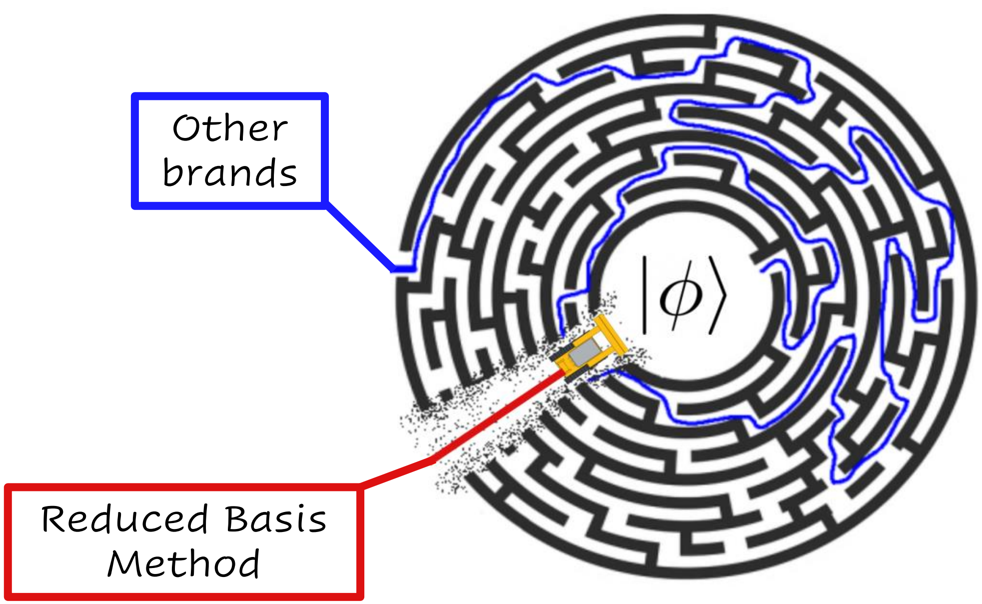
Sorry Maria, I forgot to change my title:

Dimensionality reduction for accelerating uncertainty quantification



Pablo Giuliani
giulianp@frib.msu.edu

Outline

Why → Uncertainty Quantification? ← How

The Reduced Basis Method

How it works

Applications and Results

Upcoming Highlights

Takeaways

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How →

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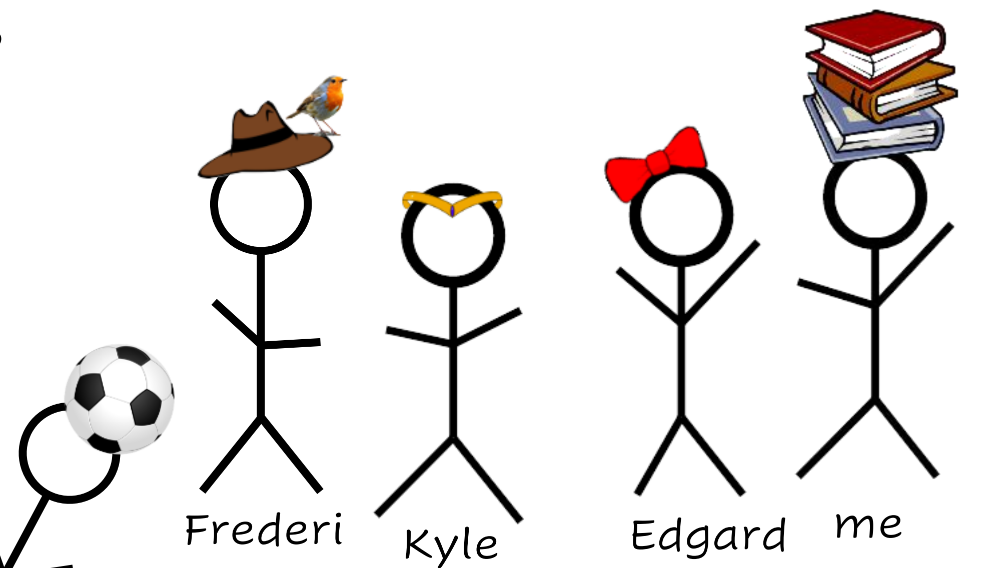
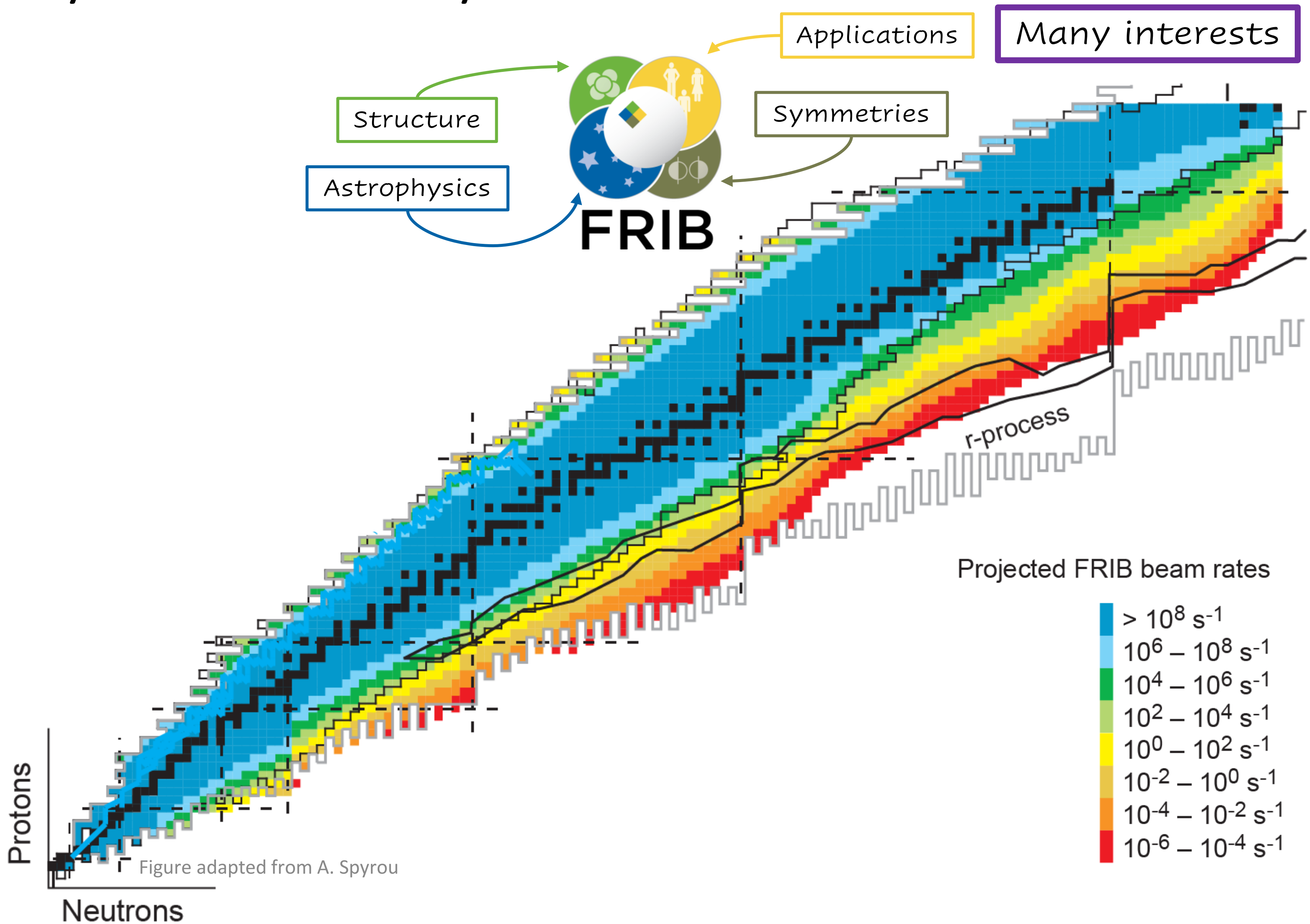


Why Uncertainty Quantification?



Why Uncertainty Quantification?

r-process

Lifetimes (Fission) (β decay)

Masses

Capture rates

...

Structure

Astrophysics

Applications

Symmetries

Many interests

Many models

UNEDF# SV-min SkM* HFB# FRDM# ...

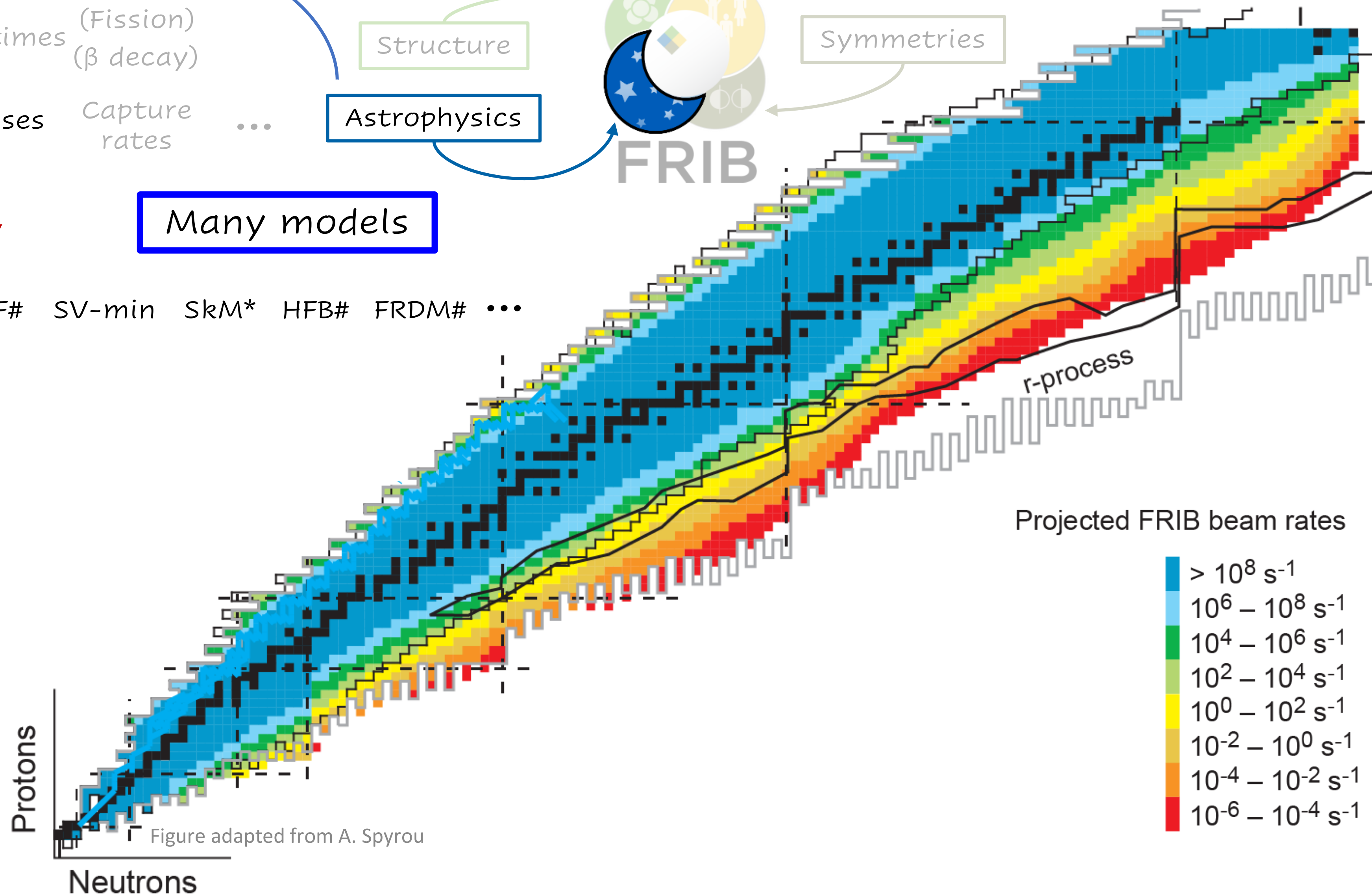


Figure adapted from A. Spyrou

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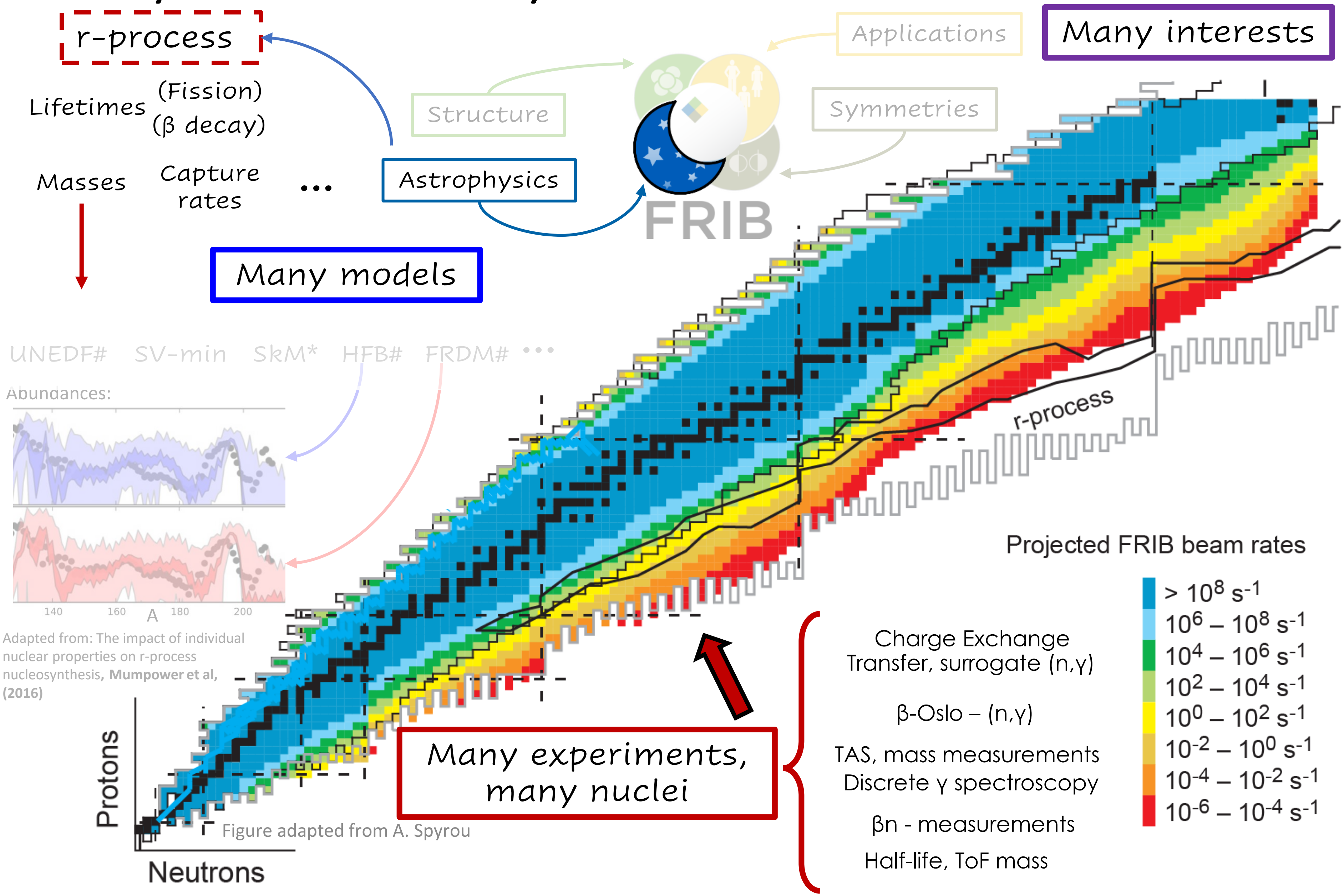

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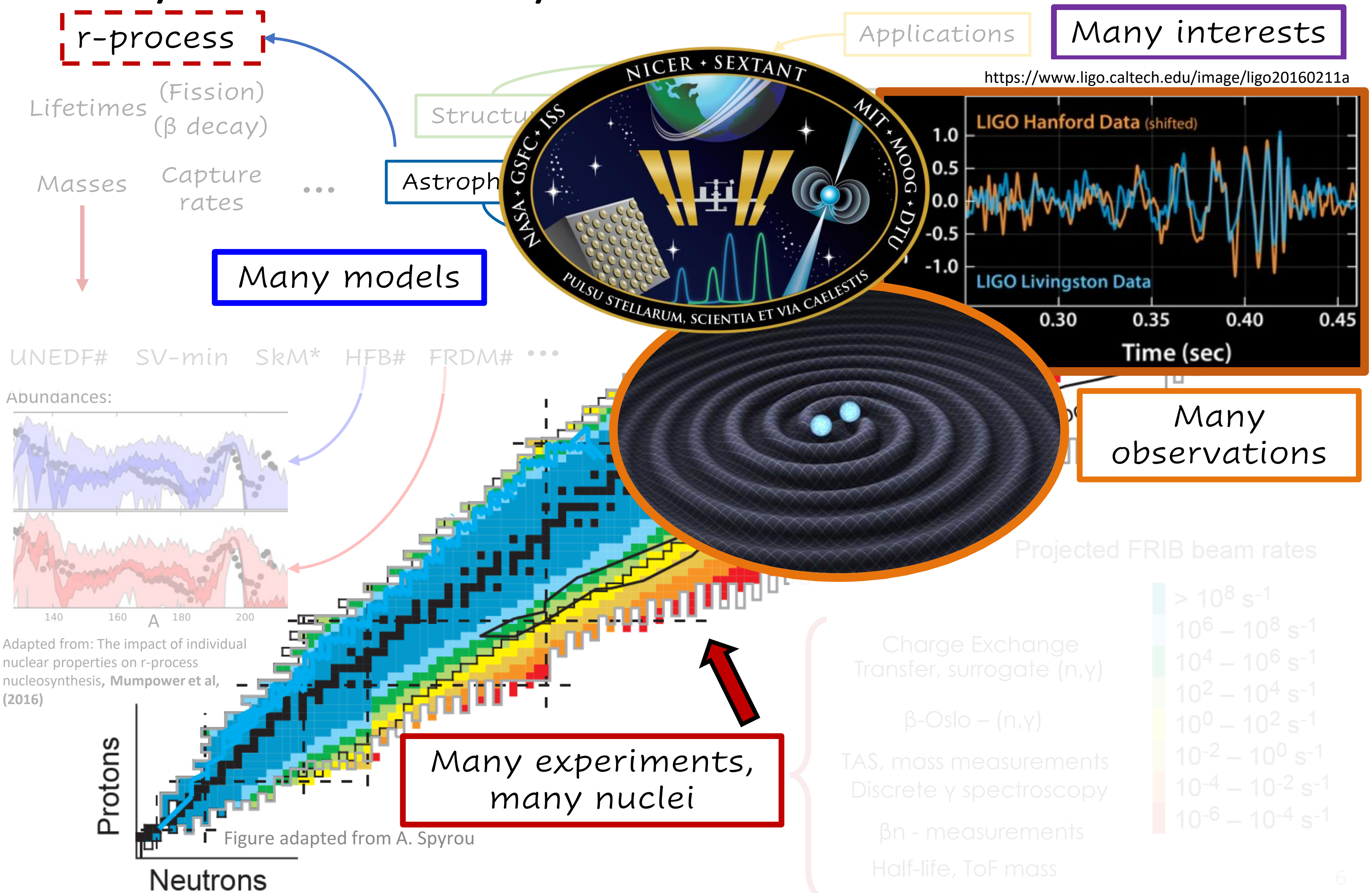

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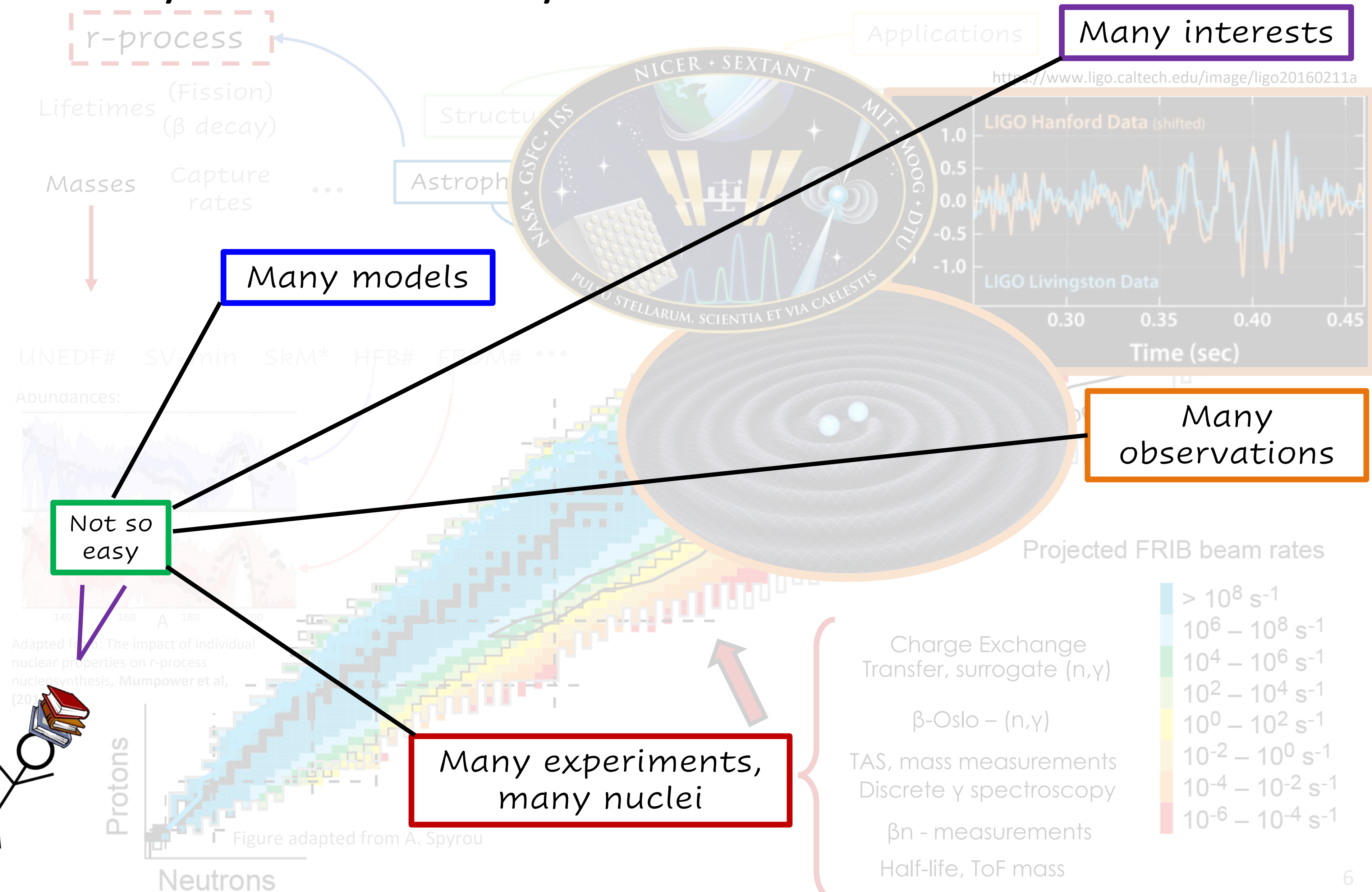

Why Uncertainty Quantification?

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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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

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Outlook and recommendations

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Quantifying model uncertainties of popular models e.g. for transfer reactions → ADWA or DWBA?

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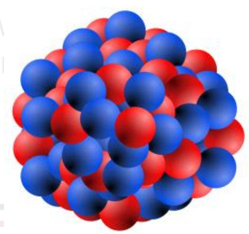

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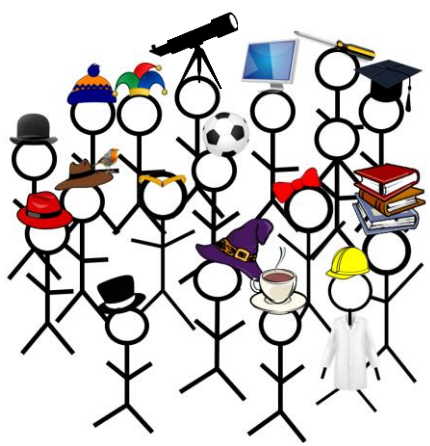

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statistics
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Work in collaboration with experts

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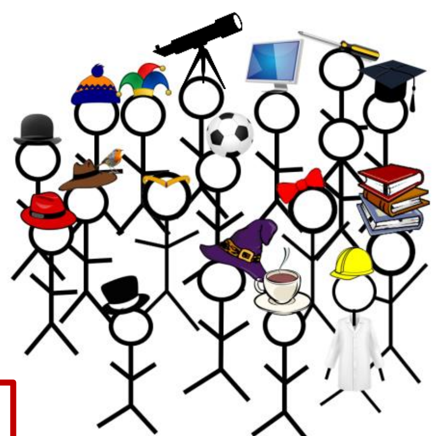

mathematics
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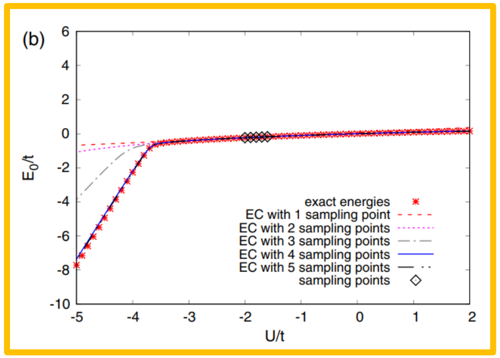
Communication

Work in collaboration with experts

Communication

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]



Google Scholar

"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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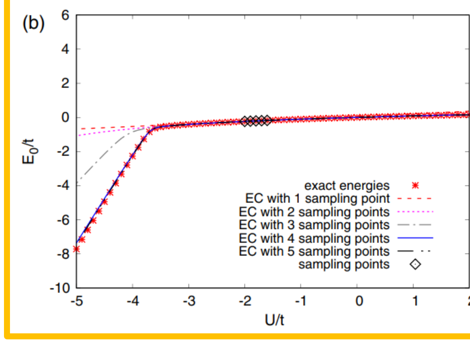

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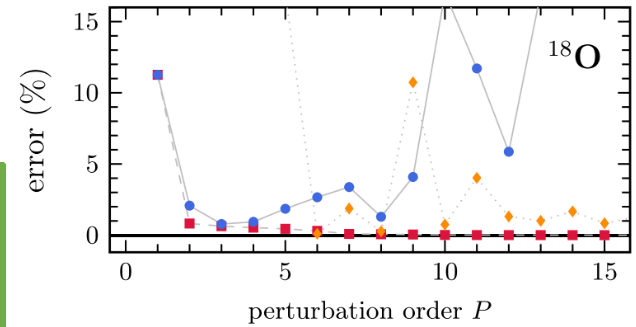
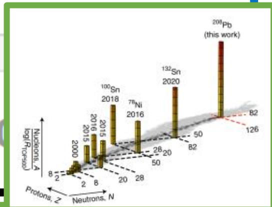


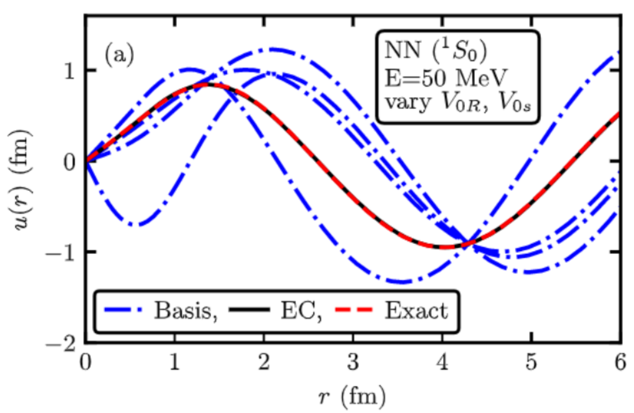


Ab initio predictions link the neutron skin of ^{208}Pb to nuclear forces (2022)

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]

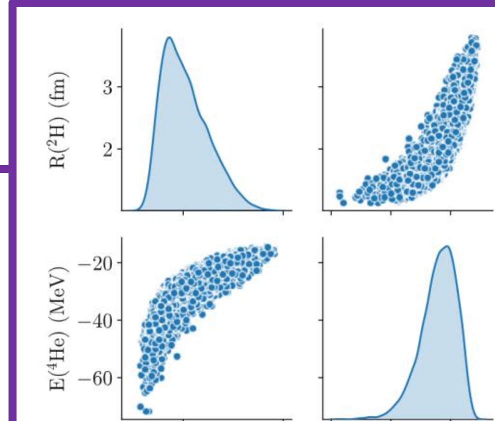
Improved many-body expansions from eigenvector continuation (2020)

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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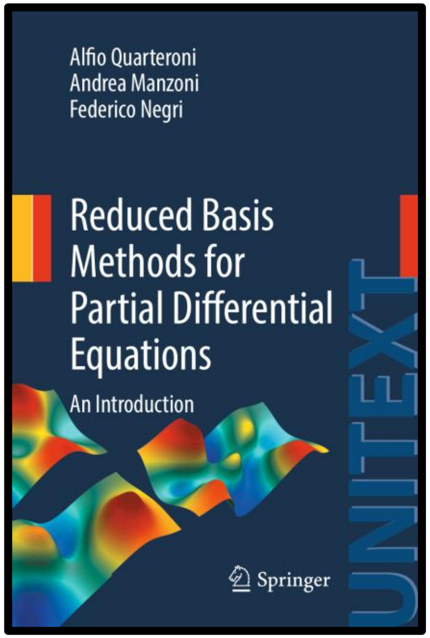

(2016)

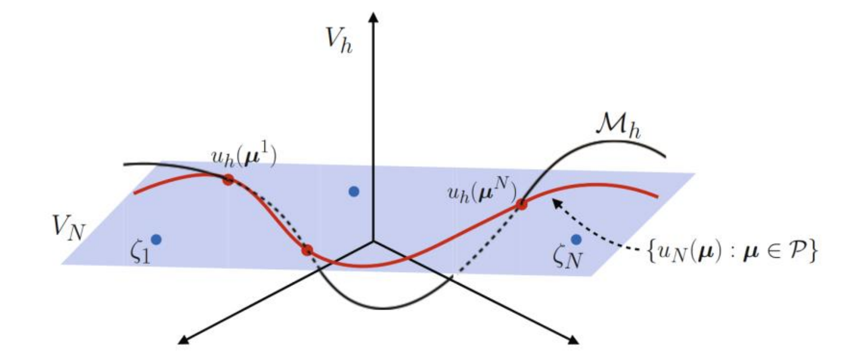

Fig. 3.1 The "snapshots" $u_h(\boldsymbol{\mu}^n), 1 \leq n \leq N$ on the parametric manifold $\mathscr{M}_h$, the RB space $V_N = \mathrm{span}\{\zeta_1, \ldots, \zeta_N\}$ = … solutions $u_N(\boldsymbol{\mu}) \in V_N$, $\boldsymbol{\mu}$ …

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]

(2009)

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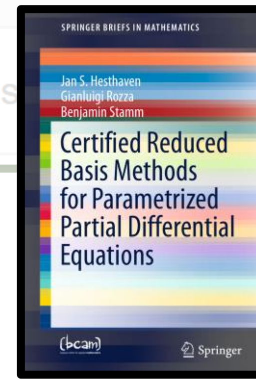
Sartori, et al



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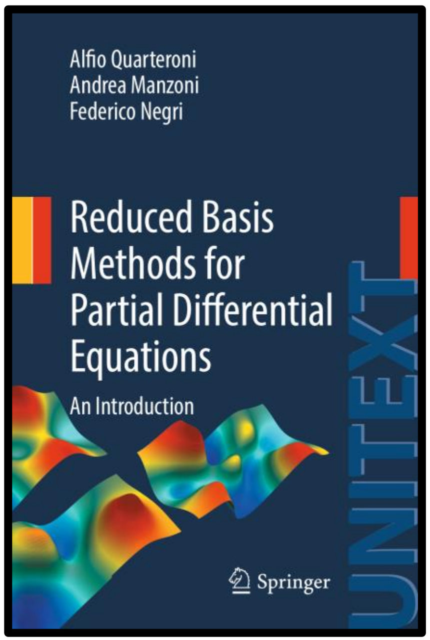

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Reduced-order modeling of time-dependent PDEs with multiple parameters in the boundary data

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

(2006)

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

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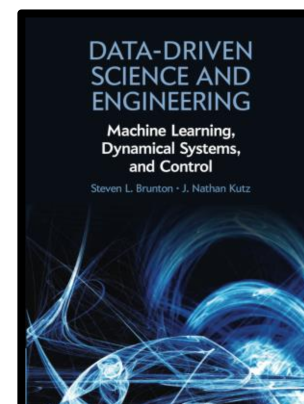

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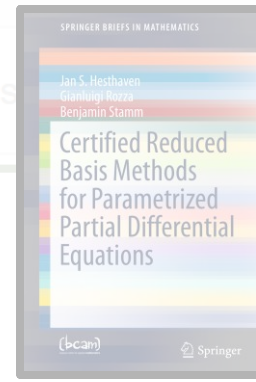

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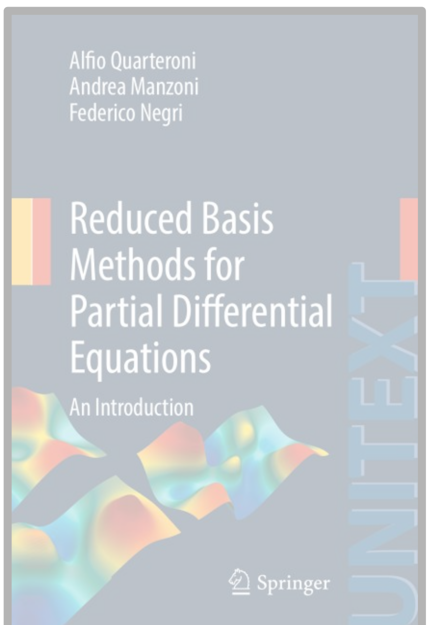

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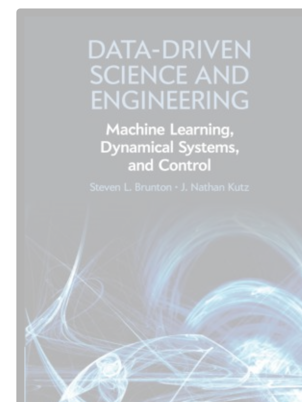

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Improved many-body expansions from eigenvector continuation

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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.

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

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

matrix. This problem can be avoided by running an orthogonalization on the EC vectors that stabilizes the subsequent numerical steps and reveals the effective dimension of the EC subspace. Since this step leads to a unit norm matrix, it also reduces the per-sample evaluation cost at the price of additional preprocessing effort (see Appendix A).

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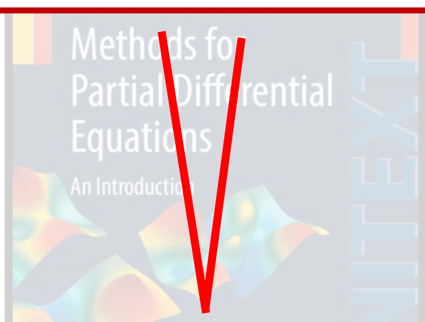
(2006)

Basis Methods for Parametrized

(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)

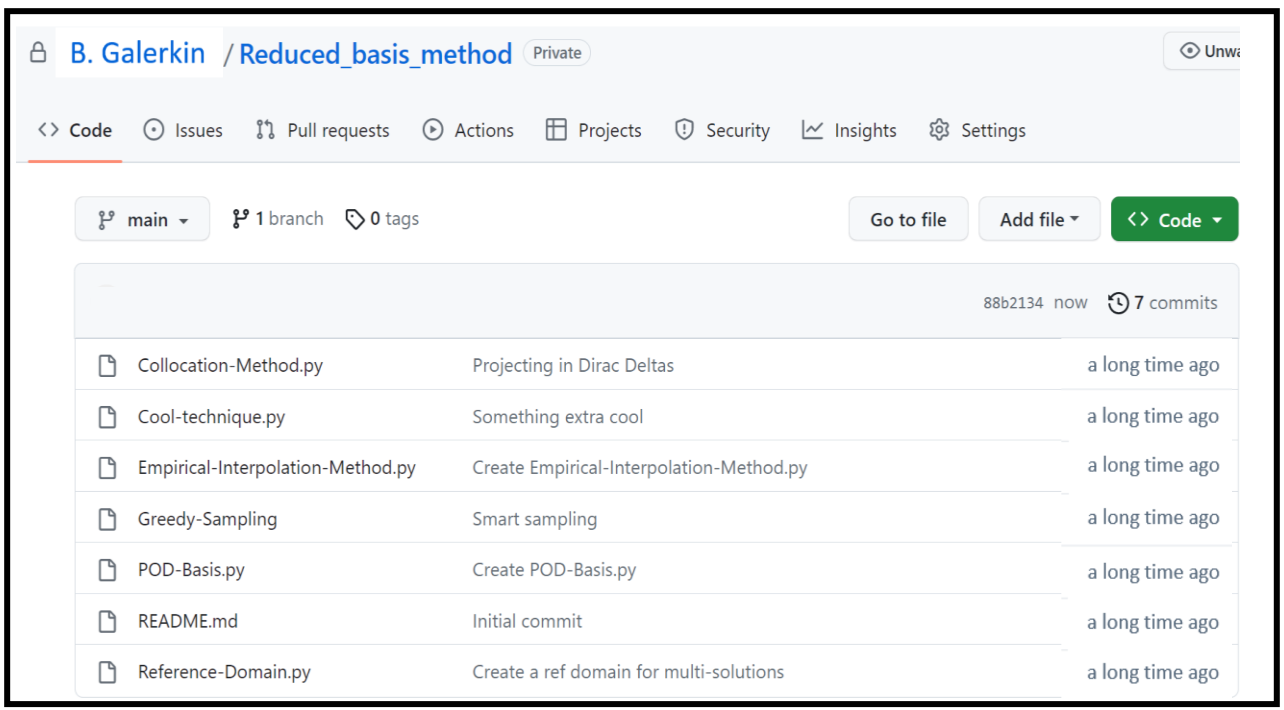
(2019)

Efficient emulators for scattering using eigenvector continuation

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

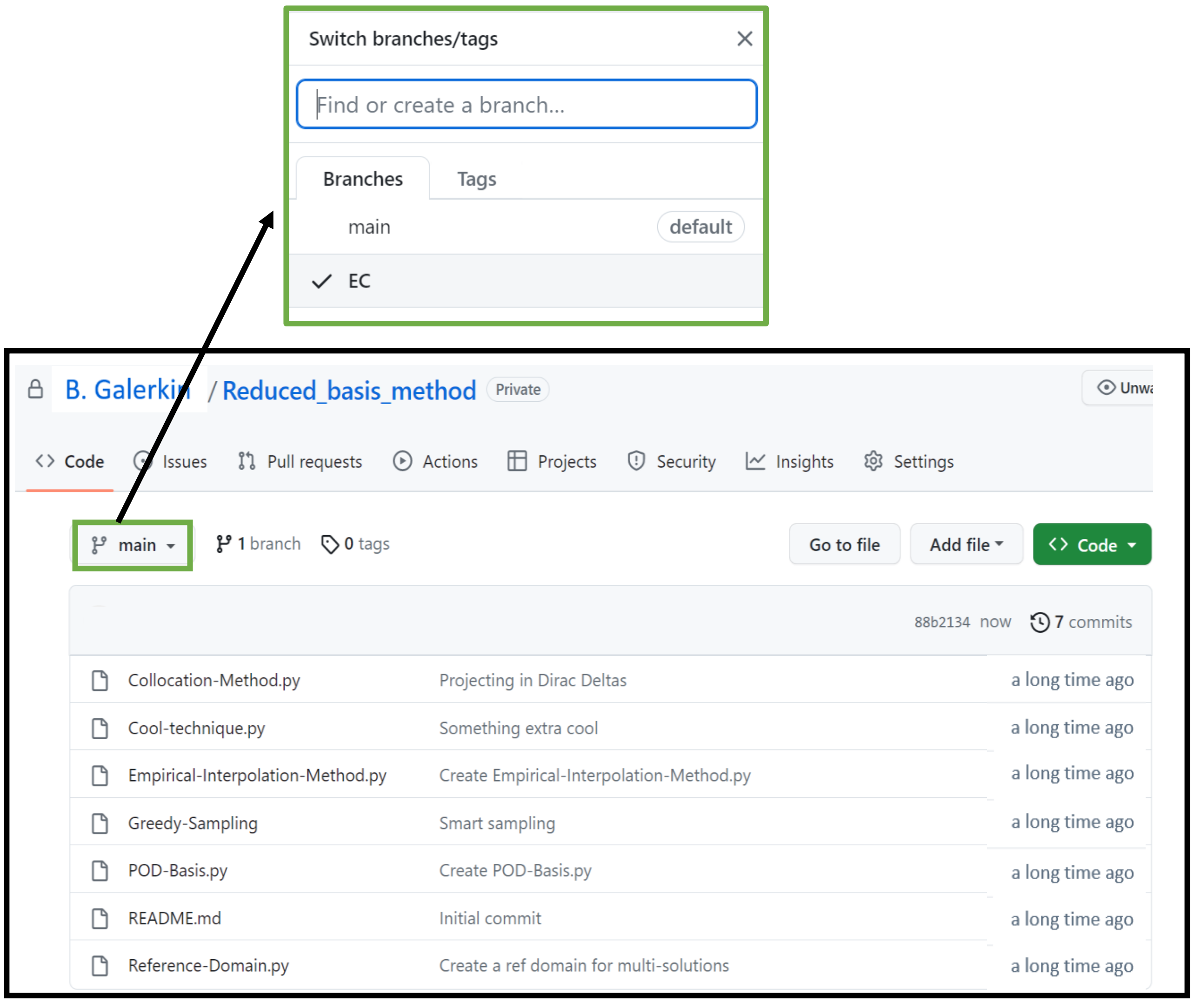
~~Why~~ Uncertainty Quantification?

How → *Communication with experts*



~~Why~~ Uncertainty Quantification?

How → *Communication with experts*



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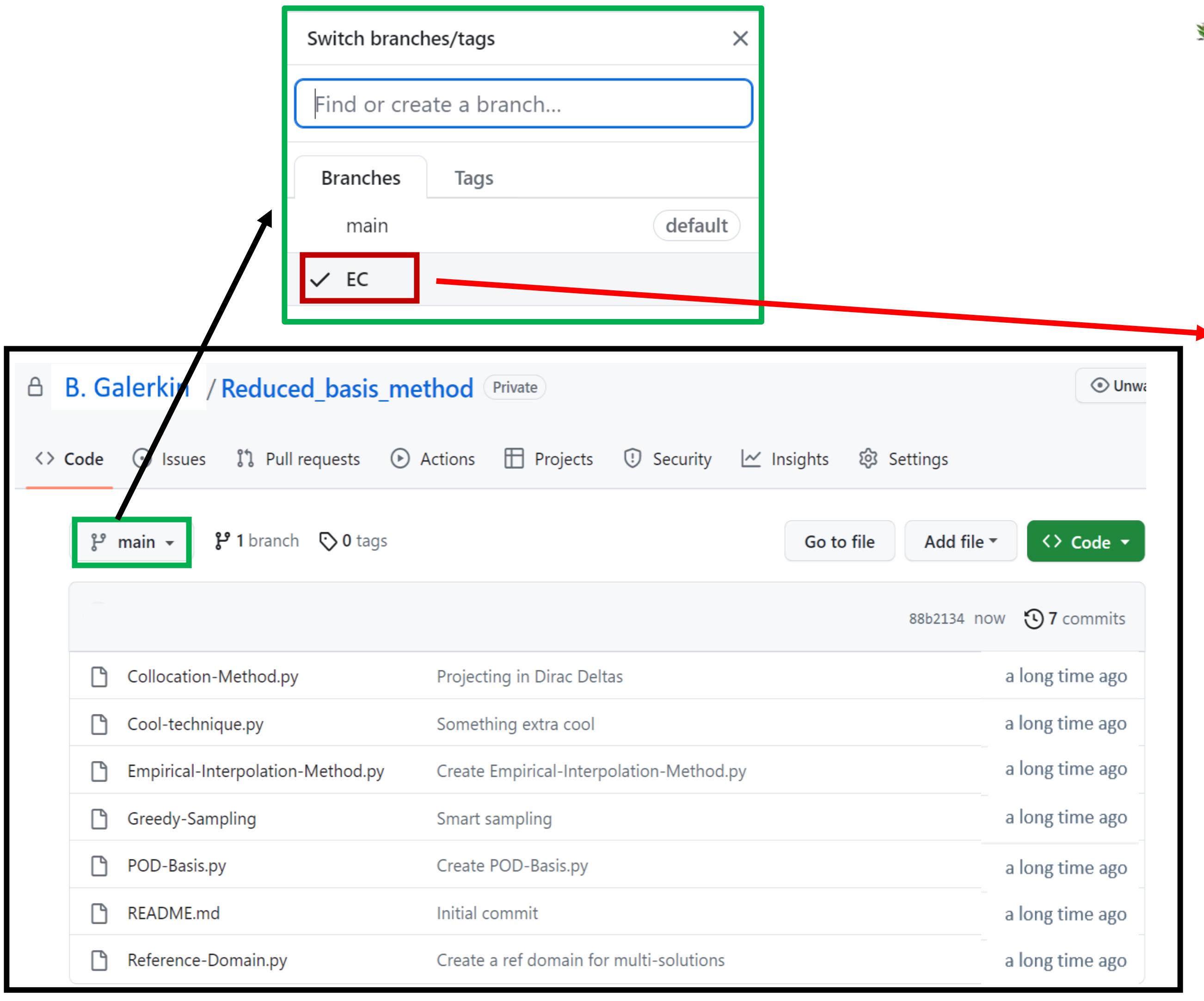

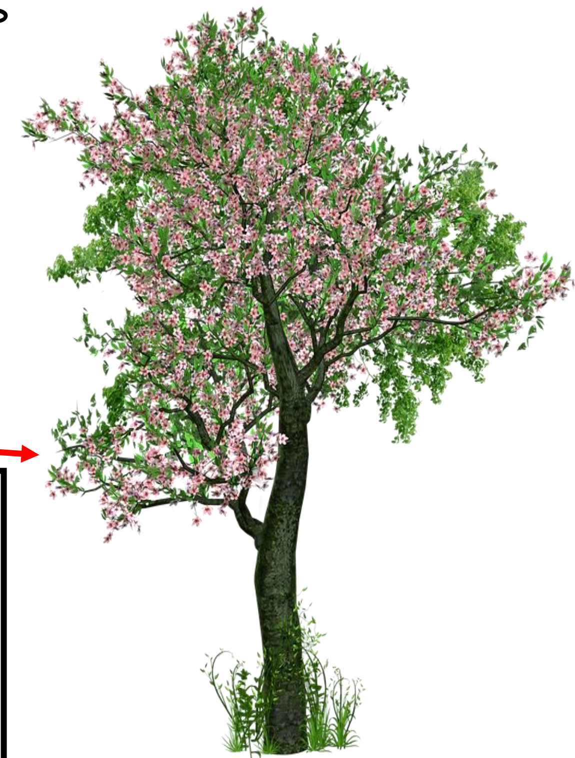

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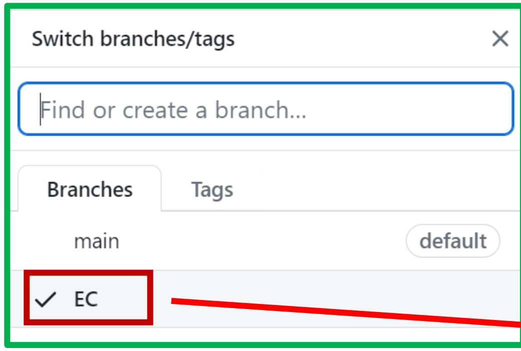
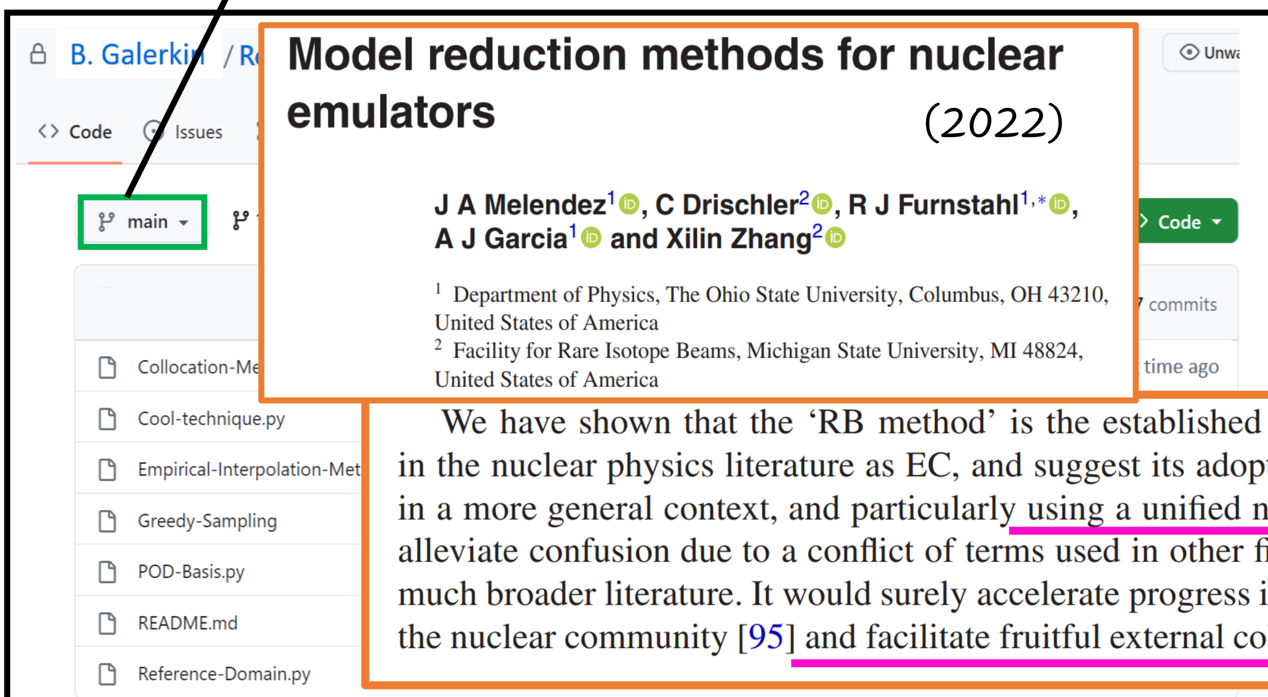




Model reduction methods for nuclear emulators

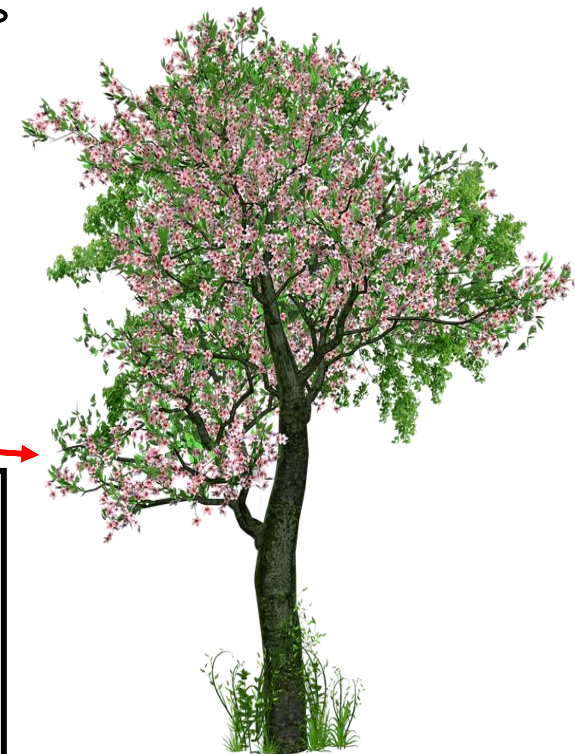
(2022)

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.



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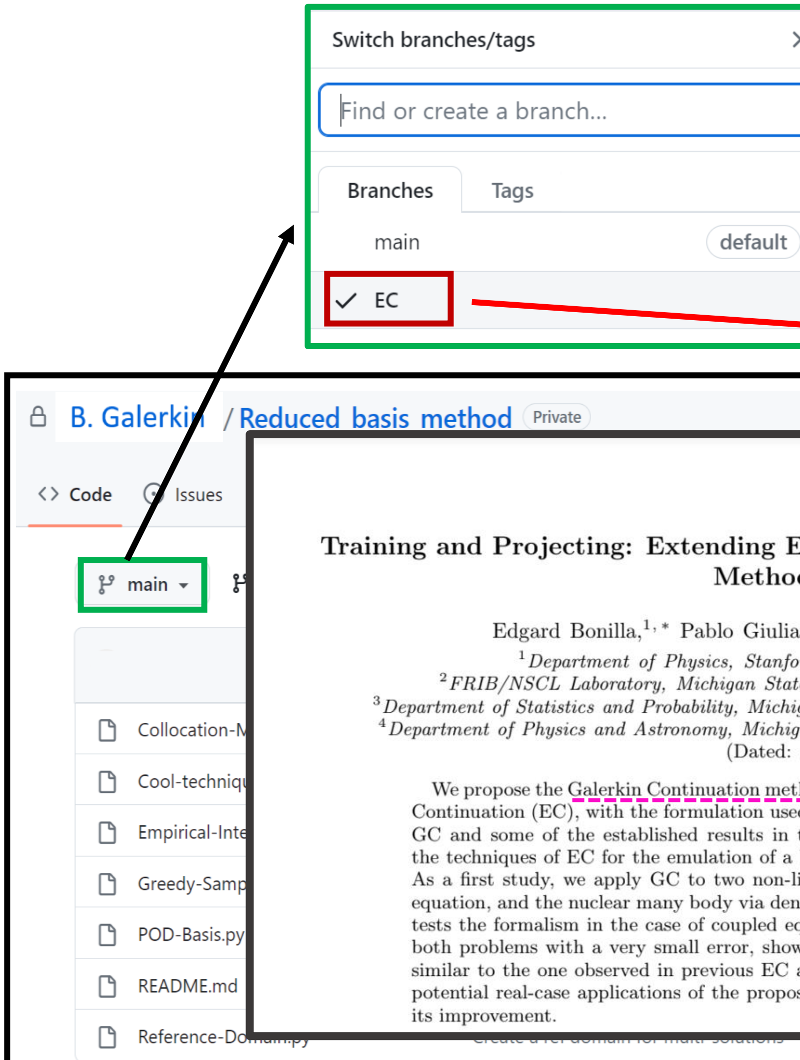
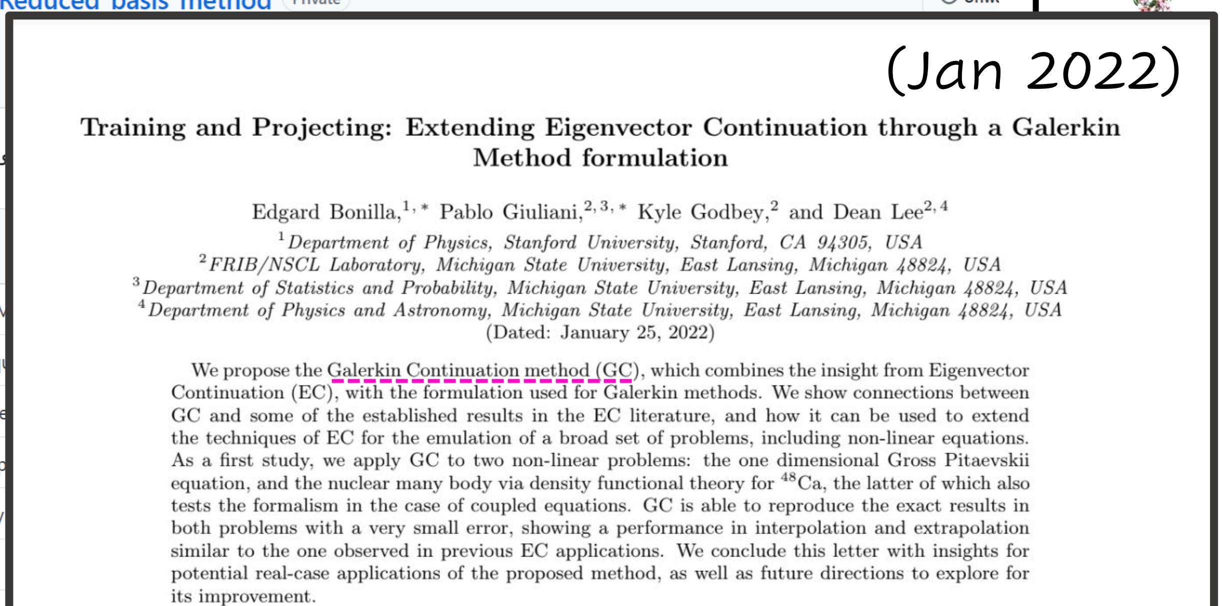
How → *Communication with experts*





(Jan 2022)

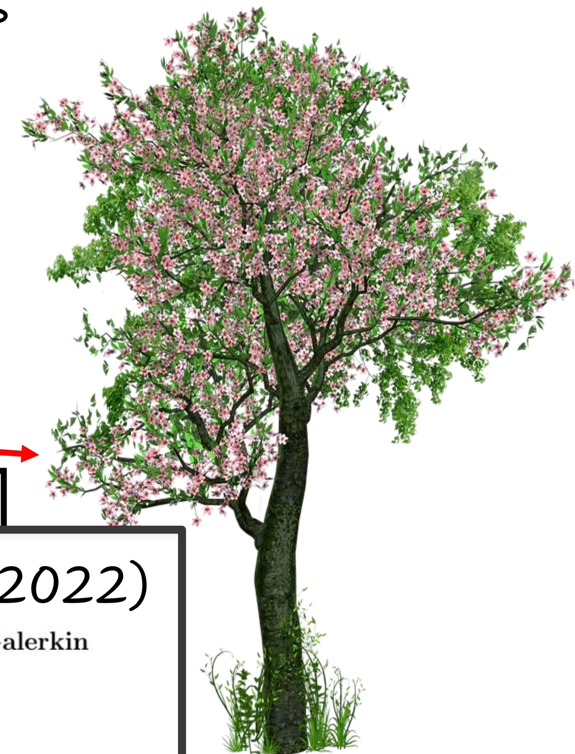
Training and Projecting: Extending Eigenvector Continuation through a Galerkin Method formulation

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*
[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)

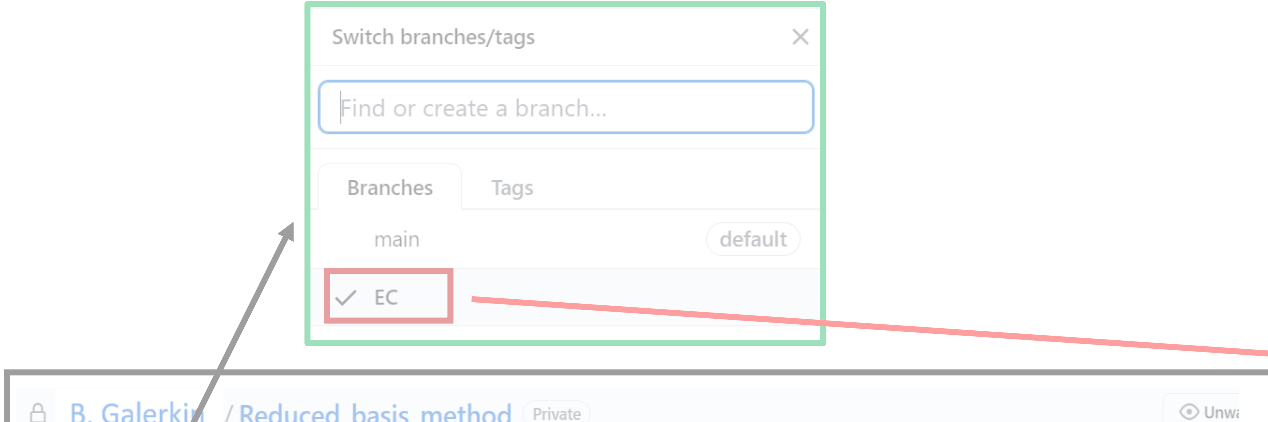
We propose the Galerkin Continuation method (GC), which combines the insight from Eigenvector Continuation (EC), with the formulation used for Galerkin methods. We show connections between GC and some of the established results in the EC literature, and how it can be used to extend the techniques of 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.



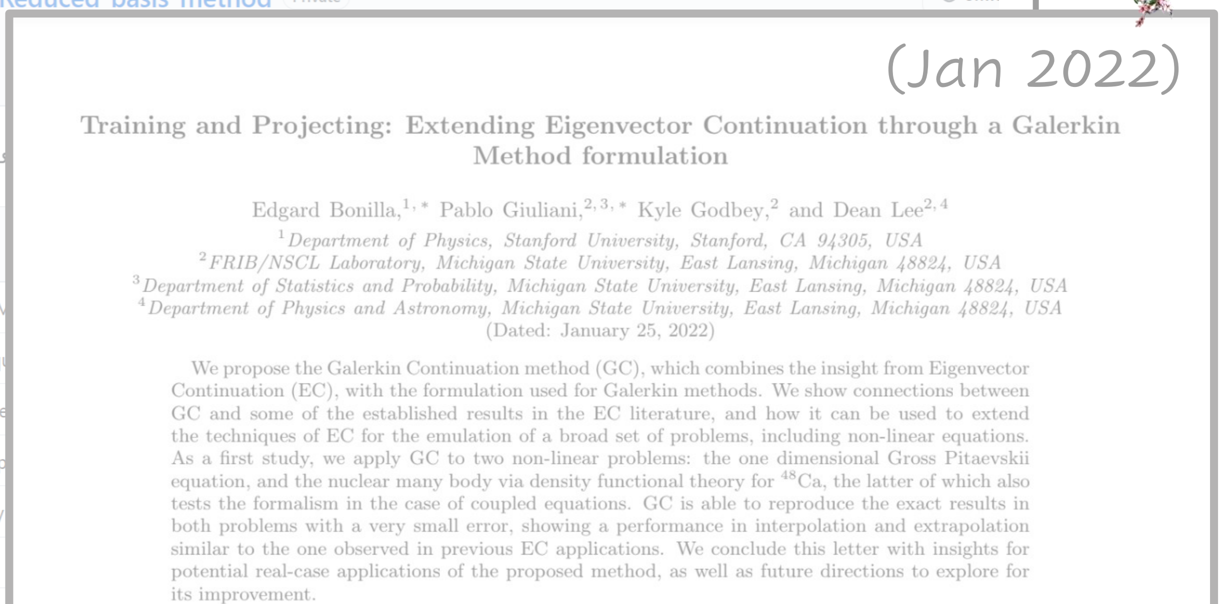
~~Why~~ Uncertainty Quantification?

How → *Communication with experts*

This is very important to us



(Jan 2022)



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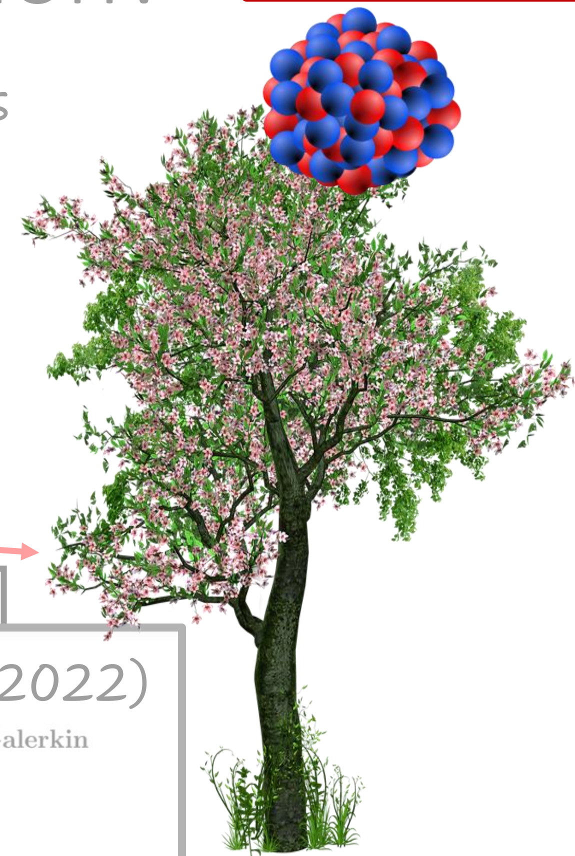


Outline

Why

Uncertainty Quantification?

How

The Reduced Basis Method

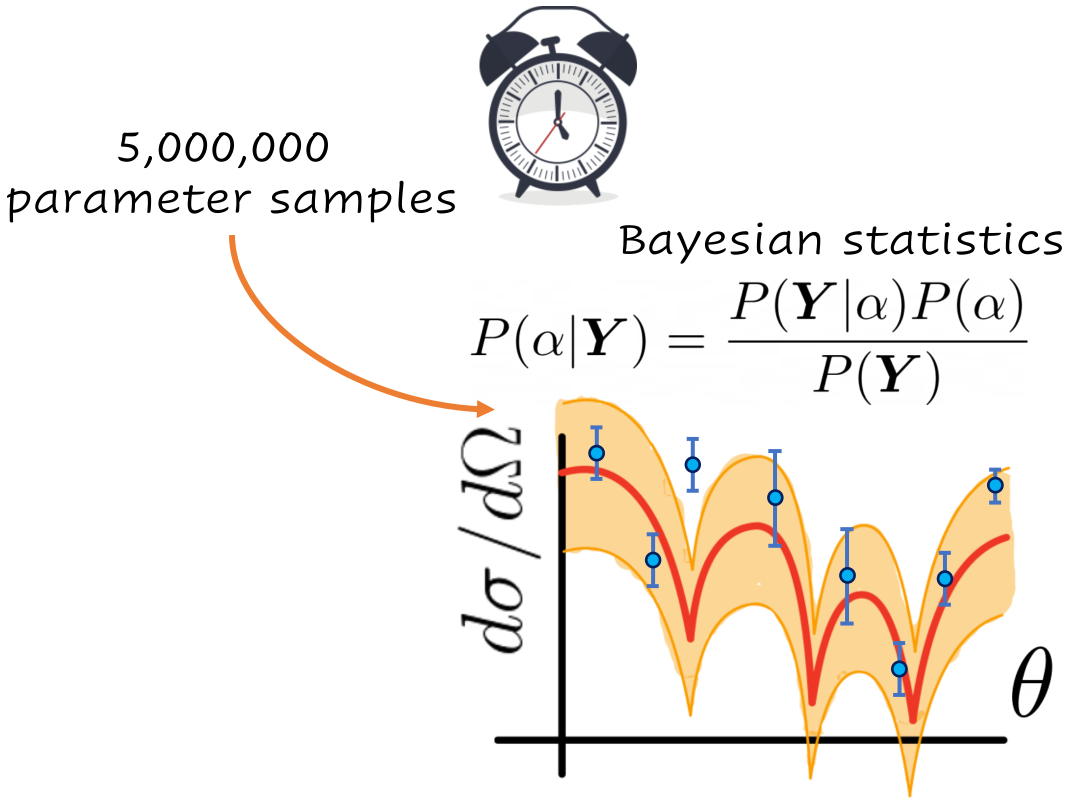
How it works

Applications and Results

Upcoming Highlights

Takeaways

Emulators



5,000,000
parameter samples
Bayesian statistics
$P(\alpha|\boldsymbol{Y}) = \frac{P(\boldsymbol{Y}|\alpha)P(\alpha)}{P(\boldsymbol{Y})}$
$d\sigma/d\Omega$
θ

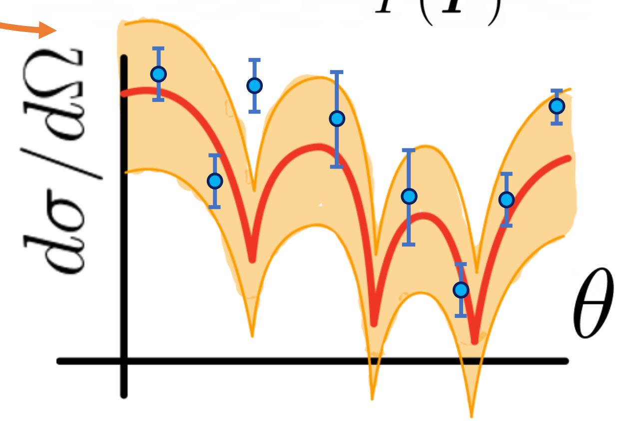
$$f(\alpha, x) \longrightarrow \hat{f}(\alpha, x)$$

"Exact" "Emulated"

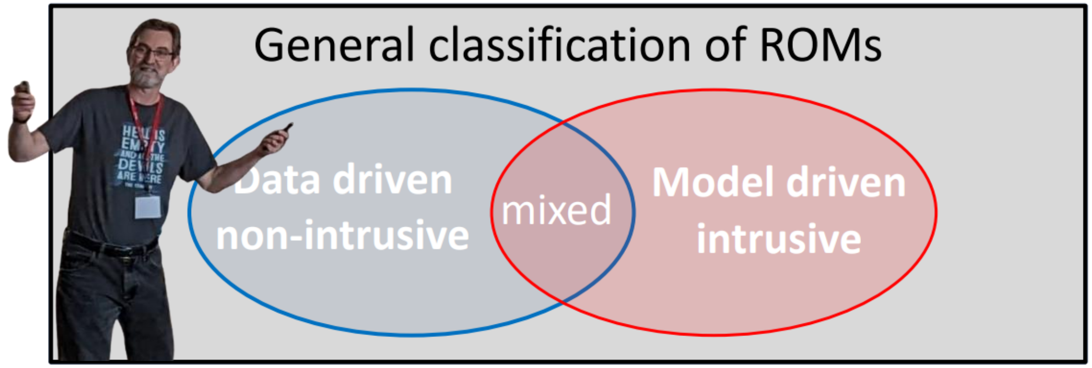
5,000,000
parameter samples

Bayesian statistics

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



Emulators



Dick's talk this morning

High fidelity computation → Emulator

Emulator → Gaussian Process

Emulator → Neural Networks

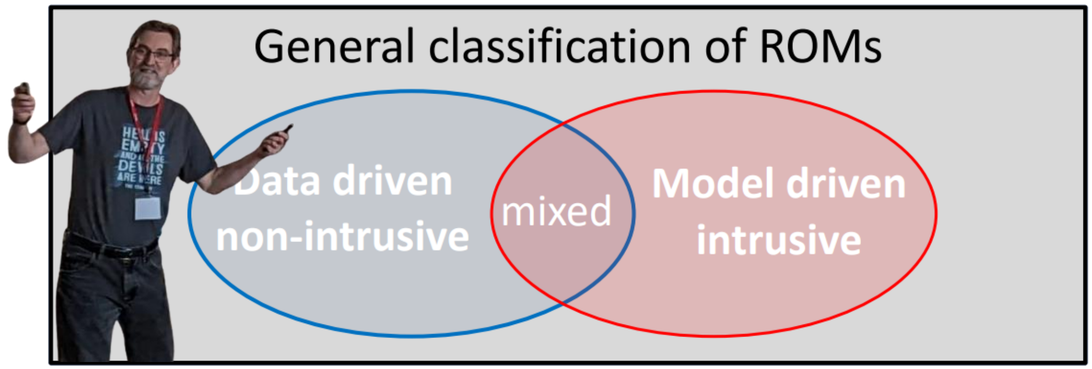
Emulator → Reduced Basis Method


→



→


Emulators



Dick's talk this morning

High fidelity computation → Emulator

Emulator → Gaussian Process

Emulator → Neural Networks

Emulator → Reduced Basis Method

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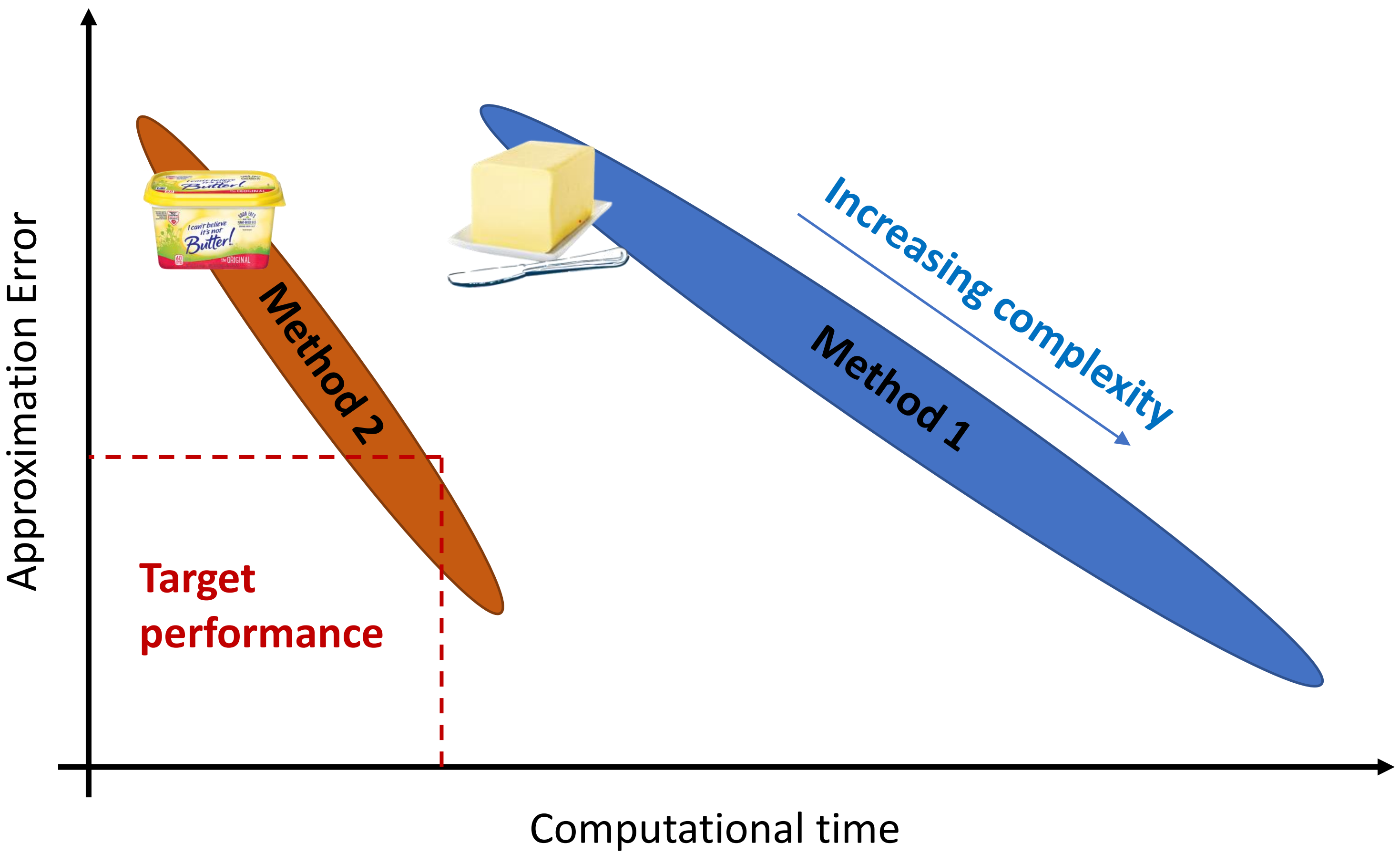
Reduced Order Models

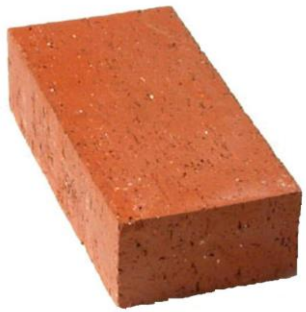
Reduced Basis Method

Computation Accuracy vs Time

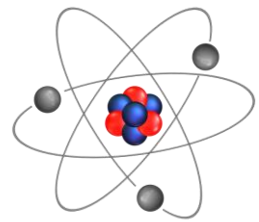


The Reduced Basis Method

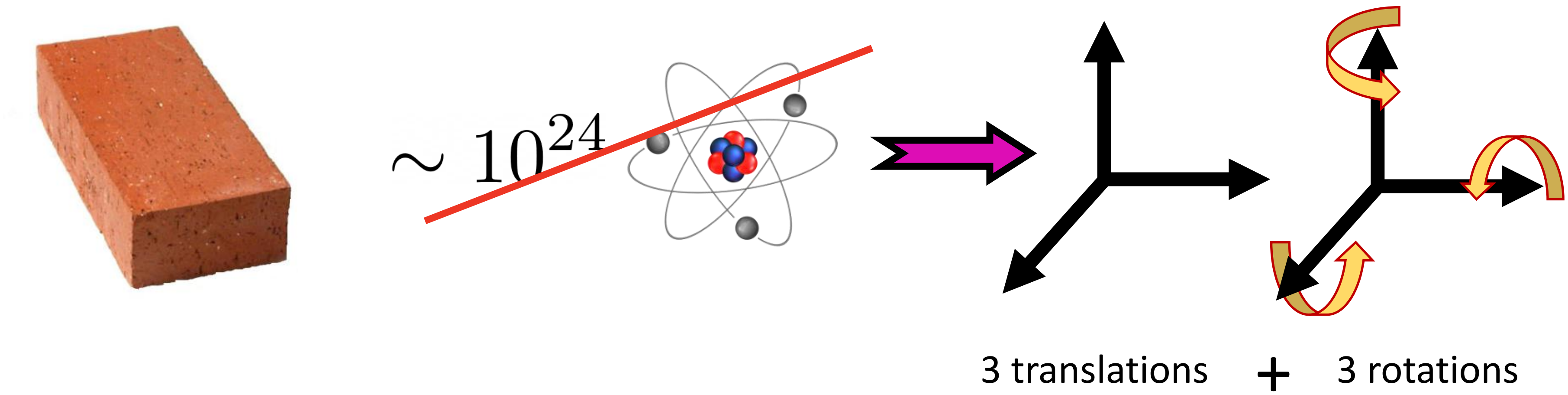
The Reduced Basis Method



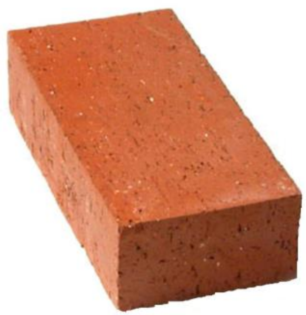
$\sim 10^{24}$



The Reduced Basis Method



The Reduced Basis Method



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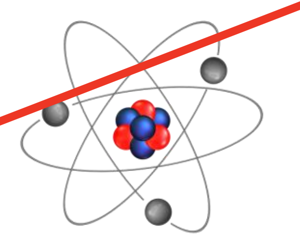
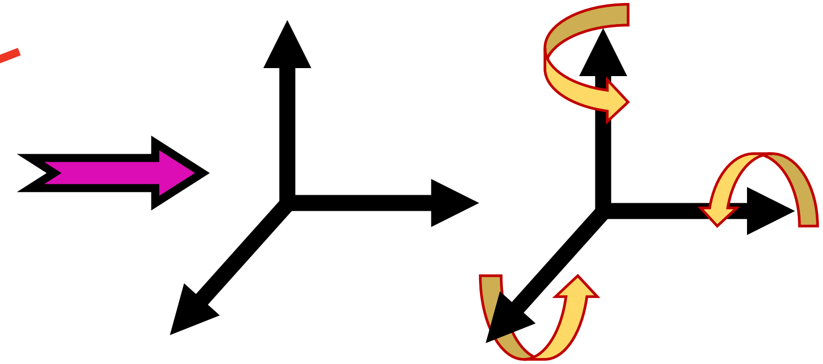
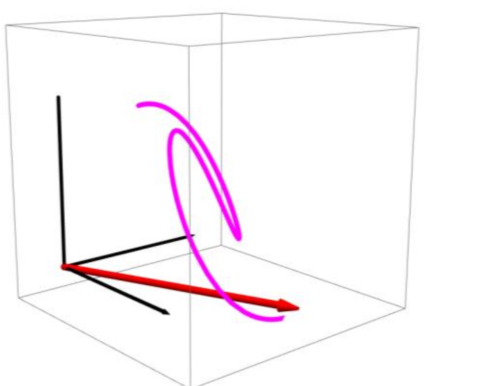


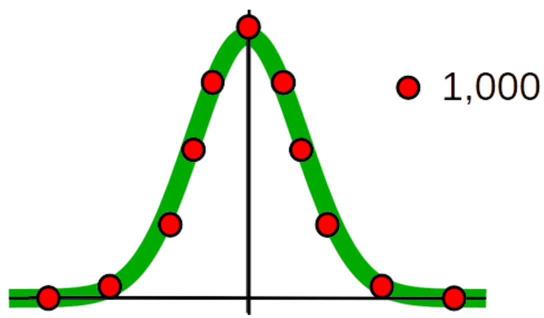


3 translations + 3 rotations

parameters

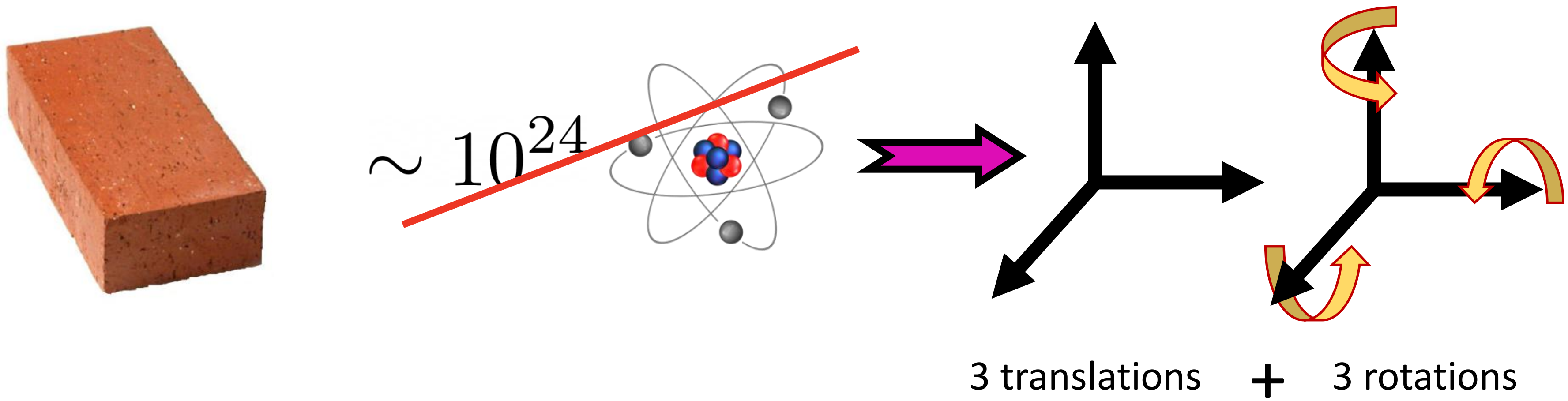
$$\mathcal{H}_\alpha \phi(x) = \lambda \phi(x)$$





Finite element

The Reduced Basis Method



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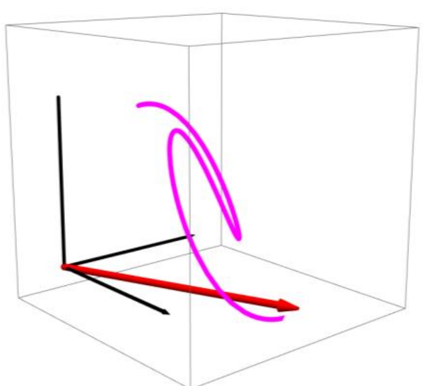

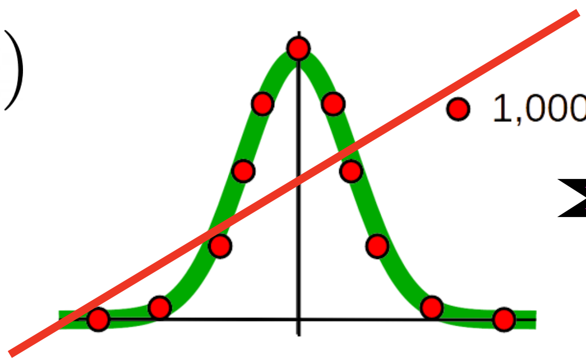

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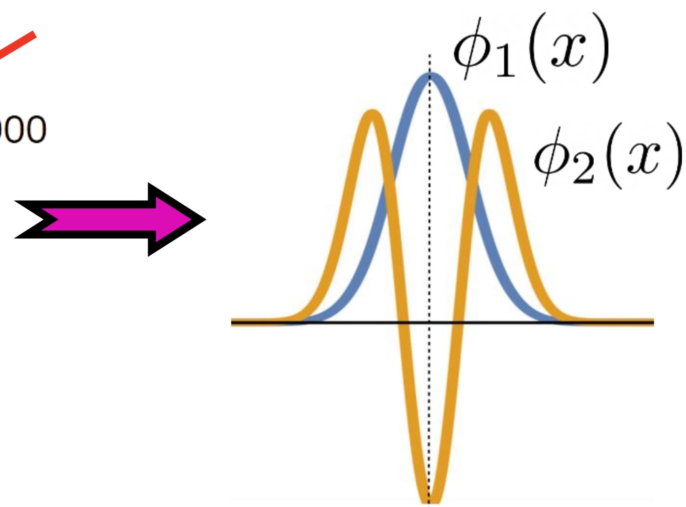
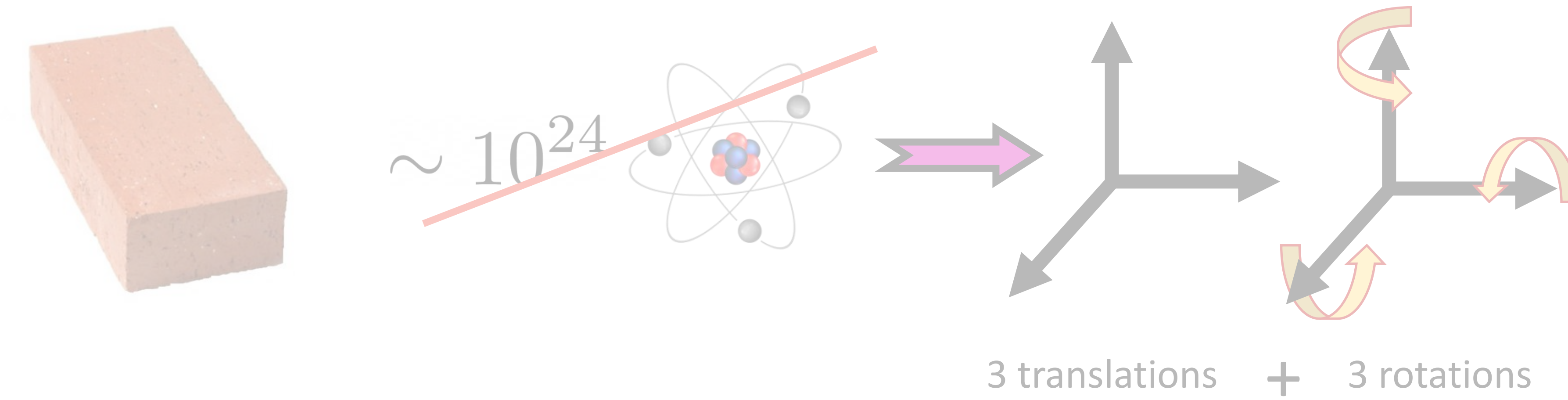
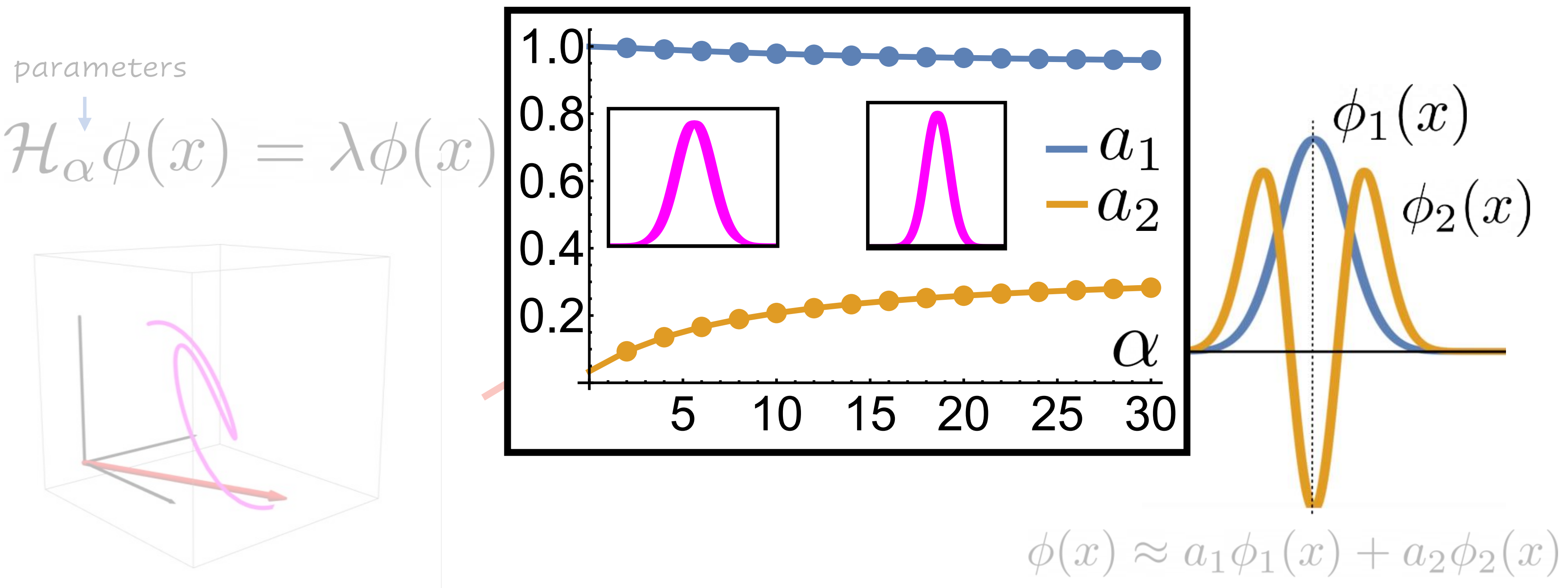
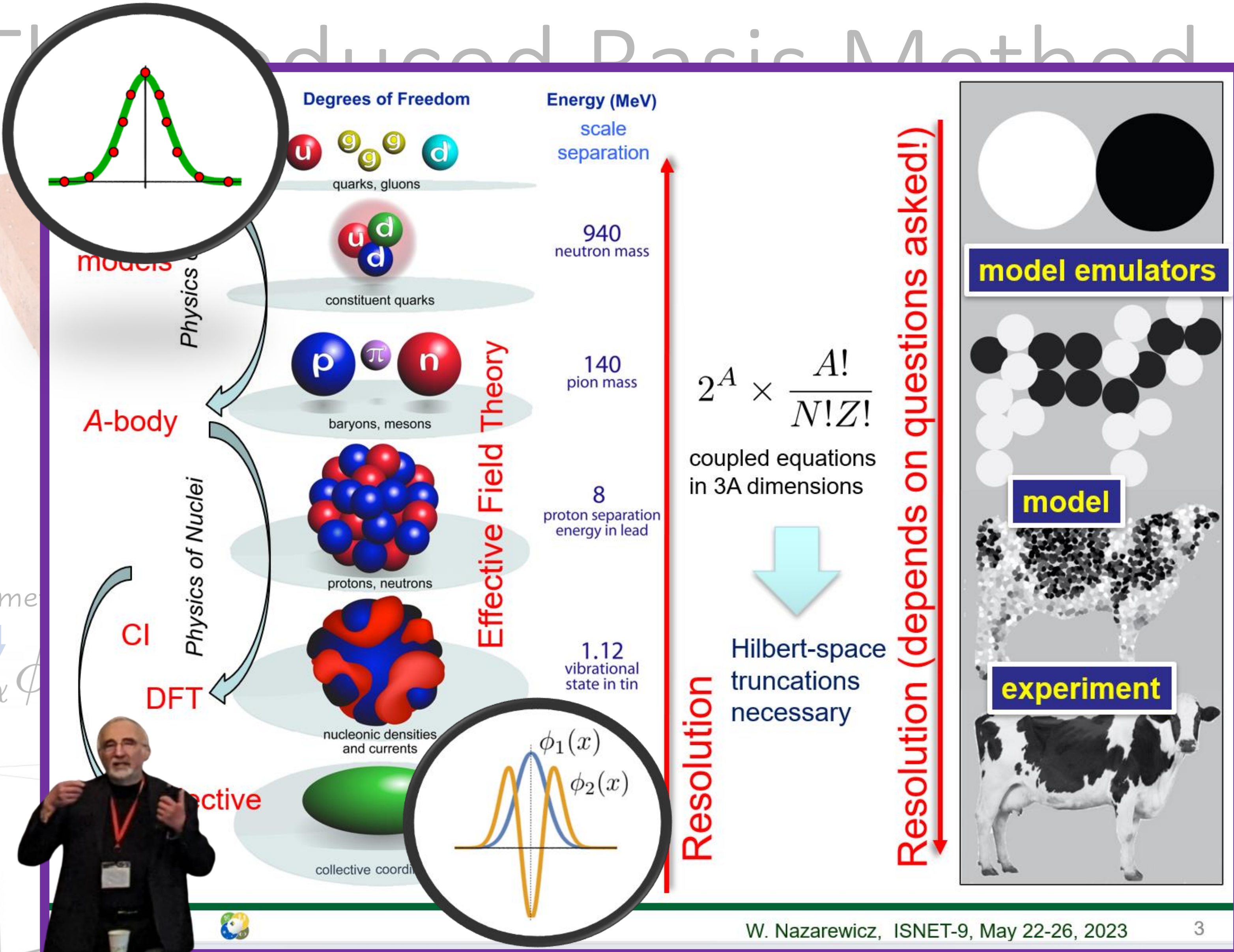


$$\phi(x) \approx a_1\phi_1(x) + a_2\phi_2(x)$$

The Reduced Basis Method



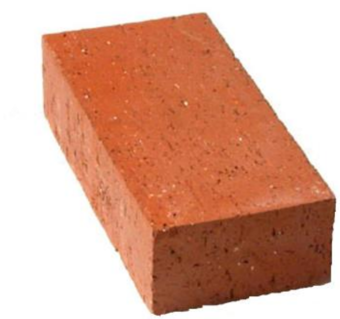


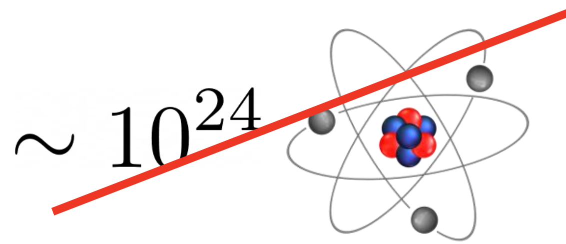


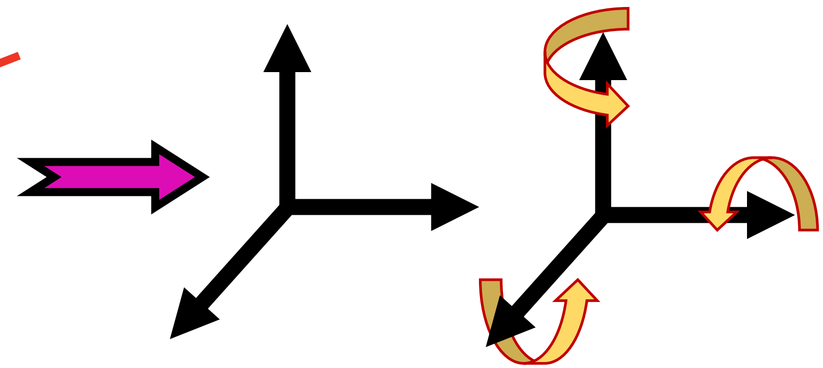
Witek's talk yesterday

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

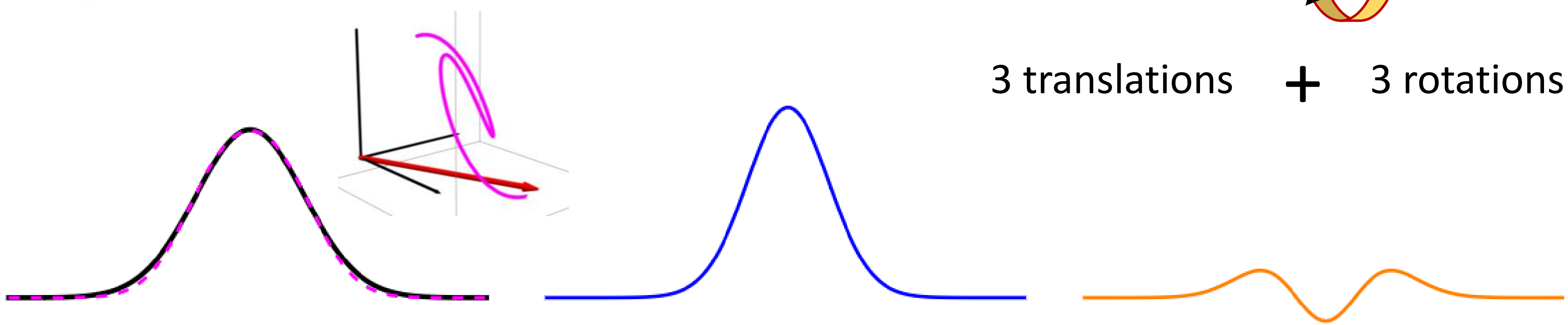
The Reduced Basis Method







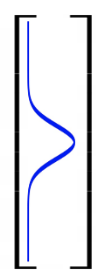
3 translations + 3 rotations



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

— $\phi(x)$

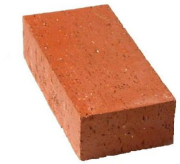
- - $\hat{\phi}(x)$

a_1 

a_2 

Changing the trapping strength α

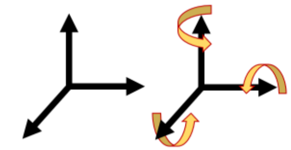
The Reduced Basis Method



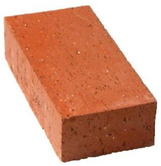
$$F_\alpha[\phi(x)] = 0$$

General differential equation

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



The Reduced Basis Method



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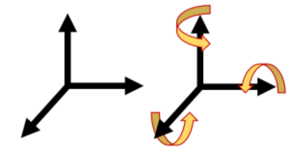
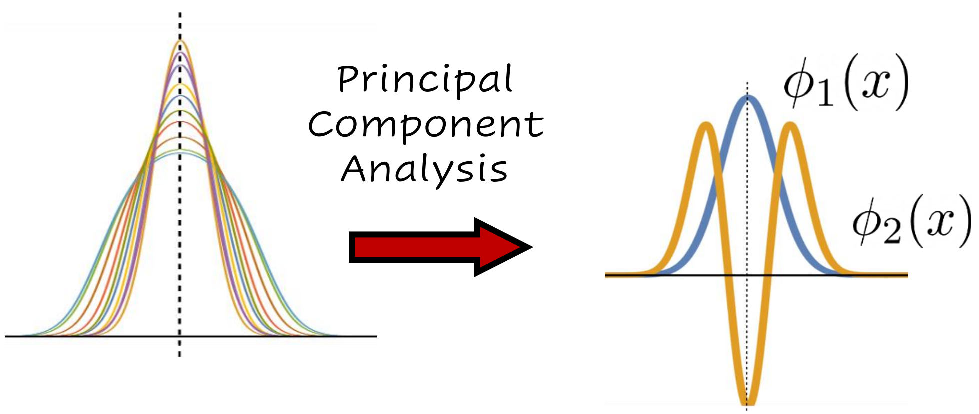
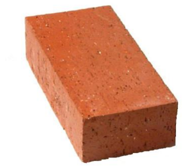


1) Choose a basis

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



The Reduced Basis Method



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General differential equation

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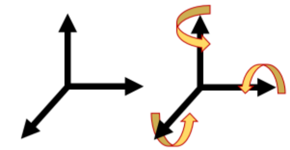

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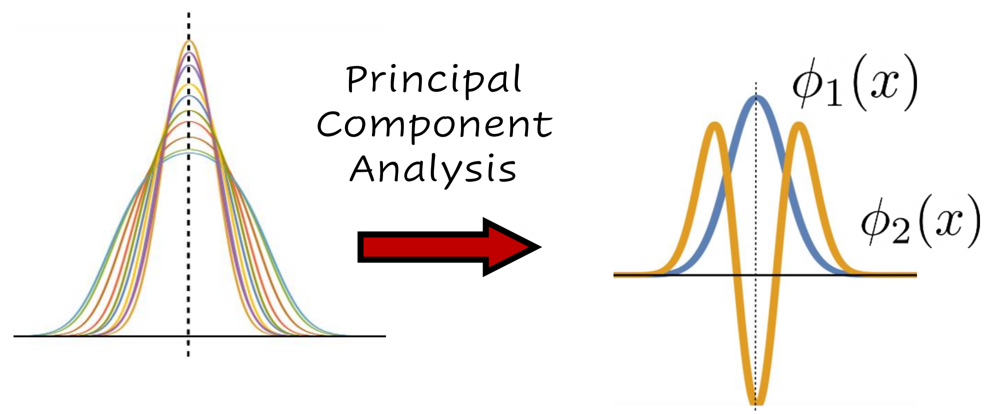
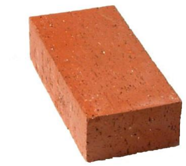


2) Project onto judges

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

One equation per coefficient

The Reduced Basis Method



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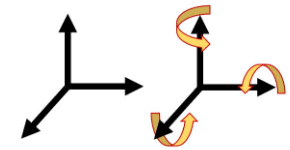

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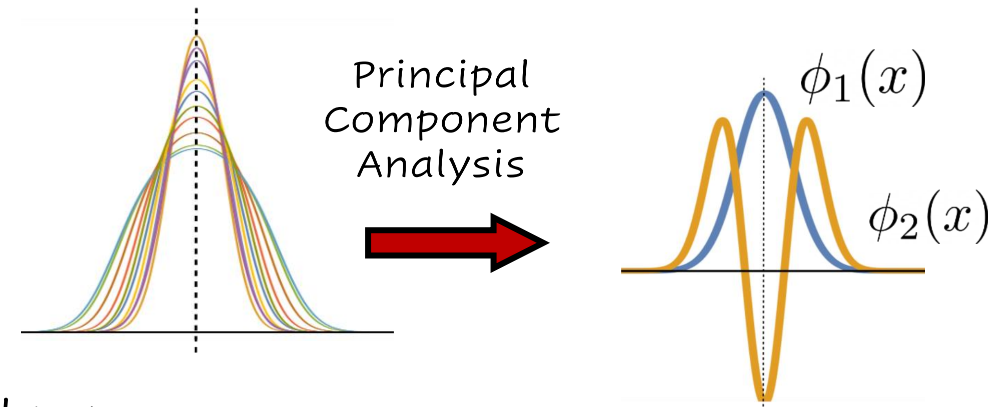


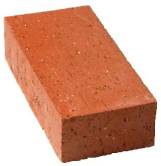
2) Project onto judges

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



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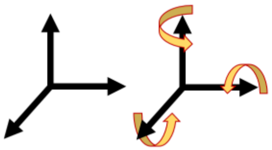

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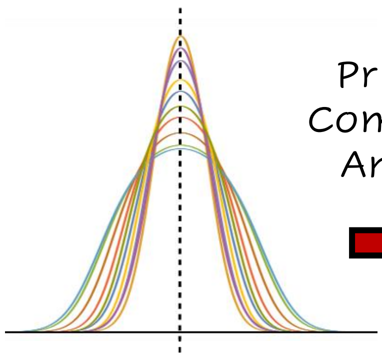
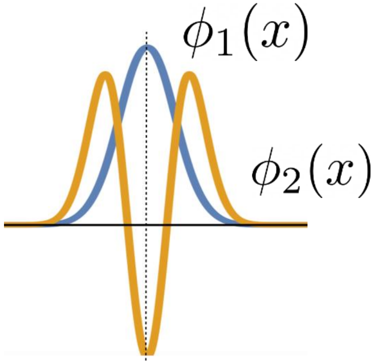


Principal Component Analysis



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

One equation per coefficient

WHY?
(ask me)

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

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, Colu... United States of America

[2] Facility for Rare Isotope Beams, Michigan State Univer... United States of America

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

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

BUQEYE Guide to Projection-Based Emulators in Nuclear Physics

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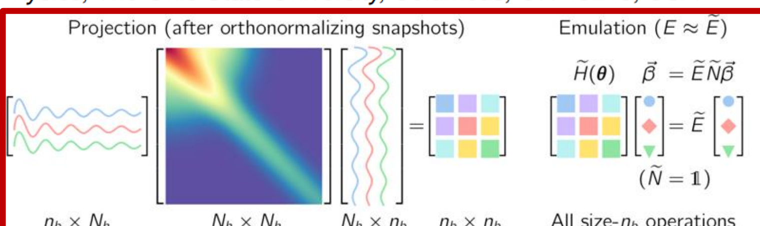
[2] *Facility for Rare Isotope Beams, Michigan State University, MI 48824, USA*

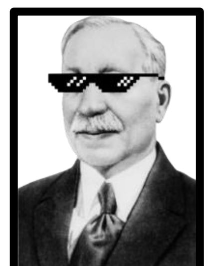
[3] *Department of Physics, The Ohio State University, Columbus, OH 43210, USA*



BAND
Bayesian Analysis of Nuclear Dynamics

and friends!

Training and Projecting



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

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

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Applications and Results

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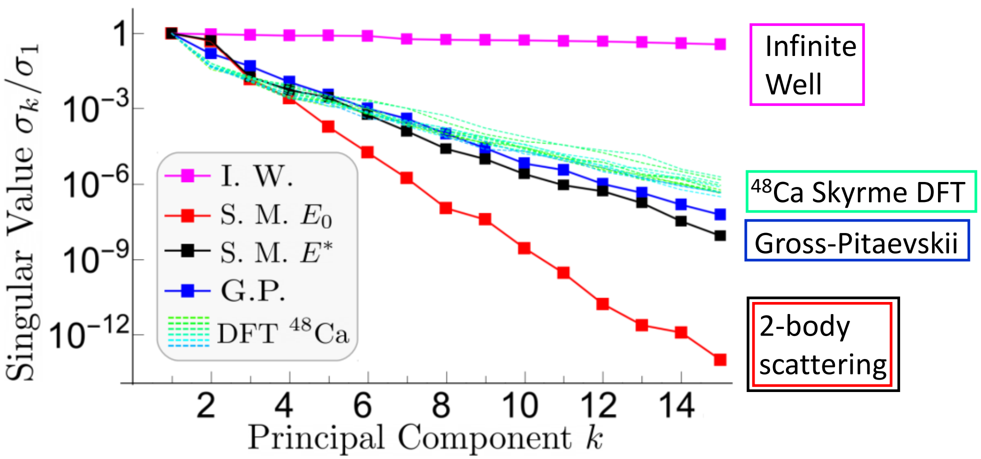
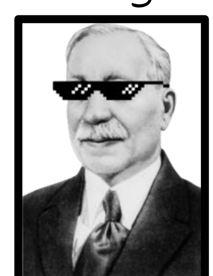
1) Broadly Applicable



Training and Projecting



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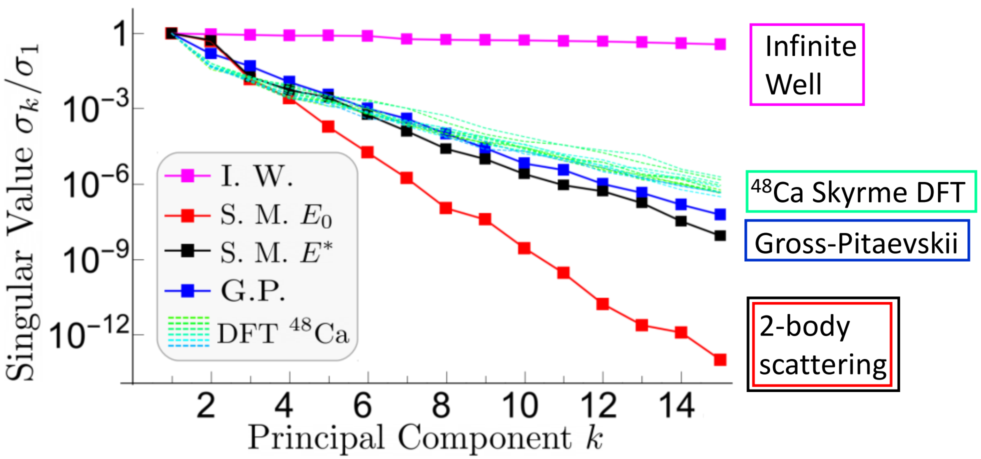
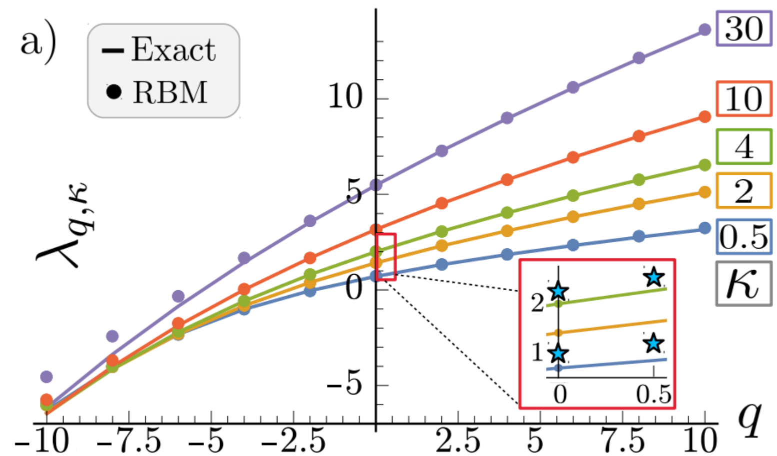
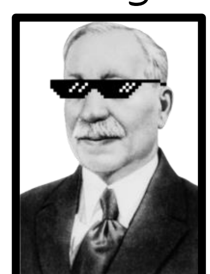


2) Very accurate



Training and Projecting



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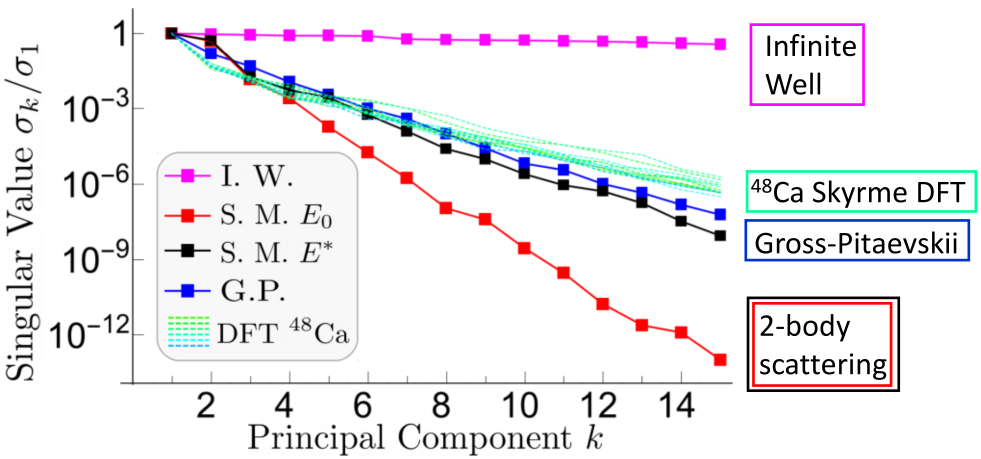

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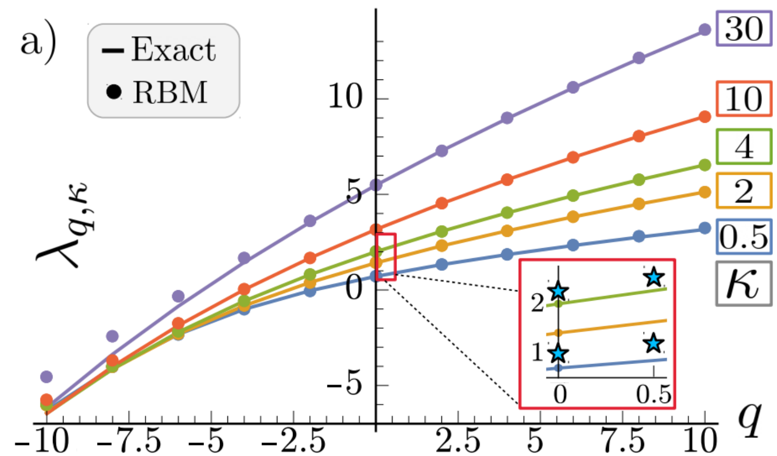
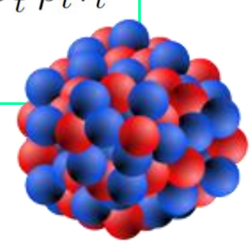


3) Very fast

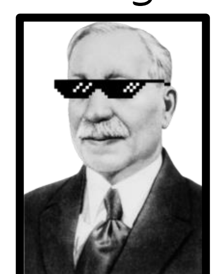
Skyrme Density Functional

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



Mili-seconds

Training and Projecting



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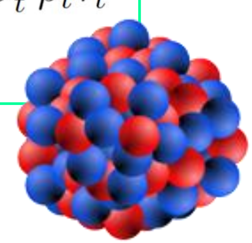

Mili-seconds

Training and Projecting

VERY non-linear

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

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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

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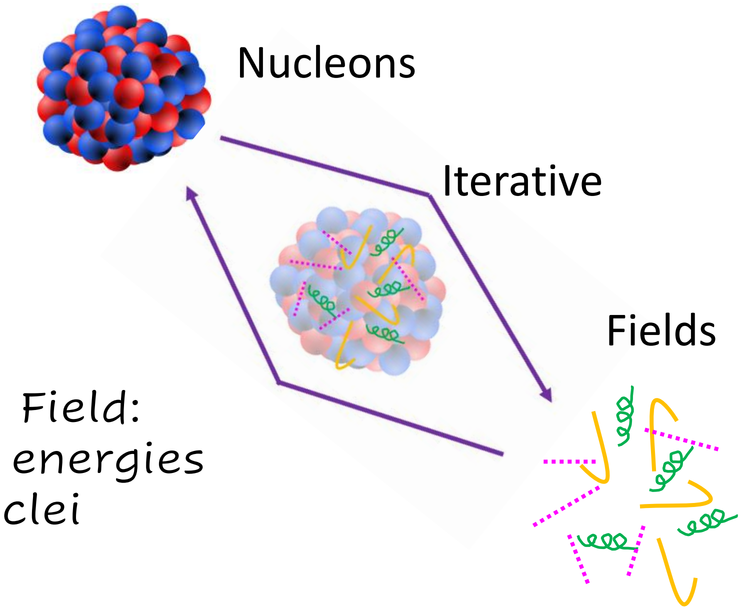
Pablo Giuliani,[1,2,*] Kyle Godbey,[1,†] Edgard Bonilla,[3,‡] Frederi Viens,[2,4,§] and Jorge Piekarewicz[5,¶]



Relativistic Mean Field:
wave functions and energies
of spherical nuclei

Bayes goes fast

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Applications and Results

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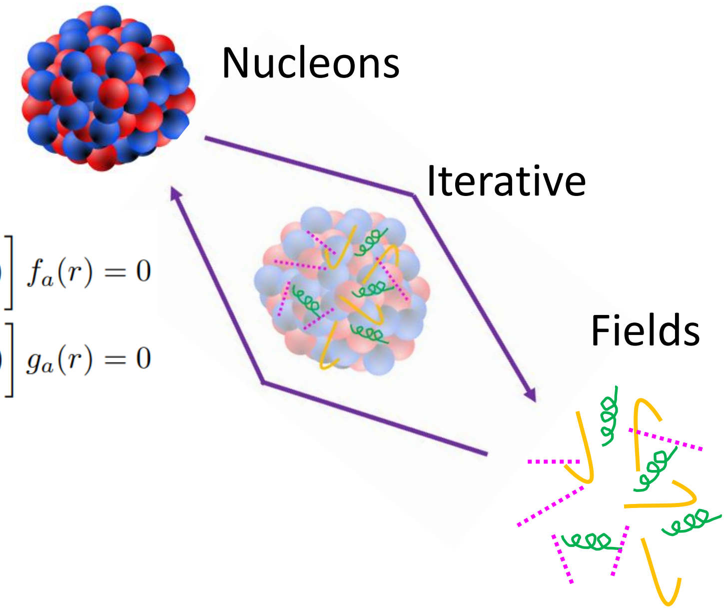

Dirac Equations

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

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

Field Equations

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

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

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

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Bayes goes fast

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Applications and Results

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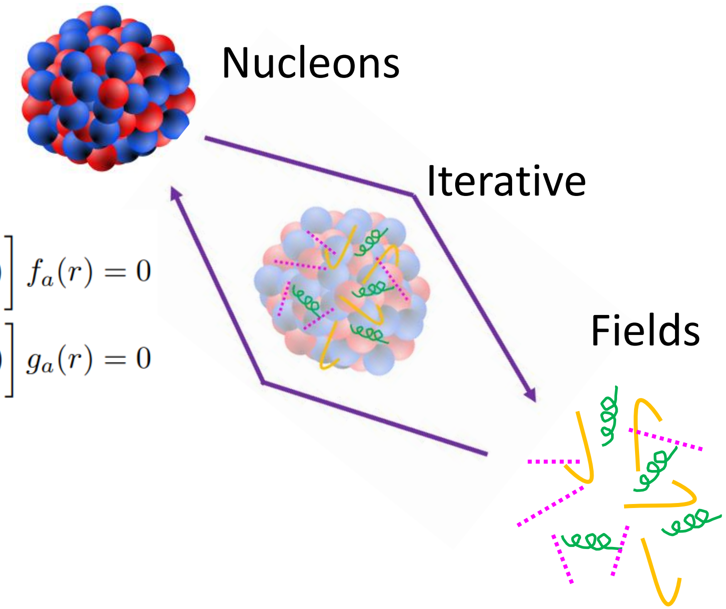

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$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_\rho^2\right)B_0(r)-2\Lambda_{\rm v}g_\rho^2W_0^2(r)B_0(r)=-\frac{g_\rho^2}{2}\big(\rho_{\rm v,p}(r)-\rho_{\rm v,n}(r)\big),$$
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Parameters α

Bayes goes fast

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Applications and Results

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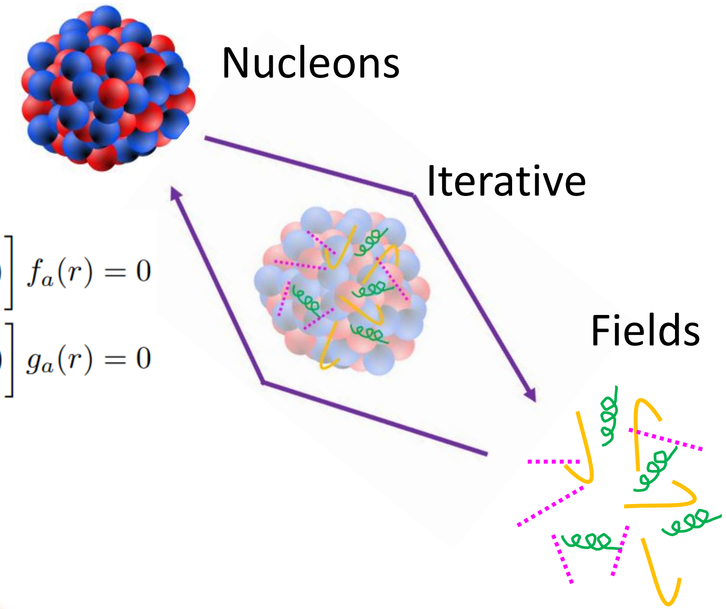

Dirac Equations

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Field Equations

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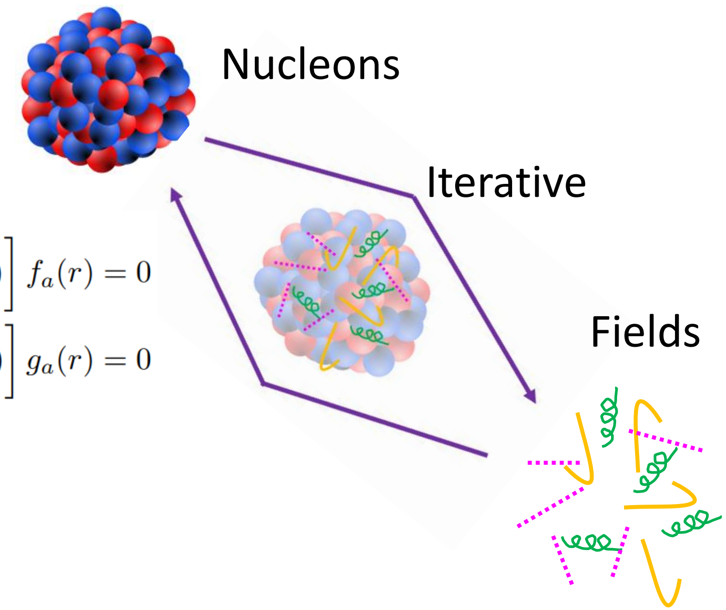

Dirac Equations

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

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

Field Equations

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

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

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

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

Bayes goes fast

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Applications and Results

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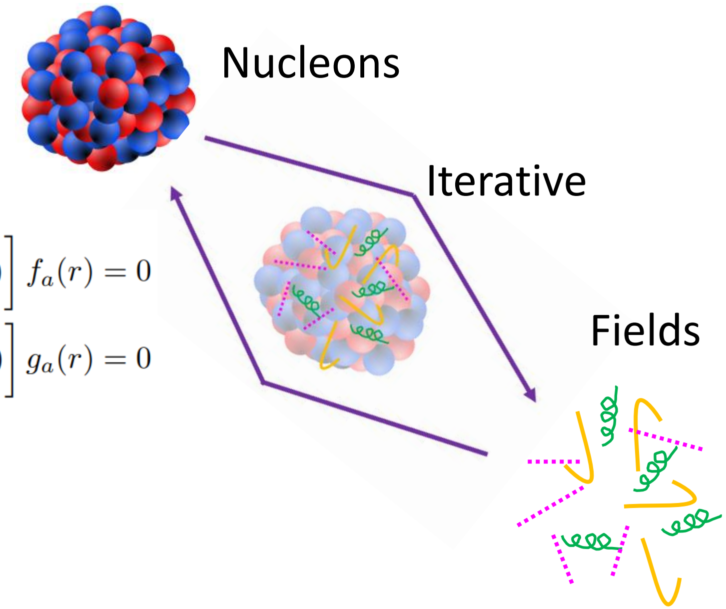


Dirac Equations

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

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

Field Equations

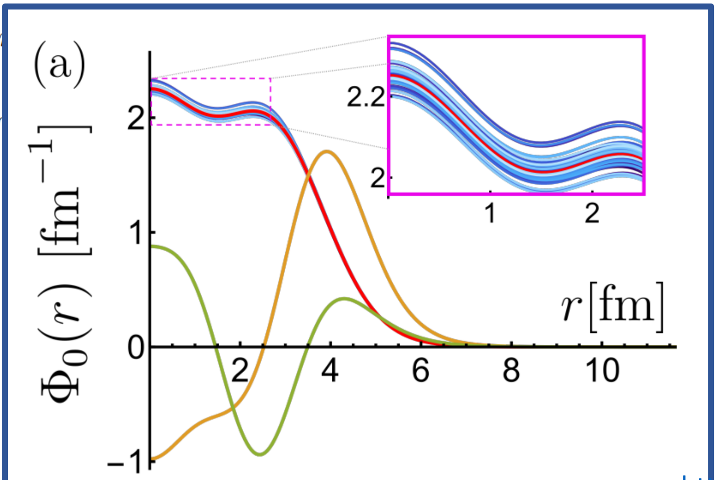
$$\langle \Phi_j(r)| \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_s^2\right)\boxed{\Phi_0(r)} - g_s^2\left(\frac{\kappa}{2}\boxed{\Phi_0^2(r)} + \frac{\lambda}{6}\Phi_0^3(r)\right) = -g_s^2\left(\rho_{s,p}(r)+\rho_{s,n}(r)\right),$$

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

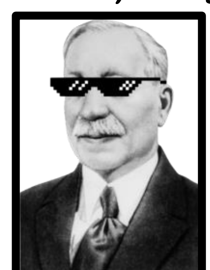
$$\langle B_j(r)| \left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-m_\rho^2\right) B_0(r) - 2\Lambda_v g_\rho^2 W_0^2(\ldots$$

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

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



Bayes goes fast



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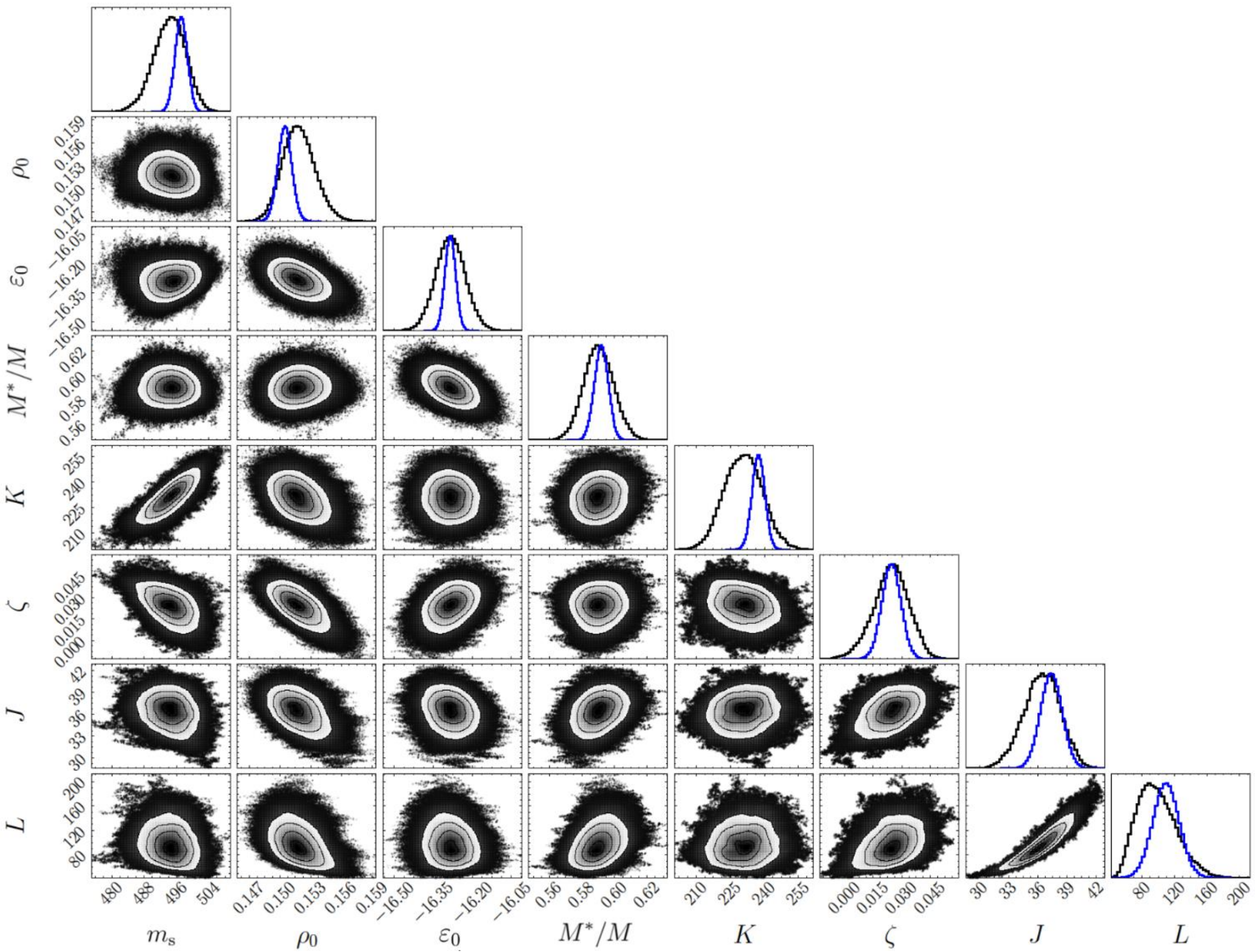
Applications and Results

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,¶]

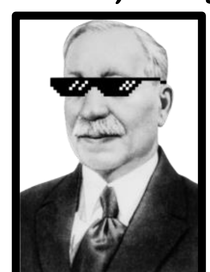
Posterior Bayesian calibration



Masses and Charge radii

^{16}O
^{40}Ca
^{48}Ca
^{68}Ni
^{90}Zr
^{100}Sn
^{116}Sn
^{132}Sn
^{144}Sm
^{208}Pb

Bayes goes fast



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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**

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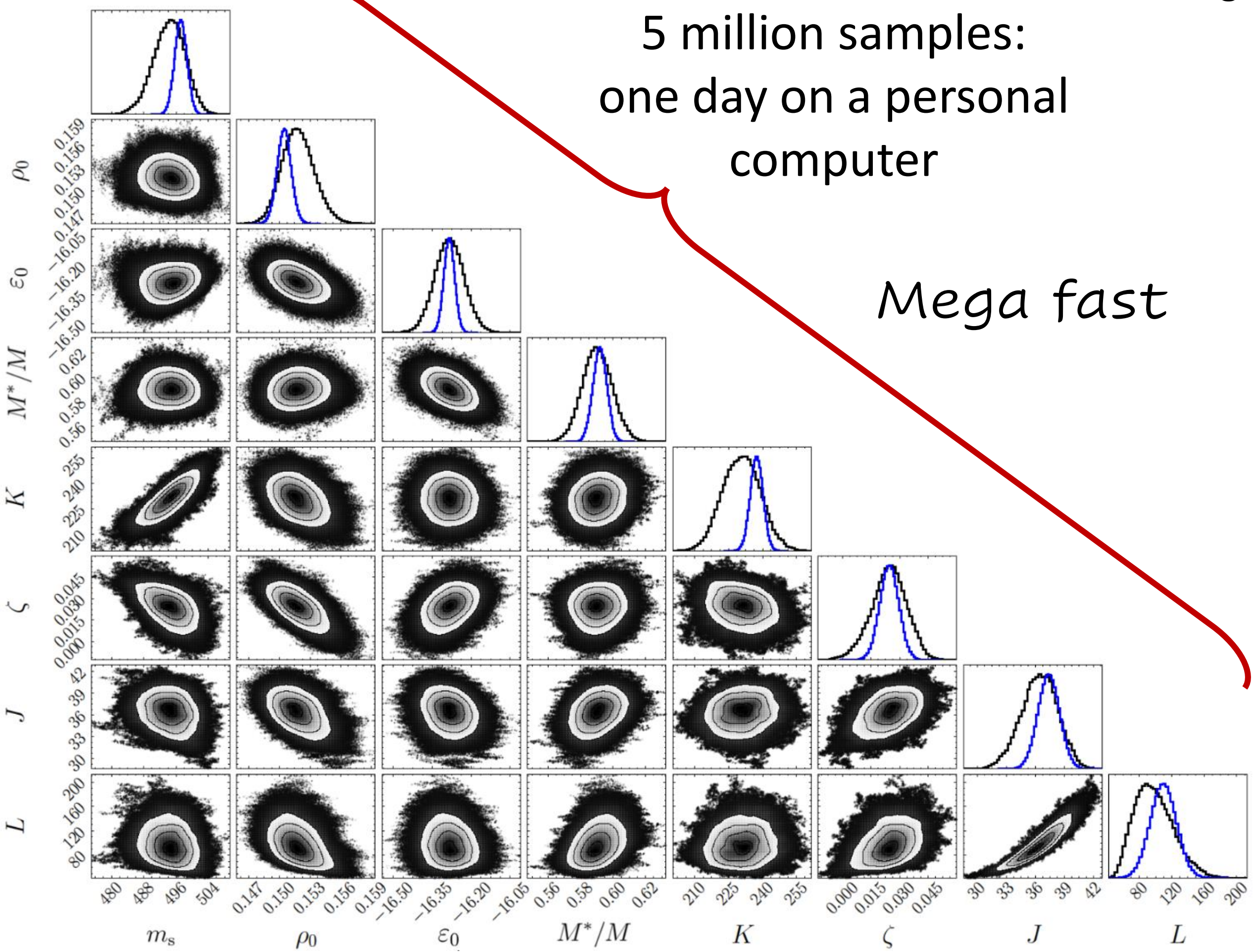

5 million samples: one day on a personal computer

Mega fast

Masses and Charge radii

^{16}O
^{40}Ca
^{48}Ca
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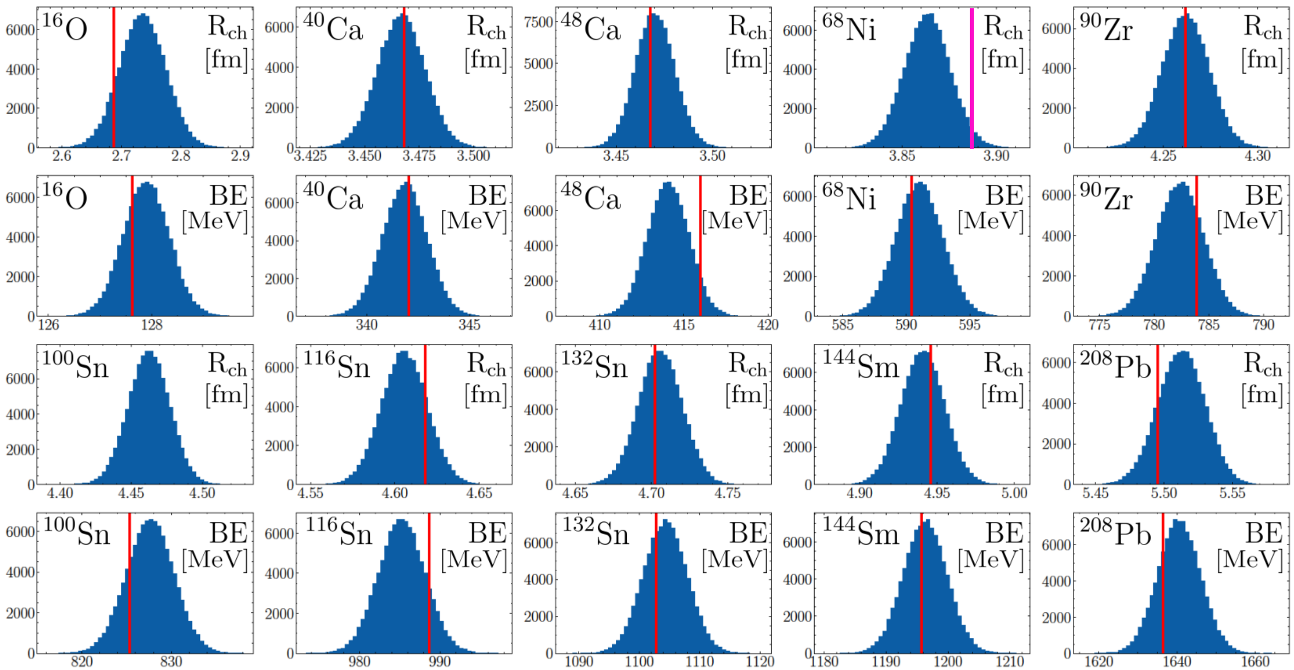

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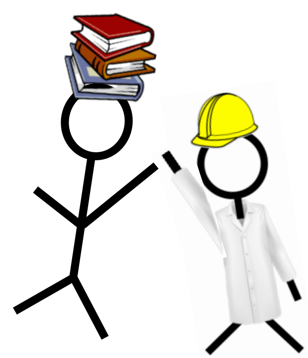
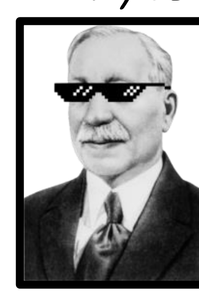
Masses and Charge radii



Bayes goes fast



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

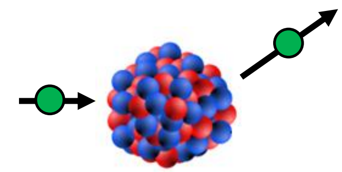
Applications and Results ❸

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

almost done....

Applications and Results ③

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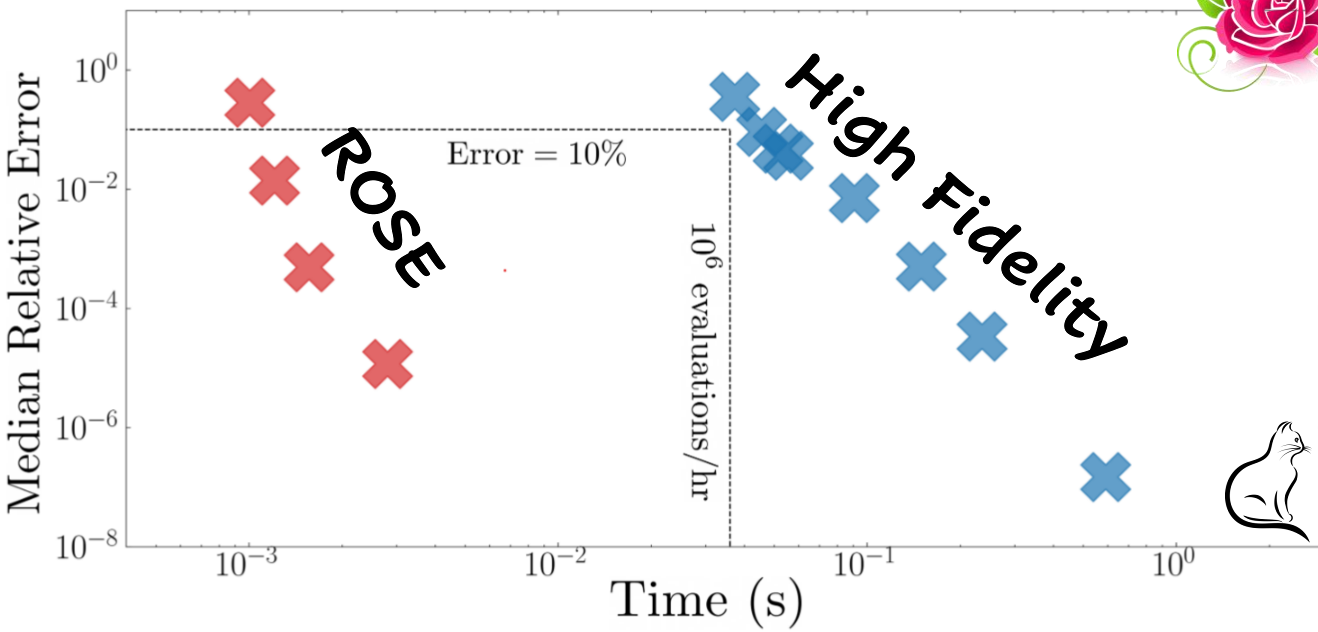

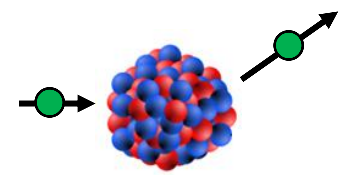

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Applications and Results ③

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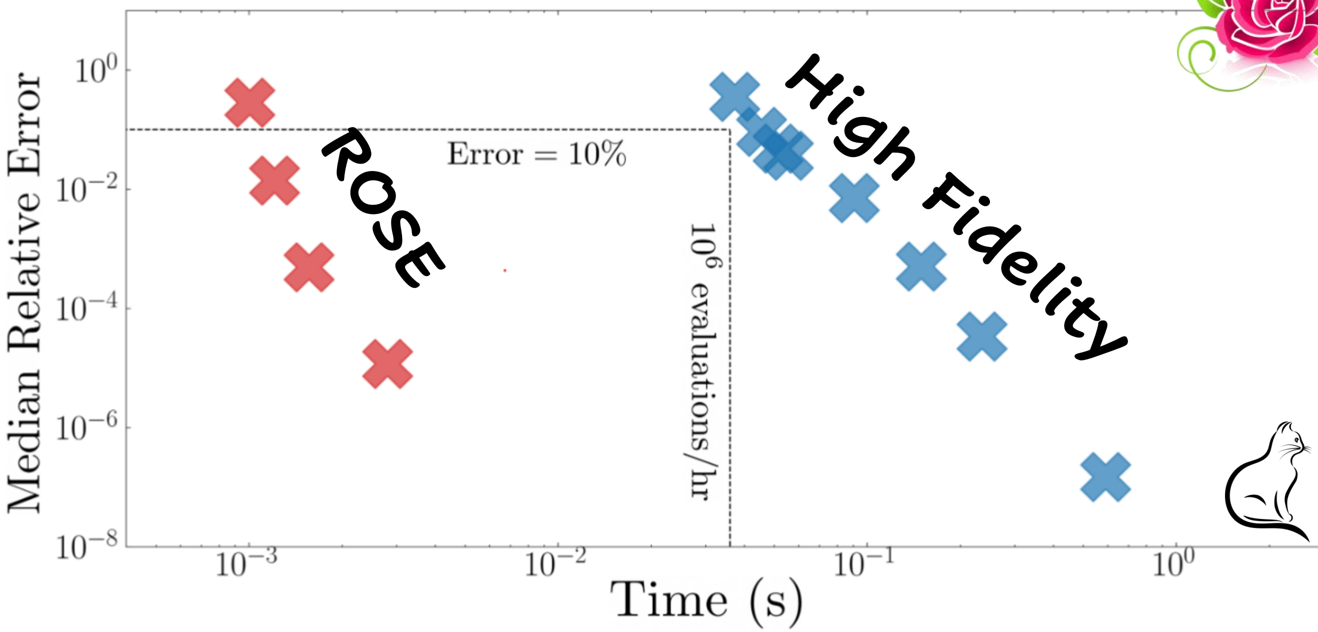

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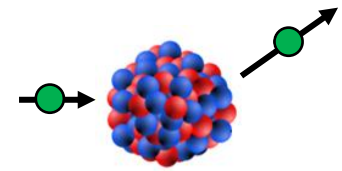

Cornerstones:

1) Free solution and principal components
2) Energy re-scaling (reference domain)
3) Non-affinity (Empirical Interpolation)

The roses

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Applications and Results ③

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Daniel Odell

Cornerstones:

Usually, a challenge

1) Free solution and principal components

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

2) Energy re- ... e domain)

3) Non-affinity (Empirical Interpolation)

The roses

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

Applications and Results

3

almost done....

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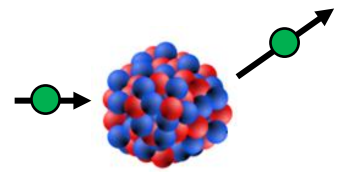

Optical Potential

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

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

The roses

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Applications and Results ③

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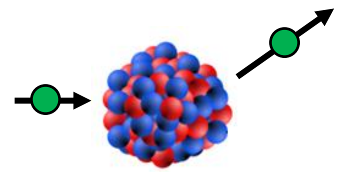

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The roses

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almost done....

Applications and Results ❸

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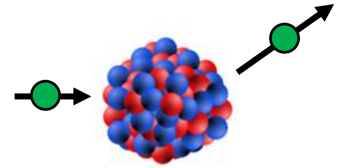

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Non-affine problem

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

The roses

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Applications and Results

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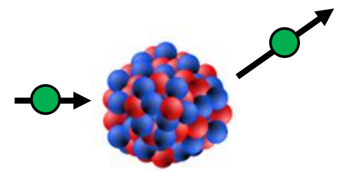

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$$\langle\psi_j|F_\alpha[\hat{\phi}(r)]\rangle = \int \psi_j(r)F_\alpha[\hat{\phi}(r)]dr = 0$$

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

Empirical Interpolation Method: one work-around

The roses

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Applications and Results ❸

almost done....

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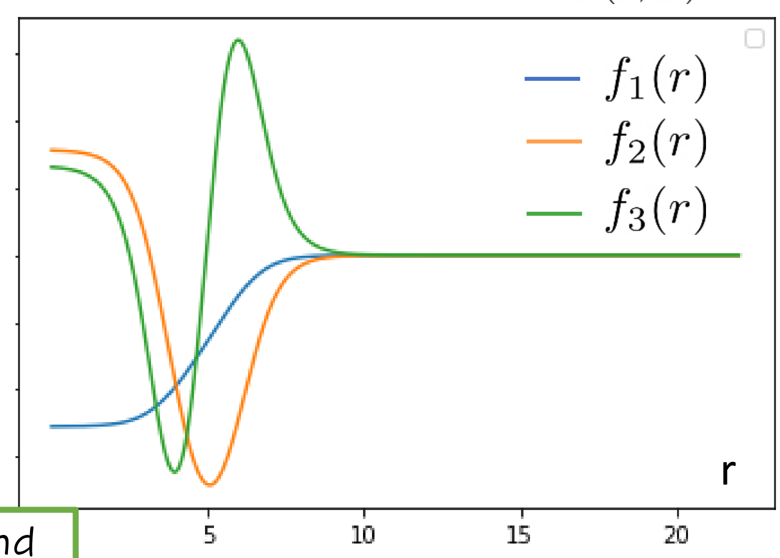
Principal components of $U(r,\alpha)$



1) Choose a basis

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

Empirical Interpolation Method: one work-around

almost done....

Applications and Results

3

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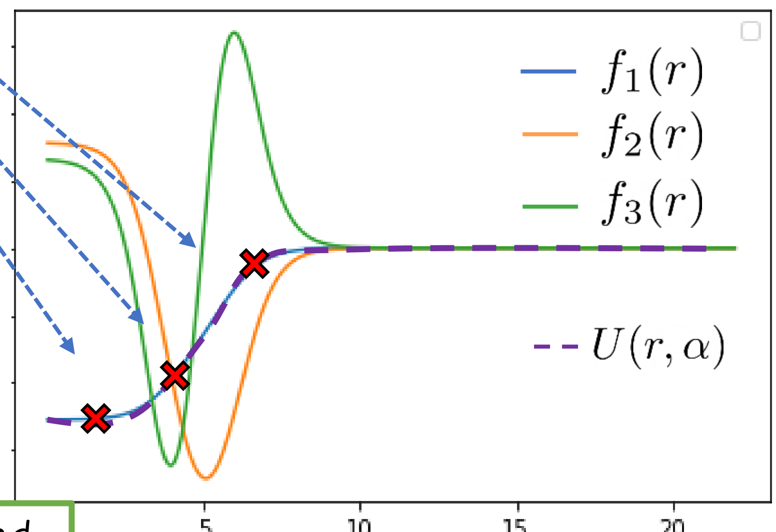
$$U(r_j, \alpha) - \sum_i^m b_i(\alpha) f(r_j) = 0$$

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

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



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Empirical Interpolation Method: one work-around

Applications and Results

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almost done....

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Dirac

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

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

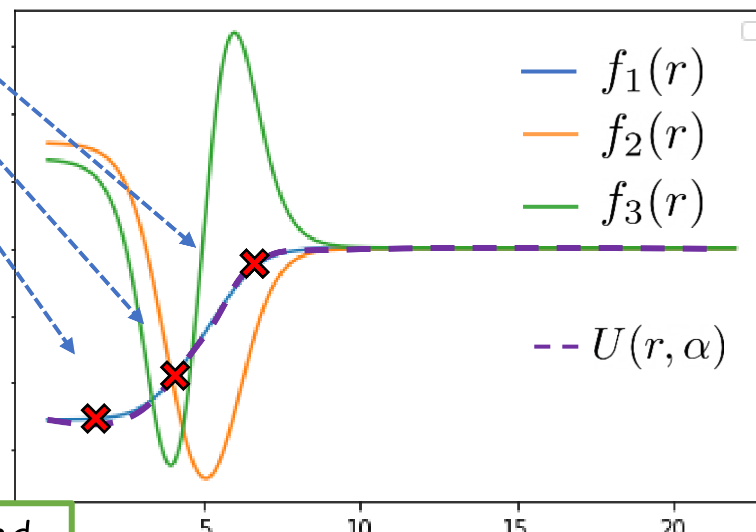
2) Project onto judges

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

Obtained by interpolation

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

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



1) Choose a basis

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Empirical Interpolation Method: one work-around

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]

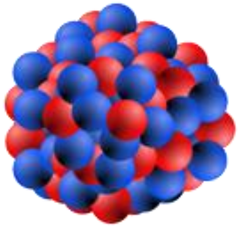
Coming soon

3) Very fast

Skyrme Density Functional

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

Mili-seconds



VERY non-linear

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

Applications and Results

4

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

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

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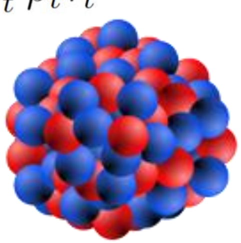

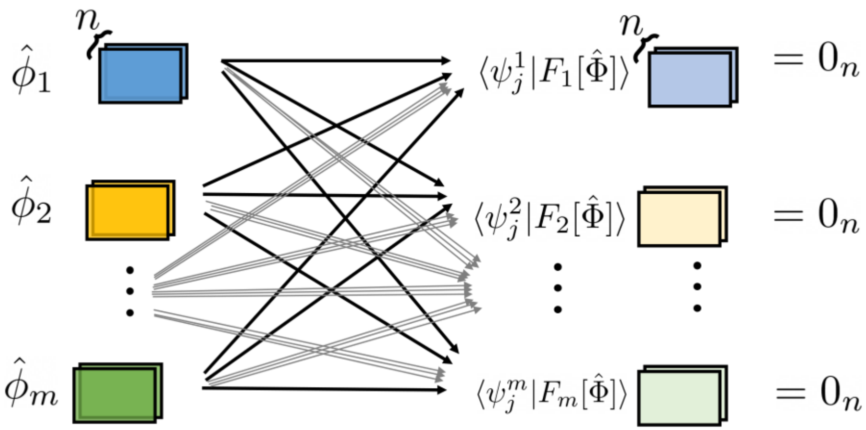

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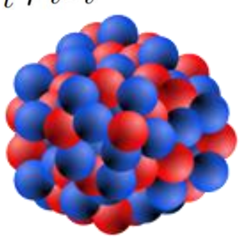
Skyrme Density Functional



Mili-seconds

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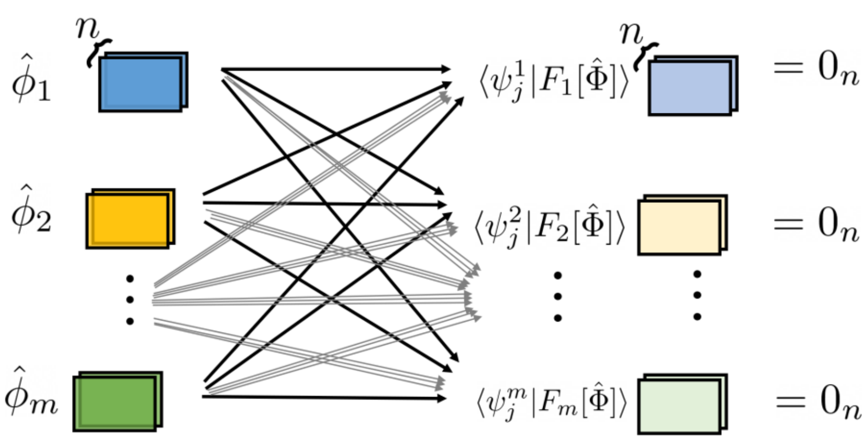
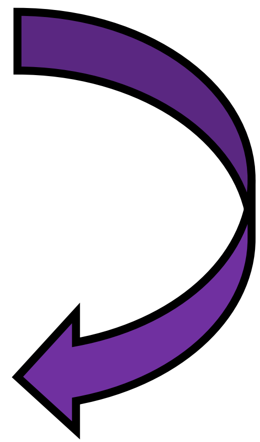
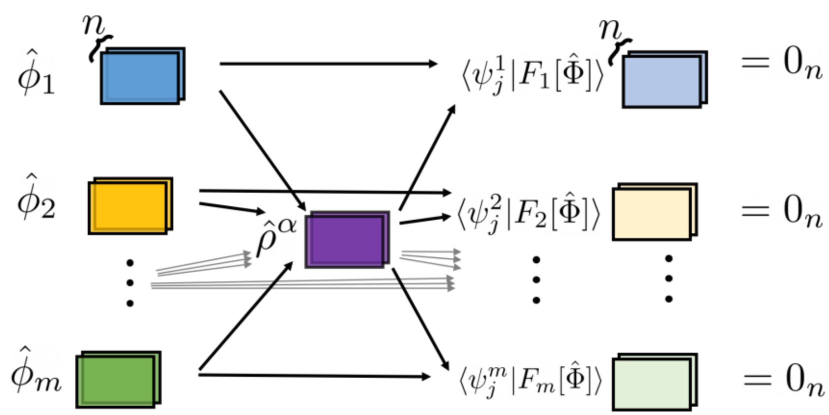




Faster



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

3) Very fast

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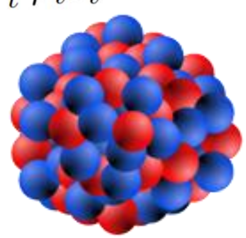
Mili-seconds



VERY non-linear

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

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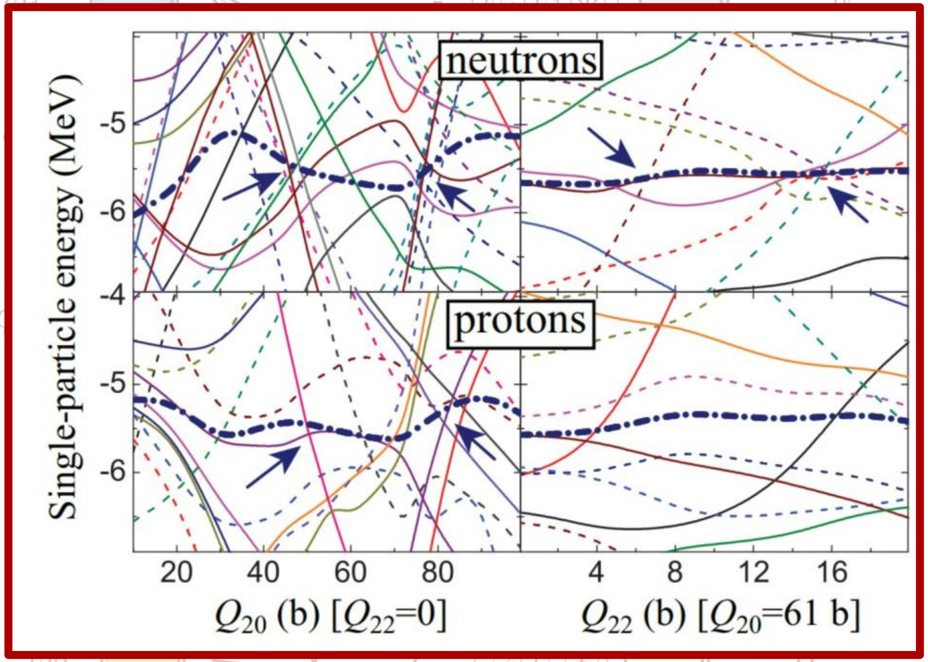
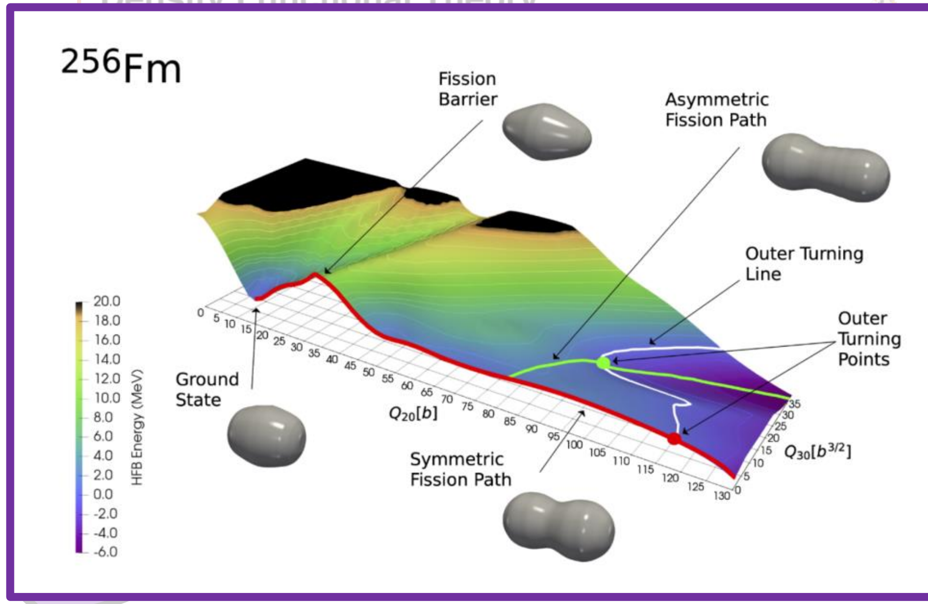


Level crossing is a problem



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

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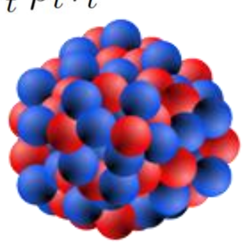

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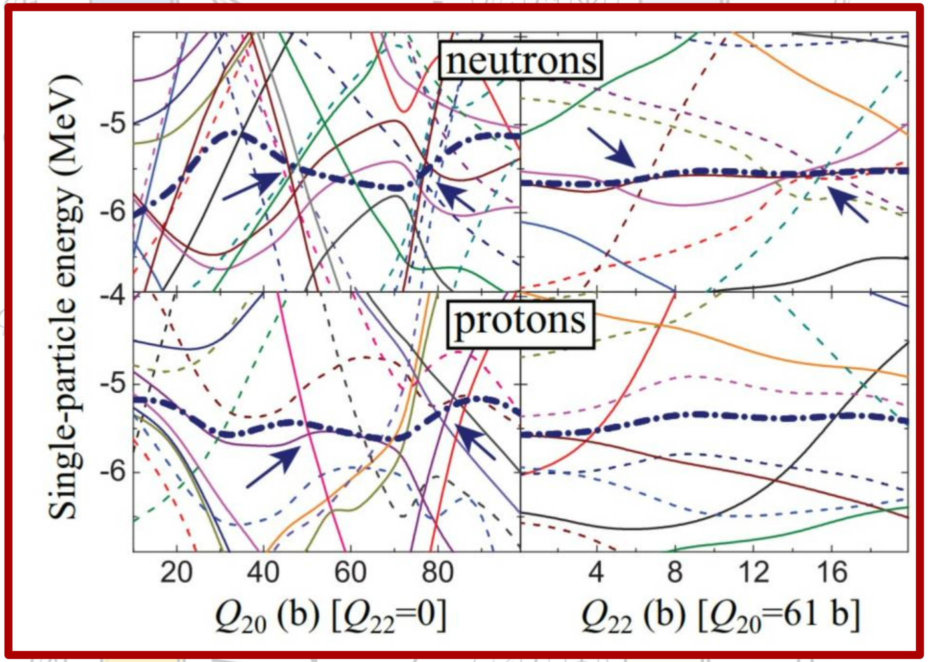

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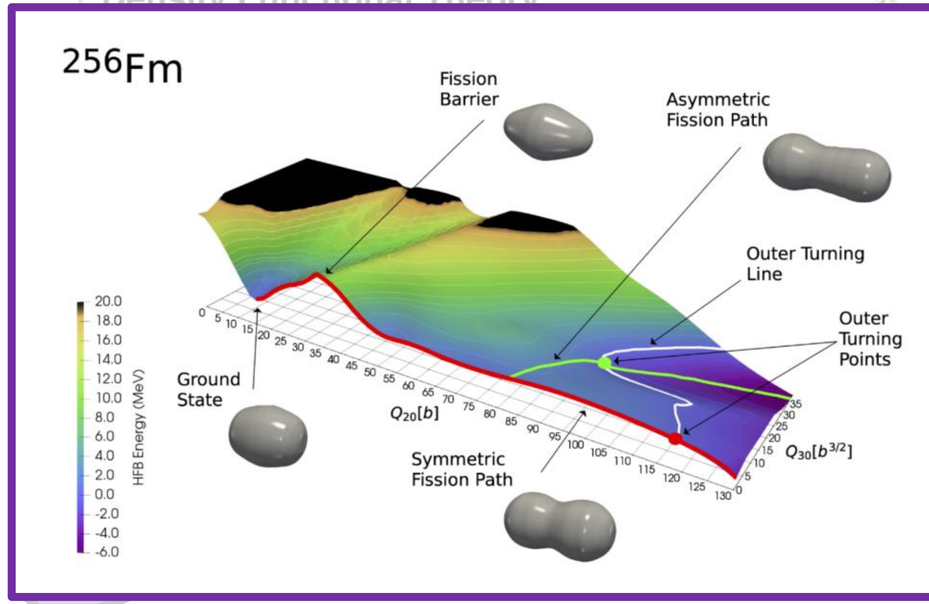

Fission is next

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

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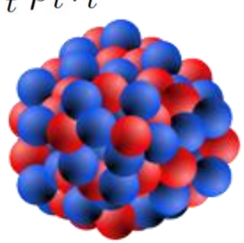

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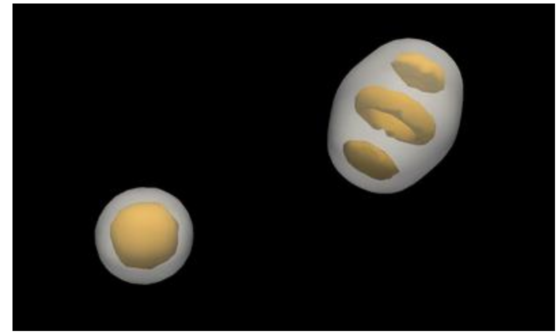
$$\rho(r)^\alpha$$

Applications and Results

5 Dynamical systems

(Time Dependent Density Functional Theory)

Kyle Godbey



big N

$$\frac{\partial}{\partial t}\phi(x,t) = -i\mathcal{H}_{\mathcal{N}\times\mathcal{N}}\phi(x,t)$$

$$\phi(x,t) \approx$$

$$\hat{\phi}(x,t) = \phi_0(x) + \sum_{k}^{n} a_k(t)\phi_k(x)$$

Projection

$$\langle\psi_j|$$

tiny n

$$\frac{d}{dt}a_j(t) = -i\mathcal{H}_{n\times n}\boldsymbol{a}(t)$$

$$e^{-it\mathcal{H}_{n\times n}}$$

Reduced dynamical system

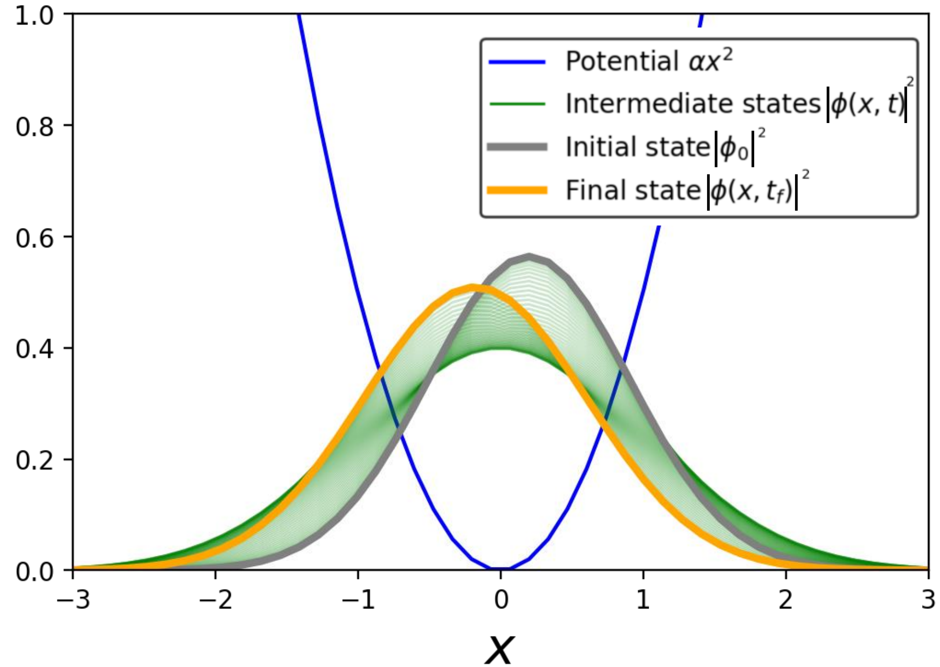
Size = n << N

Applications and Results

5 Dynamical systems

Quantum Harmonic Oscillator

$$\mathcal{H} = -\frac{\partial^2}{\partial x^2} + \alpha x^2$$



Applications and Results

5 Dynamical systems

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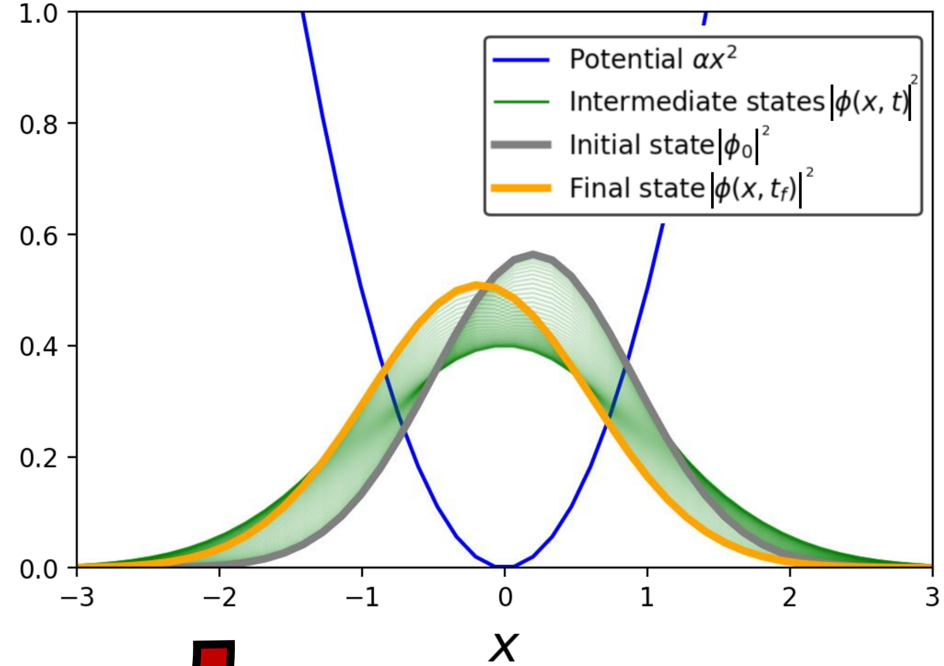
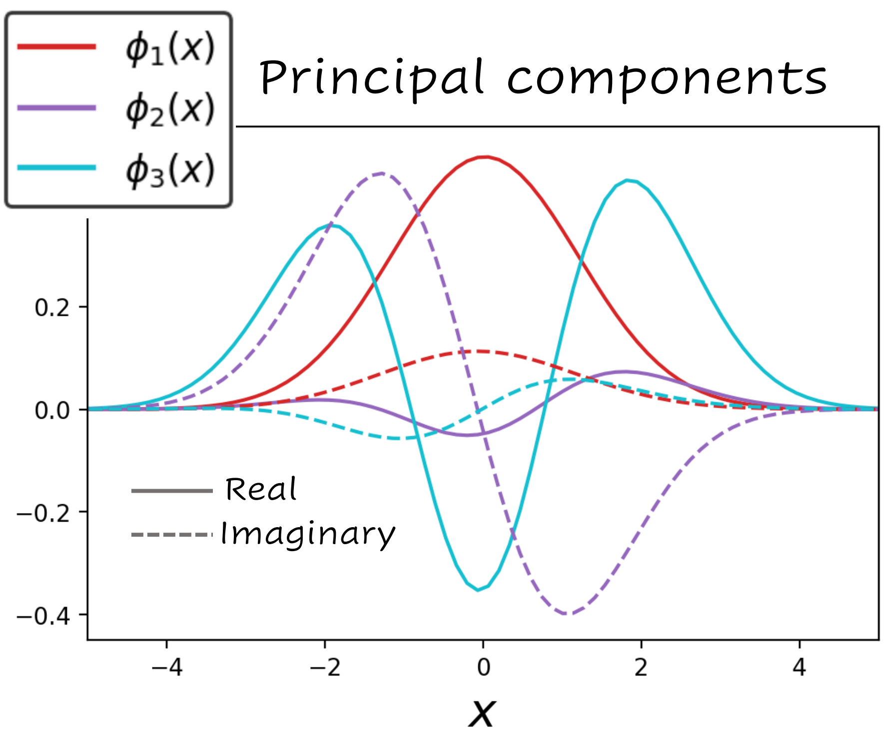


$$\hat{\phi}(x,t) = \sum_{k}^{n} a_k(t)\phi_k(x)$$

Principal components



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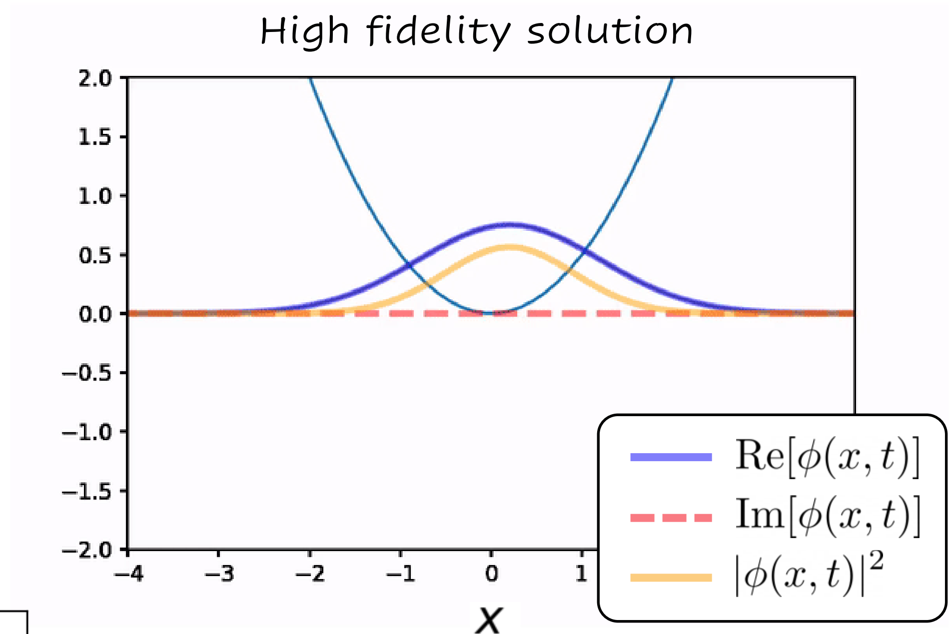

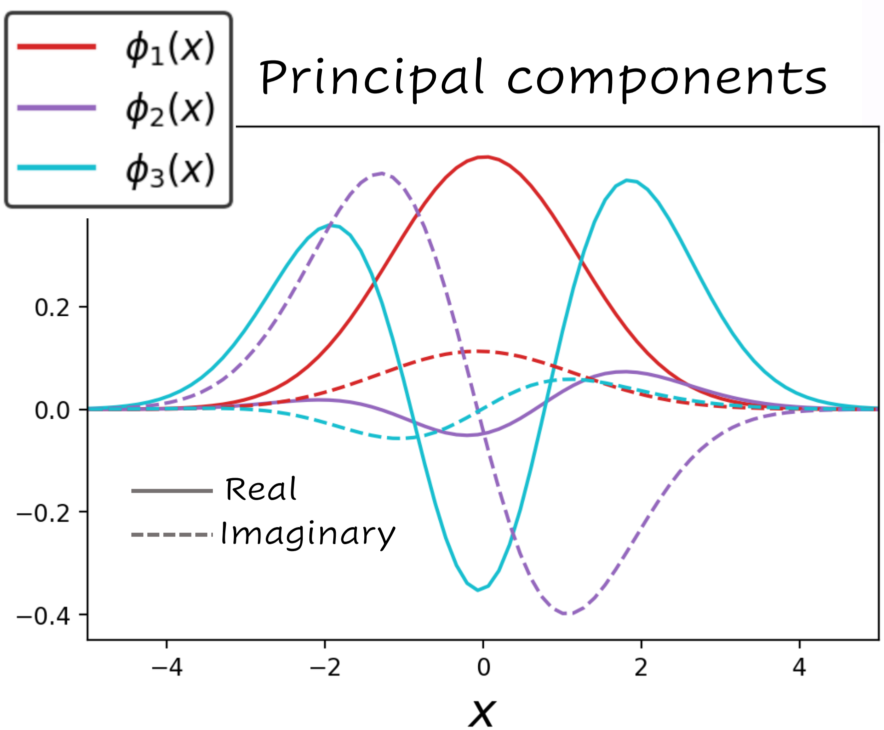

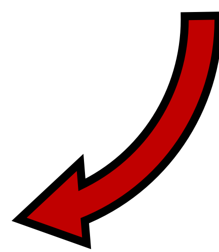

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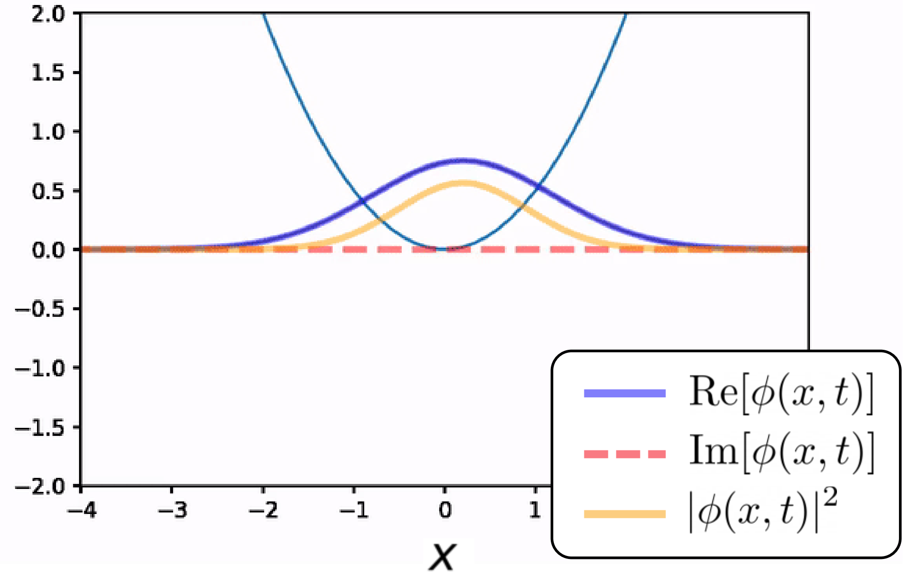
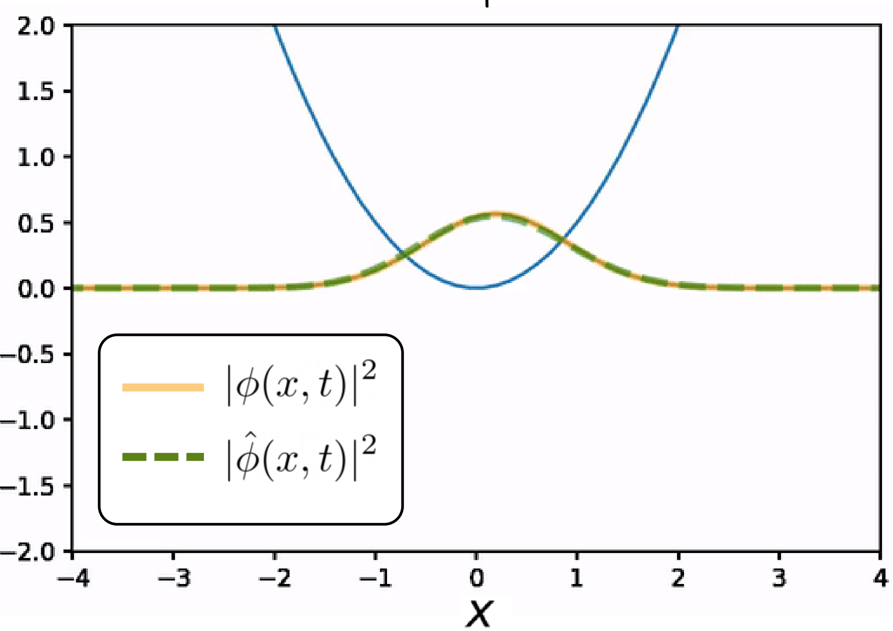
$$\mathcal{H} = -\frac{\partial^2}{\partial x^2} + \alpha x^2$$

High fidelity solution



$$\hat{\phi}(x,t) = \sum_{k}^{n} a_k(t)\phi_k(x)$$

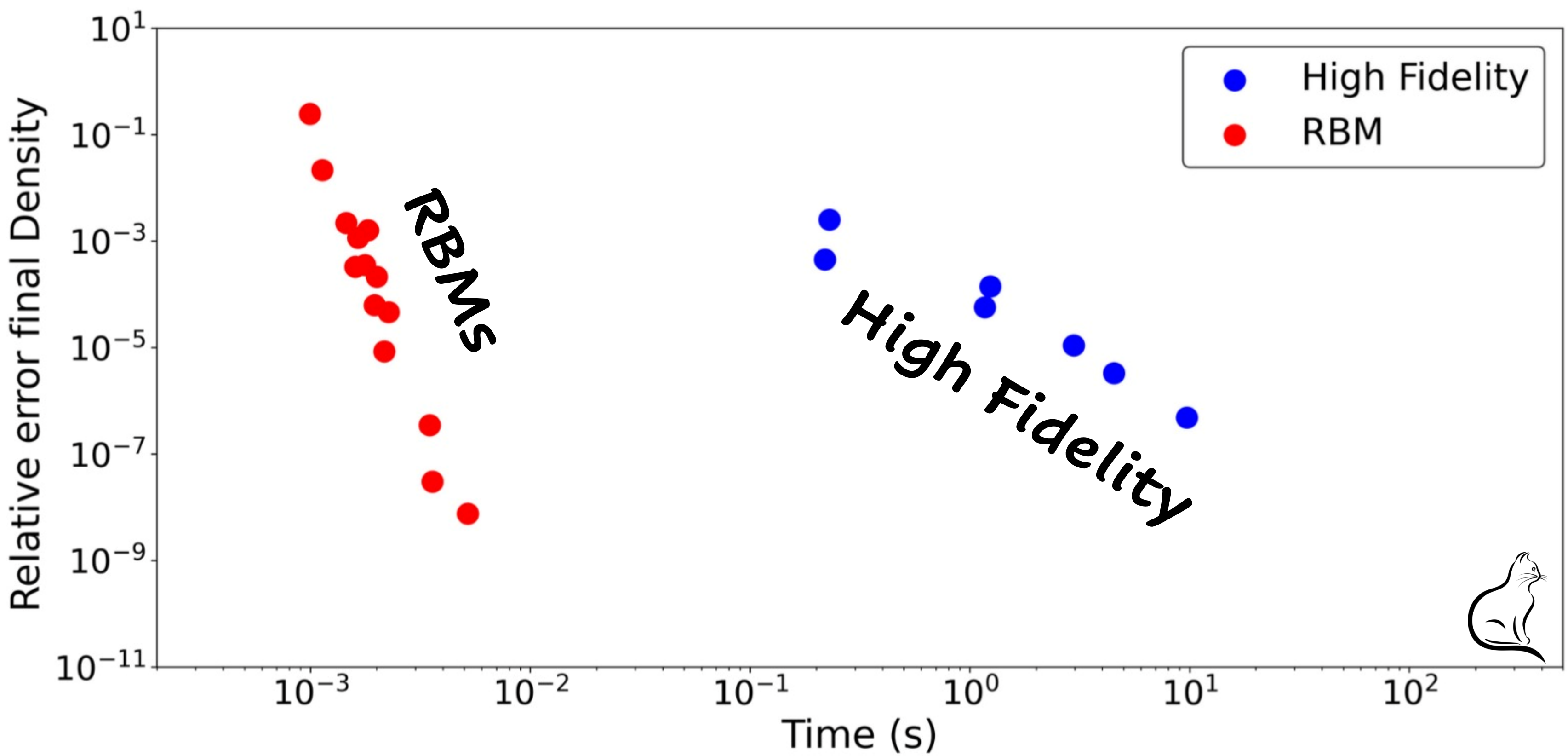
RBMs comparison



Applications and Results

5 Dynamical systems

Quantum Harmonic Oscillator



Applications and Results

5 Dynamical systems

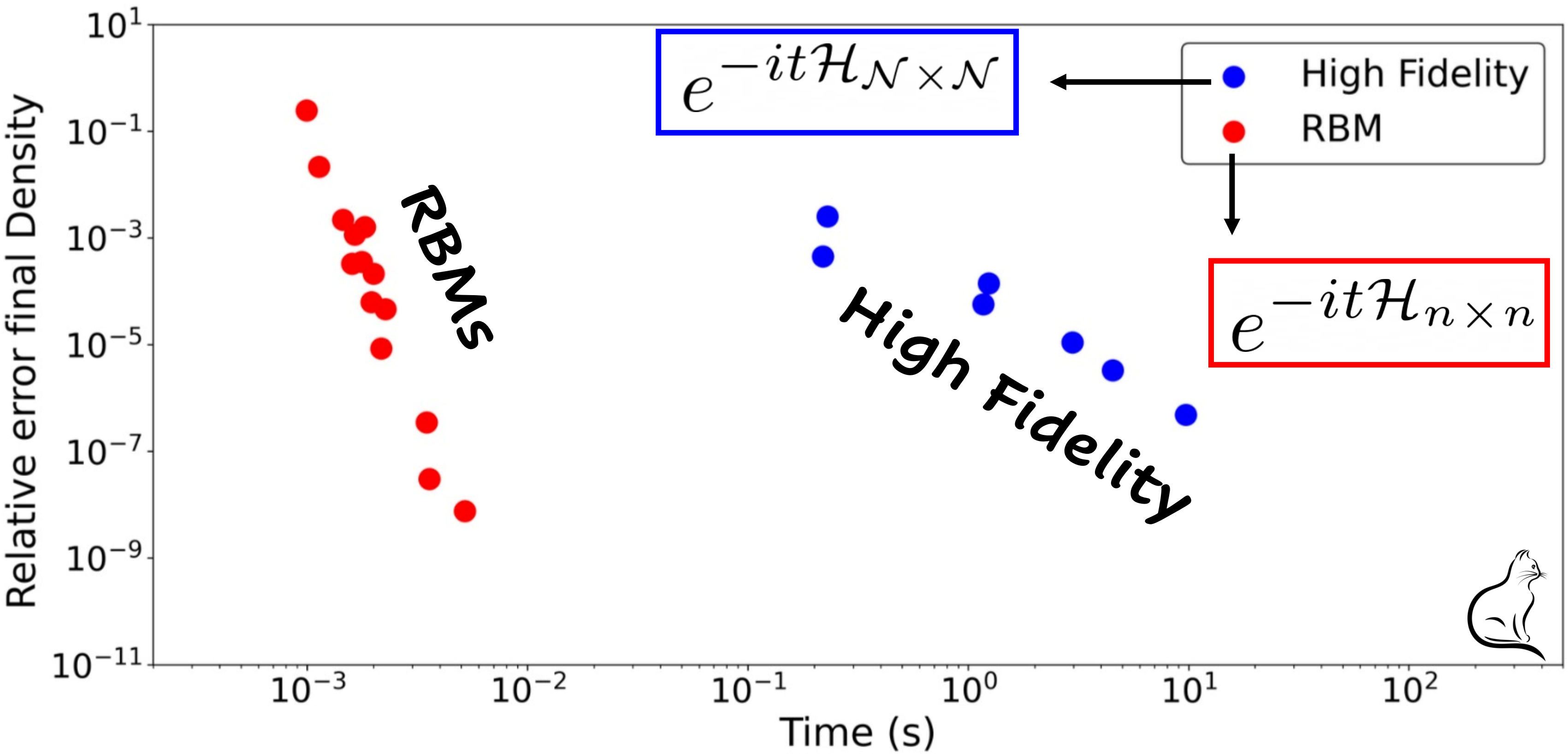
Gains from:

1) Smaller systems

2) More stable systems

$$e^{-i\Delta t\mathcal{H}} \approx 1 - i\Delta t\mathcal{H} - \frac{1}{2}\Delta t^2\mathcal{H}^2 + \dots$$

Quantum Harmonic Oscillator



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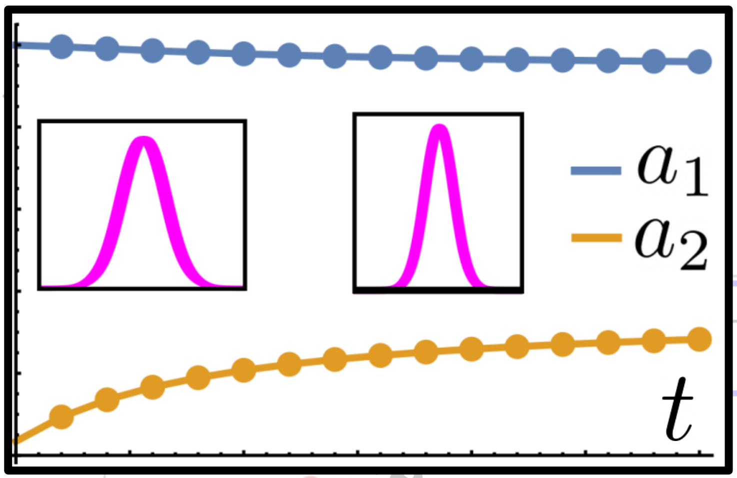
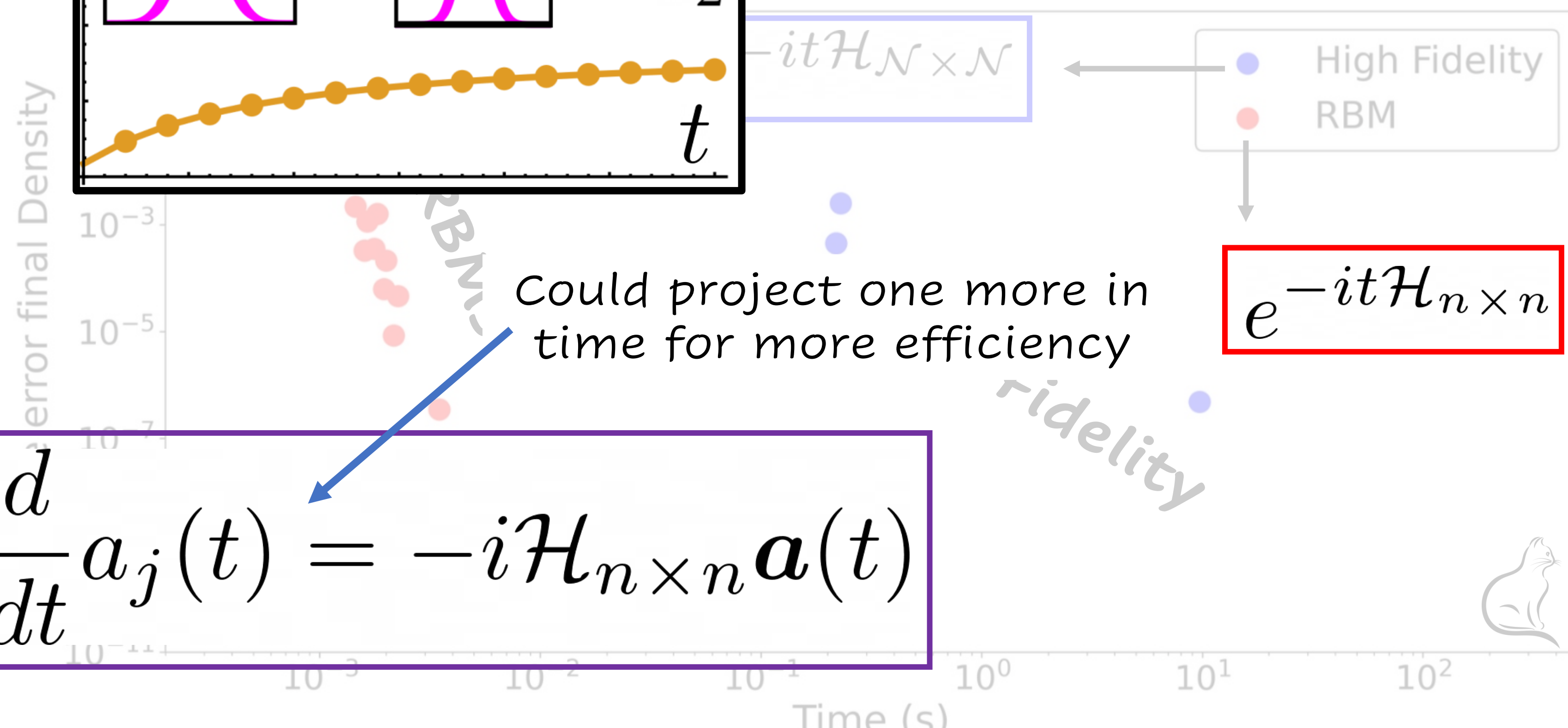
Quan





$e^{-it\mathcal{H}_{\mathcal{N}\times\mathcal{N}}}$

$$e^{-it\mathcal{H}_{n\times n}}$$

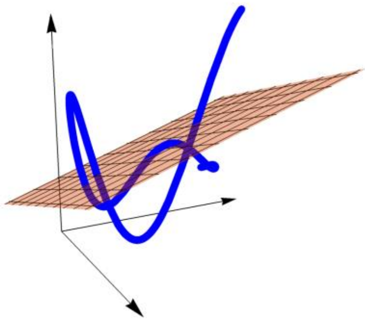
Could project one more in time for more efficiency

$$\frac{d}{dt}a_j(t) = -i\mathcal{H}_{n\times n}\boldsymbol{a}(t)$$

Applications and Results

5 Dynamical systems

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



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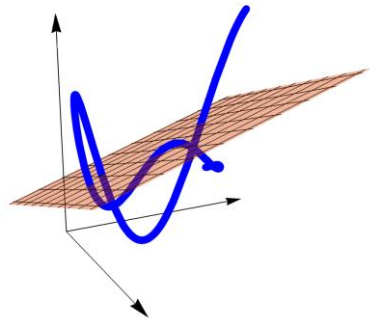
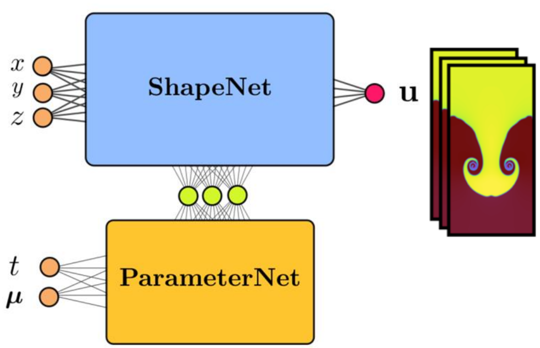


Neural Networks!



https://github.com/pswpswpsw/nif

Neural Implicit Flow: a mesh-agnostic dimensionality reduction paradigm of spatio-temporal data

Shaowu Pan Steven L. Brunton J. Nathan Kutz

Applications and Results

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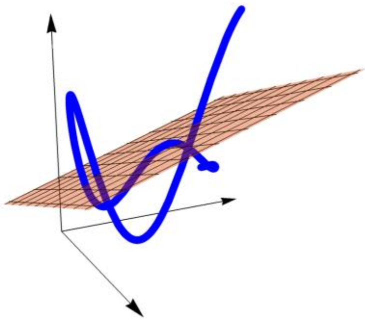

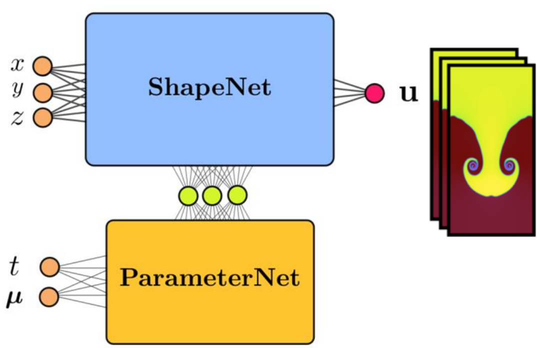

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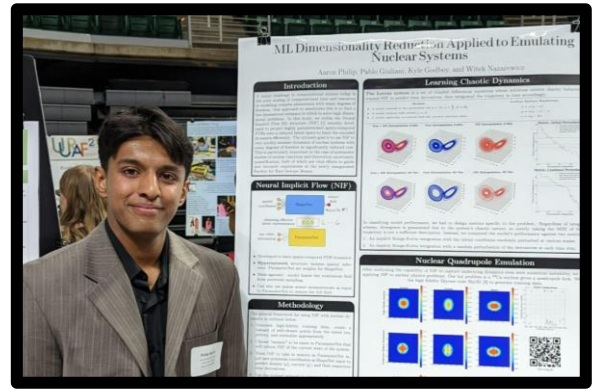
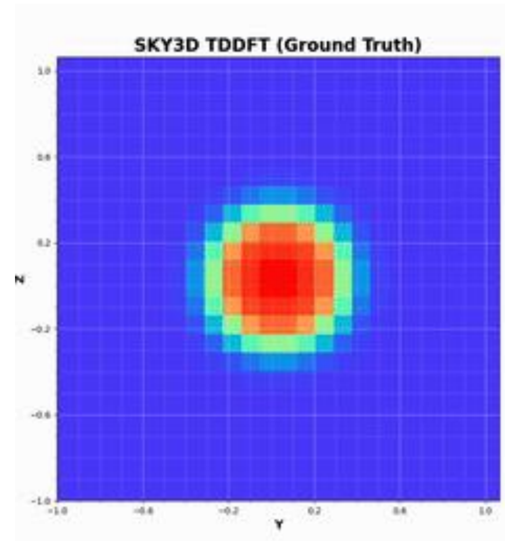


Aaron Phillip

$^{40}\mathrm{Ca}$ Quadrupole vibrations



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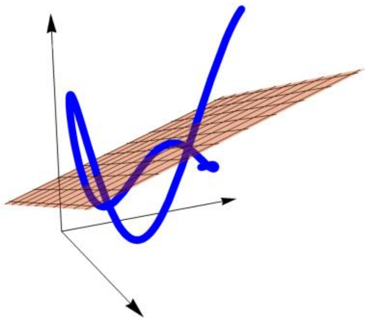

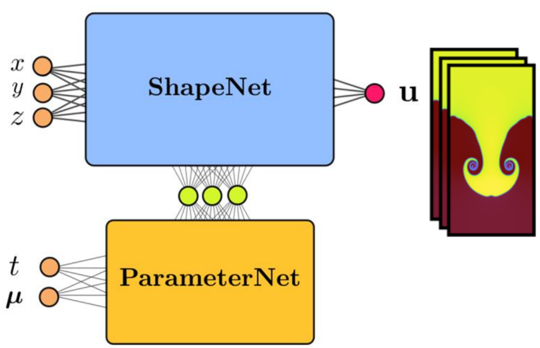

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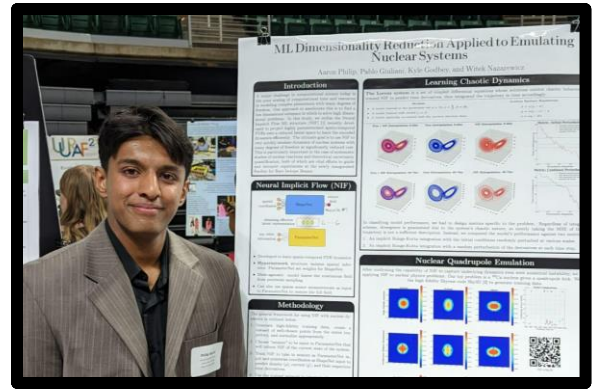

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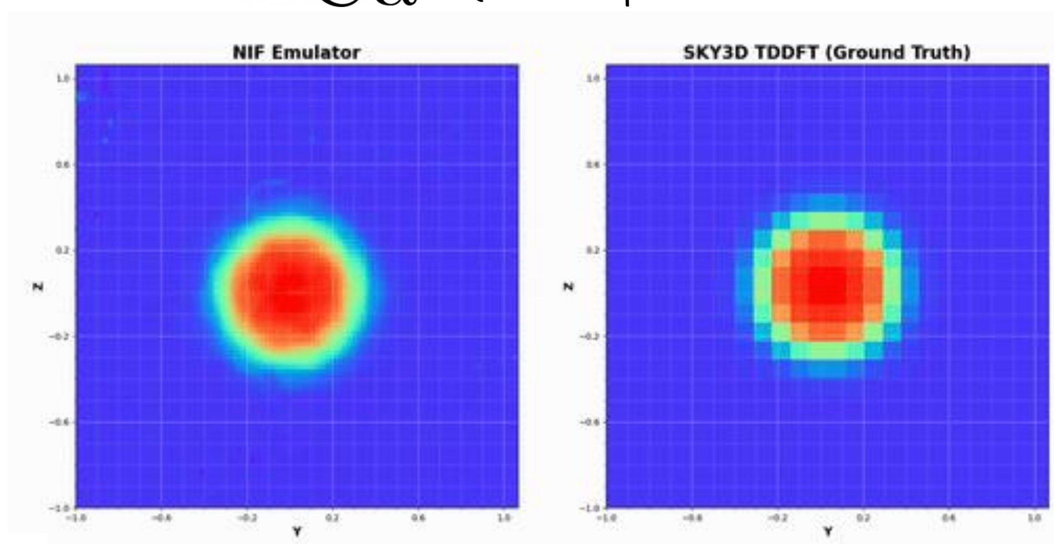

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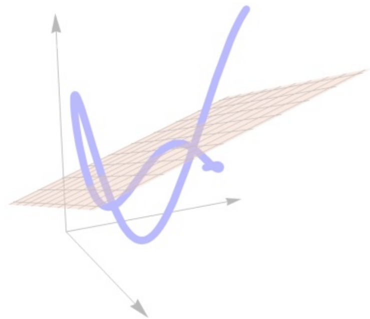

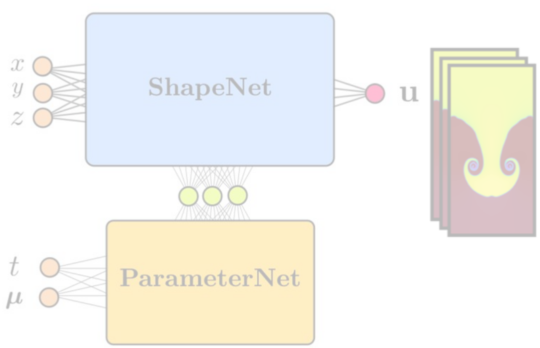

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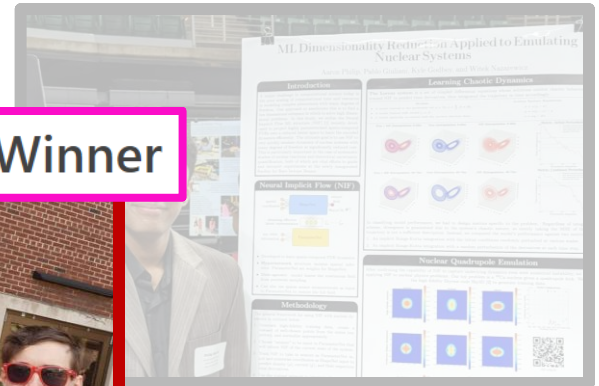
Neural Implicit Flow: a mesh-agnostic dimensionality reduction paradigm of spatio-temporal data
Shaowu Pan Steven L. Brunton J. Nathan Kutz

UURAF 2023 Award Winner

5 Dynamical systems



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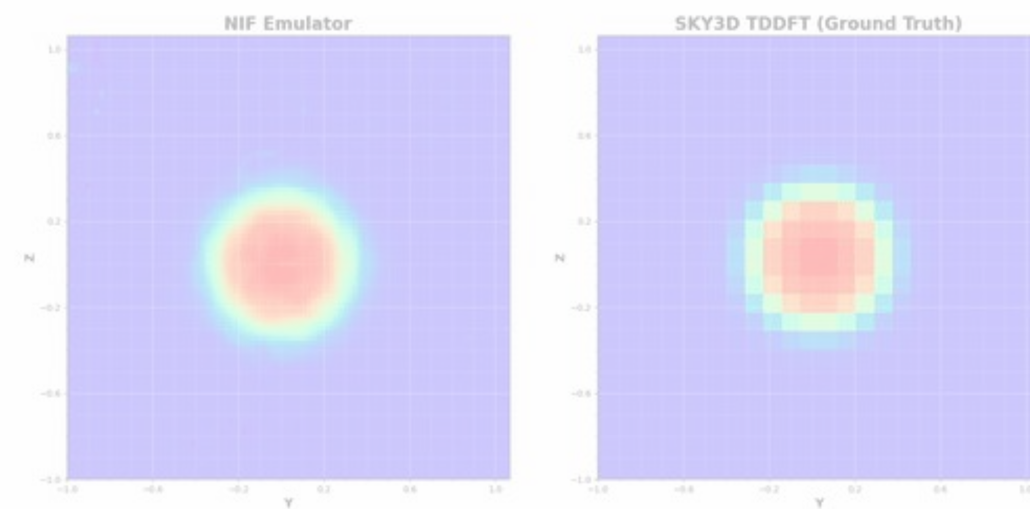


Outline

Why → Uncertainty Quantification? ← How

The Reduced Basis Method

How it works

Applications and Results

Upcoming Highlights

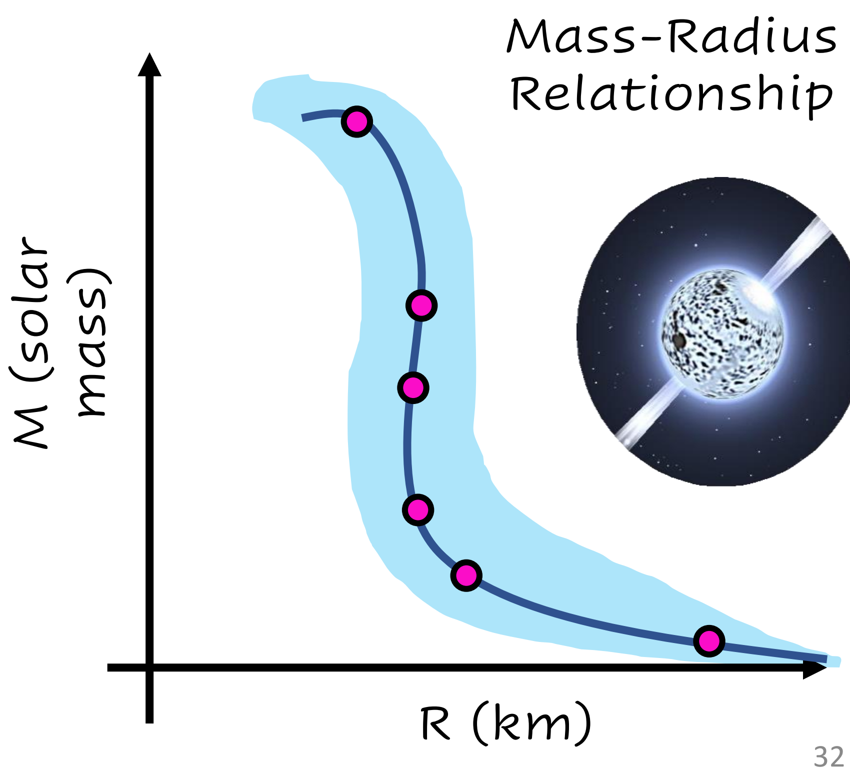
Takeaways

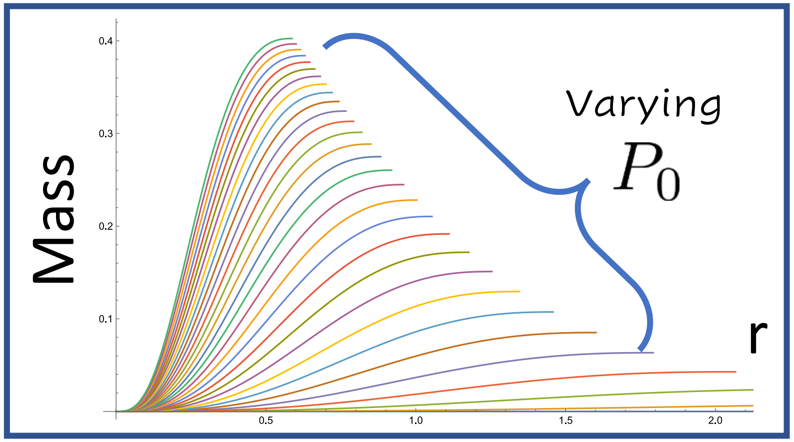
Upcoming highlights

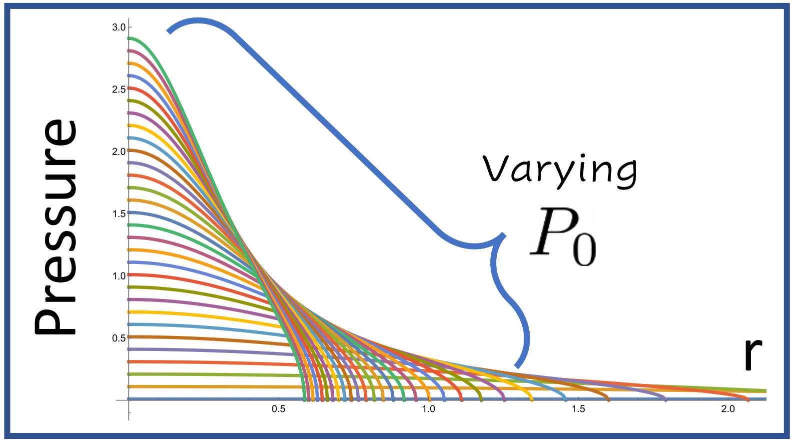
1 **Application of reduced basis methods to compact stars**

Amy Anderson,[1,*] Pablo Giuliani,[2,†] and J.Piekarewicz[1,‡]
[1]Department of Physics, Florida State University, Tallahassee, FL 323
[2]FRIB/NSCL Laboratory, Michigan State University, East Lansing, Michiga

Amy Anderson







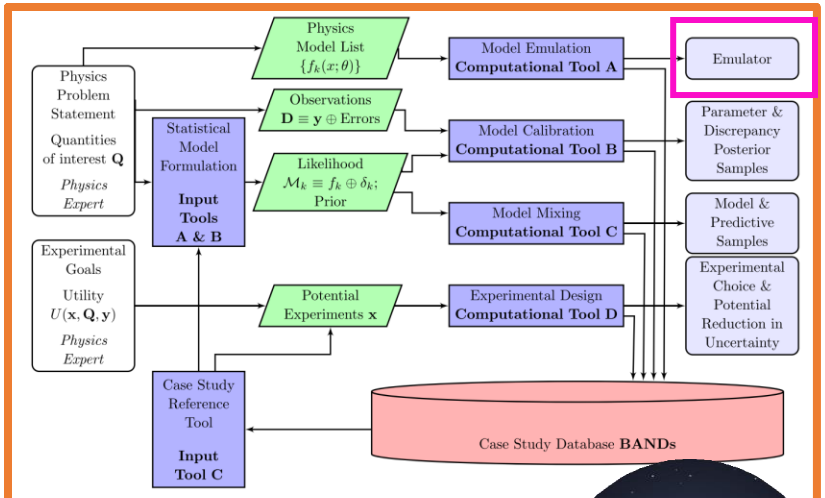
Upcoming highlights

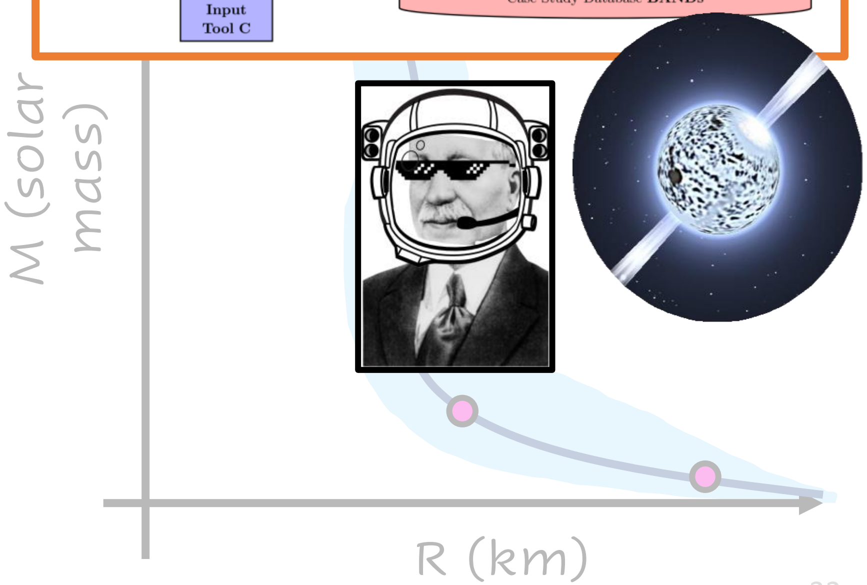
(1) Application of reduced basis methods to compact stars

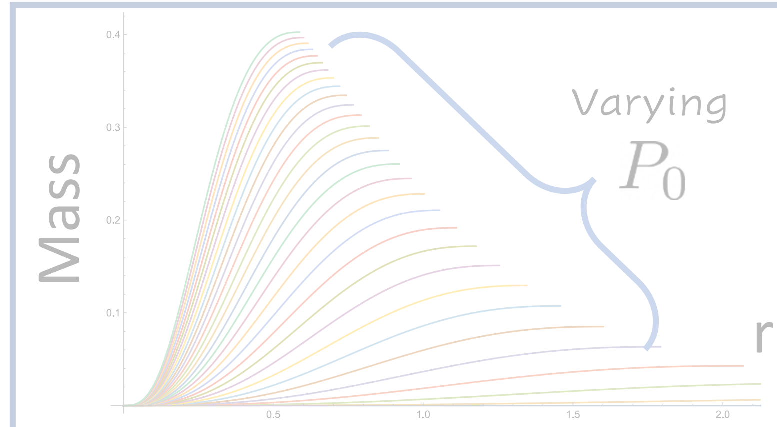
Amy Anderson,[1,*] Pablo Giuliani,[2,†] and J.Piekarewicz[1,‡]
[1]Department of Physics, Florida State University, Tallahassee, FL 323
[2]FRIB/NSCL Laboratory, Michigan State University, East Lansing, Michiga

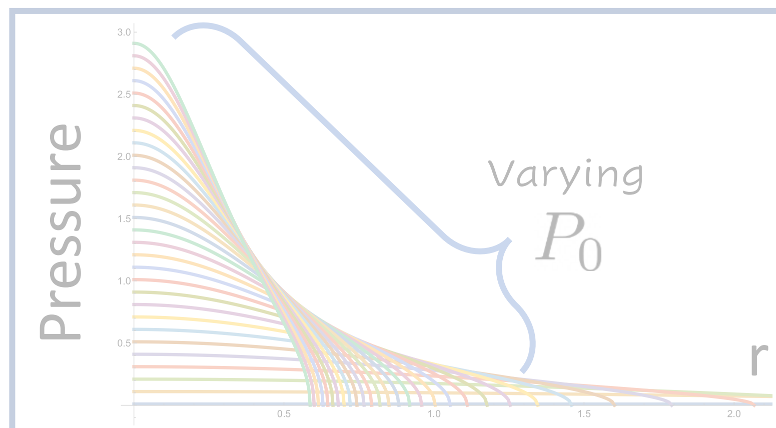
BAND Bayesian Analysis of Nuclear Dynamics Fellow 2023

Amy Anderson



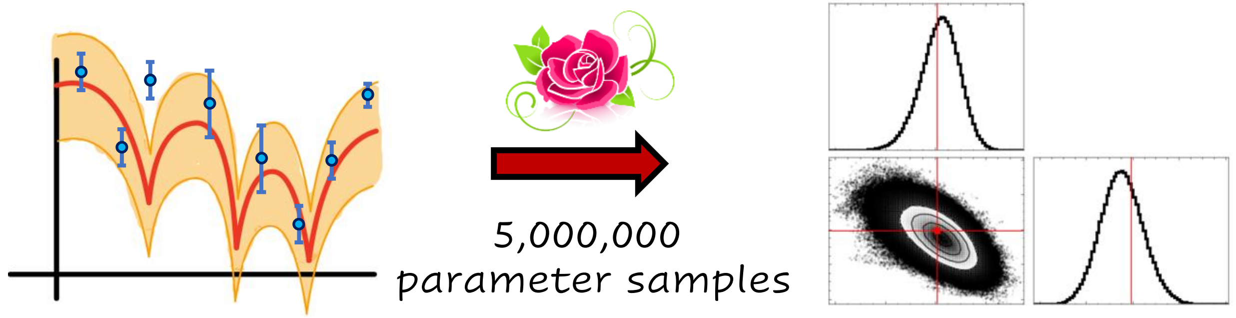






Upcoming highlights

2 Smart posterior handling



Upcoming highlights

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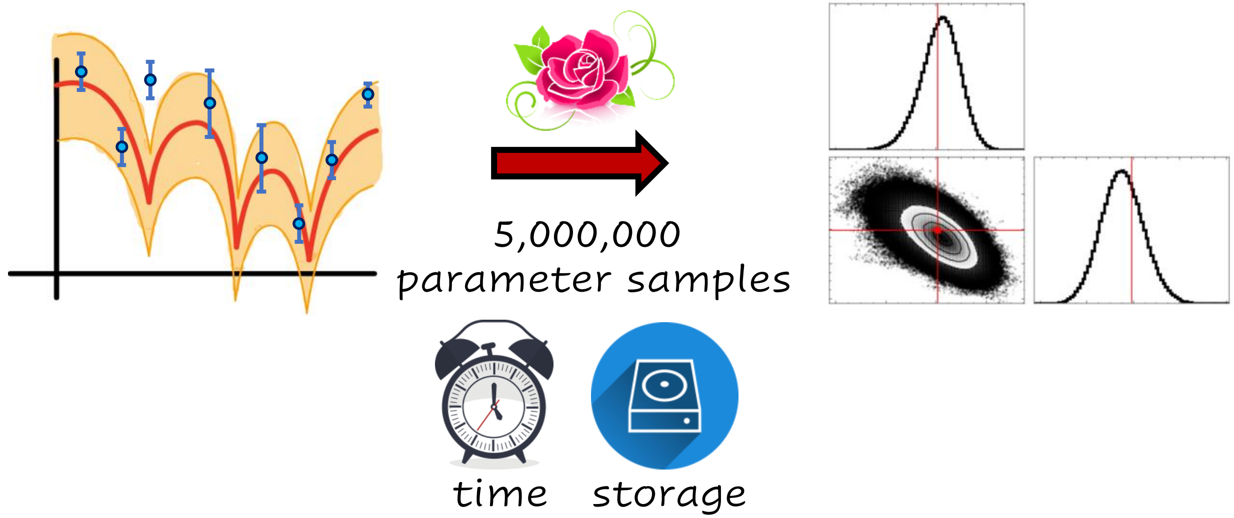

Upcoming highlights

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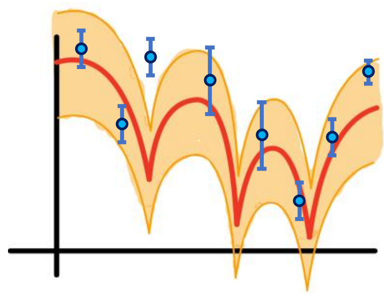
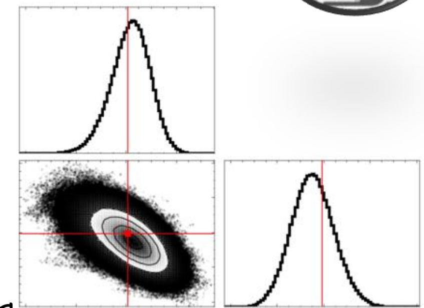


(Frederi Viens
Edgard Bonilla)

Chaos expansion

Normalizing flows



(Yukari Yamauchi
Landon Buskirk)

Upcoming highlights

Landon Buskirk

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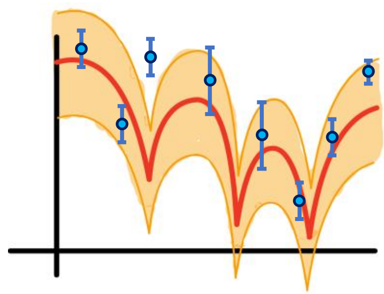

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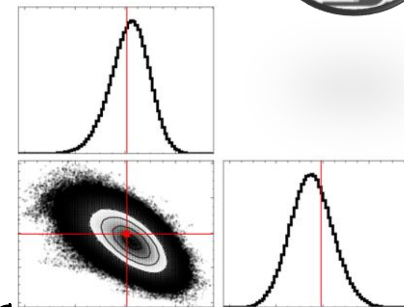

(Yukari Yamauchi
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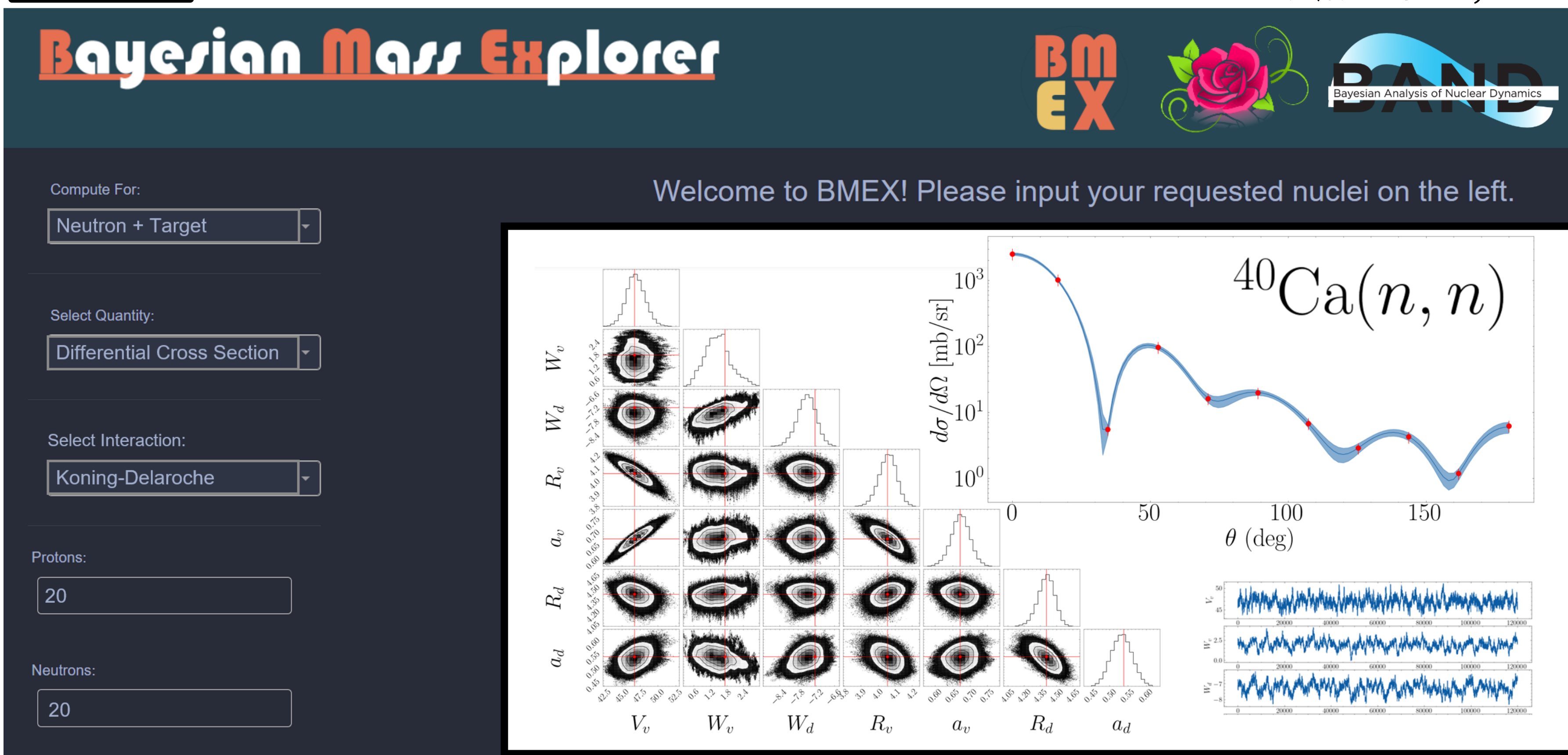

Upcoming highlights

Landon Buskirk

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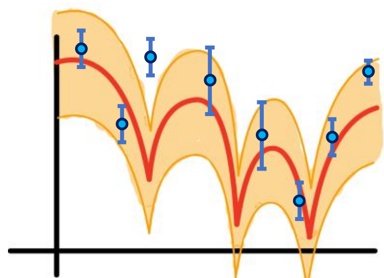

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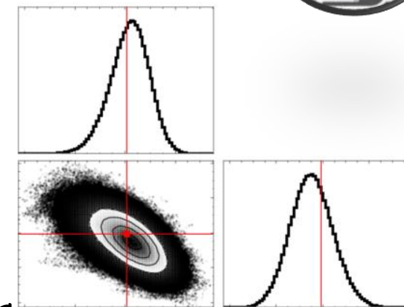


(Yukari Yamauchi Landon Buskirk)

Bayesian Mass Explorer

BMEX

Bayesian Analysis of Nuclear Dynamics

Compute For:

Neutron + Target

Select Quantity:

Differential Cross Section

Select Interaction:

Koning-Delaroche

Protons:

20

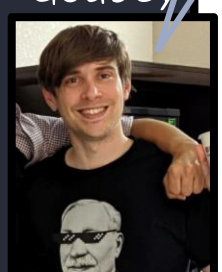
Neutrons:

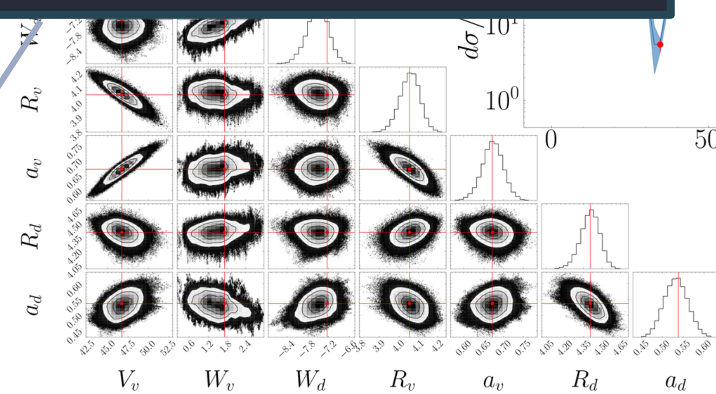
20

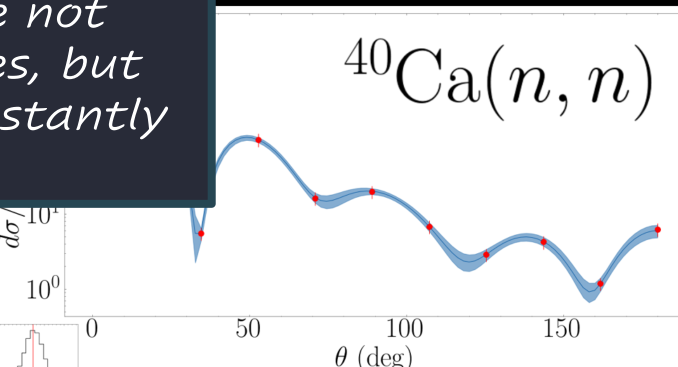
Welcome to BMEX! Please input your requested nuclei on the left.

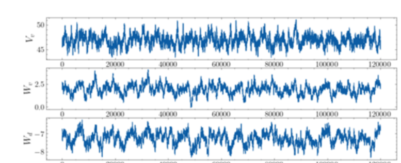
“A future where models are not defined by parameter values, but rather by distributions constantly updated with new data”

Kyle Godbey



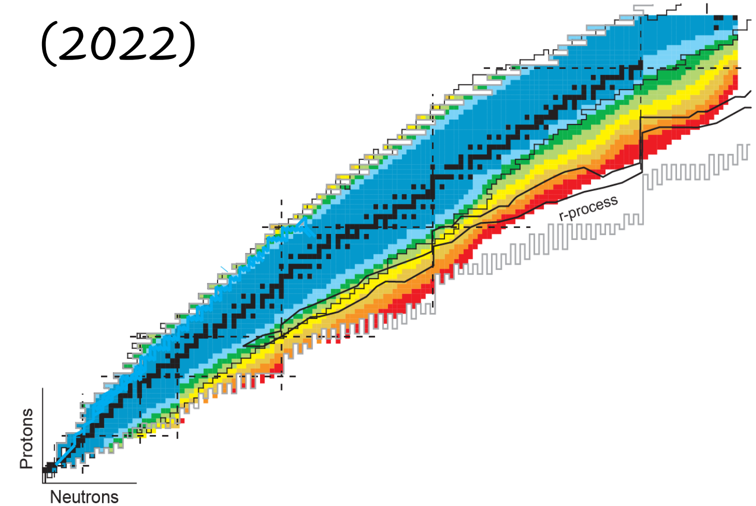


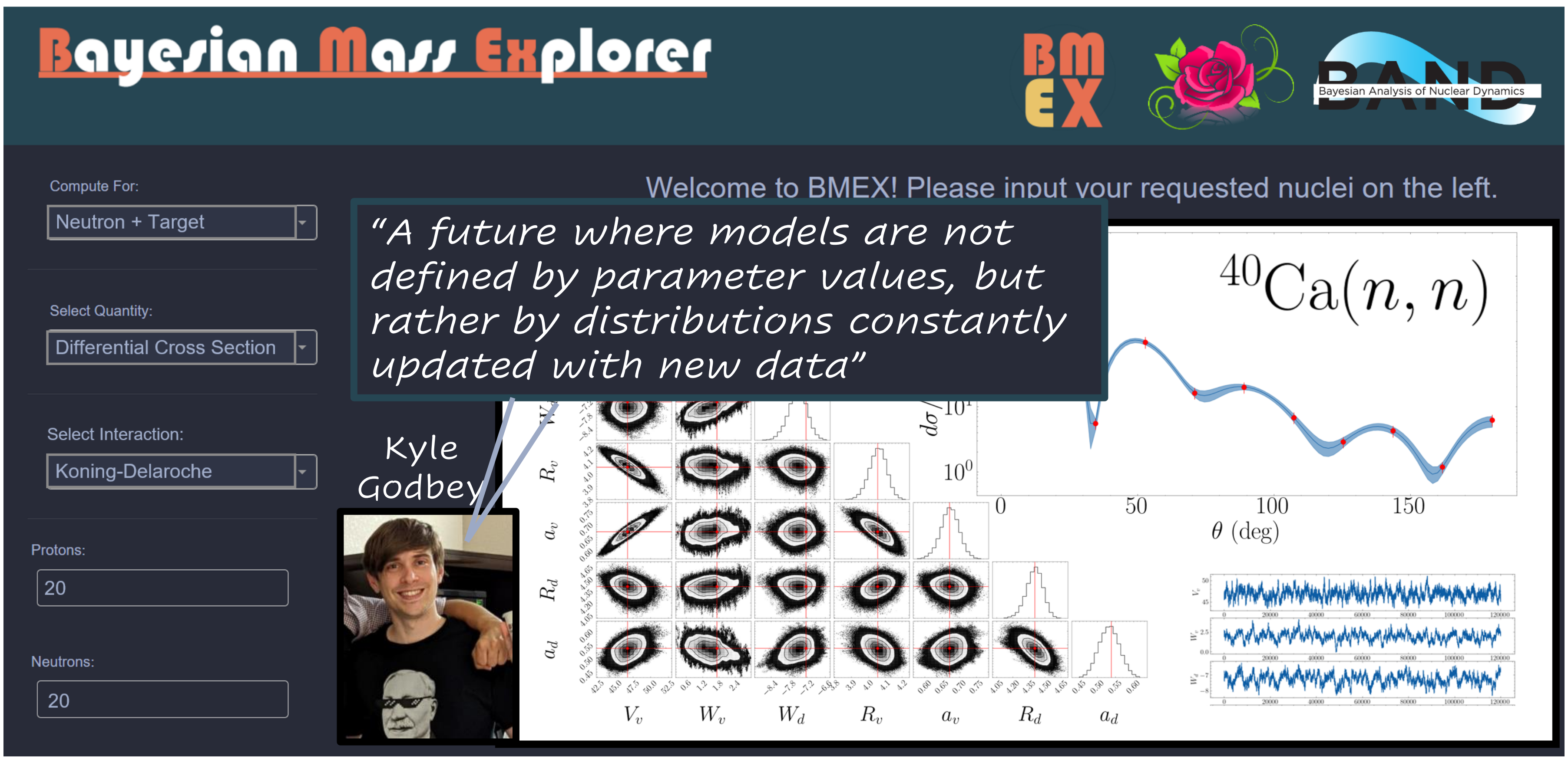




Optical potentials for the rare-isotope beam era (2022)

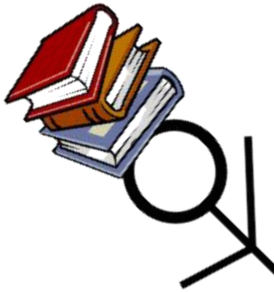
In regions of the nuclear chart away from stability, which represent a frontier in nuclear science over the coming decade and which will be probed at new rare-isotope beam facilities worldwide, there is a targeted ***need to quantify and reduce theoretical reaction model uncertainties****, especially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





Takeaways

I have two



Takeaways

1) These methods are SO cool

Takeaways

1) These methods are SO cool

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

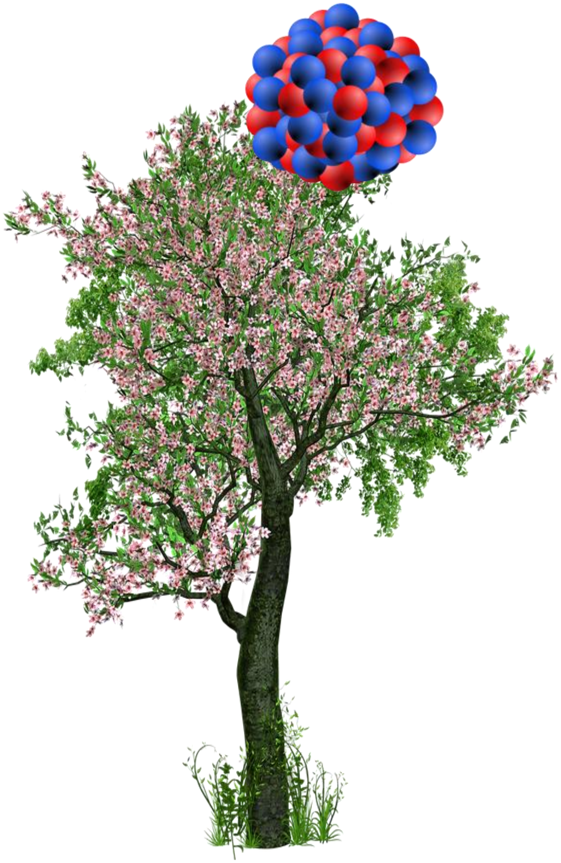
BUQEYE Guide to Projection-Based Emulators in Nuclear Physics

Takeaways

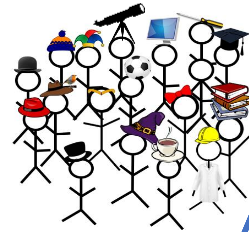
1) These methods are SO cool

2) UQ needs multidisciplinary efforts

This is very important to us



Takeaways



mathematics
statistics
computational
experimental

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Work in collaboration with experts

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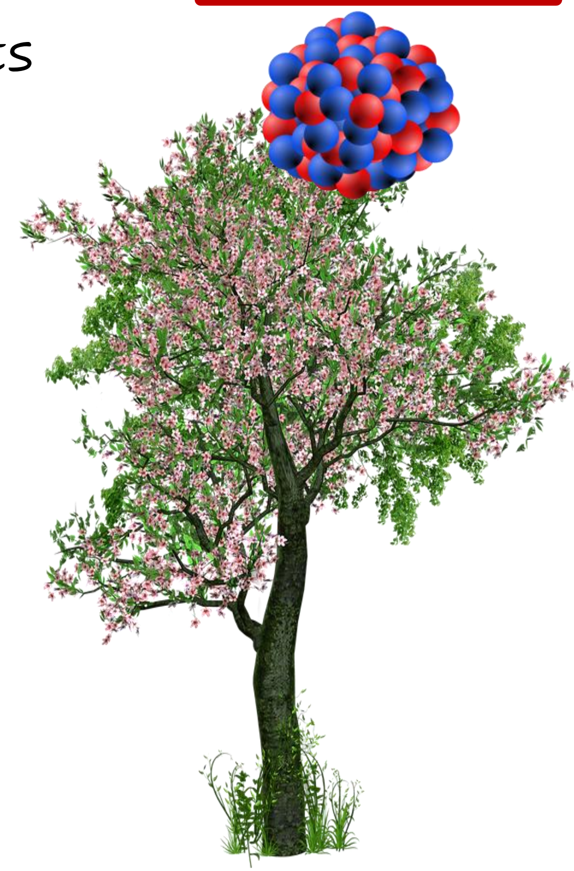
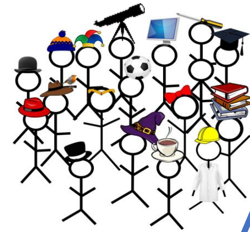


Takeaways



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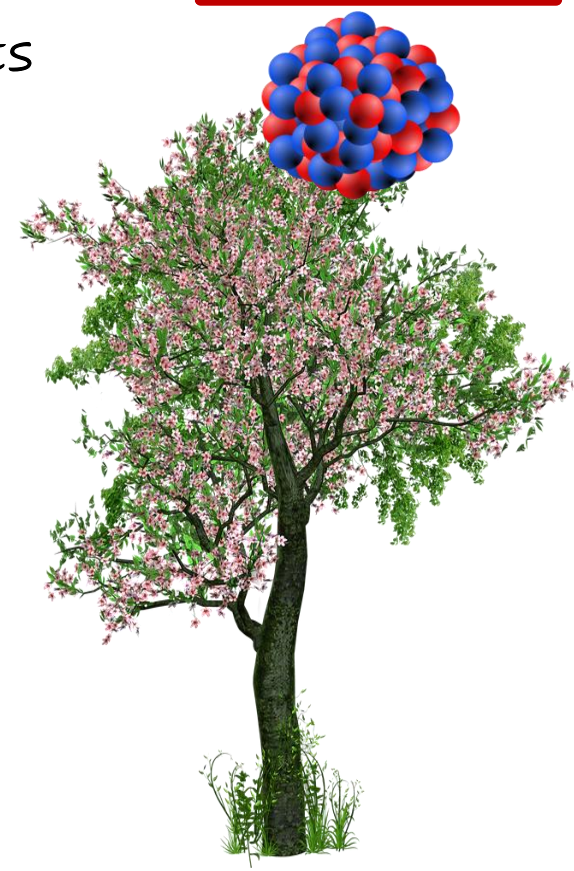

ASCSN

Advanced Scientific Computing and Statistics Network

Takeaways

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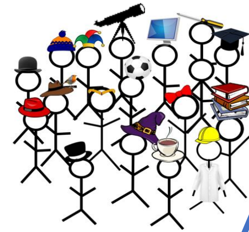

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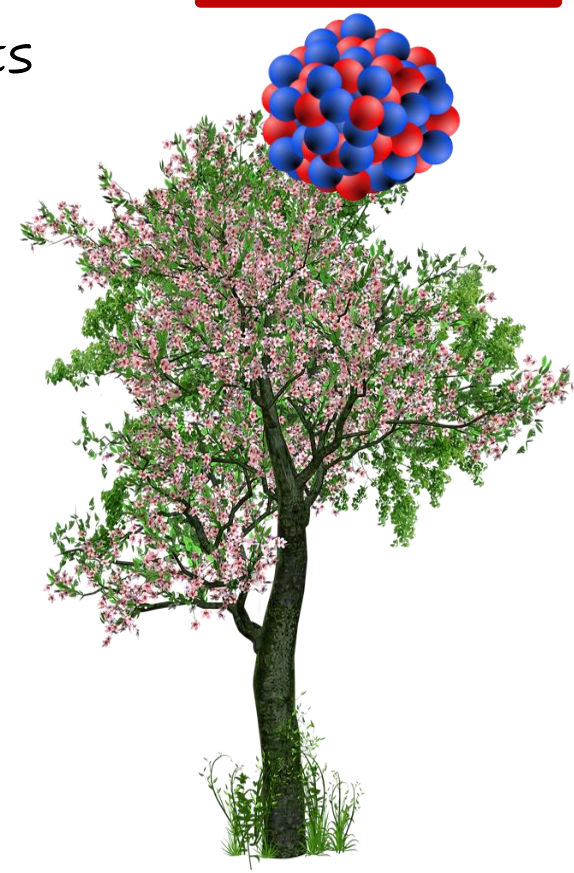
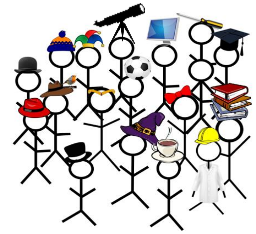


ASCSN

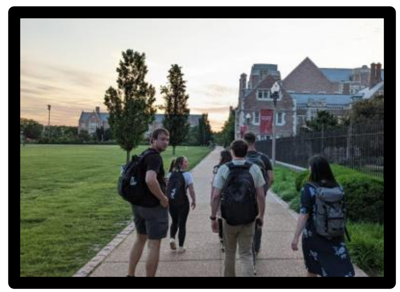
Advanced Scientific Computing and Statistics Network

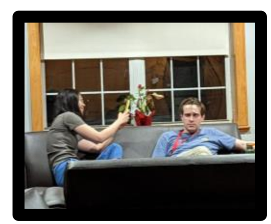
See Kyle's talk tomorrow

Takeaways



Work in collaboration with experts …





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