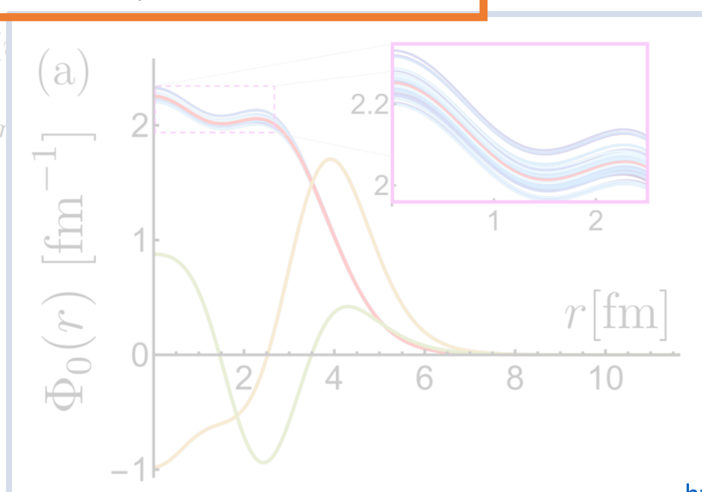
1

$$\langle \Phi_j(r)| \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_s^2\right)\Phi_0(r) - g_s^2\left(\frac{\kappa}{2}\Phi_0^2(r)+\frac{\lambda}{6}\Phi_0^3(r)\right) = -g_s^2\left(\rho_{s,p}(r)+\rho_{s,n}(r)\right),$$

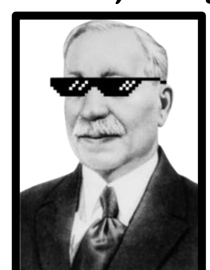
$$\langle W_j(r)| \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_v^2\right)W_0(r) - g_v^2\left(\frac{\zeta}{6}W_0^3 \ldots\right.$$

$$\langle B_j(r)| \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_\rho^2\right)B_0(r) - 2\Lambda_v g_\rho^2 W_0^2 \ldots$$

$$\langle A_j(r)| \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)A_0(r) = -e\rho_{v,p}(r),$$



Bayes goes fast



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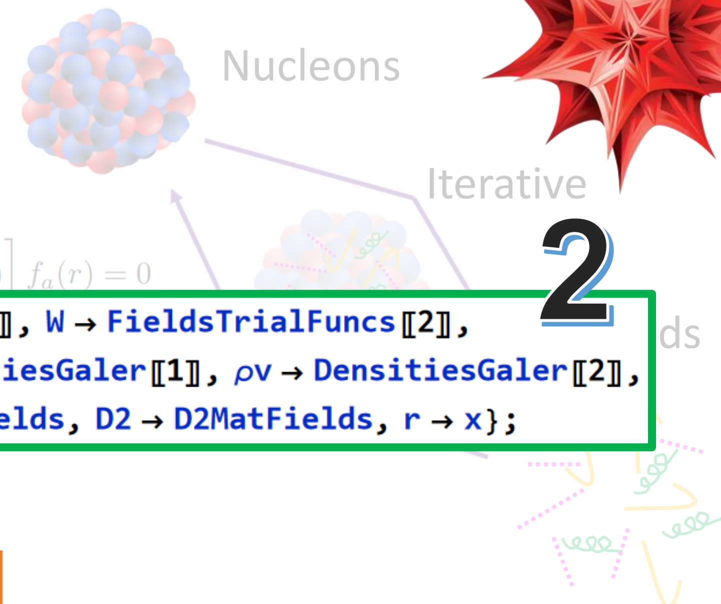


1

```
ΦEq = ((D2).Φ - ms^2*Φ + 2/r*(D1.Φ) -
   gs^2*(κ/2*Φ^2 + λ/6*Φ^3 - 2*Λs*B^2*Φ) +
   gs^2*ρs)
```

$$\langle g^{(j)}_{a,k}| \left(\frac{d}{dr} + \frac{\kappa}{r}\right) g_a(r) - \left[E_a + M - \Phi_0(r) - W_0(r) \mp \tfrac{1}{2}B_0(r) - e\left\{\begin{matrix}1\\0\end{matrix}\right\} A_0(r)\right] f_a(r) = 0$$

$$\langle f^{(j)}_{a,k}| \left(\frac{d}{dr} - \frac{\kappa}{r}\right) f_a(r)$$

2

```
ΦEqGaler = ΦEq /. {Φ → FieldsTrialFuncs[[1]], W → FieldsTrialFuncs[[2]],
    B → FieldsTrialFuncs[[3]], ρs → DensitiesGaler[[1]], ρv → DensitiesGaler[[2]],
    ρ3 → DensitiesGaler[[3]], D1 → D1MatFields, D2 → D2MatFields, r → x};
```

Field Equations

1

$$\langle \Phi_j(r)| \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - m_s^2\right)\Phi_0(r) - g_s^2\left(\frac{\kappa}{2}\Phi_0^2(r) + \frac{\lambda}{6}\Phi_0^3(r)\right) = -g_s^2\left(\rho_{s,p}(r) + \rho_{s,n}(r)\right),$$

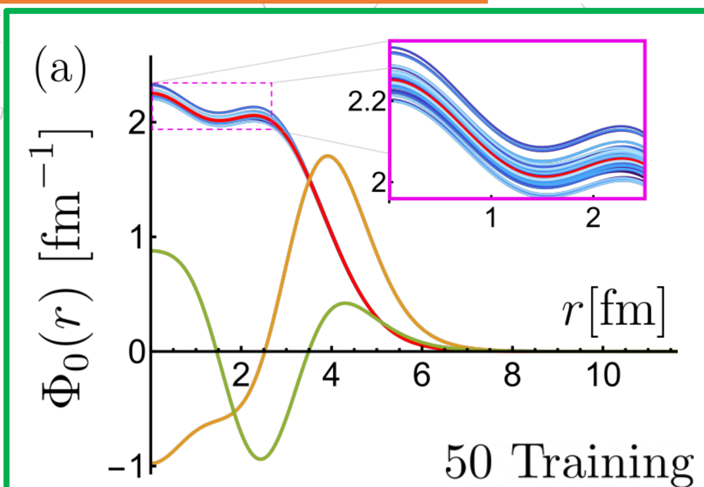
$$\langle W_j(r)| \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - m_v^2\right) W_0(r) - g_v^2\left(\frac{\zeta}{6}W_0^3 \ldots\right.$$

$$\langle B_j(r)| \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - m_\rho^2\right) B_0(r) - 2\Lambda_v g_\rho^2 W_0^2 \ldots$$

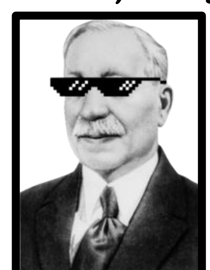
$$\langle A_j(r) \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) A_0(r) = -e\rho_{v,p}(r),$$

$$\Phi_0(r) \approx \hat{\Phi}_0(r) = \sum_{k=1}^{n_\Phi} a_k^\Phi\ \Phi_k(r)$$

2



Bayes goes fast



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```
ΦEq = ((D2).Φ - ms^2*Φ + 2/r*(D1.Φ) -
   gs^2*(κ/2*Φ^2 + λ/6*Φ^3 - 2*Λs*B^2*Φ) +
   gs^2*ρs)
```

2

```
ΦEqGaler = ΦEq /. {Φ → FieldsTrialFuncs[[1]], W → FieldsTrialFuncs[[2]],
     B → FieldsTrialFuncs[[3]], ρs → DensitiesGaler[[1]], ρv → DensitiesGaler[[2]],
    ρ3 → DensitiesGaler[[3]], D1 → D1MatFields, D2 → D2MatFields, r → x};
```

3

```
(*Fields cycle*)
For[hbasis = 1, hbasis ≤ NumberBasis, hbasis++,

  AppendTo[FinalEquationsGaler,
    Expand[ΦEqGaler.BasisFieldsSVD[[1]][[hbasis]]] == 0];
 ];
```

Field Equations

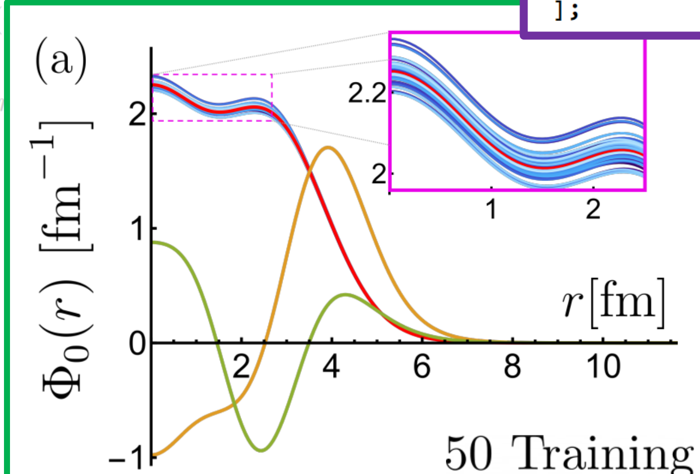
3 1

$$\langle\Phi_j(r)| \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - m_s^2\right)\Phi_0(r) - g_s^2\left(\frac{\kappa}{2}\Phi_0^2(r) + \frac{\lambda}{6}\Phi_0^3(r)\right) = -g_s^2\left(\rho_{s,p}(r) + \rho_{s,n}(r)\right),$$

$$\langle A_j(r)| \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) A_0(r) = -e\rho_{v,p}(r),$$

2

$$\Phi_0(r) \approx \hat{\Phi}_0(r) = \sum_{k=1}^{n_\Phi} a_k^\Phi \; \Phi_k(r)$$



Bayes goes fast

https://doi.org/10.3389/fphy.2022.1054524

Applications and Results

September 2022

2 **Bayes goes fast: Uncertainty Quantification for a Covariant Energy Density Functional emulated by the Reduced Basis Method**

Pablo Giuliani,[1,2,*] Kyle Godbey,[1,†] Edgard Bonilla,[3,‡] Frederi Viens,[2,4,§] and Jorge Piekarewicz[5,¶]

Name	Date modified	Type	Size
Basis	9/21/2022 11:11 AM	File folder	
Performance	9/21/2022 11:11 AM	File folder	
Nucleus_48Ca_CoeffEquations.txt	9/21/2022 11:11 AM	Text Document	1,474 KB
Nucleus_48Ca_Jacobian.txt	9/21/2022 11:11 AM	Text Document	2,404 KB
Nucleus_48Ca_JacobianKyle.txt	9/21/2022 11:11 AM	Text Document	2,404 KB
Nucleus_48Ca_NeutronSkin.txt	9/21/2022 11:11 AM	Text Document	13 KB
Nucleus_48Ca_ProtonRadius.txt	9/21/2022 11:11 AM	Text Document	7 KB
Nucleus_48Ca_TotalEnergyFields.txt	9/21/2022 11:11 AM	Text Document	513 KB
Nucleus_48Ca_TotalEnergyNucleons.txt	9/21/2022 11:11 AM	Text Document	1 KB
Nucleus_48CaBasisNumbers.txt	9/21/2022 11:11 AM	Text Document	1 KB

September 2022

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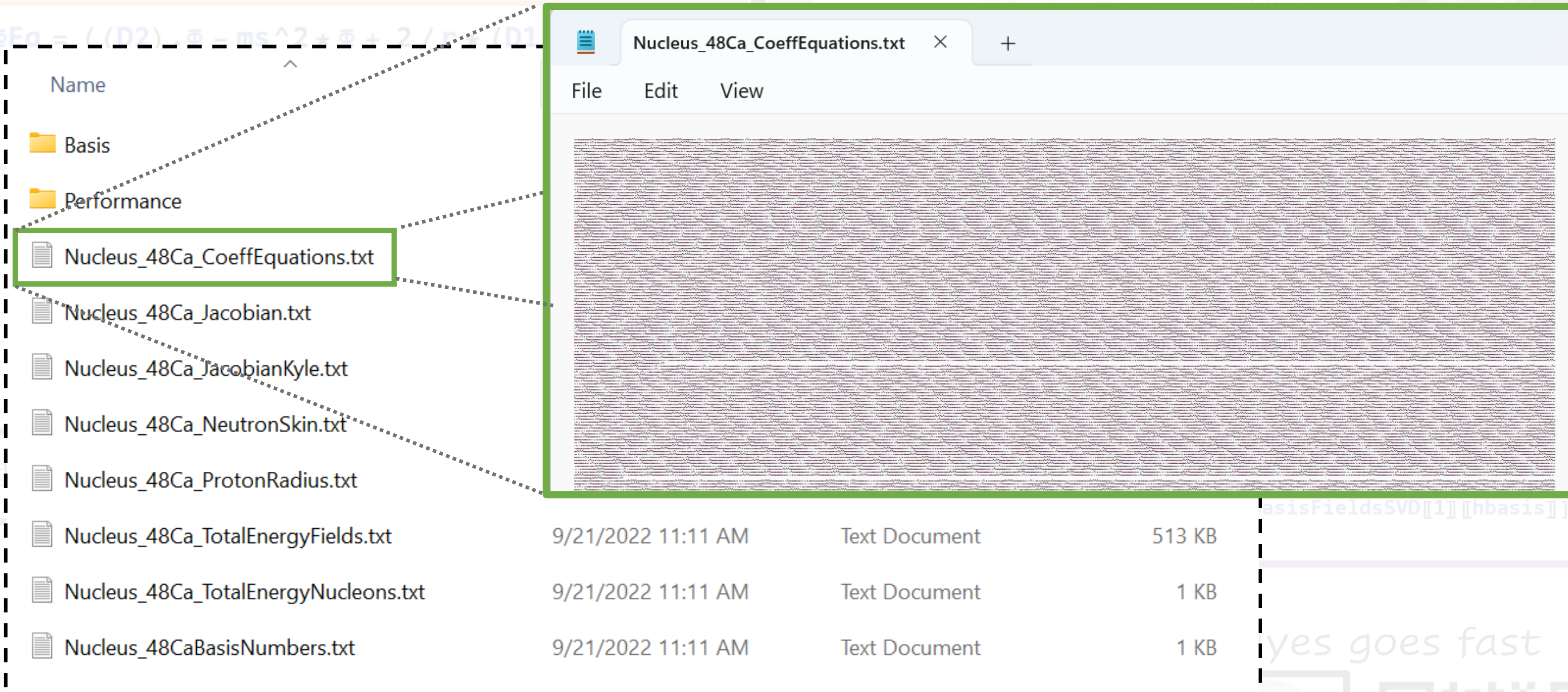

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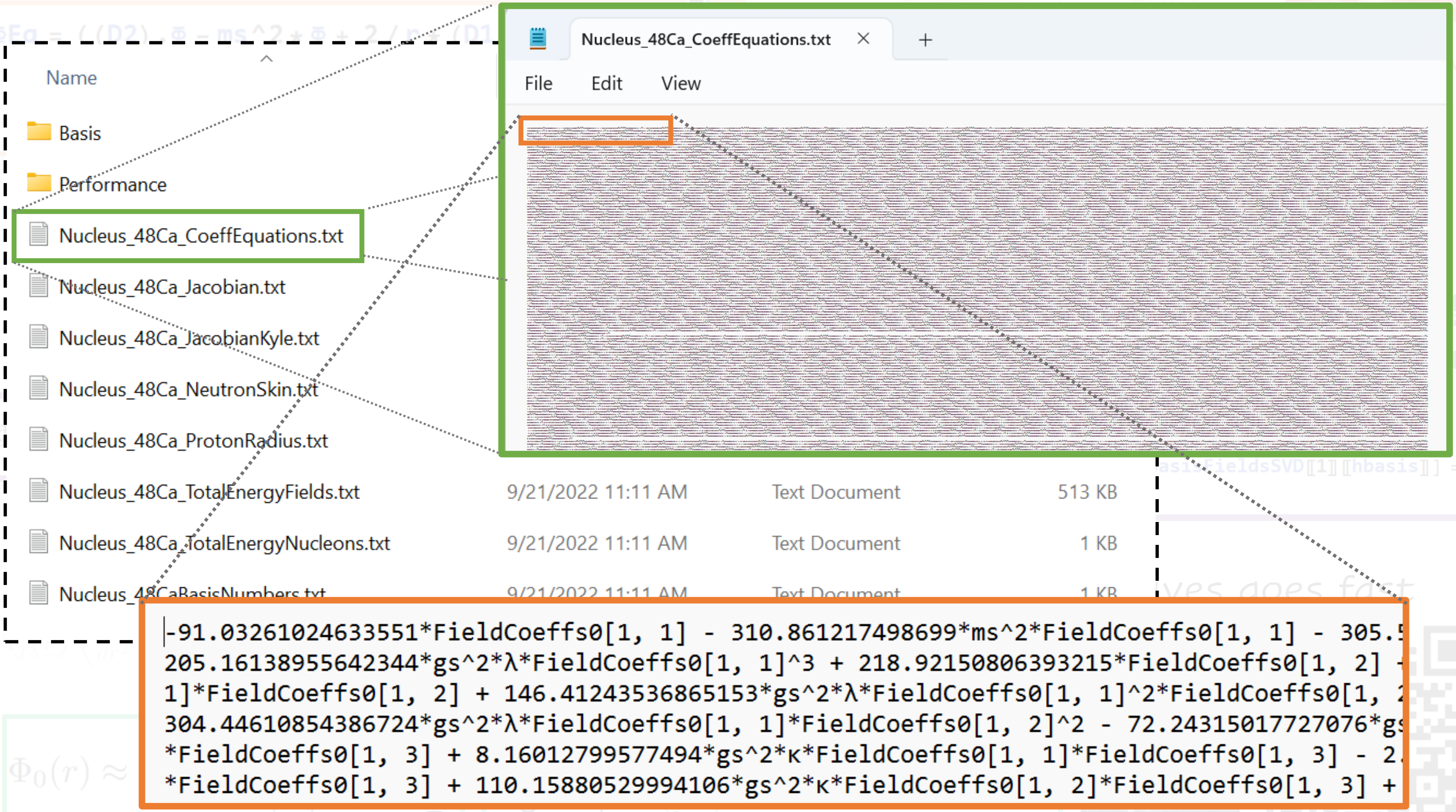

September 2022

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Nucleus_48CaBasisNumbers.txt	9/21/2022 11:11 AM	Text Document	1 KB

Compile with Cython

rmf_rbm_hybrid.so 85,499 KB

Applications and Results

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BAND
Bayesian Analysis of Nuclear Dynamics

Name	Date modified	Type	Size
Basis	…/20… 11:…	File folder	
Performance		File folder	
	9/21/2022 …	Text Document	1,474 KB
	9/21/2022 11:11 AM	Text Document	2,404 KB
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	9/21/2022 11:11 AM	Text Document	13 KB
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	…21/2022 11:11 AM	Text Document	513 KB
	…21/2022 11:11 AM	Text Document	1 KB
	…21/2022 11:11 AM	Text Document	1 KB

surmise

A Python package that is designed to provide a surrogate model interface for calibration, uncertainty quantification, and other tools.

O. Surer, M. Plumlee, S. Wild

surmise Read the Docs

```
def rbm_emulator(x,theta):

    func = [rmf_rbm.rmf_poly_16O_0,
        rmf_rbm.rmf_poly_40Ca_0,
        rmf_rbm.rmf_poly_48Ca_0,
        rmf_rbm.rmf_poly_68Ni_0,
        rmf_rbm.rmf_poly_90Zr_0,
        rmf_rbm.rmf_poly_100Sn_0,
        rmf_rbm.rmf_poly_116Sn_0,
        rmf_rbm.rmf_poly_132Sn_0,
        rmf_rbm.rmf_poly_144Sm_0,
        rmf_rbm.rmf_poly_208Pb_0,
        ]

    jacfunc = [rmf_rbm.rmf_poly_16O_0_jac,
          rmf_rbm.rmf_poly_40Ca_0_jac,
          rmf_rbm.rmf_poly_48Ca_0_jac,
```

Compile with Cython

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Applications and Results

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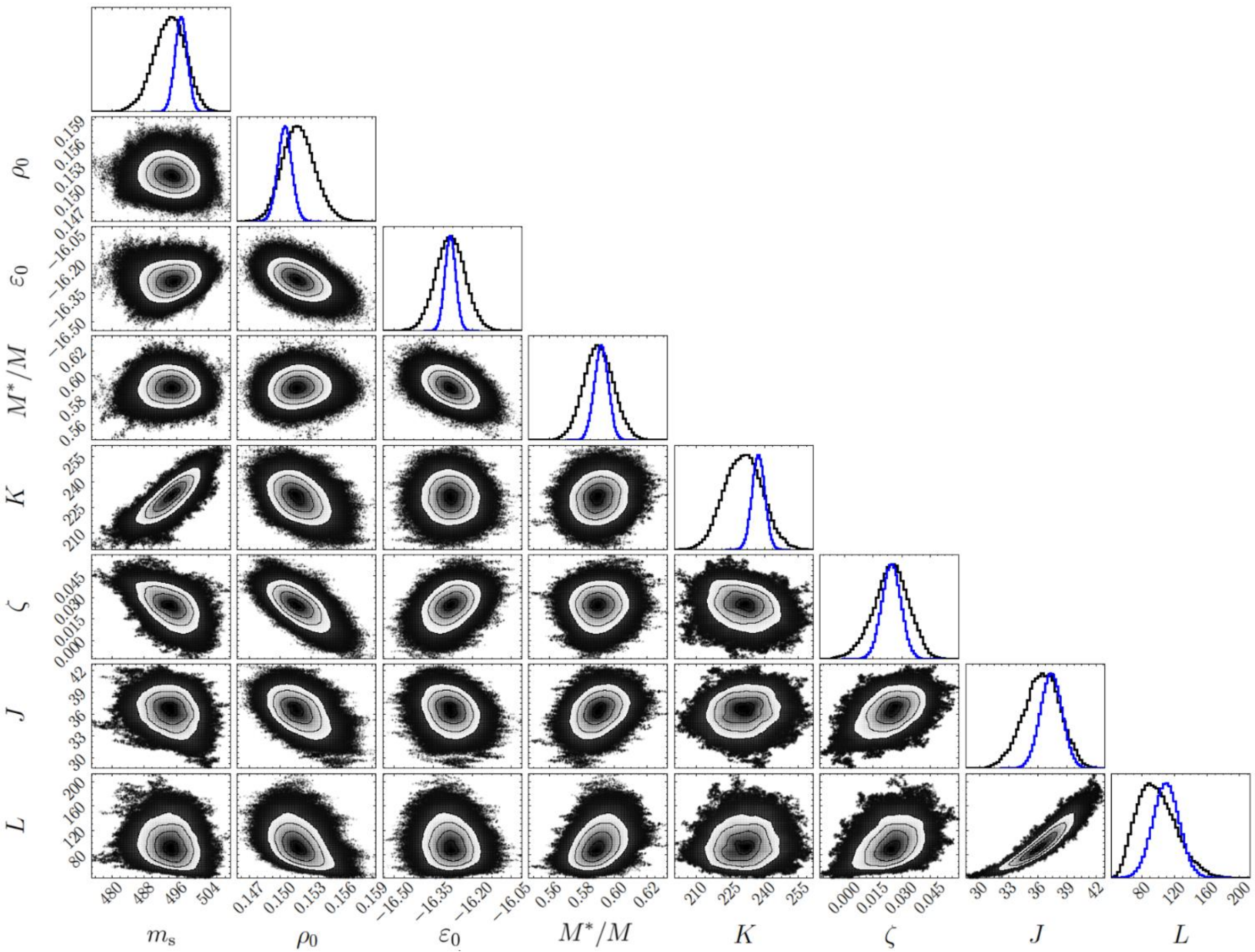
Posterior Bayesian calibration



Masses and Charge radii

^{16}O
^{40}Ca
^{48}Ca
^{68}Ni
^{90}Zr
^{100}Sn
^{116}Sn
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^{144}Sm
^{208}Pb

Bayes goes fast

https://doi.org/10.3389/fphy.2022.1054524

Applications and Results

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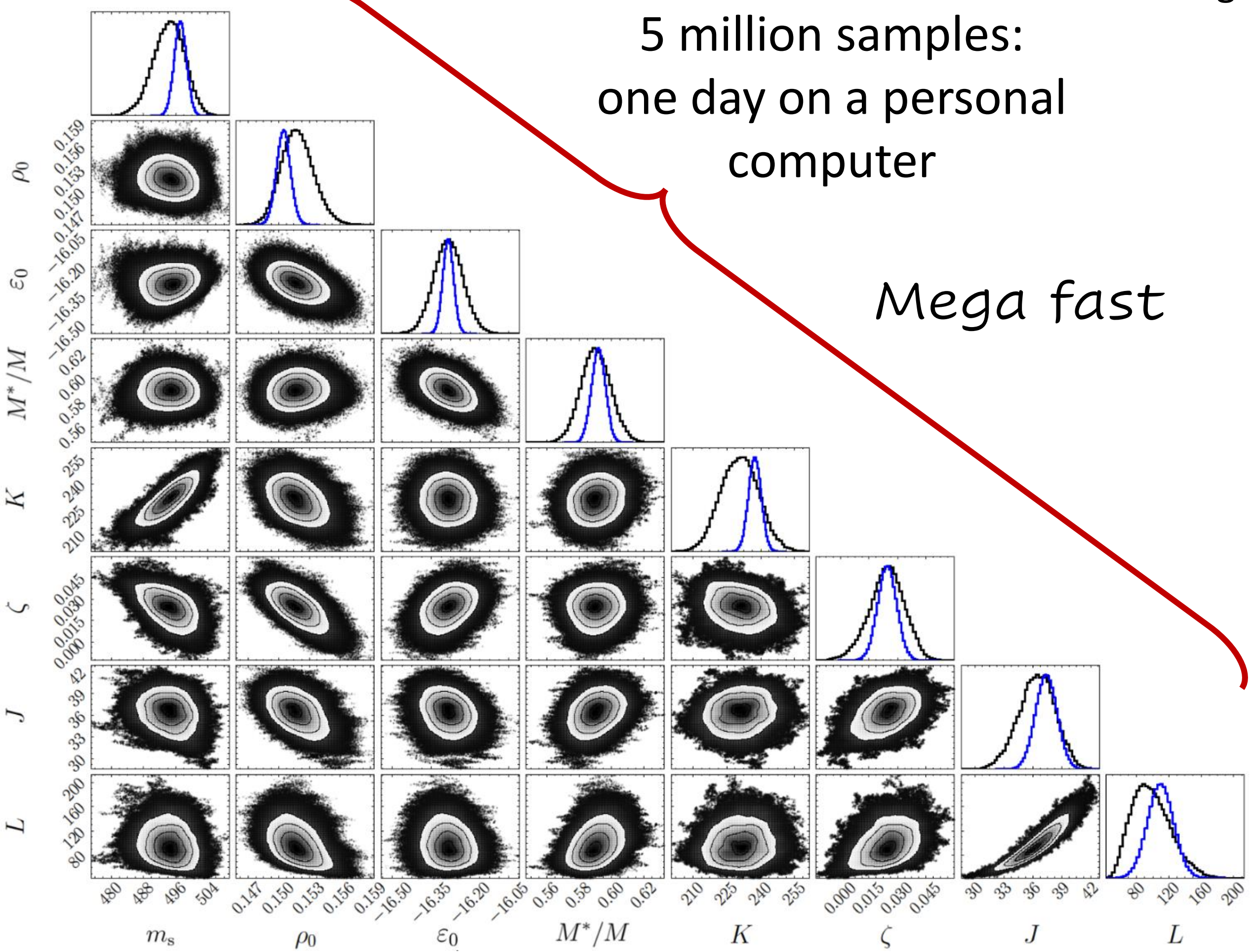

5 million samples: one day on a personal computer

Mega fast

Masses and Charge radii

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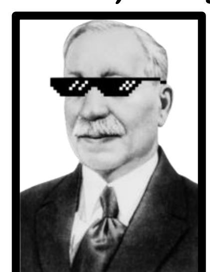

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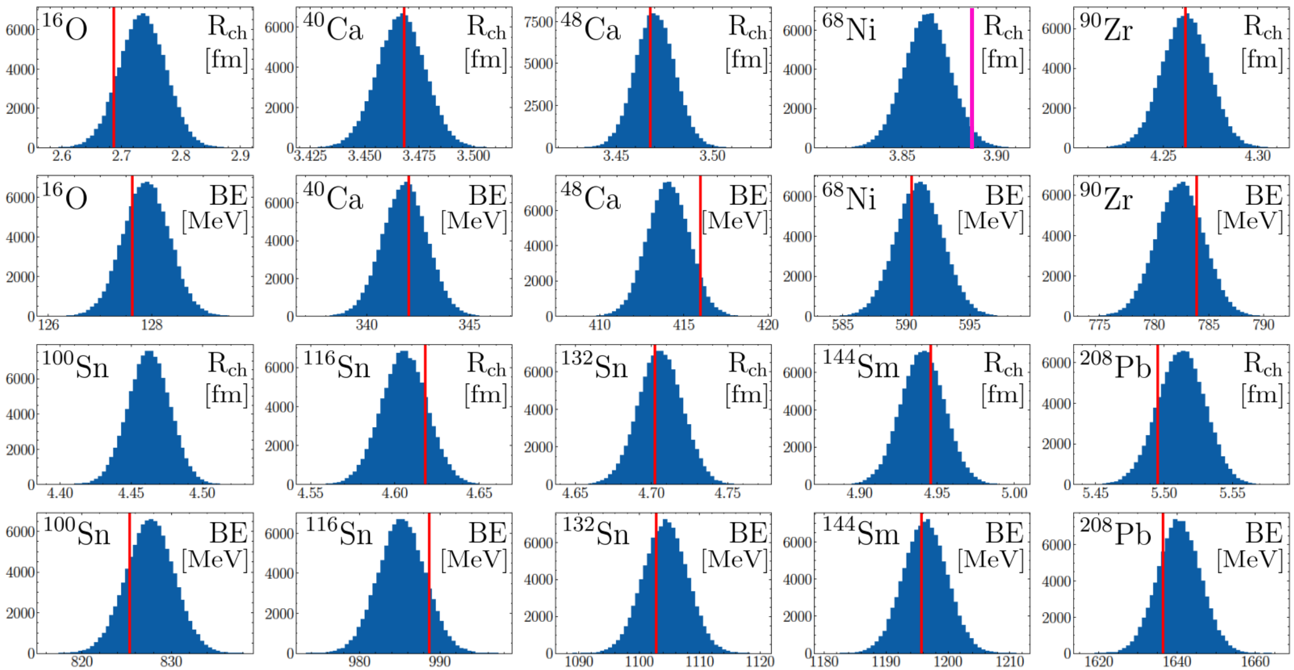

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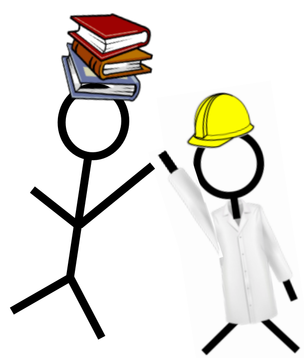
Masses and Charge radii



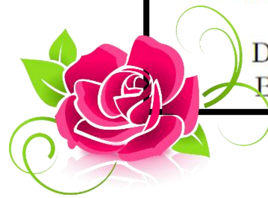
Bayes goes fast

https://doi.org/10.3389/fphy.2022.1054524

Applications and Results

3

almost done....



Presenting ROSE, a Reduced Order Scattering Emulator

D. Odell,[1,*] P. Giuliani,[2,3] M. Catacora-Rios,[2,4] M. Chan,[5] E. Bonilla,[6] K. Godbey,[2] R. J. Furnstahl,[7] and F. M. Nunes[2,4,†]

Daniel Odell

The roses

https://github.com/odell/rose

Applications and Results

3

almost done....

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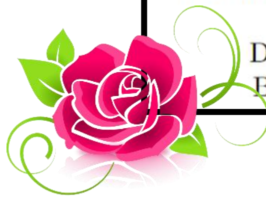
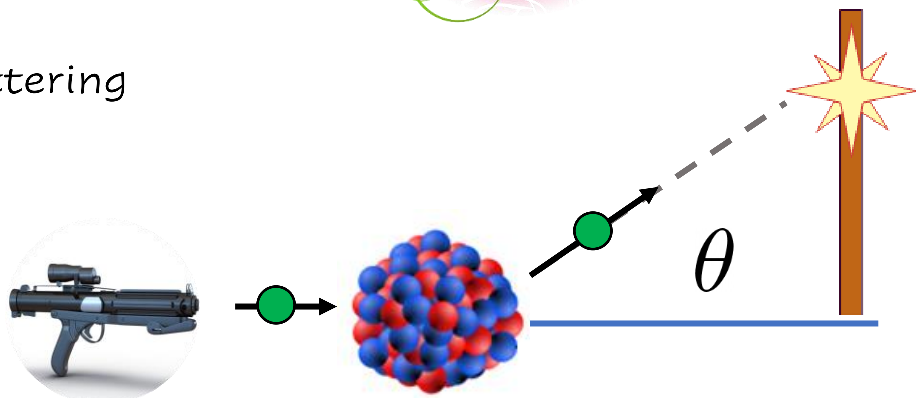


Daniel Odell

2-body scattering



$$F_\alpha(\phi) = \left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + \frac{2\eta k}{r} + U(r,\alpha) - k^2\right)\phi(r) = 0$$

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almost done....

Applications and Results

3

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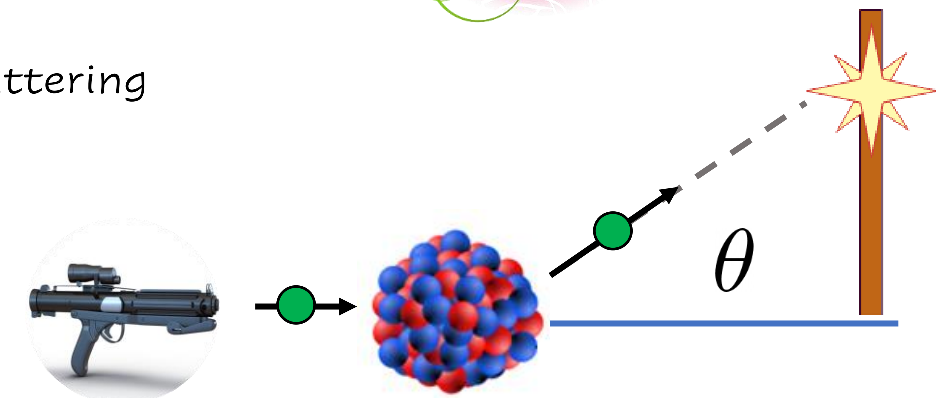

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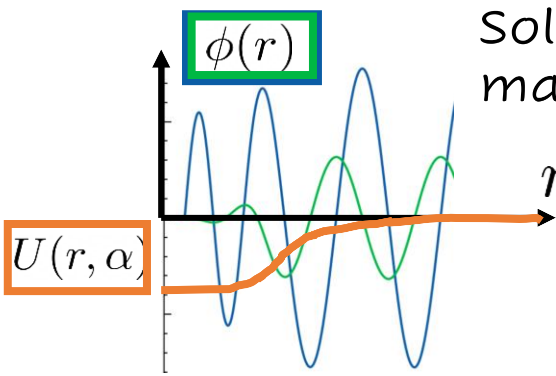

Solve for many ℓ

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Applications and Results

3

almost done....

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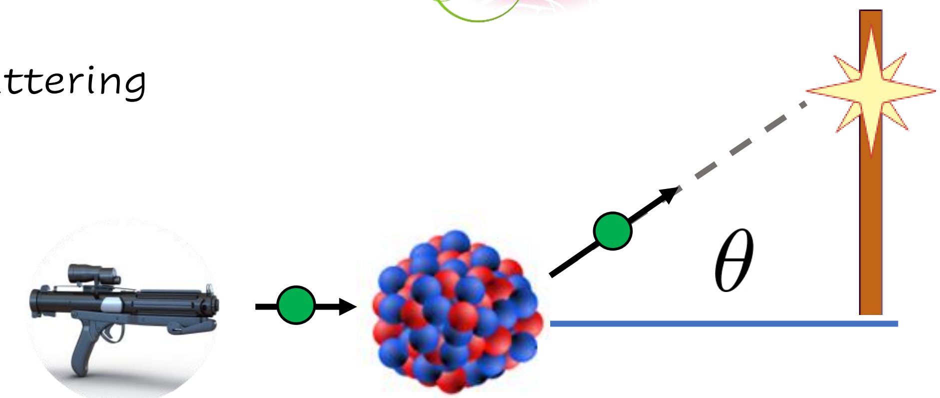

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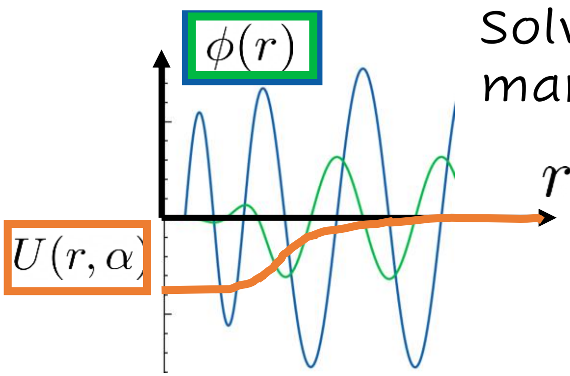
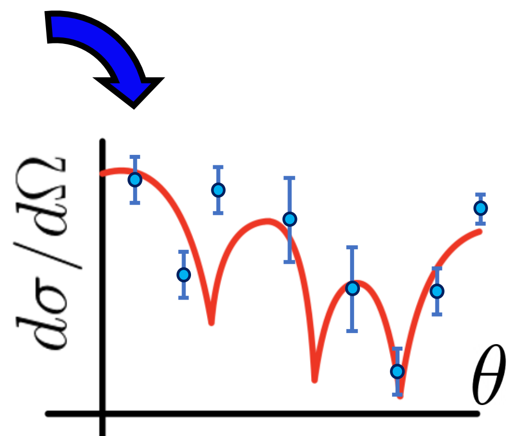


Solve for many ℓ



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Applications and Results

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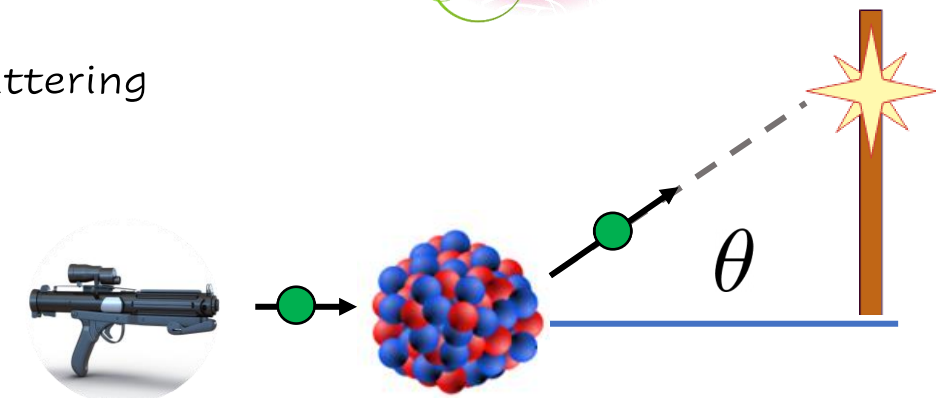

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Challenges:

1) Boundary conditions
2) Anomalies
3) Energy dependence
4) Non-affine potentials

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Applications and Results

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almost done....

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Required for the vanilla Kohn variational principle

$$\phi(r)_{r\to\infty} \to \frac{1}{p}\Big(\sin(pr - \ell\pi/2) + \tan(\delta_\ell)\cos(pr - \ell\pi/2)\Big)$$

Challenges:

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Efficient emulators for scattering using eigenvector continuation

R.J. Furnstahl, A.J. Garcia, P.J. Millican, Xilin Zhang *

Toward emulating nuclear reactions using eigenvector continuation

C. Drischler [a,*], M. Quinonez [a,b], P.G. Giuliani [a,c], A.E. Lovell [d], F.M. Nunes [a,b]

(complex Kohn variational principle)

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Applications and Results 3

almost done....

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$$\phi(r)_{r\to\infty} \to \frac{1}{p}\Big(\sin(pr - \ell\pi/2) + \tan(\delta_\ell)\cos(pr - \ell\pi/2)\Big)$$

Can be problematic

Basis of snapshots

$$\hat{\phi}(r) = \sum_k^N a_k \phi_k(r) \qquad \sum_k^N a_k = 1$$

Challenges:

1) Boundary conditions
2) Anomalies
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Applications and Results ❸

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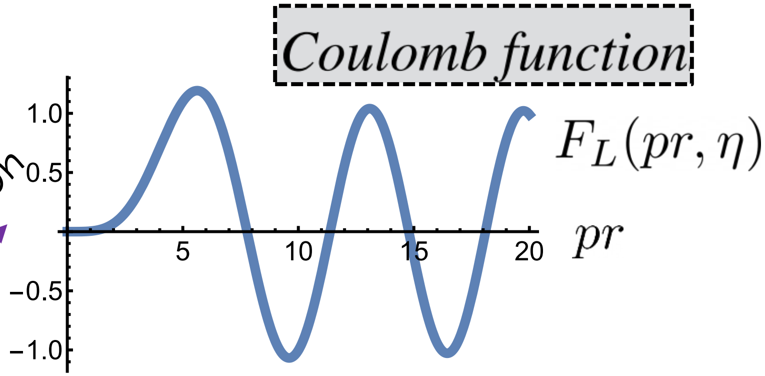

Free solution

POD Basis

$$\hat{\phi}(r) = \phi_0(r) + \sum_k^n a_k \phi_k(r)$$

Challenges:

1) Boundary conditions
2) Anomalies
3) Energy dependence
4) Non-affine potentials

The roses

https://github.com/odell/rose

almost done....

Applications and Results

3

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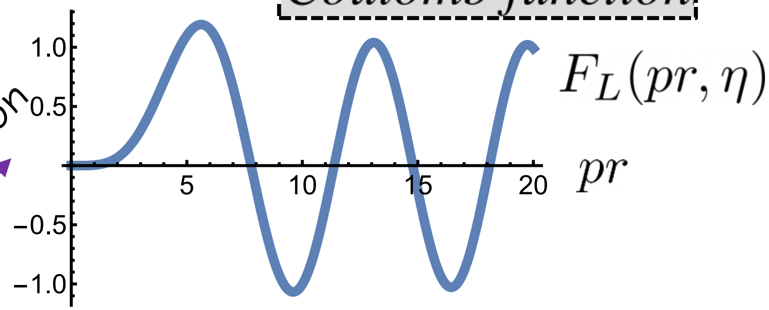
Coulomb function



Free solution

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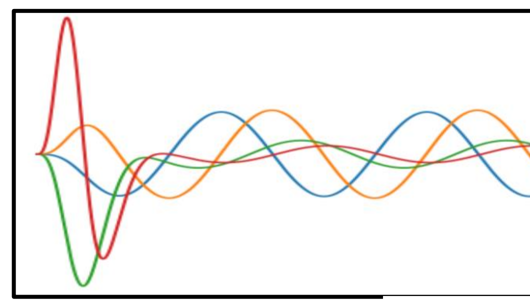
$$\hat{\phi}(r) = \phi_0(r) + \sum_k^n a_k \phi_k(r)$$

Principal components of the differences of snapshots with $\phi_0(r)$



Challenges:

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Applications and Results ③

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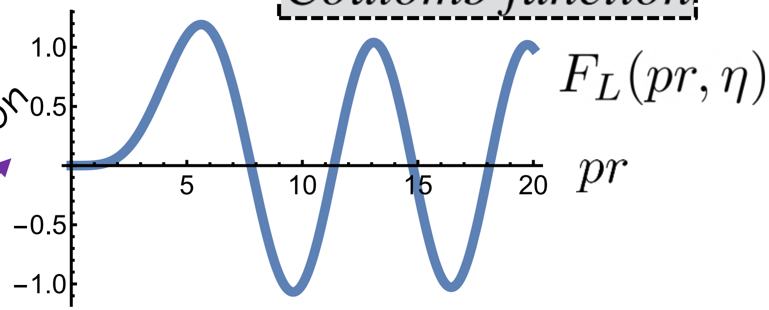
Daniel Odell

Coulomb function



Free solution

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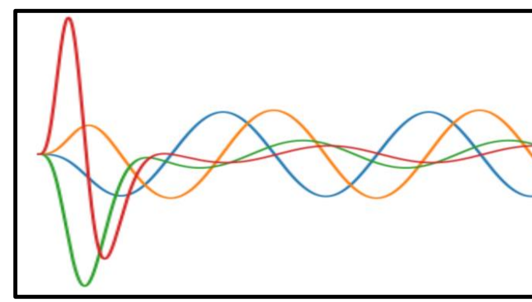
Principal components of the differences of snapshots with $\phi_0(r)$



Challenges:

1) Boundary conditions

$$\hat{\phi}(r)_{r\to 0} \sim r^{\ell+1}$$

2) Anomalies

3) Energy dependence

4) Non-affine potentials

https://colab.research.google.com/drive/1Vtg11apJy0o4D2MloDz1D0WbxbxlwW8H

Applications ③ and Results

almost done....

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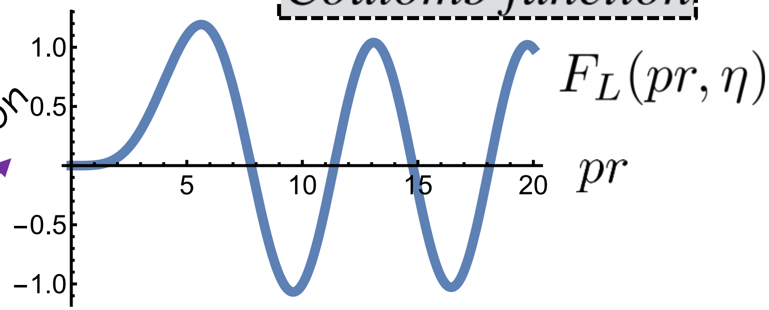

Free solution

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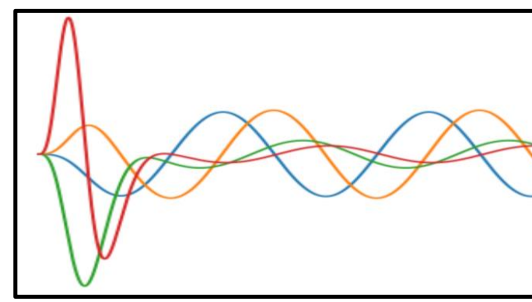


Challenges:

1) Boundary conditions

2) Anomalies

3) Energy dependence

4) Non-affine potentials

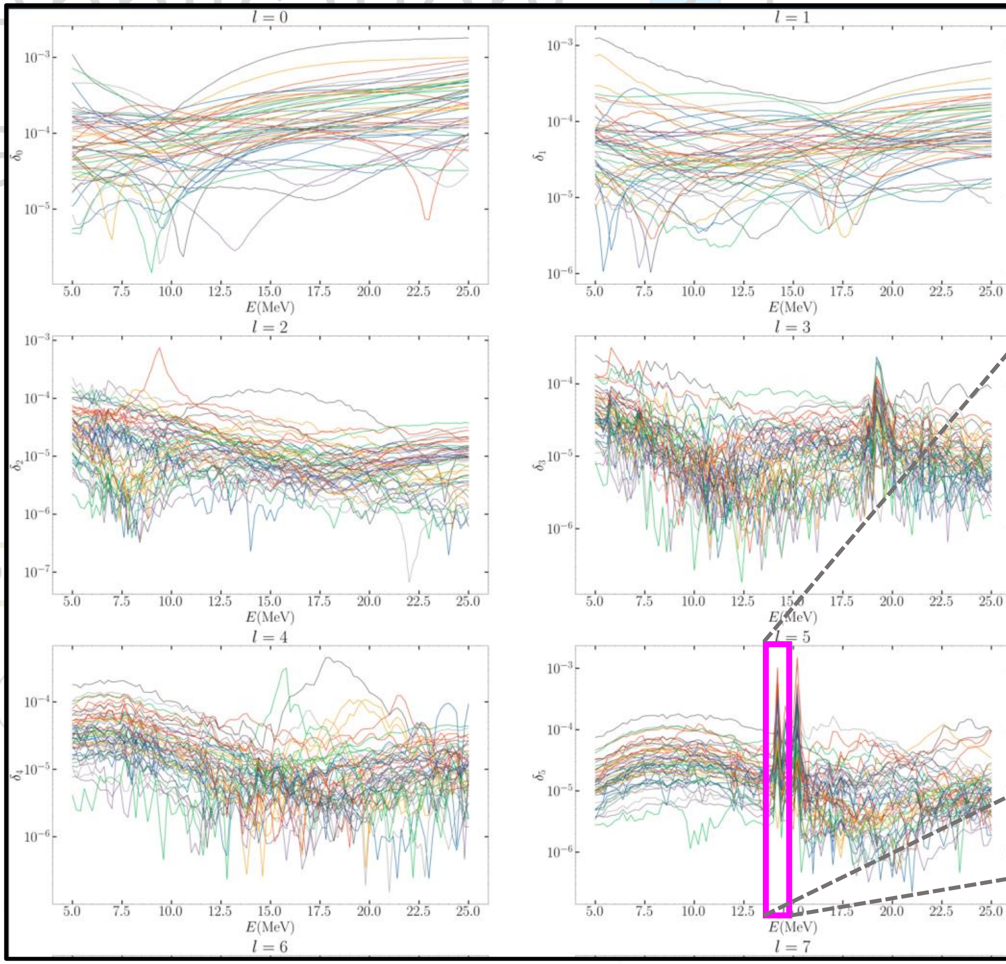
1) No ``normalization"/ constrain on coefficients

2) POD basis instead of snapshots

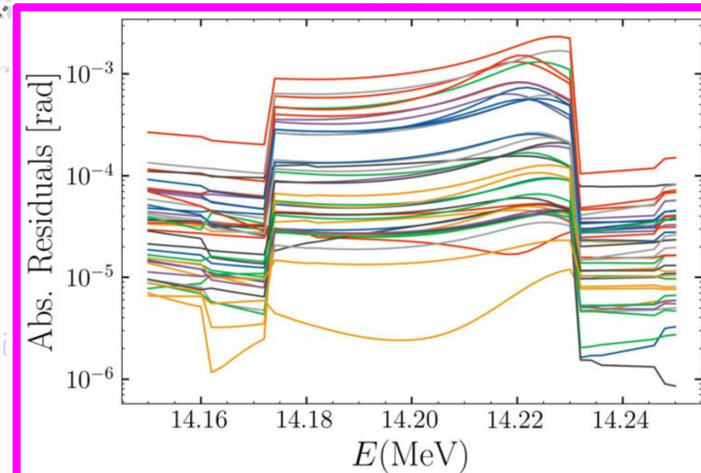
3) Not searching stationary point

Conjectures

https://colab.research.google.com/drive/1Vtg11apJy0o4D2MloDz1D0WbxbxlwW8H



Results



2) Anomalies

1) No ``normalization"/ constrain on coefficients

2) POD basis instead of snapshots

3) Not searching stationary point

Conjectures

Fast & accurate emulation of two-body scattering

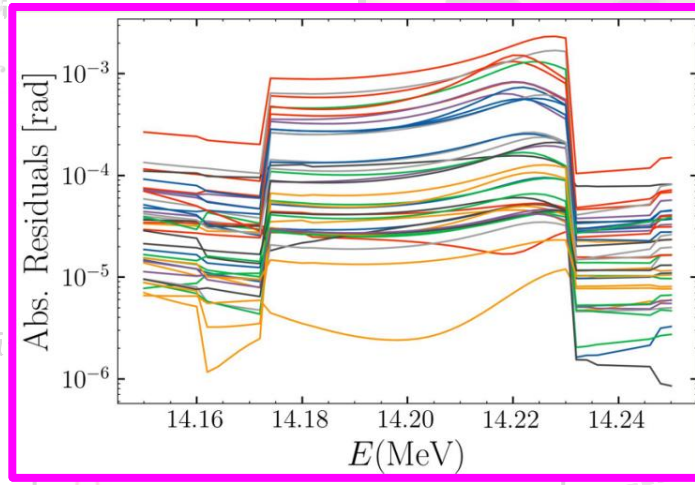
Christian Drischler (drischler@ohio.edu)

Christian's talk yesterday

Anomaly detection and removal

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

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



Might be needed if emulator acts funny

Applications and Results ③

almost done....

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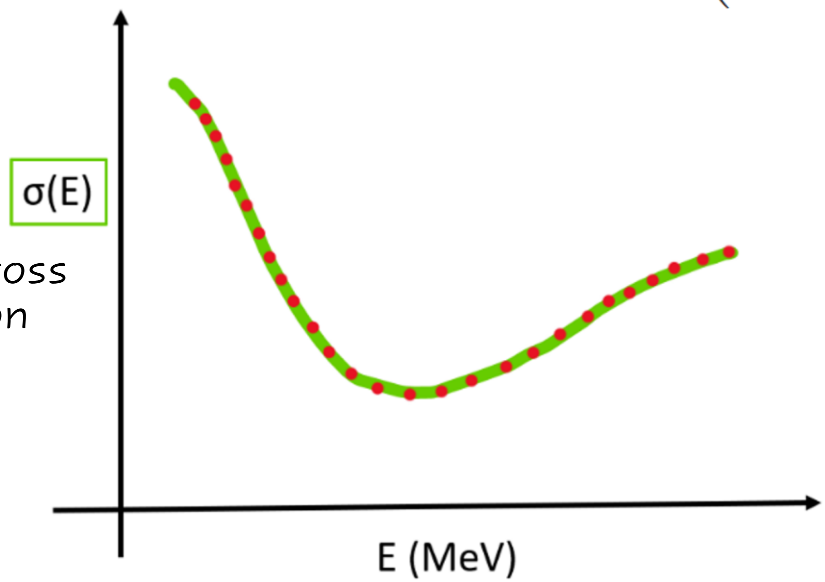
$$\left(-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}+U(r,\alpha)-p^2\right)\phi(r)$$

Total cross section



Challenges:

1) Boundary conditions
2) Anomalies
3) Energy dependence
4) Non-affine potentials

The roses

https://github.com/odell/rose

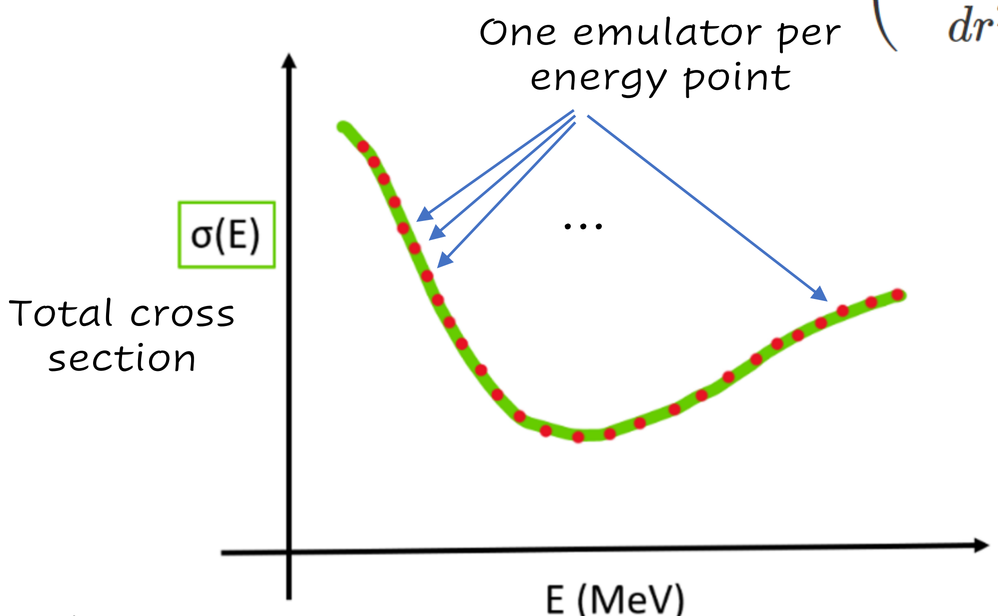
almost done....

Applications ③ and Results

Presenting ROSE, a Reduced Order Scattering Emulator

D. Odell,[1,*] P. Giuliani,[2,3] M. Catacora-Rios,[2,4] M. Chan,[5] E. Bonilla,[6] K. Godbey,[2] R. J. Furnstahl,[7] and F. M. Nunes[2,4,†]

$$\left(-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}+U(r,\alpha)-p^2\right)\phi(r)$$



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Applications and Results ❸

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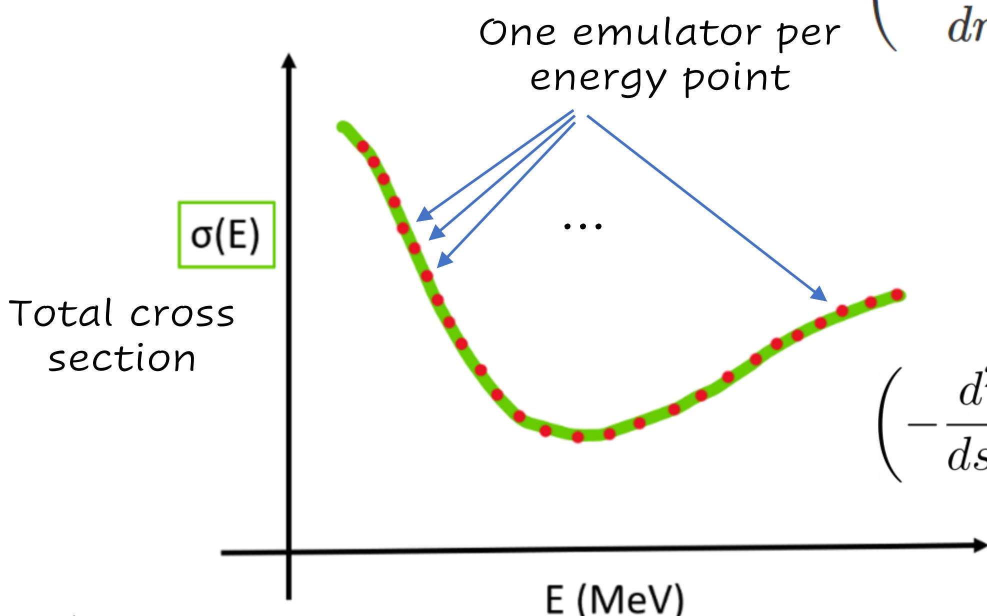

Re-scale:
$pr = s$

$$\left(-\frac{d^2}{ds^2}+\frac{\ell(\ell+1)}{s^2}+U(s,\alpha,p)-1\right)\phi(s)$$

Energy dependent

Challenges:

1) Boundary conditions
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Applications a…

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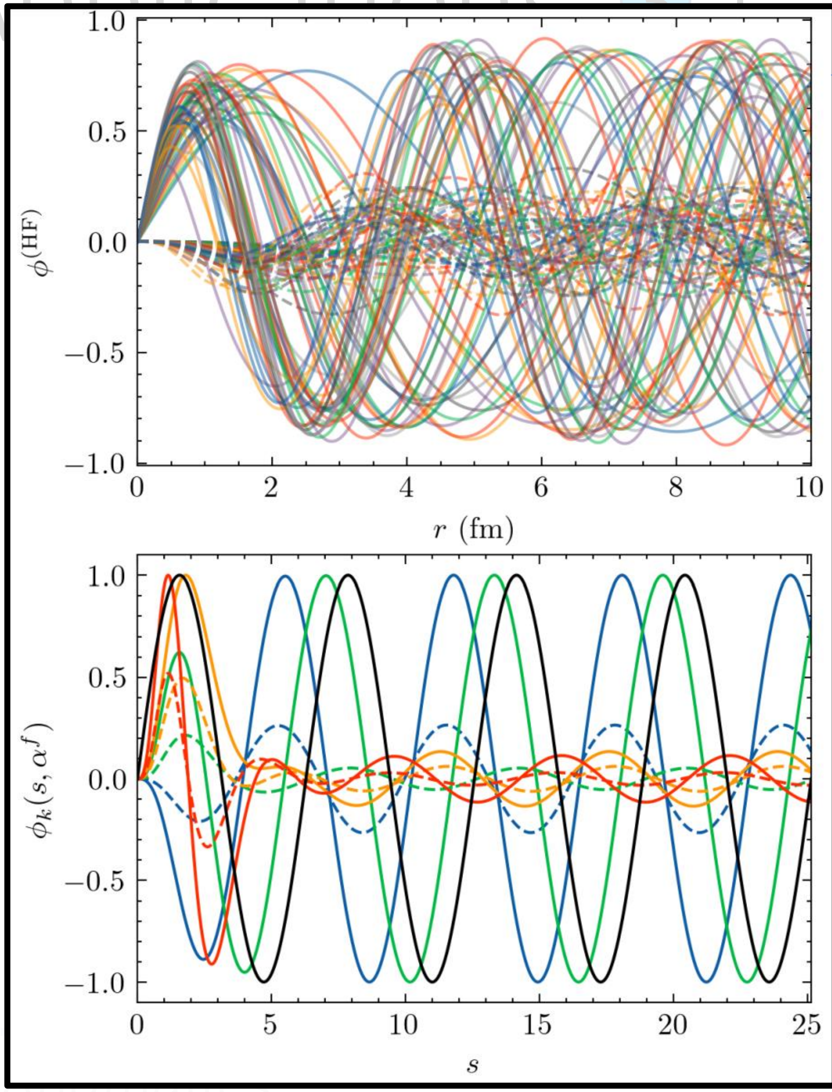

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Re-scale:
$pr = s$

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Energy dependent

Cha…

1)

2) Anomalies

3) Energy dependence

4) Non-affine potentials

The roses

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Applications and Results

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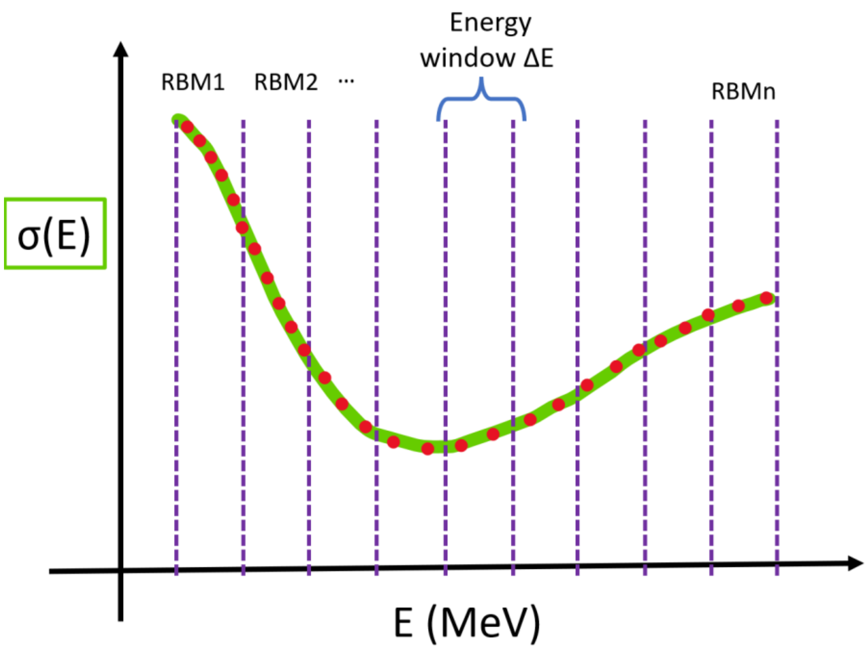

Challenges:

1) Boundary conditions
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The roses

https://colab.research.google.com/drive/1Vtg11apJy0o4D2MloDz1D0WbxbxlwW8H

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Applications and Results

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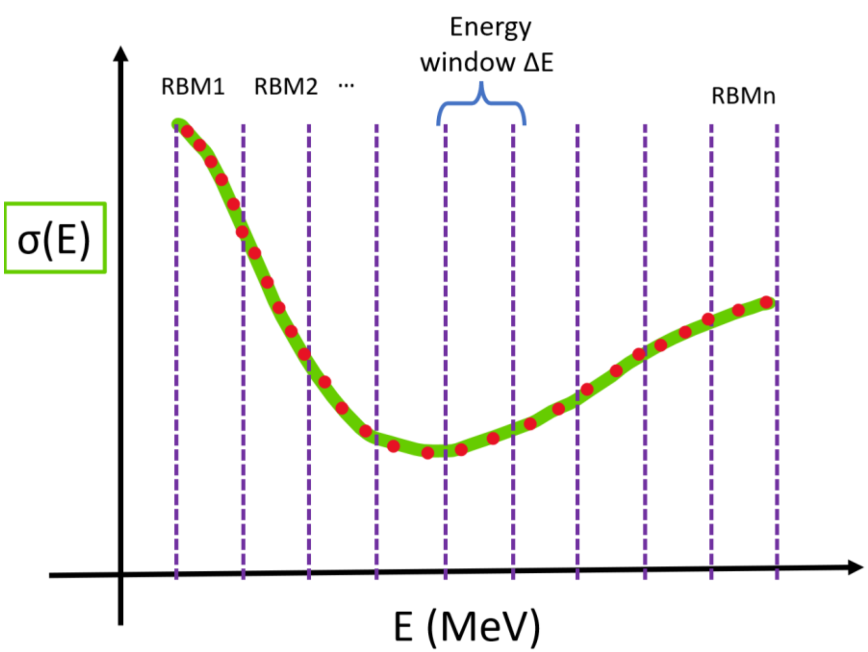

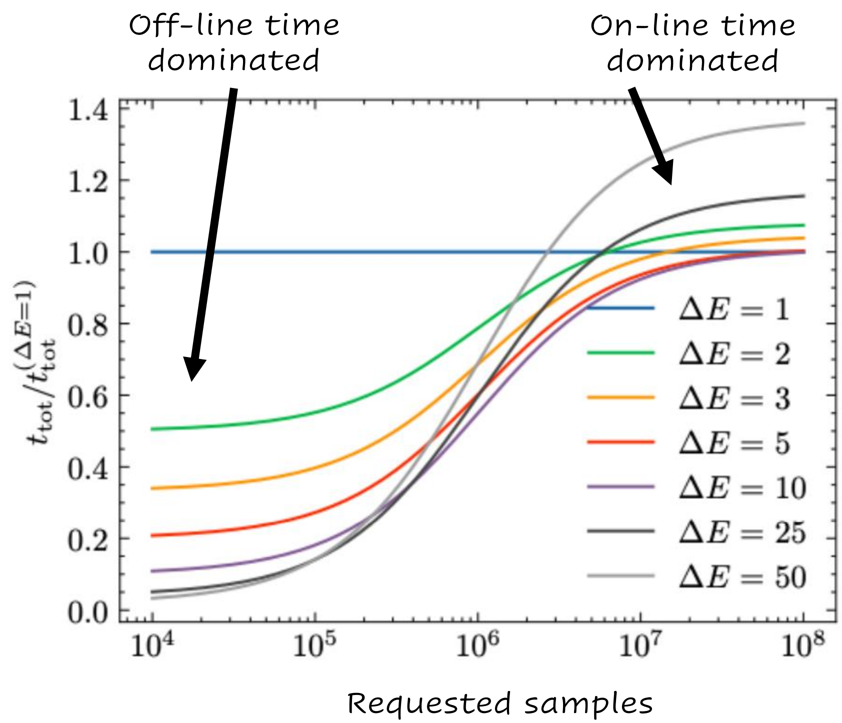

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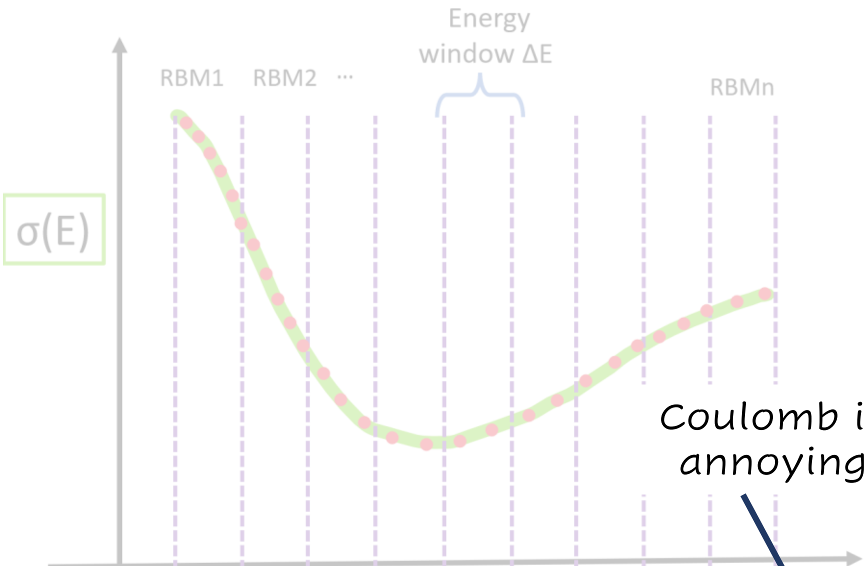

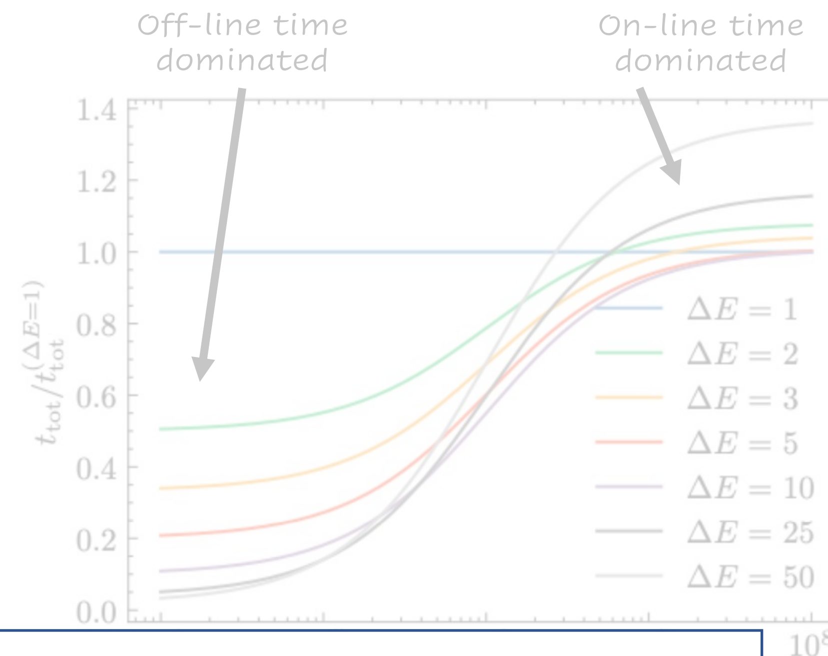

Coulomb is annoying

$$\left(-\frac{d^2}{ds^2}+\frac{\ell(\ell+1)}{s^2}+\frac{\eta^*}{s}+U(s,\alpha,p)-1\right)\phi(s)$$

Challe

1) Bo

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Applications and Results

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almost done....

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$$F_\alpha(\phi) = \left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + U(r,\alpha) - p^2\right)\phi(r) = 0$$

$$\underbrace{\begin{pmatrix} & & \\ & & \\ & & \end{pmatrix}}_{\mathcal{N}\times\mathcal{N}} \underbrace{\begin{bmatrix} \phi(r_1) \\ \phi(r_2) \\ \vdots \end{bmatrix}}_{\mathcal{N}} = \underbrace{\begin{bmatrix} 0 \\ 0 \\ \vdots \end{bmatrix}}_{\mathcal{N}}$$

High Fidelity

Applications and Results ③

almost done....

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High Fidelity

RBM

$$\hat{\phi}(r) = \phi_0(r) + \sum_k^n a_k \phi_k(r) \qquad \hat{\phi} = \begin{bmatrix}a_1\\a_2\\ \vdots\end{bmatrix}_n$$

$$\langle\psi_j|F_\alpha[\hat{\phi}(r)]\rangle = 0$$

$$j = \{1, n\}$$

$$\Big(\quad\Big)_{n\times n} \begin{bmatrix}a_1\\a_2\\ \vdots\end{bmatrix}_n = \begin{bmatrix}\cdot\\ \cdot\\ \cdot\end{bmatrix}_n$$

almost done....

Applications and Results 3

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High Fidelity

Same for local or non-local $U(r,\alpha)$

$$\langle \psi_j | F_\alpha | \phi_k \rangle = \int \psi_j^*(s) F_\alpha \phi_k(s) ds$$

RBM

$$\hat{\phi}(r) = \phi_0(r) + \sum_k^n a_k \phi_k(r) \qquad \hat{\phi} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix}_n$$

$$\langle \psi_j | F_\alpha[\hat{\phi}(r)] \rangle = 0$$

$$j = \{1, n\}$$

$$\Big(\quad\Big)_{n\times n} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix}_n = \begin{bmatrix} \cdot \\ \cdot \\ \cdot \end{bmatrix}_n$$

Applications and Results 3

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$$F_\alpha(\phi) = \left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + U(r,\alpha) - p^2\right)\phi(r) = 0$$

Offline-Online separation

Same for local or non-local $U(r,\alpha)$

$$\left(\textbf{BIG matrix} \right)_{\mathcal{N}\times\mathcal{N}} \begin{pmatrix} \phi(r_1) \\ \phi(r_2) \\ \vdots \end{pmatrix}_{\mathcal{N}} = \begin{pmatrix} 0 \\ 0 \\ \vdots \end{pmatrix}_{\mathcal{N}}$$

$$\langle \psi_j | F_\alpha | \phi_k \rangle = \int \psi_j^*(s) F_\alpha \phi_k(s) ds$$

High Fidelity

RBM

$$\hat{\phi}(r) = \phi_0(r) + \sum_k^n a_k \phi_k(r) \quad \hat{\phi} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}_n$$

$$\langle \psi_j | F_\alpha [\hat{\phi}(r)] \rangle = 0$$

$$j = \{1, n\}$$

$$\left(\text{small matrix} \right)_{n\times n} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}_n = \begin{pmatrix} \cdot \\ \cdot \\ \cdot \end{pmatrix}_n$$

almost done....

Applications and Results 3

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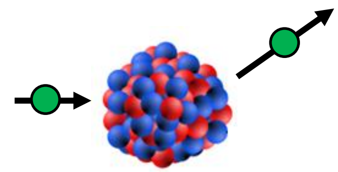

Optical Potential

$$U(r,\alpha) = -V_v\left[1+\exp\left(\frac{r-R_v}{a_v}\right)\right] - iW_v\left[1+\exp\left(\frac{r-R_w}{a_w}\right)\right] -i4a_dW_d\frac{d}{dr}\left[1+\exp\left(\frac{r-R_d}{a_d}\right)\right]$$

$$F_\alpha(\phi) = \left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + U(r,\alpha) - p^2\right)\phi(r) = 0$$

The roses

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Applications and Results

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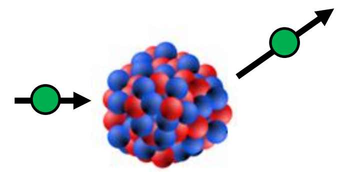

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$$\langle\psi_j|F_\alpha[\hat{\phi}(r)]\rangle = \int \psi_j(r)F_\alpha[\hat{\phi}(r)]dr = 0$$

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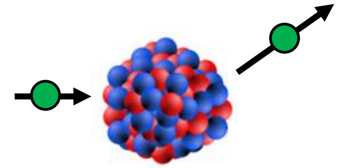

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$$F_\alpha(\phi) = \left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + U(r,\alpha) - p^2\right)\phi(r) = 0$$

Non-affine problem

$$\langle\psi_j|F_\alpha[\hat{\phi}(r)]\rangle = \int \psi_j(r) F_\alpha[\hat{\phi}(r)]dr = 0$$

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almost done....

Applications and Results ③

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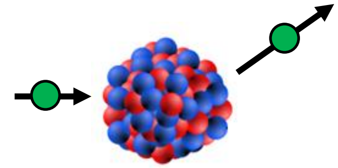

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Non-affine problem

$$\langle\psi_j|F_\alpha[\hat{\phi}(r)]\rangle = \int \psi_j(r)F_\alpha[\hat{\phi}(r)]dr = 0$$

$$U(r,\alpha) \approx \sum_i^m b_i(\alpha)f(r)$$

Empirical Interpolation Method: one work-around

The roses

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Applications and Results

almost done....

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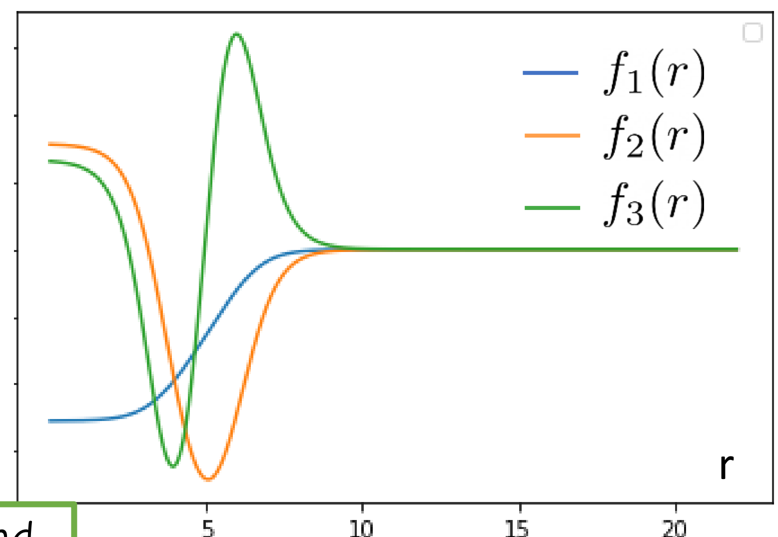
Principal components of $U(r,\alpha)$



1) Choose a basis

$$U(r,\alpha) \approx \sum_{i}^{m} b_i(\alpha) f(r)$$

Empirical Interpolation Method: one work-around

Applications and Results ③

almost done....

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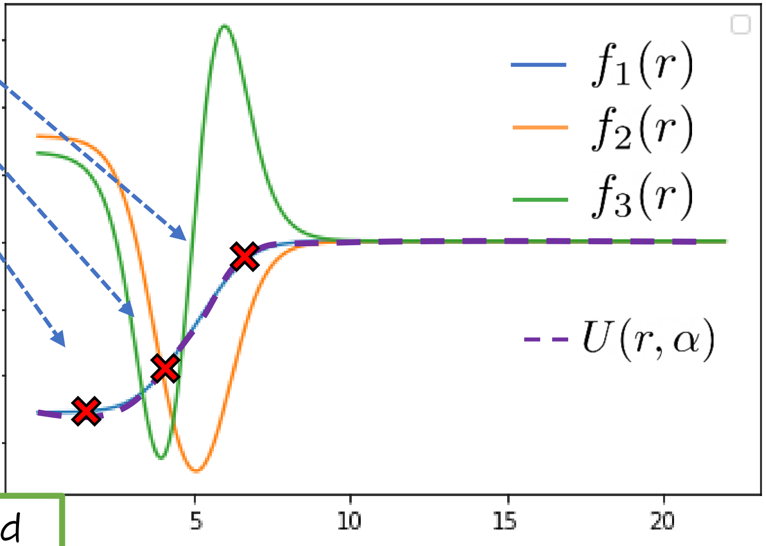
$$U(r_j,\alpha) - \sum_i^m b_i(\alpha) f(r_j) = 0$$

Obtained by interpolation $\quad j = \{1, m\}$

1) Choose a basis

$$U(r,\alpha) \approx \sum_i^m b_i(\alpha) f(r)$$

Principal components of $U(r,\alpha)$



Empirical Interpolation Method: one work-around

almost done....

Applications and Results ③

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Dirac

$$\psi_j(r) = \delta(r - r_j)$$

$$\langle \psi_j | F_\alpha[\hat{\phi}(r)] \rangle = F_\alpha[\hat{\phi}(r_j)]$$

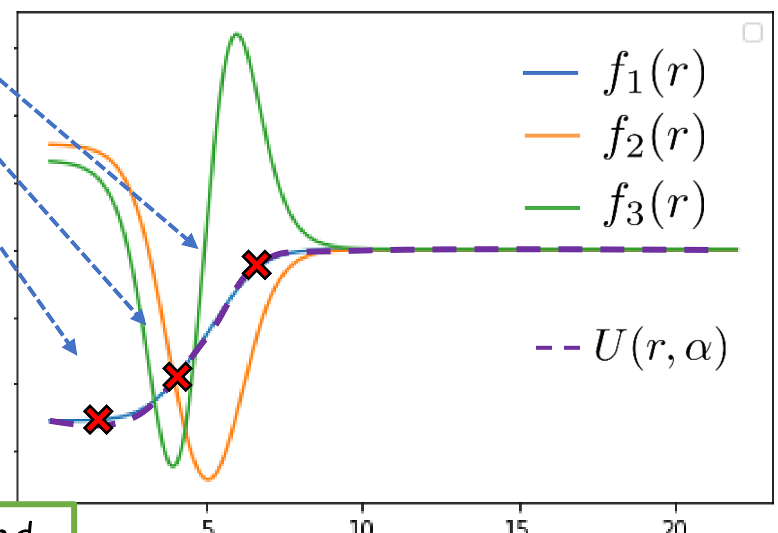
(collocation method)

2) Project

$$U(r_j, \alpha) - \sum_i^m b_i(\alpha) f(r_j) = 0$$

Obtained by interpolation $\quad j = \{1, m\}$

Principal components of $U(r, \alpha)$



1) Choose a basis

$$U(r, \alpha) \approx \sum_i^m b_i(\alpha) f(r)$$

Empirical Interpolation Method: one work-around

Applications and Results ③

almost done….

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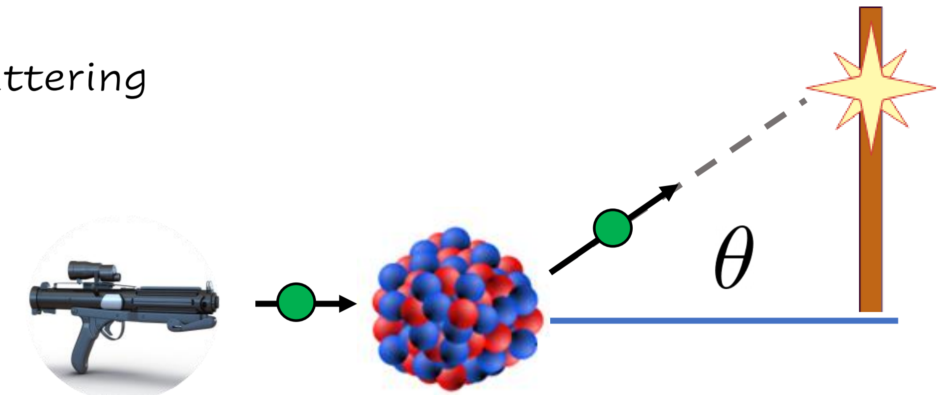
2-body scattering



$$F_\alpha(\phi) = \left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + \frac{2\eta k}{r} + U(r,\alpha) - k^2\right)\phi(r) = 0$$

Challenges:

1) Boundary conditions ✓
2) Anomalies ✓
3) Energy dependence ✓ *
4) Non-affine potentials ✓

The roses

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almost done....

Applications and Results ③

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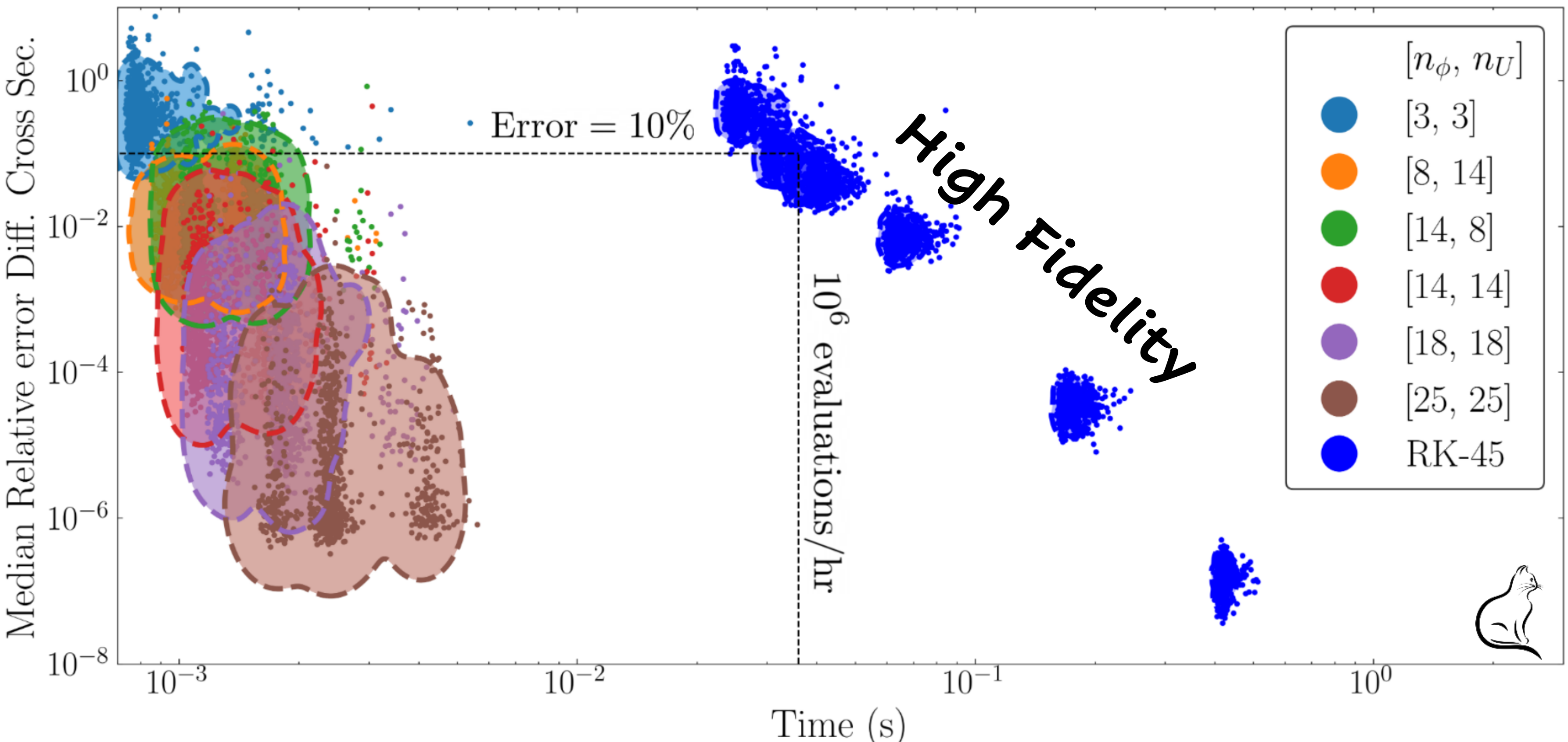
ROSE



CAT plot

almost done....

Applications and Results ③

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$$\hat{\phi}(x) = \phi_0 + \sum_k^n a_k \phi_k(x)$$

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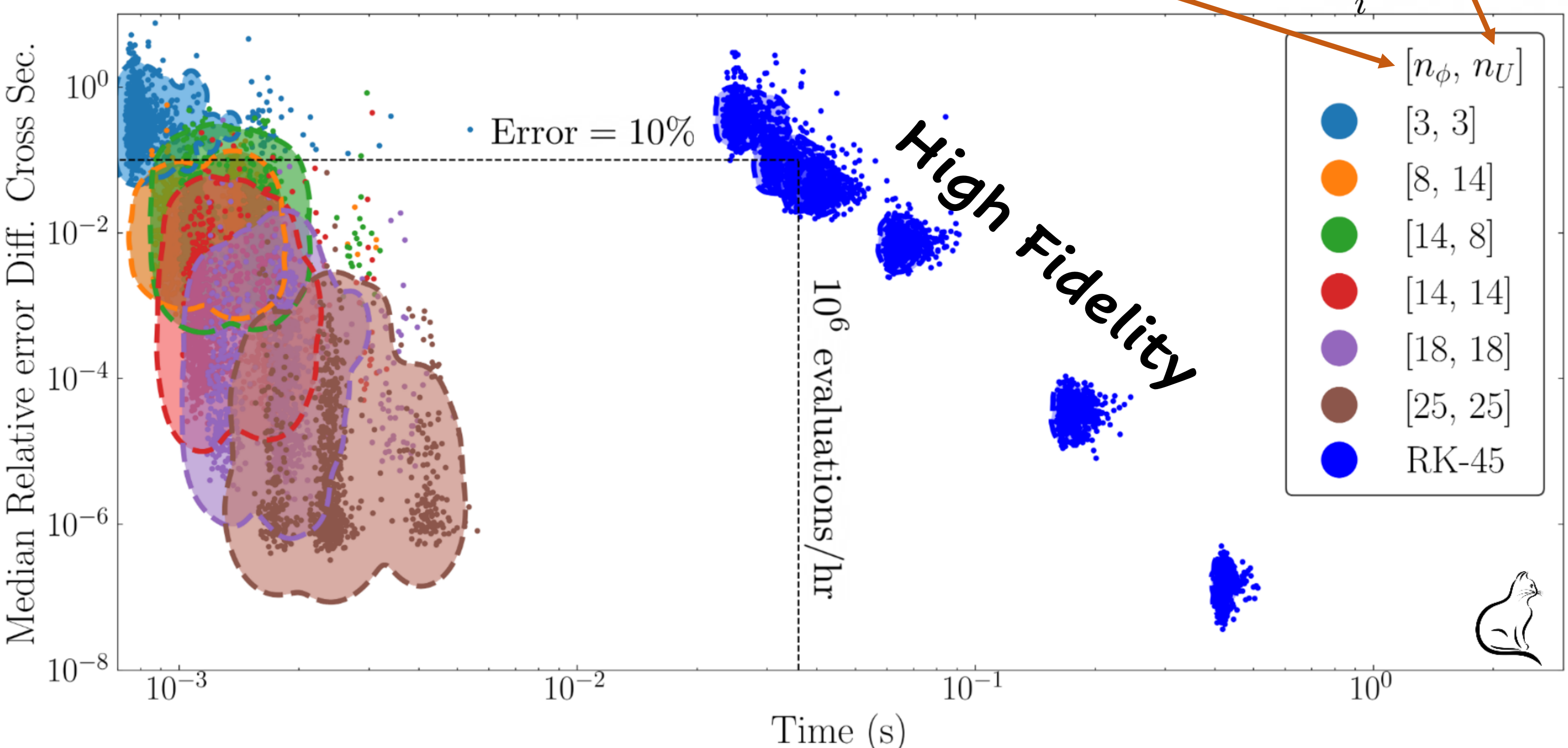
ROSE



CAT plot

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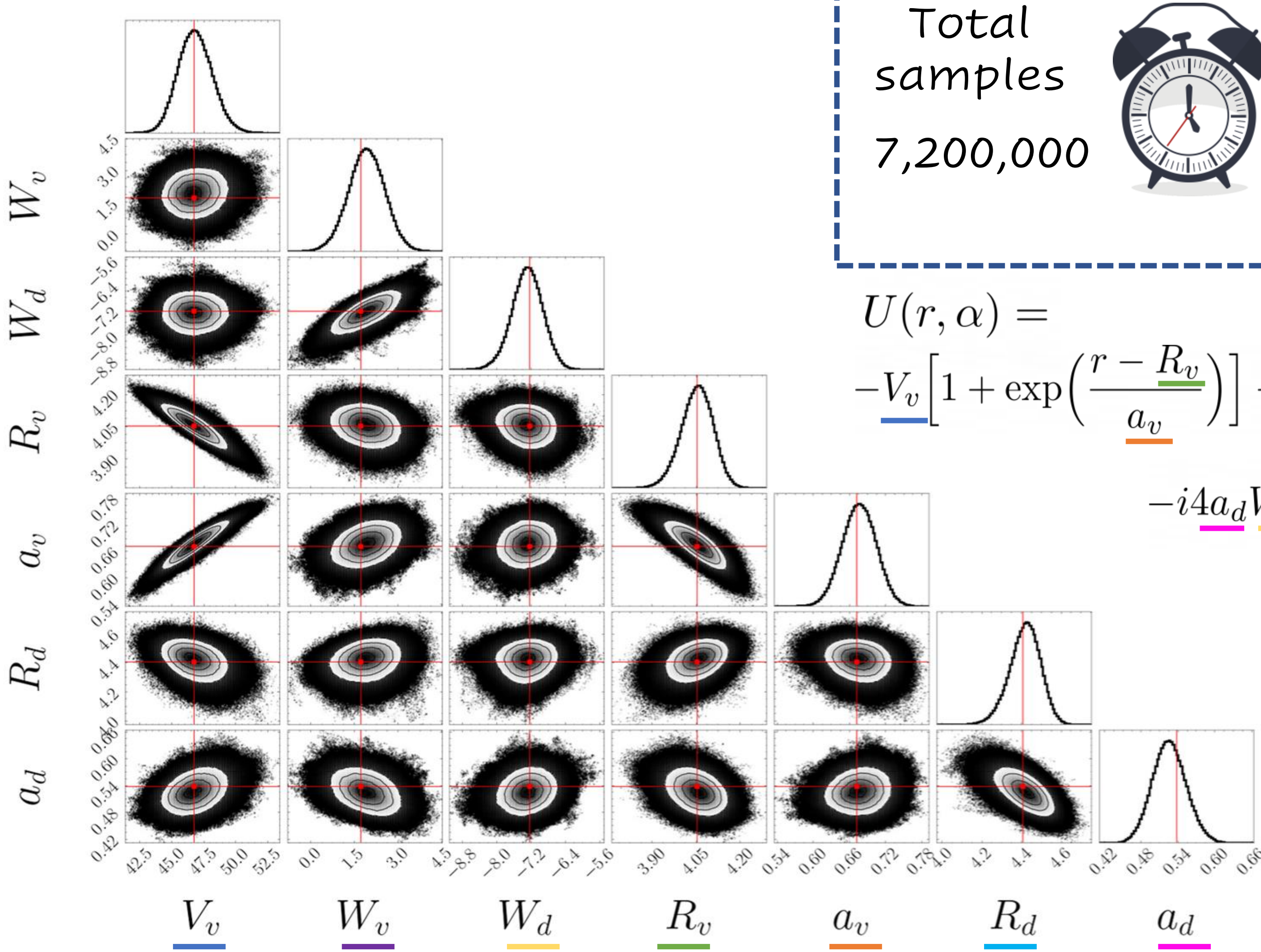

Total samples

7,200,000

High Fidelity:
2 months*

ROSE:
2 hours

$$U(r,\alpha) = -V_v\left[1+\exp\left(\frac{r-R_v}{a_v}\right)\right] - iW_v\left[1+\exp\left(\frac{r-R_v}{a_v}\right)\right] - i4a_dW_d\frac{d}{dr}\left[1+\exp\left(\frac{r-R_d}{a_d}\right)\right]$$

Applications and Results

3

almost done....

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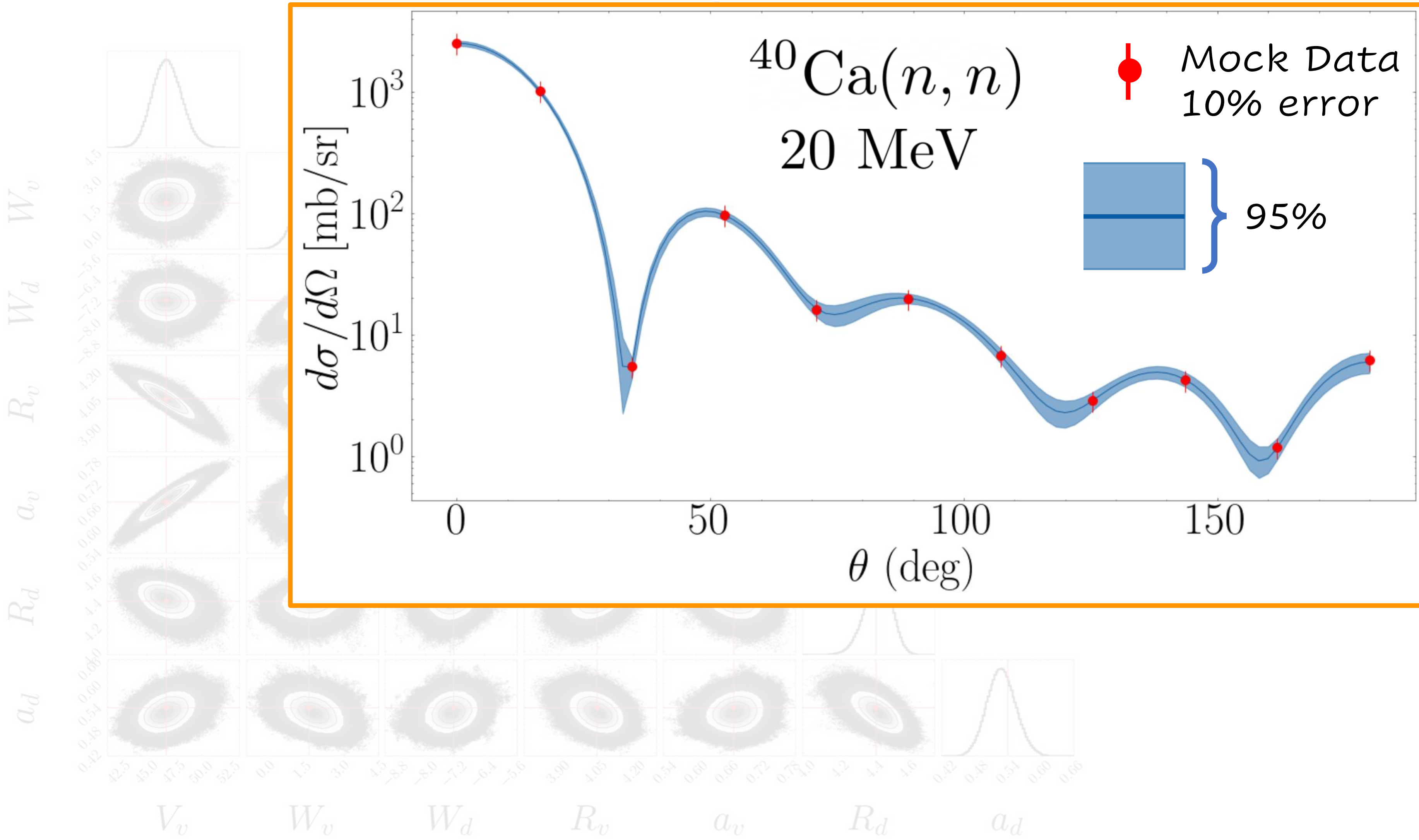

Applications and Results 3

almost done....

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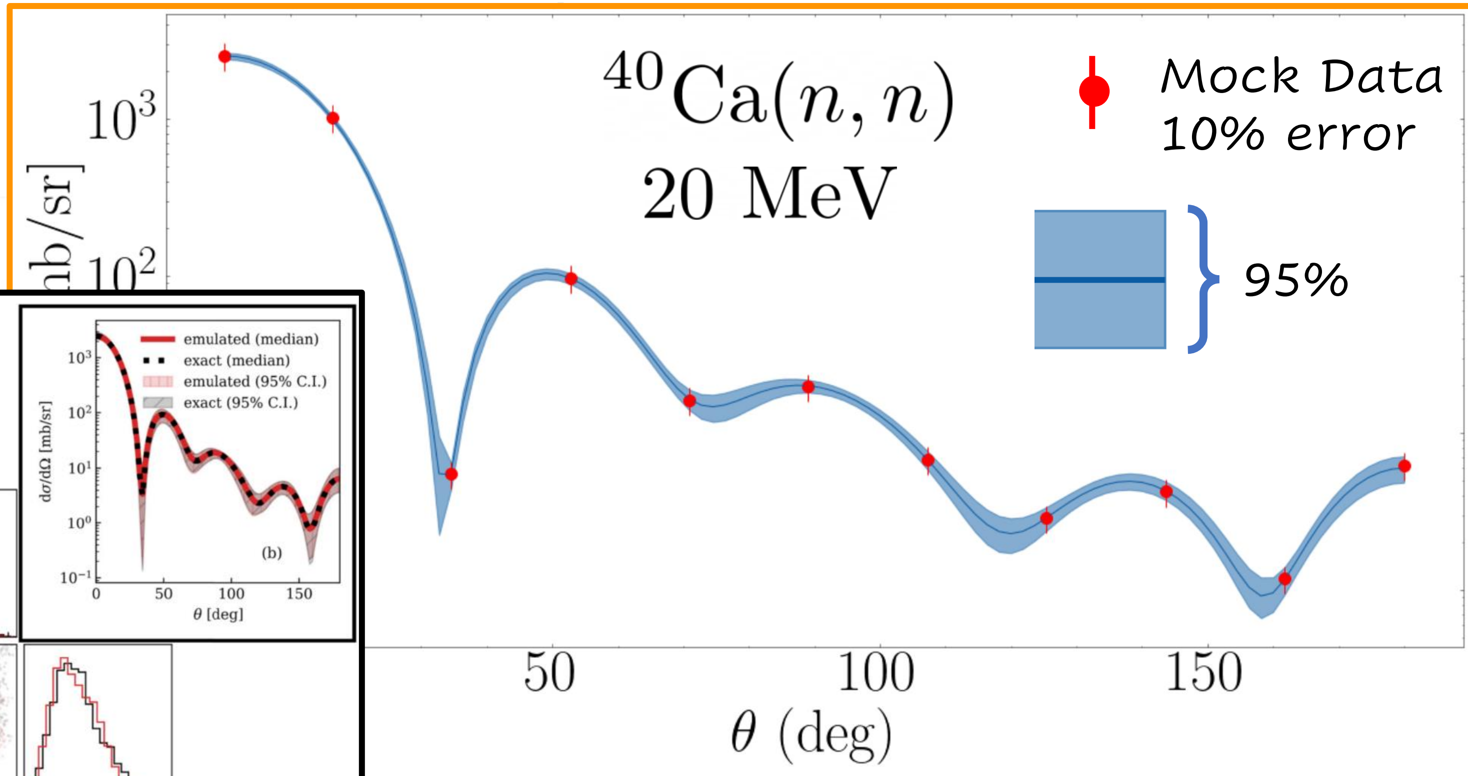
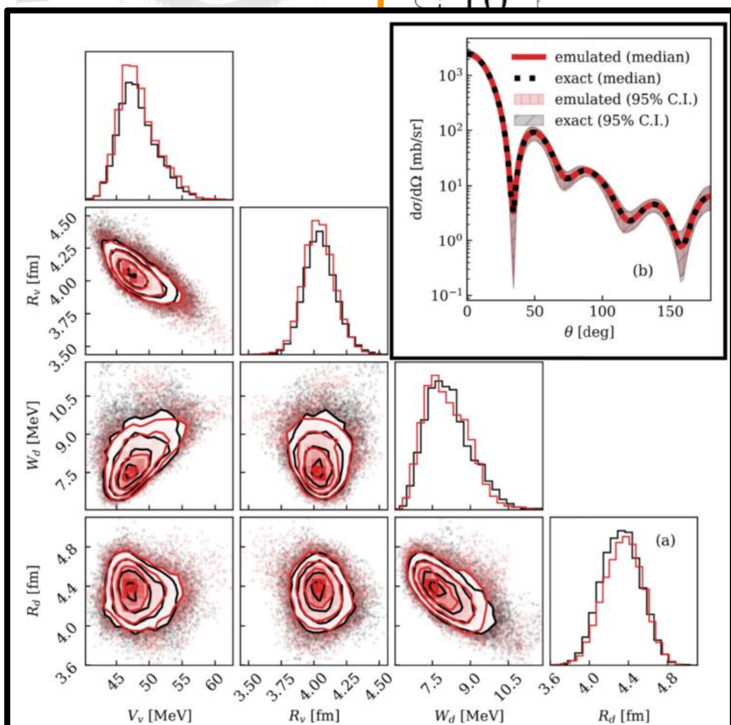




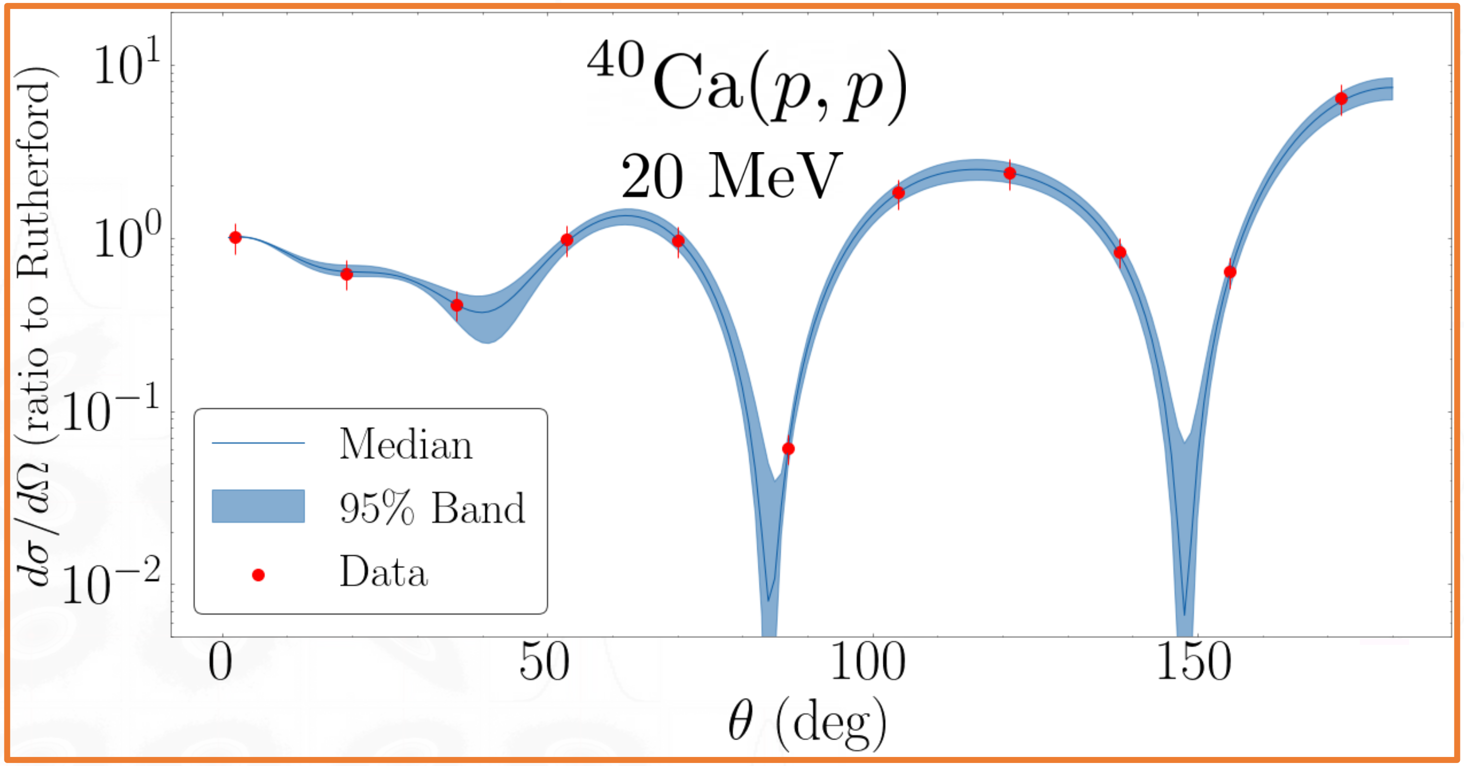
[2021 paper, Christian and friends]

almost done....

Applications and Results ❸

Presenting ROSE, a Reduced Order Scattering Emulator

D. Odell,[1,*] P. Giuliani,[2,3] M. Catacora-Rios,[2,4] M. Chan,[5] E. Bonilla,[6] K. Godbey,[2] R. J. Furnstahl,[7] and F. M. Nunes[2,4,†]



almost done....

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Most important outcome:

Software useful for the community

rose

- Reduced-Order Scattering Emulator
- Python
- BAND Framework v0.3
- Supports local, complex, non-affine interactions.
- Designed to be user-friendly.
  - See pseudo-code ➡
  - Supports user-supplied solutions

BAND
Bayesian Analysis of Nuclear Dynamics

```
import rose

def potential(r, alpha):
    alpha0, alpha1, … = alpha
    return alpha0 *
        woods_saxon(
            r, alpha1, alpha2
        ) + 1j*…

interaction = InteractionEIM(
    potential,
    num_params,
    reduced_mass,
    energy, Z_1, Z_2,
    is_complex=True
)

sae = ScatteringAmplitudeEmulator(
    interaction,
    training_points,
    l_max
)

cross_section = sae.emulate(alpha)
```

almost done....

Applications and Results ③

Presenting ROSE, a Reduced Order Scattering Emulator

D. Odell,[1,*] P. Giuliani,[2,3] M. Catacora-Rios,[2,4] M. Chan,[5] E. Bonilla,[6] K. Godbey,[2] R. J. Furnstahl,[7] and F. M. Nunes[2,4,†]

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BAND
Bayesian Analysis of Nuclear Dynamics

```
import rose
...
    l_max
)

cross_section = sae.emulate(alpha)
```

Future

- E emulation with Coulomb
  - works below threshold (AB)
- nonlocal potentials
- 3-body scattering 💵
  - T instead of t
- Coupled channels

almost done....

Applications and Results ③

Presenting ROSE, a Reduced Order Scattering Emulator

D. Odell,[1,*] P. Giuliani,[2,3] M. Catacora-Rios,[2,4] M. Chan,[5] E. Bonilla,[6] K. Godbey,[2] R. J. Furnstahl,[7] and F. M. Nunes[2,4,†]

4) Boundary conditions → Independent term

5) Incompatible domains → Reference domain

6) Non-affine operators → Empirical Interpolation Method

Challenges:

1) Boundary conditions ✓
2) Anomalies ✓
3) Energy dependence ✓ *
4) Non-affine potentials ✓

The roses

https://github.com/odell/rose

Applications and Results

3

almost done....

Presenting ROSE, a Reduced Order Scattering Emulator

D. Odell,[1,*] P. Giuliani,[2,3] M. Catacora-Rios,[2,4] M. Chan,[5] E. Bonilla,[6] K. Godbey,[2] R. J. Furnstahl,[7] and F. M. Nunes[2,4,†]

4) Boundary conditions → Independent term

$$\hat{\phi}(r) = \phi_0(r) + \sum_k^n a_k \phi_k(r)$$

1) Boundary conditions

Applications and Results ③

almost done....

Presenting ROSE, a Reduced Order Scattering Emulator

D. Odell,[1,*] P. Giuliani,[2,3] M. Catacora-Rios,[2,4] M. Chan,[5] E. Bonilla,[6] K. Godbey,[2] R. J. Furnstahl,[7] and F. M. Nunes[2,4,†]

5) Incompatible domains → Reference domain

$$\left(-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}+U(r,\alpha)-p^2\right)\phi(r)$$

Re-scale:
$pr = s$

$$\left(-\frac{d^2}{ds^2}+\frac{\ell(\ell+1)}{s^2}+U(s,\alpha,p)-1\right)\phi(s)$$

3) Energy dependence

Applications and Results ❸

almost done....

Presenting ROSE, a Reduced Order Scattering Emulator

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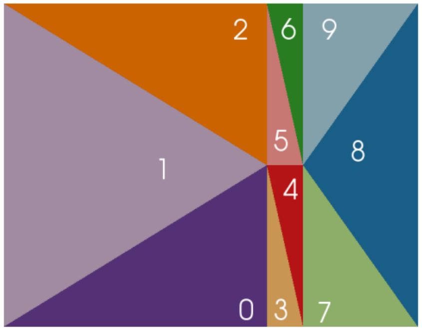

FIGURE 7: RB triangulation of the reference domain.

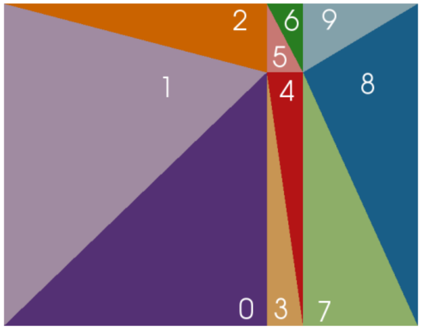

FIGURE 6: RB triangulation when the control rod is withdrawn.

$$\left(-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}+U(r,\alpha)-p^2\right)\phi(r)$$

Re-scale: $pr = s$

$$\left(-\frac{d^2}{ds^2}+\frac{\ell(\ell+1)}{s^2}+U(s,\alpha,p)-1\right)\phi(s)$$

A REDUCED ORDER MODEL FOR MULTI-GROUP TIME-DEPENDENT PARAMETRIZED REACTOR SPATIAL KINETICS (2014)

Sartori, et al

almost done....

Applications and Results

3

Presenting ROSE, a Reduced Order Scattering Emulator

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PHYSICAL REVIEW C **106**, L031302 (2022)

Letter

Applications of reduced-basis methods to the nuclear single-particle spectrum

Amy L. Anderson,[*] Graham L. O'Donnell,[†] and J. Piekarewicz[‡]
Department of Physics, Florida State University, Tallahassee, Florida 32306, USA

(Received 1 July 2022; accepted 20 September 2022; published 30 September 2022)

Reduced-basis methods provide a powerful framework for building efficient and accurate emulators. Although widely applied in many fields to simplify complex models, reduced-basis methods have only been recently introduced into nuclear physics. In this Letter we build an emulator to study the single-particle structure of atomic nuclei. By scaling a suitable mean-field Hamiltonian, a "universal" reduced basis is constructed capable of accurately and efficiently reproduce the entire single-particle spectrum of a variety of nuclei. Indeed, the reduced-basis model reproduces both ground- and excited-state energies as well as the associated wave functions with remarkable accuracy. Our results bode well for more demanding applications that use Bayesian optimization to calibrate nuclear energy density functionals.

...e domain

$$+ U(r,\alpha) - p^2 \Big) \phi(r)$$

Re-scale:
$pr = s$

(s)

FIGURE 6: RB triangulation when the control rod is withdrawn.

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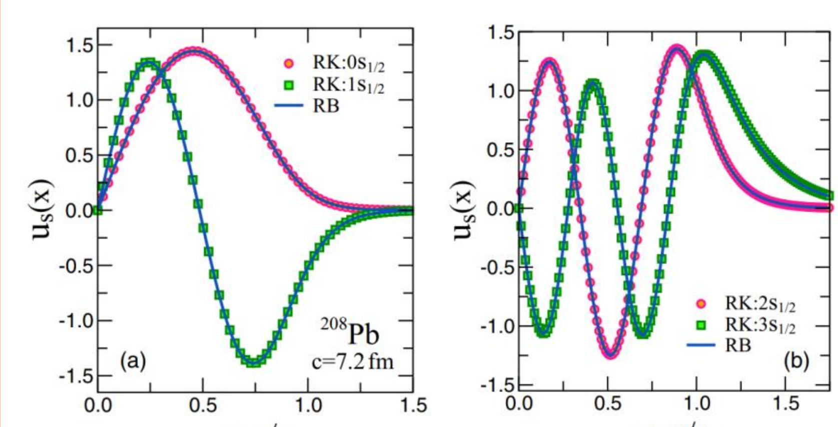

Applications and Results ③

almost done....

Presenting ROSE, a Reduced Order Scattering Emulator

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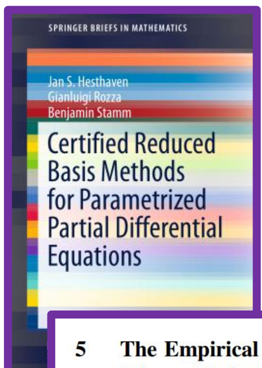
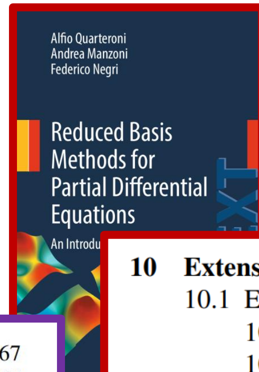
6) Non-affine operators → Empirical Interpolation Method



(2016)

(2016)



$$U(r,\alpha) \approx \sum_{i}^{m} b_i(\alpha) f(r)$$

An 'empirical interpolation' method: application to efficient reduced-basis discretization of partial differential equations

Maxime Barrault[a], Yvon Maday[b], Ngoc Cuong Nguyen[c], Anthony T. Patera[d]

(2004)

4) Non-affine potentials

Applications and Results

4

Non-affinity and Beyond: Mitigating non-linear and non-affine structures for the efficient emulation of Density Functional Theory

Kyle Godbey[1,*,+], Edgard Bonilla[2,+], Pablo Giuliani[1,3], and Yanlai Chen[4]

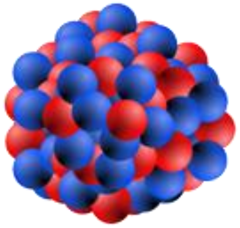
Coming soon

3) Very fast

Skyrme Density Functional

$$\mathcal{H}_t(r) = C_t^{\rho}\rho_t^2 + C_t^{\rho\Delta\rho}\rho_t\Delta\rho_t + C_t^{\tau}\rho_t\tau_t + C_t^{J}\overleftrightarrow{J}_t^2 + C_t^{\rho\nabla J}\rho_t\nabla\cdot\mathbf{J}_t,$$

Mili-seconds



VERY non-linear

$$\rho(r)^{\alpha}$$

Applications and Results

4

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Coming soon

Usually, a challenge

$$\langle \psi_j | F_\alpha[\hat{\phi}(r)] \rangle$$

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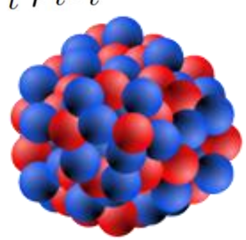

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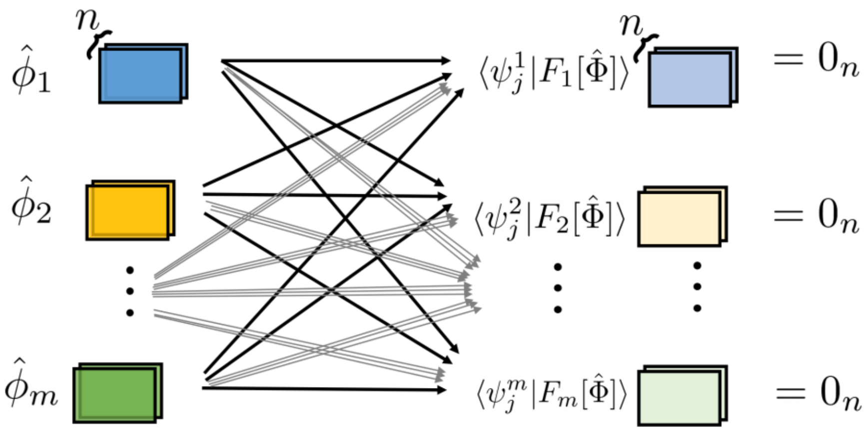

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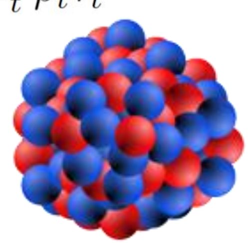
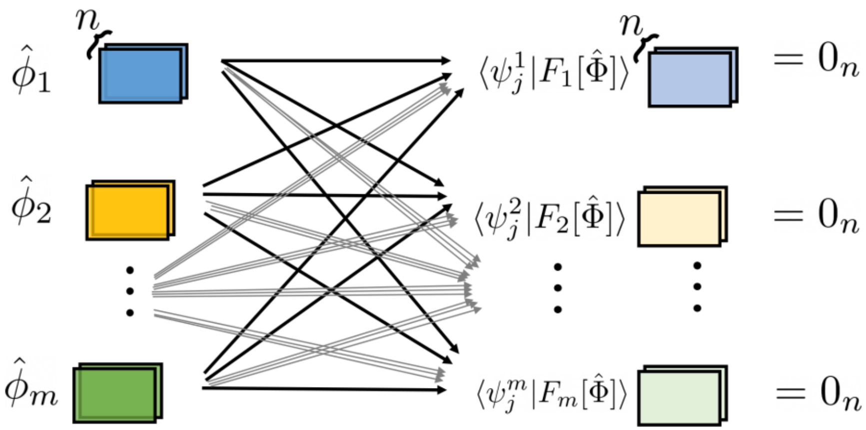
Mili-seconds





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Kyle Godbey[1,*,+], Edgard Bonilla[2,+], Pablo Giuliani[1,3], and Yanlai Chen[4]

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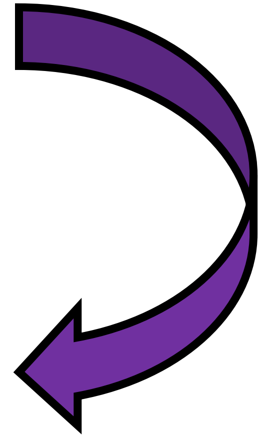
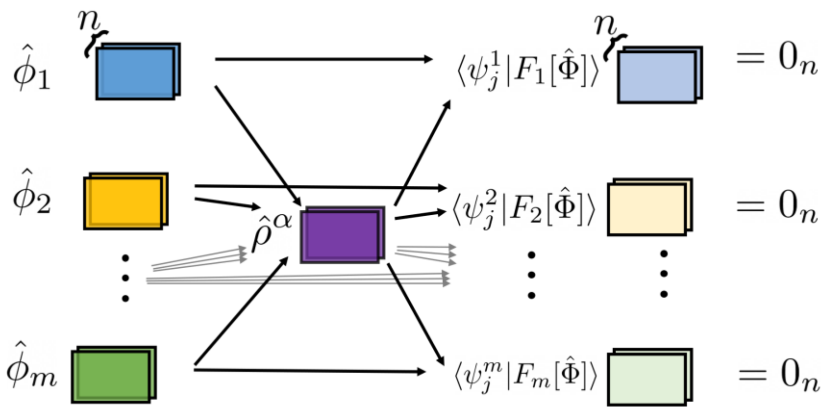


Faster



$$\left(\phi^{(1)}(r)^2 + \phi^{(2)}(r)^2 + \ \dots \ \right)^\alpha$$

3) Very fast

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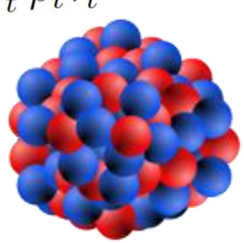
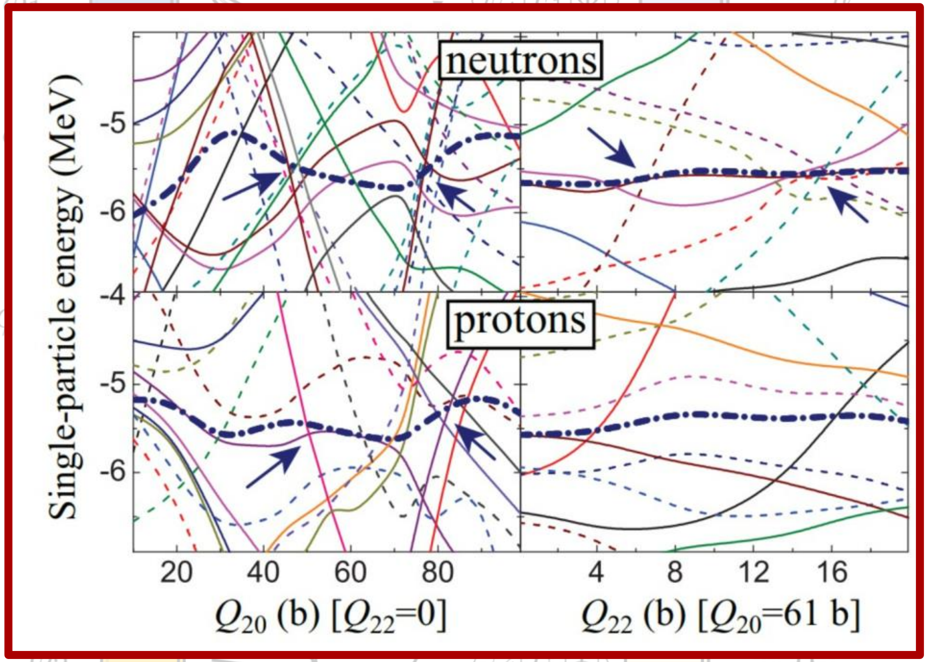
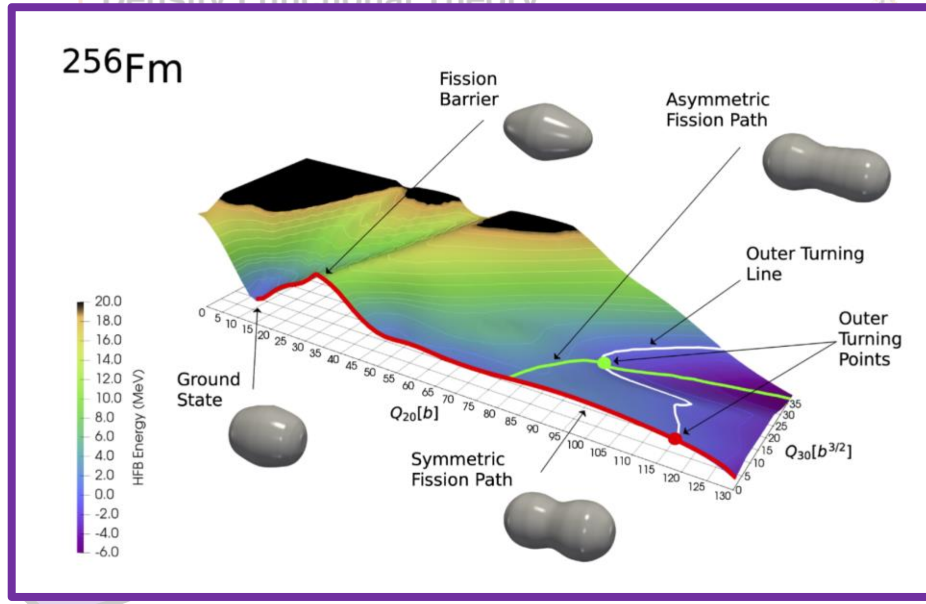


VERY non-linear

$$\rho(r)^\alpha$$

Non-affinity and Beyond: Mitigating non-linear and non-affine structures for the efficient emulation of Density Functional Theory





Level crossing is a problem

$$\left(\phi^{(1)}(r)^2 + \phi^{(2)}(r)^2 + \ \dots \ \right)^{\alpha}$$

3) Very fast

Skyrme Density Functional

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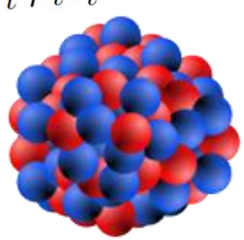
Mili-seconds



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$$\rho(r)^{\alpha}$$

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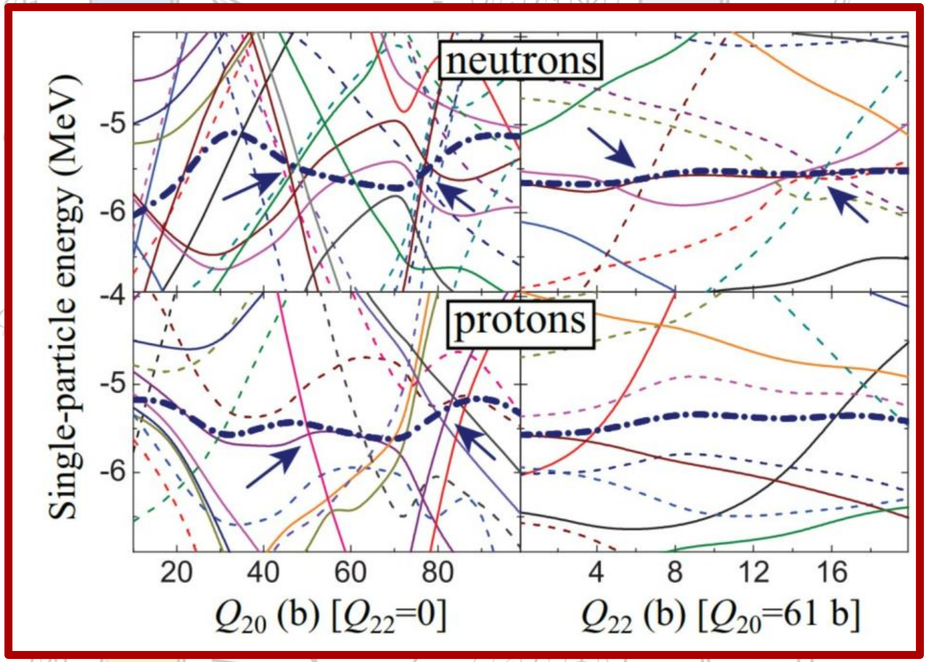

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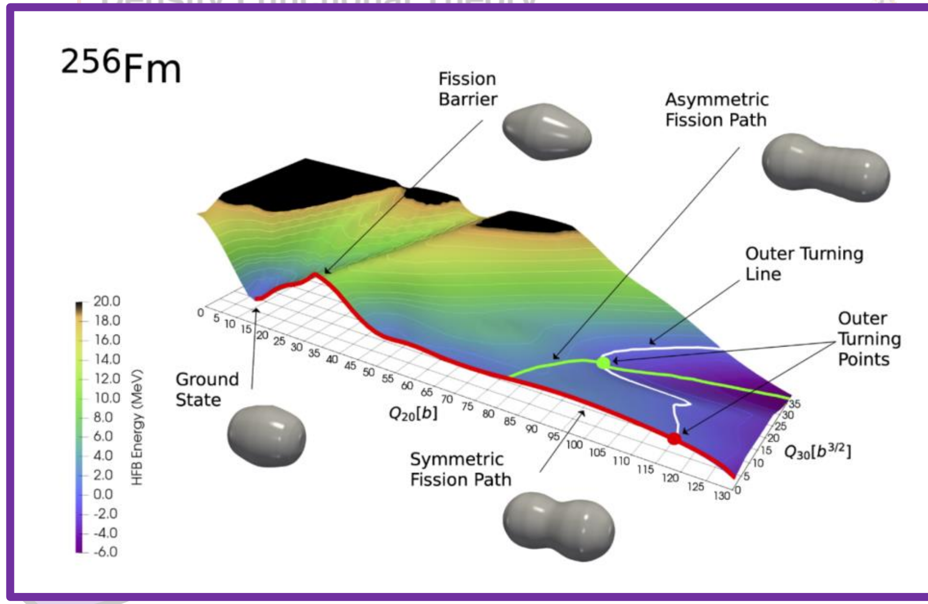

Fission is next 

$$\left(\phi^{(1)}(r)^2 + \phi^{(2)}(r)^2 + \ \dots \ \right)^\alpha$$

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Skyrme Density Functional

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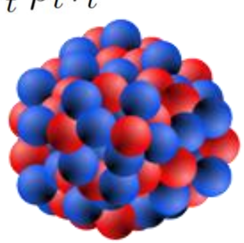


VERY non-linear

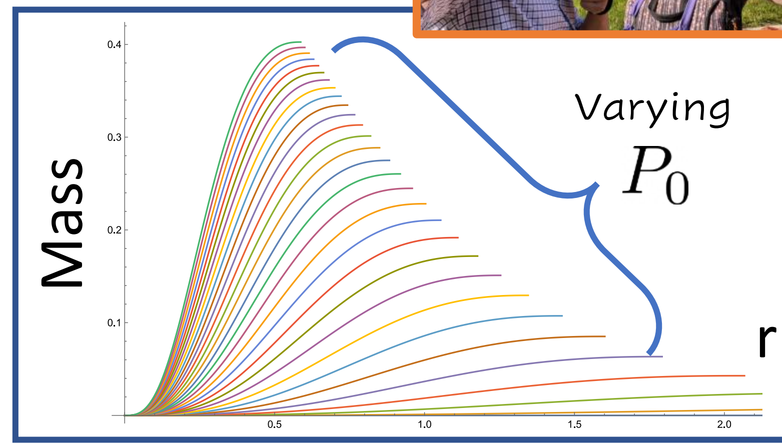
 $\rho(r)^\alpha$

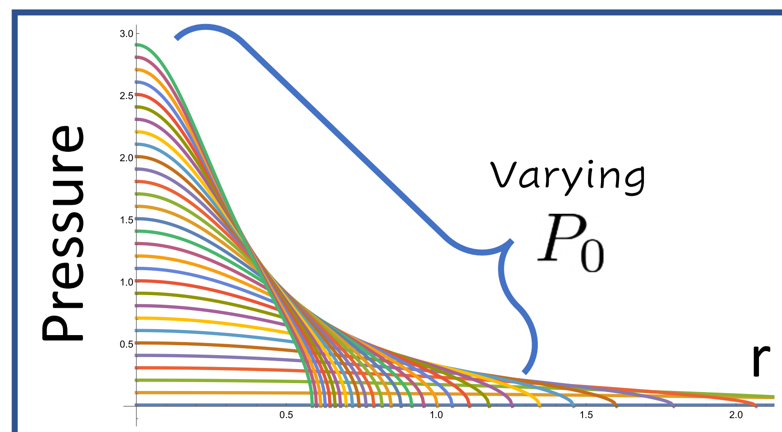
Applications and Results

5 **Application of reduced basis methods to compact stars**

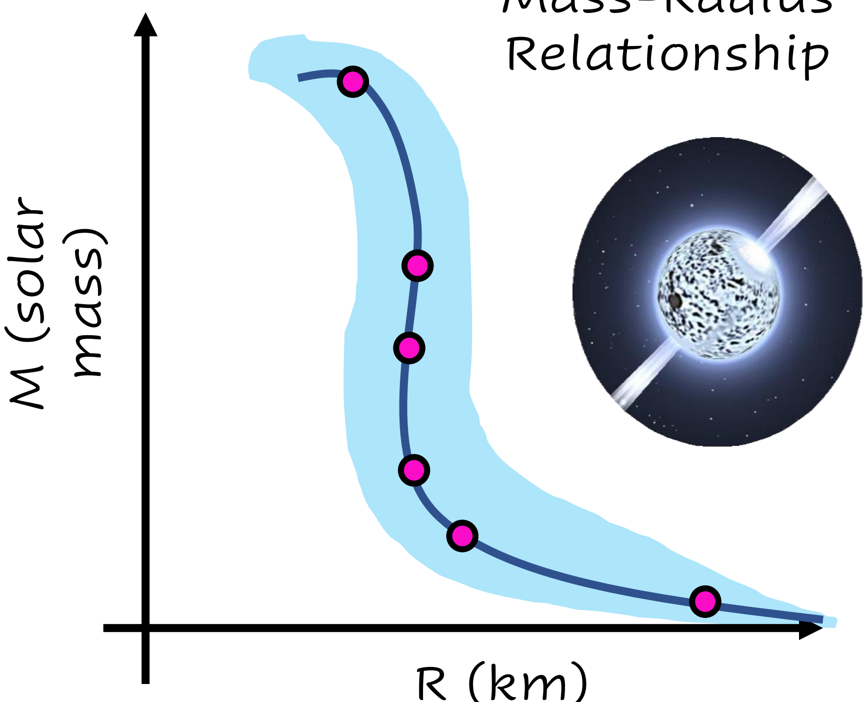
Amy Anderson,[1,*] Pablo Giuliani,[2,†] and J.Piekarewicz[1,‡]
[1] *Department of Physics, Florida State University, Tallahassee, FL 32306, USA*
[2] *FRIB/NSCL Laboratory, Michigan State University, East Lansing, Michigan 48824, USA*

Amy Anderson





Mass-Radius Relationship

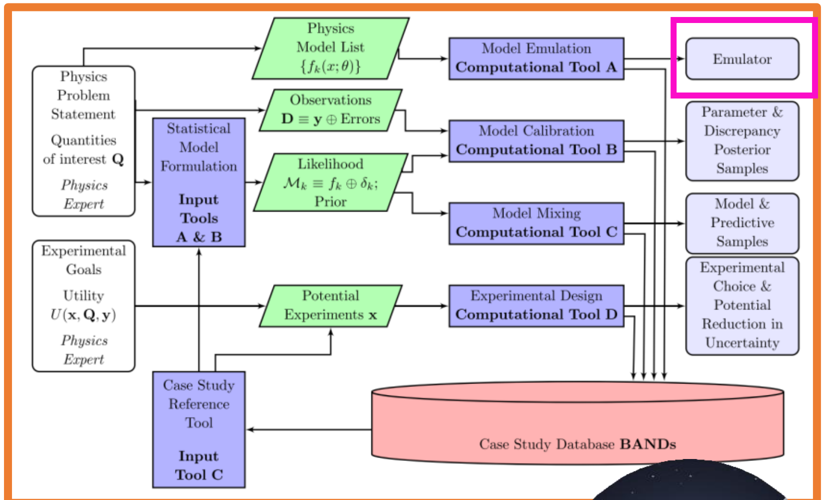


Applications and Results

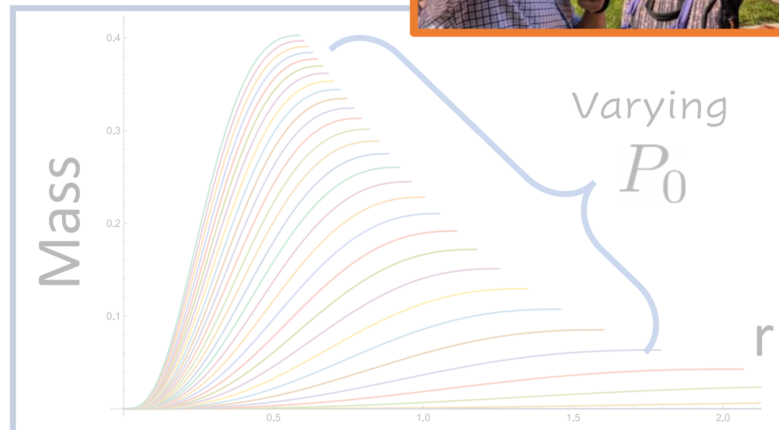
Application of reduced basis methods to compact stars

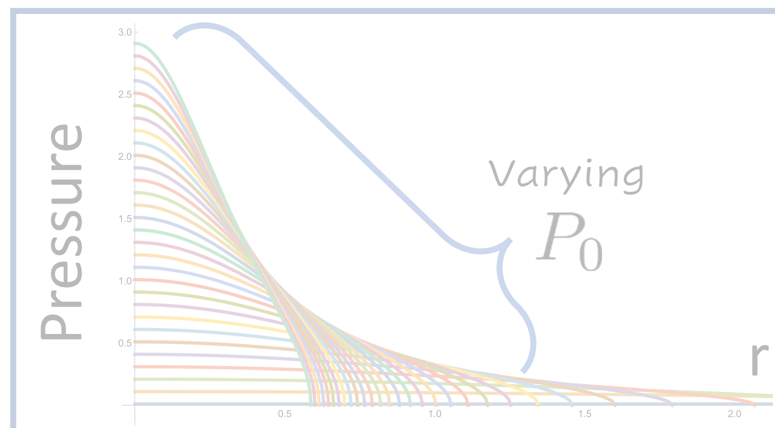
Amy Anderson,[1,*] Pablo Giuliani,[2,†] and J.Piekarewicz[1,‡]
[1] Department of Physics, Florida State University, Tallahassee, FL 32306, USA
[2] FRIB/N... ...atory, Michigan State University, East Lansing, Michigan 48824, USA

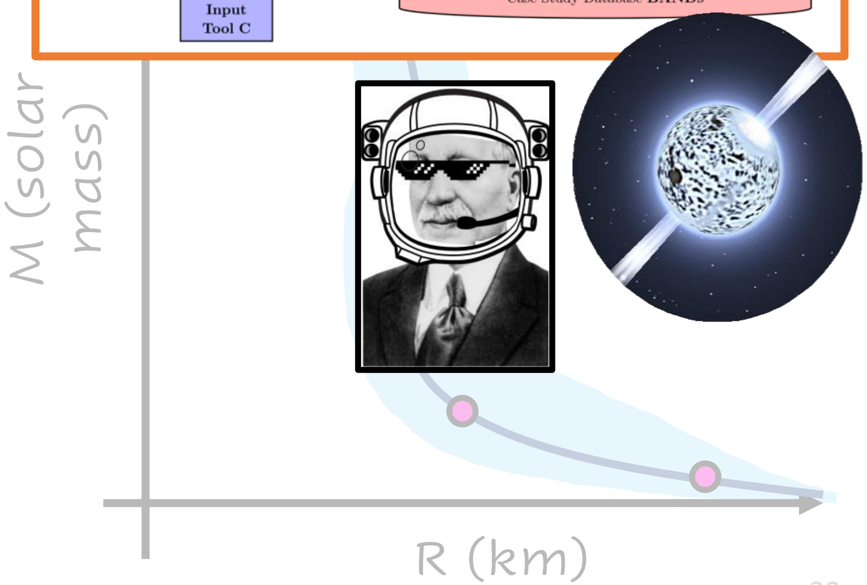
BAND Bayesian Analysis of Nuclear Dynamics



Amy Anderson Fellow 2023

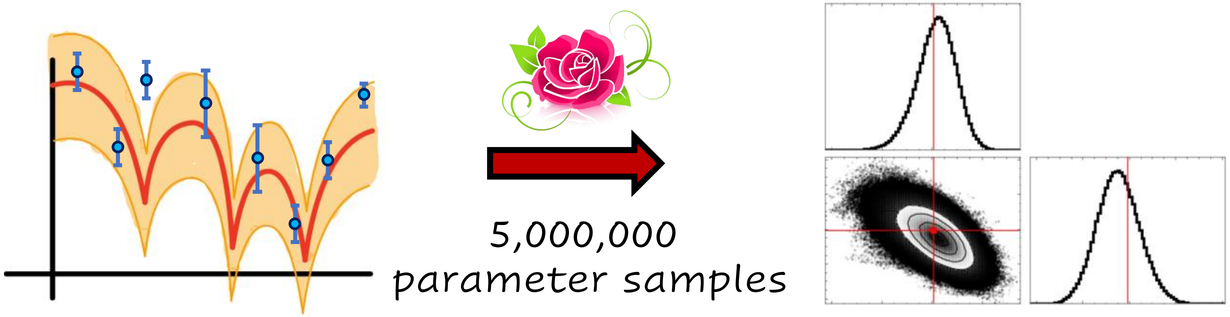






Upcoming highlight

1 Smart posterior handling



Upcoming highlights

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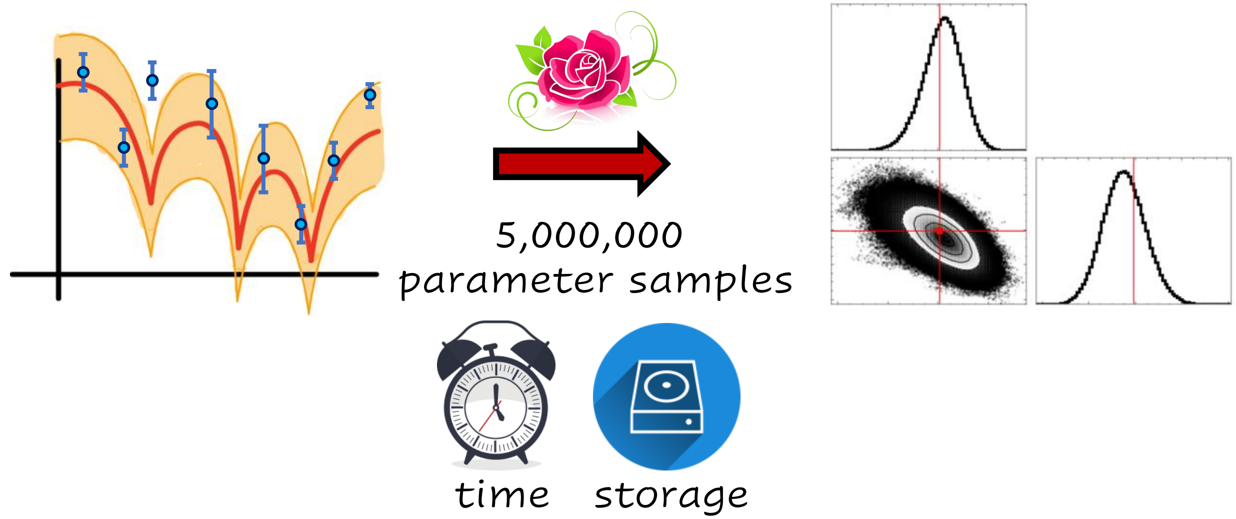

Upcoming highlights

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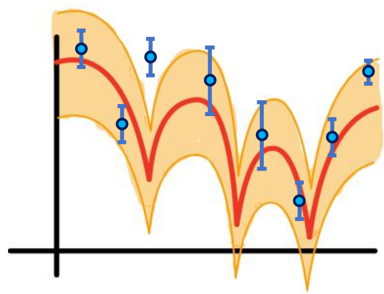
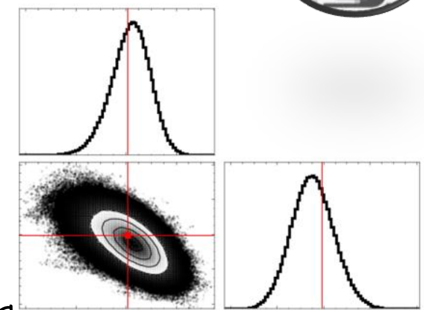


(Frederi Viens
Edgard Bonilla)

Chaos expansion

Normalizing flows



(Yukari Yamauchi
Landon Buskirk)

Upcoming highlights

Landon Buskirk

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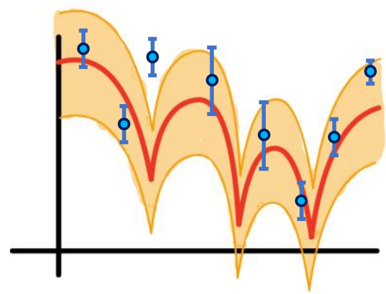

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Chaos expansion

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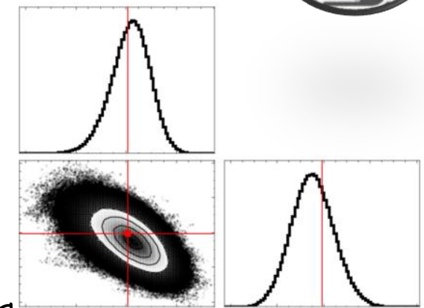
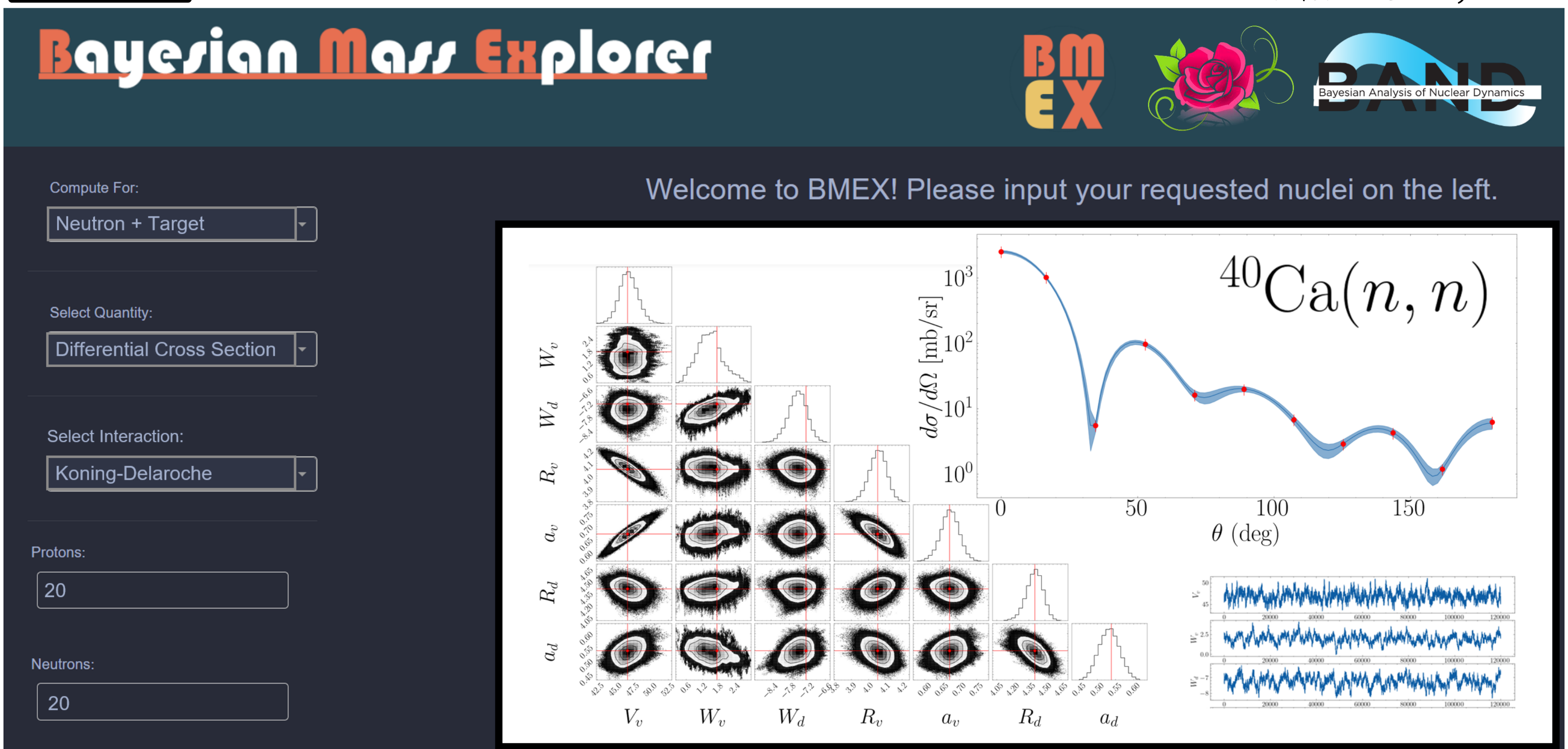


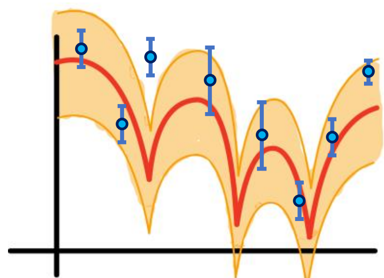
(Yukari Yamauchi Landon Buskirk)



Upcoming highlights

1 Smart posterior handling

Landon Buskirk



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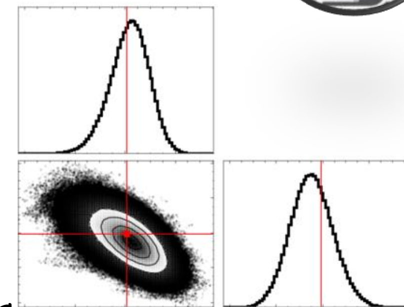


(Yukari Yamauchi Landon Buskirk)

Bayesian Mass Explorer

BMEX

Bayesian Analysis of Nuclear Dynamics

Welcome to BMEX! Please input your requested nuclei on the left.

Compute For:

Neutron + Target

Select Quantity:

Differential Cross Section

Select Interaction:

Koning-Delaroche

Protons:

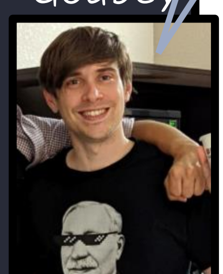
20

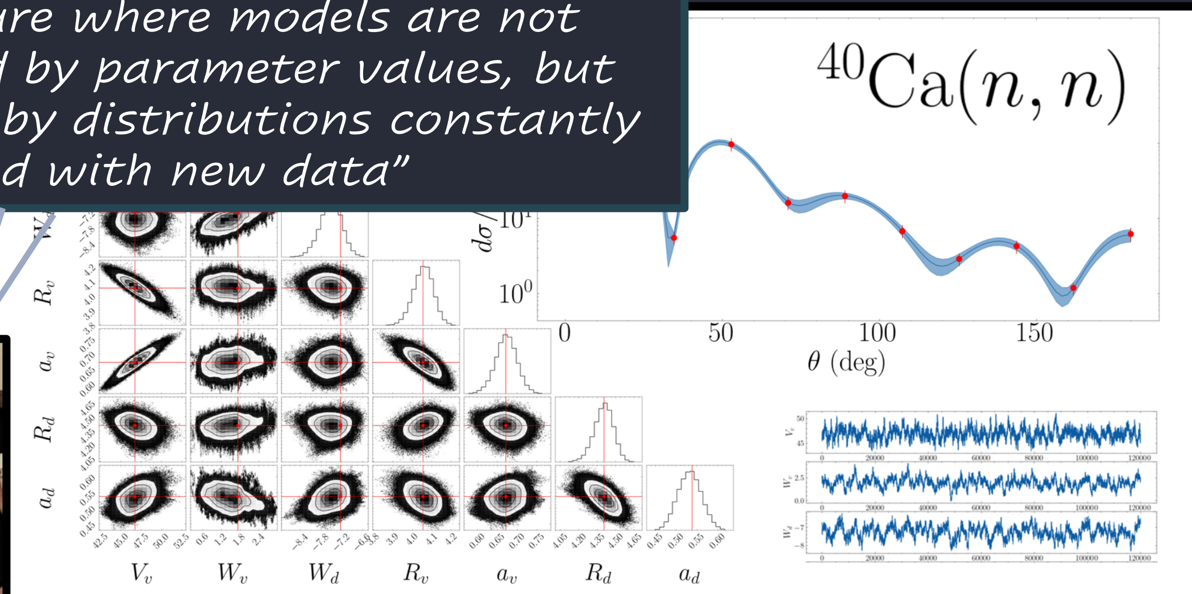
Neutrons:

20

"A future where models are not defined by parameter values, but rather by distributions constantly updated with new data"

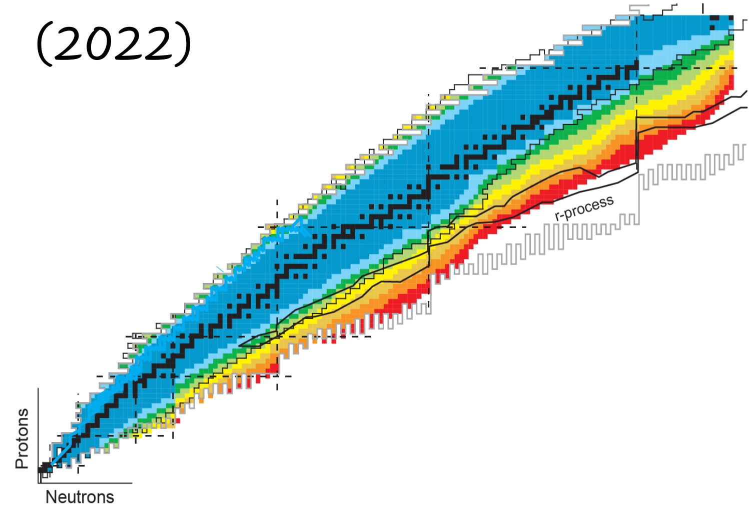
Kyle Godbey

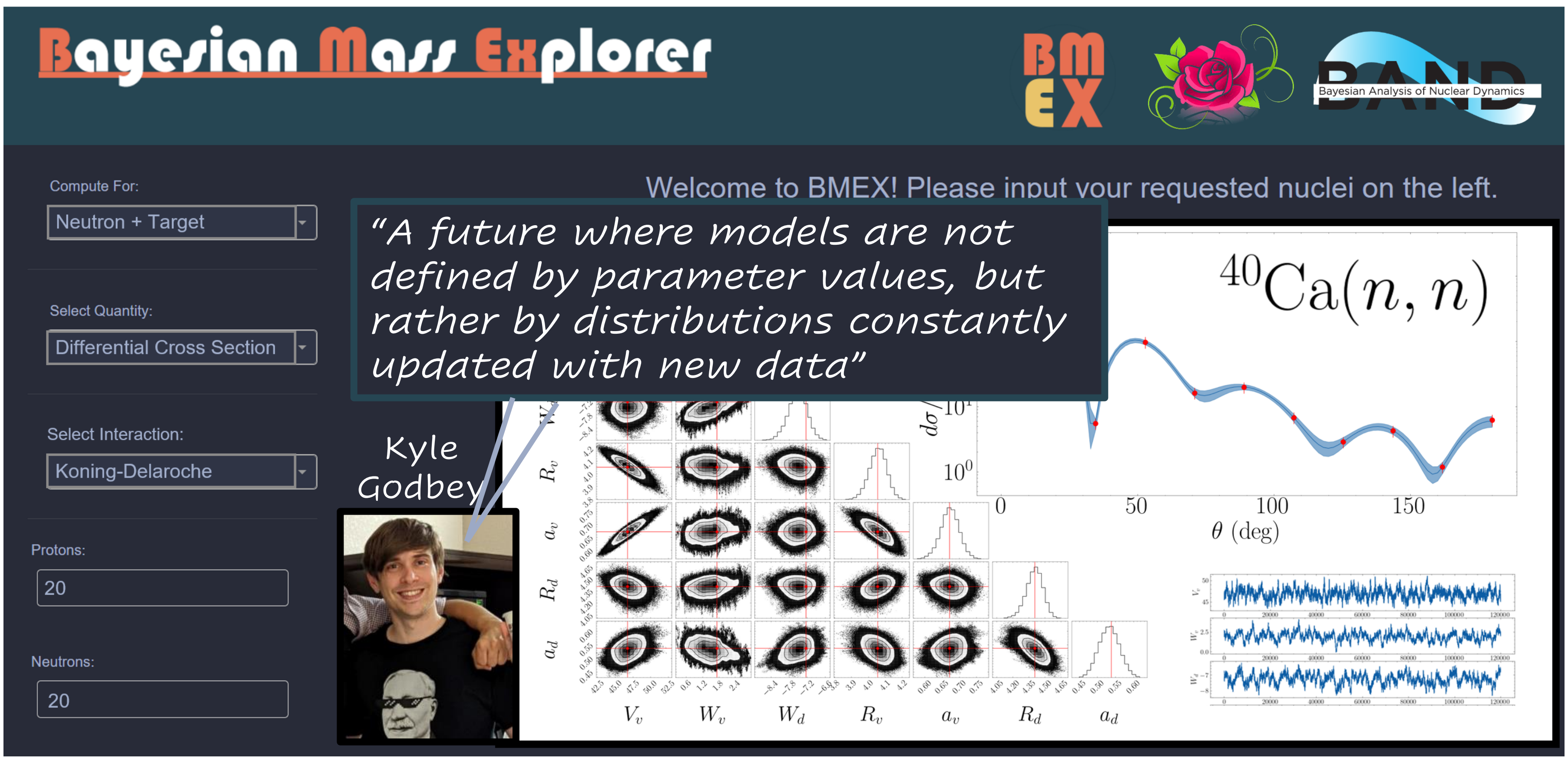




Optical potentials for the rare-isotope beam era (2022)

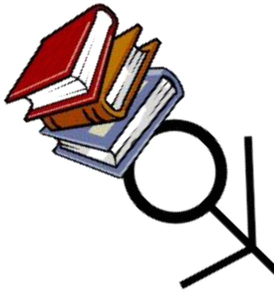
*In regions of the nuclear chart away from stability, which represent a frontier in nuclear science over the coming decade and which will be probed at new rare-isotope beam facilities worldwide, there is a targeted **need to quantify and reduce theoretical reaction model uncertainties**, especially with respect to nuclear optical potentials.*





Takeaways

I have two



Takeaways

1) These methods are SO cool

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Reduced Basis Method

Super Efficient →

Straightforward and broadly applicable

$$\hat{\phi}(x) = \phi_0 + \sum_k^n a_k \phi_k(x)$$ Training

$$\langle \psi_j | F_\alpha[\hat{\phi}(x)] \rangle = 0$$ Projecting

Accessible from all levels

jupyter {book}

Reduced Basis Methods in Nuclear Physics

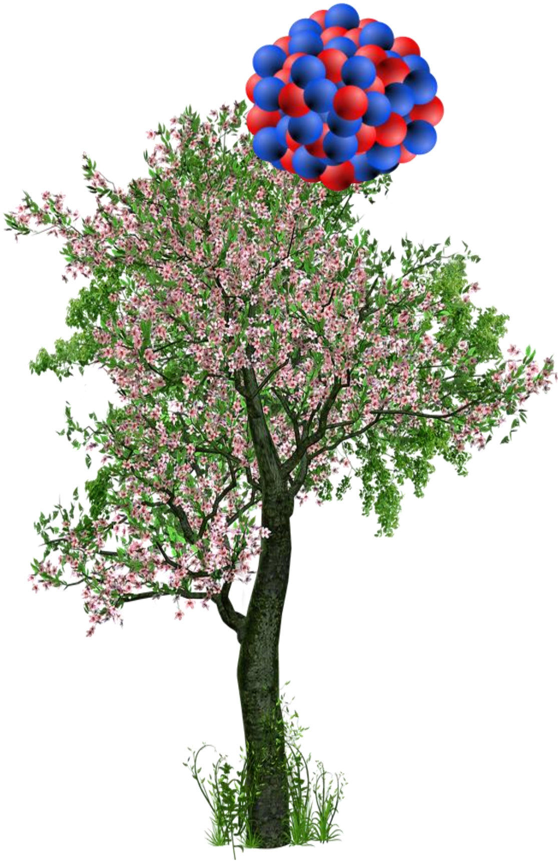
BUQEYE Guide to Projection-Based Emulators in Nuclear Physics

Takeaways

1) These methods are SO cool

2) UQ needs multidisciplinary efforts

This is very important to us



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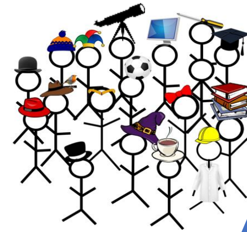

mathematics
statistics
computational
experimental

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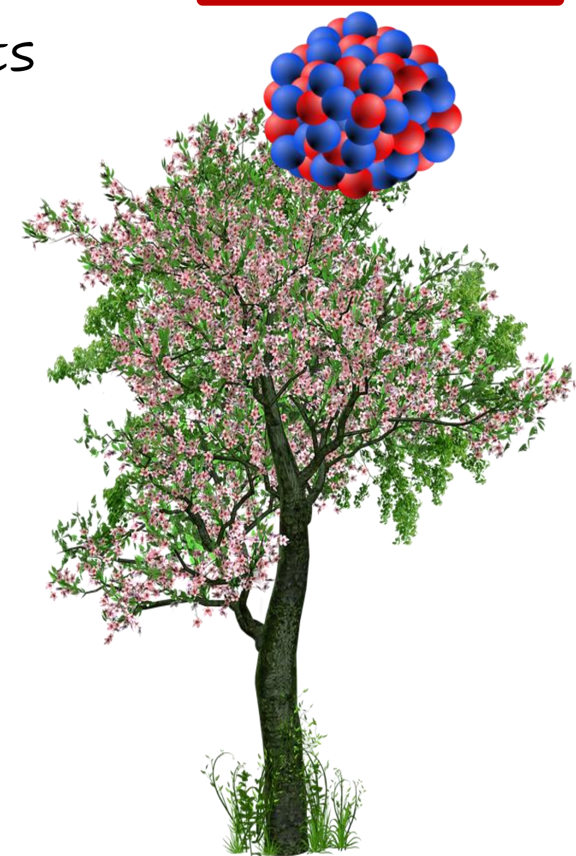
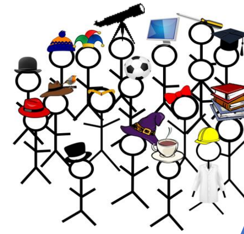


Takeaways



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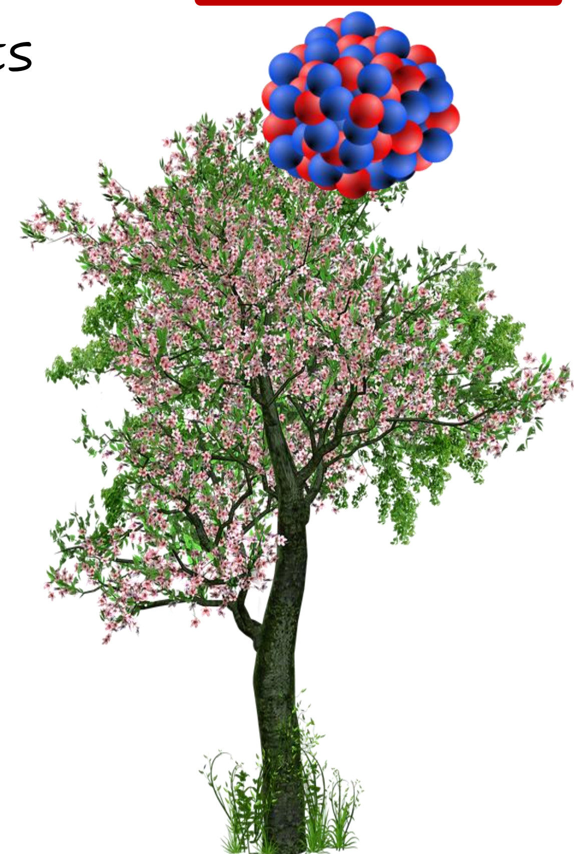
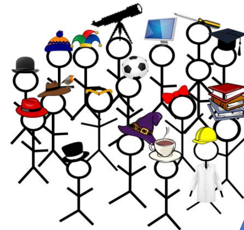
ASCSN

Advanced Scientific Computing and Statistics Network



Takeaways



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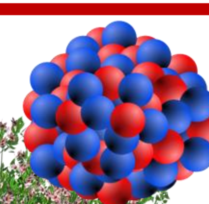
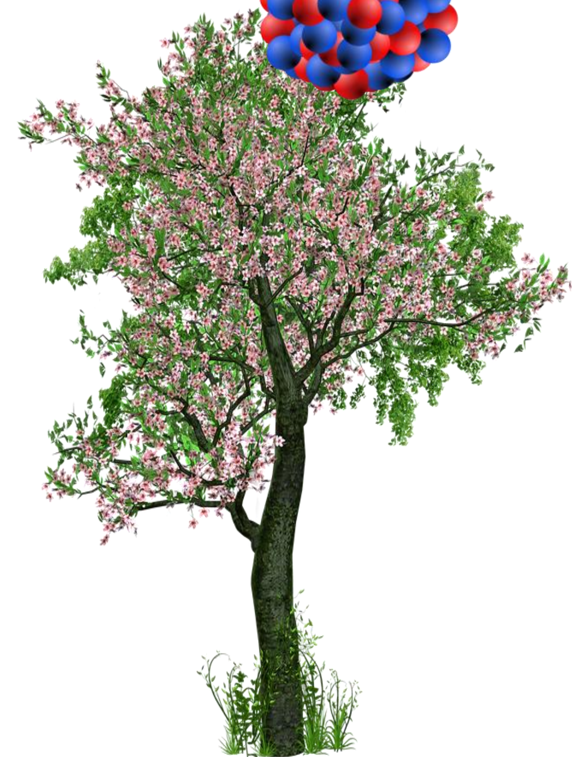


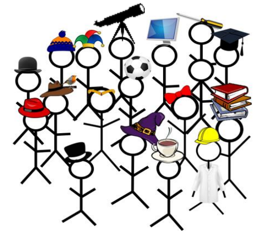
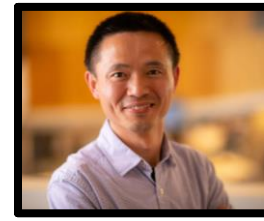
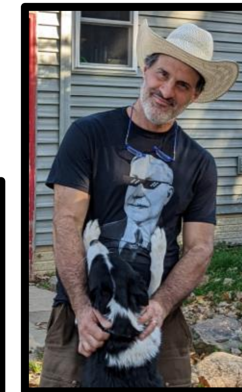


ASCSN

Advanced Scientific Computing and Statistics Network

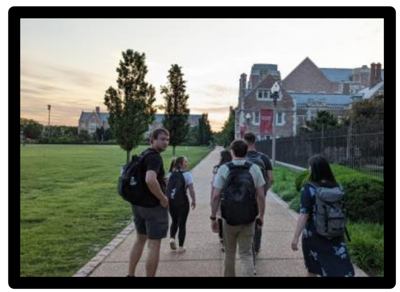
See Kyle's talk tomorrow

Takeaways

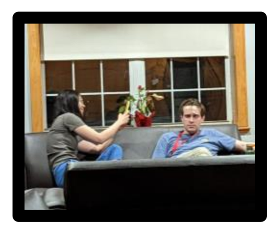
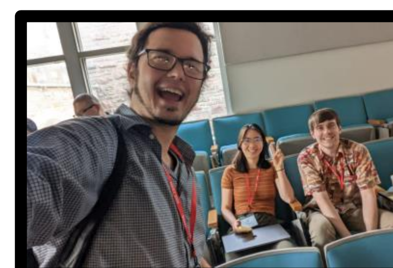






Work in collaboration with experts ...







... and find that the real UQ is the friends you made along the way