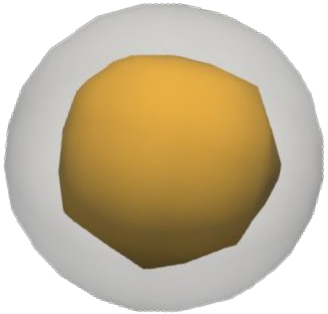
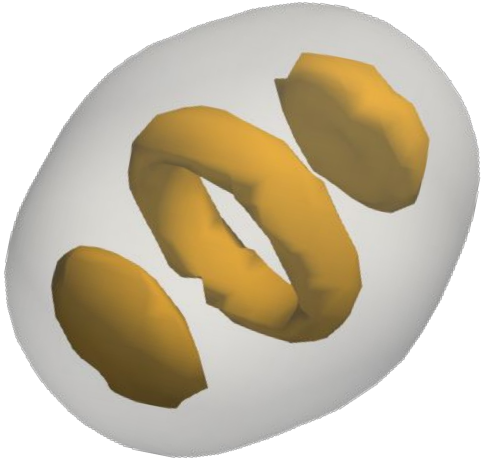
Dimensionality Reduction Techniques in Time-Dependent Problems

Kyle Godbey

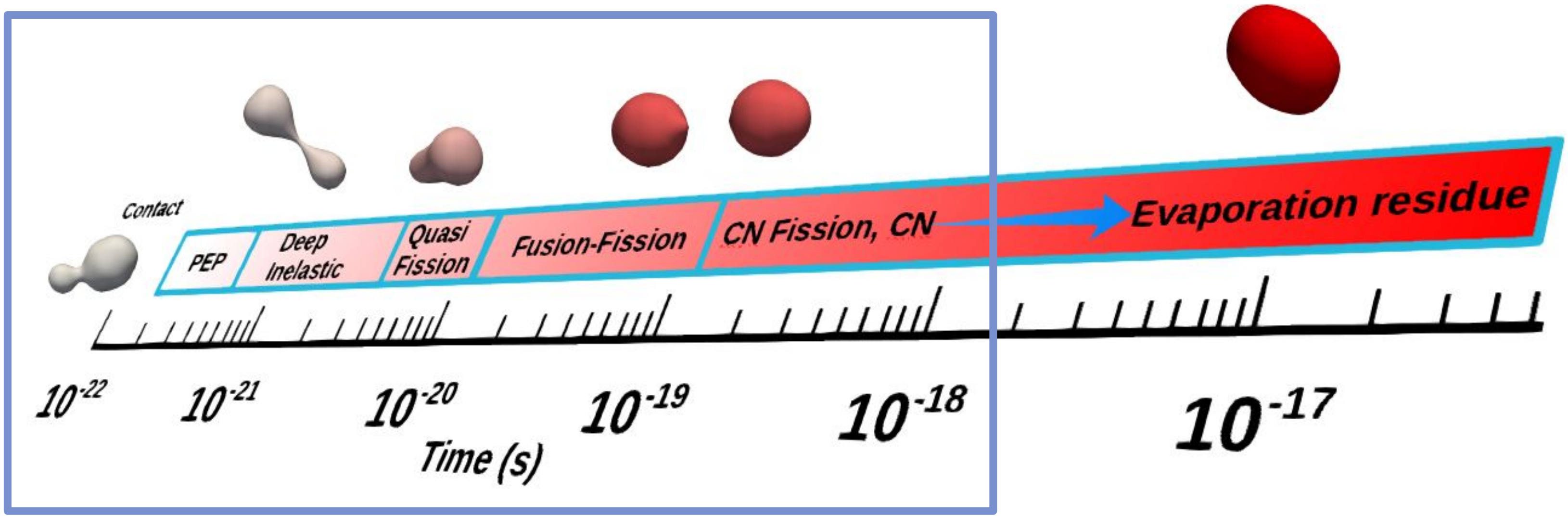




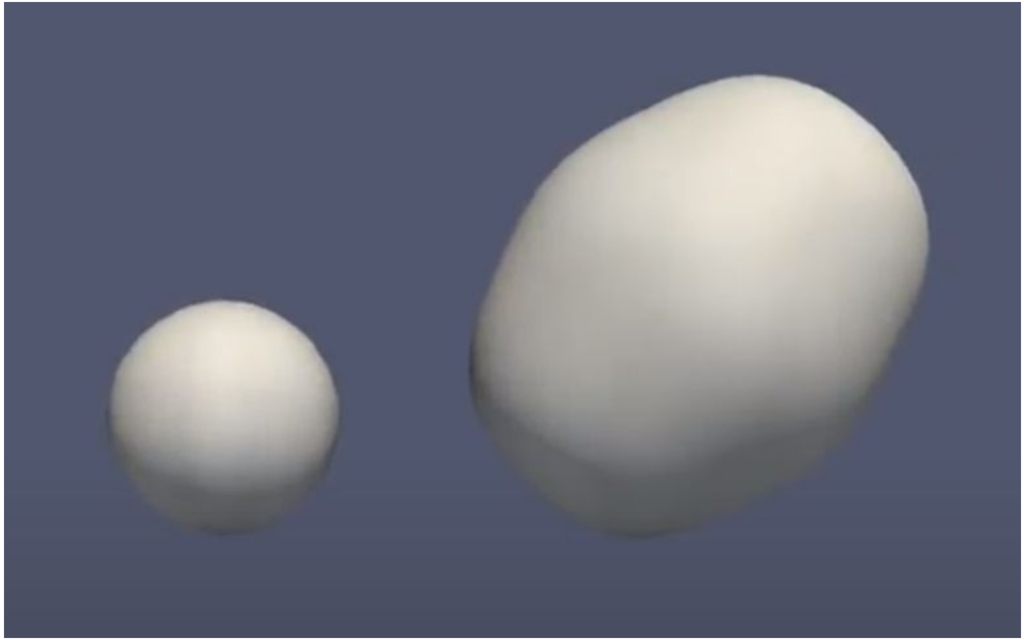
EC Workshop Eigenvector Continuation Workshop
May 2023, CEA Saclay

Google slides link with videos:
https://docs.google.com/presentation/d/1Sb7K9YqziprNxiLm4-eh1KPUfJvl1bDevW2S6ZV2L84/edit?usp=sharing

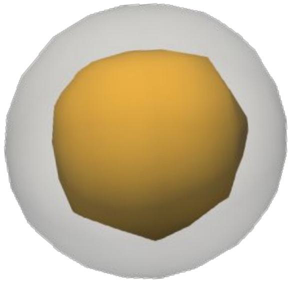
My Theoretical Bias: Real-Time Dynamics

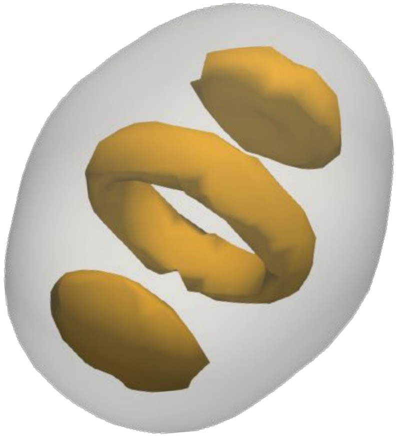


Features of DFT: Structure

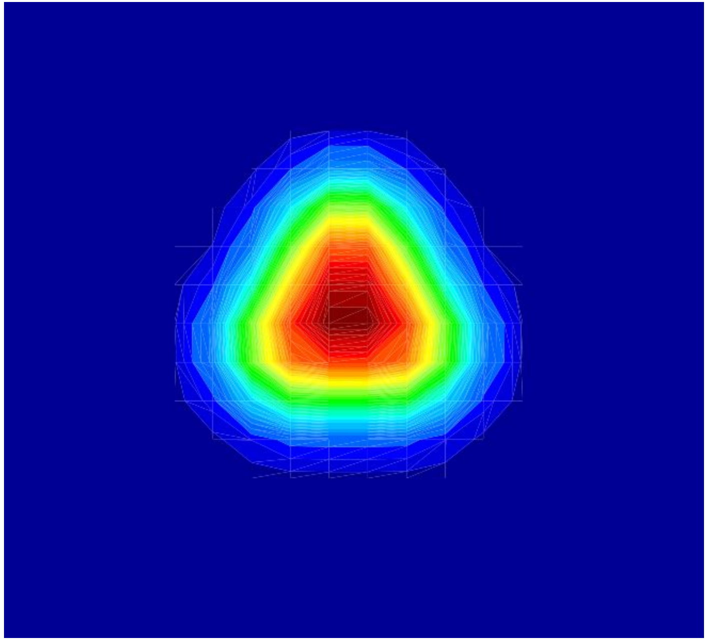


Features of DFT: Structure

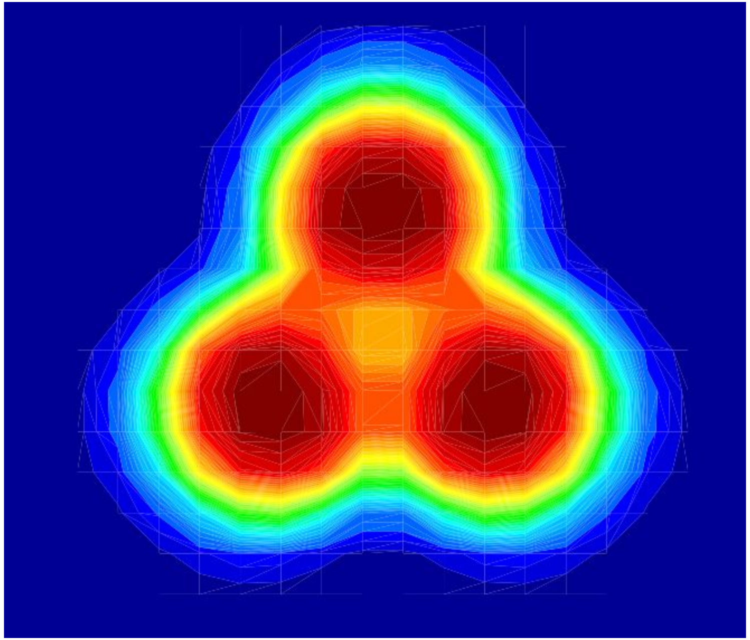




Features of DFT: Structure

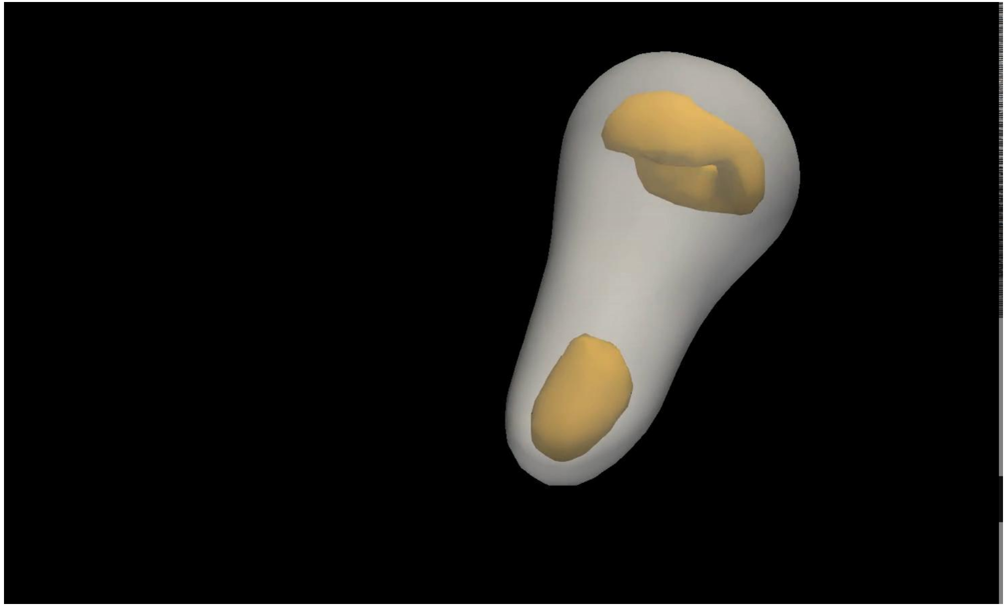


Density, $\varrho(r)$

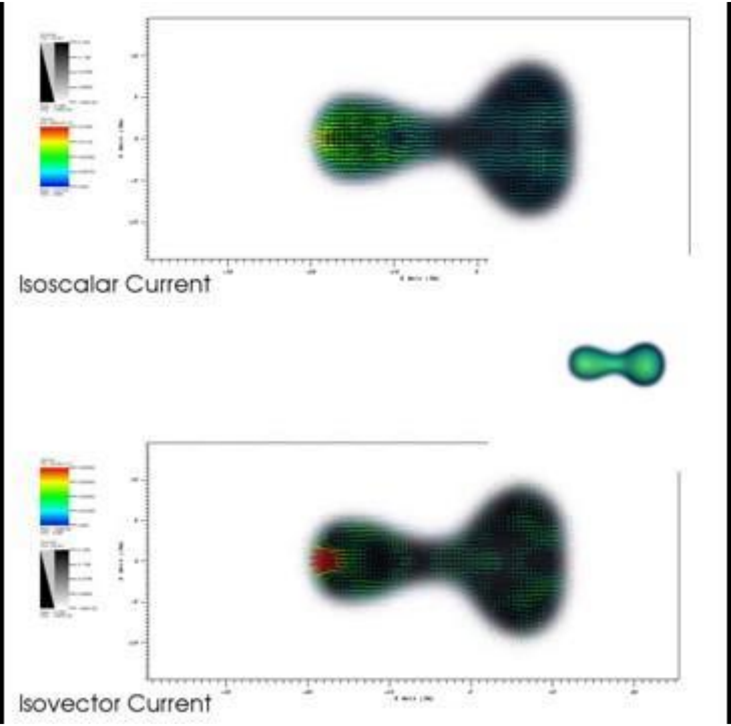


Nucleon localization function

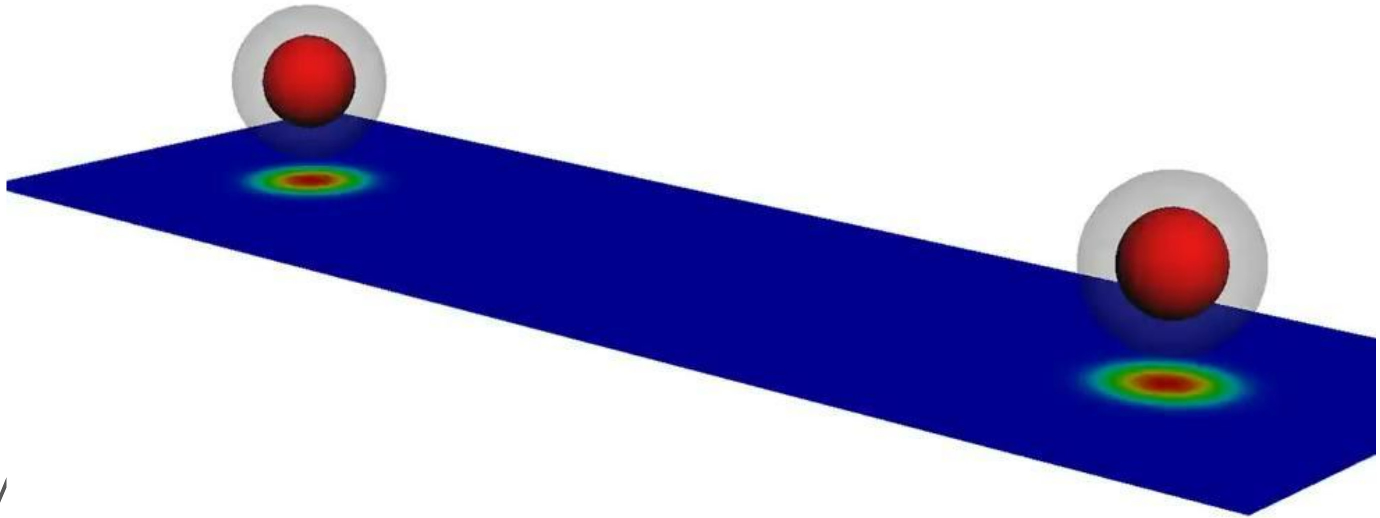
Features of DFT: Dynamics



Features of DFT: Dynamics



Features of DFT: Sensitivity



Case Study: Heavy-ion Fusion

When calibrating our models, we want to choose data that is 1) abundant and 2) informative

Near-barrier fusion turns out to be a very rich data source to mine information on ill-constrained features

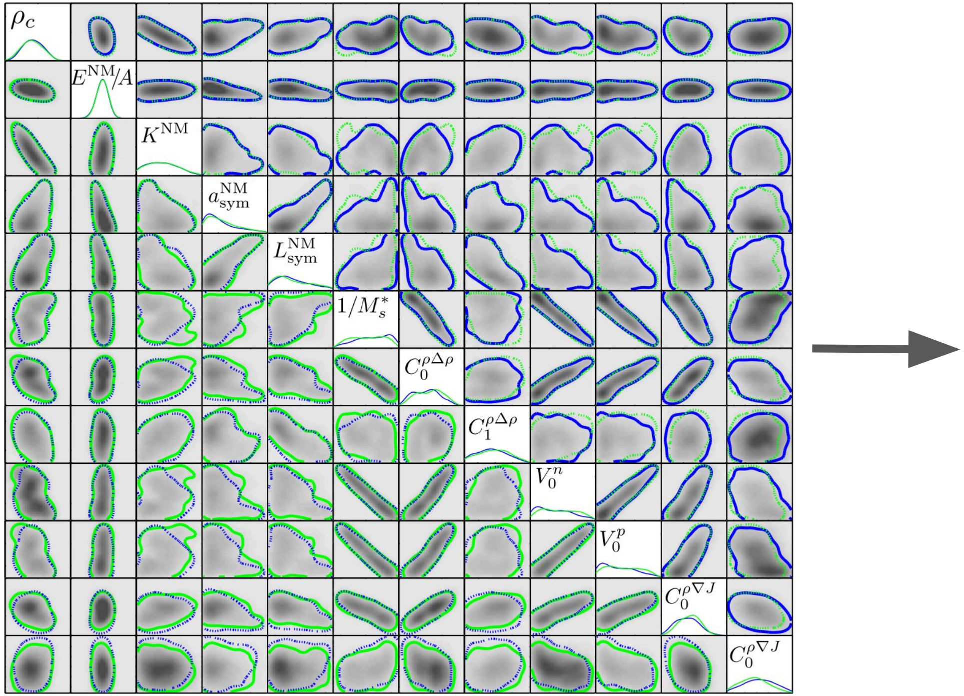
$$\mathcal{H}_{\mathrm{I}}(\mathbf{r}) = C_{\mathrm{I}}^{\rho}\rho_{\mathrm{I}}^2 + C_{\mathrm{I}}^{s}\mathbf{s}_{\mathrm{I}}^2 + C_{\mathrm{I}}^{\Delta\rho}\rho_{\mathrm{I}}\Delta\rho_{\mathrm{I}} + C_{\mathrm{I}}^{\Delta s}\mathbf{s}_{\mathrm{I}}\cdot\Delta\mathbf{s}_{\mathrm{I}} + C_{\mathrm{I}}^{\tau}\left(\rho_{\mathrm{I}}\tau_{\mathrm{I}} - \mathbf{j}_{\mathrm{I}}^2\right) + C_{\mathrm{I}}^{T}\left(\mathbf{s}_{\mathrm{I}}\cdot\mathbf{T}_{\mathrm{I}} - \overleftrightarrow{J}_{\mathrm{I}}^2\right) + C_{\mathrm{I}}^{\nabla J}\left(\rho_{\mathrm{I}}\nabla\cdot\mathbf{J}_{\mathrm{I}} + \mathbf{s}_{\mathrm{I}}\cdot(\nabla\times\mathbf{j}_{\mathrm{I}})\right)$$

Case Study: Heavy-ion Fusion

The recipe:

- Take samples from EDF posterior
- Perform time-dependent simulation
- Extract ion-ion fusion barrier
- Compute capture cross sections

Case Study: Heavy-ion Fusion



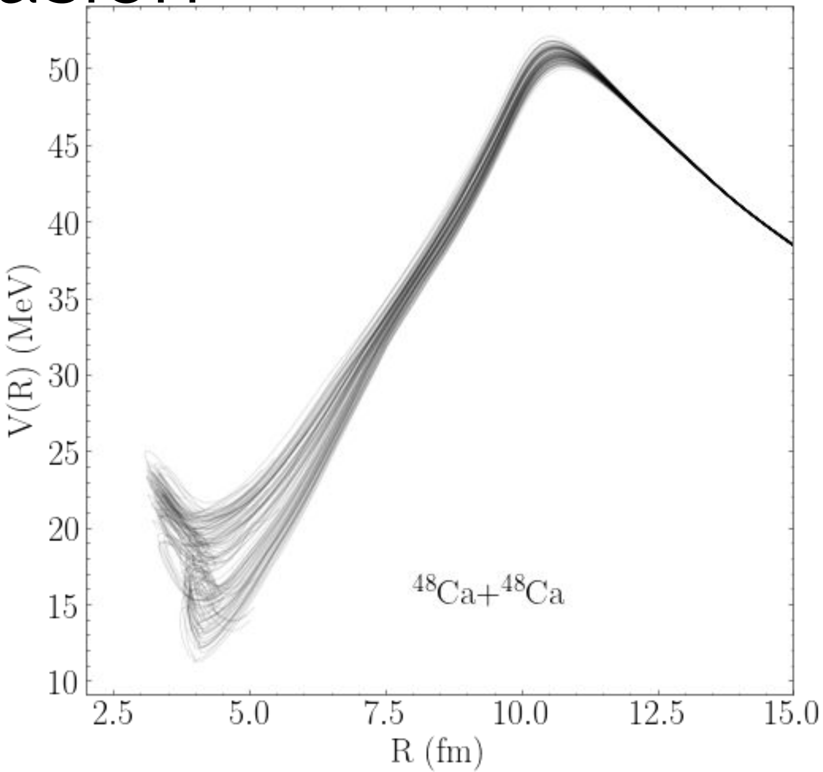
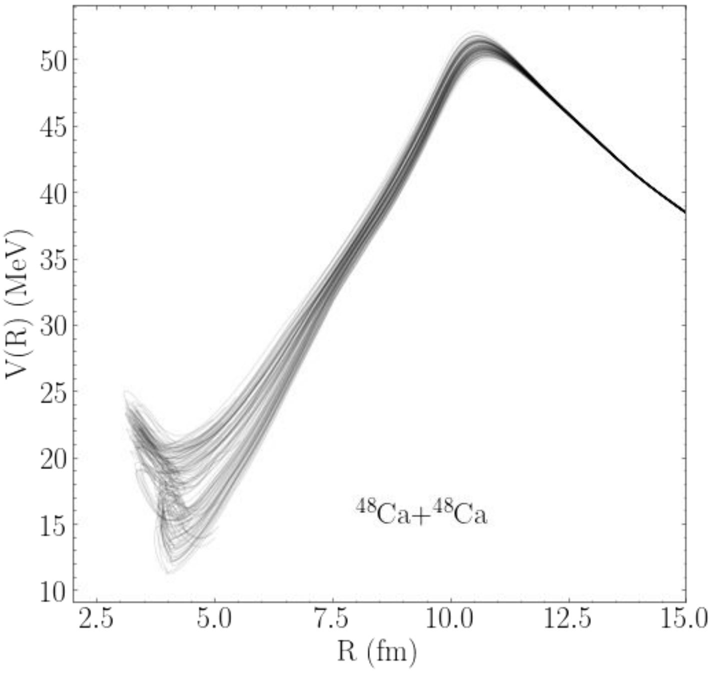
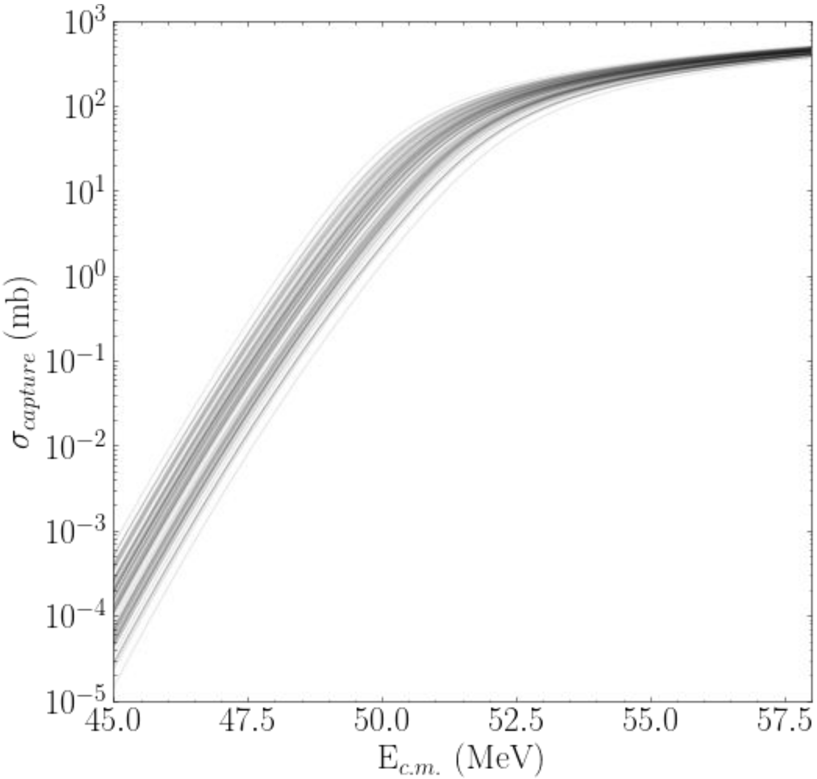


Image Credit:
J. D. McDonnell, N. Schunck, D. Higdon, J. Sarich, S. M. Wild, and W. Nazarewicz, Uncertainty Quantification for Nuclear Density Functional Theory and Information Content of New Measurements, Phys. Rev. Lett.114, 122501 (2015).

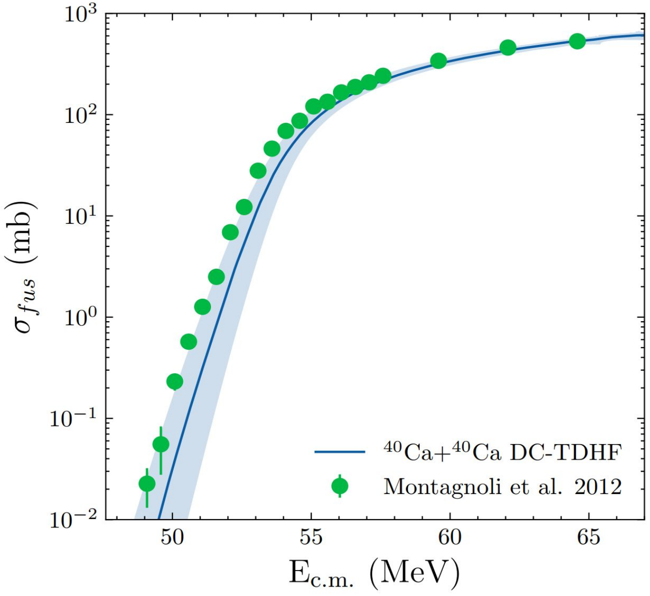
Case Study: Heavy-ion Fusion





Case Study: Heavy-ion Fusion

^{40}Ca + ^{40}Ca



^{48}Ca + ^{48}Ca

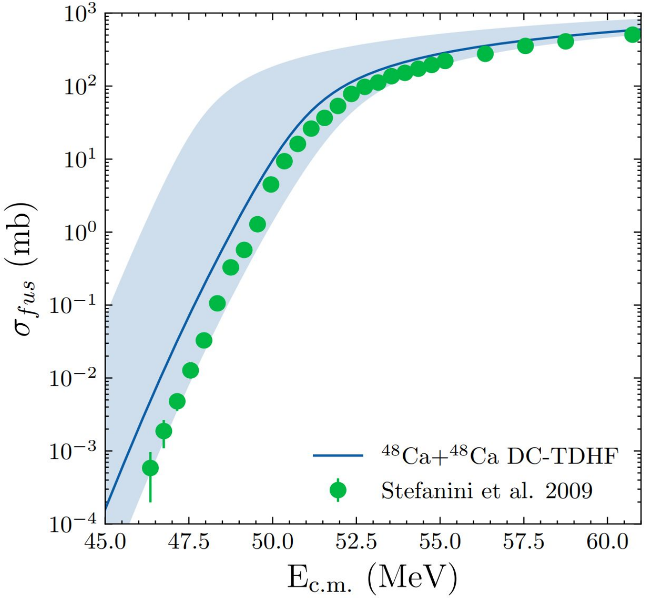
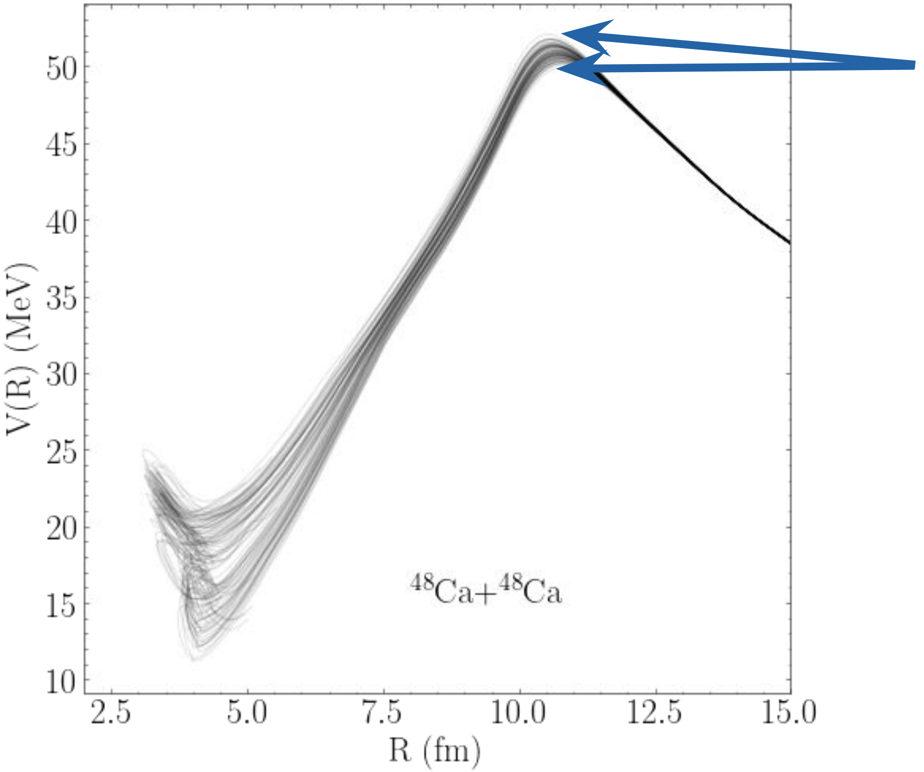


Image Credit:
K. Godbey, A. S. Umar, and C. Simenel, Uncertainty quantification in microscopic heavy-ion fusion simulations Phys. Rev. C 106, L051602 (2022) (Editors Suggestion),

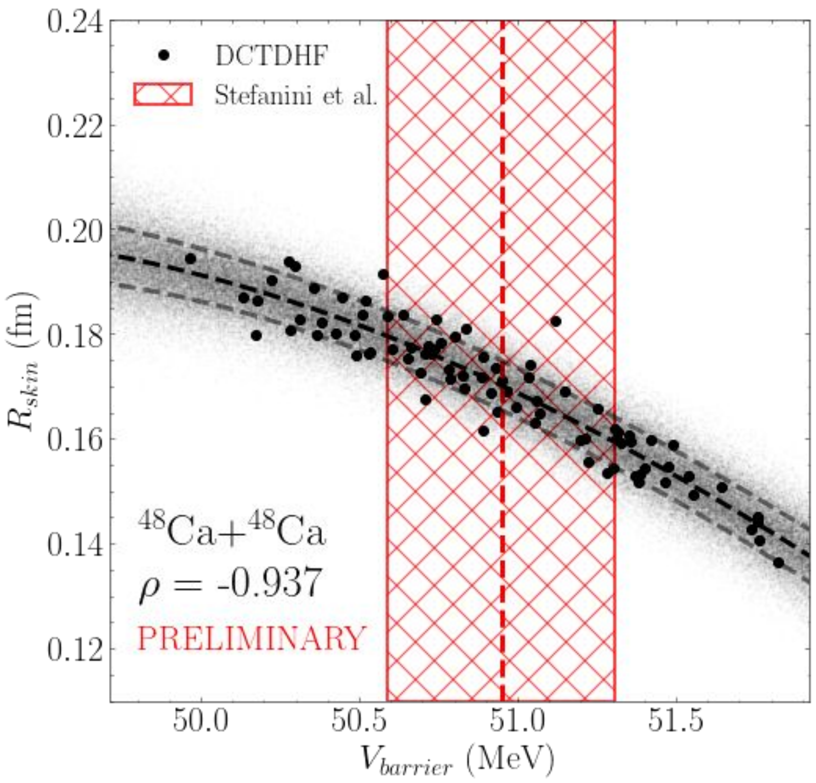
Case Study: Heavy-ion Fusion



Effect primarily driven by difference in height of the effective fusion barrier

We also see a large spread for other properties — let's check for correlations!

Case Study: Heavy-ion Fusion



These quantities are extremely correlated in the physical model!

Is this Accessible in Calibration?

With Gaussian processes, sure!

Time-dependent emulators that better capture the rich dynamics would be preferred, however

Perspectives for Time-Dependent Emulation

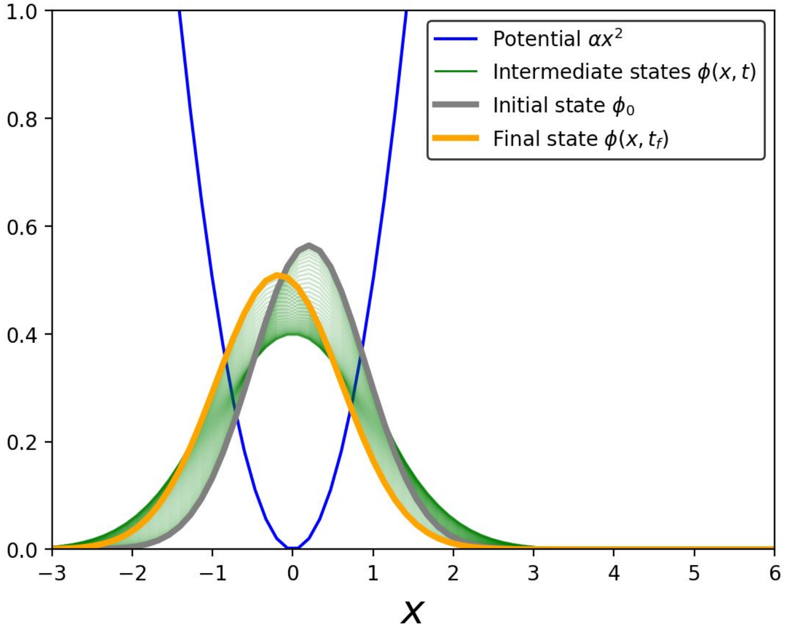
Two large classes: data-driven and model-driven

Model-driven:

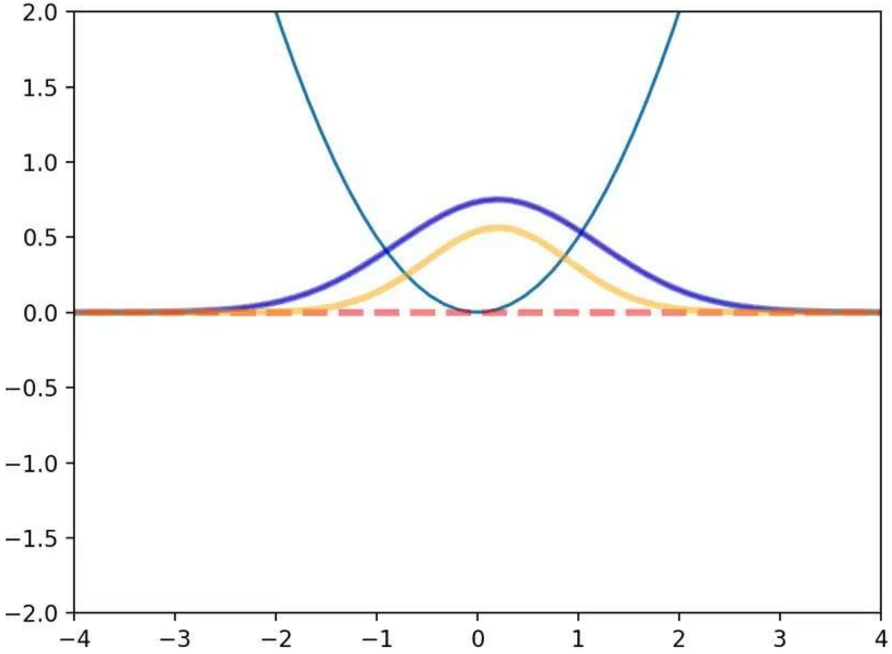
- RBMs strike again! Along with other technology mentioned by Christian and Pablo

TDRBM Examples - Particle in a HO Trap

In general, we need to inform our basis with information across time for our system:

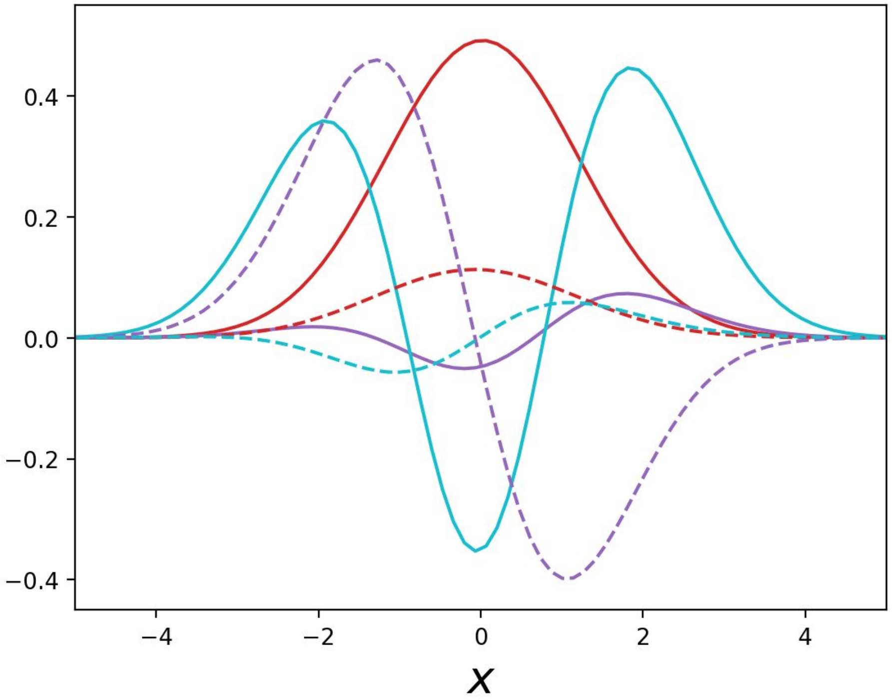


TDRBM Examples - Particle in a HO Trap



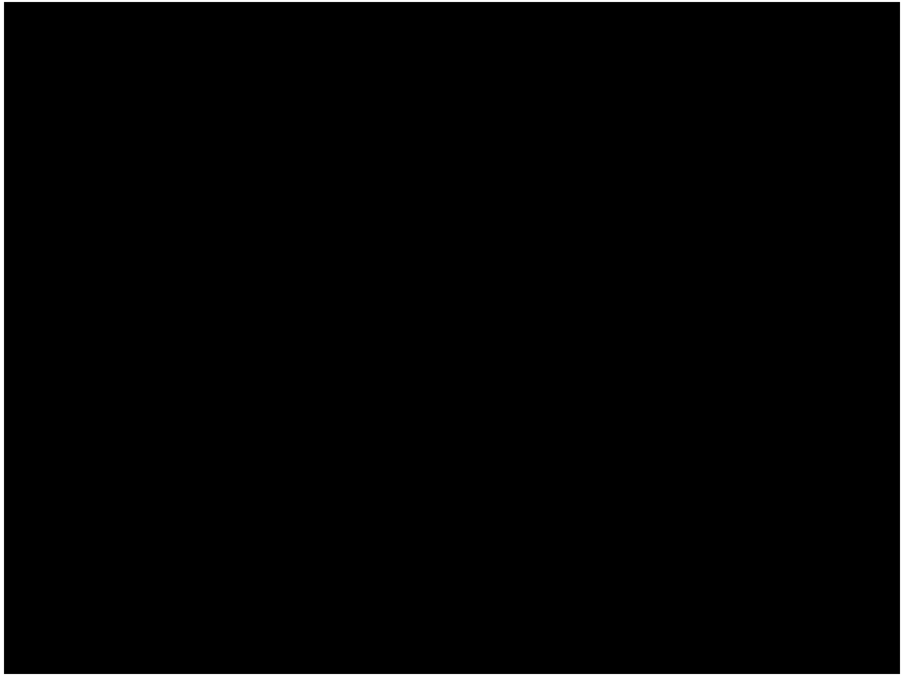
TDRBM Examples - Particle in a HO Trap

We take our snapshots across time and parameter space and generate our POD basis:

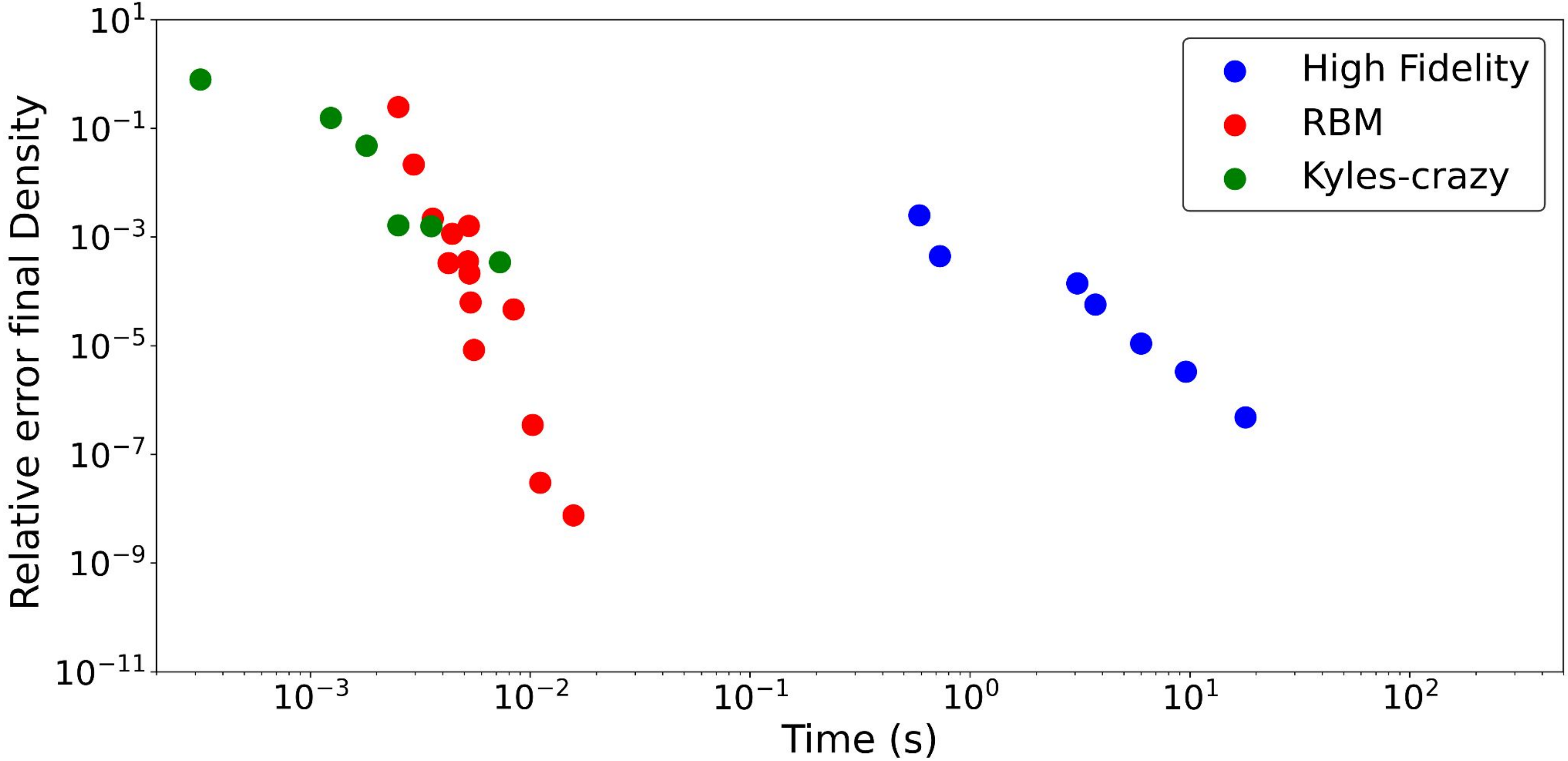


TDRBM Examples - Particle in a HO Trap

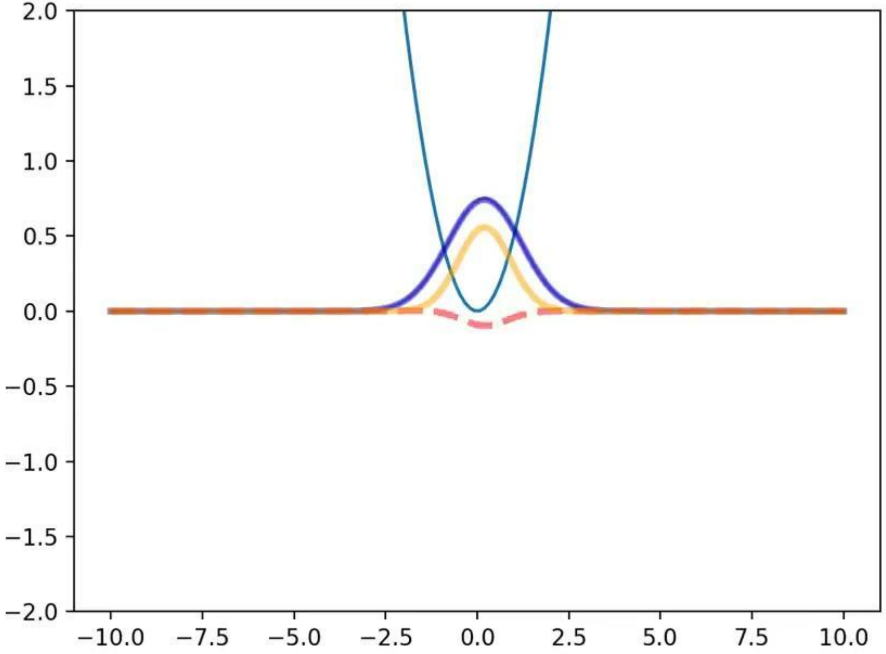
And, in the simplest RBM implementation, we can just propagate in time with our reduced Hamiltonian:



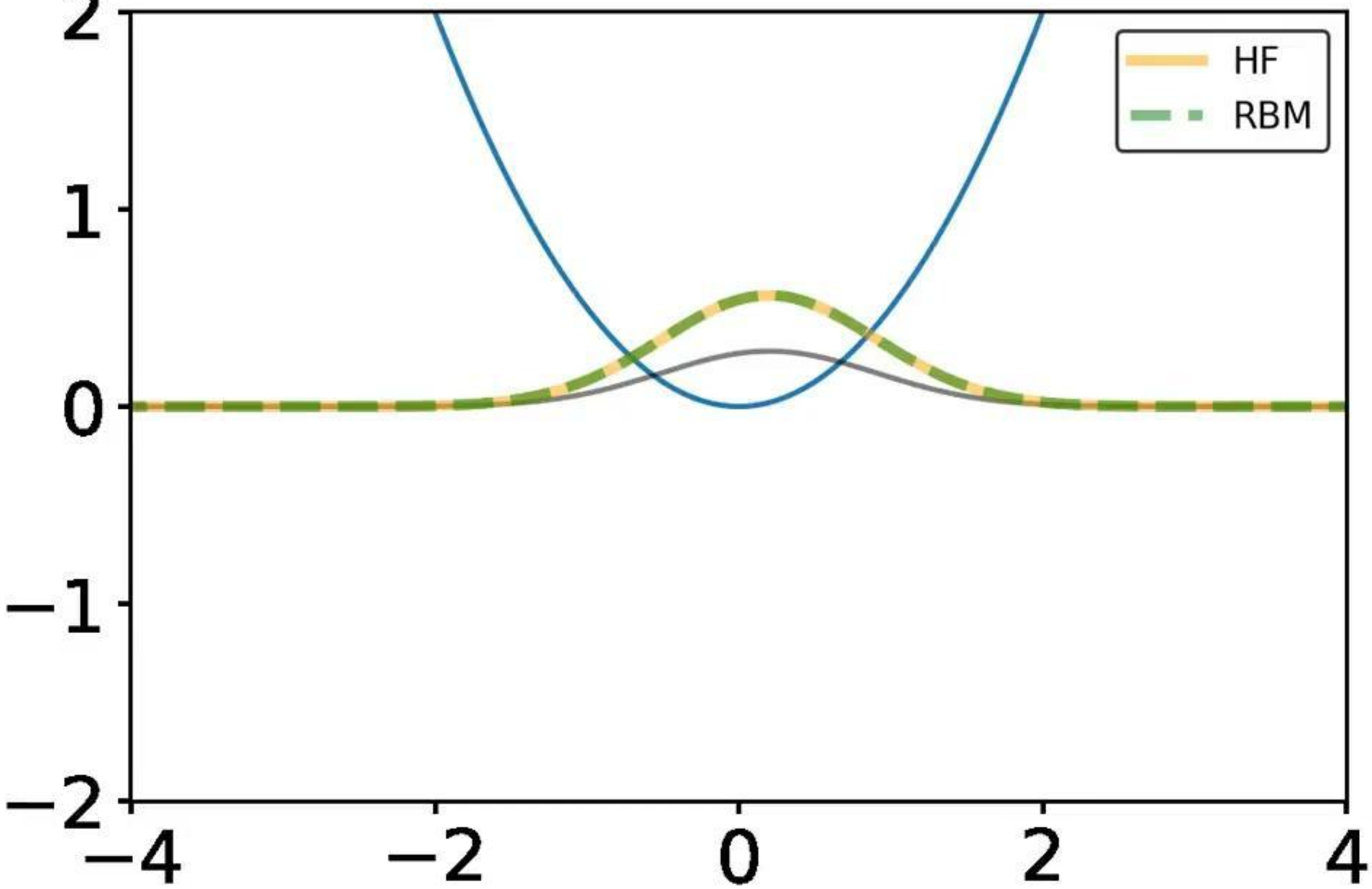
TDRBM Examples - Particle in a HO Trap



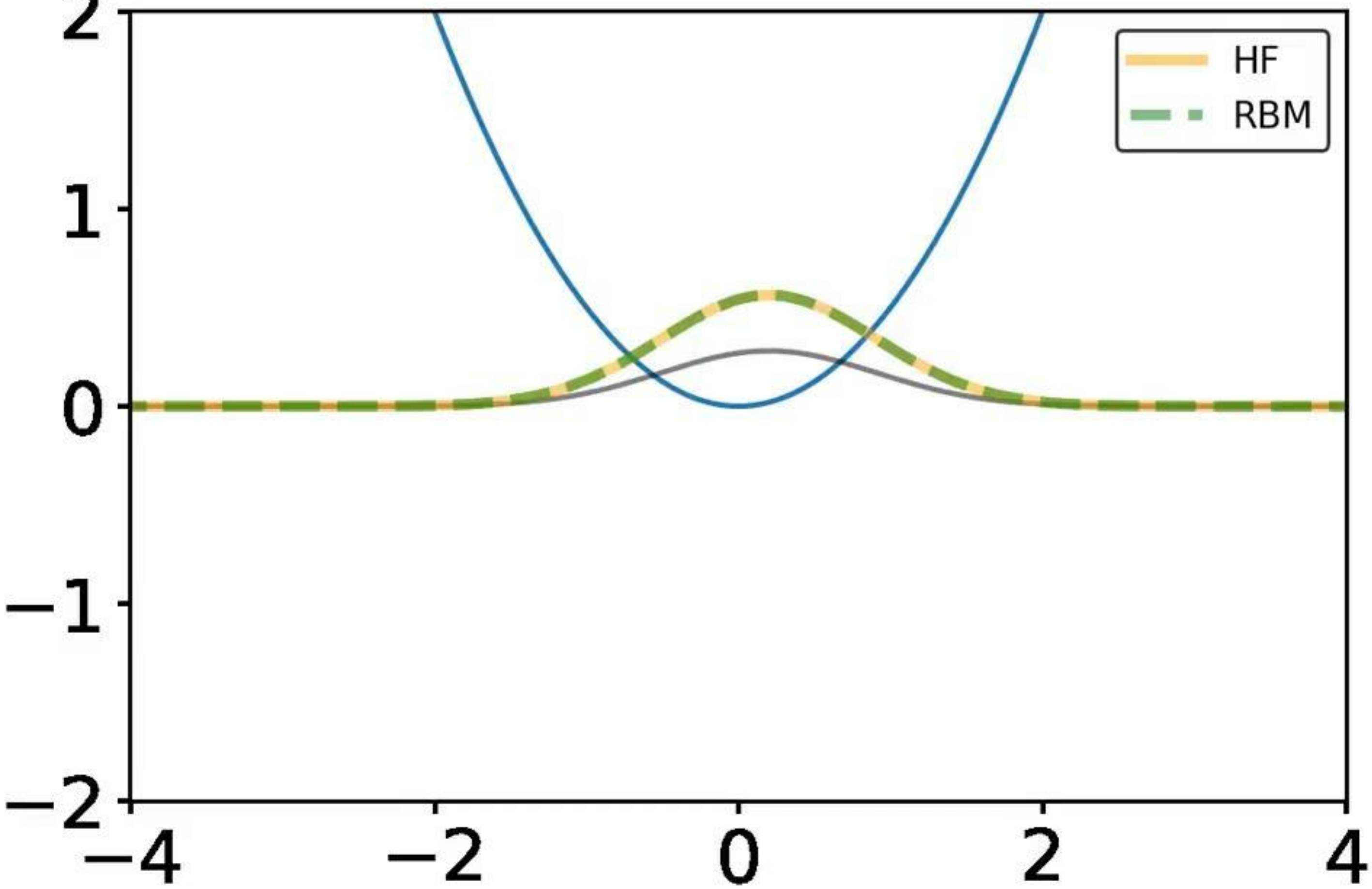
TDRBM Examples - Adding Nonlinearity



New term that depends on ϱ!



$q\varrho$ with $q < 0$



$q\varrho$ with $q > 0$

TDRBM Roundup

In general we need a bigger basis, but we get away with larger time steps thanks to the increased stability

This is for a periodic system, albeit a complicated one.

Ultimate goal of collision emulator is likely difficult for RBMs in this naive implementation

Perspectives for Time-Dependent Emulation

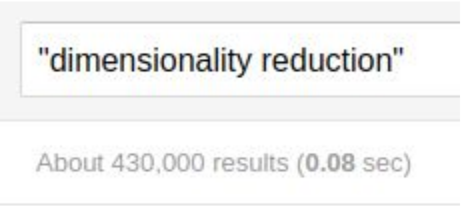
Data-driven:

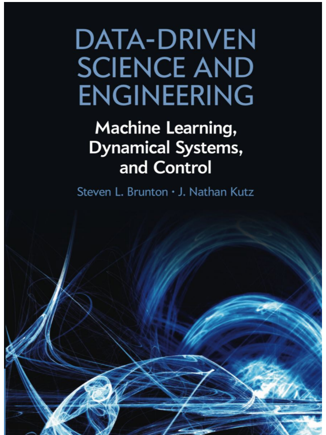
Dynamic Mode Decomposition (DMD)

Sparse Identification of Nonlinear Dynamics (SINDy)

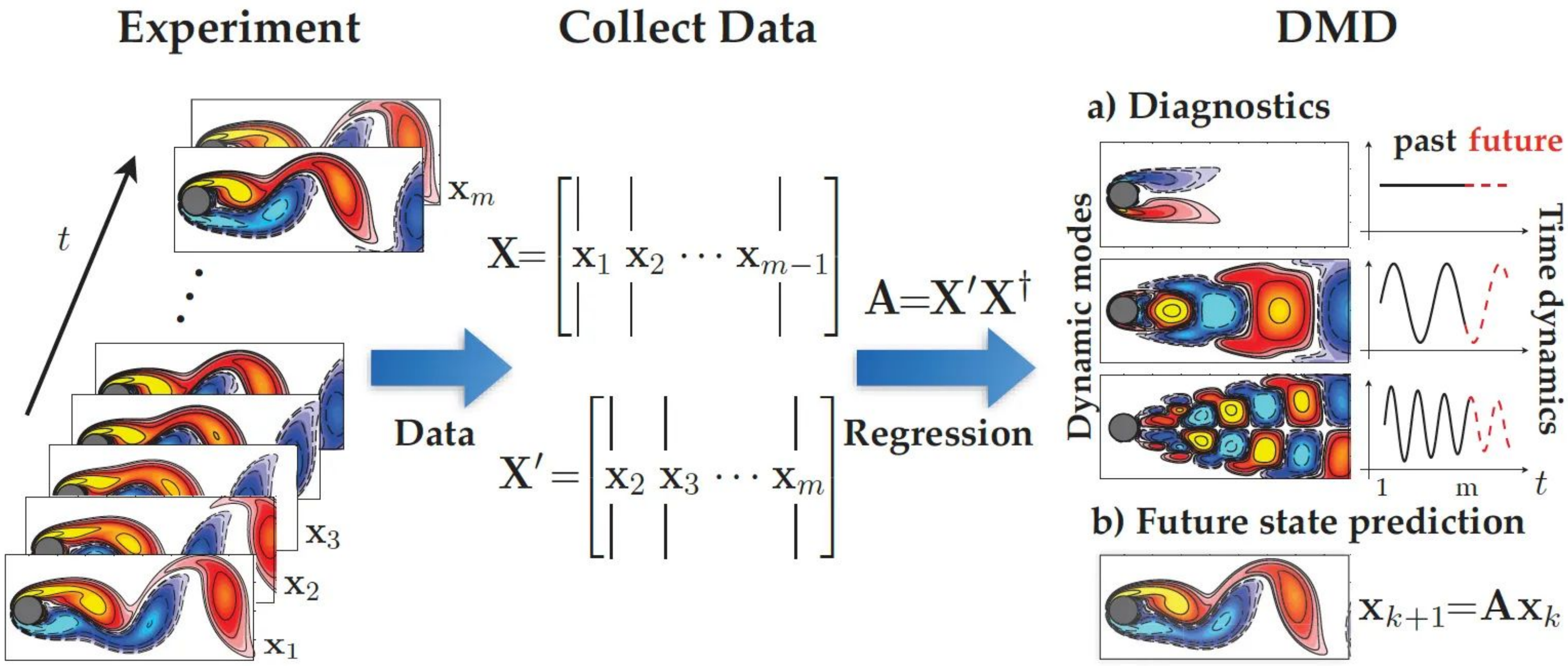
Neural Implicit Flow (NIF)

\+ a whole zoo...





Dynamic Mode Decomposition



Dynamic Mode Decomposition

S. L. Brunton et al., arXiv:2102.12086
Kutz et al., "Dynamic Mode Decomposition" (SIAM, 2016), https://www.dmdbook.com

- create snapshot matrices of discretized dynamic system

$$\mathbf{X} = \left(\mathbf{h}_0 \quad \cdots \mathbf{h}_{n-1}\right), \qquad \mathbf{X}' = \left(\mathbf{h}_1 \quad \cdots \mathbf{h}_n\right)$$

- express evolution with the help of the **Koopman operator** $\mathbf{K}$

$$\mathbf{h}_{i+1} = \mathbf{K}\mathbf{h}_i \qquad \rightarrow \qquad \mathbf{X}' = \mathbf{K}\mathbf{X}$$

- take the Moore-Penrose pseudo-inverse $\mathbf{X}^+$ to compute an (approximate) matrix representation of $\mathbf{K}$:

$$\mathbf{K} = \mathbf{X}'\mathbf{X}^+$$

- solve **eigenvalue problem** for Koopman operator to construct **reduced basis** of **dynamic modes**

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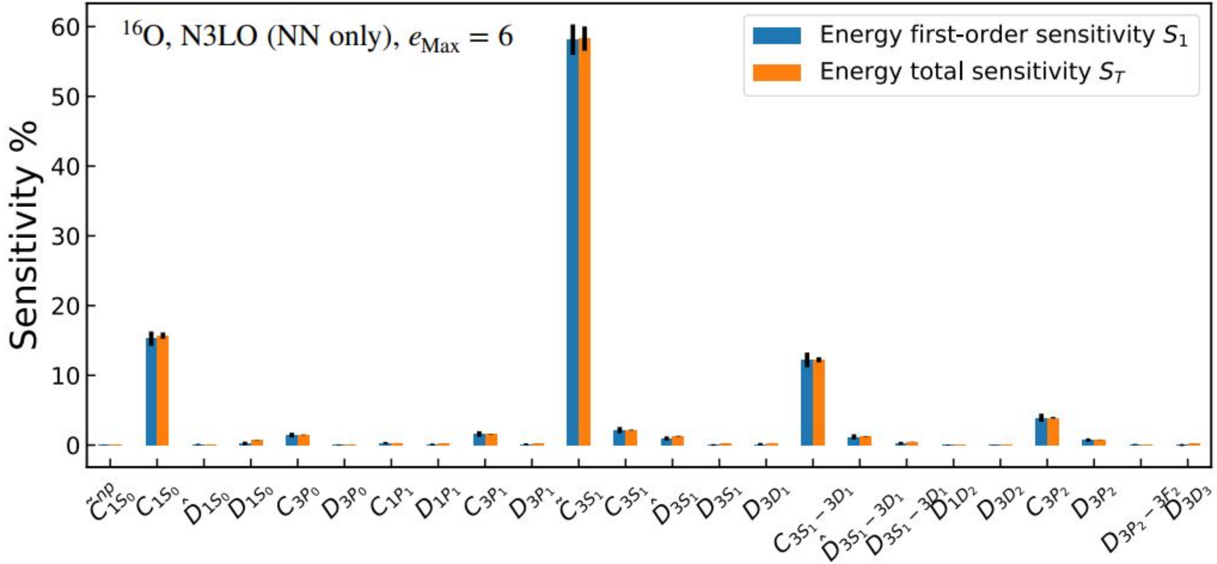
Application: Sensitivity Analysis & UQ

***J. Davison, J. Crawford**, S. Bogner, HH, in preparation*

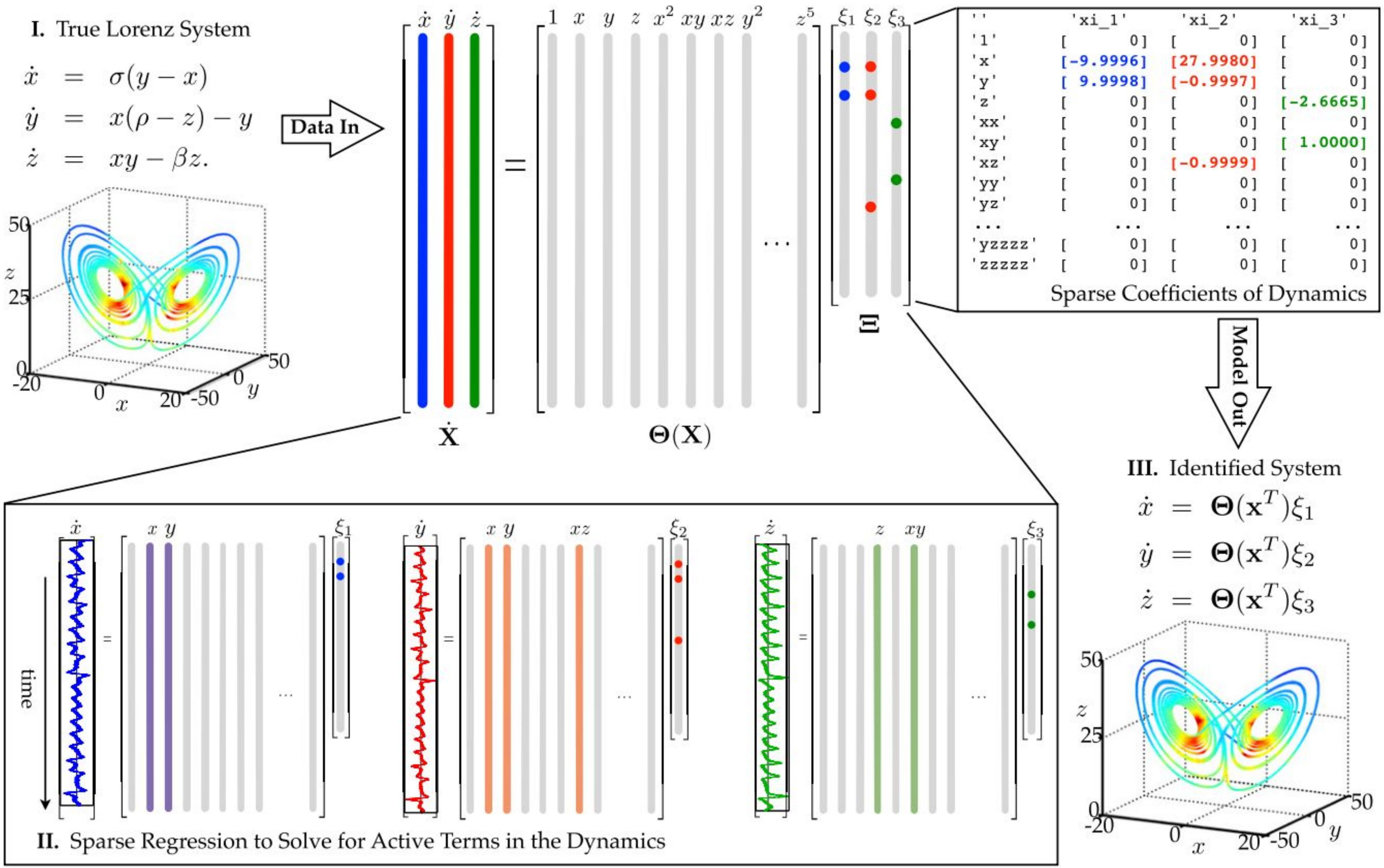


- reduction to **dominant DMD modes** allows sensitivity studies & uncertainty quantification (**while still generating full H(s)**)
- showing 200k+ Monte Carlo samples in LEC parameter space: **4-5 order of magnitude computing time reduction**

EC Workshop

Sparse Identification of Nonlinear Dynamics

What if we could mine the form of the time dynamics directly from the data?


I. True Lorenz System
$\dot{x} = \sigma(y - x)$
$\dot{y} = x(\rho - z) - y$
$\dot{z} = xy - \beta z.$
Data In
$\dot{x}$ $\dot{y}$ $\dot{z}$
1 x y z x^2 xy xz y^2 z^5
ξ_1 ξ_2 ξ_3
$\dot{\mathbf{X}}$
$\mathbf{\Theta}(\mathbf{X})$
$\mathbf{\Xi}$
'' 'xi_1' 'xi_2' 'xi_3'
'1' [0] [0] [0]
'x' [-9.9996] [27.9980] [0]
'y' [9.9998] [-0.9997] [0]
'z' [0] [0] [-2.6665]
'xx' [0] [0] [0]
'xy' [0] [0] [1.0000]
'xz' [0] [-0.9999] [0]
'yy' [0] [0] [0]
'yz' [0] [0] [0]
'yzzzz' [0] [0] [0]
'zzzzz' [0] [0] [0]
Sparse Coefficients of Dynamics
Model Out
III. Identified System
$\dot{x} = \mathbf{\Theta}(\mathbf{x}^T)\xi_1$
$\dot{y} = \mathbf{\Theta}(\mathbf{x}^T)\xi_2$
$\dot{z} = \mathbf{\Theta}(\mathbf{x}^T)\xi_3$
time
II. Sparse Regression to Solve for Active Terms in the Dynamics

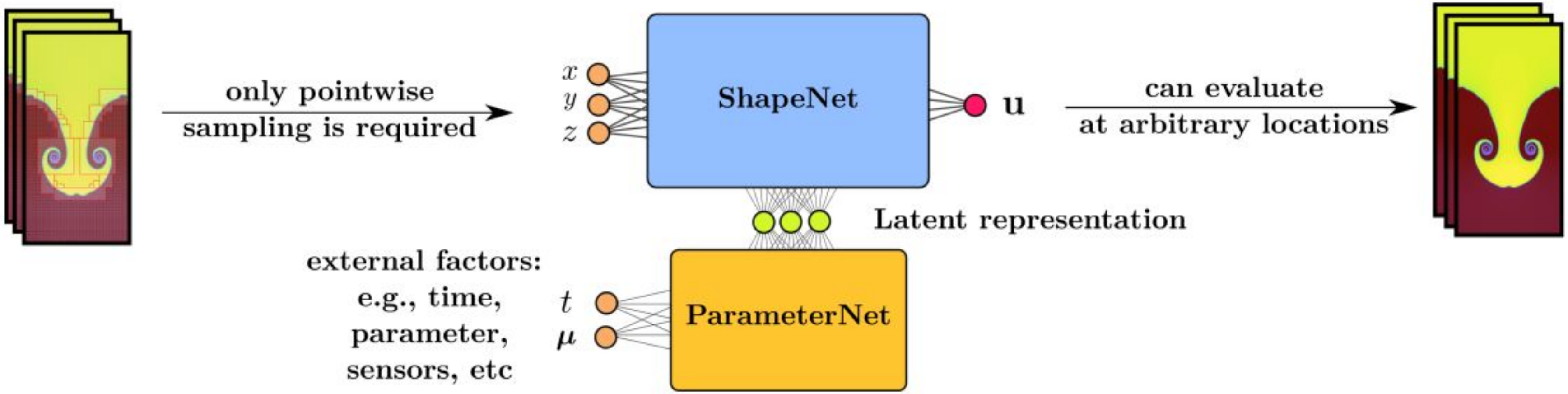
Sparse Identification of Nonlinear Dynamics

Also good candidate for model discovery even beyond time dynamics!

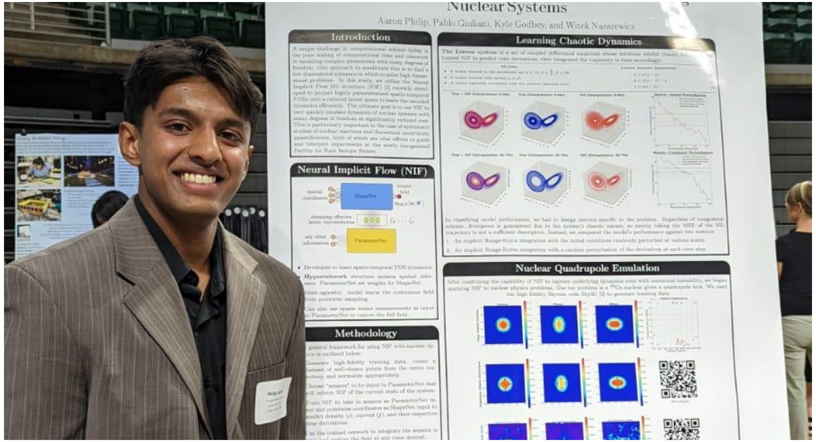
Neural Implicit Flow

Even more data-driven: let's look at hypernetworks for learning dynamics

Neural Implicit Flow

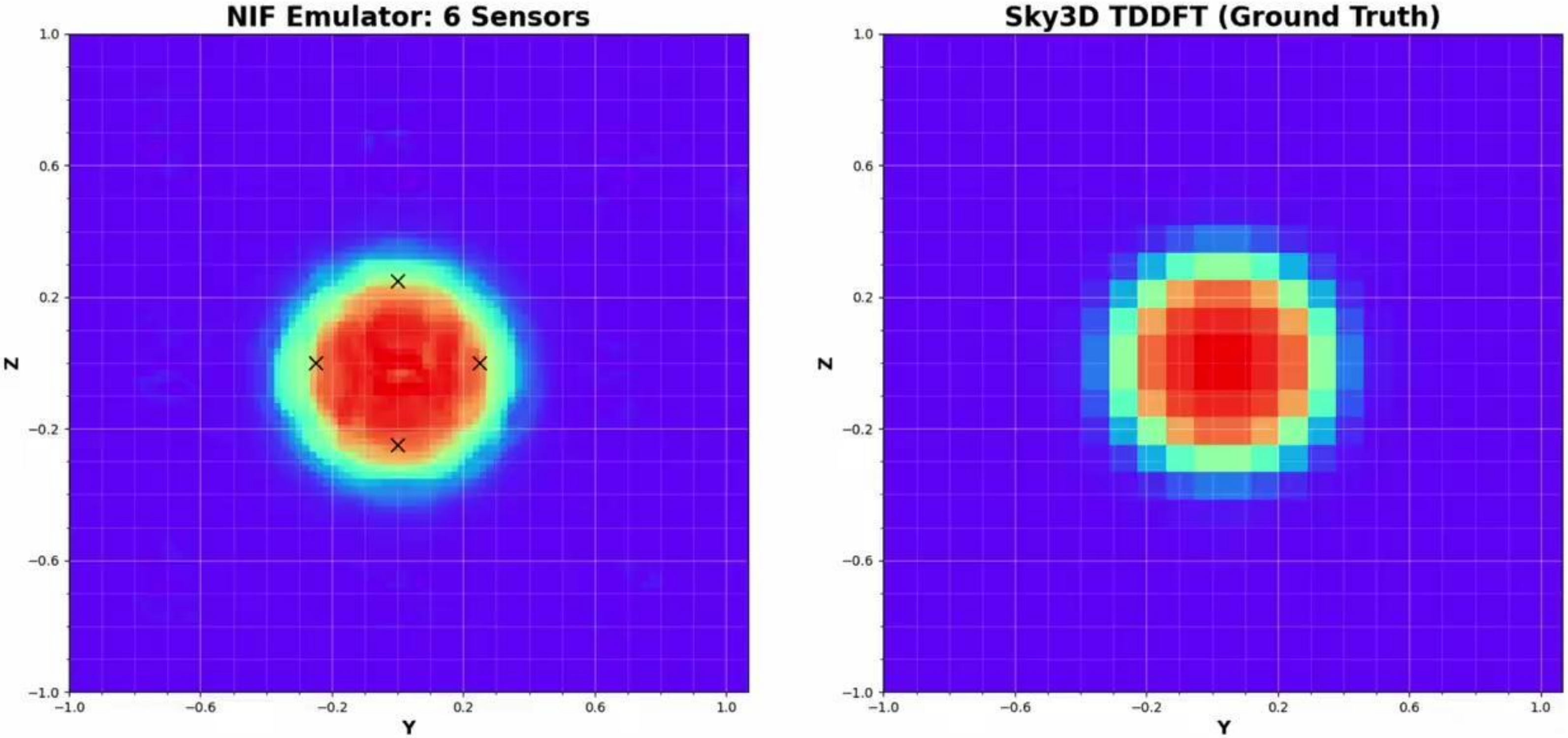


Neural Implicit Flow



Student Aaron Philip making good headway for applications to TDDFT! First step is to see how much we can reduce the dimensionality per time step

Neural Implicit Flow (as an interpolator)



Where to Next?

A potential gain on the statistical side is to apply dimensionality reduction techniques in that realm

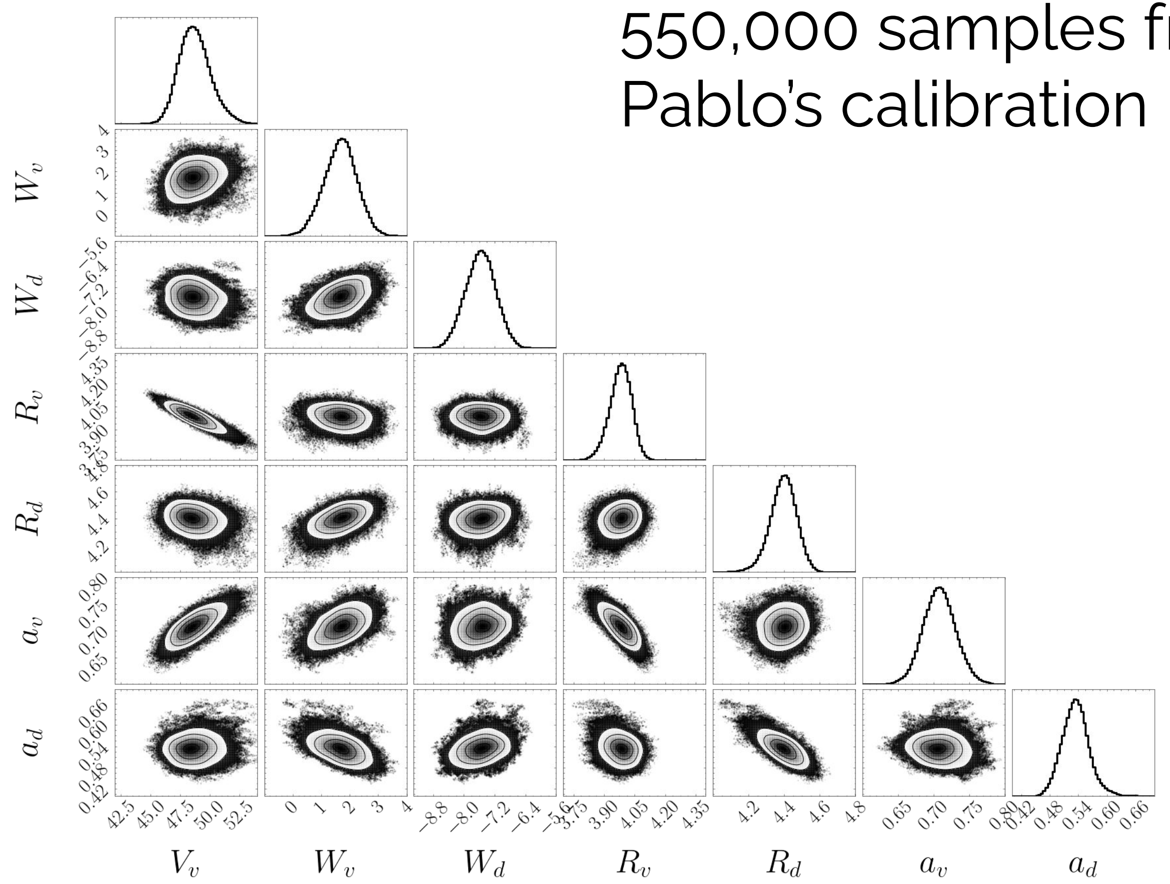
One avenue is the polynomial chaos expansion – a sort of RBM for your probability distribution – but we're still in the early days of theoretical development here

Enter: Normalizing Flows

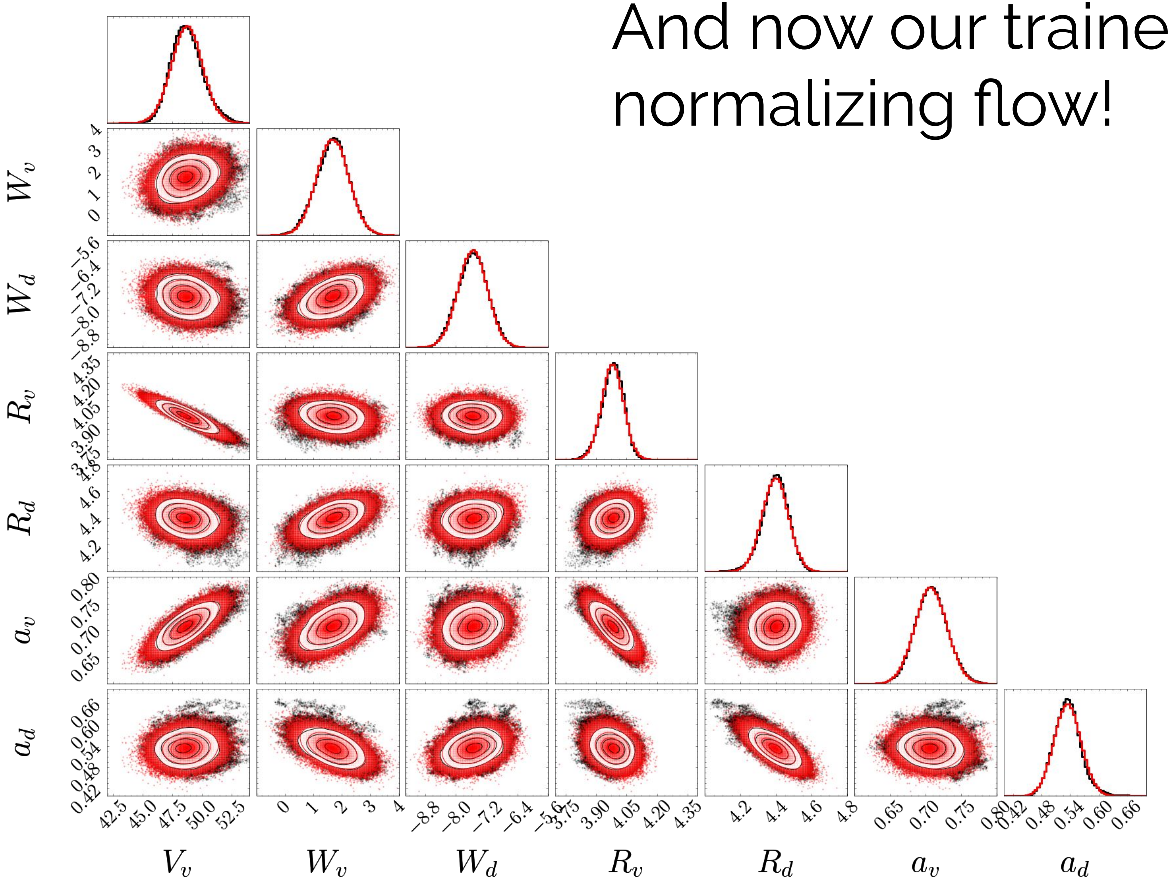
"A Normalizing Flow is a transformation of a simple probability distribution (e.g., a standard normal) into a more complex distribution by a sequence of invertible and differentiable mappings."

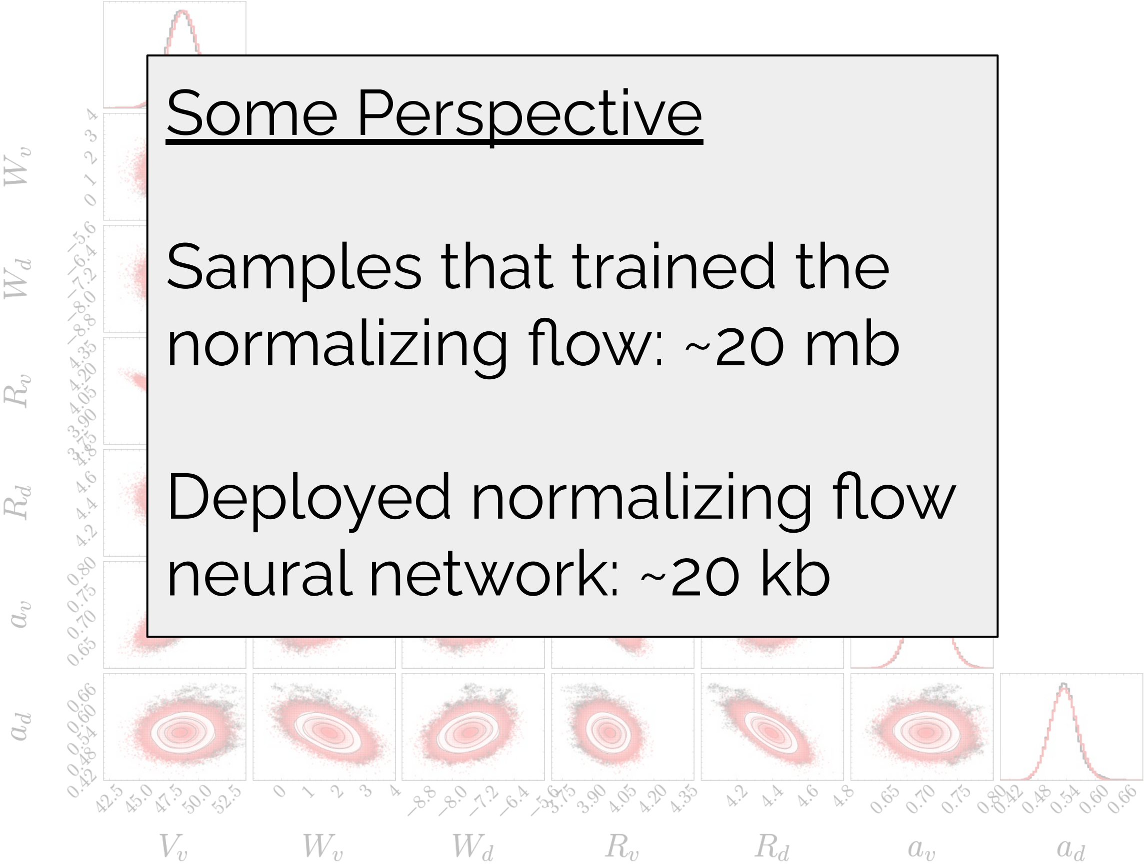
Ivan Kobyzev et al, . Normalizing flows: An introduction and review of current methods. IEEE Transactions on Pattern Analysis and Machine Intelligence, 2020.

550,000 samples from Pablo's calibration



And now our trained normalizing flow!





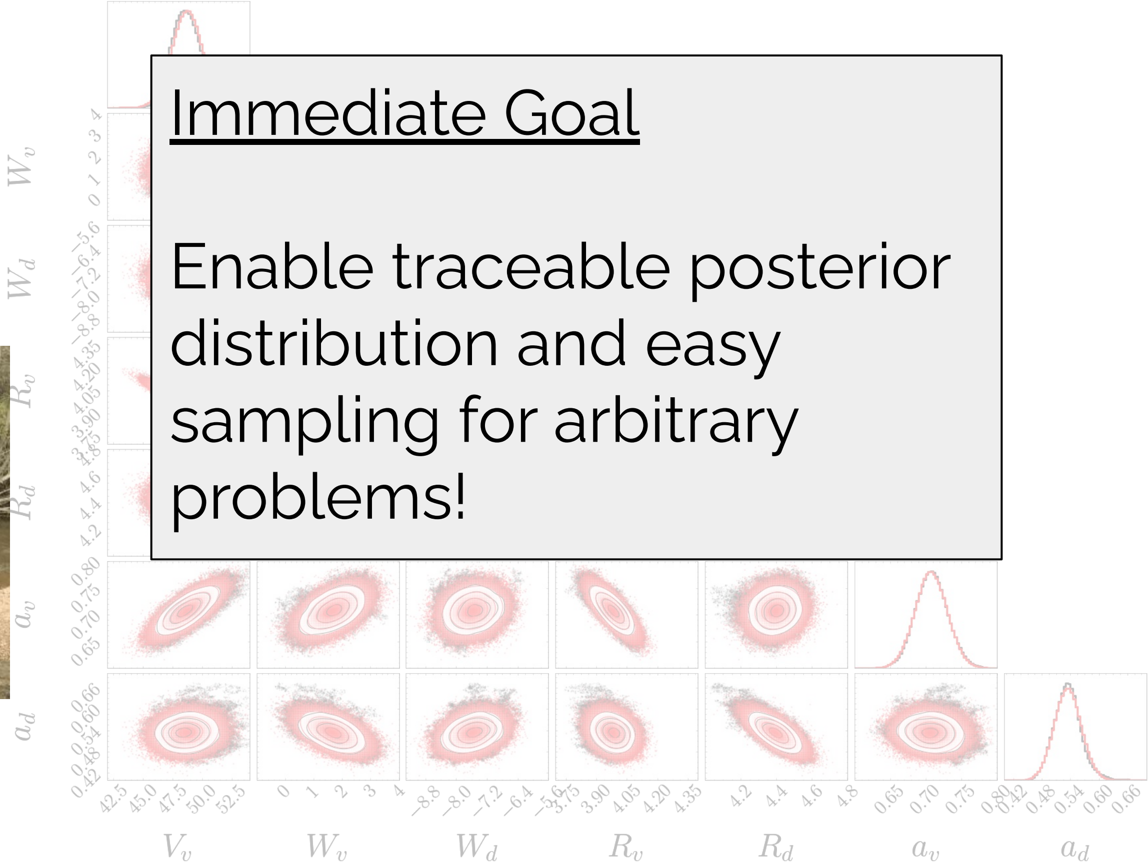
Some Perspective

Samples that trained the normalizing flow: ~20 mb

Deployed normalizing flow neural network: ~20 kb

Landon Buskirk

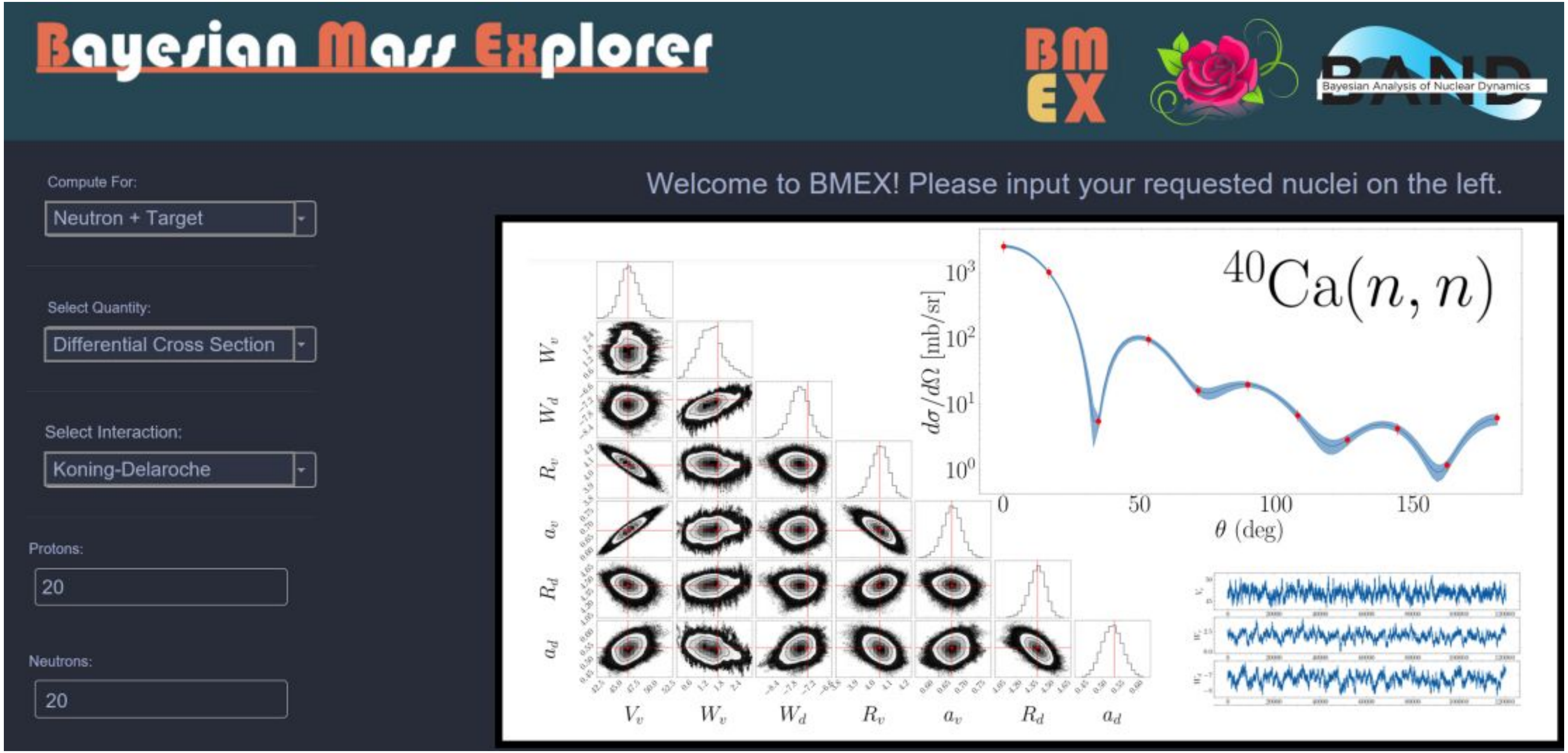
Yukari Yamauchi



Immediate Goal

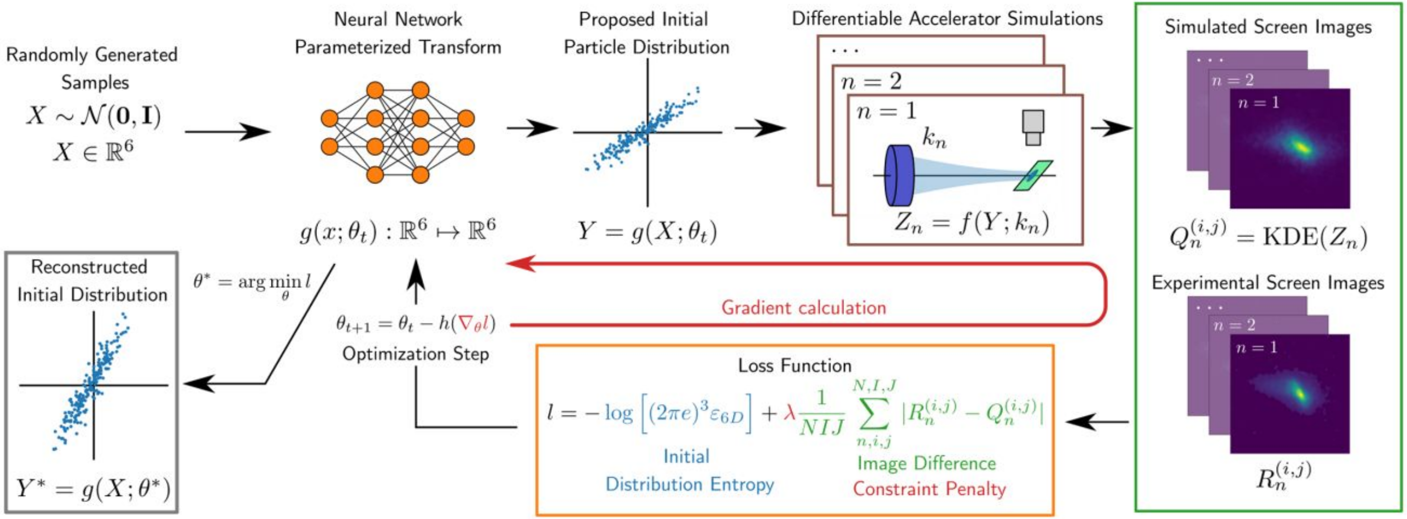
Enable traceable posterior distribution and easy sampling for arbitrary problems!

Deployable Emulators



https://bmex.dev

Deployable Emulators - Perspectives for Experimental Design and Control?



R. Roussel et al, Phys. Rev. Lett. 130, 145001

Challenges?

Let's discuss! Each application domain has its own – as a community we should try to identify common issues and their solutions

It's gonna be a long journey, so please share what you learn along the way!

https://rbm.ascsn.net

Forum is coming soon!
Check https://ascsn.net
for details