The Fast and the Fewer

Speeding up and orthogonalizing nuclear models for UQ

FRIB

BAND — Bayesian Analysis of Nuclear Dynamics

STREAMLINE

ASCSN

AD REDIGENDUM DIMENSIO — VIDEAMUS OBUMBRATIO

LANL

Few Body Reactions Group

July 2024

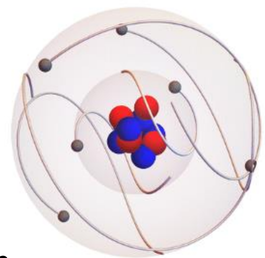
Pablo Giuliani
giulianp@frib.msu.edu

[Watch the recording](#) [Link to these slides](#)

Outline

My context

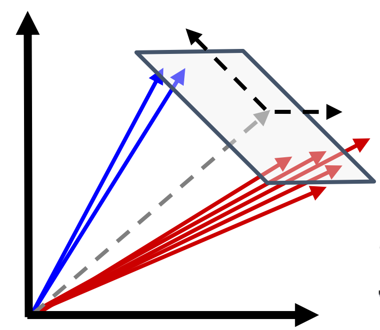
Bayes and Nuclei



Two challenges

Computational paradigm

Dimensionality Reduction



Model Order Reduction (Faster)

Model Combination (Fewer)

Takeaways

Objectives:

1) Excite and lower barrier
2) Draw connections

Disclaimer on:

1) Content
2) Teamwork

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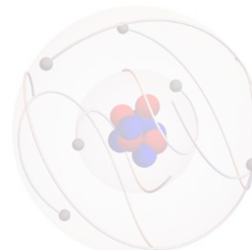

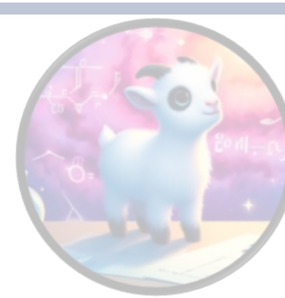

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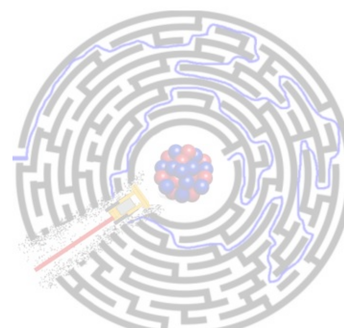

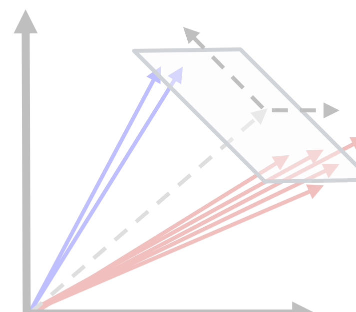

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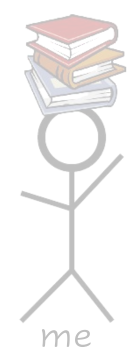

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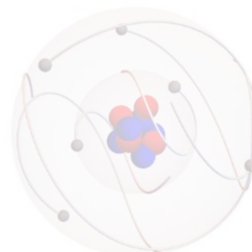

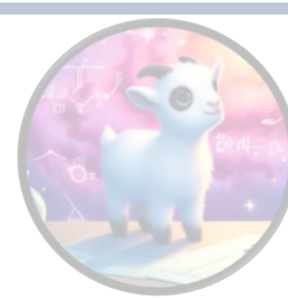

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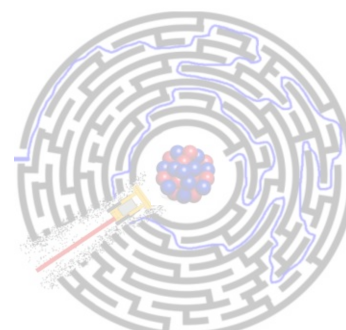

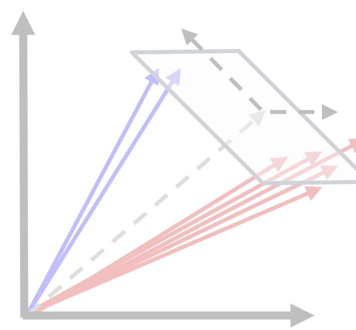

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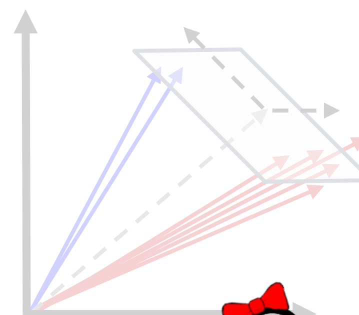


Model Order Reduction (Faster)

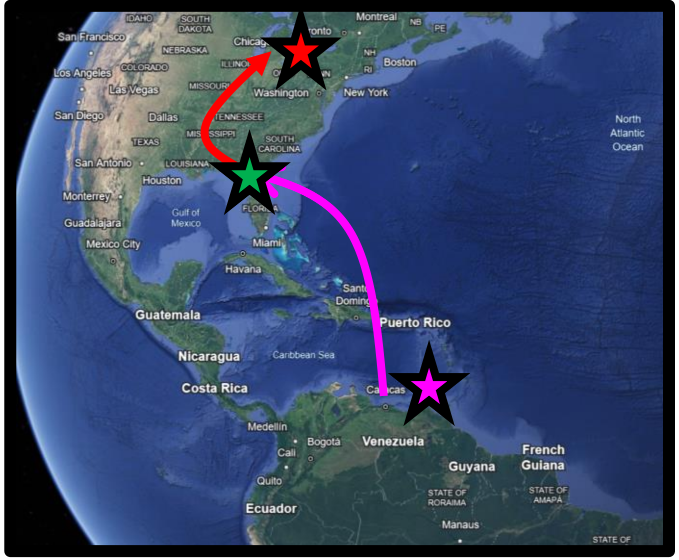
Model Combination (Fewer)

Takeaways

Paul Filomena Remco Rachel Vojta Witek Daniel Dean Casey Brendan Rahul Ingo Megan ChatGPT … Aaron Andrew An Lauren Diogenes Jorge Frederi Kyle Edgard me

My context

My co t



Venezuela

Universidad Simon Bolivar

Undegrad

Florida State University

PhD

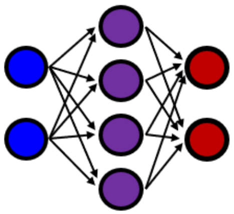
Postdoc

FRIB

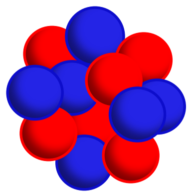
Michigan

My co t

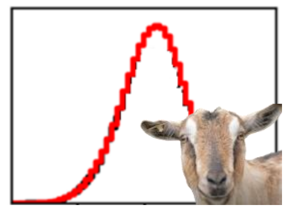
Venezuela



Machine Learning



Nuclear Physics



Bayesian Statistics

Research

Education

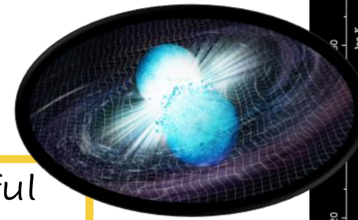
Outreach

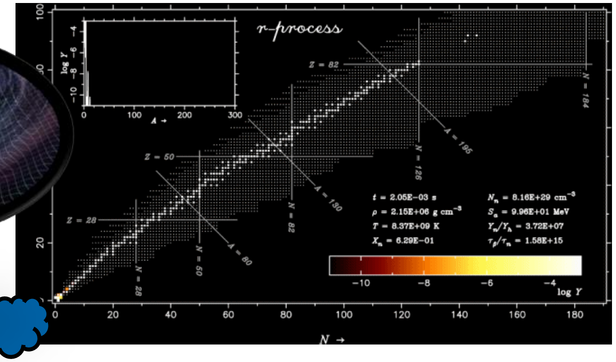
Community

FRIB

Michigan

Big questions





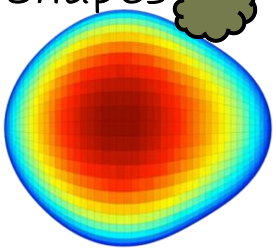
What structures form at the extremes?

Can we make useful things?

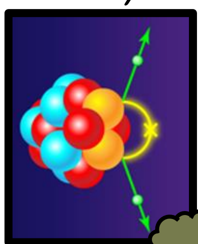
Where do heavy elements come from?

What's up with neutrinos?

Shapes



Decays



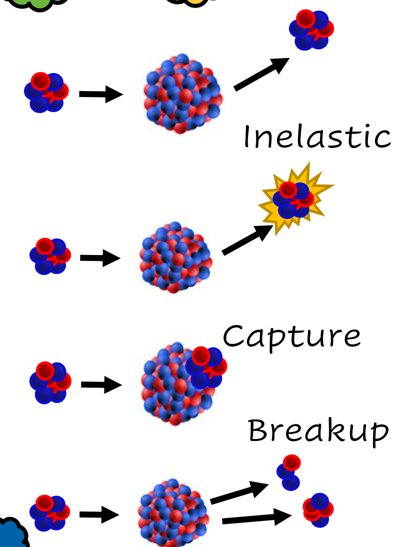
Applications

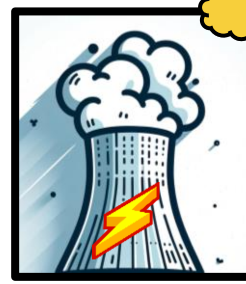
Structure

Symmetries

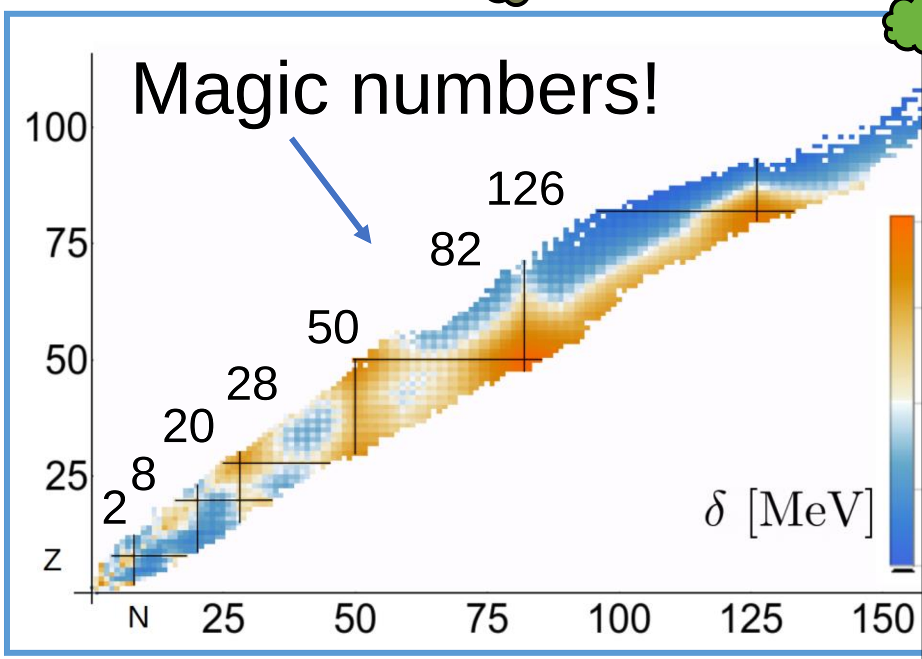
Astrophysics

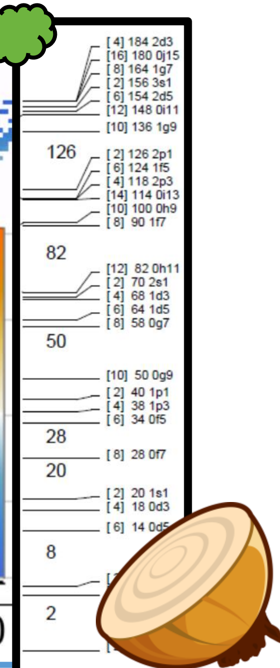
FRIB

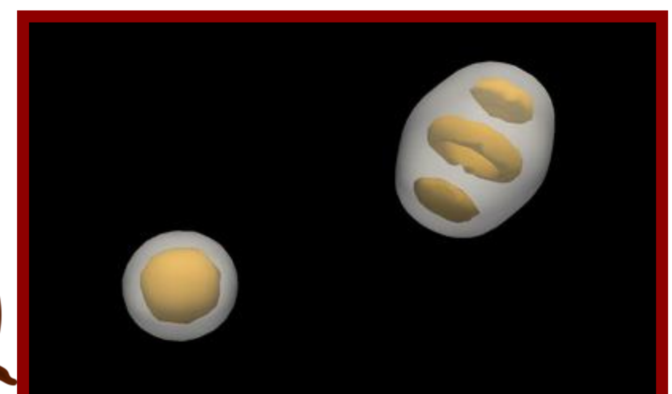




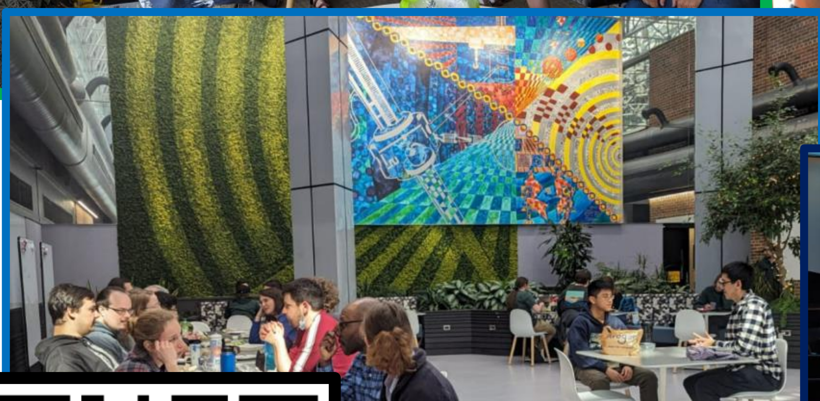
Power





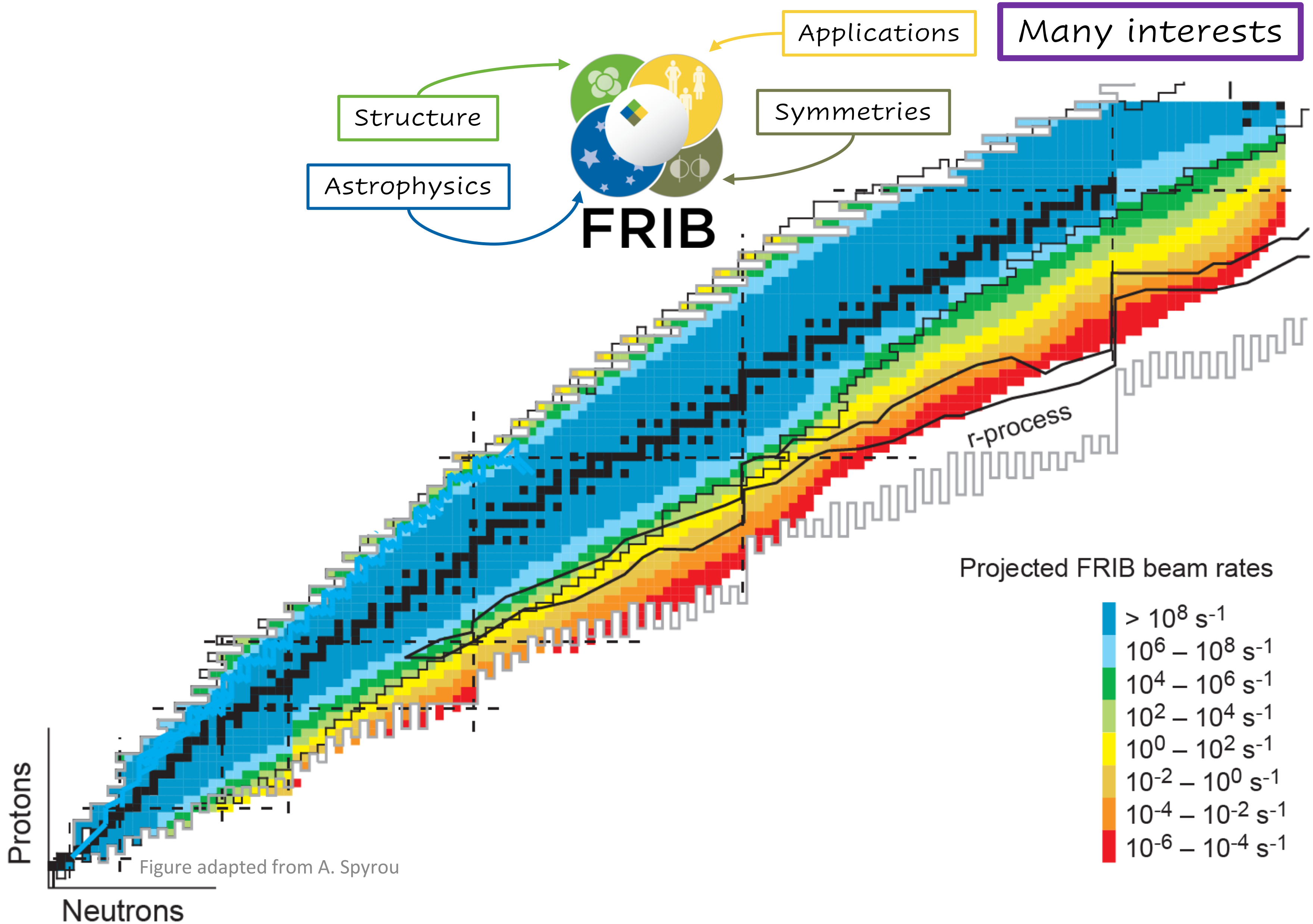


We have fun



Teaser

Cycle example



Cycle example

r-process

Lifetimes (β decay)

(Fission)

Masses

Capture rates

...

Astrophysics

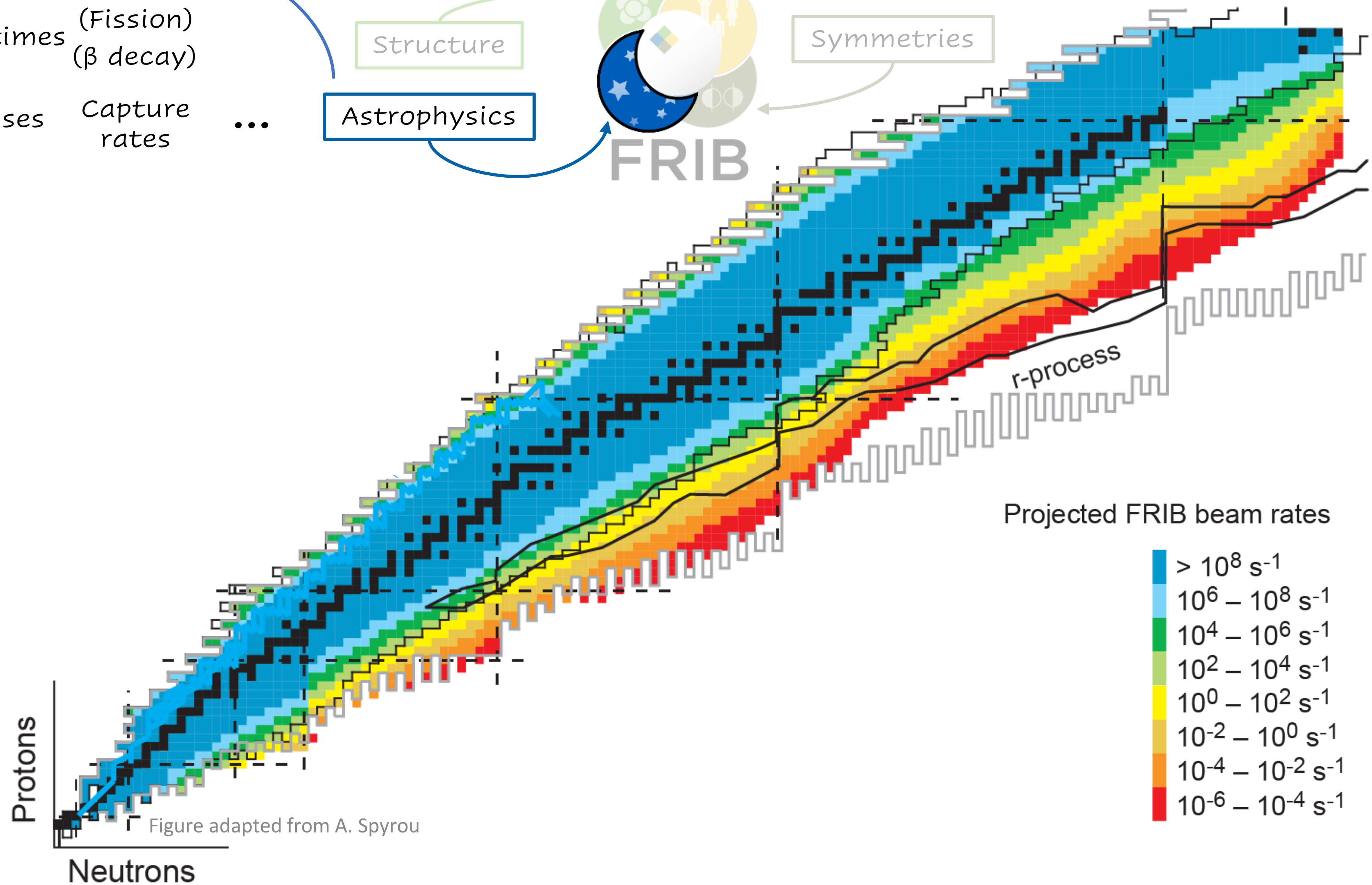
Structure

Applications

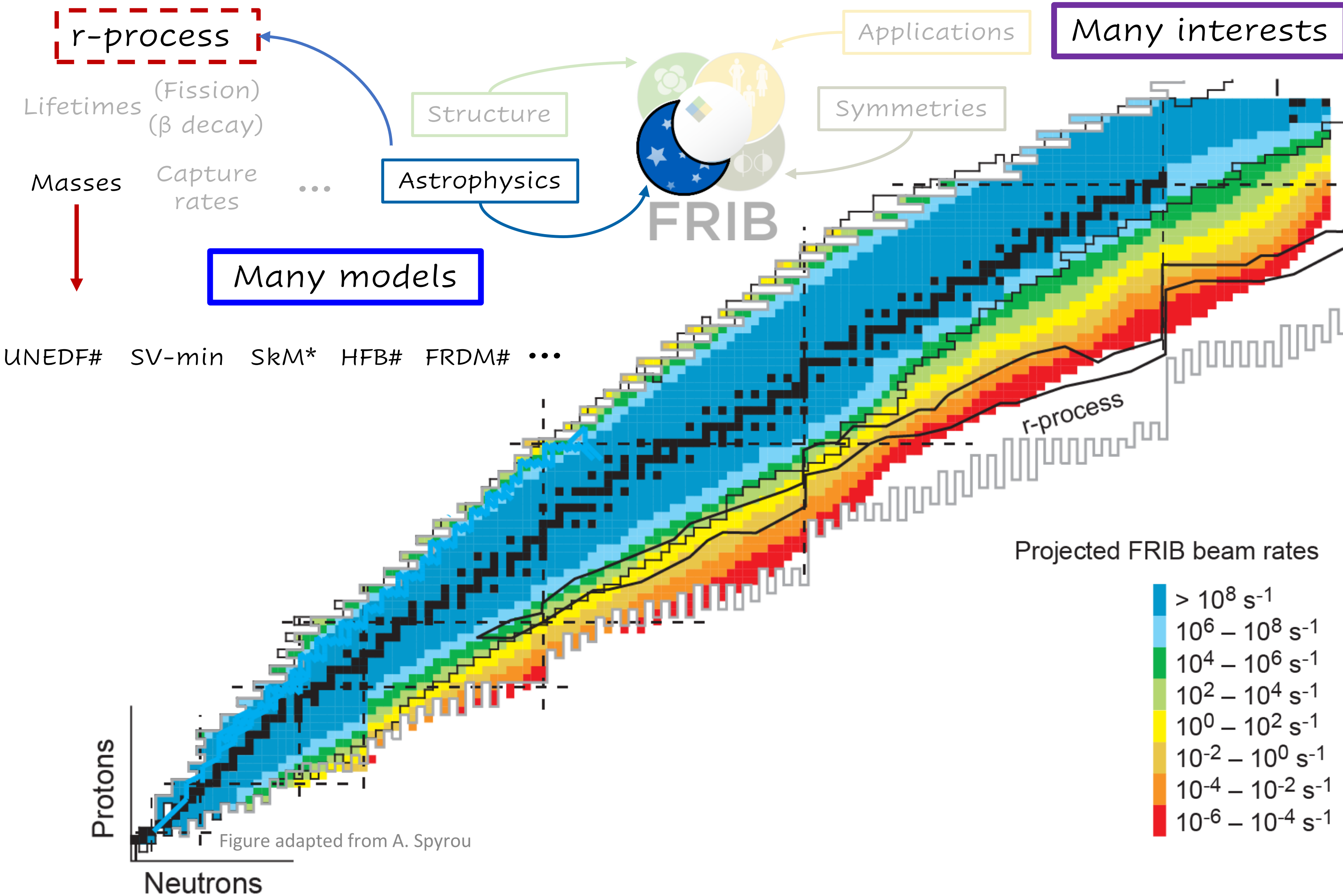
Symmetries

FRIB

Many interests



Cycle example



Cycle example

r-process

Lifetimes (Fission) (β decay)

Masses Capture rates ...

Astrophysics

Structure

Applications

Symmetries

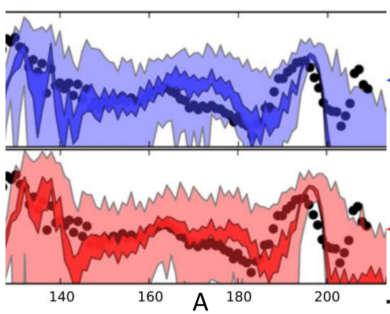
FRIB

Many interests

Many models

UNEDF# SV-min SkM* HFB# FRDM# •••

Abundances:



Adapted from: The impact of individual nuclear properties on r-process nucleosynthesis, **Mumpower et al, (2016)**

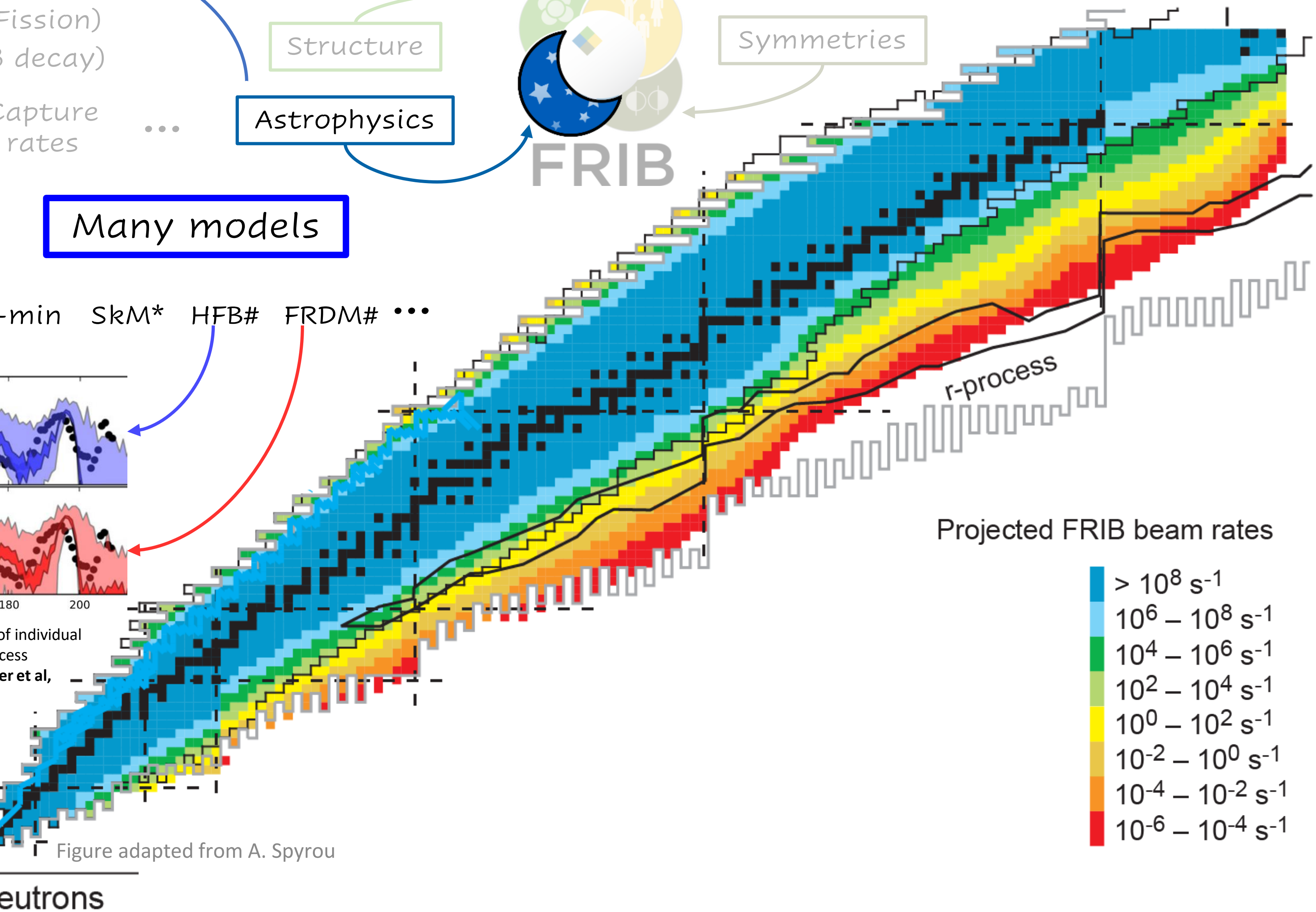


Figure adapted from A. Spyrou

Cycle example

r-process

Lifetimes (Fission) (β decay)

Masses Capture rates …

Astrophysics

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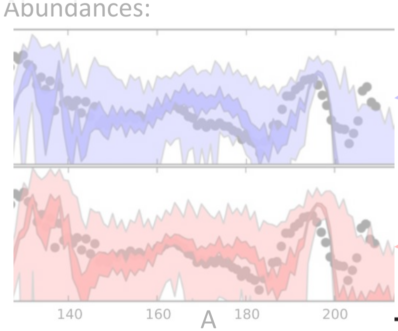
UNEDF# SV-min SkM* HFB# FRDM# …



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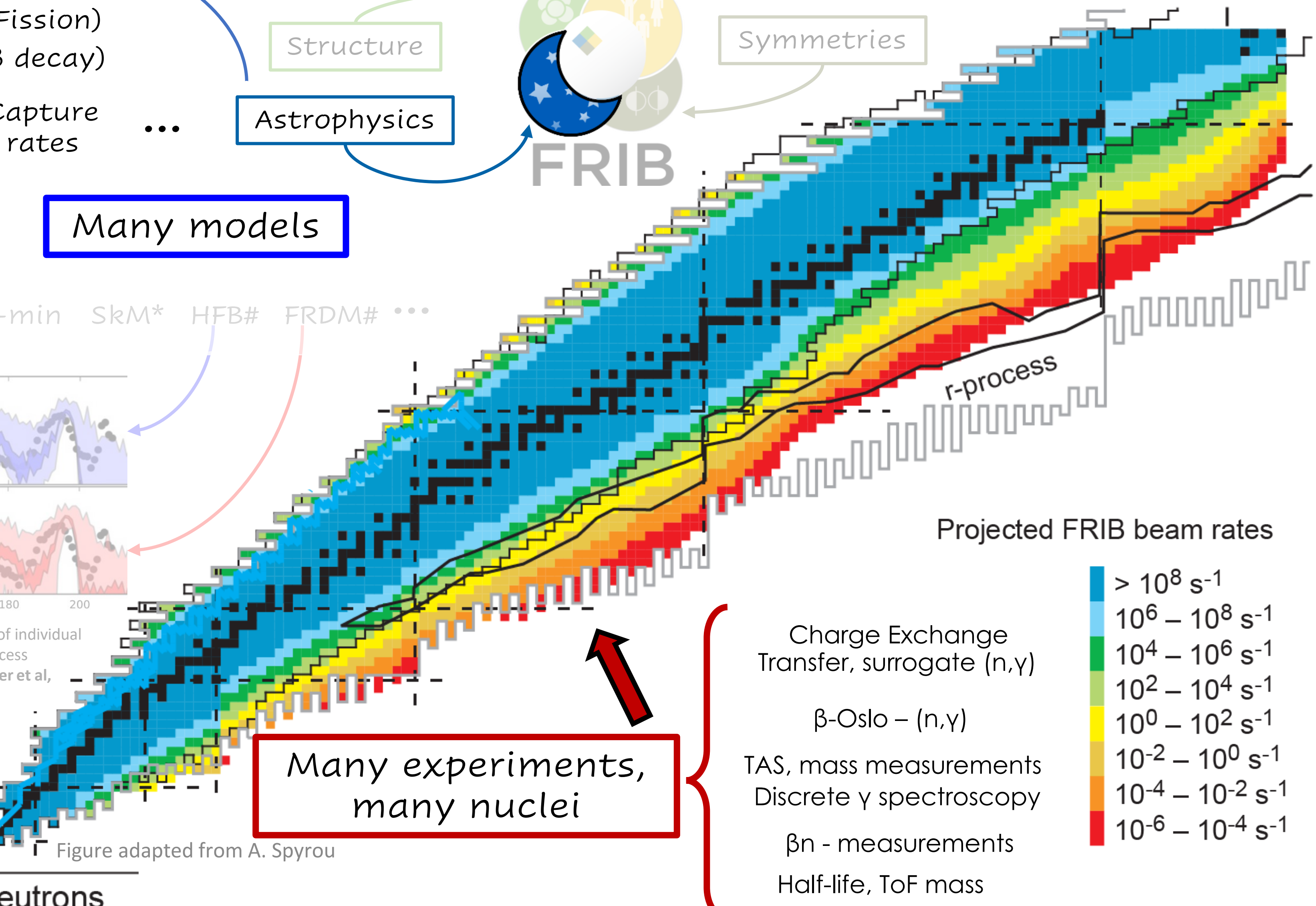


Many experiments, many nuclei

Charge Exchange
Transfer, surrogate (n,γ)

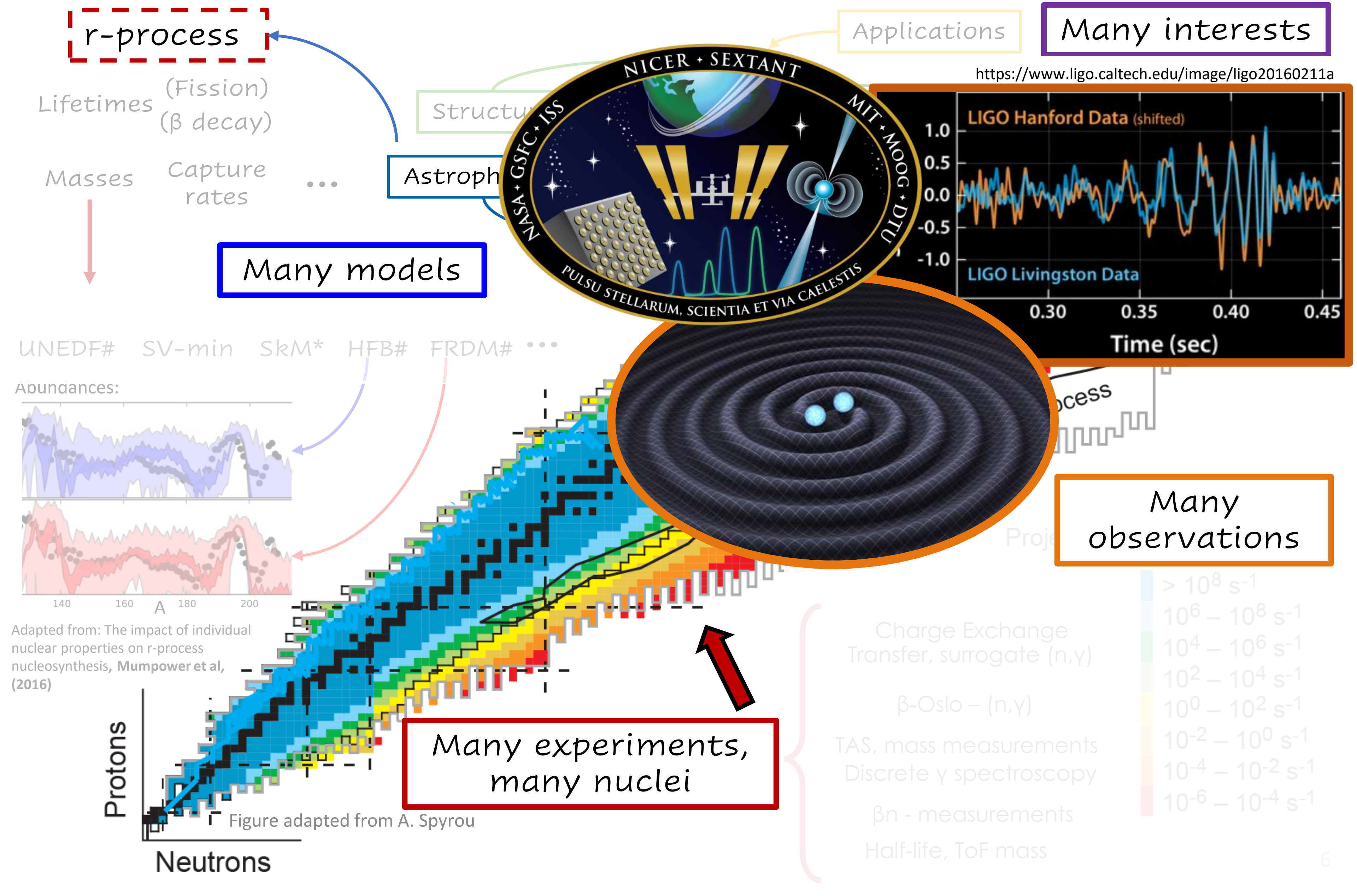
β-Oslo – (n,γ)

TAS, mass measurements
Discrete γ spectroscopy

βn - measurements

Half-life, ToF mass

Cycle example



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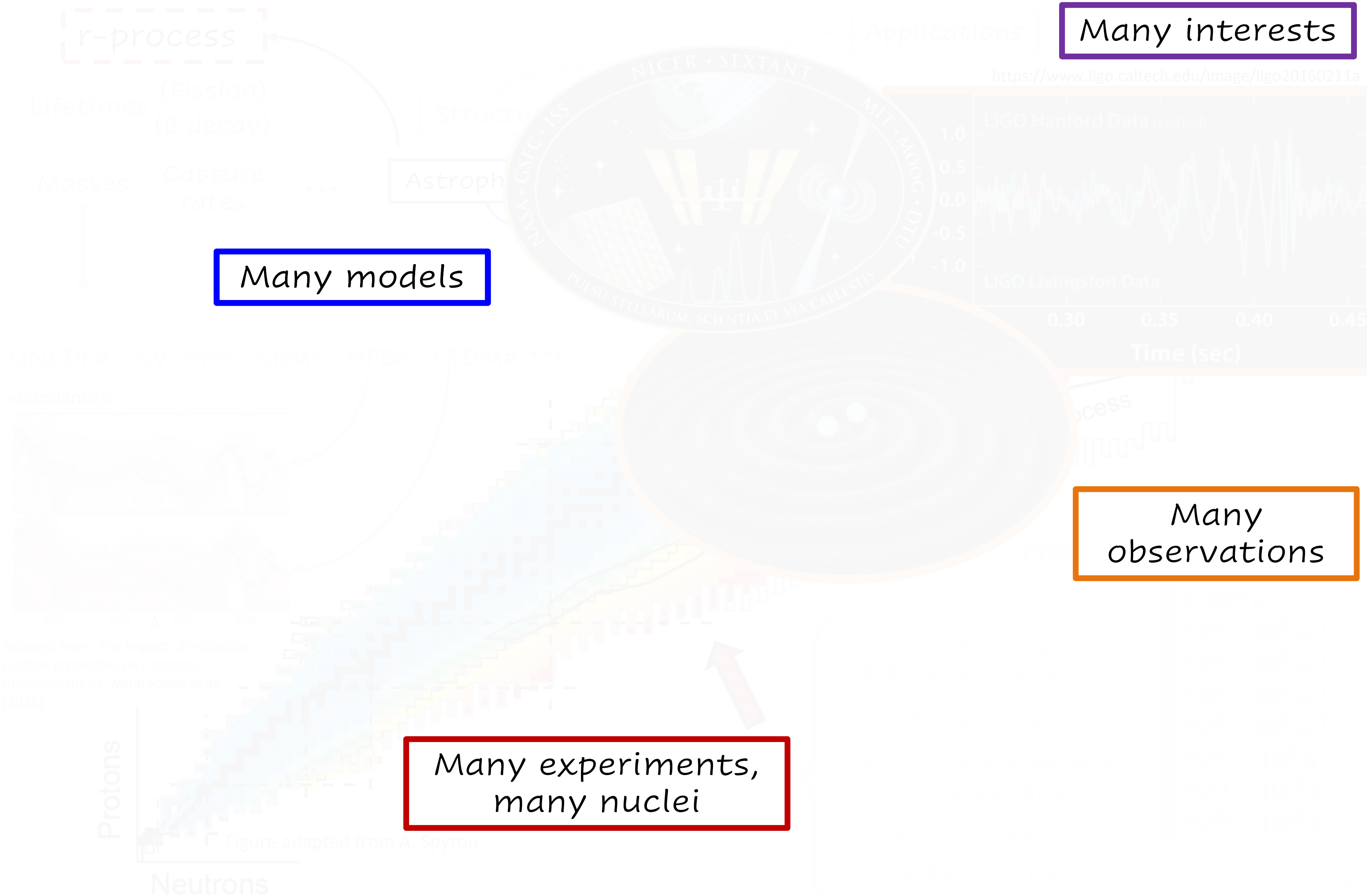


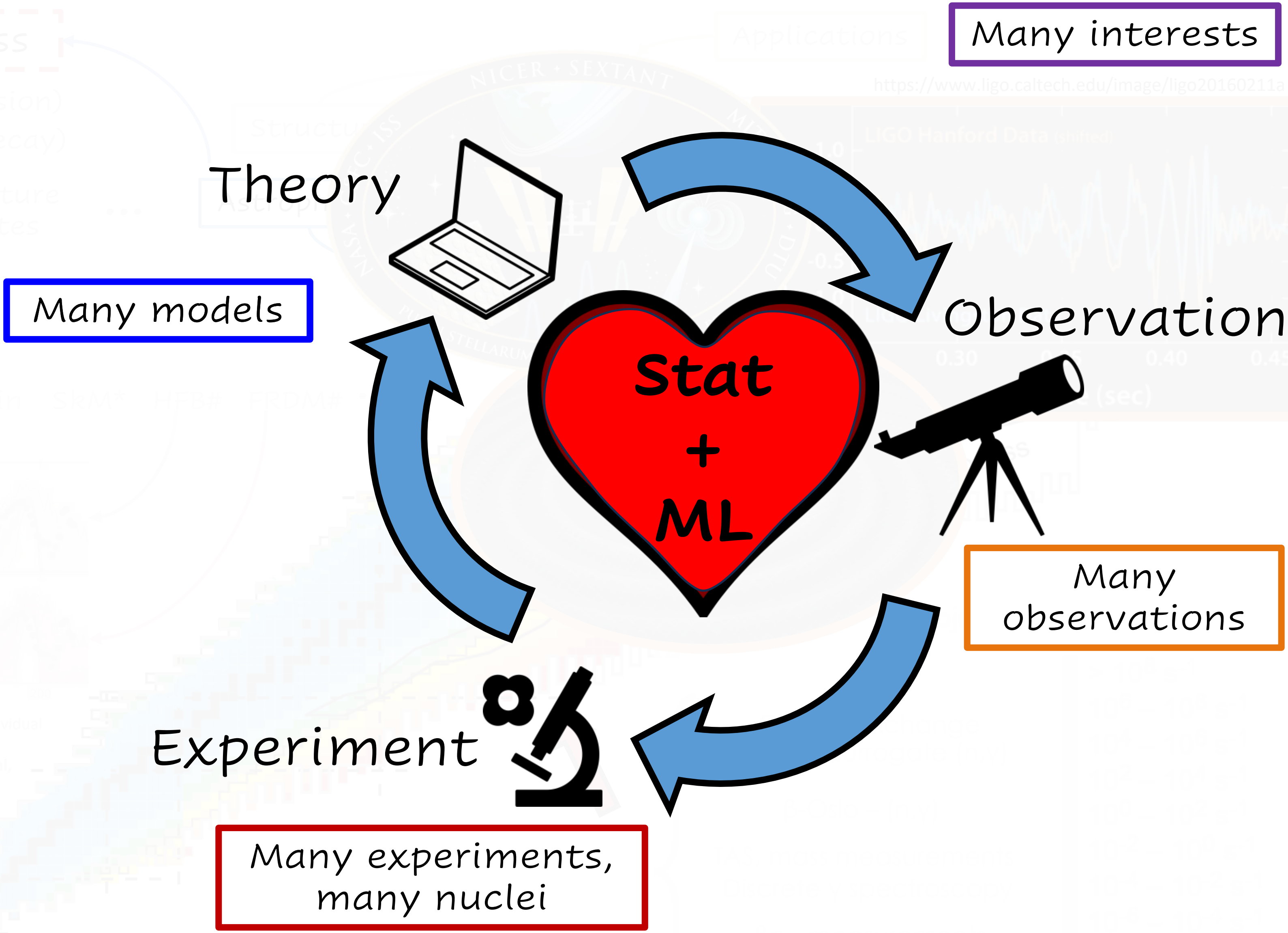
Many interests

Many models

Many observations

Many experiments, many nuclei

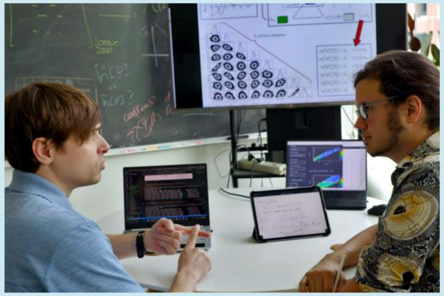
Cycle example



Cycle example

Sidebar 7.2 How Nuclear Theory Fosters Innovation

The nuclear theory ecosystem functions holistically to guide and support experimental programs, develop the theoretical and computational directions of the future, and communicate and integrate new results with other science and technology domains. It also provides invaluable workforce to critical areas of the US economy. Universities and national laboratories are the engines that drive us toward these intertwined short-, medium-, and long-term goals. The last decade has seen several advances that have sprouted in small local research groups, flourishing there until the ideas and methods could be widely adopted and incorporated into the priorities of larger parts of the ecosystem. Here we discuss two representative examples.



[S55]

Full quantification of uncertainties in predictions Around the time of the last LRP, several researchers in university and laboratory groups began using data-intensive Bayesian statistical methods to systematically include nuclear physics model uncertainties in predictions and in parameter inference. The resulting methods have improved our ability to compare theory with experiment in all subfields of nuclear science. One science application is the Bayesian analysis of the transport particles of dense nuclear matter. These methods are now part of the toolkit employed in many larger efforts (e.g., topical collaborations) and are being disseminated through multi-institutional collaborations such as the Bayesian Analysis of Nuclear Dynamics Cyberinfrastructure for Sustained Scientific Innovation (CSSI) software framework. The ability to better fit and compare theory with data is also beneficial to the nuclear data enterprise. Because research in this area involves data analysis and machine learning tools, students working on these projects have proven highly employable beyond nuclear physics, proceeding, for example, to careers in quantum computing, to data-driven activities in other research fields such as medical science, and throughout the private sector.

8 DEVELOPING A NUCLEAR WORKFORCE FOR THE BENEFIT OF SOCIETY

8.1 INTRODUCTION

People are central to the scientific enterprise. A discussion of the compelling nuclear science for the next decade must inherently include a discussion of the people—at every level—who will pursue that science and the skills and societal applications that spring from it.

A skilled nuclear science workforce contributes substantially to US innovation and economic growth, including the development of new machine learning tools for finance, the careful and state-of-the-art treatment of cancer patients, and the education of the next generation (Sidebars 8.1 and 2.1 highlight some of these individuals). However, the number of

FRIB-TA Summer School: Practical Uncertainty Quantification and Emulator Development in Nuclear Physics

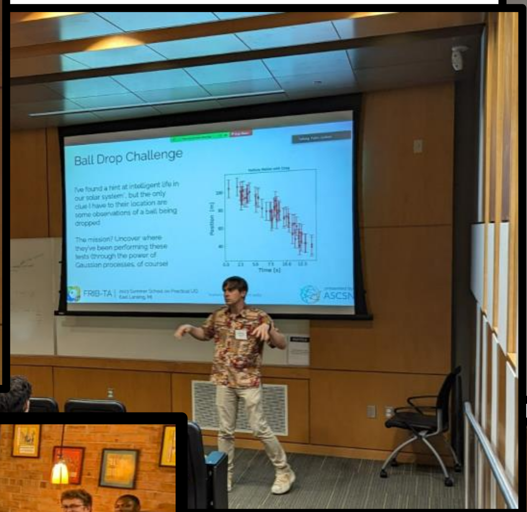
Theory Alliance
FACILITY FOR RARE ISOTOPE BEAMS

Edgard B. | Rahul J.
Me G. | Fernando M.
Kyle G. | Alexandra S.
Morten H. | Frederi V.

June 26 – June 28 2023

https://forum.ascsn.net/t/about-the-2023-frib-ta-summer-school/42

Link to recordings



"This was a very holistic and humane Summer School. I didn't just grow as a physicist, but as a person!"

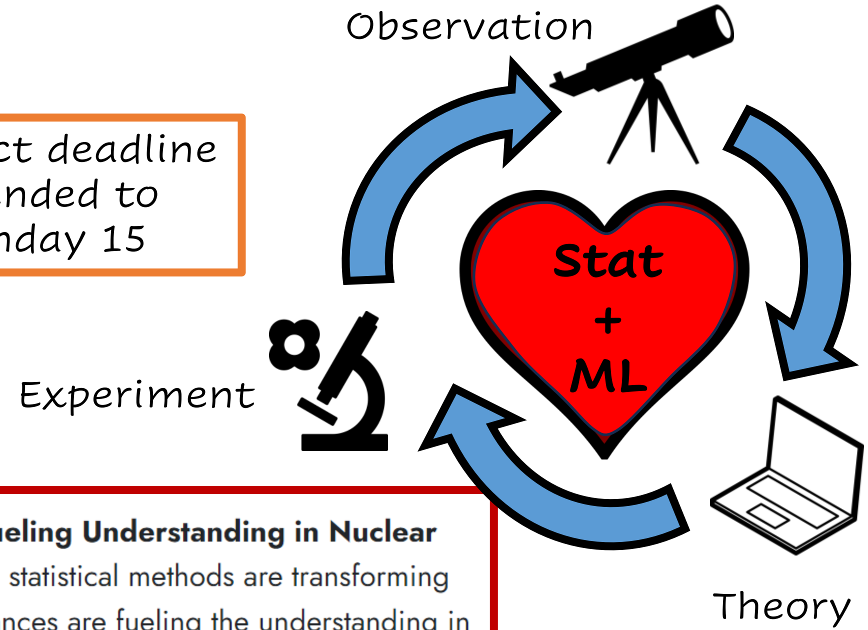
-Anonymous (feedback)

DNP 2024

Fall Meeting of the APS
Division of Nuclear Physics

October 7-10

Abstract deadline extended to Monday 15



From Data to Discovery: How Machine Learning and Statistics are Fueling Understanding in Nuclear Physics - Recent advances in cutting-edge machine learning and advanced statistical methods are transforming science across all disciplines. The lead speaker will discuss how these advances are fueling the understanding in nuclear physics and the role that open-source science and community-driven development plays in lowering the barrier for participation in the computational sciences. The speaker will also describe efforts to build inclusive online collaboration spaces and share resources for kickstarting the uptake of advanced scientific computing. All contributed speakers and the audience in the session will have the opportunity to collaborate and participate in this endeavour.

DNP 2024

Fall Meeting of the APS
Division of Nuclear Physics

October 7-10

Let's normalize the conversation

Lifting the Shadows: DEI Panel - This session aims to create an open space to discuss the impact that disruptive behaviors – including sexual harassment and general mistreatment – have on the workforce, and to identify community-driven efforts we can adopt to better protect those that are most vulnerable. After the presentations the speakers and audience will engage in a panel discussion directly addressing these issues in an attempt to foster alliances, share ideas, and work together to lift the shadows disrupting our community.

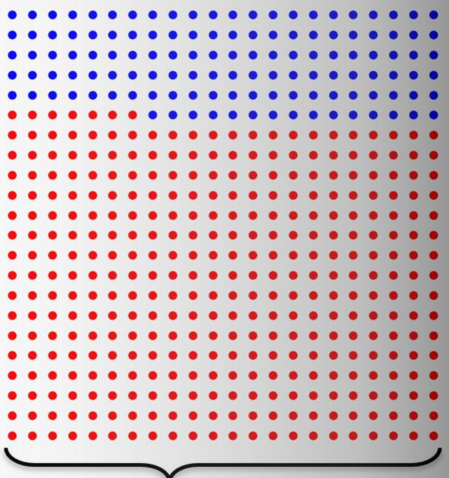
RECOMMENDATION 1

… to capitalize on the extraordinary opportunities for scientific discovery… ***We must draw on the talents of all in the nation to achieve this goal.***

- Expanding policy and resources to ensure a safe and respectful environment for everyone, realizing the full potential of the US nuclear workforce.

Yes, Sexual Harassment Still Drives Women Out of Physics

by Julie Libarkin, 2019

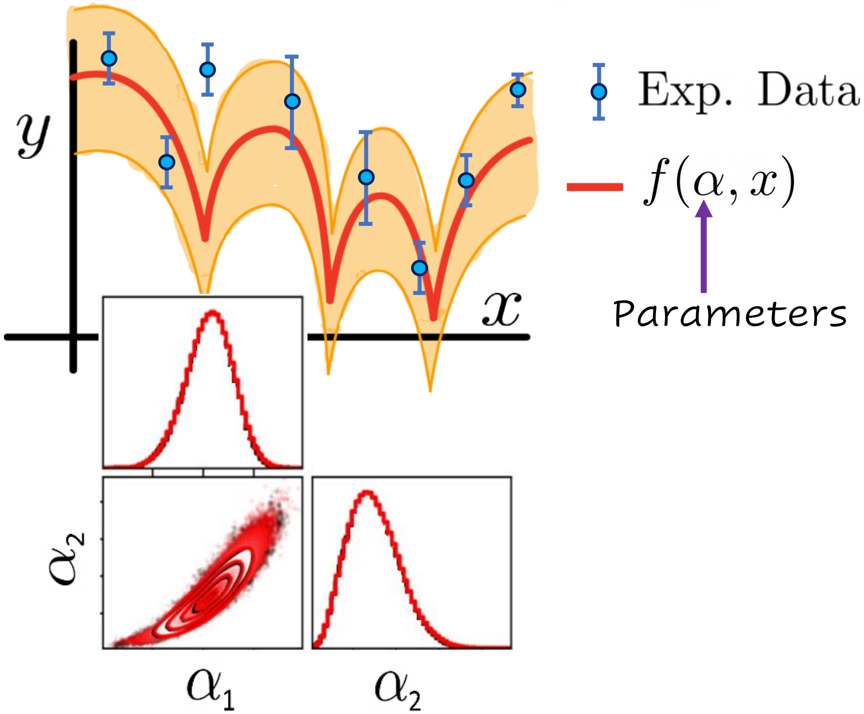


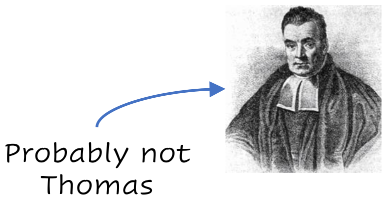
Nearly ***three-quarters*** of the roughly **500** undergraduate respondents **experienced some form of sexual harassment.**

https://github.com/ascsn/2023-FRIB-TA-Summer-School

Bayesian Formulation

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





https://github.com/ascsn/2023-FRIB-TA-Summer-School

Bayesian Formulation

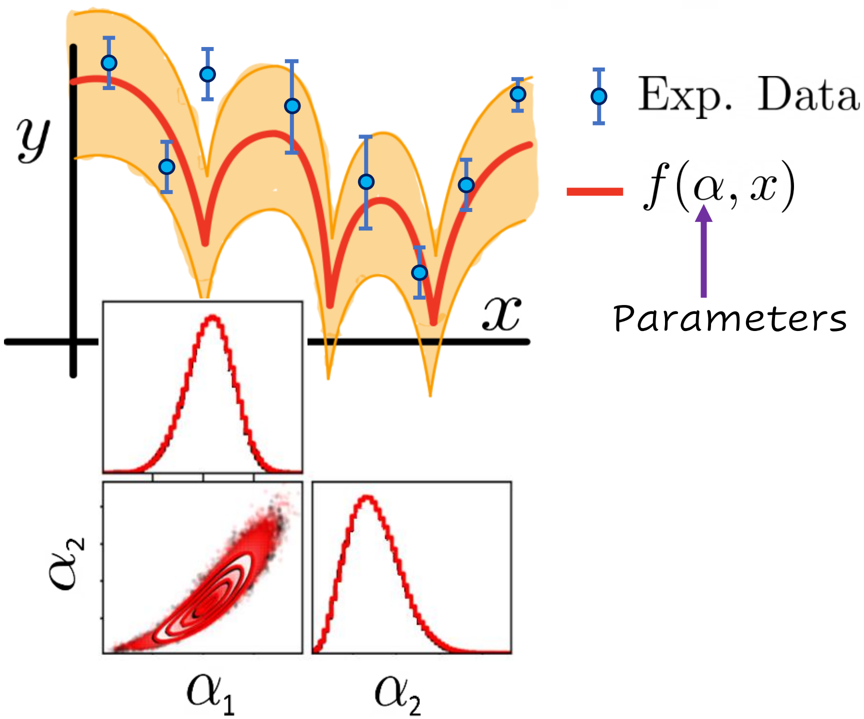
(what we want)
Posterior

(what we think happened)
Likelihood

(what we think we know)
Prior

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

Evidence
(how much sense all makes)



Bayesian Formulation

(what we want) **Posterior**

(what we think happened) **Likelihood**

(what we think we know) **Prior**

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

Evidence (how much sense all makes)

Advantages:

1) Assumptions are clearly stated

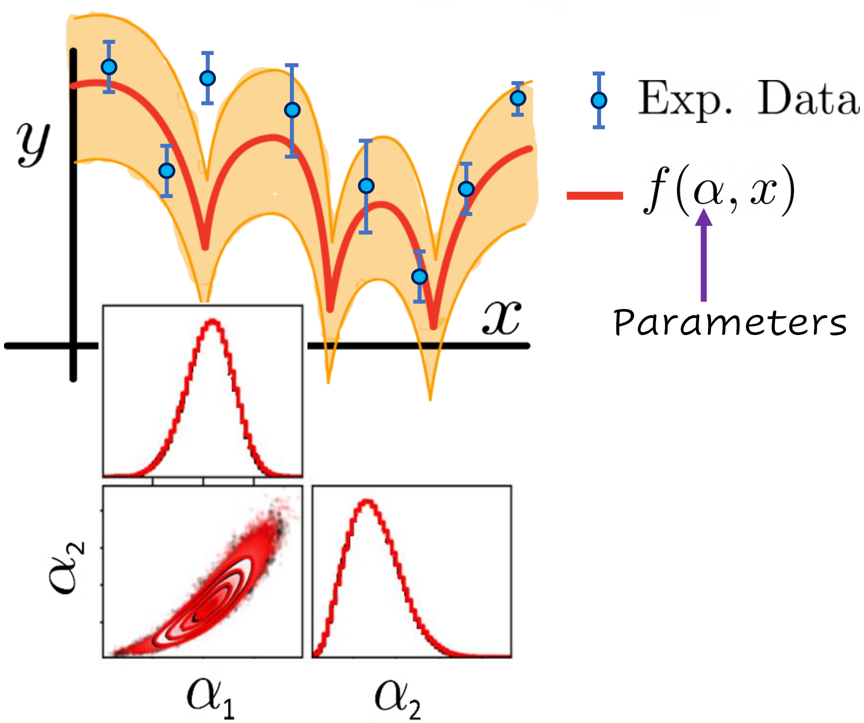
2) Allows for natural continuous learning

Probably not Thomas

Challenge 1: repeated evaluations

Likelihood

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



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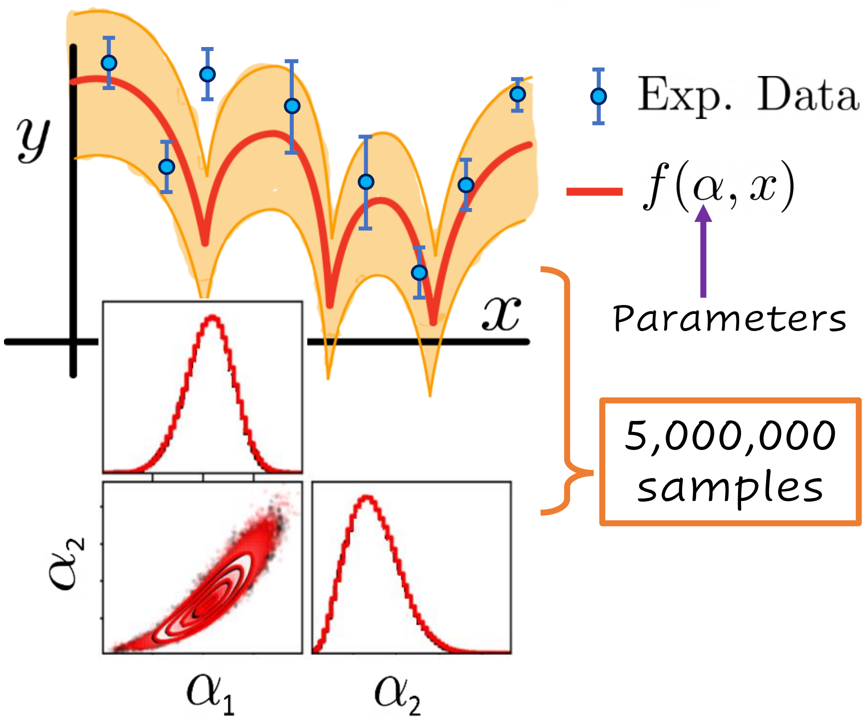

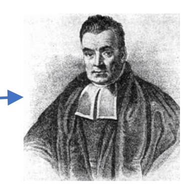

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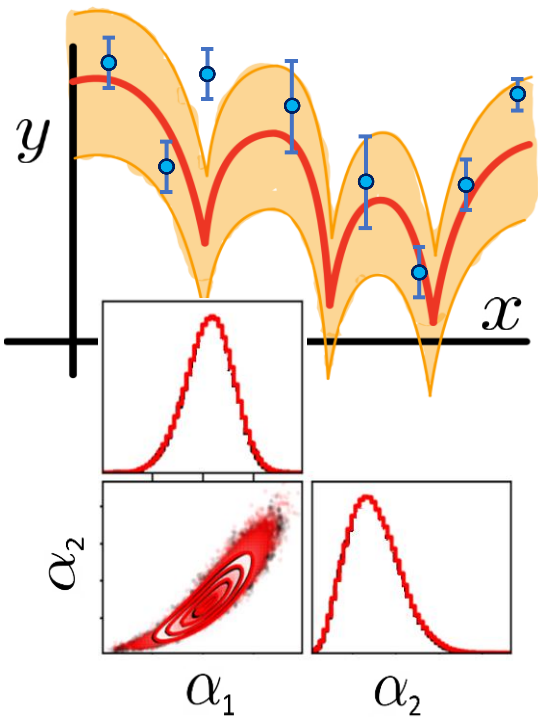


Exp. Data

$f(\alpha, x)$

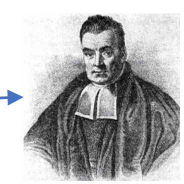
Parameters

5,000,000 samples

$f(\alpha, x)$

1 second → 2 months

1 hour → 1/2 century



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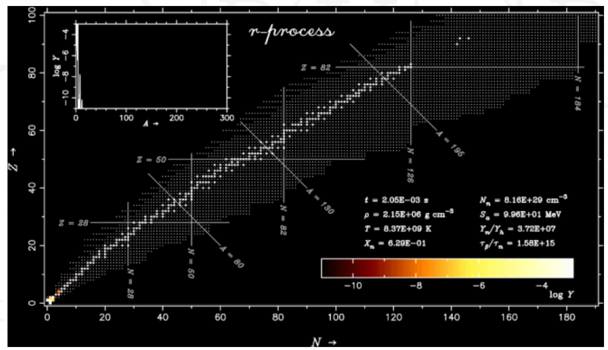
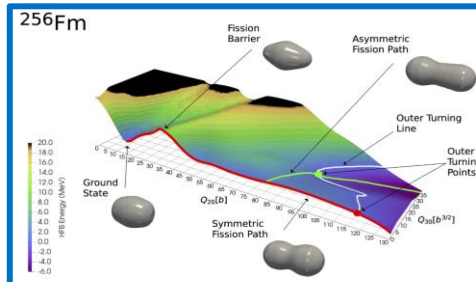
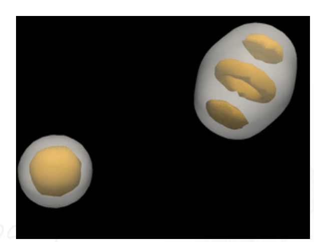


R-process abundances

Potential Energy Surfaces



Time dependent density functional theory



1/2 century

1 hour

$f(\alpha, x)$

Challenge 1: repeated evaluations

Jean-François Paquet

- For one choice of model parameters:
  - Simulate 10^3-10^4 collisions (expt: 10^6) [model is stochastic]
  - Simulation: a few core-minute/collision
  - = ~100-1000 core-hours per param
- 1k param samples → ~ 10^5-10^6 core-hour
- 10k param samples → ~ 10^6-10^7 core-hour

Heavy ion collisions

Many-body problem

Andreas Ekström

Computing nuclei: an HPC problem

Solving the Schrödinger equation for a large collection of strongly interacting nucleons typically requires substantial high-performance computing resources.

Carla Fröhlich

Core-collapse super novae

Self-consistent 3D simulations
- The ultimate goal
- Computationally expensive → can do O(10)

Neutron stars

Dense matter physics in a nutshell

Bayesian inference requires ~10^7 model evaluations

Rahul Somasundaram

$f(\alpha, x)$

MORE

The more accurate PCGP and PCSK emulators give tighter posterior on model parameters than that from the Scikit GP

Open Science Grid delivered 5 million CPU hours for the data generation

Relativistic collisions

Chun Shen

Challenge 1: repeated evaluations

"High Fidelity" → "Emulated"

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

Posterior distribution $P(\alpha|\mathbf{Y}) \longrightarrow \hat{P}(\alpha|\mathbf{Y})$

Challenge 1: repeated evaluations

Dimensionality Reduction

"High Fidelity"

"Emulated"

Physical model $f(\alpha, x) \rightarrow \hat{f}(\alpha, x)$

Posterior distribution $P(\alpha|\mathbf{Y}) \rightarrow \hat{P}(\alpha|\mathbf{Y})$

Model Order Reduction:

- Reduced basis methods (~eigenvector continuation)
- Dynamic Mode Decomposition
- SINDy and NIF
- ...

Gaussian Process

Neural Networks

...

Normalizing flows

Chaos expansion

Variational Bayes

...

Challenge 1: repeated evaluations

Dimensionality Reduction

"High Fidelity"

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- Normalizing flows
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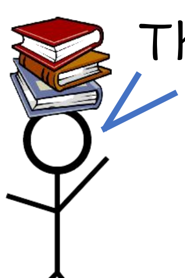
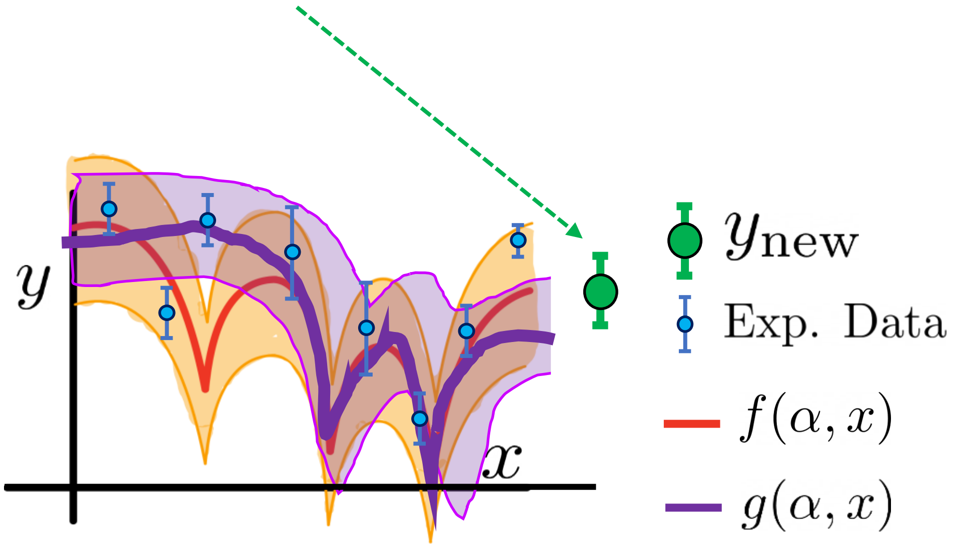


The Fast

Challenge 2: repeated models

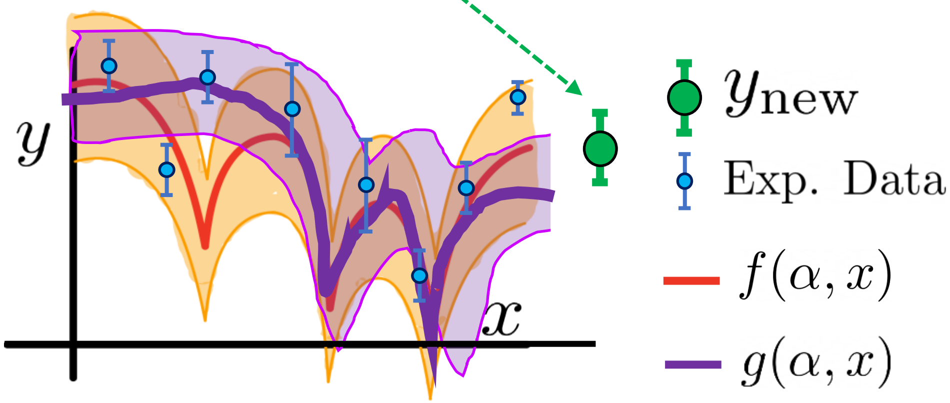
$$P(y_{\text{new}}|\boldsymbol{Y}) = \quad ?$$



Challenge 2: repeated models

$$P(y_{\text{new}}|\mathbf{Y}) = \begin{array}{c} P(y_{\text{new}}|\underline{f}, \mathbf{Y})P(\underline{f}|\mathbf{Y}) \\ + \\ P(y_{\text{new}}|\underline{g}, \mathbf{Y})P(\underline{g}|\mathbf{Y}) \end{array}$$

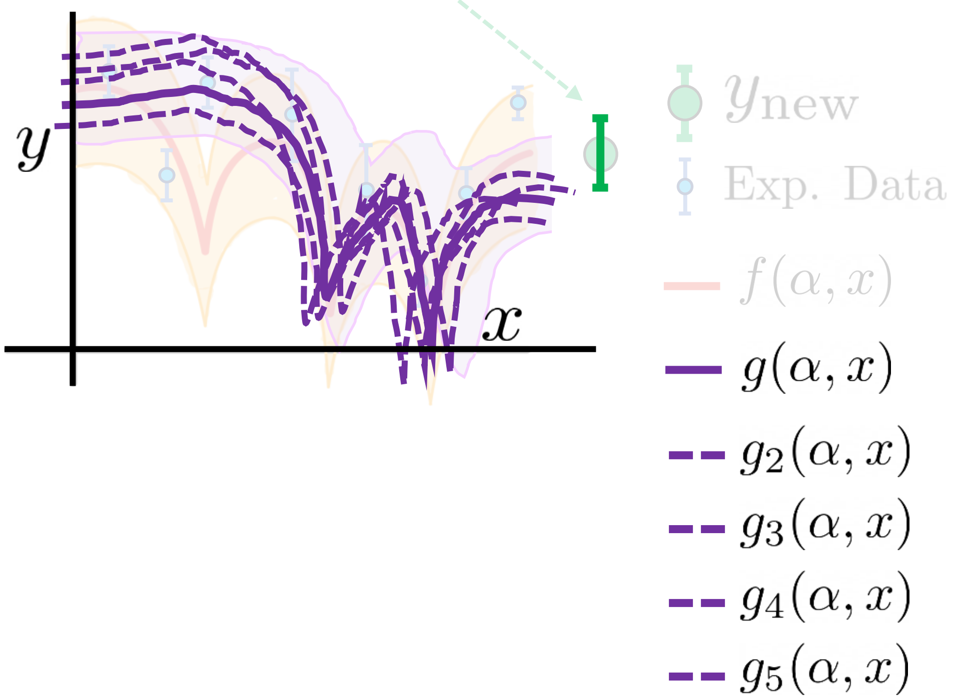
Bayesian Model Averaging



Challenge 2: repeated models

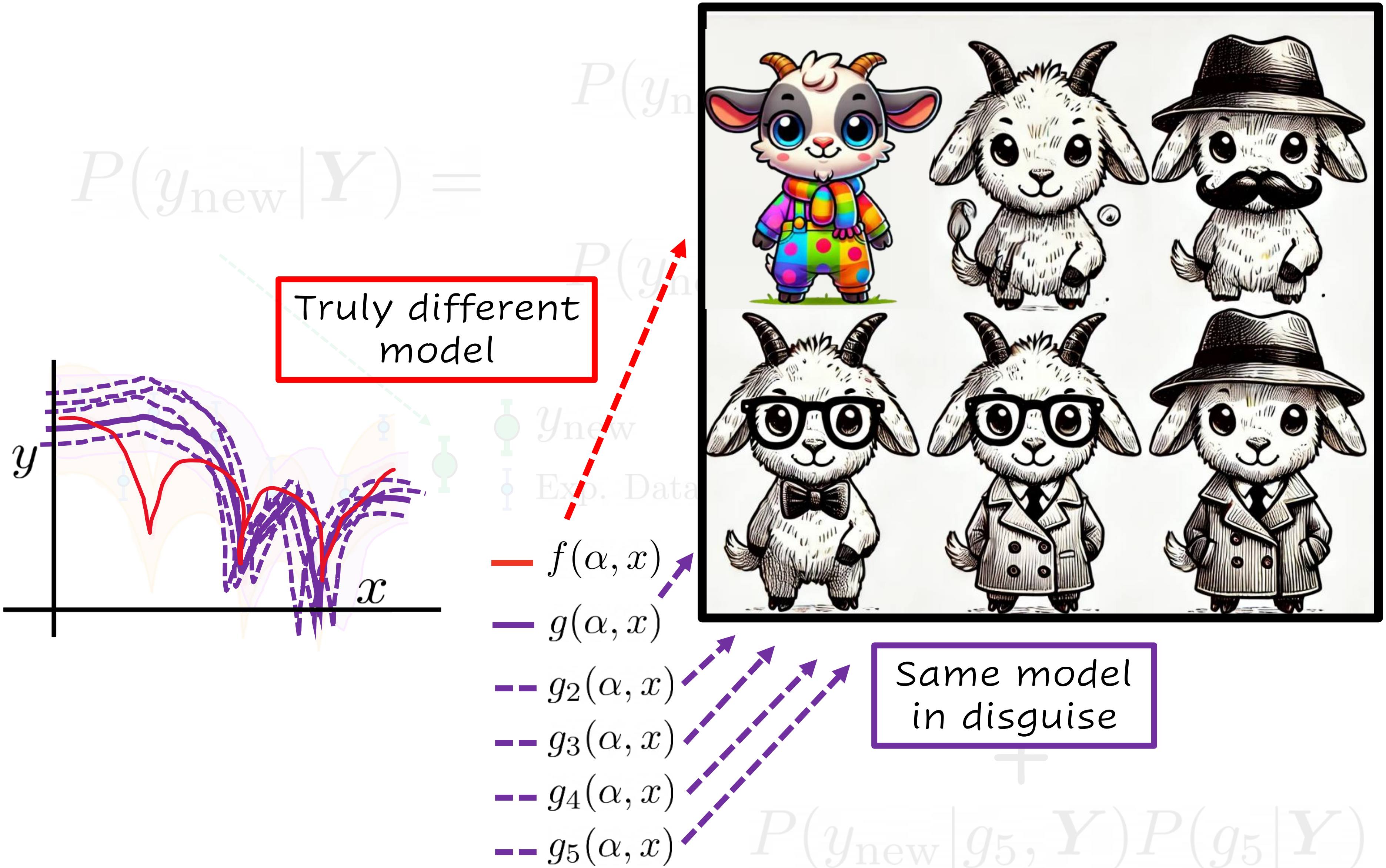
$$P(y_{\text{new}}|\mathbf{Y}) = P(y_{\text{new}}|f,\mathbf{Y})P(f|\mathbf{Y}) + P(y_{\text{new}}|g,\mathbf{Y})P(g|\mathbf{Y})$$

Bayesian Model Averaging

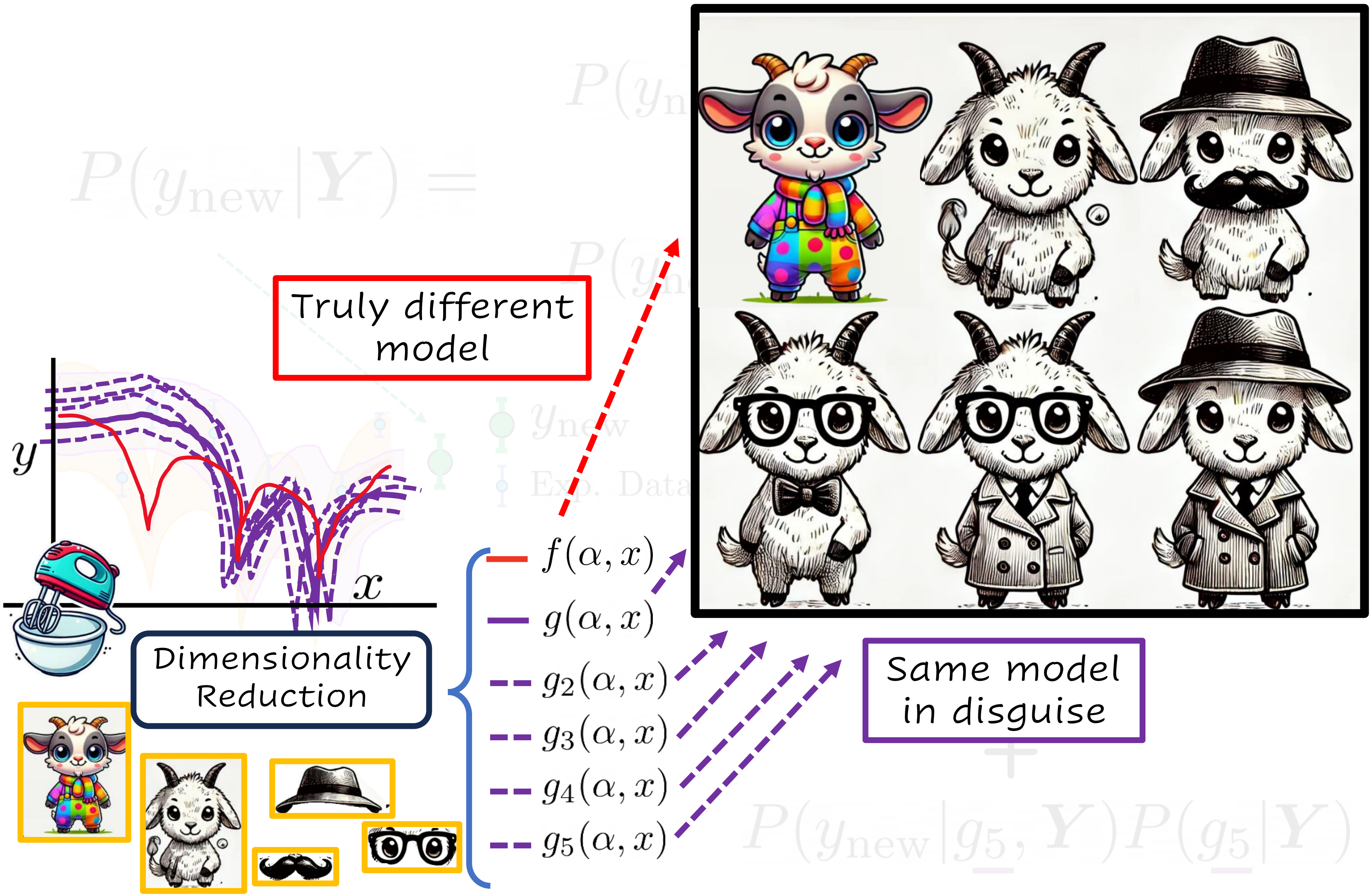


$$P(y_{\text{new}}|g_2,\mathbf{Y})P(g_2|\mathbf{Y}) + \cdots + P(y_{\text{new}}|g_5,\mathbf{Y})P(g_5|\mathbf{Y})$$

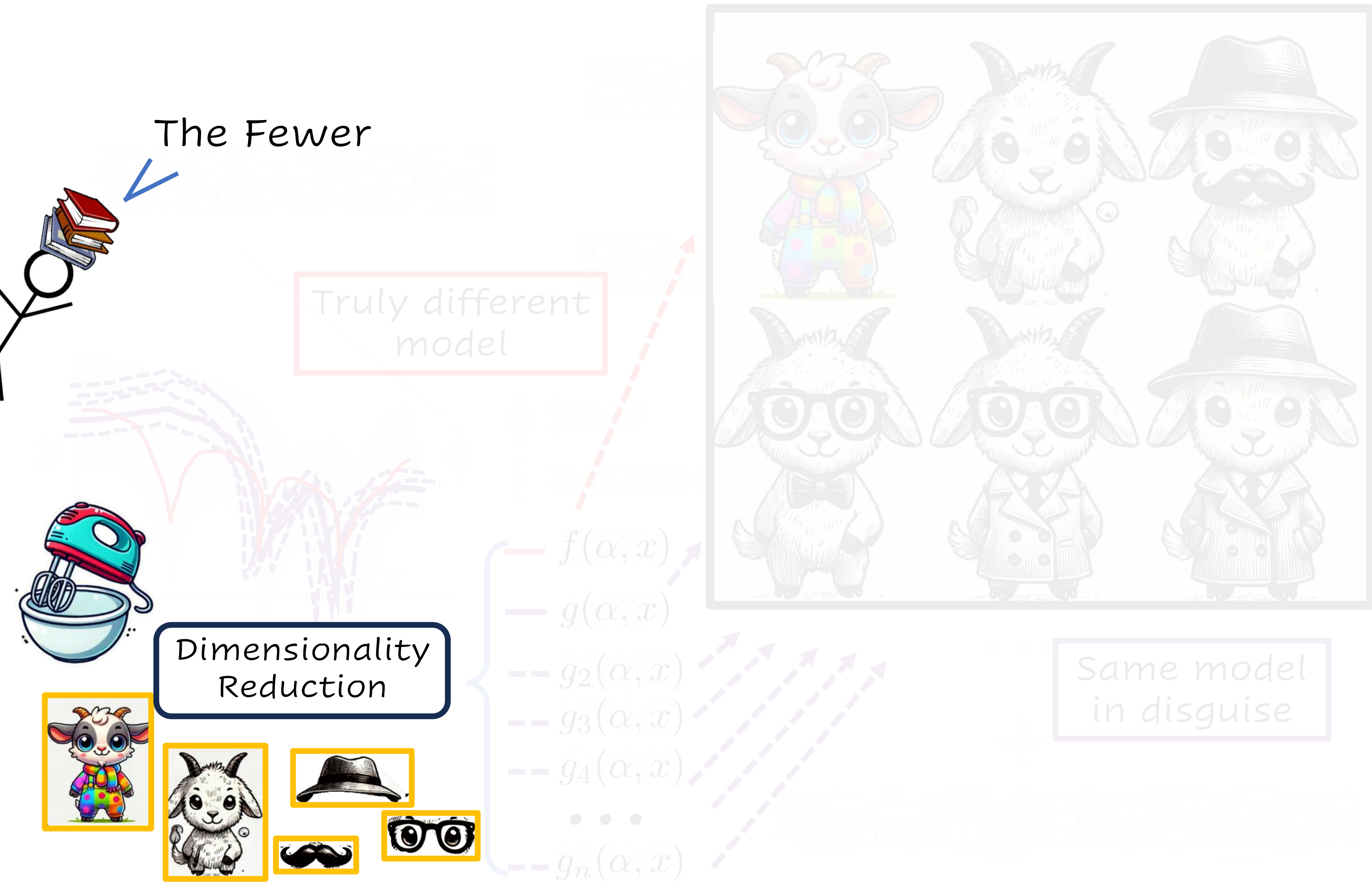
Challenge 2: repeated models



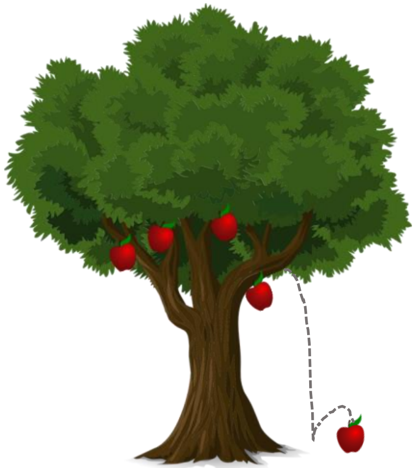
Challenge 2: repeated models

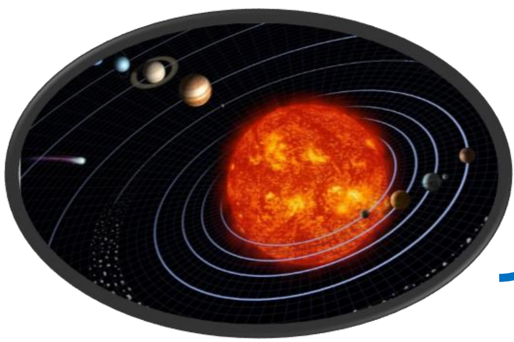


Challenge 2: repeated models



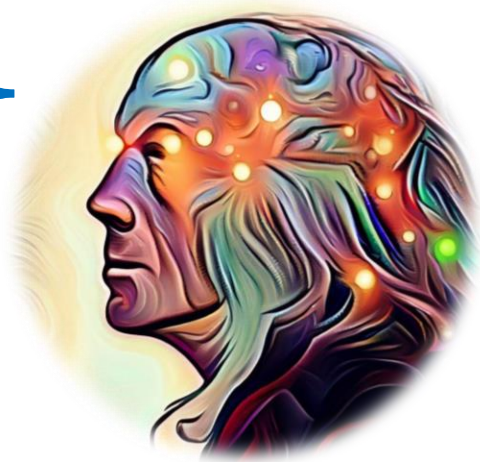
Computation paradigm





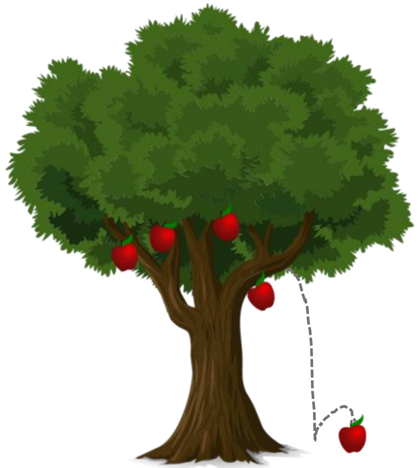
Nature

(created by DALL-E)



Newton
(XVII century)

Computation paradigm



Nature

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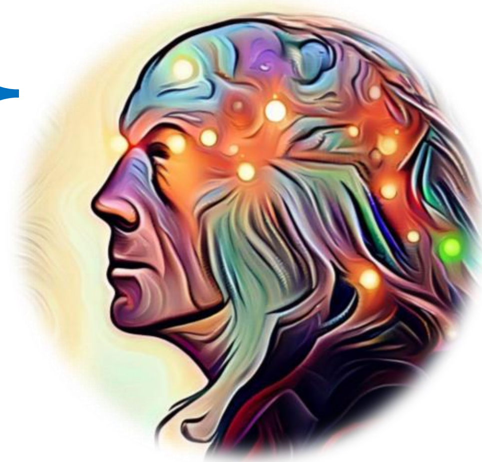


Newton
(XVII century)

$$F = G\frac{m_1 m_2}{r^2}$$

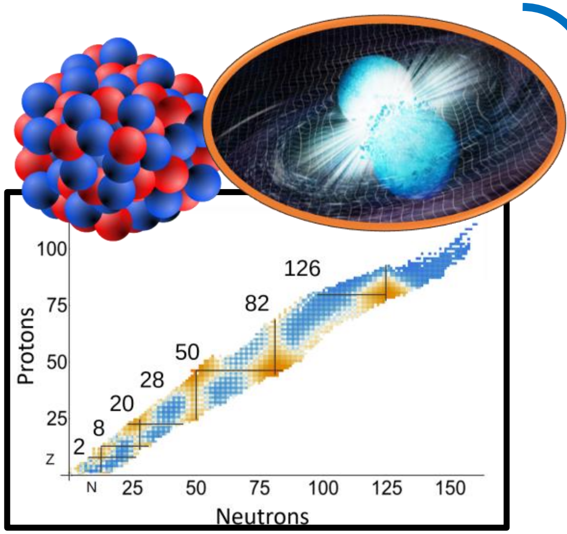
Calculations

Explain

Predict

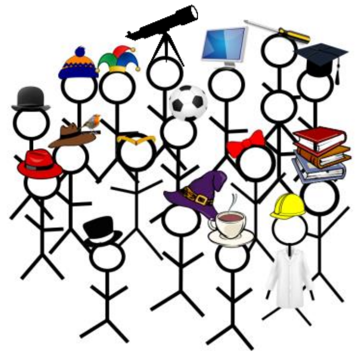
Build

Computation paradigm



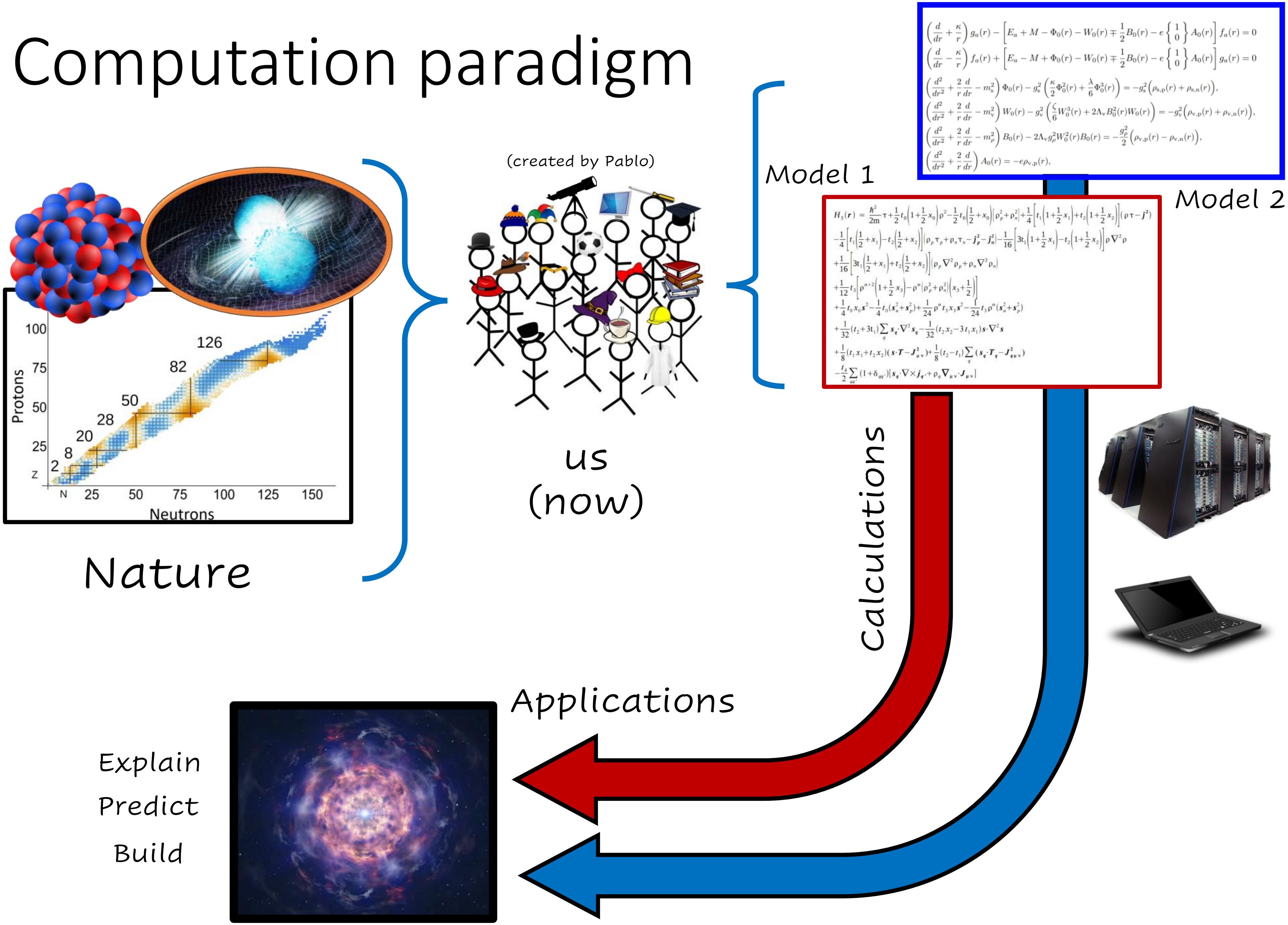
Nature

(created by Pablo)

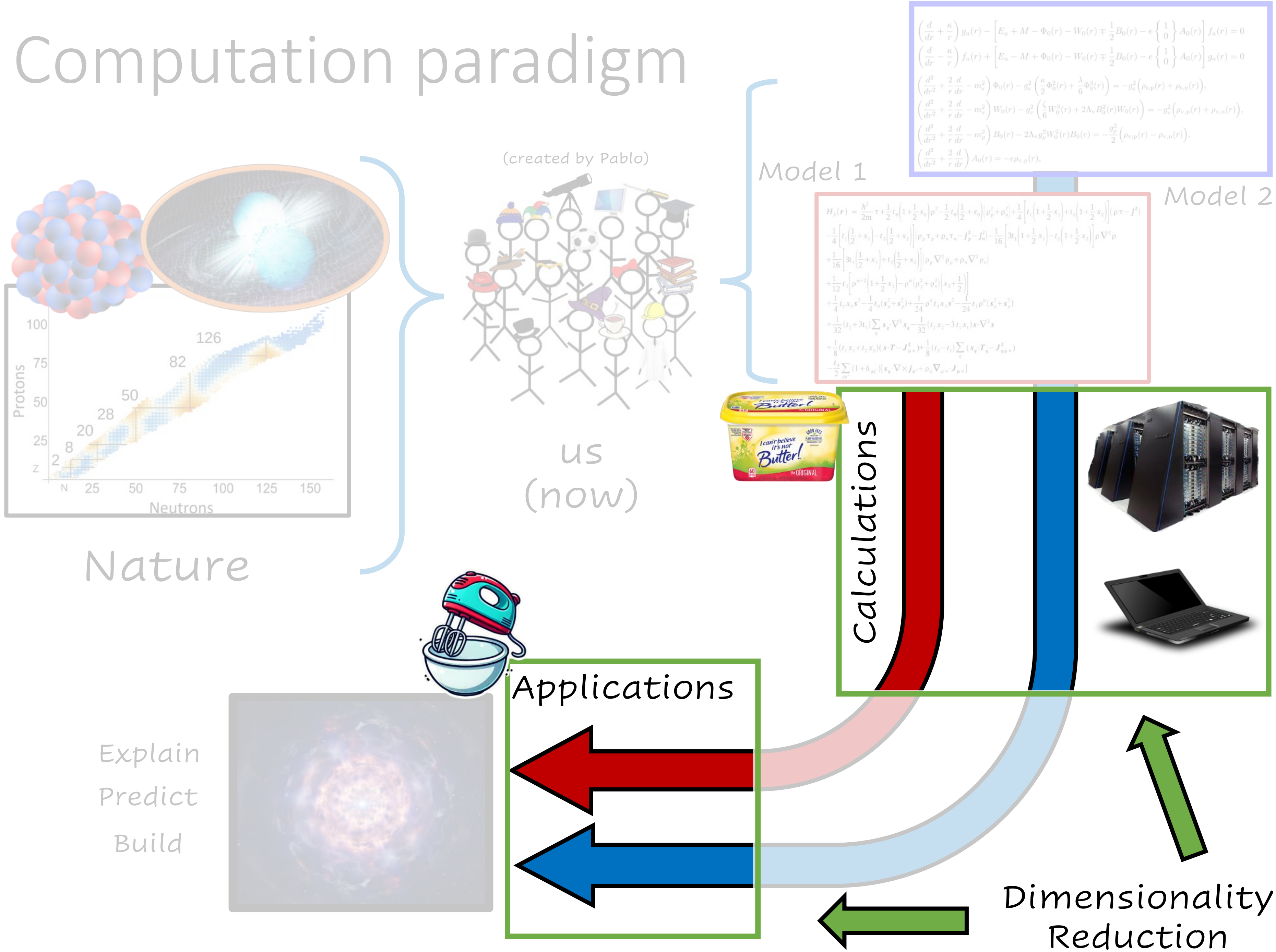


us
(now)

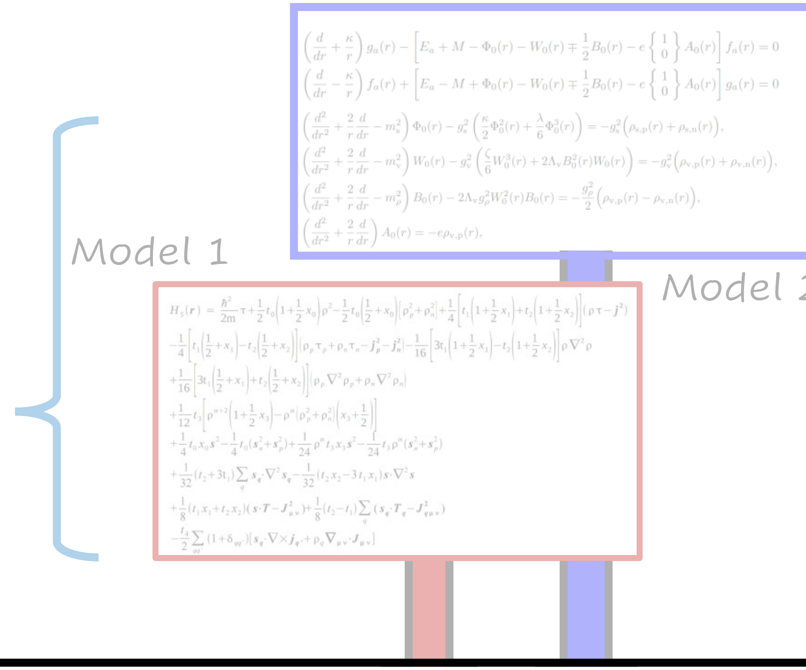
Computation paradigm



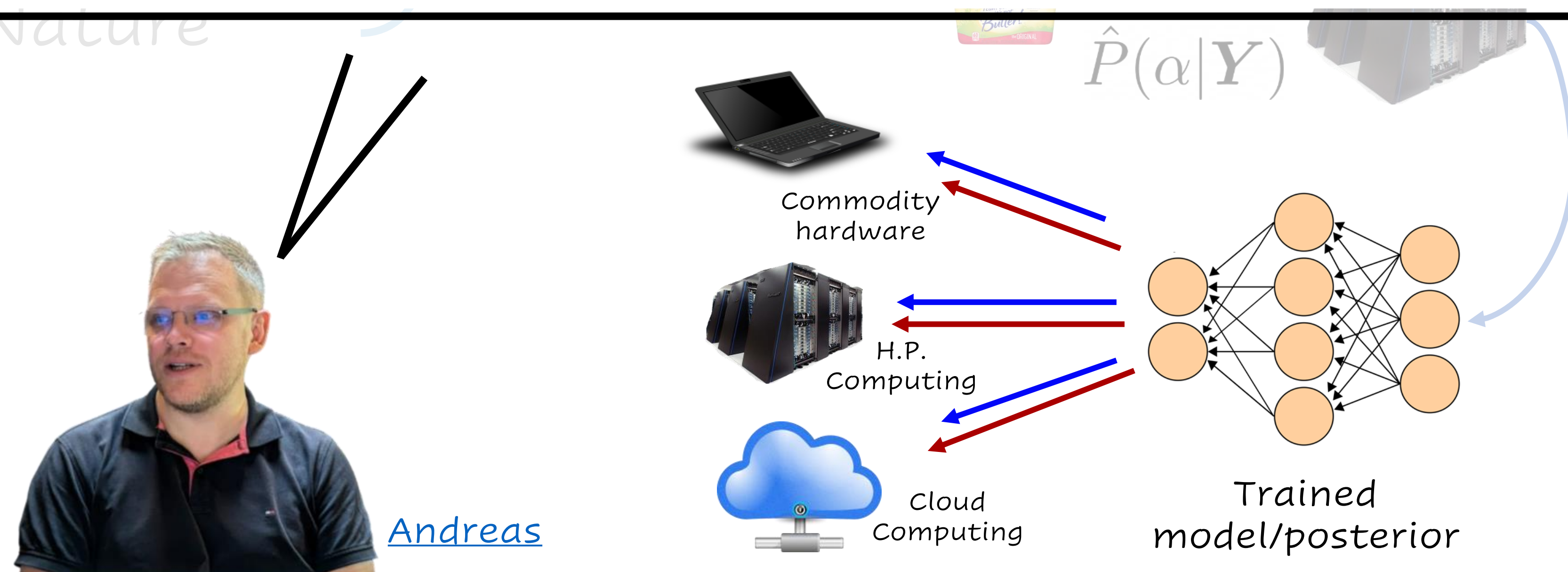
Computation paradigm



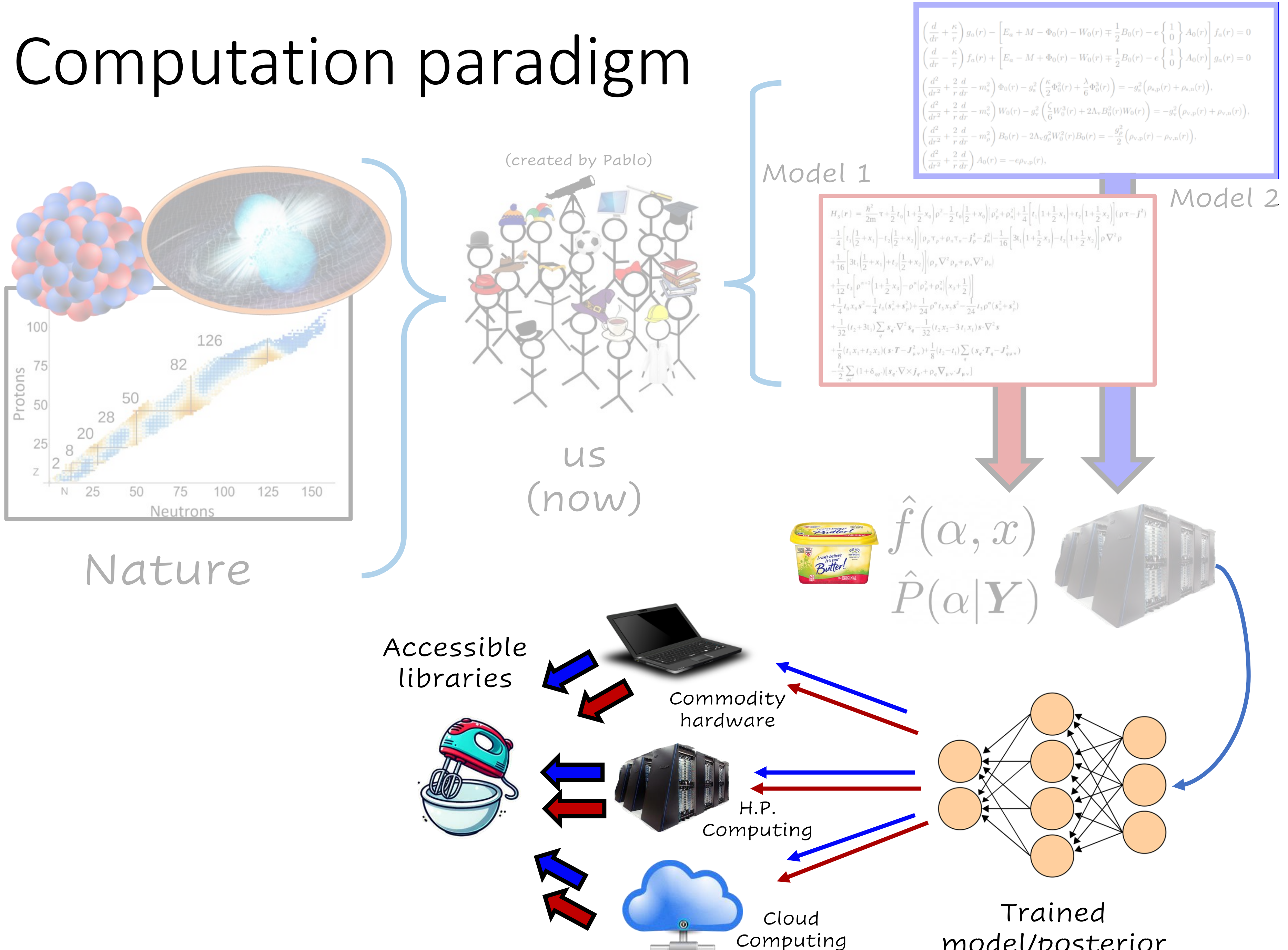
Computation paradigm

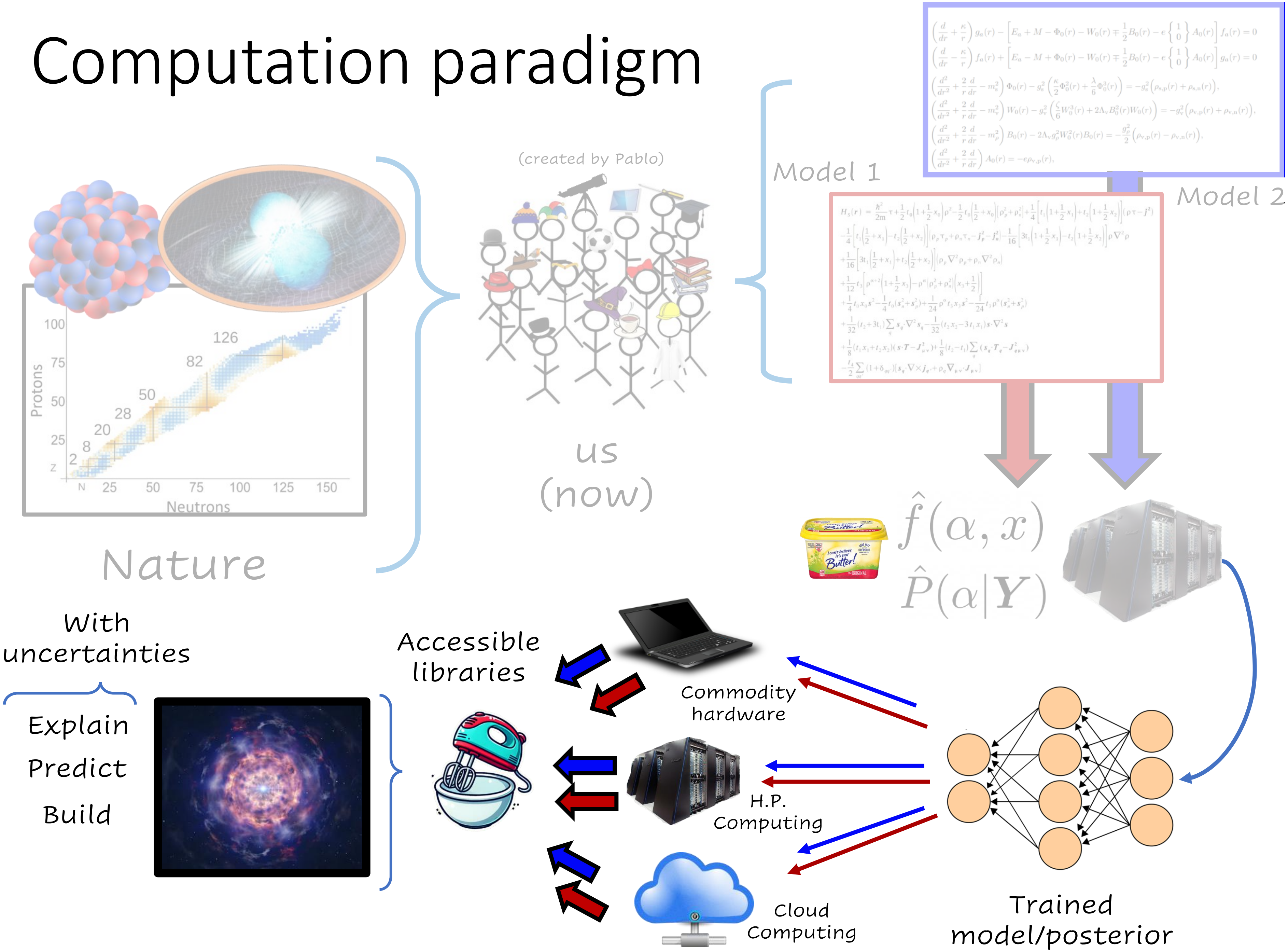


develop (and share!) emulators for managing computational costs and facilitating model mixing for comprehensive inference and better predictive performance.



Computation paradigm

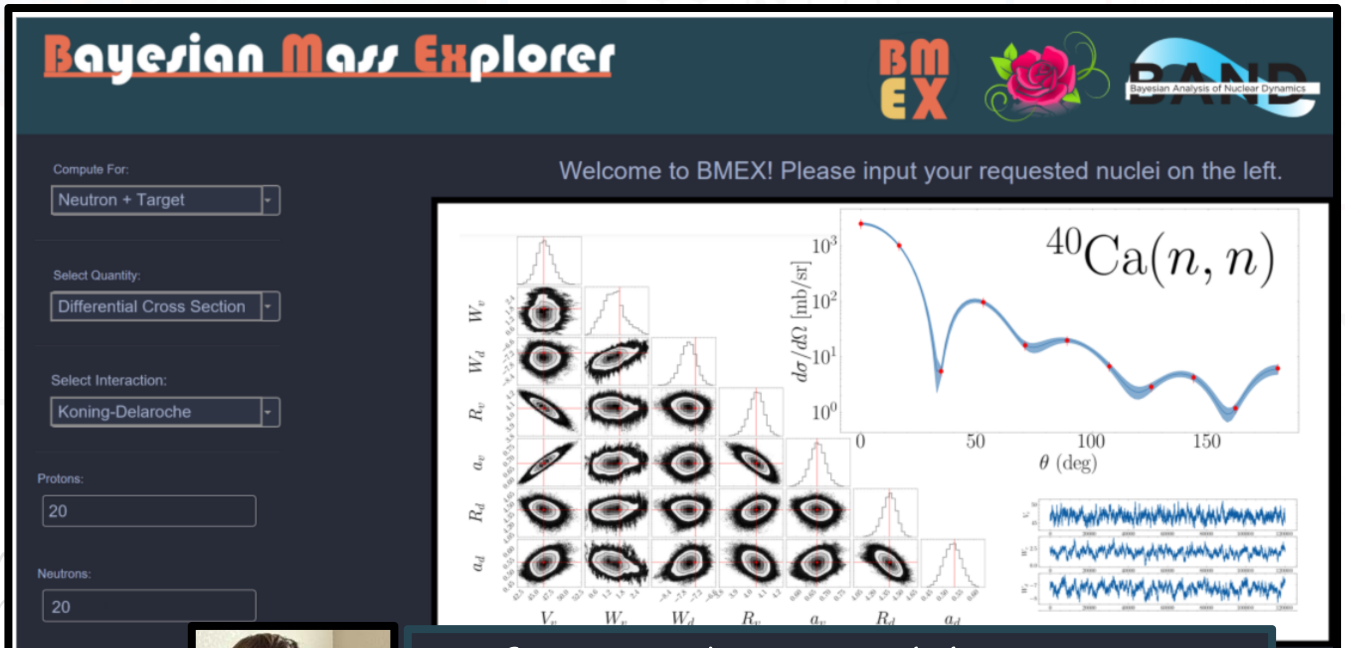




Computation paradigm
(created by Pablo)
Model 1
Model 2
Protons
Neutrons
Nature
us
(now)
$\hat{f}(\alpha, x)$
$\hat{P}(\alpha|\mathbf{Y})$
With
uncertainties
Explain
Predict
Build
Accessible
libraries
Commodity
hardware
H.P.
Computing
Cloud
Computing
Trained
model/posterior

Computation paradigm

https://bmex.dev/



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

Perspectives for Accessible and Reproducible Bayesian Workflows

[Thursday](#)

Link to these slides

Outline

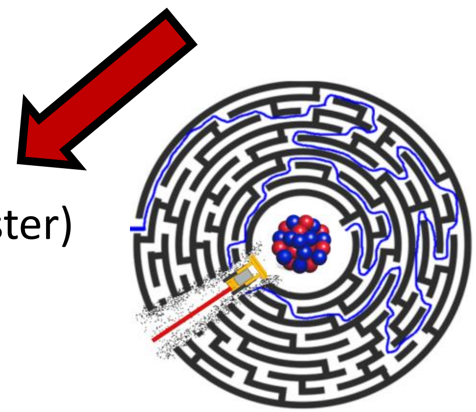
My context

Bayes and Nuclei

Two challenges

Computational paradigm

Dimensionality Reduction



Model Order Reduction (Faster)

Model Combination (Fewer)

Takeaways

How it works

$$
\begin{aligned}
H_S(\boldsymbol{r}) = {} & \frac{\hbar^2}{2m}\tau + \frac{1}{2}t_0\left(1+\frac{1}{2}x_0\right)\rho^2 - \frac{1}{2}t_0\left(\frac{1}{2}+x_0\right)\left[\rho_p^2+\rho_n^2\right] + \frac{1}{4}\left[t_1\left(1+\frac{1}{2}x_1\right)+t_2\left(1+\frac{1}{2}x_2\right)\right](\rho\tau - \boldsymbol{j}^2) \\
& -\frac{1}{4}\left[t_1\left(\frac{1}{2}+x_1\right)-t_2\left(\frac{1}{2}+x_2\right)\right]\left(\rho_p\tau_p+\rho_n\tau_n-\boldsymbol{j}_p^2-\boldsymbol{j}_n^2\right) - \frac{1}{16}\left[3t_1\left(1+\frac{1}{2}x_1\right)-t_2\left(1+\frac{1}{2}x_2\right)\right]\rho\nabla^2\rho \\
& +\frac{1}{16}\left[3t_1\left(\frac{1}{2}+x_1\right)+t_2\left(\frac{1}{2}+x_2\right)\right]\left(\rho_p\nabla^2\rho_p+\rho_n\nabla^2\rho_n\right) \\
& +\frac{1}{12}t_3\left[\rho^{\alpha+2}\left(1+\frac{1}{2}x_3\right)-\rho^{\alpha}\left(\rho_p^2+\rho_n^2\right)\left(x_3+\frac{1}{2}\right)\right] \\
& +\frac{1}{4}t_0x_0\boldsymbol{s}^2-\frac{1}{4}t_0(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2)+\frac{1}{24}\rho^{\alpha}t_3x_3\boldsymbol{s}^2-\frac{1}{24}t_3\rho^{\alpha}(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2) \\
& +\frac{1}{32}(t_2+3t_1)\sum_q \boldsymbol{s}_q\cdot\nabla^2\boldsymbol{s}_q-\frac{1}{32}(t_2x_2-3t_1x_1)\boldsymbol{s}\cdot\nabla^2\boldsymbol{s} \\
& +\frac{1}{8}(t_1x_1+t_2x_2)(\boldsymbol{s}\cdot\boldsymbol{T}-\boldsymbol{J}_{\mu\nu}^2)+\frac{1}{8}(t_2-t_1)\sum_q(\boldsymbol{s}_q\cdot\boldsymbol{T}_q-\boldsymbol{J}_{q\mu\nu}^2) \\
& -\frac{t_4}{2}\sum_{qq'}(1+\delta_{qq'})[\boldsymbol{s}_q\cdot\nabla\times\boldsymbol{j}_{q'}+\rho_q\nabla_{\mu\nu}\cdot\boldsymbol{J}_{\mu\nu}]
\end{aligned}
$$

Density Functional Theory

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

Parameters: α

$$\left\{\rho_c, E^{NM}/A, K^{NM}, a_{sym}^{NM}, L_{sym}^{NM}, M_s^*, C_t^{\rho\Delta\rho}, C_t^{\rho\nabla J}\right\}$$

How it works

$$
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& -\frac{1}{4}\left[t_1\left(\frac{1}{2}+x_1\right)-t_2\left(\frac{1}{2}+x_2\right)\right]\left(\rho_p\tau_p+\rho_n\tau_n-\boldsymbol{j}_p^2-\boldsymbol{j}_n^2\right)-\frac{1}{16}\left[3t_1\left(1+\frac{1}{2}x_1\right)-t_2\left(1+\frac{1}{2}x_2\right)\right]\rho\nabla^2\rho\\
& +\frac{1}{16}\left[3t_1\left(\frac{1}{2}+x_1\right)+t_2\left(\frac{1}{2}+x_2\right)\right]\left(\rho_p\nabla^2\rho_p+\rho_n\nabla^2\rho_n\right)\\
& +\frac{1}{12}t_3\left[\rho^{\alpha+2}\left(1+\frac{1}{2}x_3\right)-\rho^{\alpha}\left(\rho_p^2+\rho_n^2\right)\left(x_3+\frac{1}{2}\right)\right]\\
& +\frac{1}{4}t_0x_0\boldsymbol{s}^2-\frac{1}{4}t_0(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2)+\frac{1}{24}\rho^{\alpha}t_3x_3\boldsymbol{s}^2-\frac{1}{24}t_3\rho^{\alpha}(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2)\\
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\end{aligned}
$$

Density Functional Theory

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

Parameters: α

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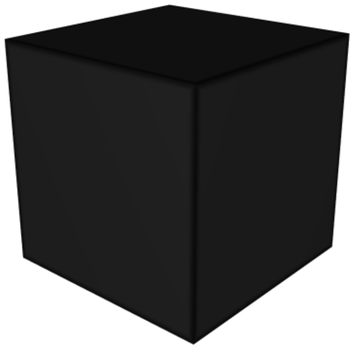
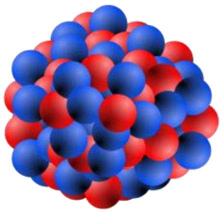
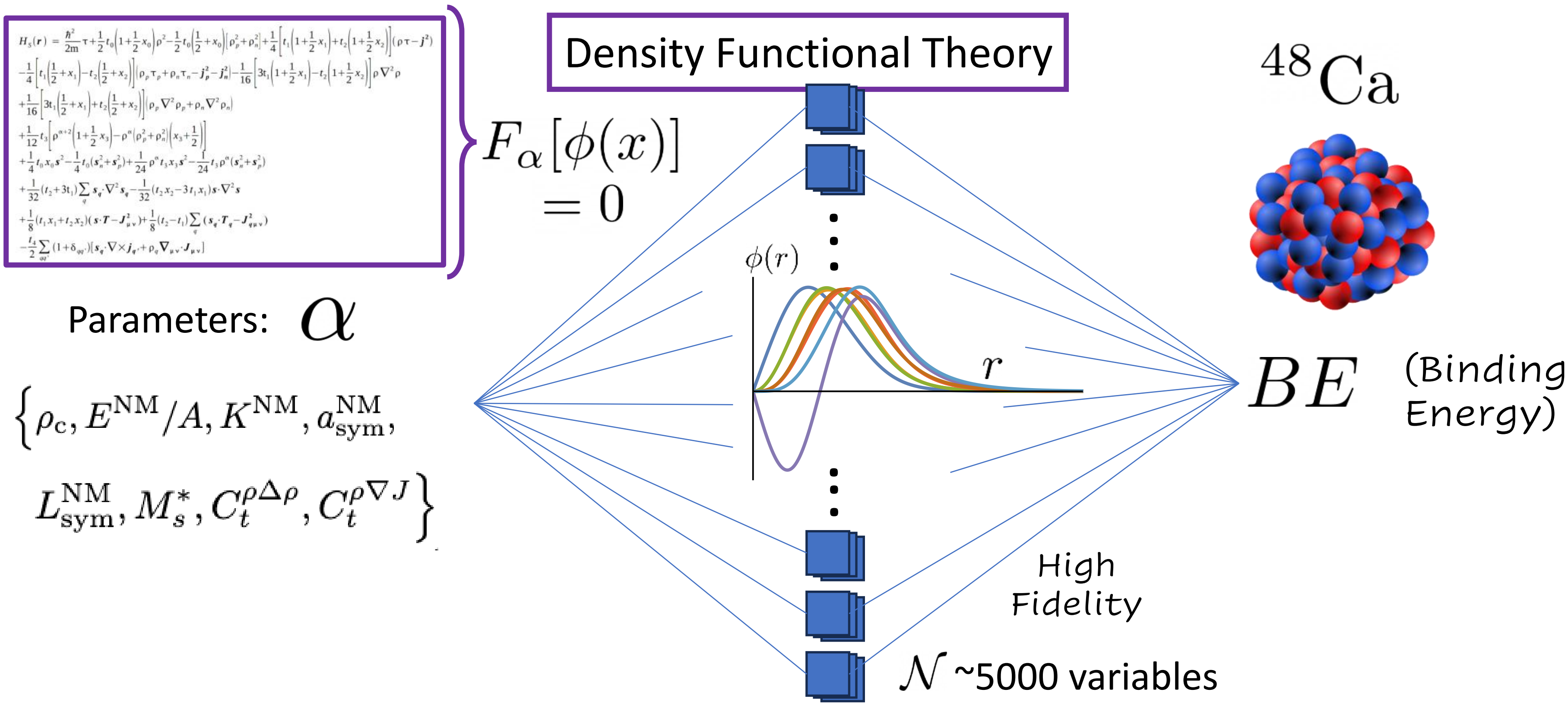


^{48}Ca

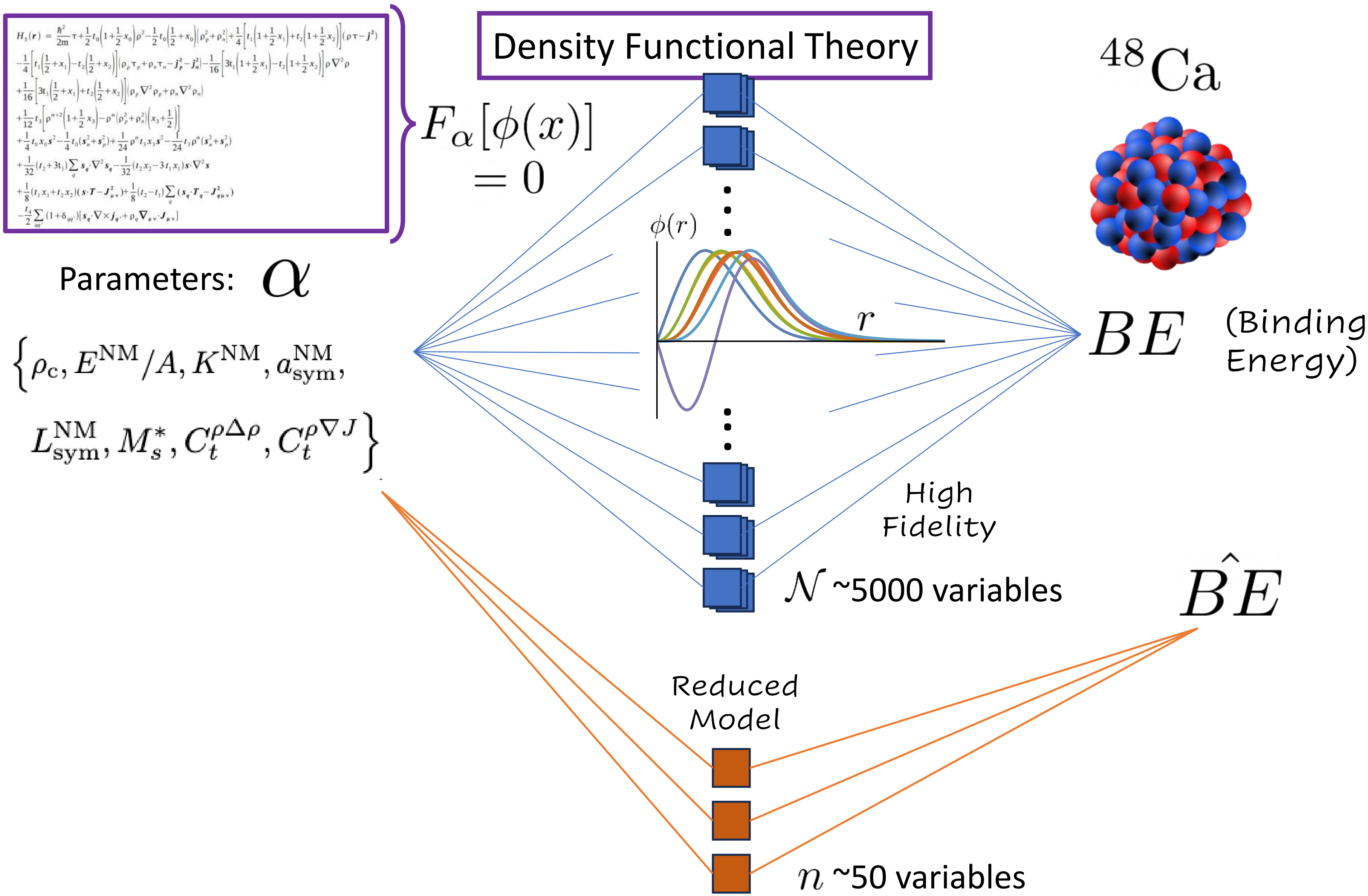


BE (Binding Energy)

How it works

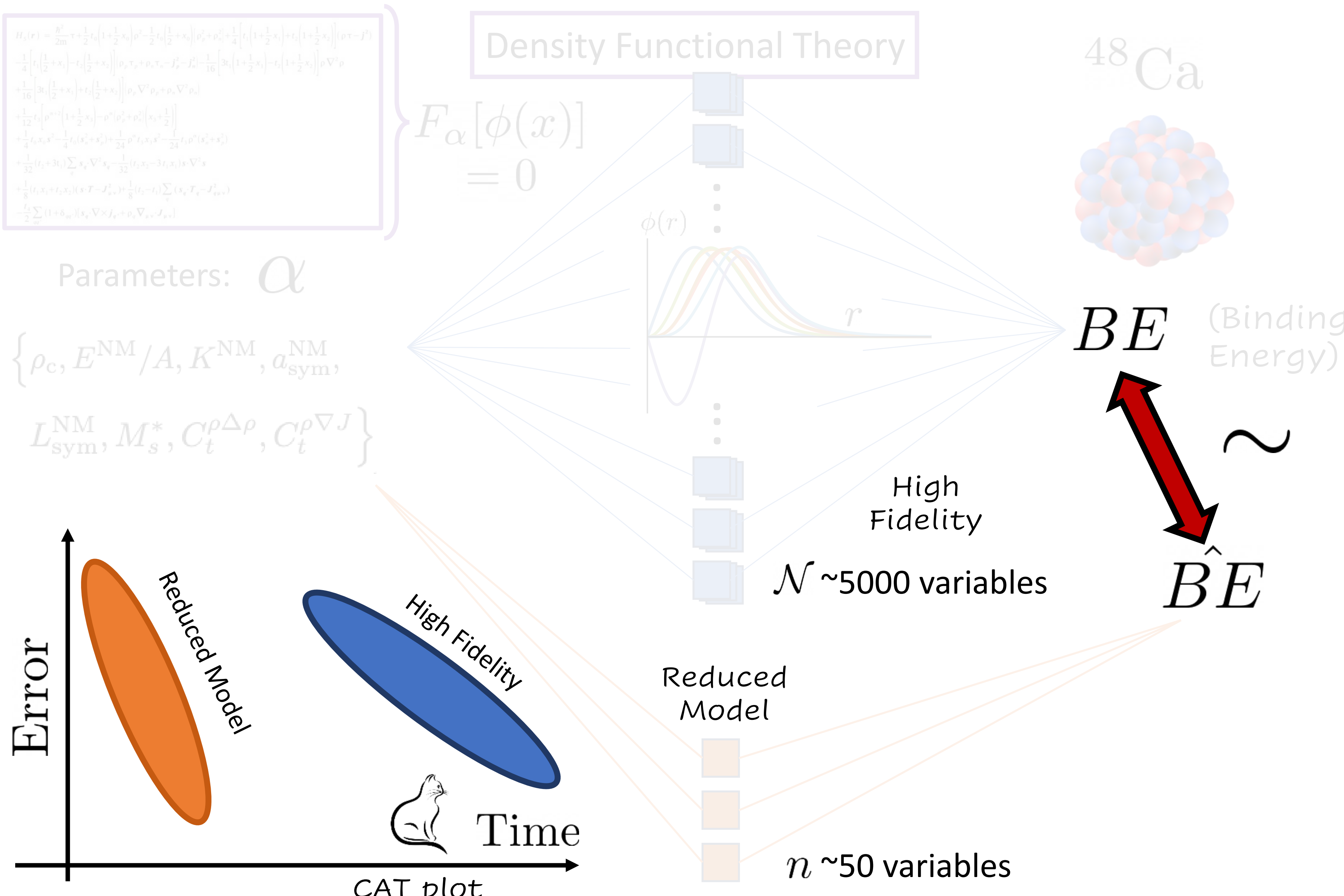

Density Functional Theory
$F_\alpha[\phi(x)] = 0$
Parameters: α
$\{\rho_c, E^{NM}/A, K^{NM}, a_{sym}^{NM}, L_{sym}^{NM}, M_s^*, C_t^{\rho\Delta\rho}, C_t^{\rho\nabla J}\}$
$\phi(r)$
r
^{48}Ca
BE
(Binding Energy)
High Fidelity
$\mathcal{N}$ ~5000 variables

How it works



Density Functional Theory
$F_\alpha[\phi(x)] = 0$
Parameters: α
$\{\rho_c, E^{NM}/A, K^{NM}, a^{NM}_{sym}, L^{NM}_{sym}, M^*_s, C^{\rho\Delta\rho}_t, C^{\rho\nabla J}_t\}$
$\phi(r)$
r
^{48}Ca
BE
(Binding Energy)
High Fidelity
$\mathcal{N}$ ~5000 variables
$\hat{BE}$
Reduced Model
n ~50 variables

How it works



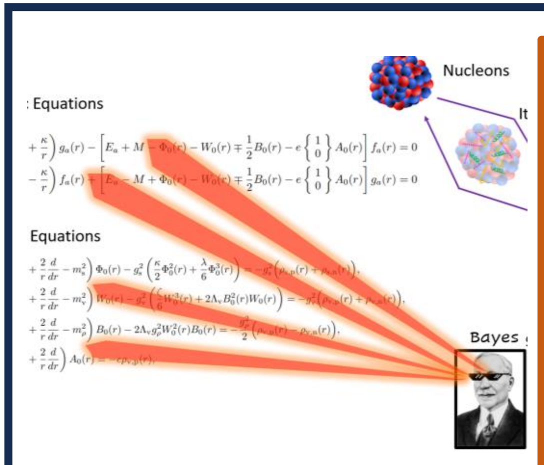
Density Functional Theory
$F_\alpha[\phi(x)] = 0$
Parameters: α
^{48}Ca
BE (Binding Energy)
$\sim$
$\hat{BE}$
High Fidelity
$\mathcal{N}$ ~5000 variables
Reduced Model
n ~50 variables
Error
Time
Reduced Model
High Fidelity
CAT plot

How it works

Reducing your model in two easy steps:

1) Find good reduced coordinates

2) Find equations for them



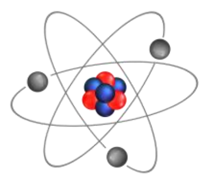
Me talking for an hour about this

How it works

Reducing your model in two easy steps:

1) Find good reduced coordinates

$\sim 10^{24}$

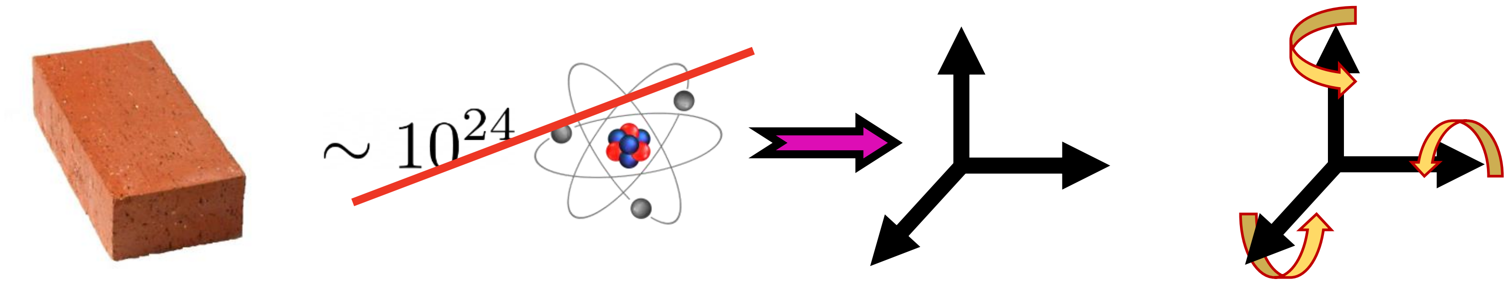


2) Find equations for them

How it works

Reducing your model in two easy steps:

1) Find good reduced coordinates



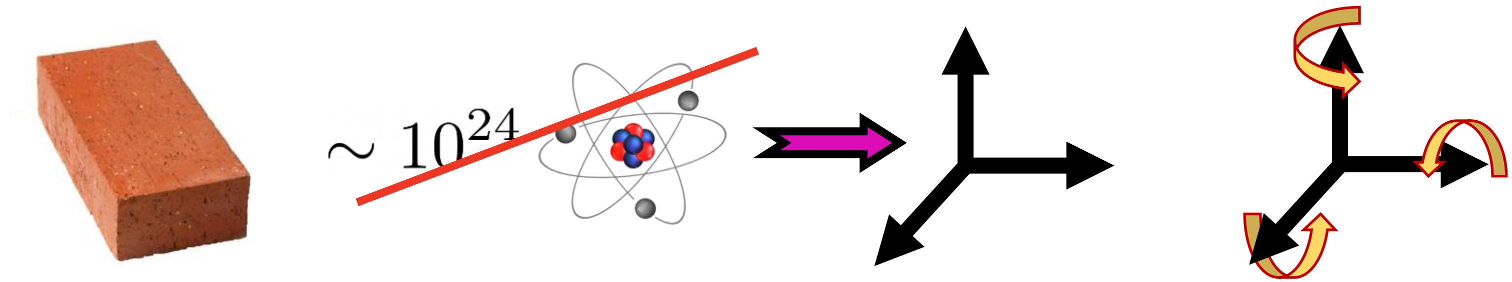
3 translations + 3 rotations

2) Find equations for them

How it works

Reducing your model in two easy steps:

1) Find good reduced coordinates



3 translations + 3 rotations

2) Find equations for them

$$\vec{F} = \frac{d\vec{p}}{dt} \qquad \vec{\tau} = \frac{d\vec{L}}{dt}$$

How it works

Quantum Harmonic Oscillator

$$H_\alpha \phi(x) \equiv \left(-\frac{d^2}{dx^2} + \alpha x^2 \right) \phi(x) = \lambda \phi(x)$$

How it works

Quantum Harmonic Oscillator

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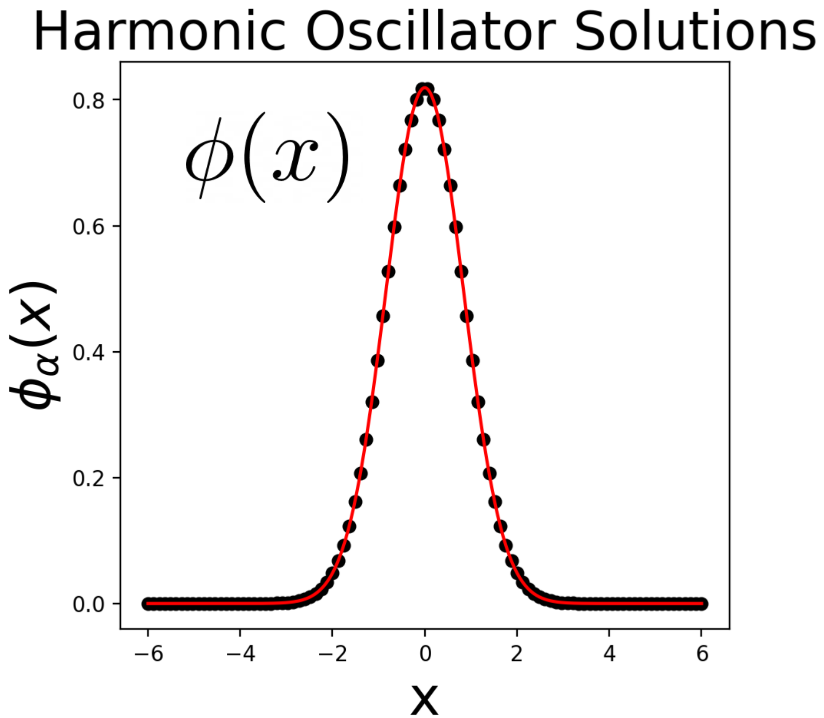

How it works

Quantum Harmonic Oscillator

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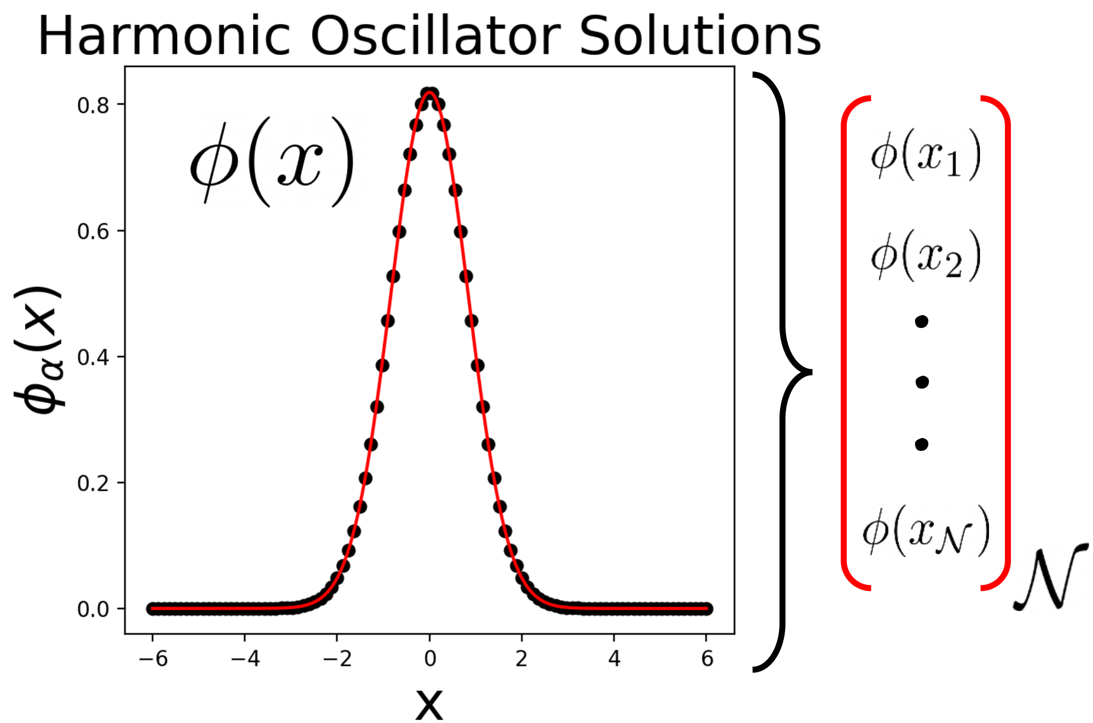

How it works

Quantum Harmonic Oscillator

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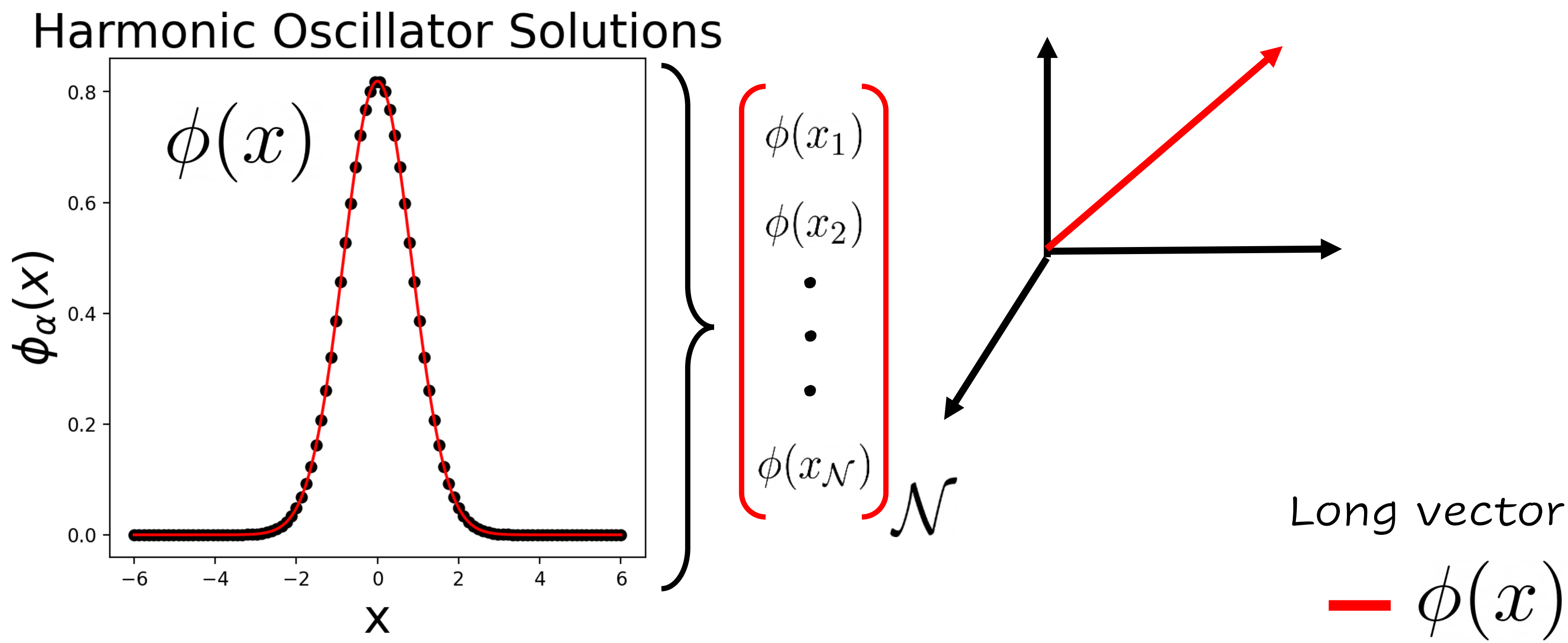

How it works

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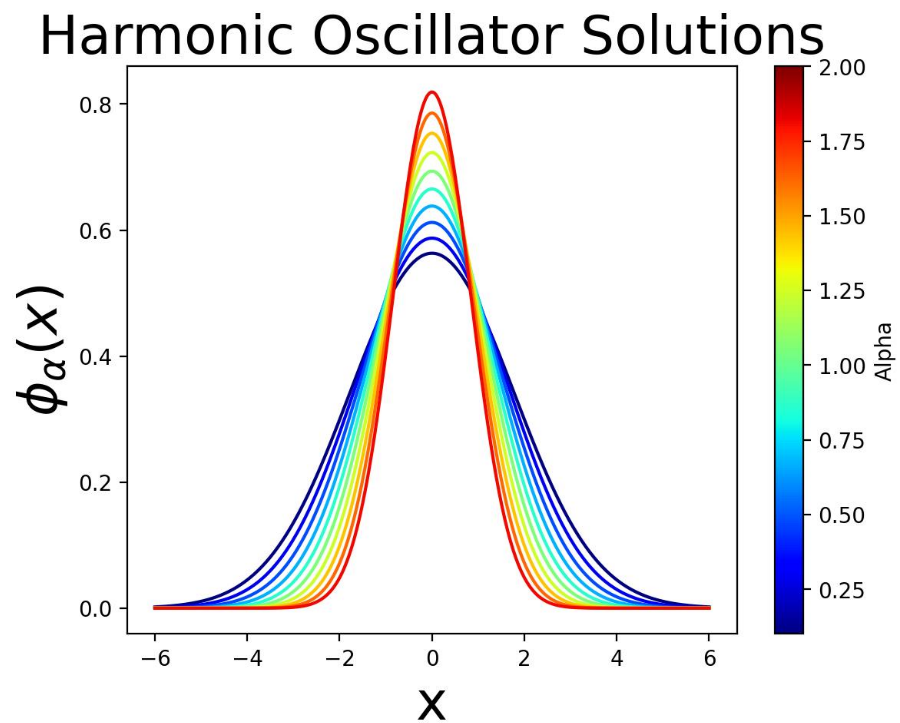
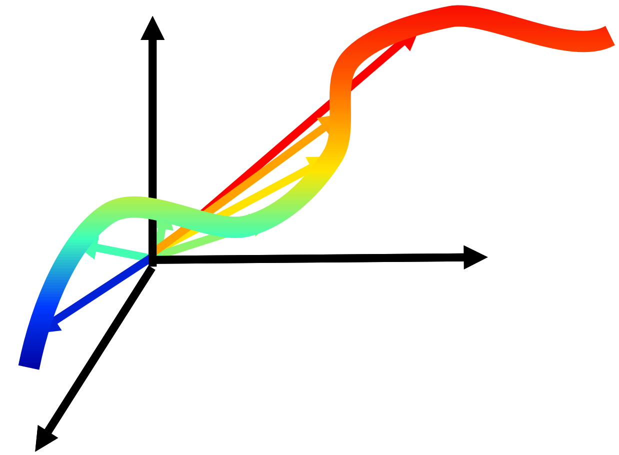




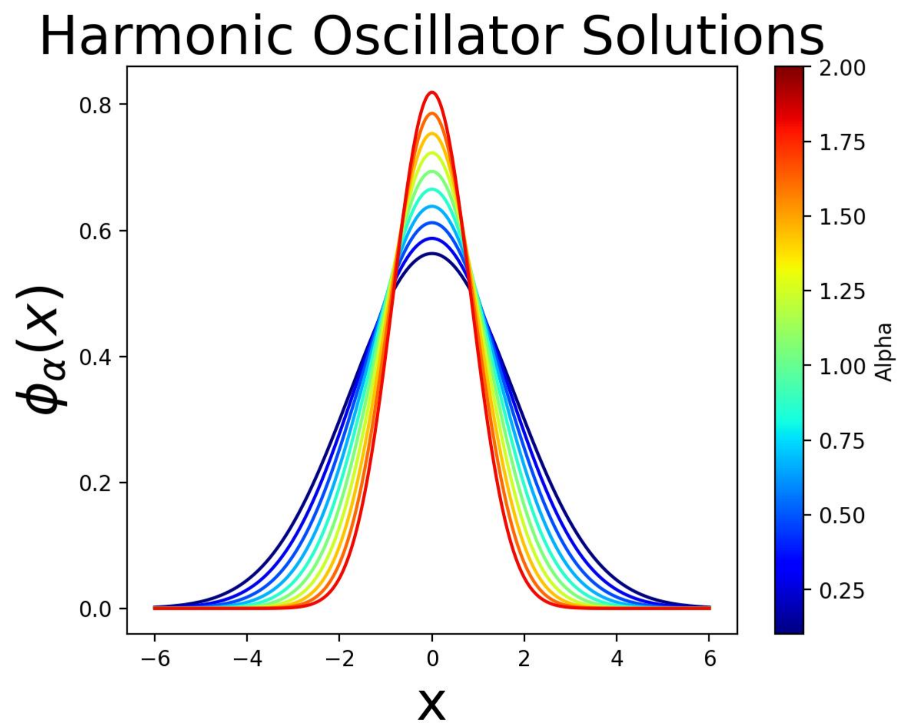
Solution Manifold

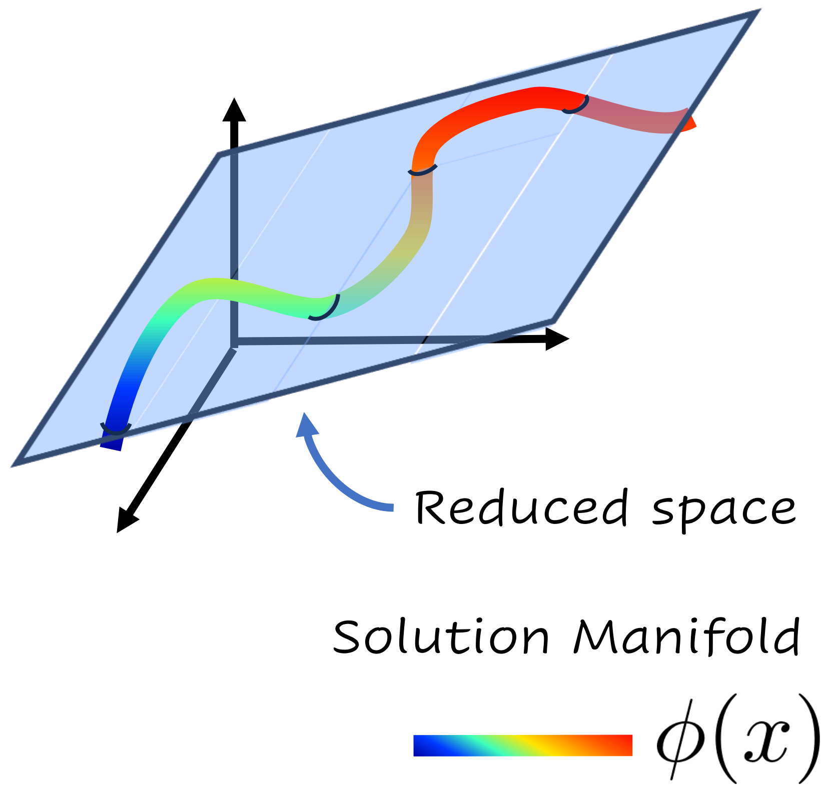
Many Long Vectors

How it works

Quantum Harmonic Oscillator

$$H_\alpha \phi(x) \equiv \left(-\frac{d^2}{dx^2} + \alpha x^2 \right) \phi(x) = \lambda \phi(x)$$

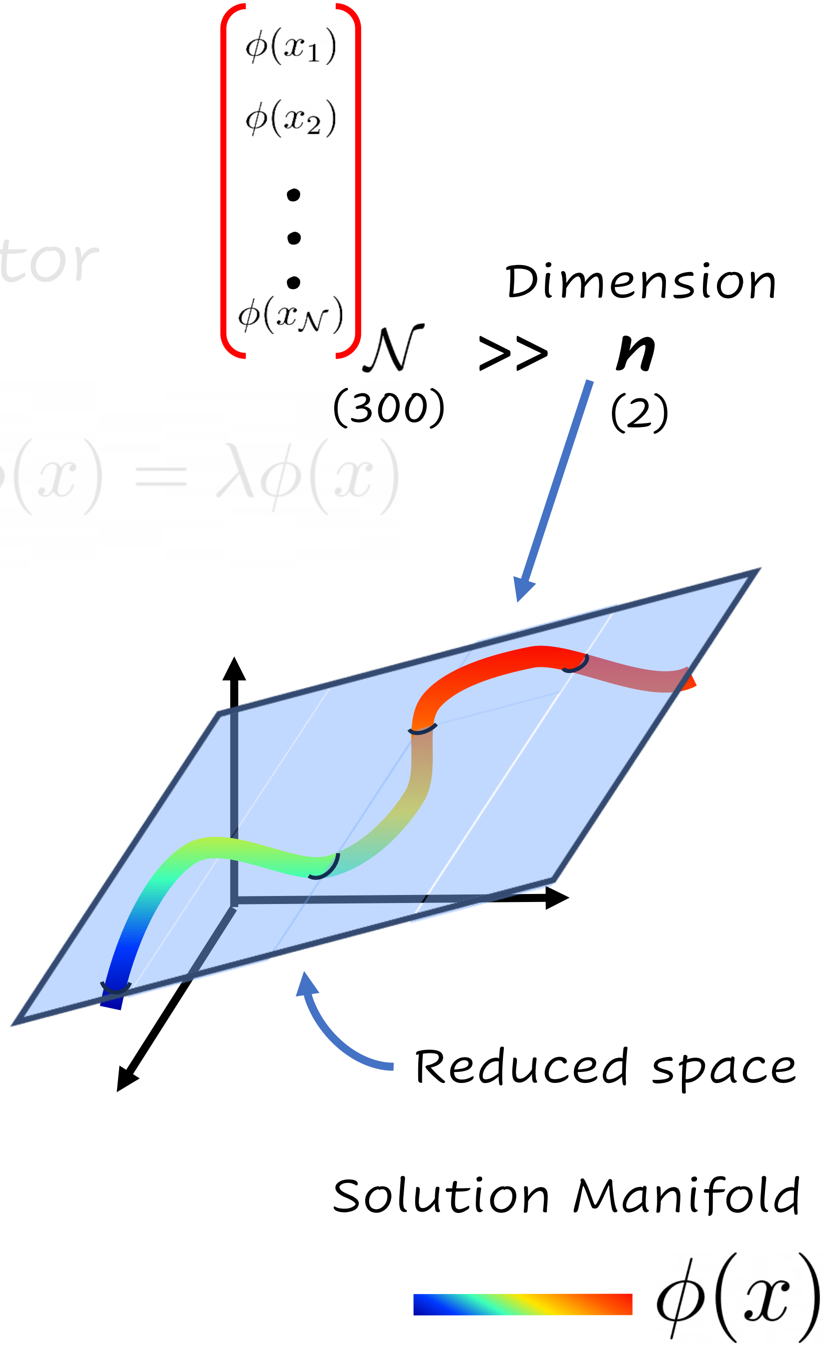




How it works

Quantum Harmonic Oscillator

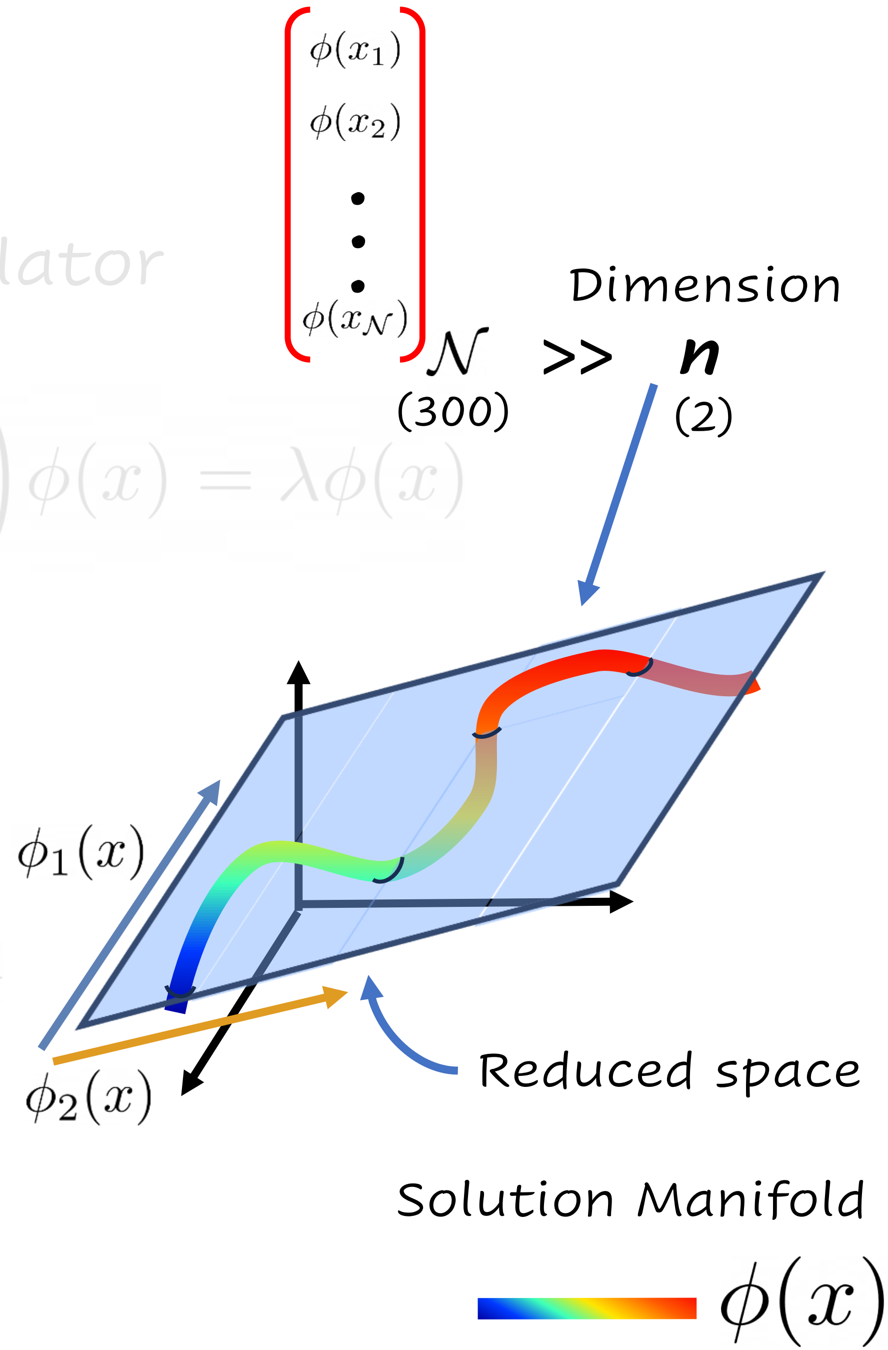
$$H_\alpha \phi(x) \equiv \left(-\frac{d^2}{dx^2} + \alpha x^2\right)\phi(x) = \lambda \phi(x)$$



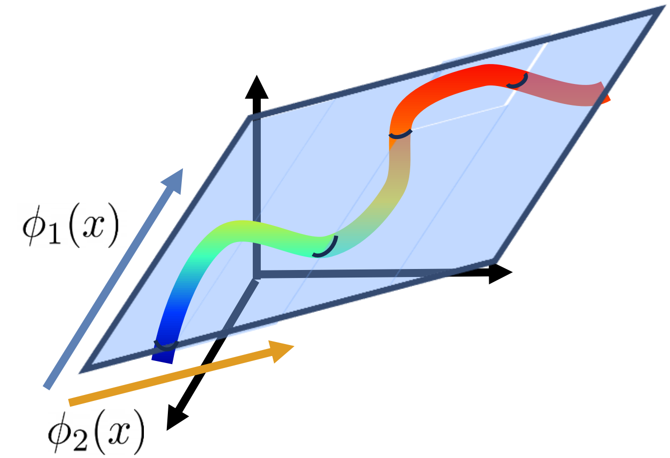
How it works

Quantum Harmonic Oscillator

$$H_\alpha \phi(x) \equiv \left(-\frac{d^2}{dx^2} + \alpha x^2\right)\phi(x) = \lambda\phi(x)$$



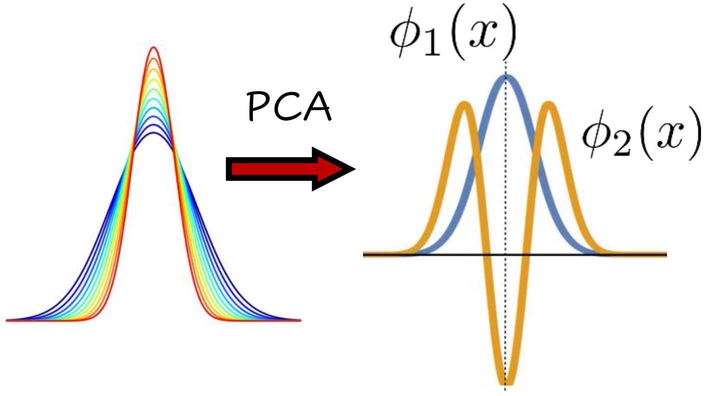
How it works



Quantum Harmonic Oscillator

Reduced Basis

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



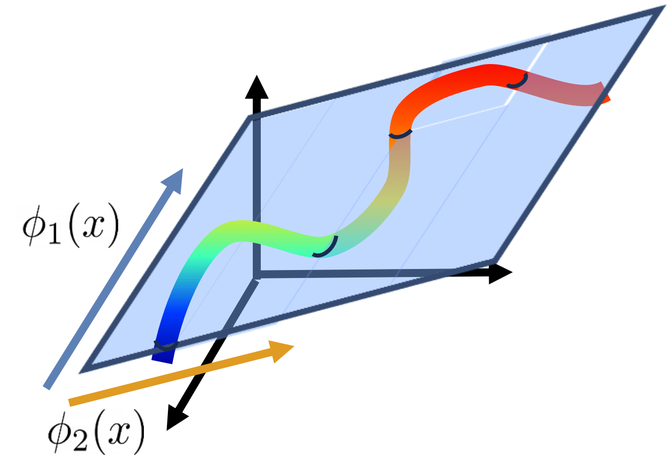
How it works

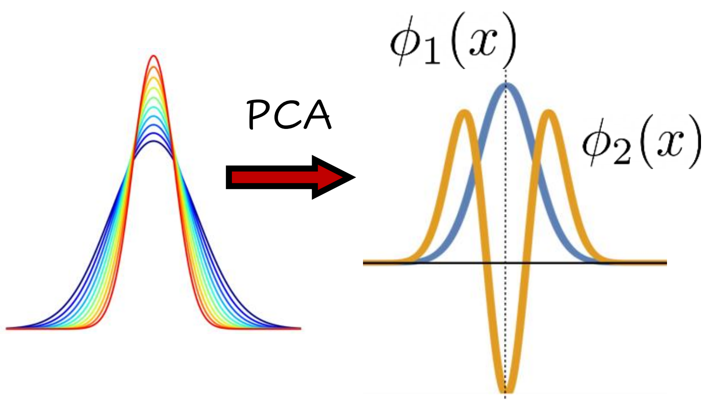
Quantum Harmonic Oscillator

Reduced Basis

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

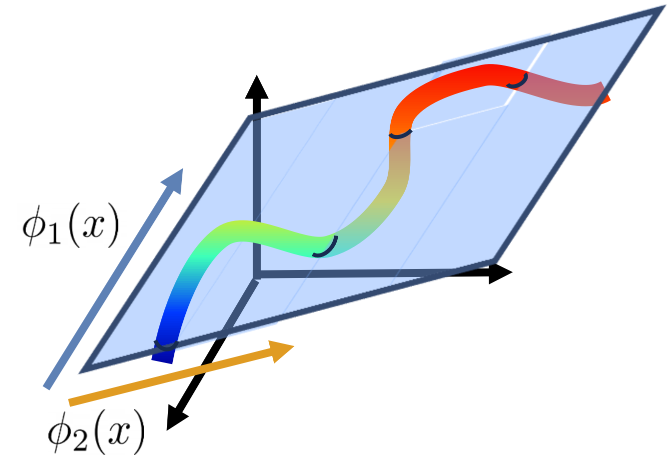
$$\underbrace{H_\alpha \phi(x) = \lambda\phi(x)}_{F_\alpha[\phi(x)] = 0}$$





How it works

Quantum Harmonic Oscillator



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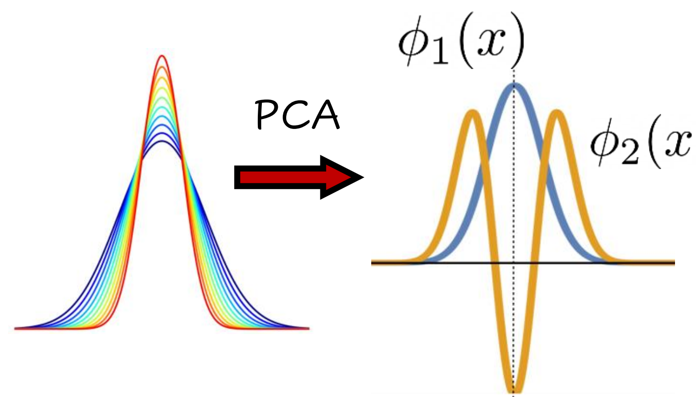
$$\underbrace{H_\alpha \phi(x) = \lambda\phi(x)}_{F_\alpha[\phi(x)] = 0}$$

$$\langle \psi_1 | F_\alpha(\hat{\phi}(x)) \rangle = 0$$

$$\langle \psi_2 | F_\alpha(\hat{\phi}(x)) \rangle = 0$$



Boris Galerkin

**Congratulations! You found the second joke

How it works

Quantum Harmonic Oscillator

Reduced Basis

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

$$H_\alpha\phi(x) = \lambda\phi(x)$$

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

Boris Galerkin

$$\langle\psi_1|F_\alpha(\hat{\phi}(x))\rangle = 0$$

$$\langle\psi_2|F_\alpha(\hat{\phi}(x))\rangle = 0$$

Two coefficients

Two equations*

*Technically, there are three equations if you count the normalization condition. Plus, there is also the eigenvalue, so yeah, there are three equations. Funny that someone would write such a long footnote, makes you wonder if this is just a joke**.

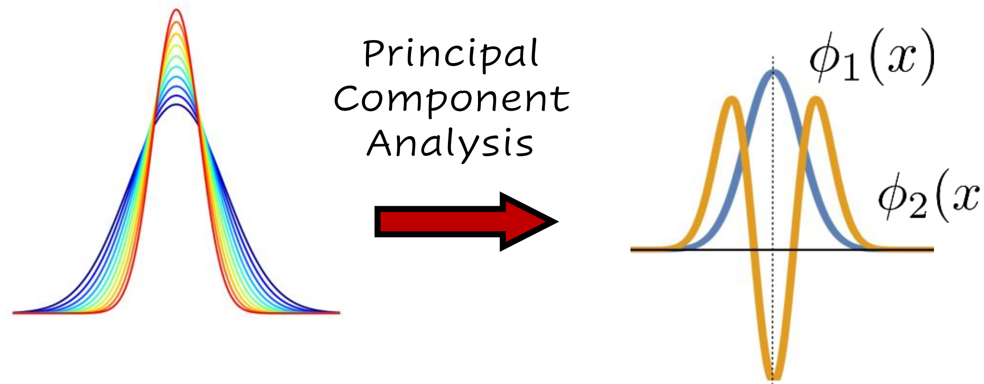
How it works

Reducing your model in two easy steps:

Reduced Basis Method

1) Find good reduced coordinates

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



2) Find equations for them

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

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

One equation per coefficient

$$\underbrace{\left[\hat{H}(\alpha) \right]}_{n \times n} \underbrace{\begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix}}_{n} = \hat{\lambda} \underbrace{\begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix}}_{n}$$

Harmonic Oscillator Example

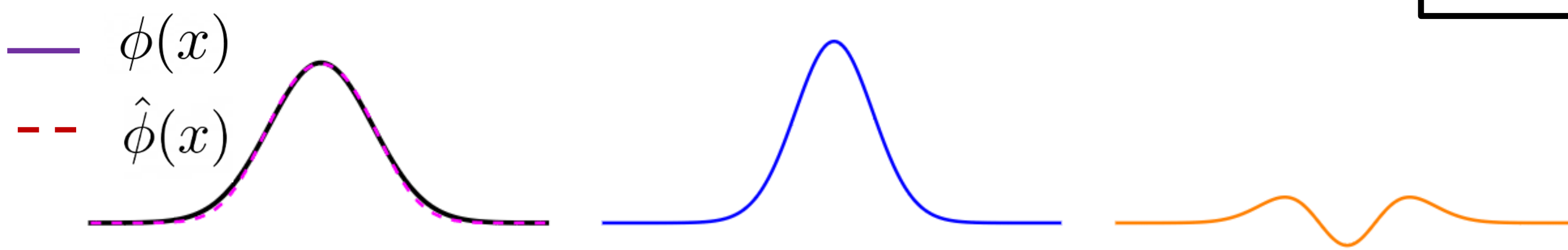
How it works

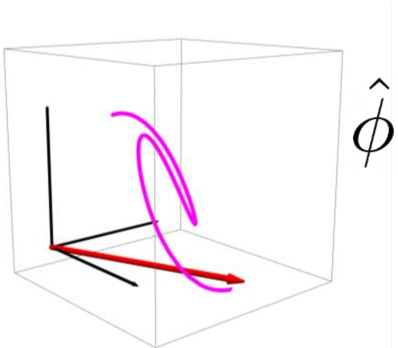
$$H_\alpha \phi(x) \equiv \left(-\frac{d^2}{dx^2} + \alpha x^2 \right) \phi(x) = \lambda \phi(x)$$

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

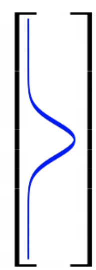
Linear Embedding

Reduced Basis Method

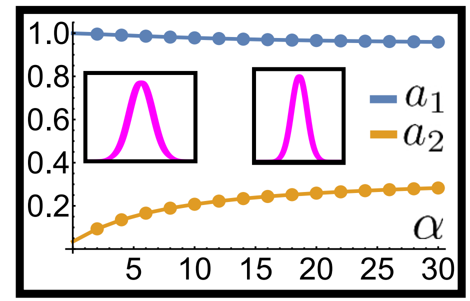




$$\hat{\phi}(x) = \quad a_1$$



$$+ \quad a_2$$

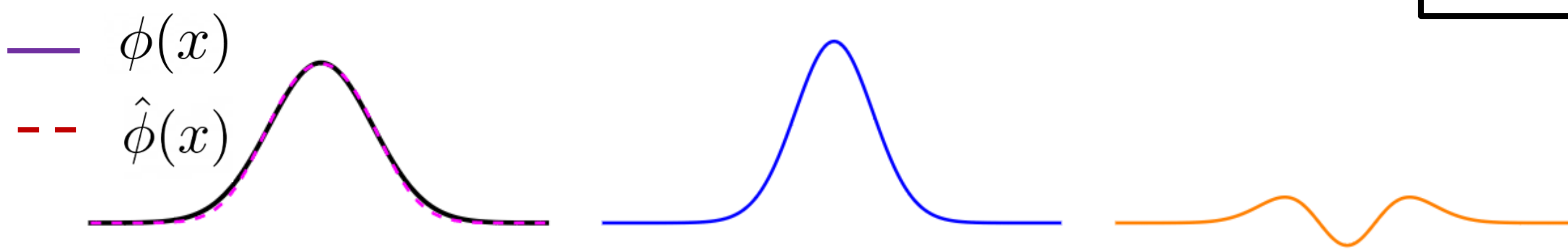


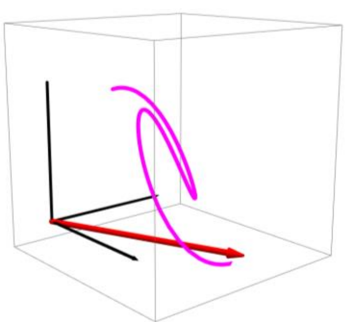
How it works

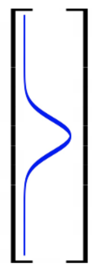
$$H_\alpha \phi(x) \equiv \left(-\frac{d^2}{dx^2} + \alpha x^2 \right) \phi(x) = \lambda \phi(x)$$

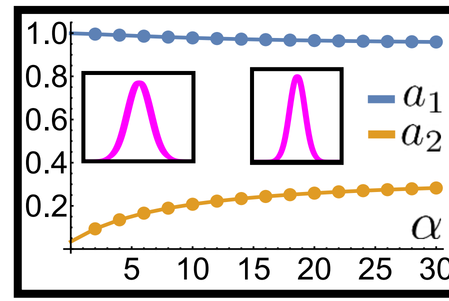
$\phi(x) \approx a_1 \phi_1(x) + a_2 \phi_2(x)$ Linear Embedding

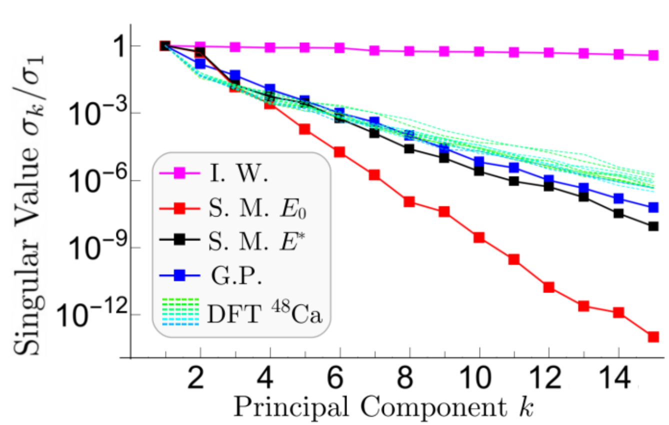
Reduced Basis Method





$\hat{\phi}(x) = a_1$  $+ a_2$ 



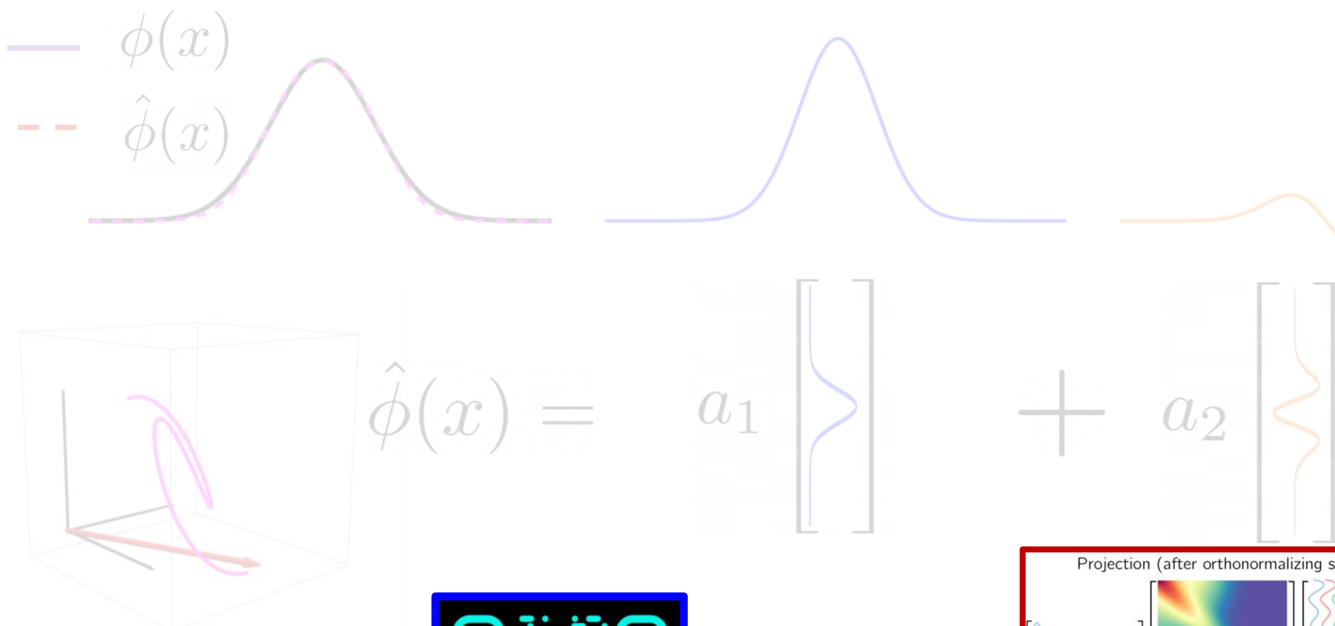


Bad

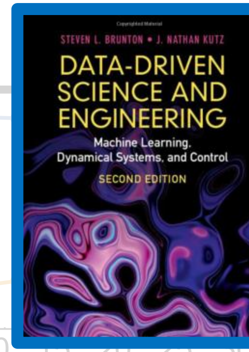
Good

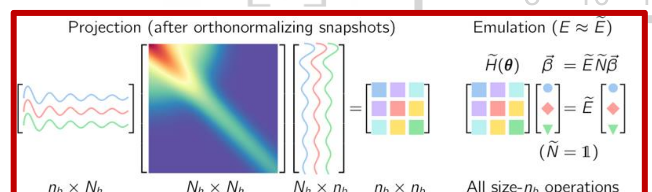
PCA Doctor

How it works



http://databookuw.com





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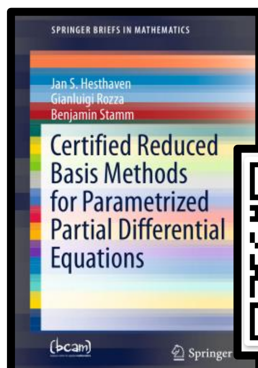
Dimensionality Reduction in Nuclear Physics
Presented by ASCSN



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 48824, USA*
[3]*Department of Physics, The Ohio State University, Columbus, OH 43210, USA*

https://link.springer.com/book/10.1007/978-3-319-22470-1

Dimensionality Reduction in
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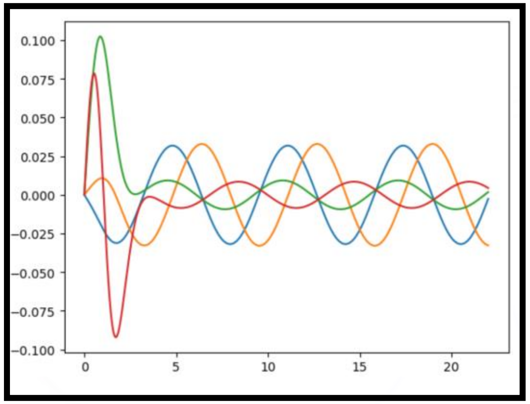
works



$$\frac{d}{dt} a_j(t) - i\hat{H}\boldsymbol{a}(t) = 0, \quad (30)$$

where $\boldsymbol{a}(t) = \{a_1(t), \dots a_n(t)\}$ and the reduced Hamiltonian is computed as:

$$\hat{H}_{j,k} = \langle \phi_j | H | \phi_k \rangle$$

```
A = np.zeros((M,M))
for j in range(M):
    A[:,j] = np.interp(
      sample_pts, s, U[:,j])
```

```
def beta(S):
    betas = np.zeros(M)
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```
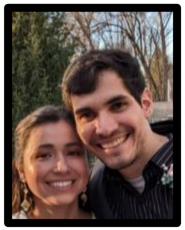

Diogenes Figueroa



Kyle Beyer

Edgard Bonilla

Kyle Godbey

Ruchi Garg

Daniel Odell

Eric Flynn

Daniel Lay

Megan Campbell

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Partial Differential Equations

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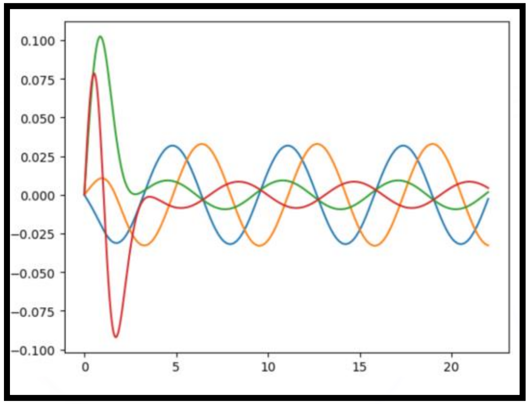

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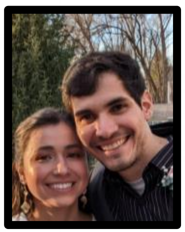
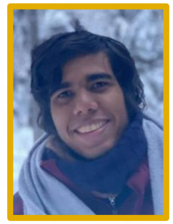


Kyle Beyer

Edgard Bonilla



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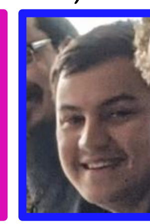


Daniel Lay

Megan Campbell

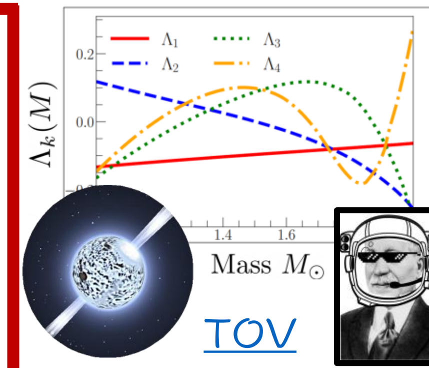
you?

Dimensionality Reduction in Nuclear Physics
Presented by ASCSN

Applications

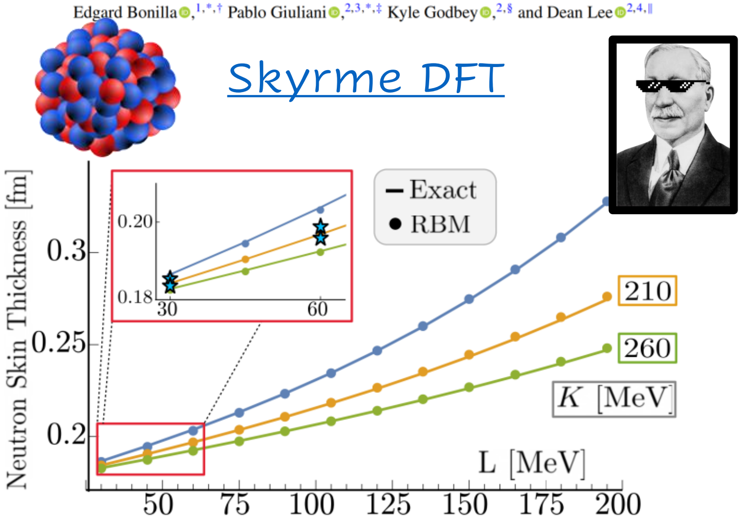
Towards accelerated nuclear-physics parameter estimation from binary neutron star mergers: Emulators for the Tolman-Oppenheimer-Volkoff equations

Brendan T. Reed,[1] Rahul Somasundaram,[1,2] Soumi De,[1] Cassandra L. Armstrong,[3] Pablo Giuliani,[4] Collin Capano,[2,5] Duncan A. Brown,[2] and Ingo Tews[1]



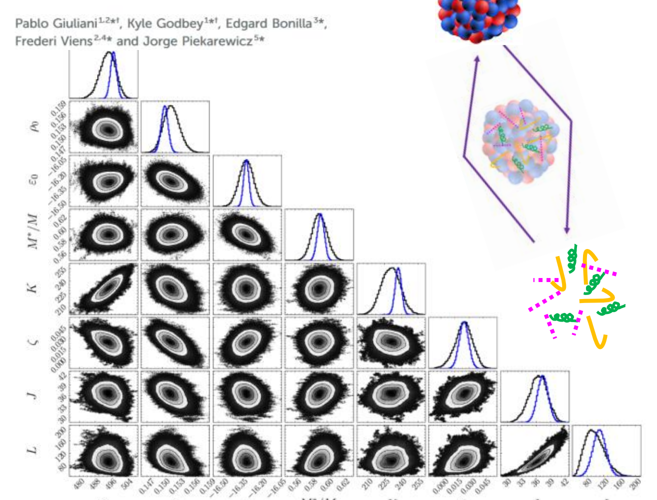
Training and projecting: A reduced basis method emulator for many-body physics

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



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*]



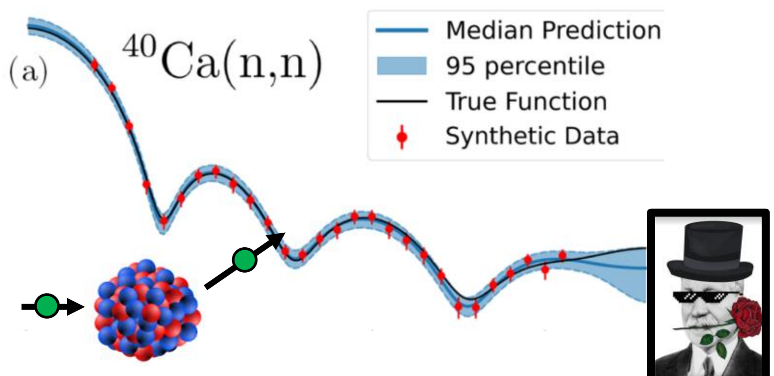
$10^2 - 10^7$

Speed-ups

ROSE: A reduced-order scattering emulator for optical models

D. Odell,[1,*] P. Giuliani,[2,3,†] K. Beyer,[4,‡] M. Catacora-Rios,[2,5] M. Y.-H. Chan,[6,§] E. Bonilla,[7,∥] R. J. Furnstahl,[8,¶] K. Godbey,[2,#] and F. M. Nunes[2,5,**]

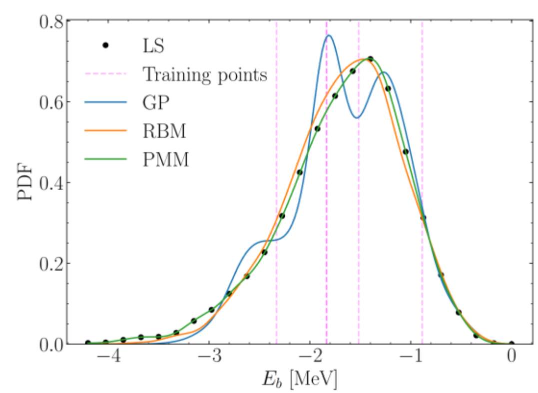
Scattering



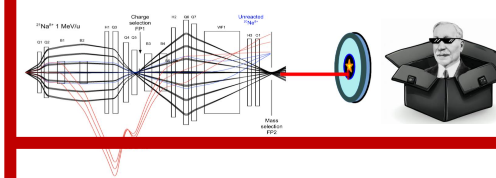
Emulators for scarce and noisy data: application to auxiliary field diffusion Monte Carlo for the deuteron

Rahul Somasundaram,[1,2,*] Cassandra L. Armstrong,[3] Pablo Giuliani,[4,5] Kyle Godbey,[4] Stefano Gandolfi,[1] and Ingo Tews[1]

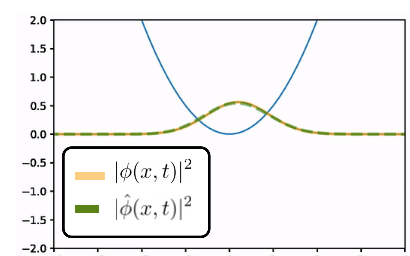
Auxiliary Field QMC



Beam Control



Time dynamics



Applications

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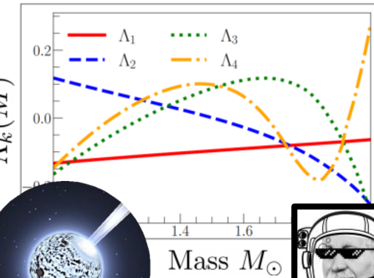

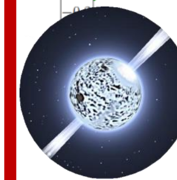

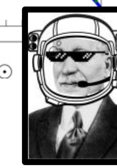

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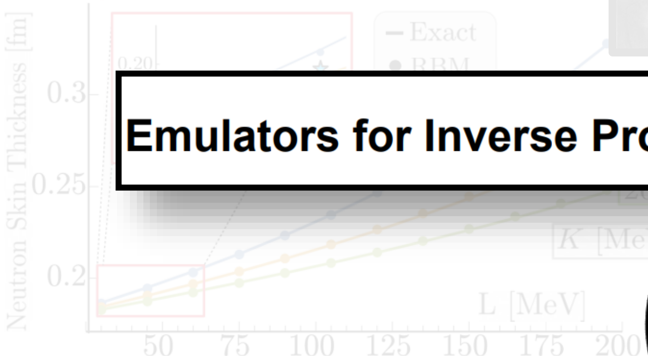
Edgard Bonilla, Pablo Giuliani, Kyle Godbey and Dean Lee

Skyrme DFT



Bayes goes fast: Uncertainty quantification for a covariant energy density functional emulated by the reduced basis method

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RMF DFT

[This morning]

Emulators for Inverse Problems in Dense Matter Physics

Rahul Somasundaram

$10^2 - 10^7$

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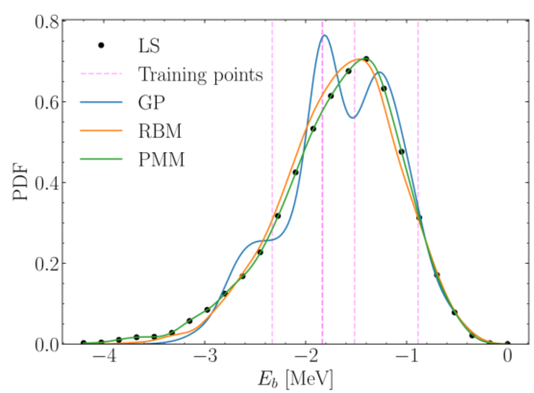


Beam Control

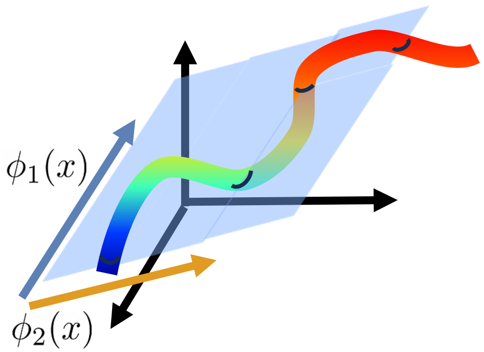
Time dynamics

Beyond the Reduced Basis Method

1) Find good reduced coordinates

2) Find equations for them

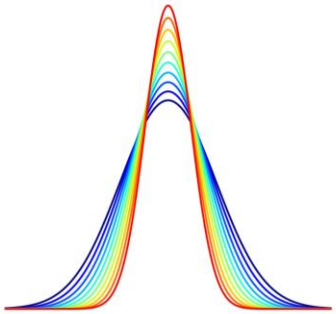
Beyond the Reduced Basis Method

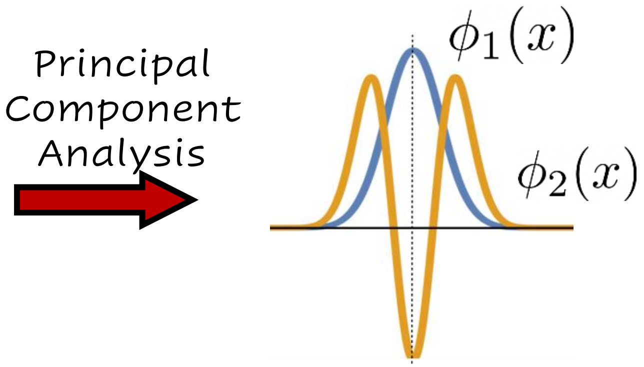


Linear embedding

1) Find good reduced coordinates

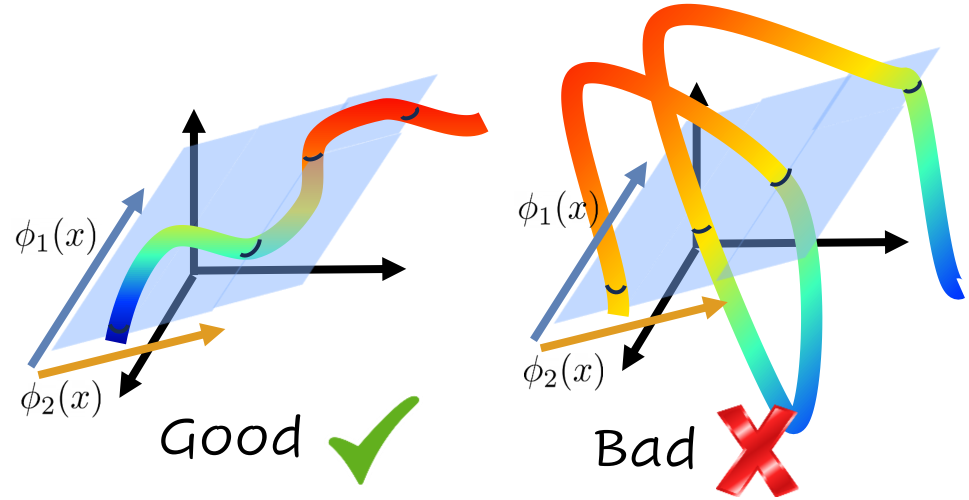
$$\hat{\phi}(x) = \phi_0 + \sum_{k}^{n} a_k \phi_k(x)$$





2) Find equations for them

Beyond the Reduced Basis Method



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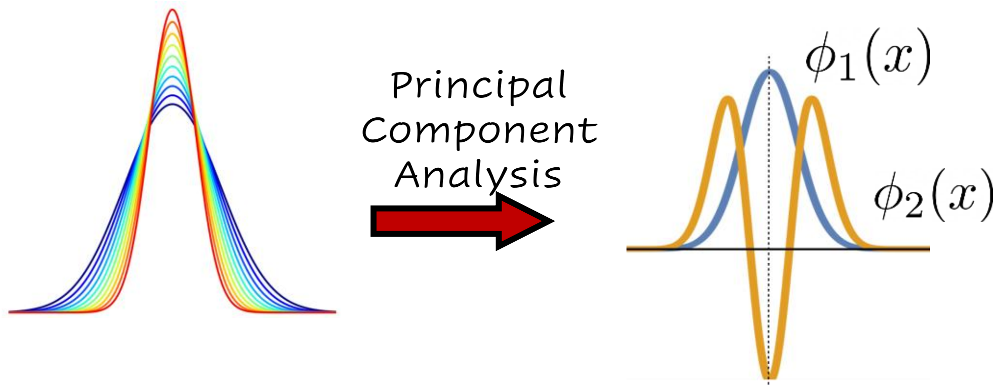

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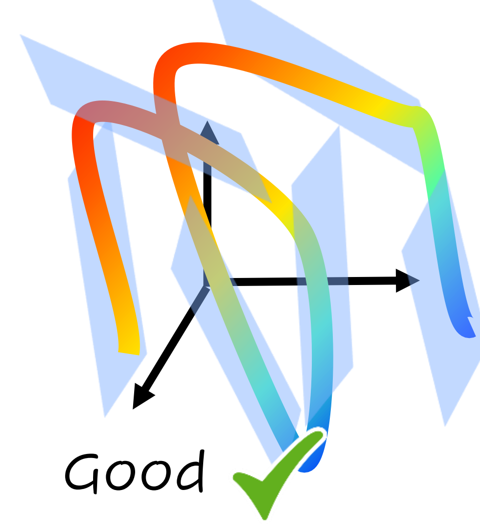
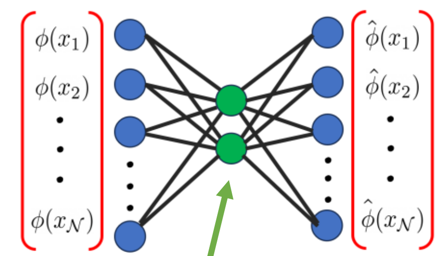
Beyond the Reduced Basis Method



Linear embedding

1) Find good reduced coordinates

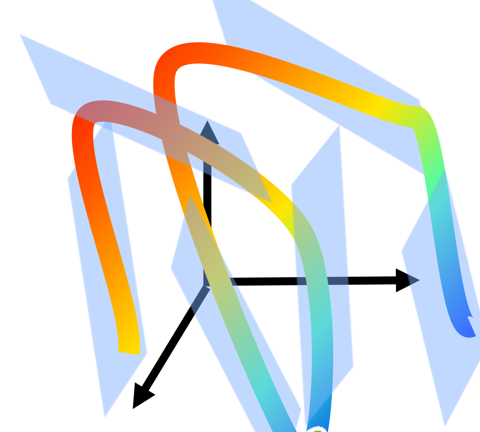
$$\hat{\phi}(x) = \phi_0 + \sum_k^n \underline{a_k} \phi_k(x) \qquad \phi(x) \approx \sum_k^n a_k \phi(x/l_k)$$



2) Find equations for them

Non-linear embedding

Beyond the Reduced Basis Method



Good ✓

Linear embedding

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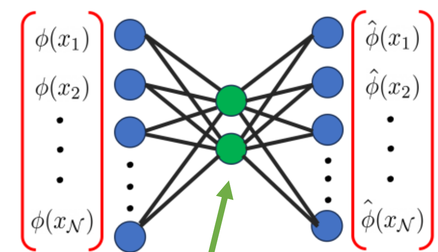


Galerkin Projection

2) Find equations for them

Non-linear embedding

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

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

Bad ✗

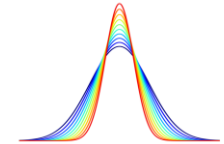
Beyond the Redu
Basis Method

Linear embedding

1) Find good reduced coordi

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

$$\left(-\frac{d^2}{dx^2} + \alpha x^2 \right) \phi(x) = \lambda \phi(x)$$



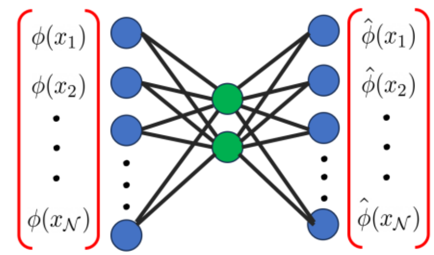
(Affine operators) Good ✓

$$\left(-\frac{d^2}{dx^2} + kx^2 + q\rho(x)^\sigma \right) \phi_i(x) = \lambda_i \phi_i(x)$$

Bad ✗

(Non-affine operators)

$$\phi(x) \approx \sum_{k}^{n} a_k \phi(x/l_k)$$



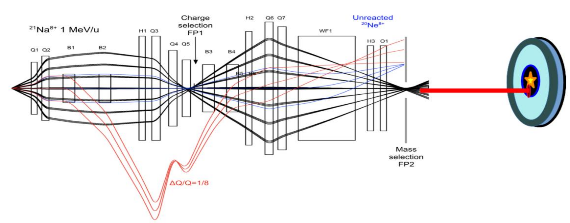
(Generalized reduced coordinates) Bad ✗

Galerkin Projection

2) Find equations for them

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

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



Bad ✗

(Experimental control)

Beyon

[Me talking for half hour about this]

Learn Equations from data

~~Galerkin Projection~~

2) Find equations for them

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

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

$$\left(-\frac{d^2}{dx^2} + \alpha x^2\right)\phi(x) = \lambda\phi(x)$$

(Affine operators) Good ✓

$$\left(-\frac{d^2}{dx^2} + kx^2 + q\rho(x)^\sigma\right)\phi_i(x) = \lambda_i\phi_i(x)$$

Bad ✗

(Non-affine operators)

$$\phi(x) \approx \sum_k^n a_k\phi(x/l_k)$$

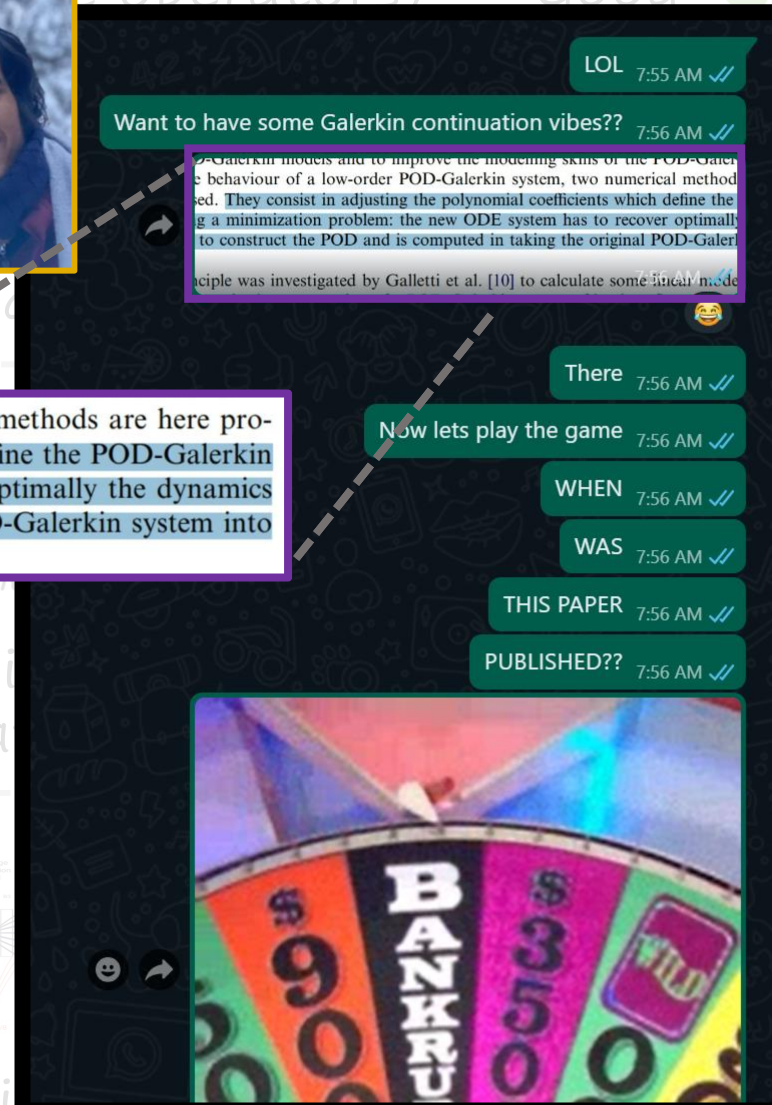
(Generalized reduced coordinates) Bad ✗

Bad ✗

(Experimental control)

[Me talking for half hour about this]

Edgard



To correct the behaviour of a low-order POD-Galerkin system, two numerical methods are here proposed and assessed. They consist in adjusting the polynomial coefficients which define the POD-Galerkin system by solving a minimization problem: the new ODE system has to recover optimally the dynamics of the data used to construct the POD and is computed in taking the original POD-Galerkin system into account.

~~Galerkin Projection~~

2) Find equations for them

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

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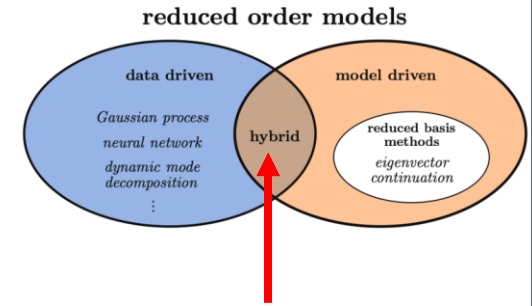
Modern Evolution Algorithms

Overview – What is Modern (3)

← Nobuo Sato



Many things here

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Calibrated reduced-order POD-Galerkin system for fluid flow modelling

M. Couplet [a,*], C. Basdevant [b], P. Sagaut [c]

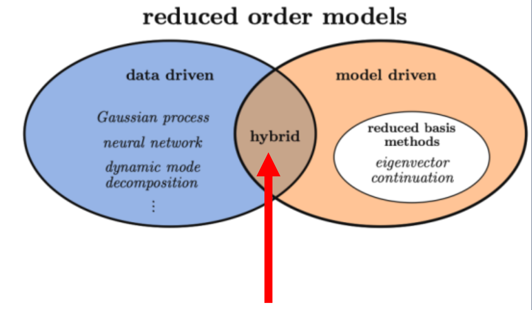
[a] *ONERA, Computational Fluid Dynamics and Aeroacoustics Department, 29 av. de la Division Leclerc, BP 72, 92322 Châtillon, France*
[b] *LMD, École Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 5, France*
[c] *LMM, Université Pierre et Marie Curie, Boîte 162, 4 place Jussieu, 75252 Paris Cedex 5, France*

Received 14 June 2004; received in revised form 19 November 2004; accepted 12 January 2005
Available online 22 February 2005

Modern Evolution Algorithms

Overview – What is Modern (3)

← Nobuo Sato



Many things here

From Data to Reduced-Order Models via Generalized Balanced Truncation

Azka Muji Burohman, Bart Besselink, *Member, IEEE*, Jacquelien M. A. Scherpen, *Fello*
and M. Kanat Camlibel, *Senior Member, IEEE*

III. Data-Driven Petrov–Galerkin Projection

Consider the linear discrete-time input/state/output system

$$\Sigma_{\text{true}}: \begin{aligned} \boldsymbol{x}(k+1) &= A_{\text{true}}\boldsymbol{x}(k) + B_{\text{true}}\boldsymbol{u}(k) + \boldsymbol{w}(k), \\ \boldsymbol{y}(k) &= C_{\text{true}}\boldsymbol{x}(k) + D_{\text{true}}\boldsymbol{u}(k) + \boldsymbol{z}(k) \end{aligned} \tag{5}$$

where $(\boldsymbol{u}, \boldsymbol{x}, \boldsymbol{y}) \in \mathbb{R}^{m+n+p}$ are the input/state/output and $(\boldsymbol{w}, \boldsymbol{z}) \in \mathbb{R}^{n+p}$ are noise terms. Throughout the article, we assume that the system matrices $(A_{\text{true}}, B_{\text{true}}, C_{\text{true}}, D_{\text{true}})$ and the noise $(\boldsymbol{w}, \boldsymbol{z})$ are *unknown*. What is known instead are a finite … f input/state/output measurements harvested from the … n (5)

REVIEW ARTICLE WILEY

A tutorial on data-driven eigenvalue identification: Prony analysis, matrix pencil, and eigensystem realization algorithm

Anas Almunif | Lingling Fan | Zhixin Miao

Summary

To identify power system eigenvalues from measurement data, Prony analysis, matrix pencil (MP), and eigensystem realization algorithm (ERA) are three major methods. This paper reviews the three methods and sheds insight on

To correct the behaviour of a low-order POD-Galerkin system, two numerical methods are here posed and assessed. They consist in adjusting the polynomial coefficients which define the POD-Ga system by solving a minimization problem: the new ODE system has to recover optimally the dyn of the data used to construct the POD and is computed in taking the original POD-Galerkin syster account.

Calibrated reduced-order POD-Galerkin system for fluid flow modelling

M. Couplet [a,*], C. Basdevant [b], P. Sagaut [c]

Methodology	Assumed dynamics	Measurements of dynamic states	Robustness to noise and errors
Prony Analysis	Linear	Not required	Non-robust
Matrix Pencil Method	Linear	Not required	Non-robust
Subspace identification	Linear	Not required	Robust
Dynamic mode decomposition (DMD)	Linear	Required	Robust
Linear operator based DMD	Nonlinear	Required	Robust
Proposed ESI Method	Nonlinear	Not required	Robust

Fig. 1. Comparison of state-of-the-art data-driven methodologies for power system dynamic characterization.

Data-Driven Identification of Nonlinear Power System Dynamics Using Output-Only Measurements

Pranav Sharma, *Student Member, IEEE*, Venkataramana Ajjarapu, *Life Fellow, IEEE*, and Umesh Vaidya, *Senior Member, IEEE*

Data-Driven Extraction of Uniformly Stable and Passive Parameterized Macromodels

TOMMASO BRADDE, (Member, IEEE), STEFANO GRIVET-TALOCIA, (Fellow, IEEE), ALESSANDRO ZANCO, (Member, IEEE), AND GIUSEPPE C. CALAFIORE, (Fellow, IEEE)
Department of Electronics and Telecommunications, Politecnico di Torino, 10129 Torino, Italy

required system outputs [1]–[3]. The intrinsic complexity of the first-principle physical laws (e.g. Maxwell's equations) is reduced to a small set of explanatory instrumental variables that are sufficient to predict the input-output relationship of interest. In particular, in the field of electronics

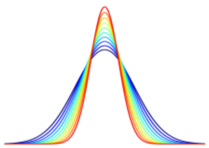
Interpolation among reduced-order matrices to obtain parameterized models for design, optimization and probabilistic analysis

Joris Degroote[1,2], Jan Vierendeels[1] and Karen Willcox[2,*,†]

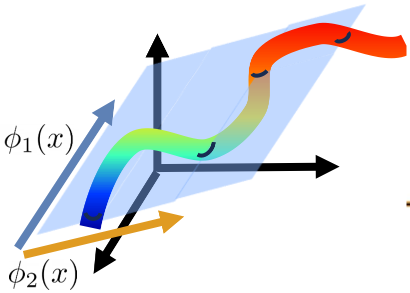
In this paper, we introduce interpolation among the system matrices of the reduced models to efficiently handle nonlinear parametric dependencies. Our approach is efficient because, once an initial set of ROMs has been derived, obtaining a ROM solution for a new parameter value avoids any computations that depend on the dimension of the full-scale model. That is, at each new

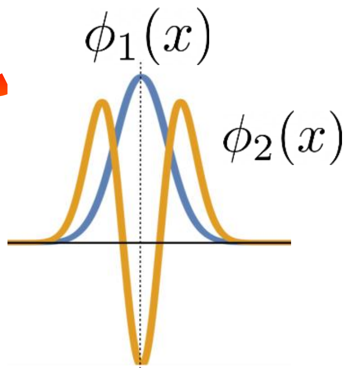
Example

$$\left(-\frac{d^2}{dx^2}+\alpha x^2\right)\phi(x)=\lambda\phi(x)$$



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





Learn Equations
from data

Galerkin Projection

2) Find equations for them

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

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

Example

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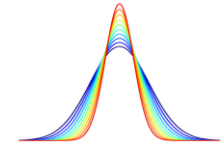

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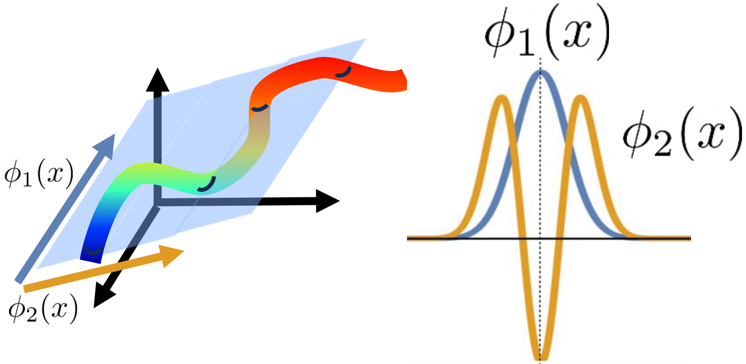

$$\langle\psi_j|\Big(H-\lambda\Big)|\hat{\phi}\rangle=0$$

$$\Big[\hat{H}(\alpha)\Big]_{2\times 2}\begin{bmatrix}a_1\\ a_2\end{bmatrix}_2=\hat{\lambda}\begin{bmatrix}a_1\\ a_2\end{bmatrix}$$

Learn Equations from data

Galerkin Projection

2) Find equations for them

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

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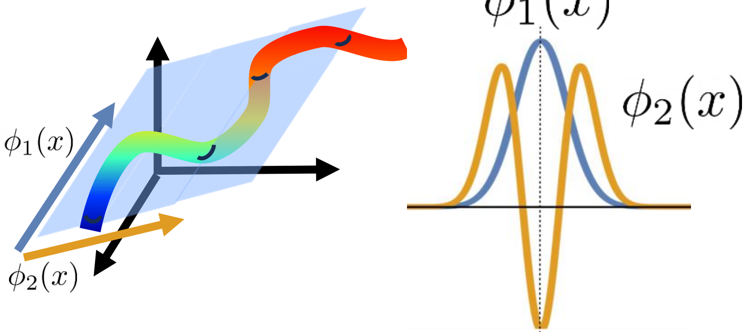
Example

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



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Galerkin Projection

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$$\left[\hat{H}(\alpha)\right]_{2\times 2}\begin{bmatrix} a_1 \\ a_2 \end{bmatrix}_2 = \hat{\lambda}\begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$$

$$\begin{pmatrix} M_{11}^{(0)} & M_{12}^{(0)} \\ M_{21}^{(0)} & M_{22}^{(0)} \end{pmatrix} + \alpha\begin{pmatrix} M_{11}^{(1)} & M_{12}^{(1)} \\ M_{21}^{(1)} & M_{22}^{(1)} \end{pmatrix}$$

$$-\langle\phi_2|\frac{d^2}{dx^2}|\phi_1\rangle$$

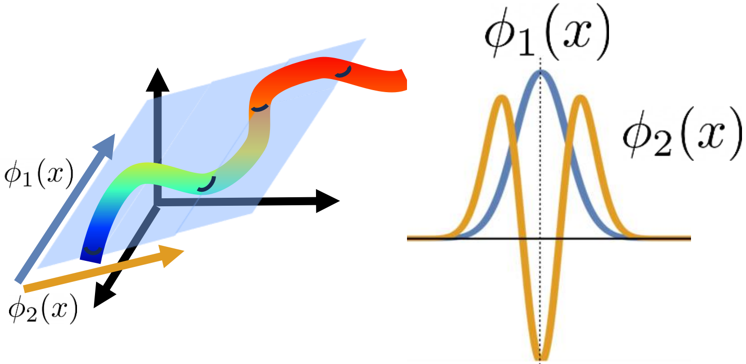
$$\langle\phi_2|x^2|\phi_1\rangle$$

Example

$$\left(-\frac{d^2}{dx^2} + \alpha x^2\right)\phi(x) = \lambda\phi(x)$$

$$\langle\psi_j|\left(H - \lambda\right)|\hat{\phi}\rangle = 0$$

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



Learn Equations
from data

$$\left[\hat{H}(\alpha)\right]_{2\times 2}\begin{bmatrix} a_1 \\ a_2 \end{bmatrix}_2 = \hat{\lambda}\begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$$

Galerkin Projection

2) Find equations for them

$$\begin{pmatrix} M_{11}^{(0)} & M_{12}^{(0)} \\ M_{21}^{(0)} & M_{22}^{(0)} \end{pmatrix} + \alpha\begin{pmatrix} M_{11}^{(1)} & M_{12}^{(1)} \\ M_{21}^{(1)} & M_{22}^{(1)} \end{pmatrix}$$

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

$$-\langle\phi_2|\frac{d^2}{dx^2}|\phi_1\rangle \qquad \langle\phi_2|x^2|\phi_1\rangle$$

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

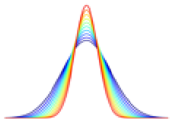
Fit from data

$$\hat{H} = \hat{H}_0 + \alpha\hat{H}_1 + \alpha^2\hat{H}_2 + \ldots$$

Learn Equations
from data

2) Find equations for them

$$\left(-\frac{d^2}{dx^2}+\alpha x^2\right)\phi(x)=\lambda\phi(x)$$



(Affine operators) Good ✓

$$\left(-\frac{d^2}{dx^2}+kx^2+q\rho(x)^\sigma\right)\phi_i(x)=\lambda_i\phi_i(x)$$

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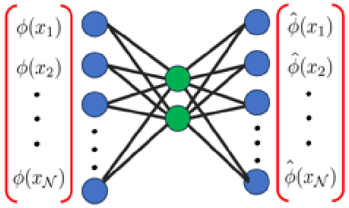
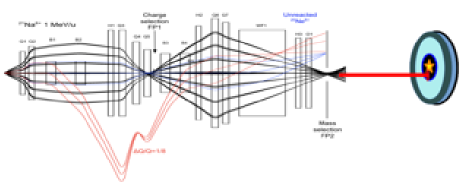


(Generalized reduced coordinates) Good ✓



(Experimental control) Good ✓

Fit from data

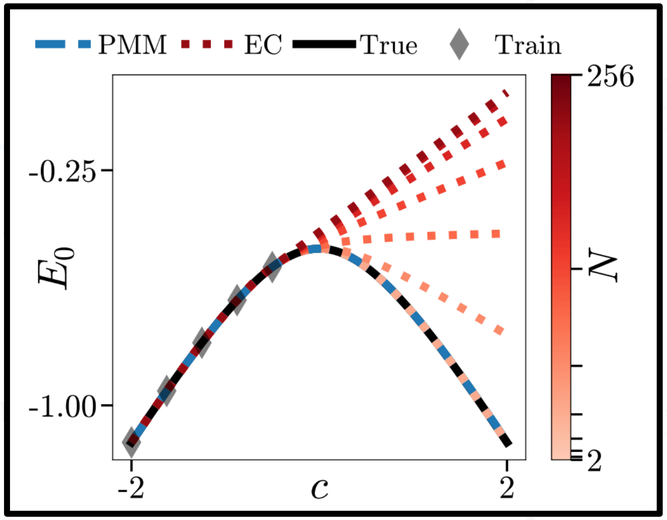
$$\hat{H}=\hat{H}_0+\alpha\hat{H}_1+\alpha^2\hat{H}_2+\ldots$$

Arxiv update!

https://arxiv.org/abs/2401.11694

Parametric Matrix Models

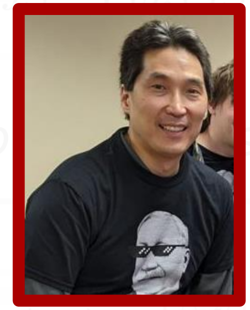
Patrick Cook[*†1,2], **Danny Jammooa**[*‡1,2], **Morten Hjorth-Jensen**[3,1,2], **Daniel D. Lee**[4], **and Dean Lee**[1,2]



defined implicitly [1–6]. Here we introduce a general class of machine learning algorithms called parametric matrix models (PMMs), where the constraint equations to be solved are matrix equations. The dependent variables can be defined implicitly or explicitly, and the equations may use algebraic, differential, or integral relations. One very simple example is $M(\vec{c}) = M_0 + \sum_i c_i M_i$, where M_0 and each M_i are Hermitian matrices, and the final outputs are eigenvalues of $M(\vec{c})$. The PMM can be designed to incor-

Danny Jammooa

Patrick Cook



Dean Lee

Daniel Lee

Morten Hjorth-Jensen

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Parametric Matrix Models

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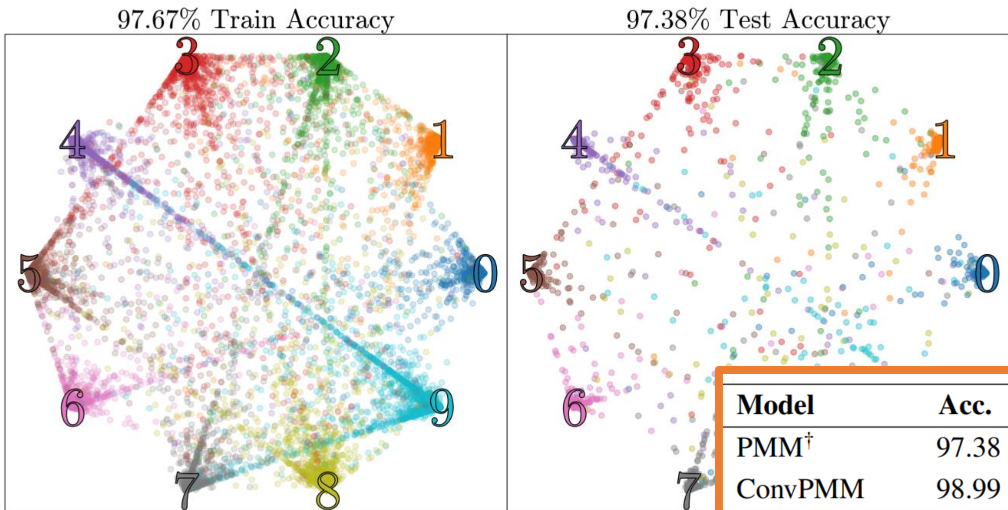
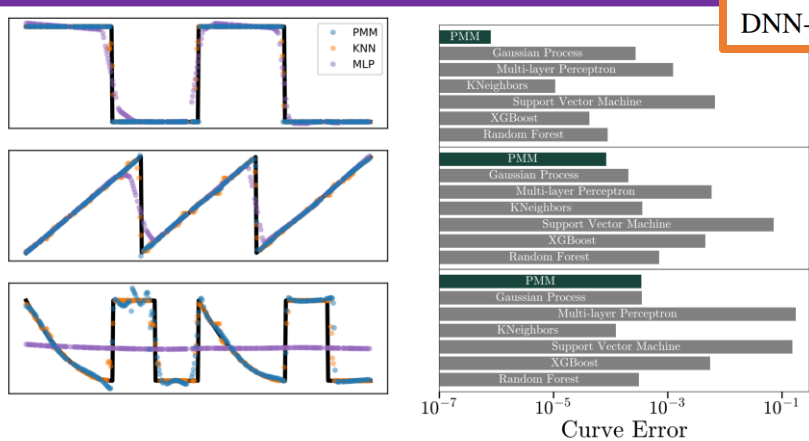
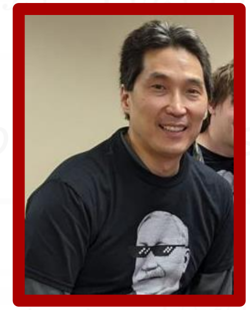


Model	Acc.	float
PMM†	97.38	4990
ConvPMM	98.99	129 416
DNN-2†[56]	96.5	∼ 311 650
DNN-3†[56]	97.0	∼ 386 718
DNN-5†[56]	97.2	∼ 575 050




Danny Jammooa


Patrick Cook


Dean Lee


Daniel Lee

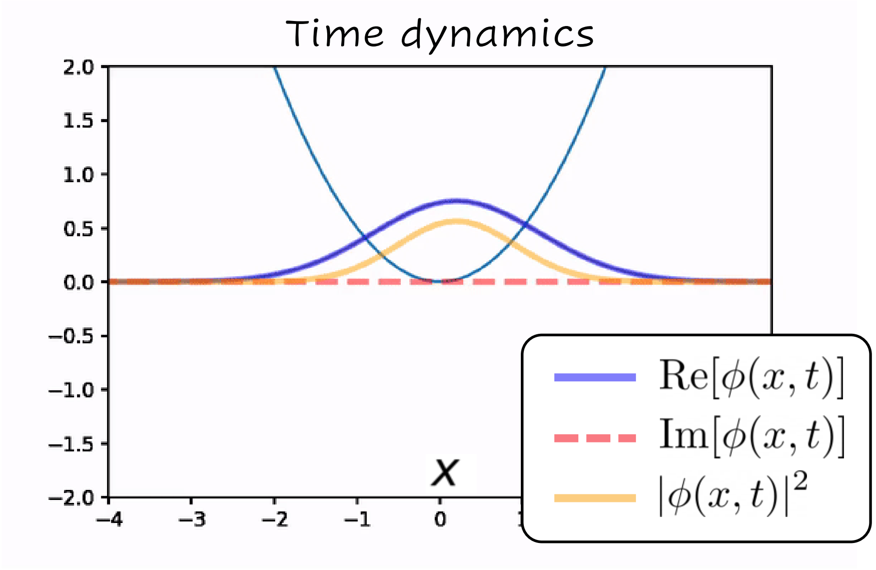

Morten Hjorth-Jensen

Classification ML!

General curve/surface fitting!

Beyond the Reduced Basis Method: applications

Beyond the Reduced Basis Method: applications



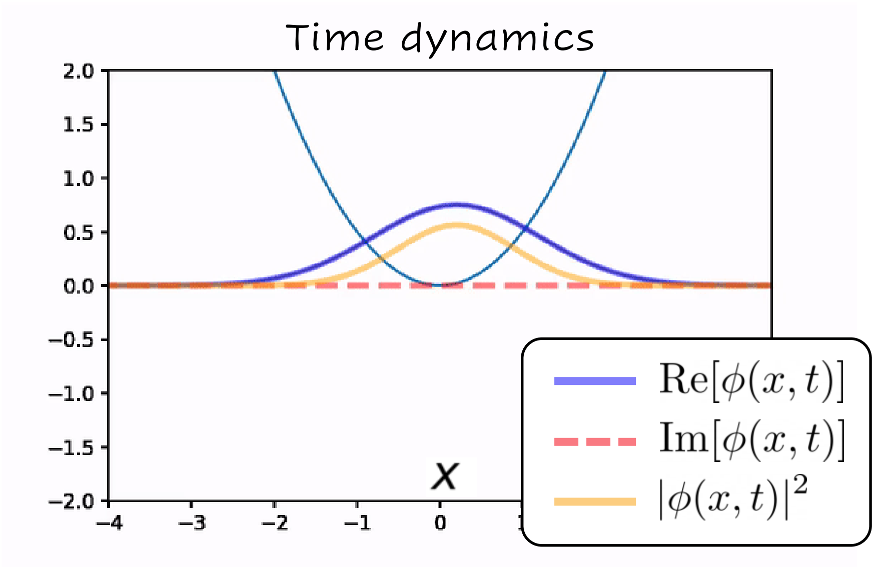
$$\mathcal{H} =$$

$$-\frac{d^2}{dx^2} + kx^2$$

big N

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

Beyond the Reduced Basis Method: applications



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big N

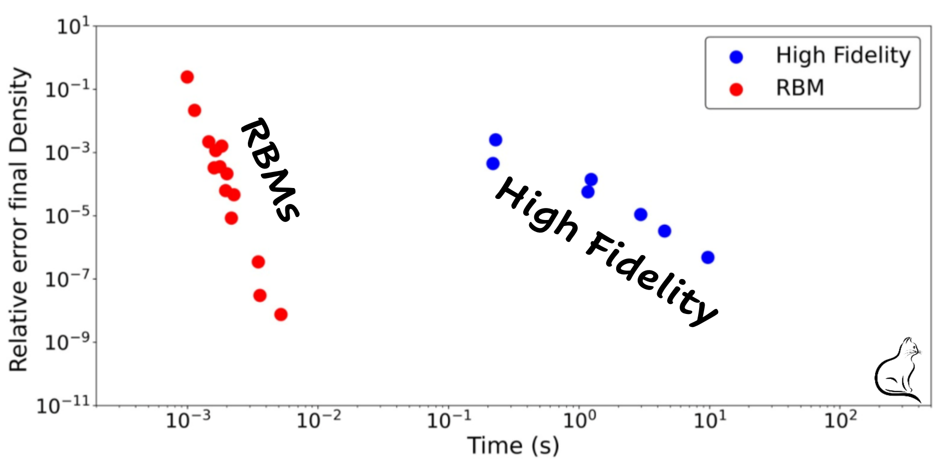
$$\frac{\partial}{\partial t}|\phi(x,t)\rangle = -i\mathcal{H}_{N\times N}|\phi(x,t)\rangle$$

Linear embedding:

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

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

tiny n



Beyond the Reduced Basis Method: applications

$$\mathcal{H} = -\frac{d^2}{dx^2} + kx^2 + q\rho(x)^\sigma$$

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

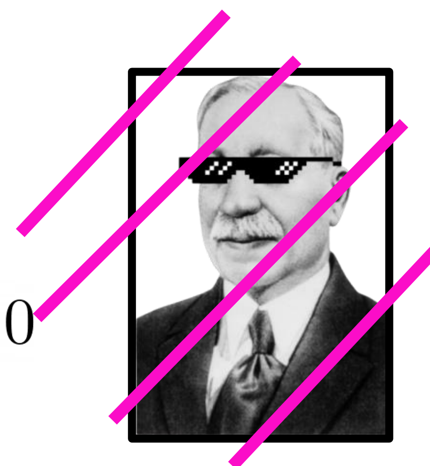
Beyond

Linear embedding:

Problem

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

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



Beyond the Reduced Basis Method: applications

Andrew

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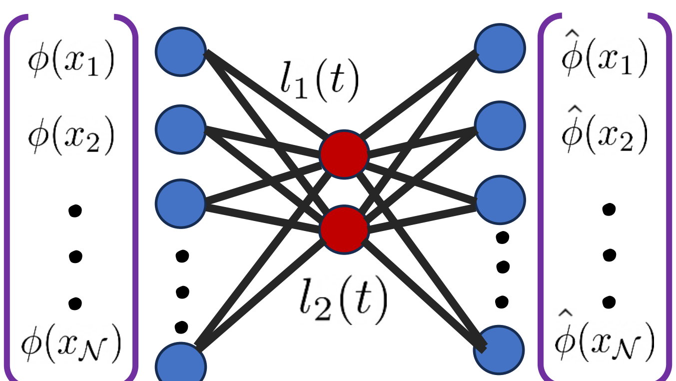
Beyond

Linear embedding:

1) Find good reduced coordinates

Autoencoder



Beyond the Reduced Basis Method: applications

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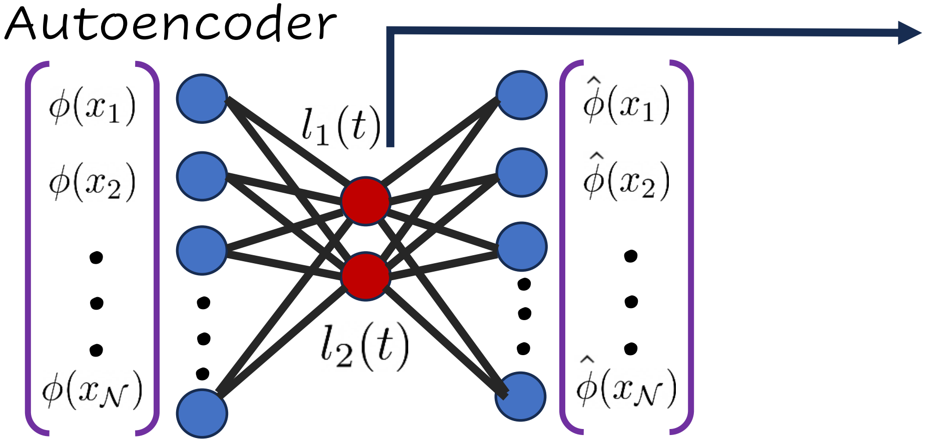

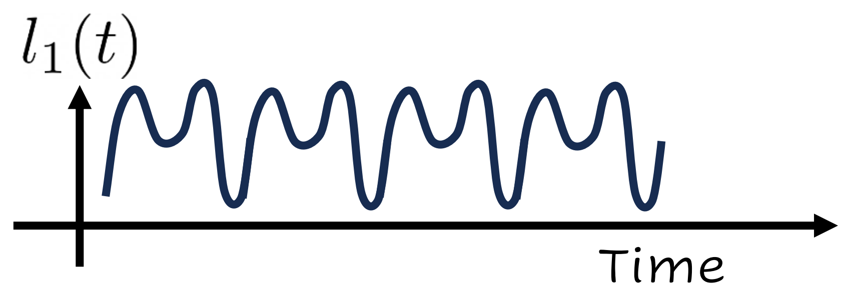

Beyond the Reduced Basis Method: applications

$$\mathcal{H} = -\frac{d^2}{dx^2} + kx^2 + q\rho(x)^\sigma$$

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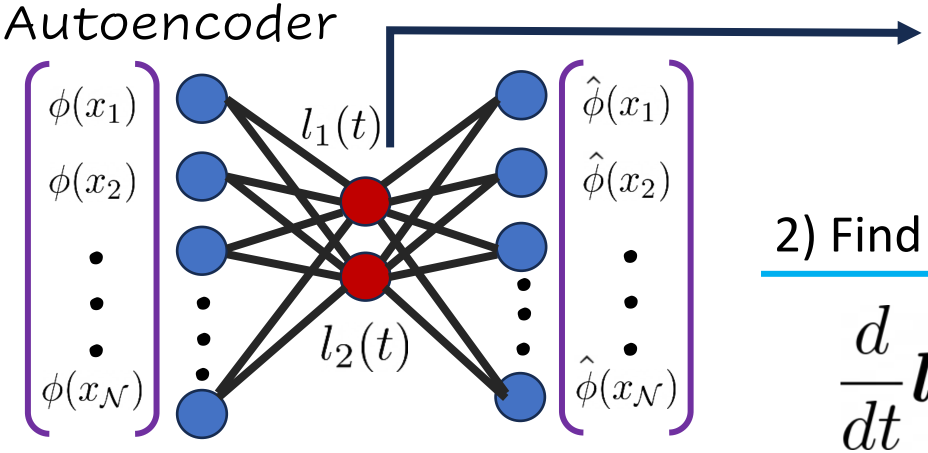
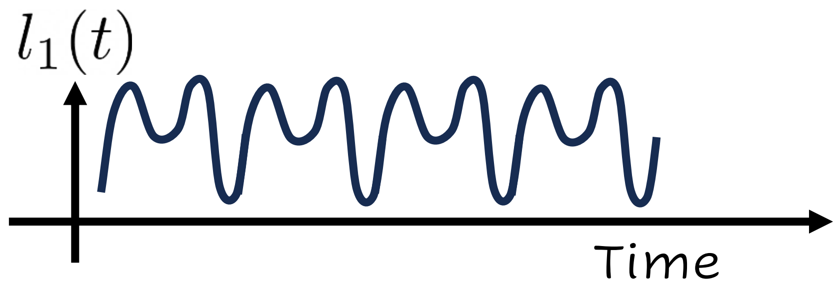
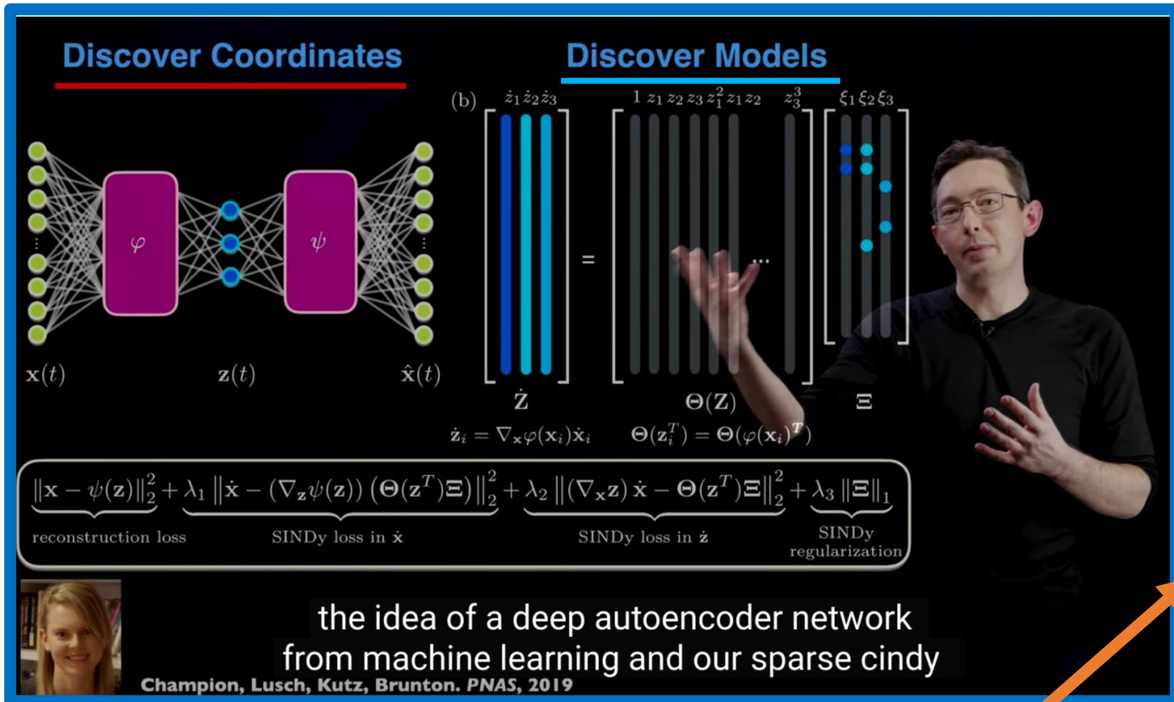


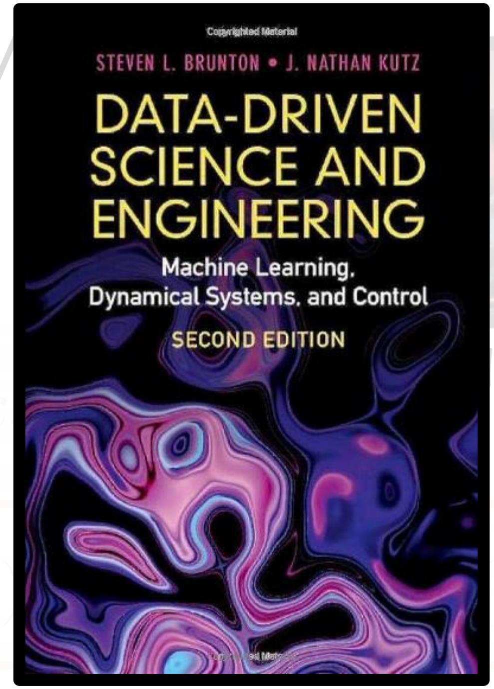


2) Find equations for them:

$$\frac{d}{dt}\boldsymbol{l(t)} = f(\boldsymbol{l(t)})$$

Sparse Identification of Nonlinear Dynamics





Right here in University of Washington!

1) Find good reduced coordinates

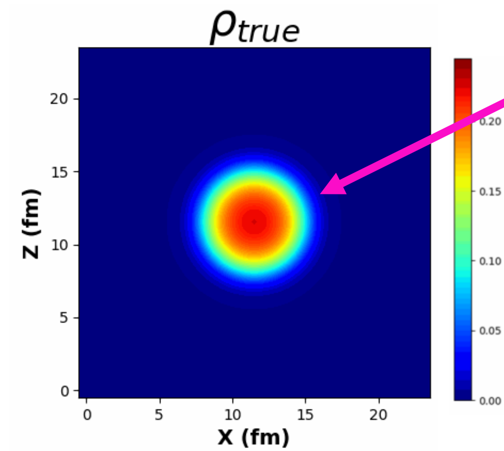
2) Find equations for them:

$$\frac{d}{dt}\boldsymbol{l(t)} = f(\boldsymbol{l(t)})$$

(SINDy)

Sparse Identification of Nonlinear Dynamics

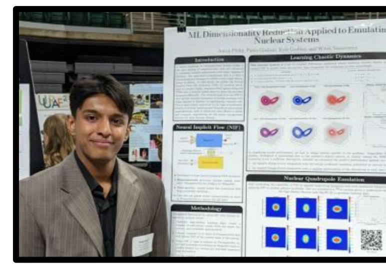
Beyond the Reduced Basis Method: applications



Vibrating Calcium

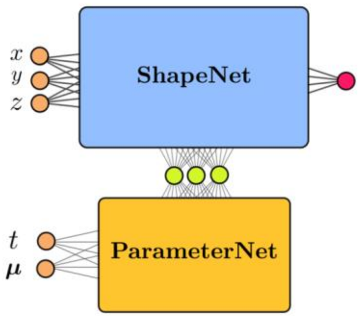
High Fidelity

$$
\begin{aligned}
H_S(\mathbf{r}) = {} & \frac{\hbar^2}{2m}\tau + \frac{1}{2}t_0\left(1+\frac{1}{2}x_0\right)\rho^2 - \frac{1}{2}t_0\left(\frac{1}{2}+x_0\right)\left[\rho_p^2+\rho_n^2\right] + \frac{1}{4}\left[t_1\left(1+\frac{1}{2}x_1\right)+t_2\left(1+\frac{1}{2}x_2\right)\right](\rho\tau-\mathbf{j}^2) \\
& -\frac{1}{4}\left[t_1\left(\frac{1}{2}+x_1\right)-t_2\left(\frac{1}{2}+x_2\right)\right]\left(\rho_p\tau_p+\rho_n\tau_n-\mathbf{j}_p^2-\mathbf{j}_n^2\right) - \frac{1}{16}\left[3t_1\left(1+\frac{1}{2}x_1\right)-t_2\left(1+\frac{1}{2}x_2\right)\right]\rho\nabla^2\rho \\
& +\frac{1}{16}\left[3t_1\left(\frac{1}{2}+x_1\right)+t_2\left(\frac{1}{2}+x_2\right)\right]\left(\rho_p\nabla^2\rho_p+\rho_n\nabla^2\rho_n\right) \\
& +\frac{1}{12}t_3\left[\rho^{\alpha+2}\left(1+\frac{1}{2}x_3\right)-\rho^{\alpha}\left(\rho_p^2+\rho_n^2\right)\left(x_3+\frac{1}{2}\right)\right] \\
& +\frac{1}{4}t_0x_0\mathbf{s}^2-\frac{1}{4}t_0(\mathbf{s}_n^2+\mathbf{s}_p^2)+\frac{1}{24}\rho^{\alpha}t_3x_3\mathbf{s}^2-\frac{1}{24}t_3\rho^{\alpha}(\mathbf{s}_n^2+\mathbf{s}_p^2) \\
& +\frac{1}{32}(t_2+3t_1)\sum_q \mathbf{s}_q\cdot\nabla^2\mathbf{s}_q-\frac{1}{32}(t_2x_2-3t_1x_1)\mathbf{s}\cdot\nabla^2\mathbf{s} \\
& +\frac{1}{8}(t_1x_1+t_2x_2)(\mathbf{s}\cdot\mathbf{T}-\mathbf{J}_{\mu\nu}^2)+\frac{1}{8}(t_2-t_1)\sum_q(\mathbf{s}_q\cdot\mathbf{T}_q-\mathbf{J}_{q\mu\nu}^2) \\
& -\frac{t_4}{2}\sum_{qq'}(1+\delta_{qq'})[\mathbf{s}_q\cdot\nabla\times\mathbf{j}_{q'}+\rho_q\nabla_{\mu\nu}\cdot\mathbf{J}_{\mu\nu}]
\end{aligned}
$$



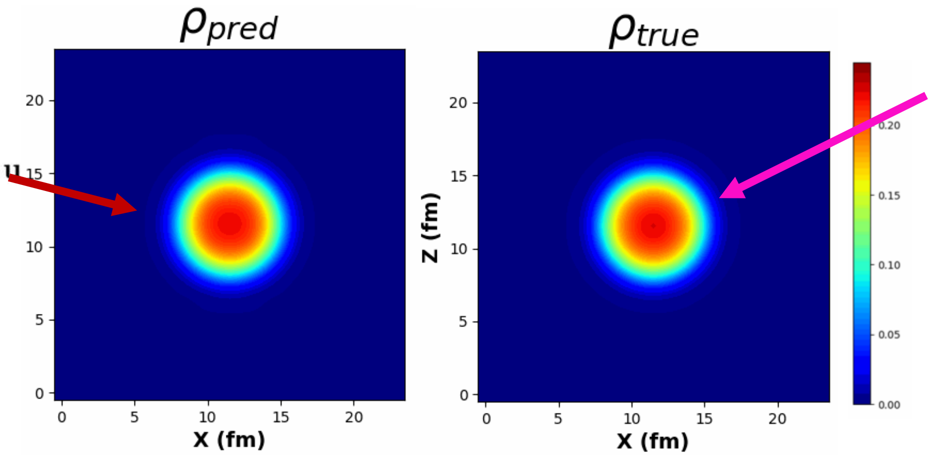
Aaron P.
Pablo G.
Kyle G.
Witek N.

Beyond the Reduced Basis Method: applications



Neural Implicit Flow

https://github.com/pswpswpsw/nif



Vibrating Calcium

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

Shaowu Pan Steven L. Brunton J. Nathan Kutz

High Fidelity

$$
\begin{aligned}
H_S(\boldsymbol{r}) = & \frac{\hbar^2}{2m}\tau + \frac{1}{2}t_0\left(1+\frac{1}{2}x_0\right)\rho^2 - \frac{1}{2}t_0\left(\frac{1}{2}+x_0\right)\left[\rho_p^2+\rho_n^2\right] + \frac{1}{4}\left[t_1\left(1+\frac{1}{2}x_1\right)+t_2\left(1+\frac{1}{2}x_2\right)\right](\rho\tau-\boldsymbol{j}^2) \\
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& +\frac{1}{16}\left[3t_1\left(\frac{1}{2}+x_1\right)+t_2\left(\frac{1}{2}+x_2\right)\right]\left(\rho_p\nabla^2\rho_p+\rho_n\nabla^2\rho_n\right) \\
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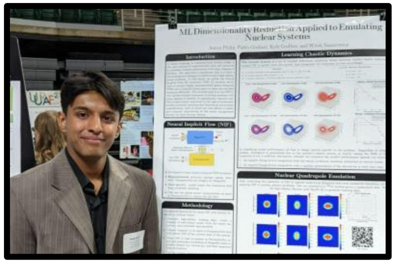
& +\frac{1}{4}t_0x_0\boldsymbol{s}^2-\frac{1}{4}t_0(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2)+\frac{1}{24}\rho^\alpha t_3x_3\boldsymbol{s}^2-\frac{1}{24}t_3\rho^\alpha(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2) \\
& +\frac{1}{32}(t_2+3t_1)\sum_q \boldsymbol{s}_q\cdot\nabla^2\boldsymbol{s}_q-\frac{1}{32}(t_2x_2-3t_1x_1)\boldsymbol{s}\cdot\nabla^2\boldsymbol{s} \\
& +\frac{1}{8}(t_1x_1+t_2x_2)(\boldsymbol{s}\cdot\boldsymbol{T}-\boldsymbol{J}_{\mu\nu}^2)+\frac{1}{8}(t_2-t_1)\sum_q(\boldsymbol{s}_q\cdot\boldsymbol{T}_q-\boldsymbol{J}_{q\mu\nu}^2) \\
& -\frac{t_4}{2}\sum_{qq'}(1+\delta_{qq'})[\boldsymbol{s}_q\cdot\nabla\times\boldsymbol{j}_{q'}+\rho_q\nabla_{\mu\nu}\cdot\boldsymbol{J}_{\mu\nu}]
\end{aligned}
$$



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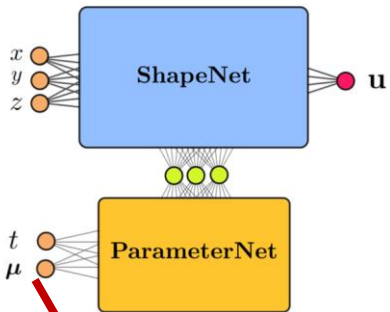
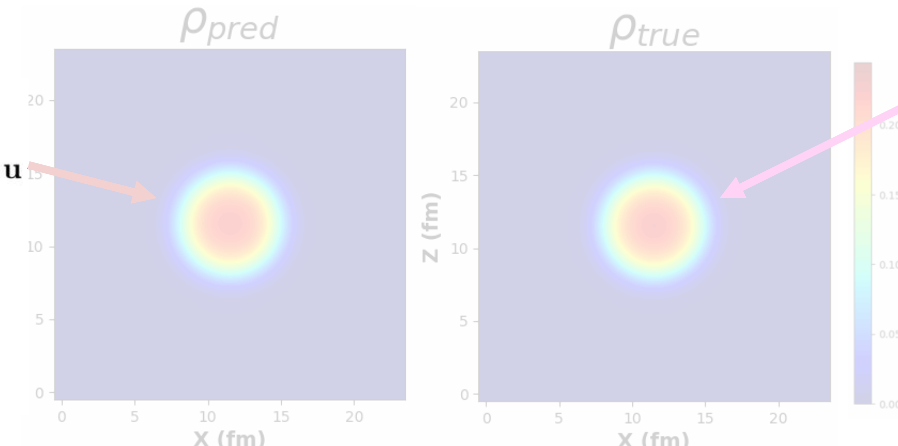
Beyond the Reduced Basis Method: applications





High Fidelity

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Vibrating Calcium

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

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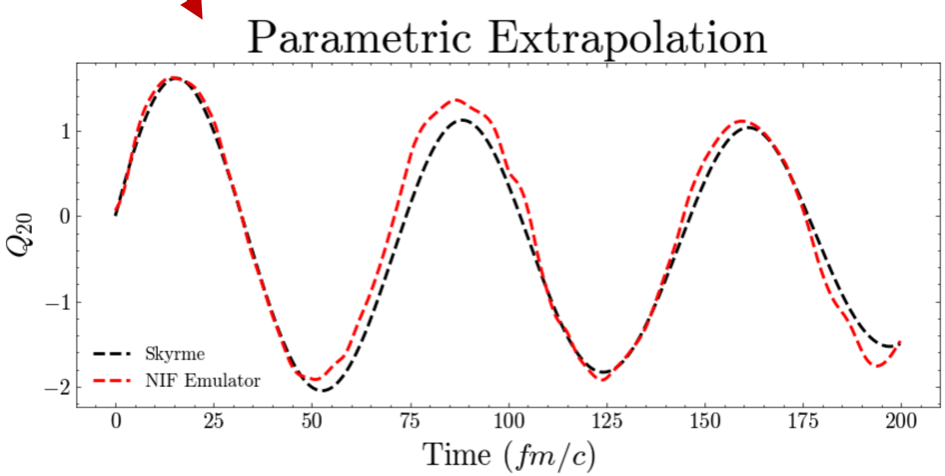
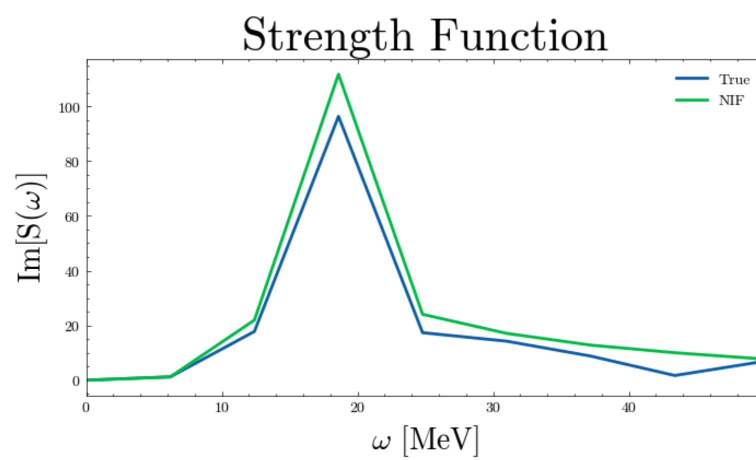
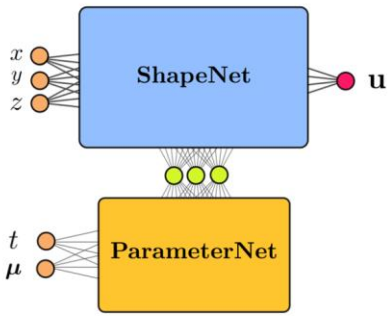
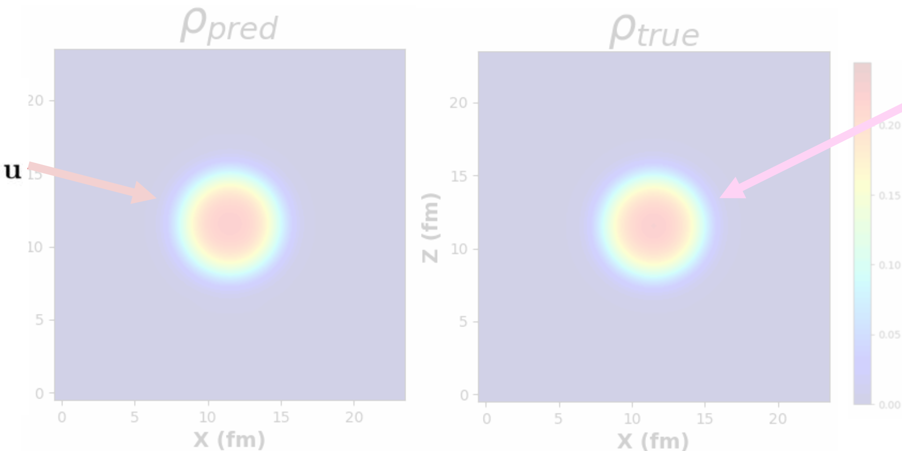




Beyond the Reduced Basis Method: applications





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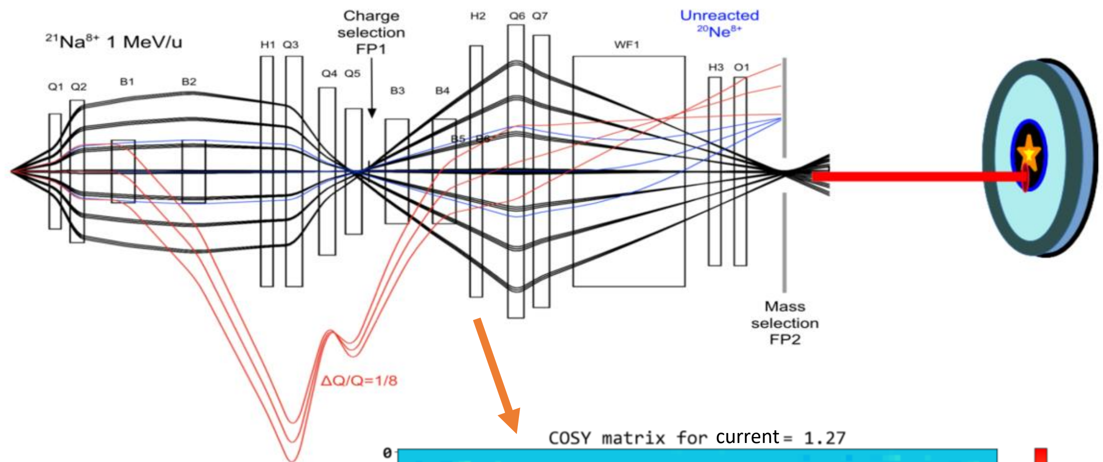
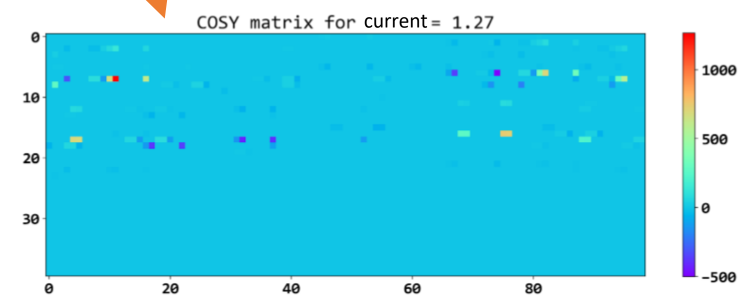
UURAF 2023 Award Winner

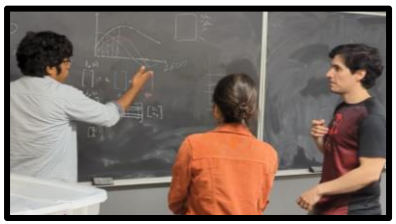
Goldwater Scholarship 2024

Beyond the Reduced Basis Method: applications





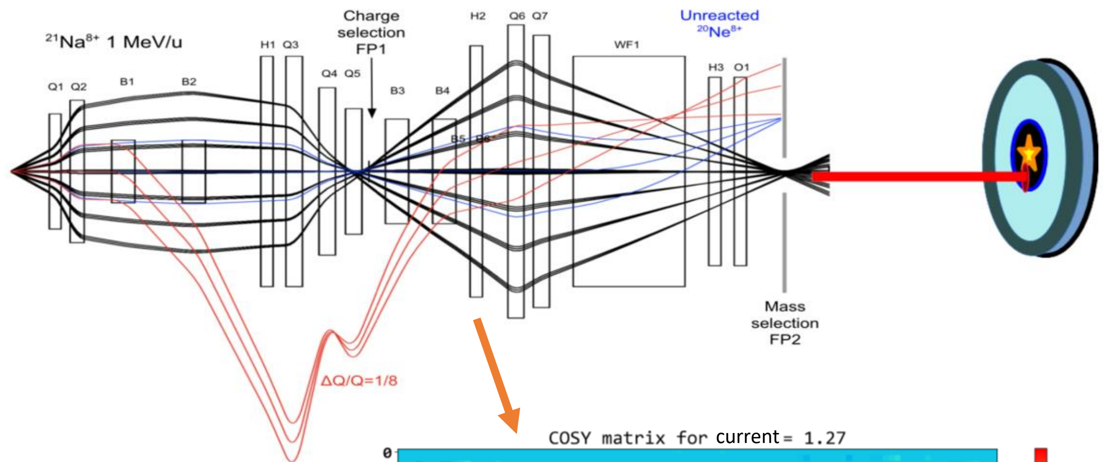
Edgard Ruchi Diogenes



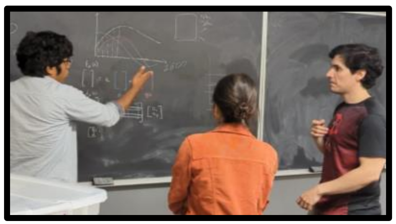
Efficient Emulation of the SECAR beam

Dimensionality Reduction in
Nuclear Physics
Presented by ASCSN

Beyond the Reduced Basis Method: applications



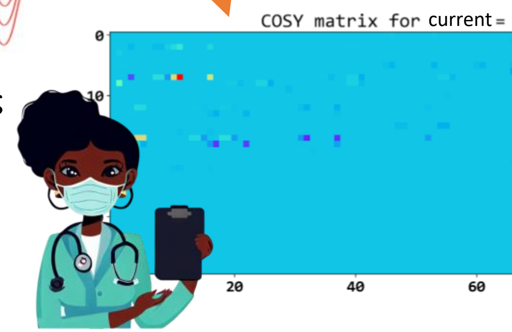
Edgard Ruchi Diogenes



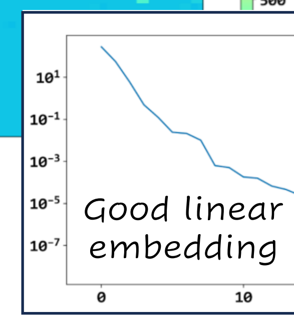
Efficient Emulation of the SECAR beam

Dimensionality Reduction in Nuclear Physics
Presented by ASCSN

Learn Equations from data



$$\hat{M}(I) = M_0 + \sum_k a_k(I) M_k$$



Beyond the Reduced Basis Method: applications

Edgard B. Ruchi G. Diogenes F.

Efficient Emulation of the SECAR beam

Dimensionality Reduction in Nuclear Physics
Presented by ASCSN

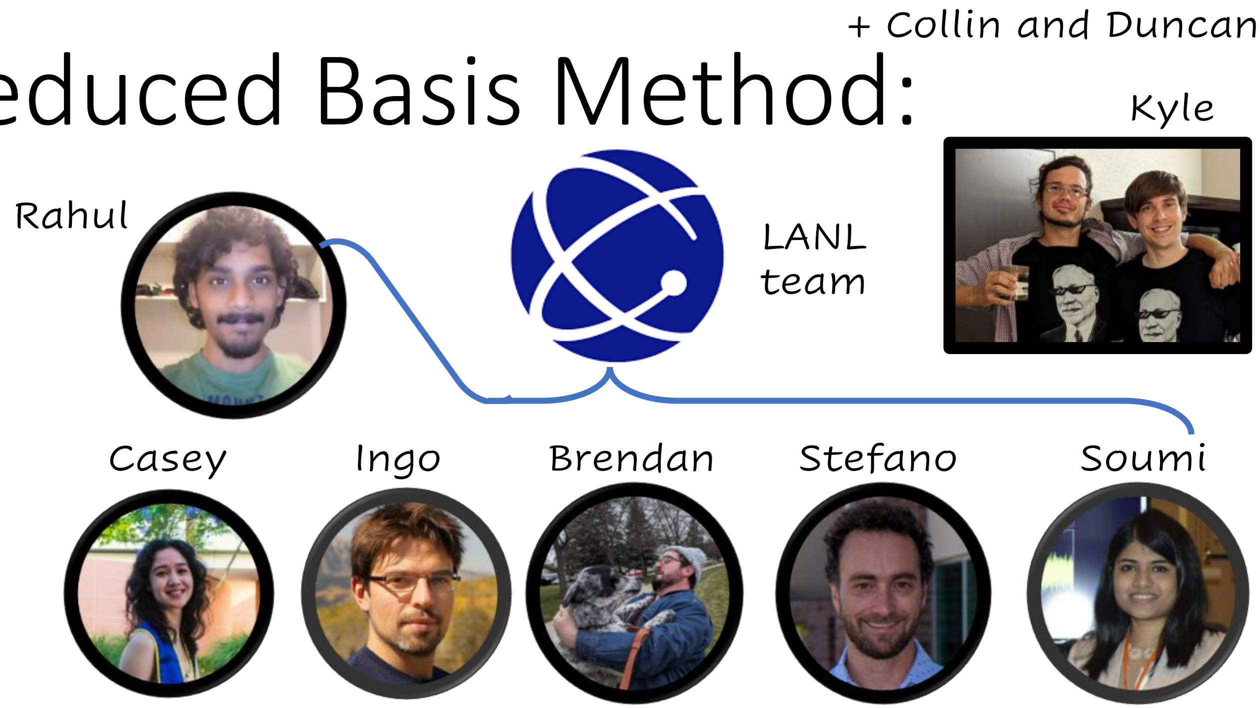
Learn Equations from data

$$\hat{M}(I) = M_0 + \sum_k a_k(I) M_k$$

~ 3,000 faster than high fidelity

# of Bases	Emulation Time (to FP1)	Max Position Error (x)	Max angular Error (ax)
3	(9.7 ± 0.3) ms*	1 μm	1 nrad
10	(10.9 ± 0.6) ms*	0.01 μm	7.5 prad
15	(12.1 ± 0.2) ms*	0.7 nm	0.3 frad

Beyond the Reduced Basis Method: applications



This morning

Emulators for Inverse Problems in Dense Matter Physics

Beyond the Reduced Basis Method: applications

+ Collin and Duncan

Rahul

LANL team

Kyle

1) Find good reduced coordinates

Linear embedding

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

Casey

Ingo

Brendan

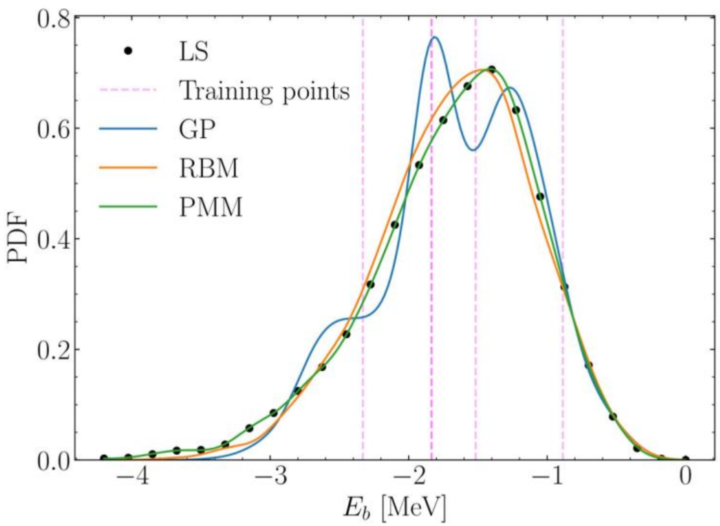
Stefano

Soumi

2) Find equations from data

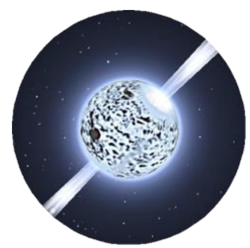
Emulators for scarce and noisy data: application to auxiliary field diffusion Monte Carlo for the deuteron

Rahul Somasundaram,[1,2,*] Cassandra L. Armstrong,[3] Pablo Giuliani,[4,5] Kyle Godbey,[4] Stefano Gandolfi,[1] and Ingo Tews[1]

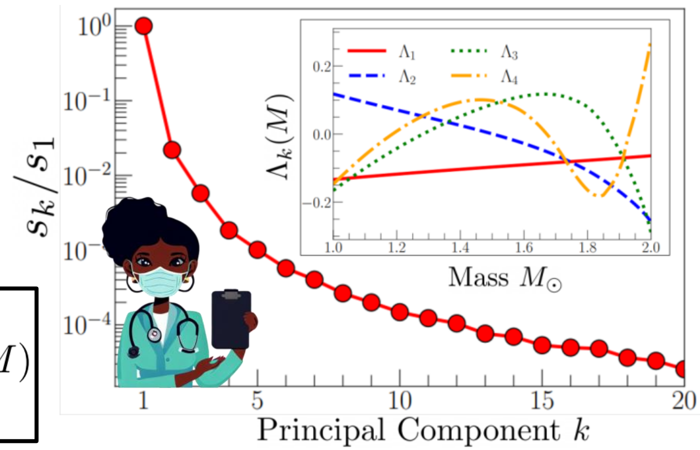


Towards accelerated nuclear-physics parameter estimation from binary neutron star mergers: Emulators for the Tolman-Oppenheimer-Volkoff equations

Brendan T. Reed,[1] Rahul Somasundaram,[1,2] Soumi De,[1] Cassandra L. Armstrong,[3] Pablo Giuliani,[4] Collin Capano,[2,5] Duncan A. Brown,[2] and Ingo Tews[1]



$$\sum_k^n a_k(\alpha)\Lambda_k(M)$$



This morning

Emulators for Inverse Problems in Dense Matter Physics

Beyond the Reduced Basis Method: applications

1) Find good reduced coordinates

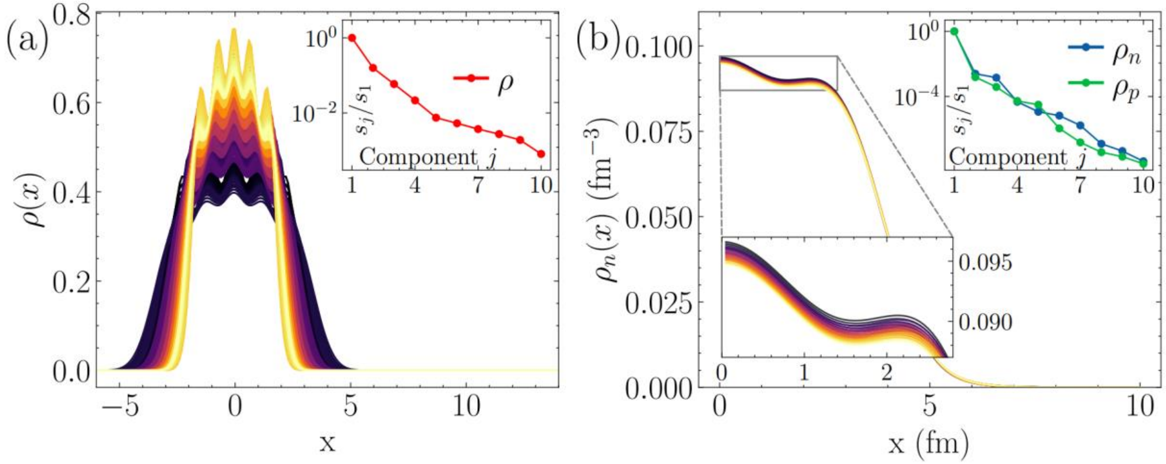
Linear embedding

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

2) Find equations from data

Non-linear toy problem

Skyrme DFT



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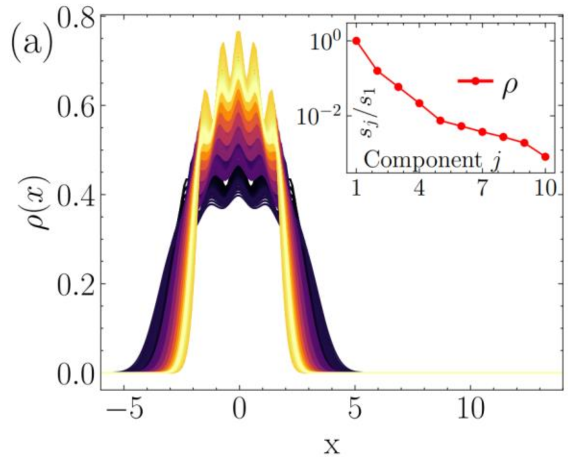
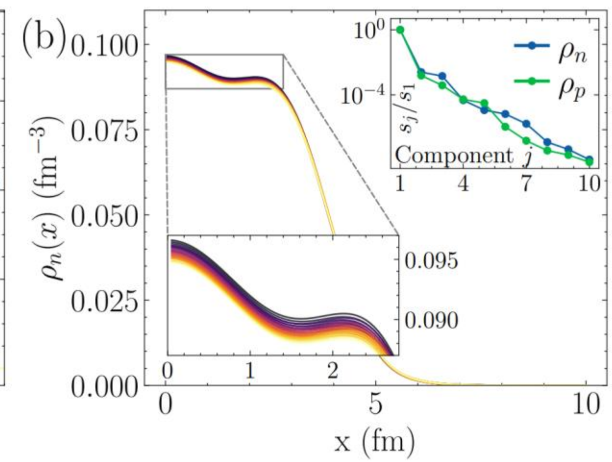
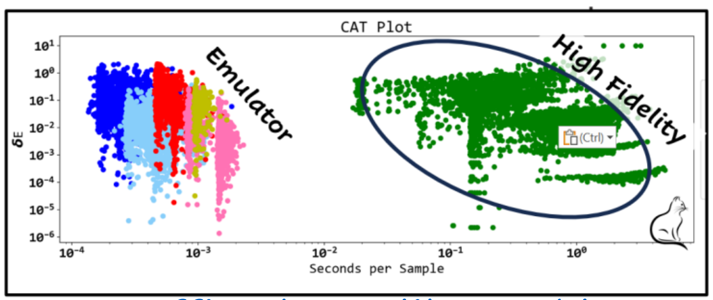


Skyrme DFT

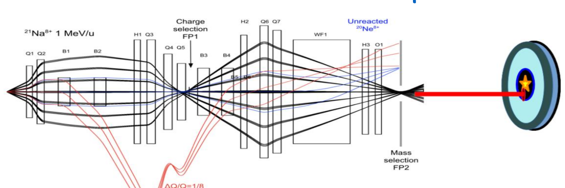


Learning Implicit Equations from data

Diógenes Figueroa,[1,*] E. Bonilla,[2] Ruchi Garg,[3] Pablo Giuliani,[3] and Kyle Godbey[3]

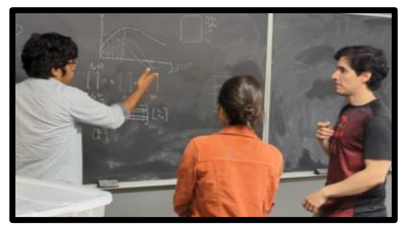


Non-affined DFT-like problems

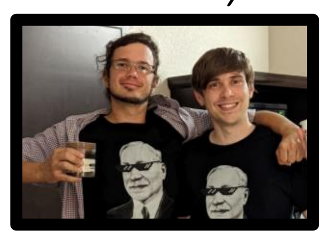


Experimental control

Edgard Ruchi Diogenes



me Kyle



Beyond the Reduced Basis Method: applications

1) Find good reduced coordinates

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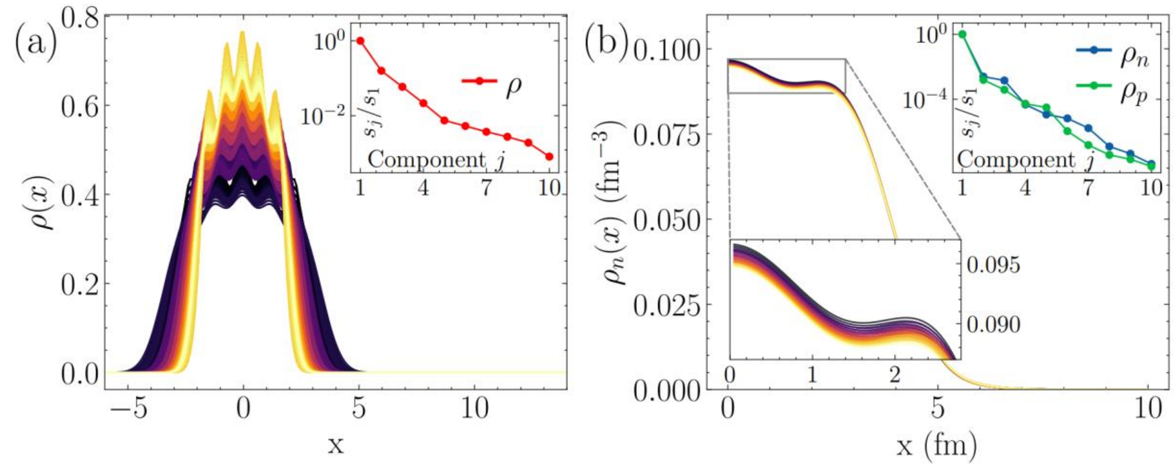
2) Find equations from data

Non-linear toy problem | Skyrme DFT



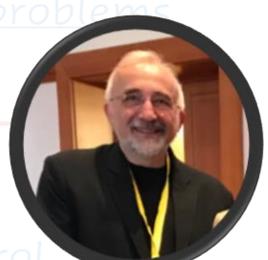
Illya

me Kyle

Nathan

Wolfgang

Witek



Discovering reduced order model equations of many-body quantum systems using genetic programming: a technical report

Illya Bakurov,[1] Pablo Giuliani,[2] Kyle Godbey,[2] Nathan Haut,[3] Wolfgang Banzhaf,[1] and Witold Nazarewicz[2,4]

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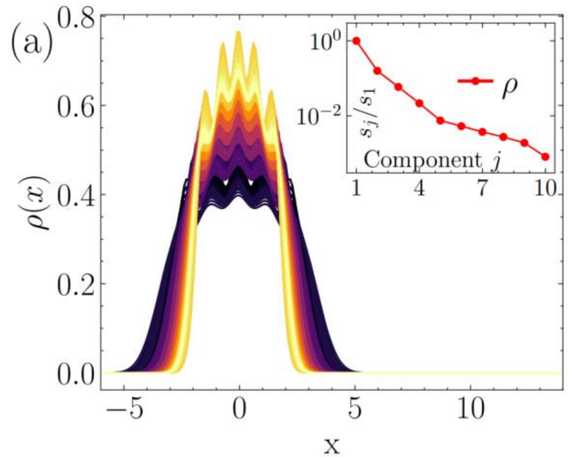
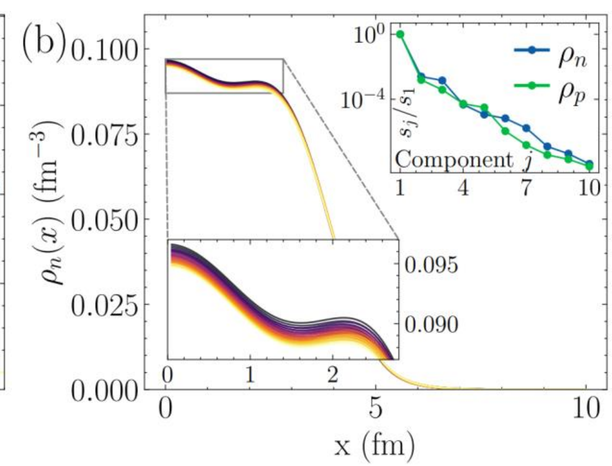


Skyrme DFT



Illya

me Kyle

Nathan

Wolfgang

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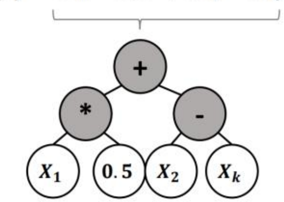
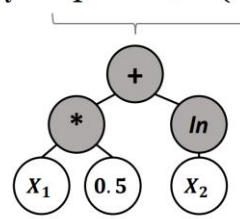
Discovering reduced order model equations of many-body quantum systems using genetic programming: a technical report

Illya Bakurov,[1] Pablo Giuliani,[2] Kyle Godbey,[2] Nathan Haut,[3] Wolfgang Banzhaf,[1] and Witold Nazarewicz[2,4]

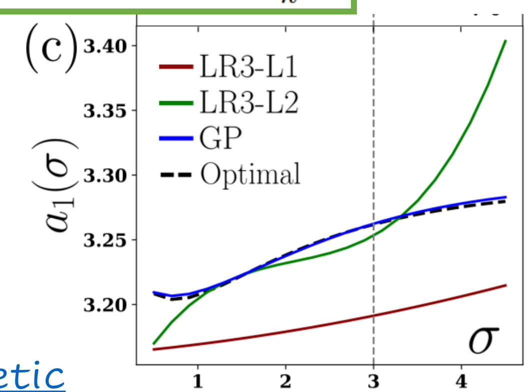
$f_i = X_1 * 0.5 + X_2 - X_k$



$f_i = X_1 * 0.5 + \ln(X_2)$

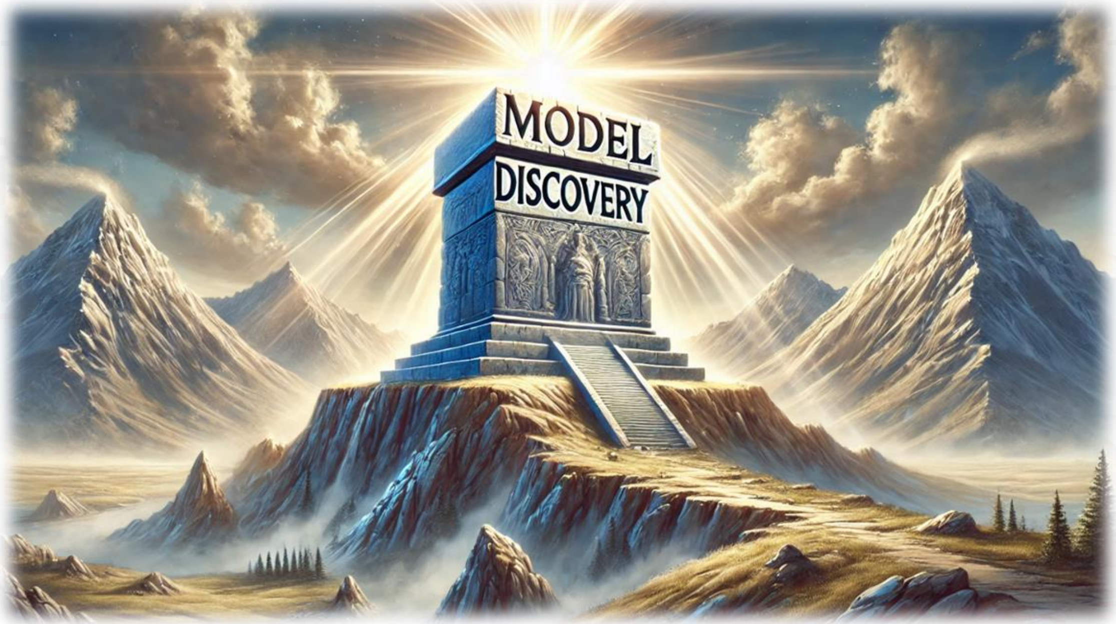


$$\hat{\rho}(x;\alpha) = \sum_k^n a_k(\alpha)\rho_k(x)$$



Genetic Programing

10,000 speed-up!



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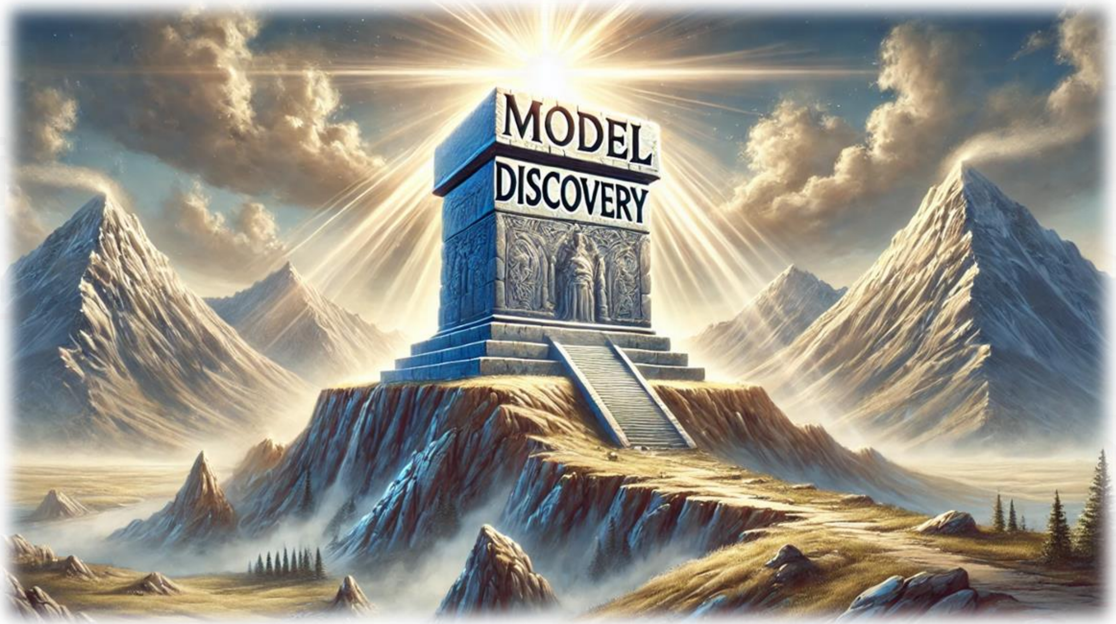

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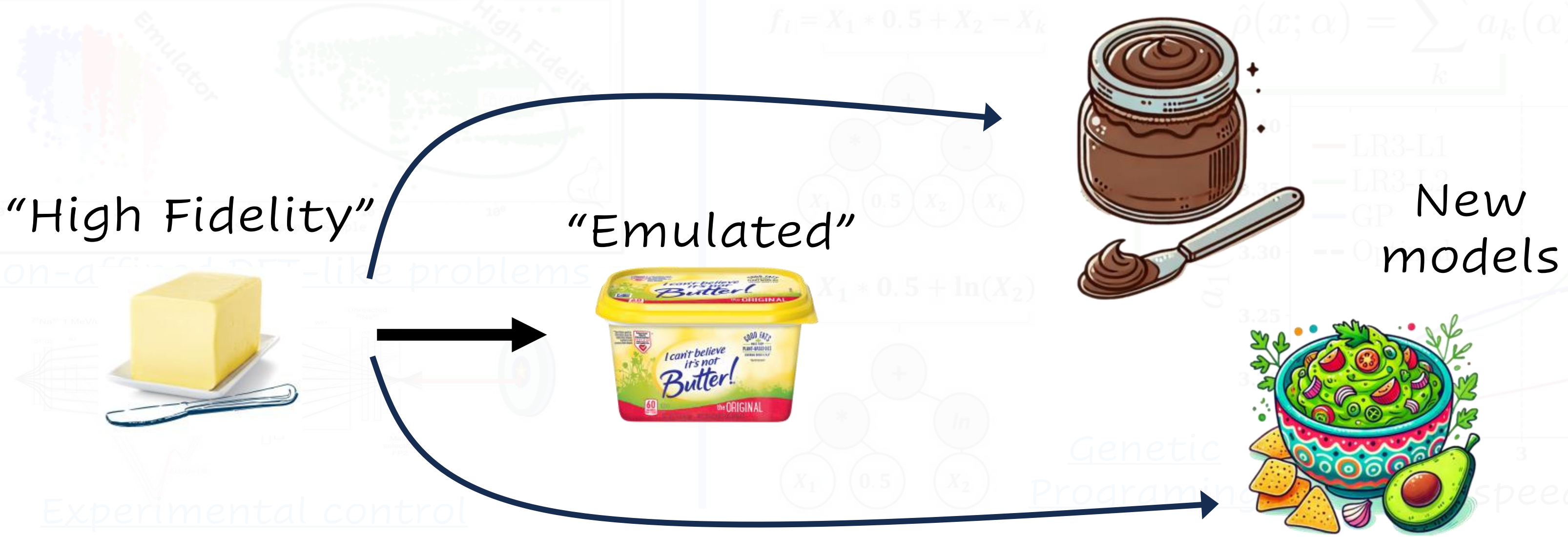


[Link to these slides]

Outline

My context

Bayes and Nuclei

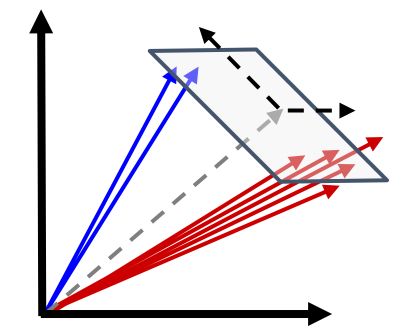
Two challenges

Computational paradigm

Dimensionality Reduction

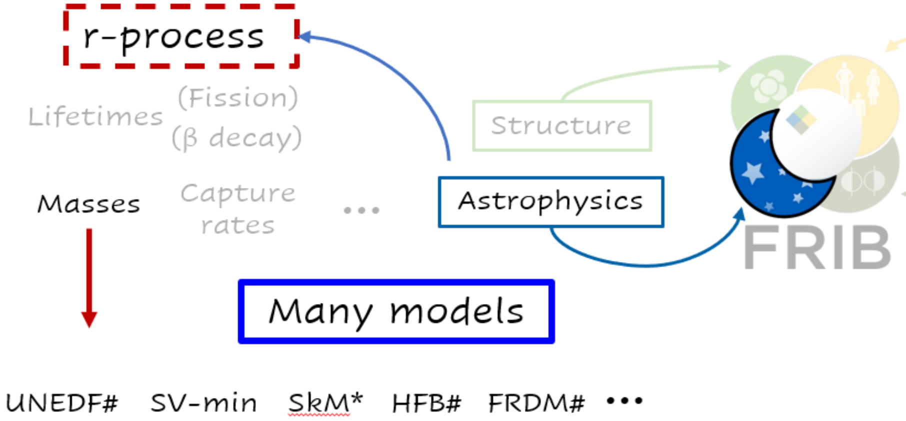
Model Order Reduction (Faster)

Model Combination (Fewer)

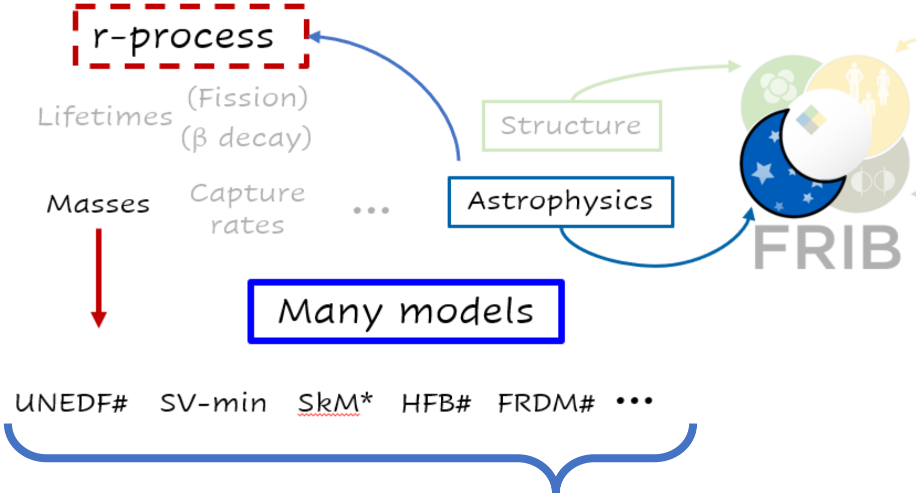


Takeaways

Combining models



Combining models



Can we combine the wisdom of all?

A congress of models

Combining models

r-process

Lifetimes (Fission) (β decay)

Masses Capture rates ...

Structure

Astrophysics

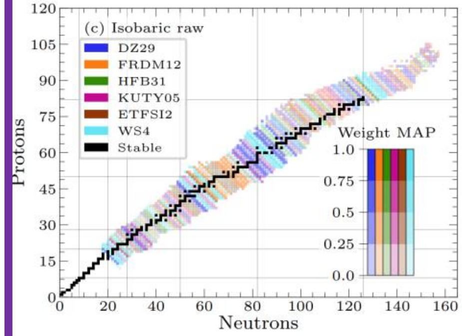
Many models

UNEDF# SV-min SkM* HFB# FRDM# •••

Can we combine the wisdom of all?

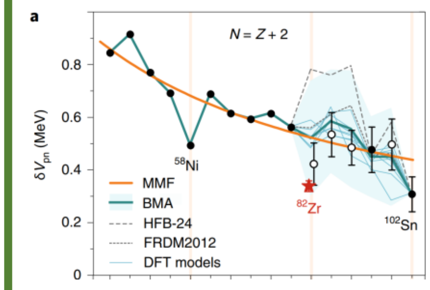
Uncertainty Quantification of Mass Models Using Ensemble Bayesian Model Averaging

Yukiya Saito,[1,2,3,4,*] I. Dillmann,[1,5] R. Krücken,[1,2,6] M. R. Mumpower,[7,8] and R. Surman[3]



Precision mass measurement of lightweight self-conjugate nucleus ^{80}Zr

A. Hamaker, E. Leistenschneider, R. Jain, G. Bollen, S. A. Giuliani, K. Lund, W. Nazarewicz, L. Neufcourt, C. R. Nicoloff, D. Puentes, R. Ringle, C. S. Sumithrarachchi and I. T. Yandow



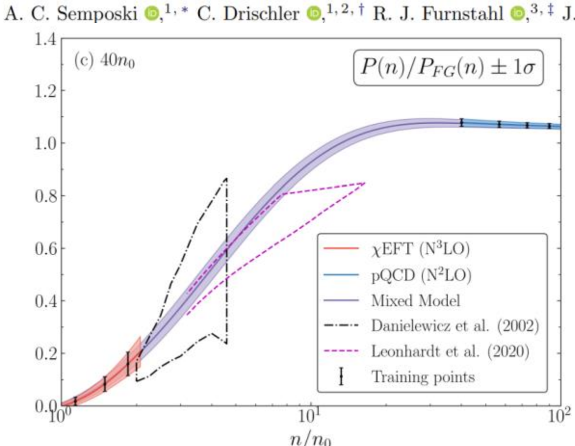
Bayesian Model Averaging

Bayesian Model Mixing

A congress of models

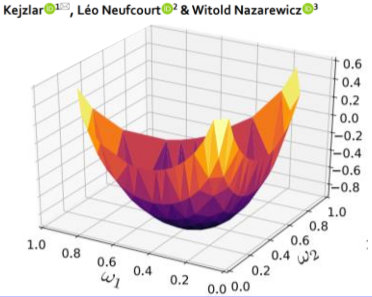
From chiral EFT to perturbative QCD: a Bayesian model mixing approach to symmetric nuclear matter

A. C. Semposki,[1,*] C. Drischler,[1,2,†] R. J. Furnstahl,[3,‡] J. A. Melendez,[3,§] and D. R. Phillips[1,4,¶]

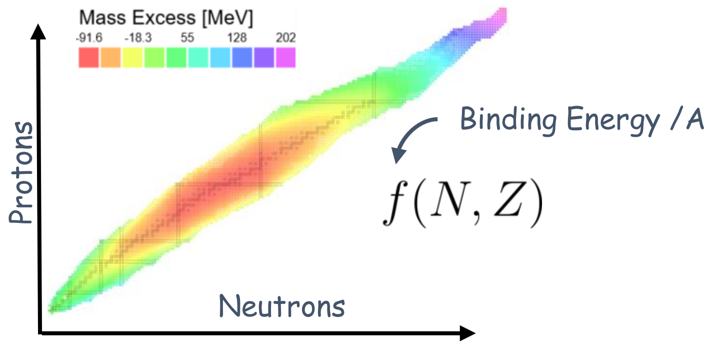


Local Bayesian Dirichlet mixing of imperfect models

Vojtech Kejzlar[1], Léo Neufcourt[2] & Witold Nazarewicz[3]



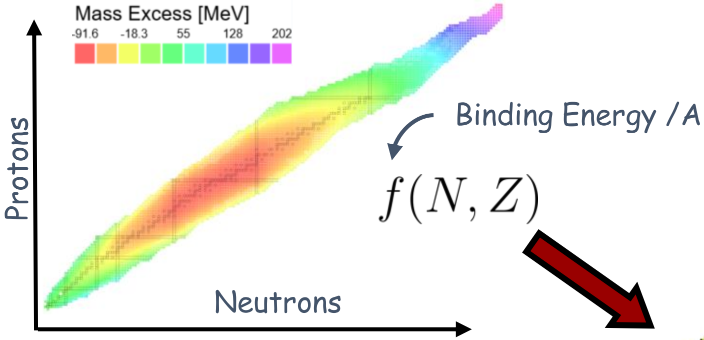
Combining models

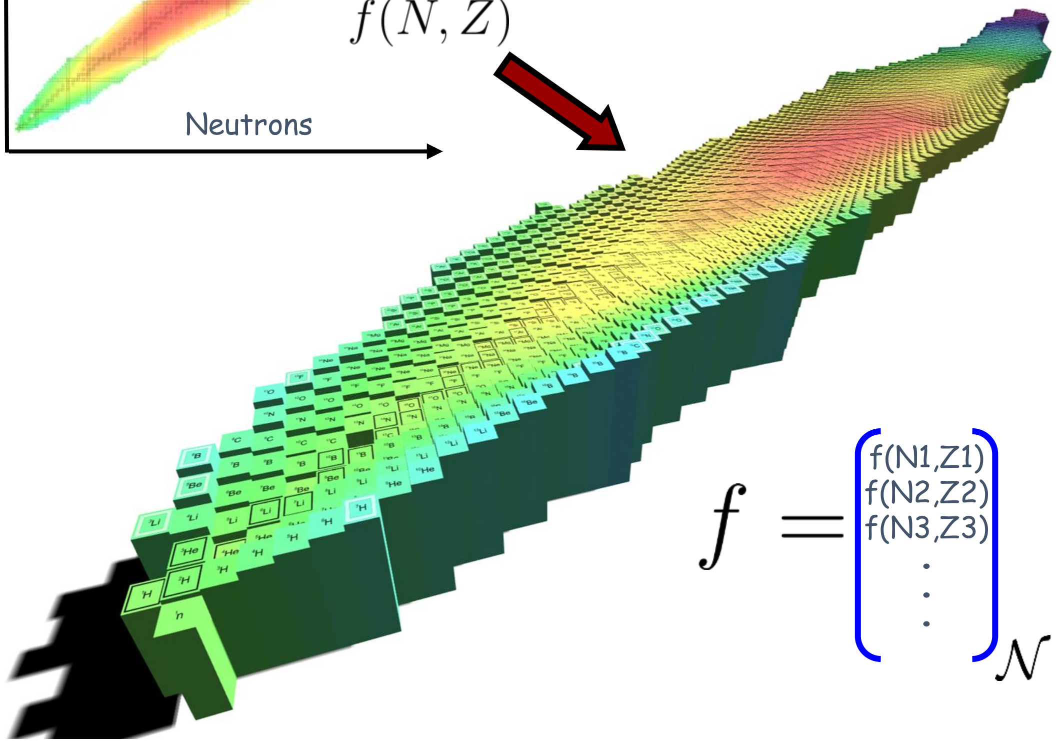


Model orthogonalization and Bayesian forecast mixing via Principal Component Analysis

Pablo Giuliani [1,+], Kyle Godbey [1,x], Vojtech Kejzlar [2,†], and Witold Nazarewicz [3,*]

Combining models





$$f = \begin{pmatrix} f(N1,Z1) \\ f(N2,Z2) \\ f(N3,Z3) \\ \vdots \end{pmatrix}_{\mathcal{N}}$$

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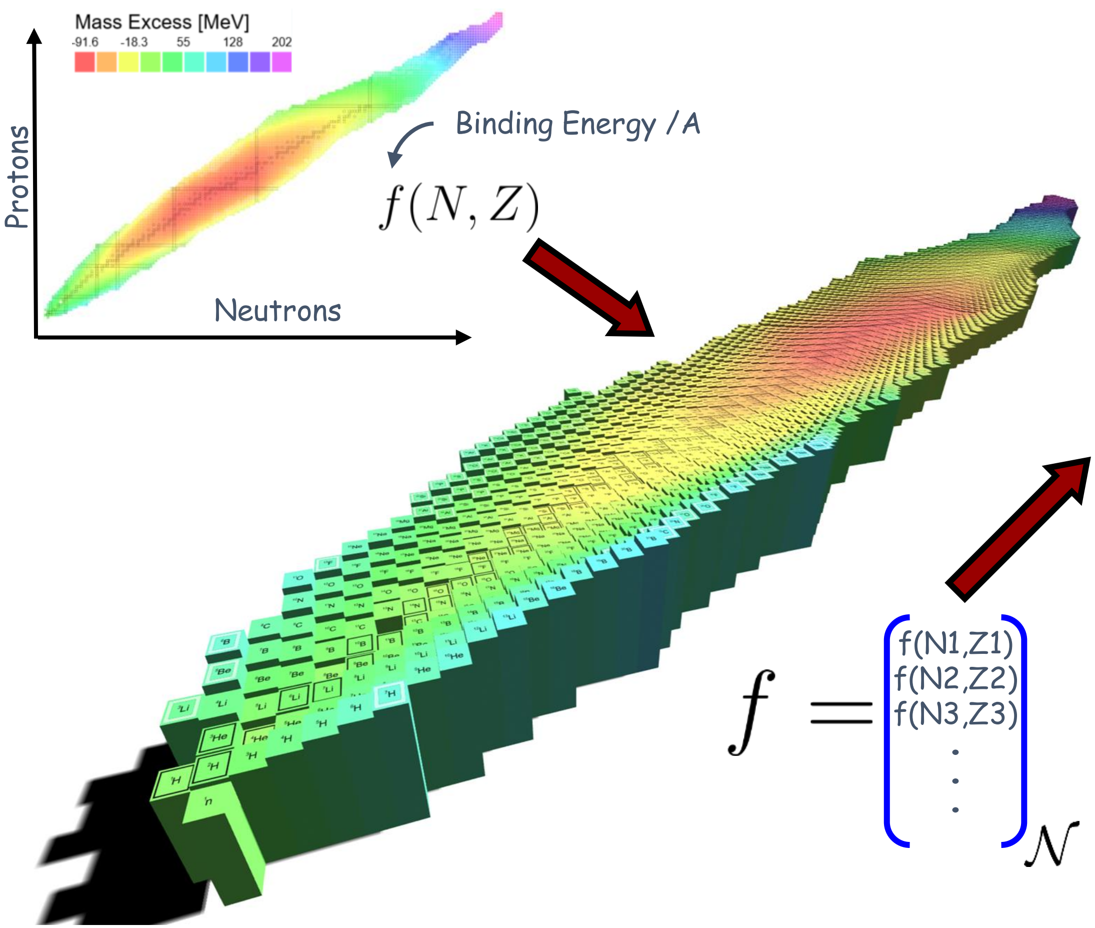

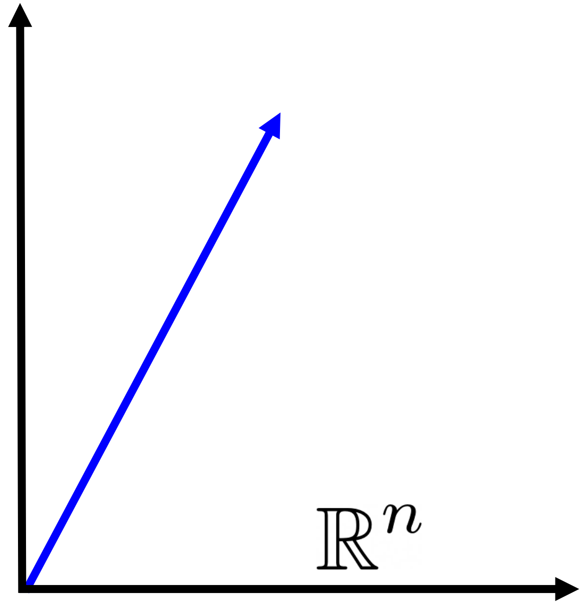

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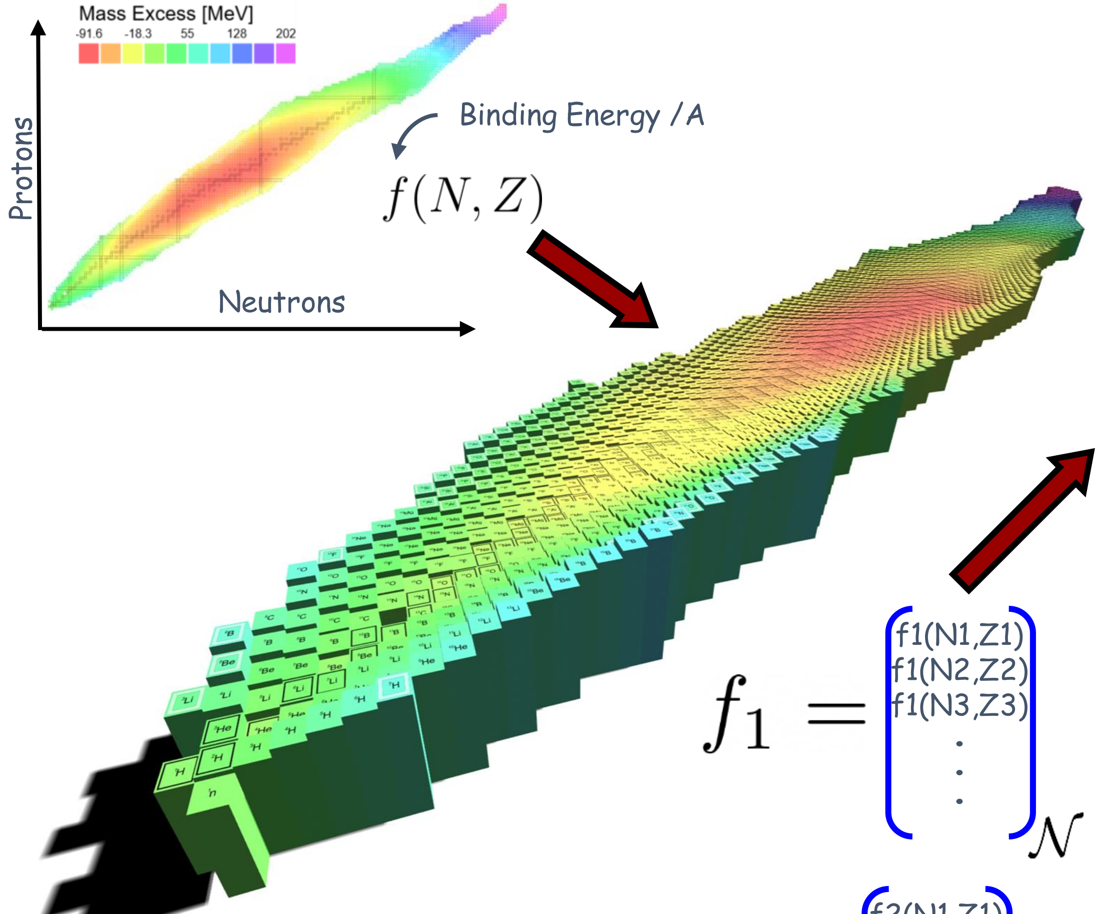
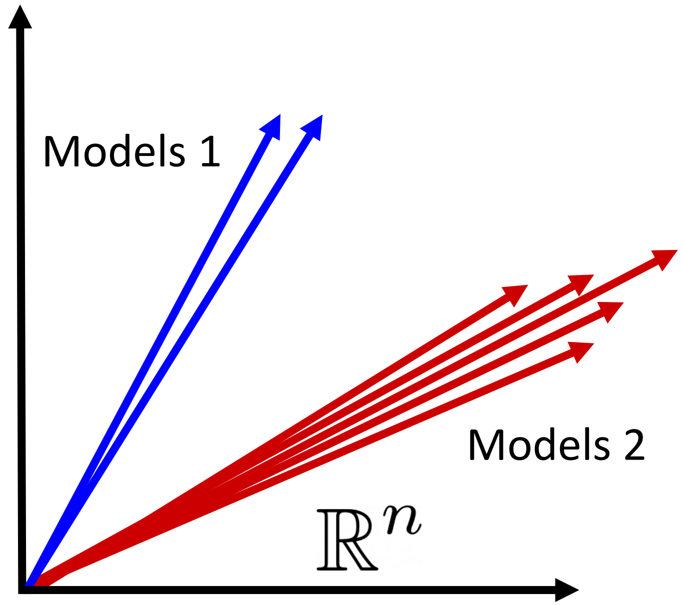
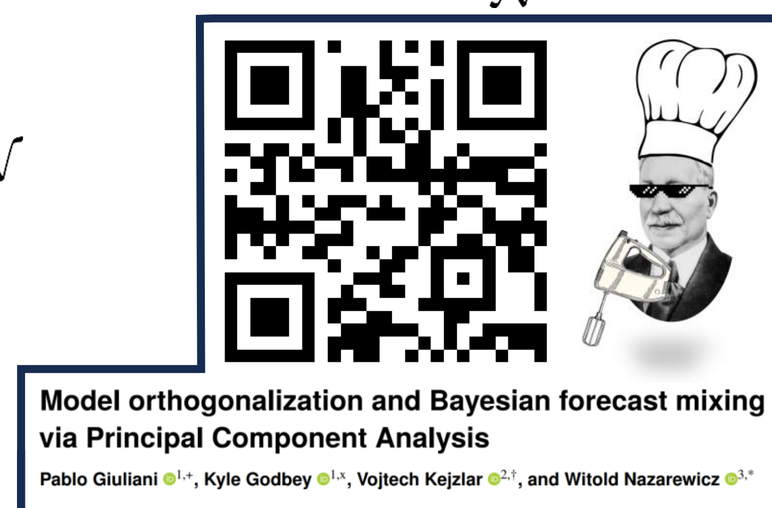




$$f_1 = \begin{pmatrix} f1(N1,Z1) \\ f1(N2,Z2) \\ f1(N3,Z3) \\ \vdots \end{pmatrix}_{\mathcal{N}}$$

$$f_2 = \begin{pmatrix} f2(N1,Z1) \\ f2(N2,Z2) \\ f2(N3,Z3) \\ \vdots \end{pmatrix}_{\mathcal{N}}$$

$$f_3 = \begin{pmatrix} f3(N1,Z1) \\ f3(N2,Z2) \\ f3(N3,Z3) \\ \vdots \end{pmatrix}_{\mathcal{N}} \quad \ldots$$



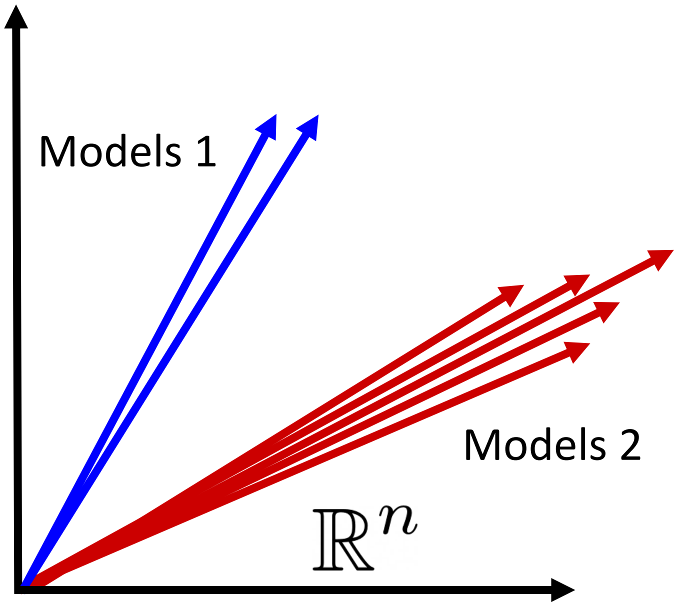
Combining models

Combined model

Weights

$$f^{\dagger}(\boldsymbol{x};\omega) = \sum_{k=1}^{m} \omega_k \, f_k(\boldsymbol{x})$$

Original models



Model orthogonalization and Bayesian forecast mixing via Principal Component Analysis

Pablo Giuliani [1,+], Kyle Godbey [1,x], Vojtech Kejzlar [2,†], and Witold Nazarewicz [3,*]

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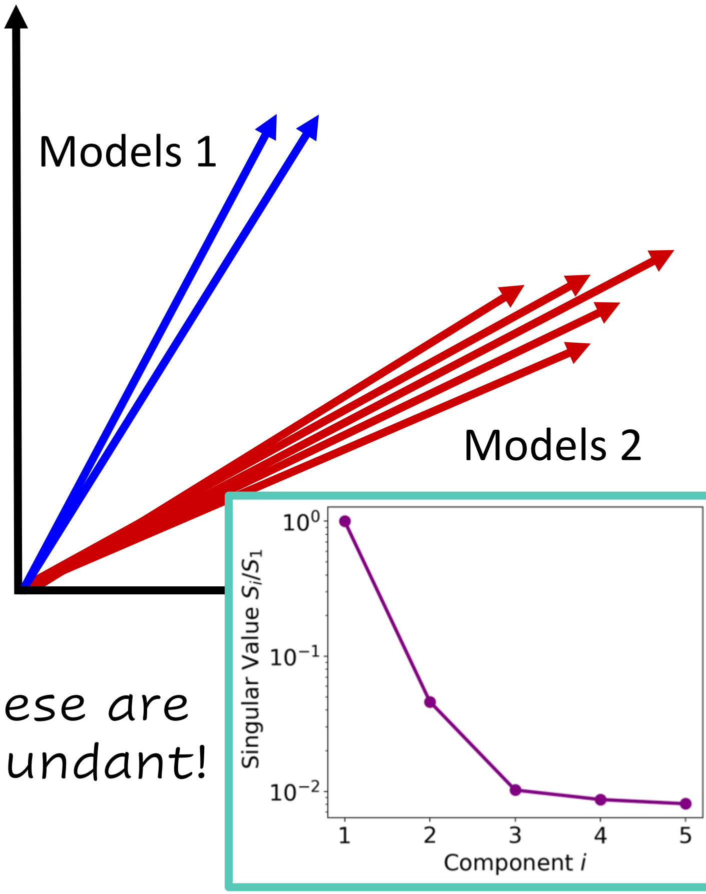

These are redundant!

PCA Doctor

Model orthogonalization and Bayesian forecast mixing via Principal Component Analysis

Pablo Giuliani [1,*], Kyle Godbey [1,×], Vojtech Kejzlar [2,†], and Witold Nazarewicz [3,*]

Combining models

Combined model

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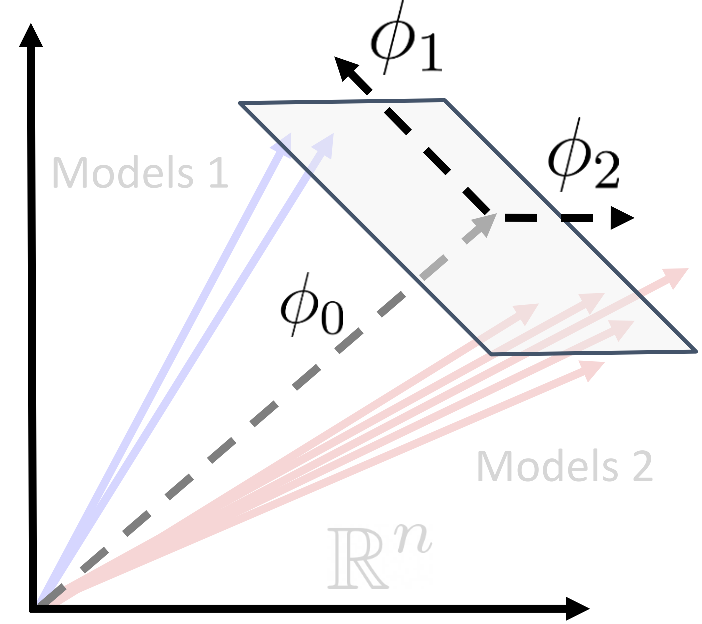
Original models

Principal Component Analysis



Principal components

$$f^{\dagger}(\boldsymbol{x};\boldsymbol{b}) = \phi_0(\boldsymbol{x}) + \sum_{j=1}^{p} b_j \phi_j(\boldsymbol{x})$$

Combined model

Latent weights

Bayesian way

$$P(\boldsymbol{b}|\boldsymbol{Y})$$

Model orthogonalization and Bayesian forecast mixing via Principal Component Analysis

Pablo Giuliani, Kyle Godbey, Vojtech Kejzlar, and Witold Nazarewicz

Combining models

Combined model →

Weights ↓

$$f^{\dagger}(\boldsymbol{x};\omega) = \sum_{k=1}^{m} \omega_k f_k(\boldsymbol{x})$$

← Original models

Principal Component Analysis

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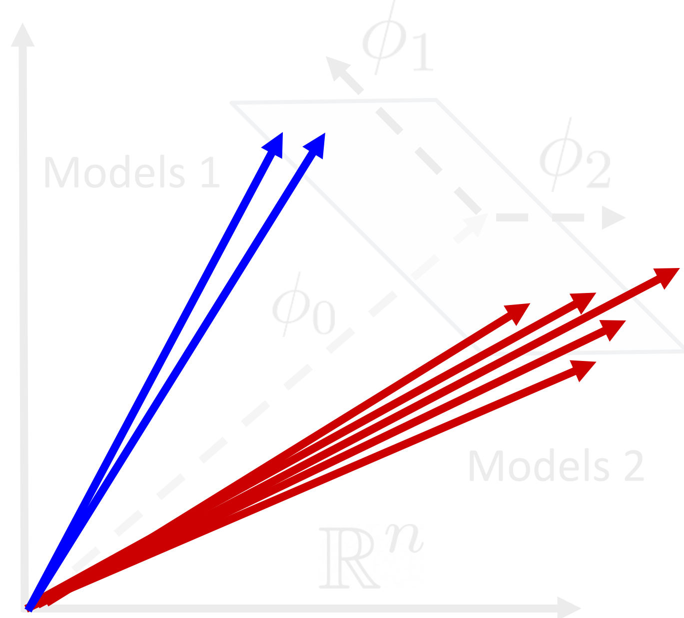

Combining models

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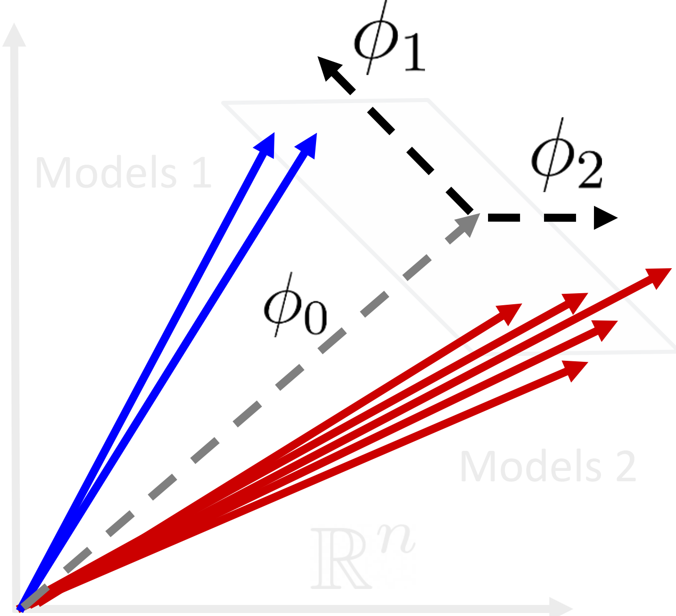
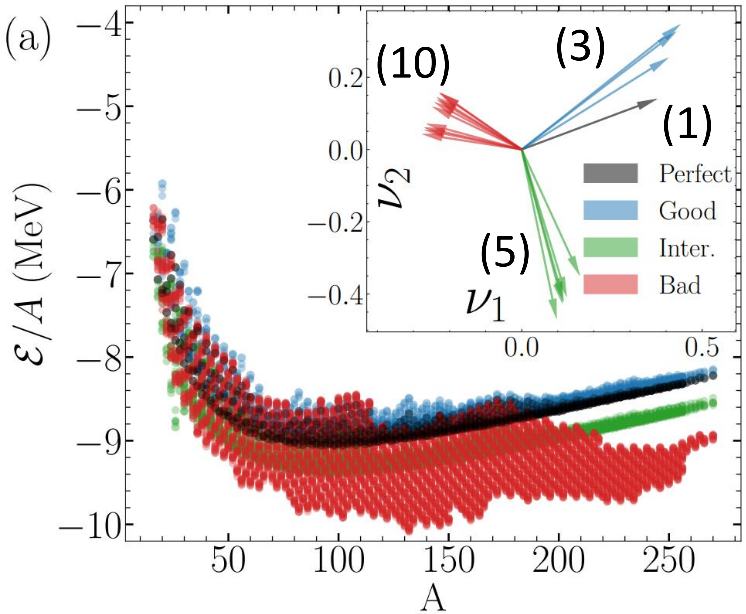


Toy example

$$f^{\dagger}(\boldsymbol{x};\boldsymbol{b}) = \phi_0(\boldsymbol{x}) + \sum_{j=1}^{p} b_j \phi_j(\boldsymbol{x})$$



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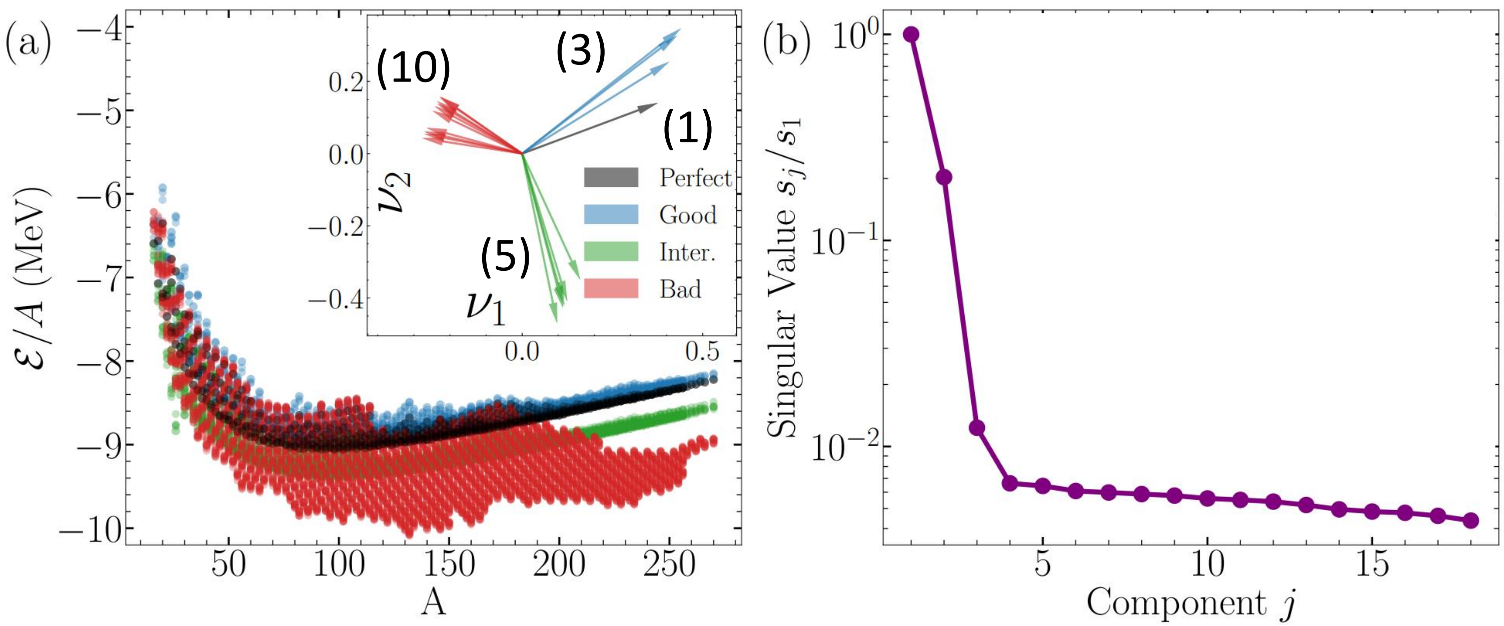

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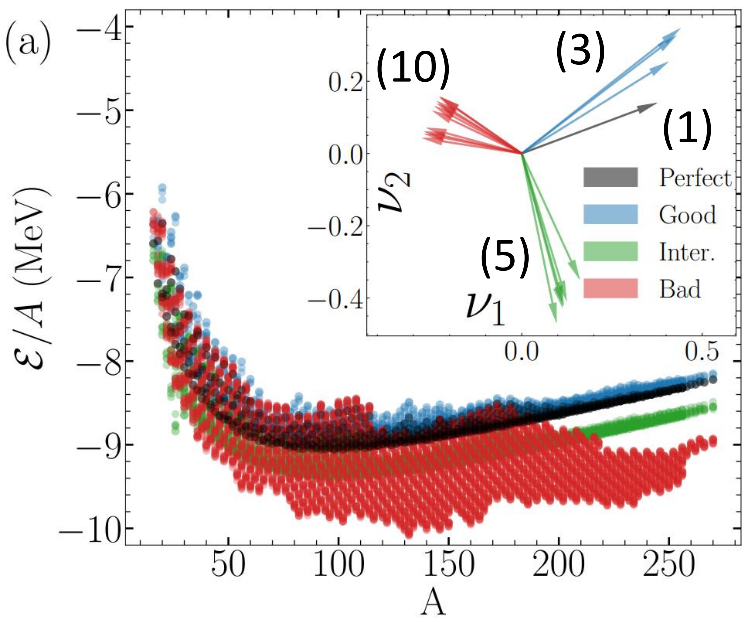
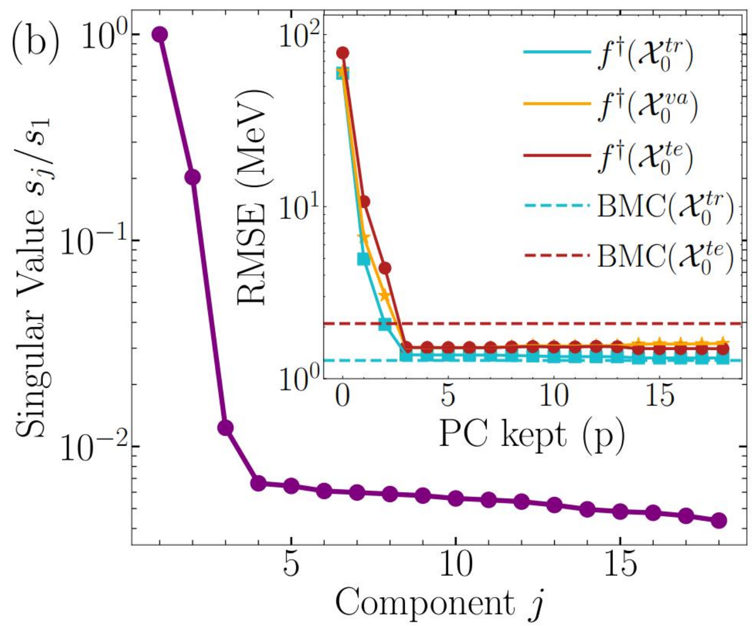
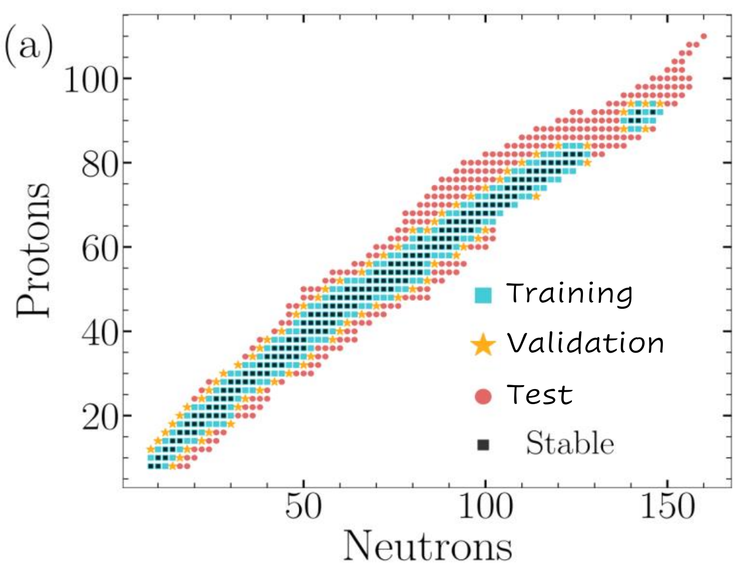
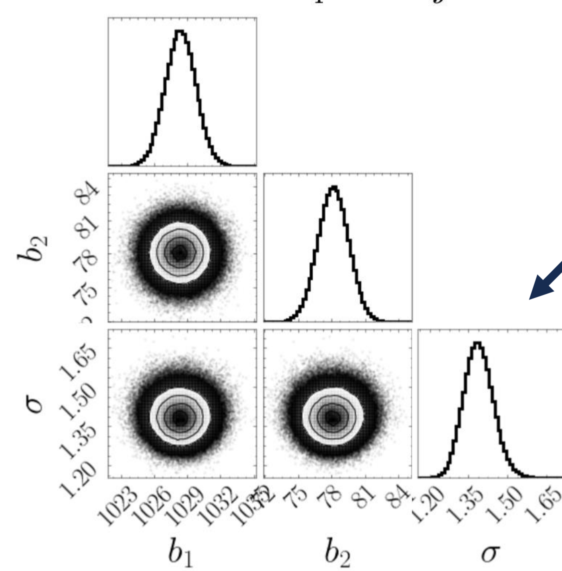








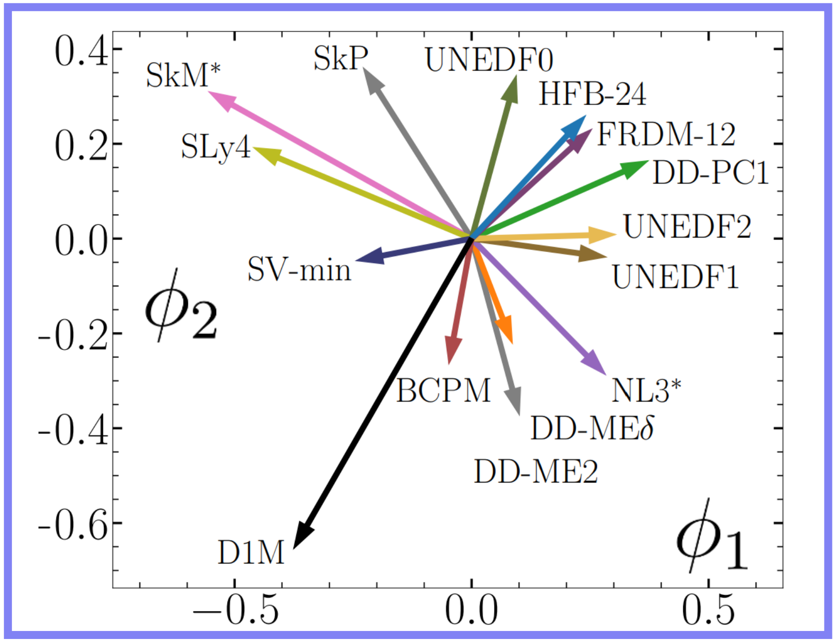
$$P(\boldsymbol{b}|\boldsymbol{Y})$$

Bayesian way

Real case

$$f^{\dagger}(\boldsymbol{x};\boldsymbol{b}) = \phi_0(\boldsymbol{x}) + \sum_{j=1}^{p} b_j \phi_j(\boldsymbol{x})$$

Identifies similarities



Real case

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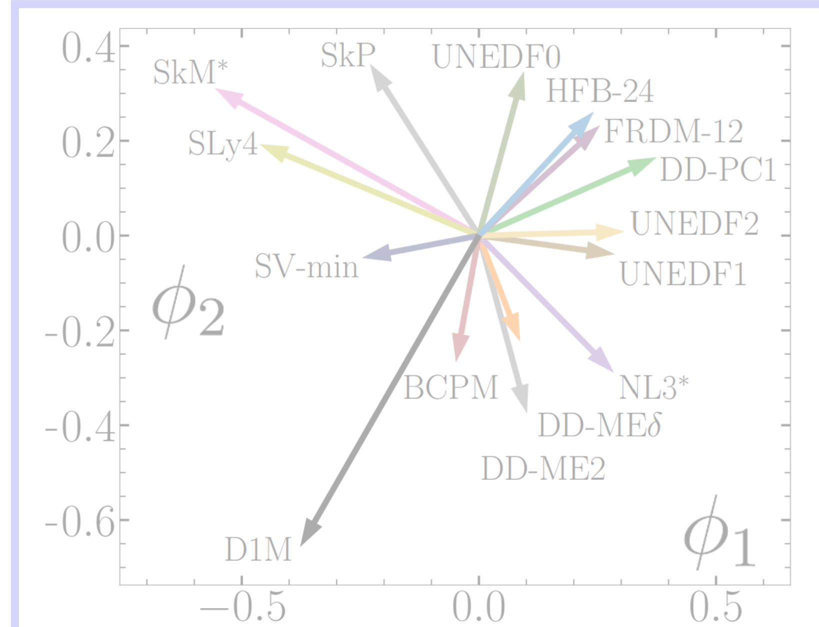
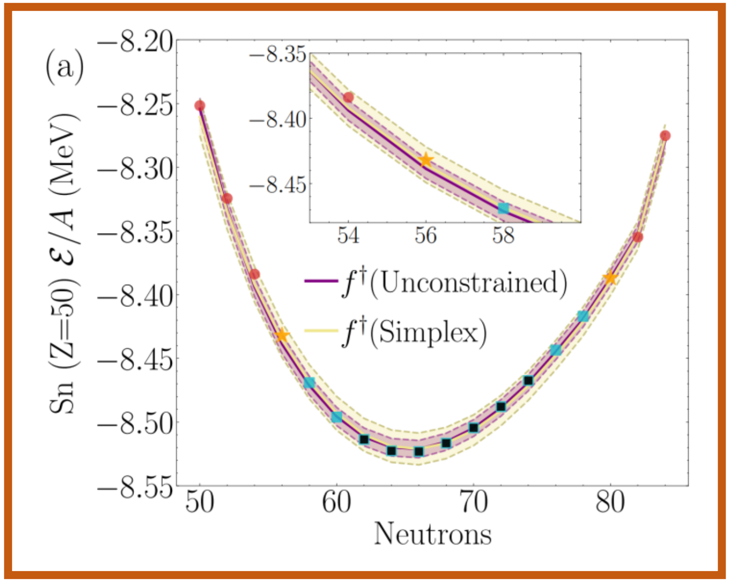
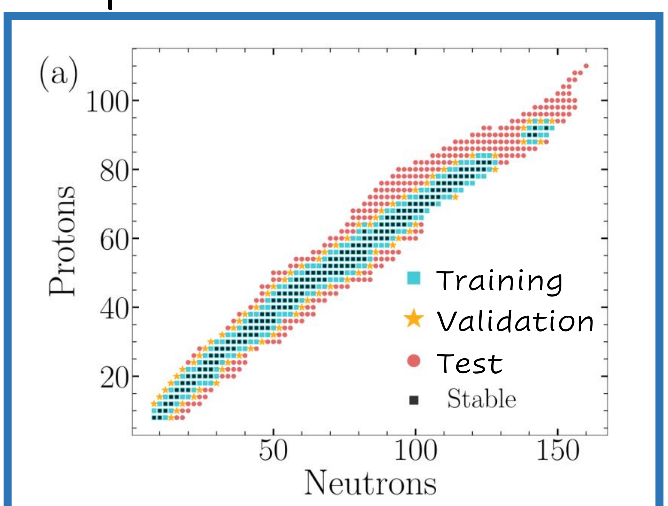


Good uncertainties



Good extrapolation

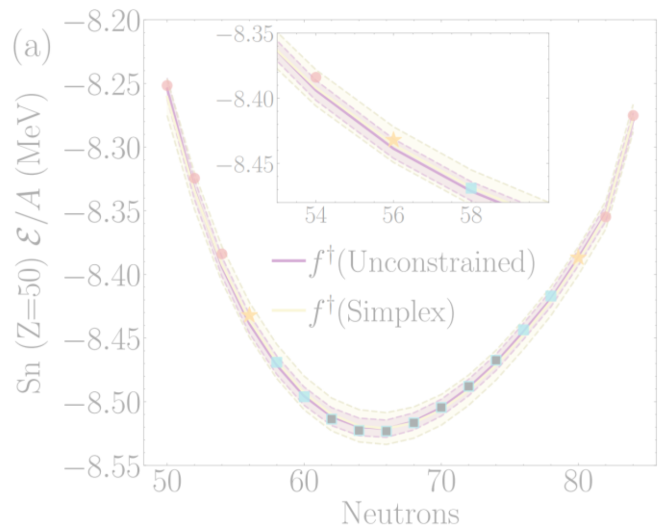


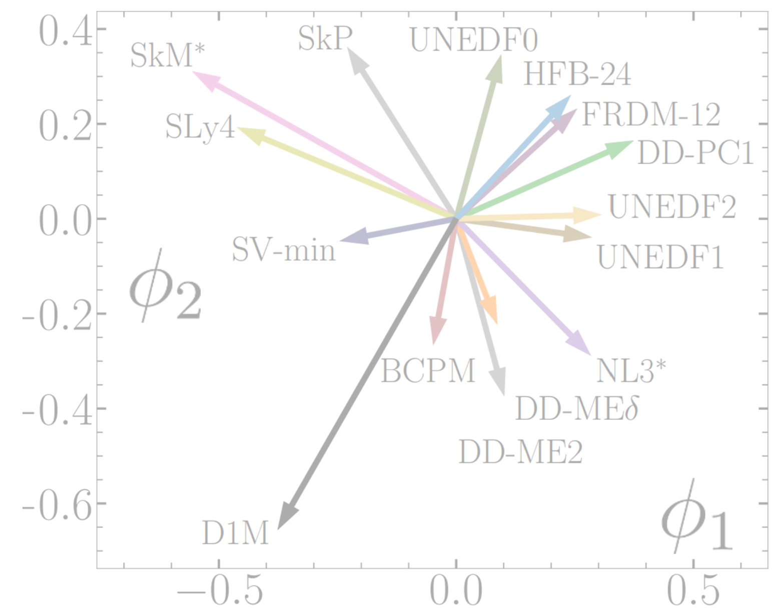
Real case

$$f^{\dagger}(\boldsymbol{x};\boldsymbol{b}) = \phi_0(\boldsymbol{x}) + \sum_{j=1}^{p} b_j \phi_j(\boldsymbol{x})$$

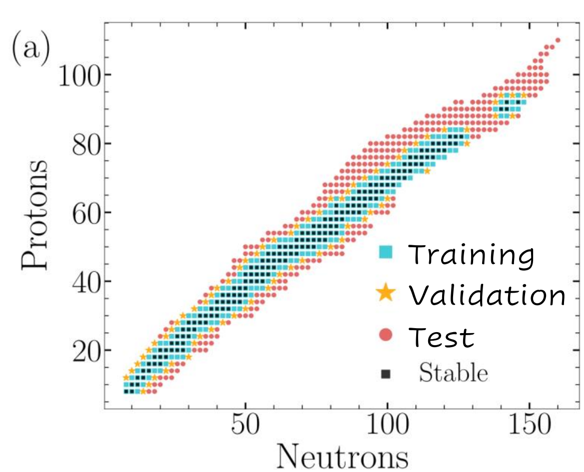
Identifies similarities

Good uncertainties

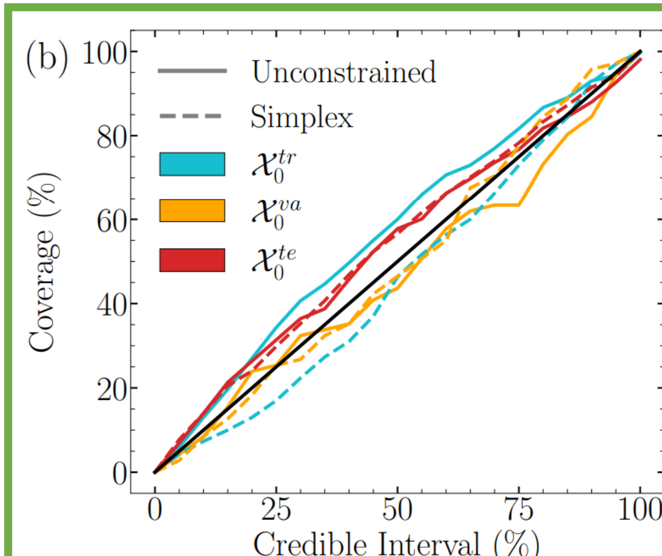




Good extrapolation



Good coverage

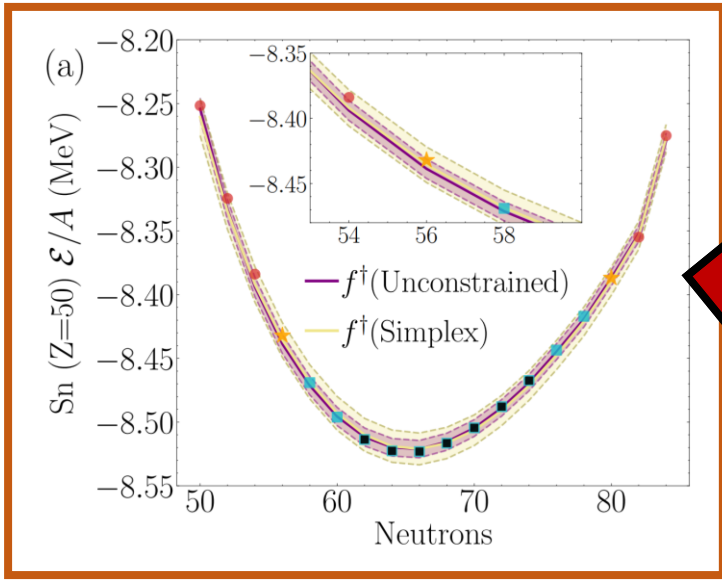


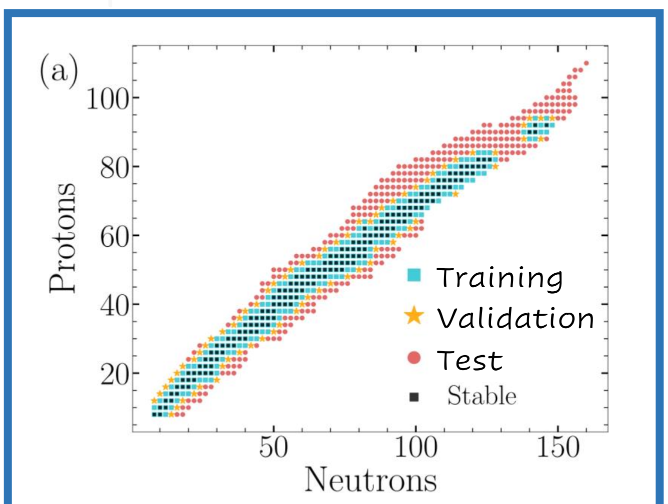
An Le

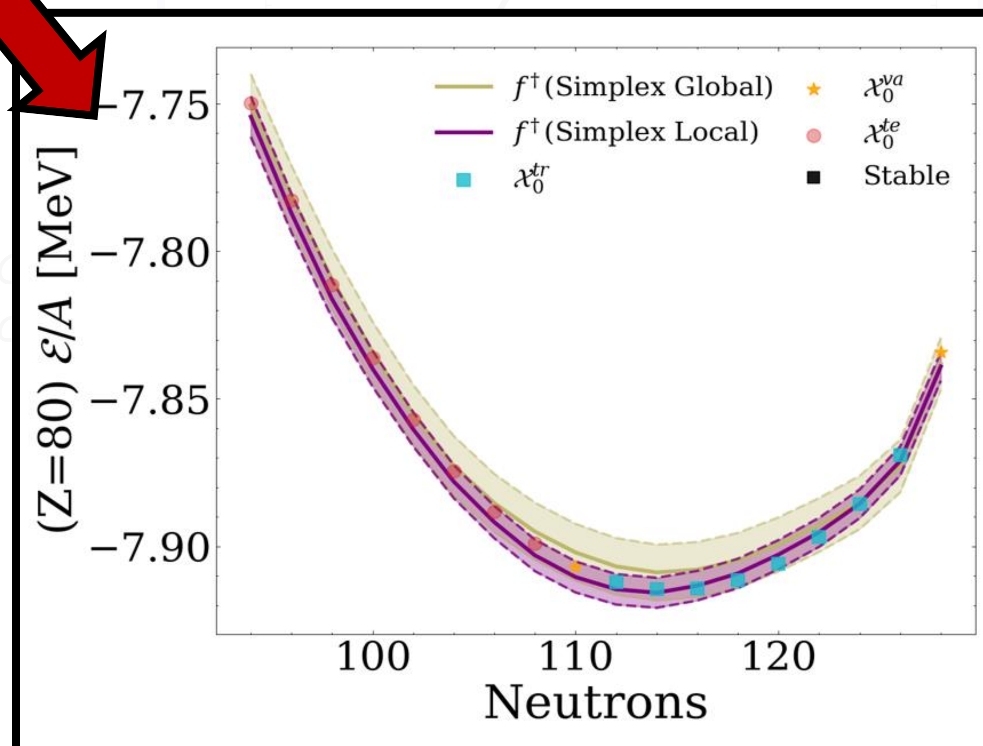
$$f^{\dagger}(\boldsymbol{x};\boldsymbol{b}) = \phi_0(\boldsymbol{x}) + \sum_{j=1}^{p} b_j \phi_j(\boldsymbol{x})$$

$b_j(\boldsymbol{x})$

Extension to local weights in progress!







Real case

Good uncertainties

Identifies similarities

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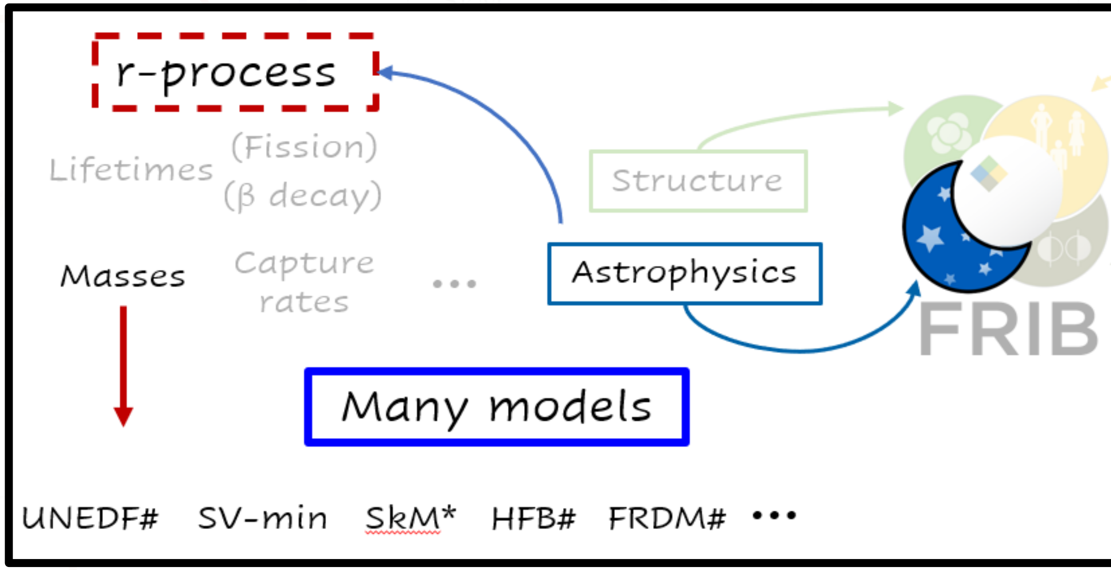
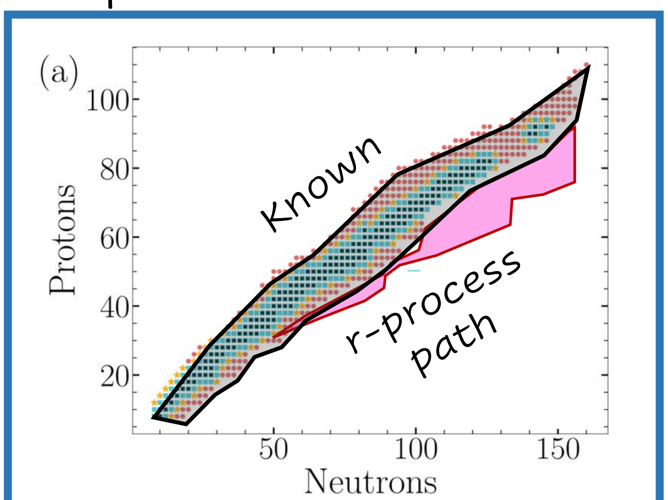
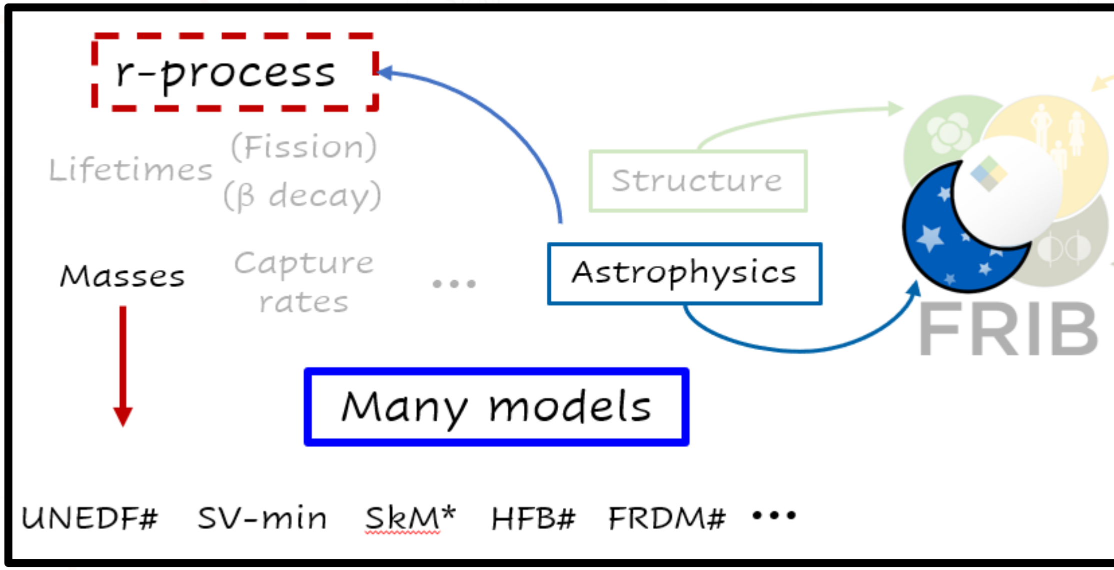


Good extrapolation

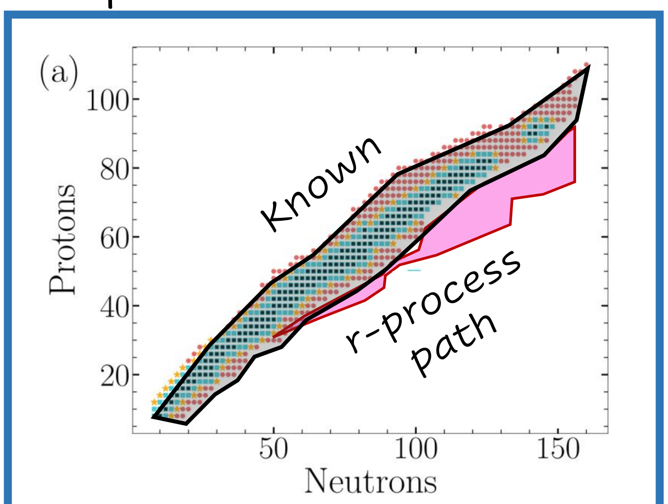


Good coverage

Make the goats proud



Good extrapolation



Good coverage

Link to these slides

Outline

My context

Bayes and Nuclei

Two challenges

Computational paradigm

Dimensionality Reduction

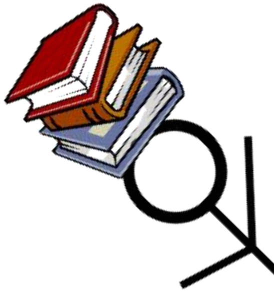
Model Order Reduction (Faster)

Model Combination (Fewer)

Takeaways

Takeaways

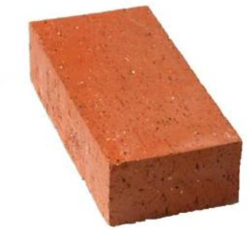
I have two-ish



Takeaways

About Dimensionality Reduction

- Two clear steps:



1) Find good reduced coordinates

2) Find equations for them

Allows you to be creative, mix and match, and **read***

*Yes, please read, we really need to read more

Takeaways

About Dimensionality Reduction

- Two clear steps:

1) Find good reduced coordinates

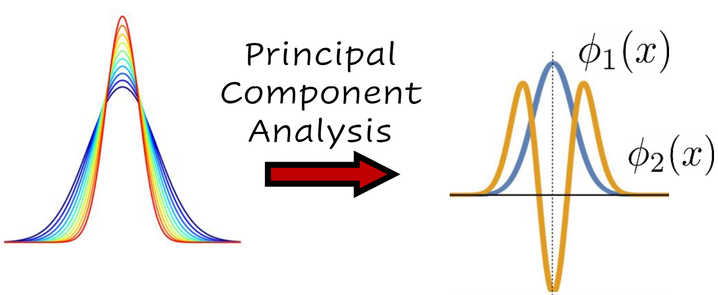
2) Find equations for them

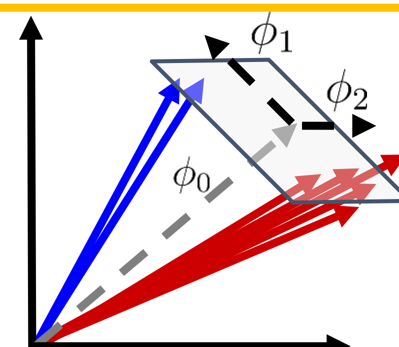
Allows you to be creative, mix and match, and **read**

- Bridge between emulation and Bayesian model combination

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

$$f^{\dagger}(\boldsymbol{x};\boldsymbol{b}) = \phi_0(\boldsymbol{x}) + \sum_{j=1}^{p} b_j \phi_j(\boldsymbol{x})$$





Takeaways

About Dimensionality Reduction

- Two clear steps
- Bridge between emulation and Bayesian model combination

About Machine learning and Statistics

Takeaways

About Dimensionality Reduction

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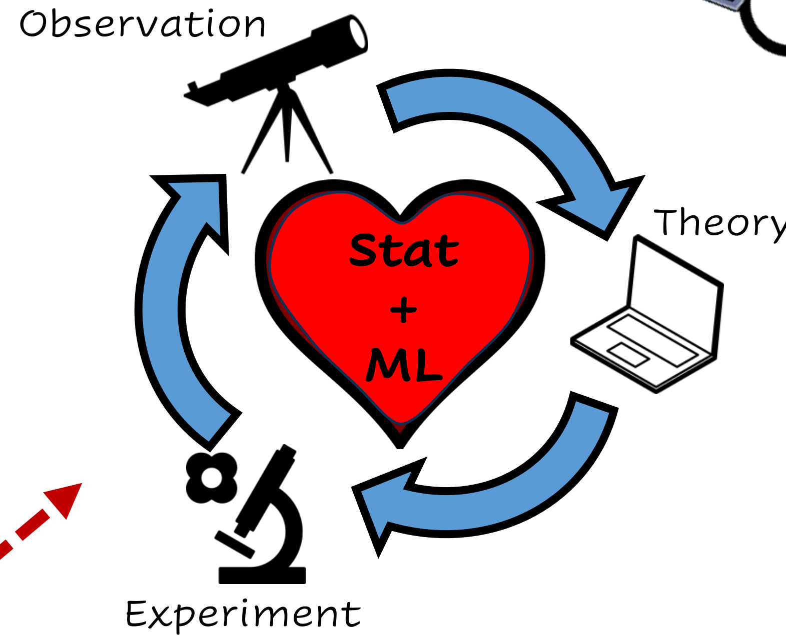
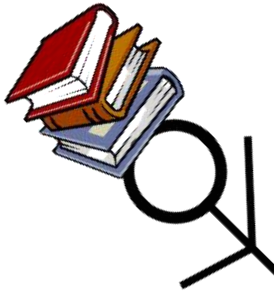
- Bridge between emulation and Bayesian model combination

About Machine learning and Statistics

1) ***Are*** propelling nuclear physics towards a new era of ***discovery***



Takeaways



About Dimensionality Reduction

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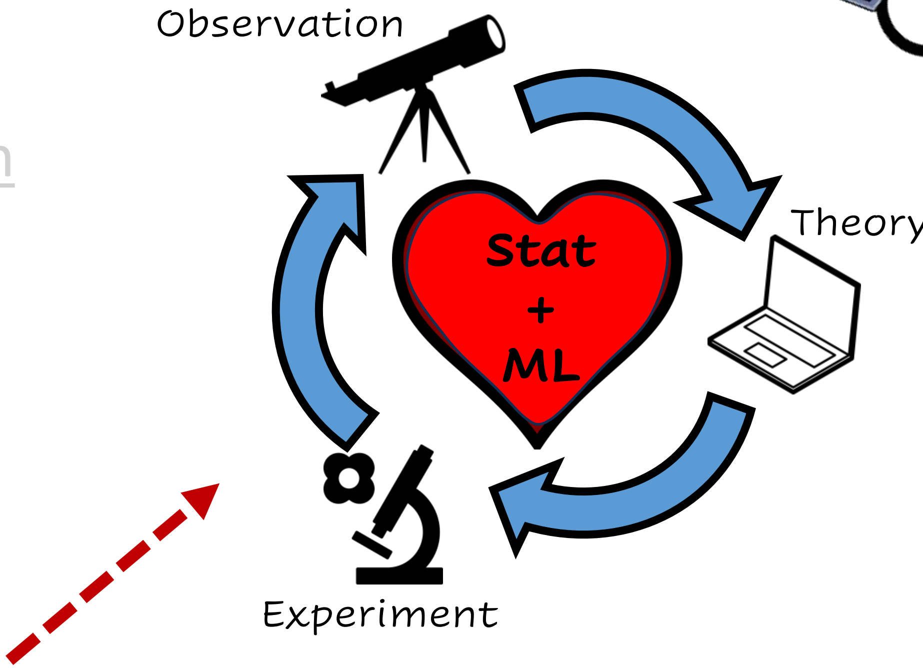
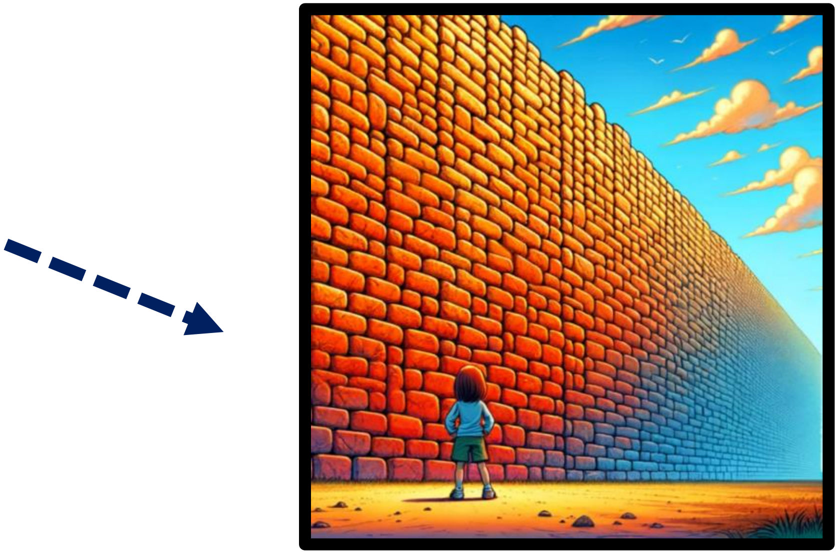


About Machine learning and Statistics

1) ***Are*** propelling nuclear physics towards a new era of ***discovery***

2) Could help to lower barriers



Lowering the Barrier

(Data-science)

Statistics &

Machine Learning

Lowering the Barrier

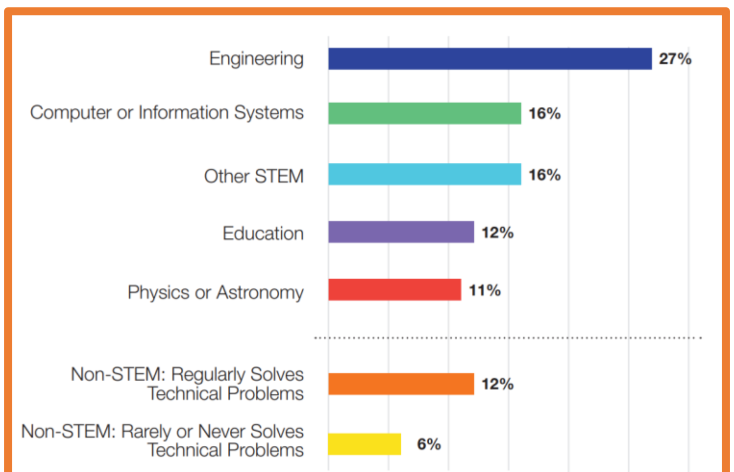
(Data-science)

Statistics &
Machine Learning

1

Widely applicable

Highly Transferable



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Lowering the Barrier

(Data-science)

Statistics &
Machine Learning

1

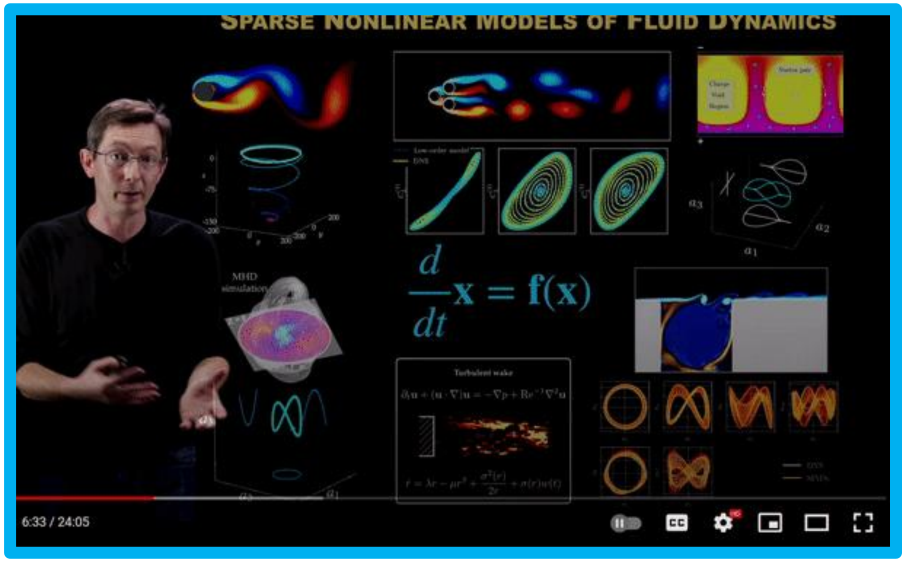
Widely applicable

Highly Transferable

2 Almost self trainable

Employment for New Physics Bachelors, AIP 2023

Sparse Identification of Nonlinear Dynamics (SINDy)



Lowering the Barrier

Forecasting the future of artificial intelligence (2023)

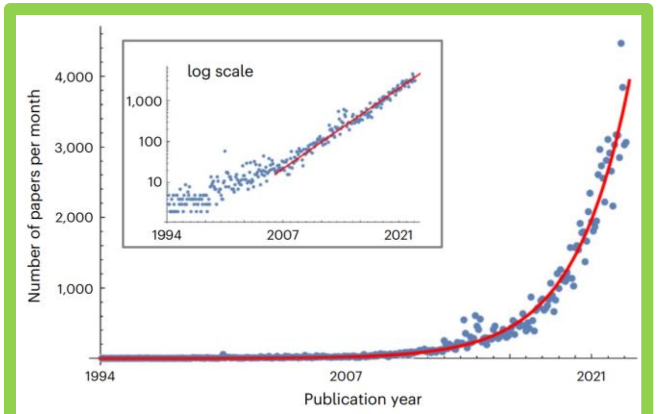


Fig. 1 | The number of papers published per month in the arXiv categories of AI and ML are growing exponentially. The doubling rate of papers per month is roughly 23 months, which might lead to problems for publishing in these fields, at some point. The categories are cs.AI, cs.LG, cs.NE and stat.ML.

(Data-science)

Statistics &

Machine Learning

3 Exponentially impactful

1 Widely applicable

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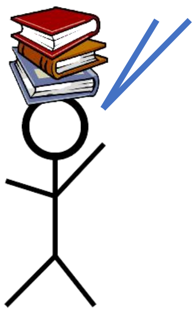
Sparse Identification of Nonlinear Dynamics (SINDy)

Employment for New Physics Bachelors, AIP 2023

Lowering the Barrier

Perfect opportunity for creating a more inclusive scientific community in the XXI century



(Data-science)

Statistics & Machine Learning

1 Widely applicable

Highly Transferable

2 Almost self trainable

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Forecasting the future of artificial intelligence (2023)

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Lowering the Barrier

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A NEW ERA OF DISCOVERY

THE 2023 LONG RANGE PLAN FOR NUCLEAR SCIENCE

2023 | VERSION 1.3

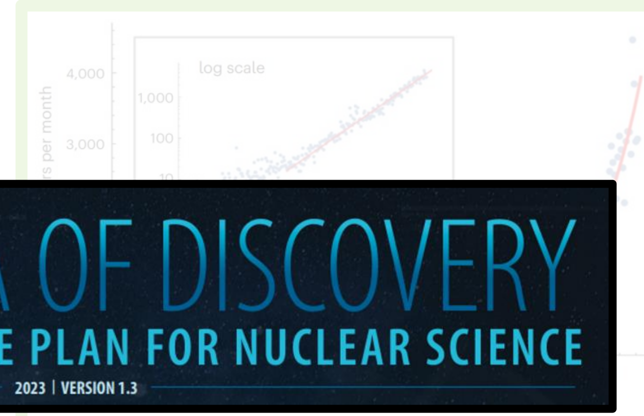


Fig. 1 | The number of papers published per month in the arXiv categories of AI and ML are growing exponentially. The doubling rate of papers per month is roughly 23 months, which might lead to problems for publishing in these fields, at some point. The categories are cs.AI, cs.LG, cs.NE and stat.ML.

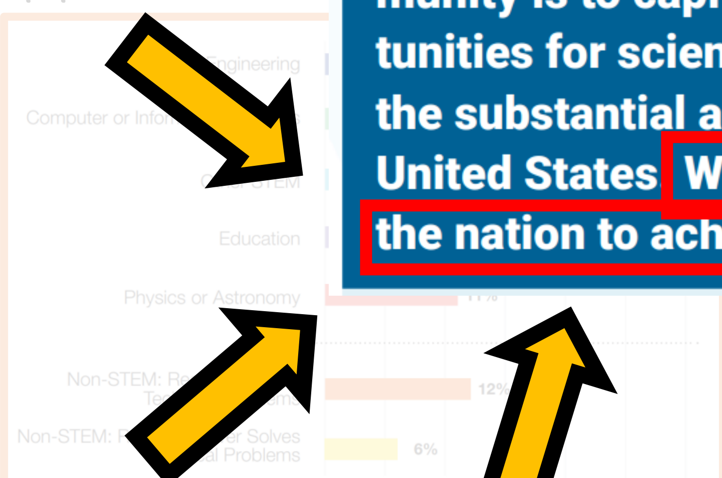
Statistics & Machine Learning

Exponentially impactful

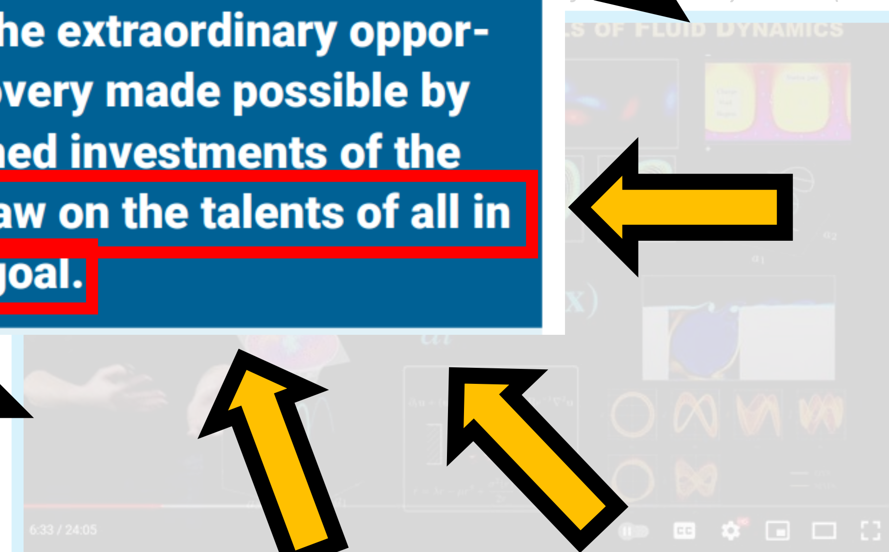
Widely applicable

RECOMMENDATION 1

The highest priority of the nuclear science community is to capitalize on the extraordinary opportunities for scientific discovery made possible by the substantial and sustained investments of the United States. We must draw on the talents of all in the nation to achieve this goal.

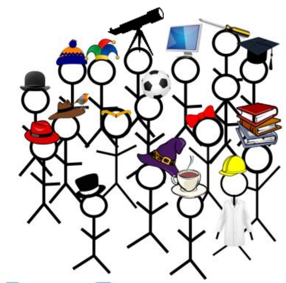


Employment for New Physics Bachelors, AIP 2023



...ar Dynamics (SINDy)

Lowering the Barrier



Kyle Godbey

ASCSN

Advanced Scientific Computing and Statistics Network

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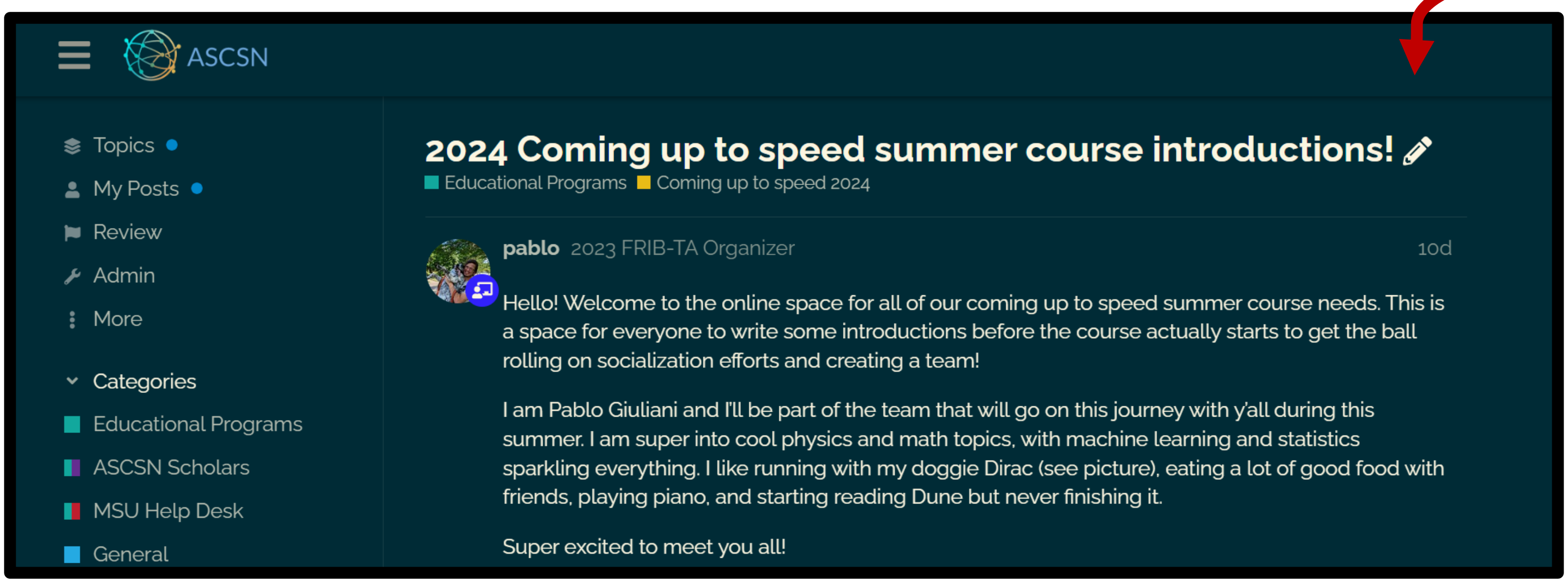


Lowering the Barrier

Kyle Godbey

ASCSN

https://ascsn.net/

Pilot with PING

Paul Gueye

Advanced Scientific Computing and Statistics Network

← ASCSN Scholars

Forum

Takeaways

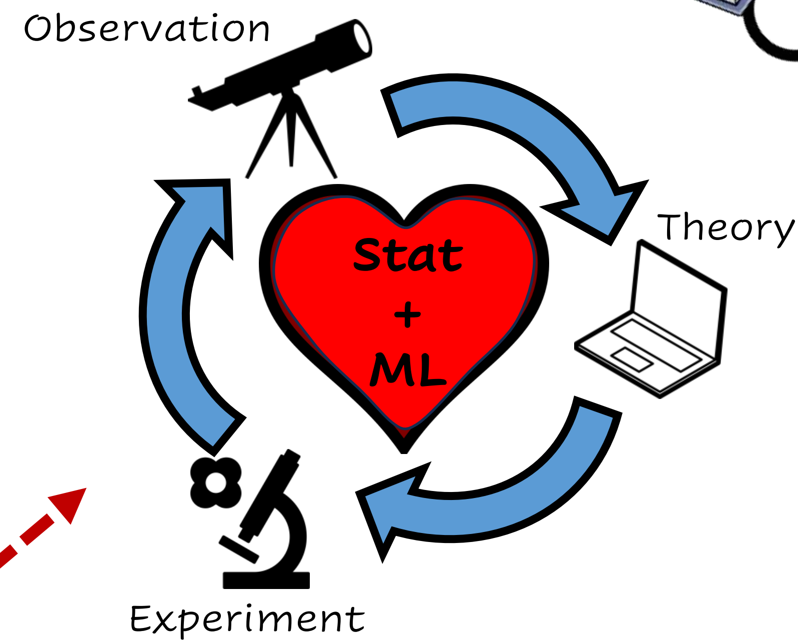
About Dimensionality Reduction

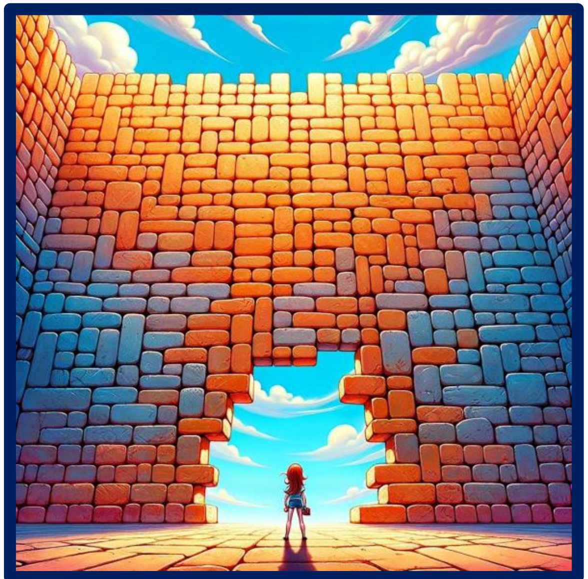
- Two clear steps
- Bridge between emulation and Bayesian model combination

About Machine learning and Statistics

1) ***Are*** propelling nuclear physics towards a new era of ***discovery***

2) ***Could*** help propel nuclear physics towards a new era of ***inclusion***





Thank-yous

STREAMLINE
BAND
Bayesian Analysis of Nuclear Dynamics
Few Body Reactions Group

People who pay my lunch and collaborations

Special thanks: ChatGPT

Conference organizers

Ingo Tews

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An Le
Andrew Yeomans-Stephenson
Aaron Philip
Landon Buskirk
Lauren JIn
George Schreibeis
Jacob Kozera
Dirac
…

And thank you, for listening

Further resources

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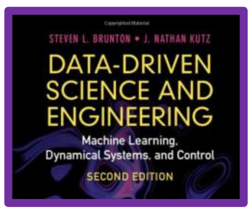

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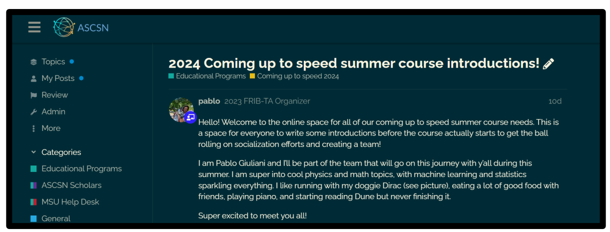
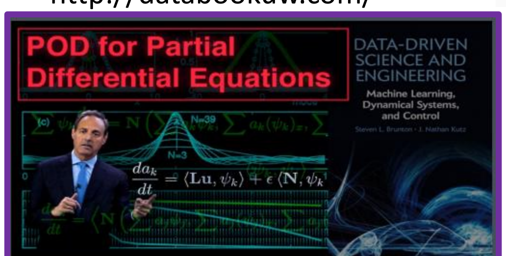


[Link to these slides]



FRIB-TA Summer School: Practical Uncertainty Quantification and Emulator Development in Nuclear Physics

https://forum.ascsn.net/t/about-the-2023-frib-ta-summer-school/42

[Watch the recording]