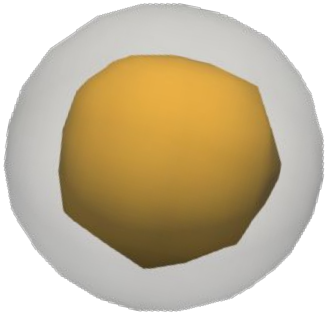
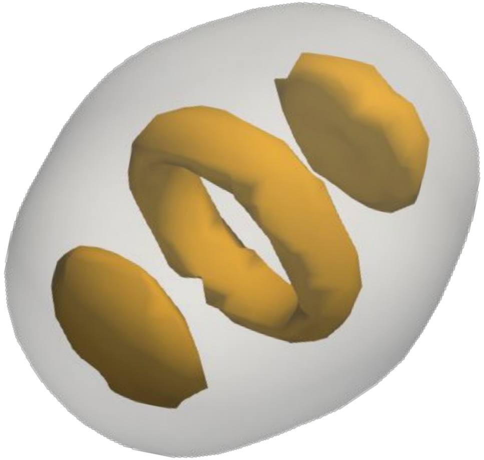
Dimensionality Reduction Techniques in Time-Dependent Problems

Kyle Godbey

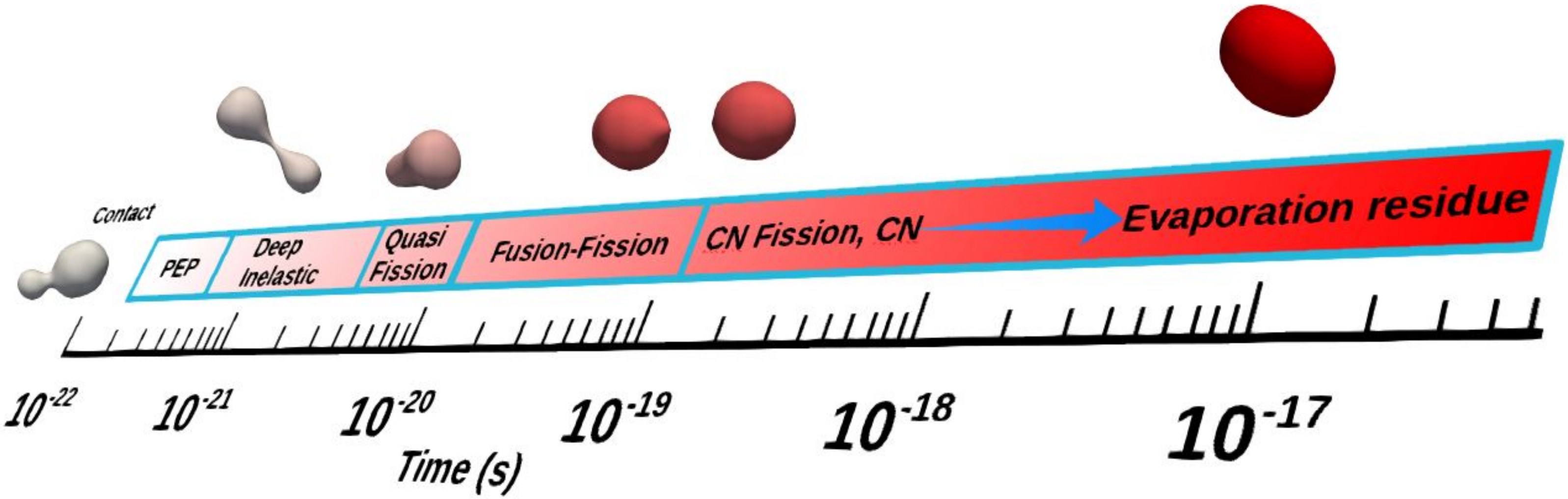




STREAMLINE
STREAMLINE Symposium
May 2024, East Lansing

Google slides link with videos:
https://docs.google.com/presentation/d/1gecxfpX7yjzau2y2dicd6F5nneVk2Xlraw4ht8wERGM/edit?usp=sharing

Dynamics Are More Than Reactions!



Dynamics Are More Than Reactions!

Reactions, resonant phenomena, decays, etc. are all governed by the dynamics of the quantum many-body problem

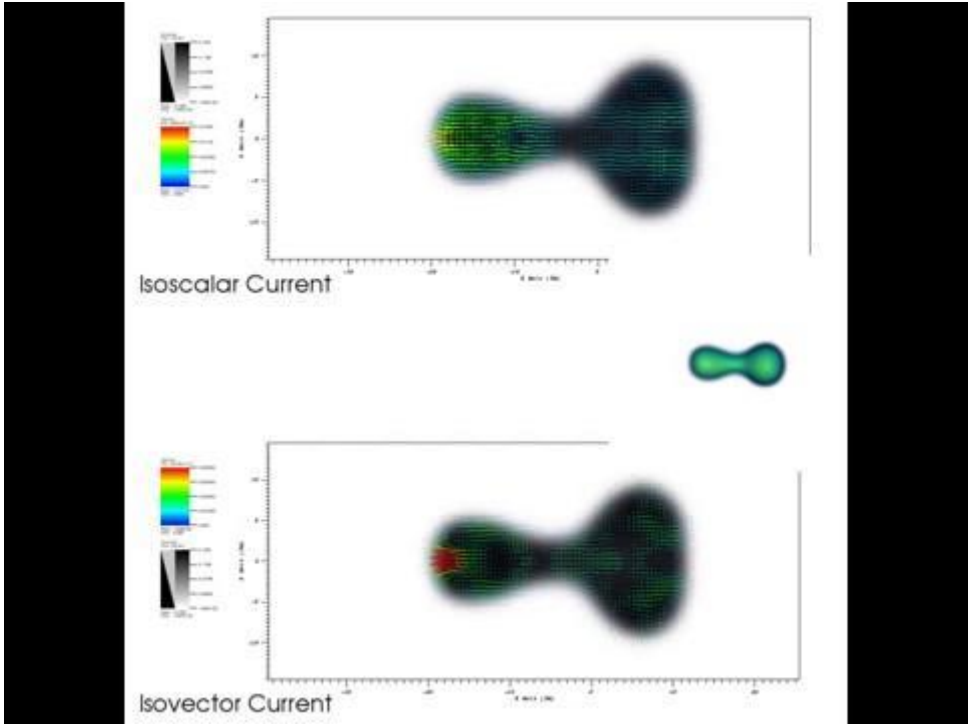
Explicit time evolution is a **very** powerful framework if you can afford it

Sensitivity to the intricacies in the nuclear structure

Explicit dynamics of shape evolution

Collective phenomena emerge from your many-body description

Don’t Forget Transfer and Equilibration



Perspectives for Time-Dependent Emulation

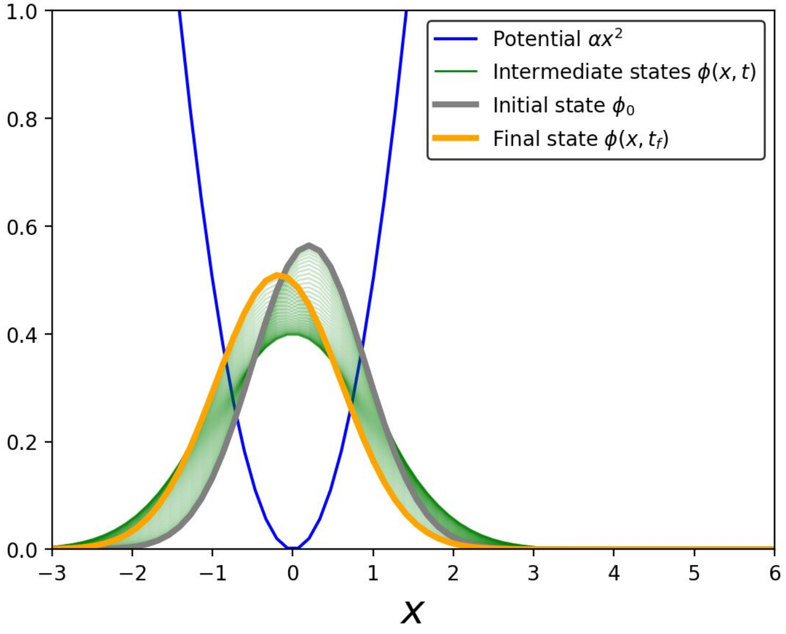
Two large classes: data-driven and model-driven

Model-driven:

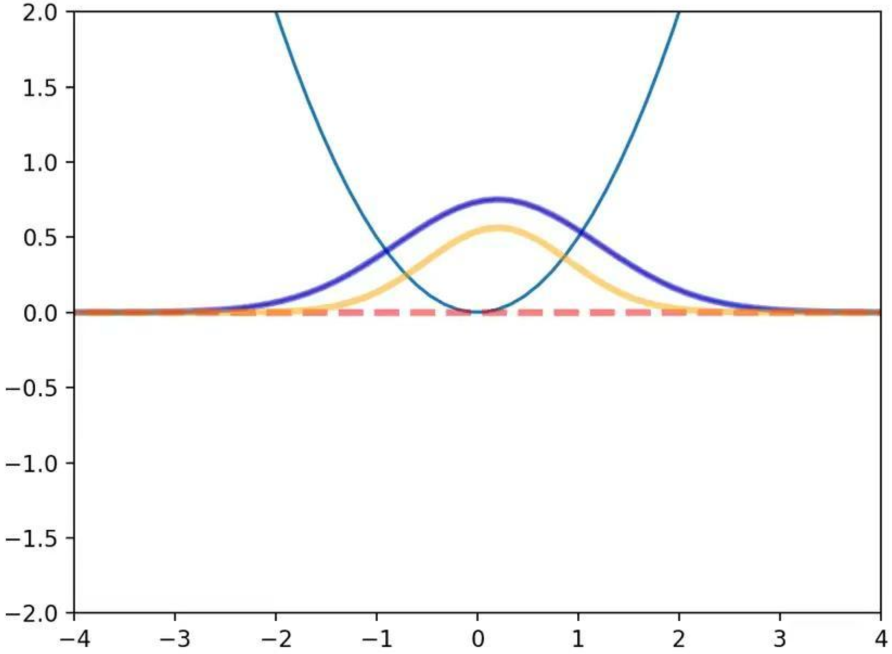
The reduced basis method (and related approaches) are a natural first place to check.

TDRBM Examples - Particle in a HO Trap

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

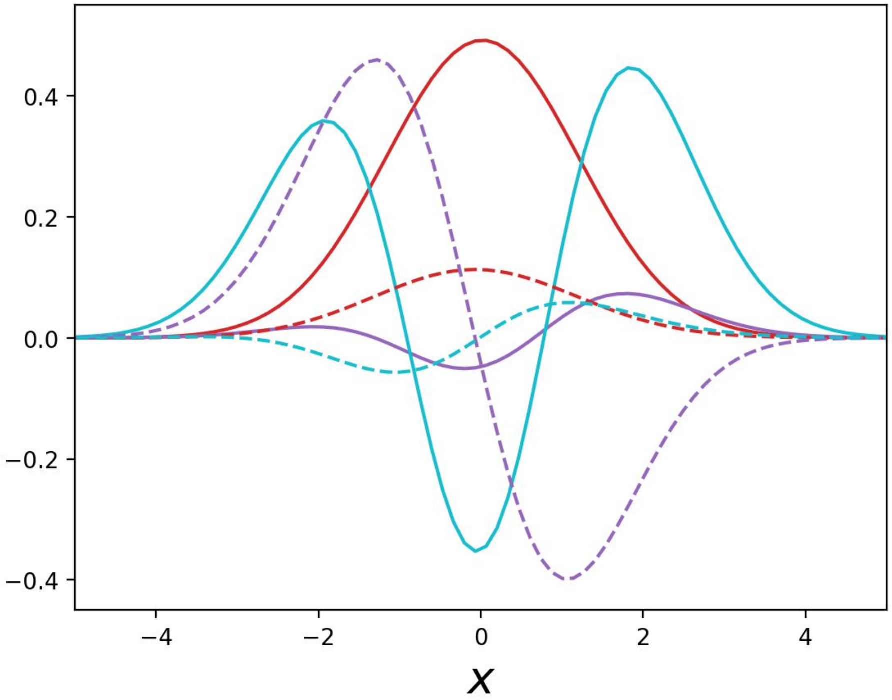


TDRBM Examples - Particle in a HO Trap



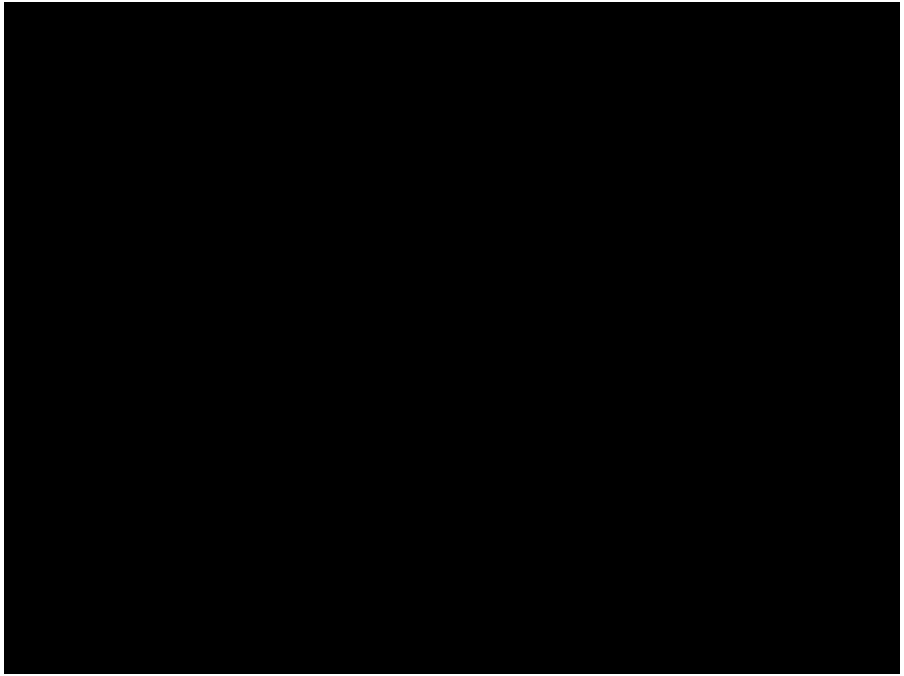
TDRBM Examples - Particle in a HO Trap

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

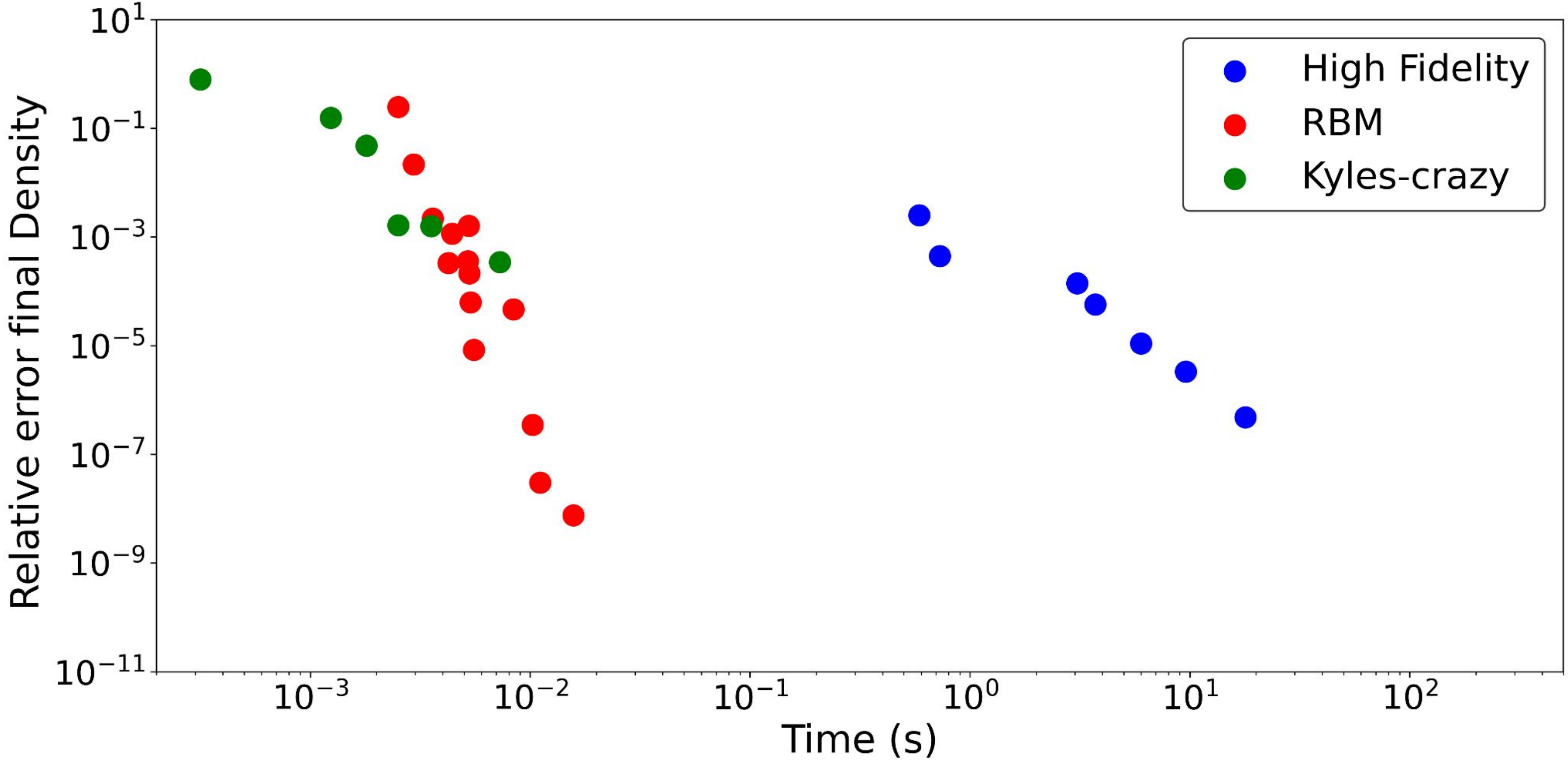


TDRBM Examples - Particle in a HO Trap

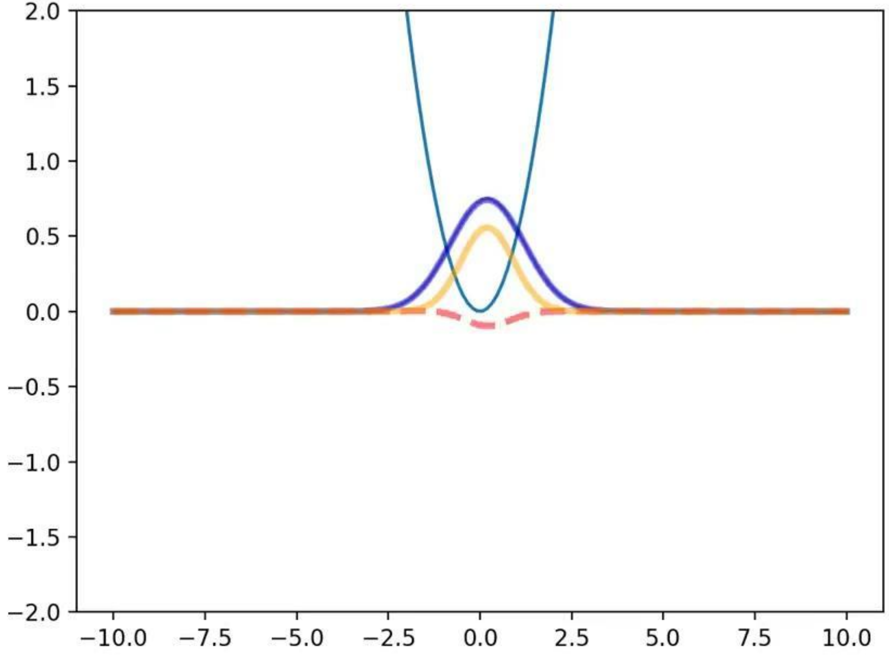
And, in the simplest RBM implementation, we can just propagate in time with our reduced Hamiltonian:



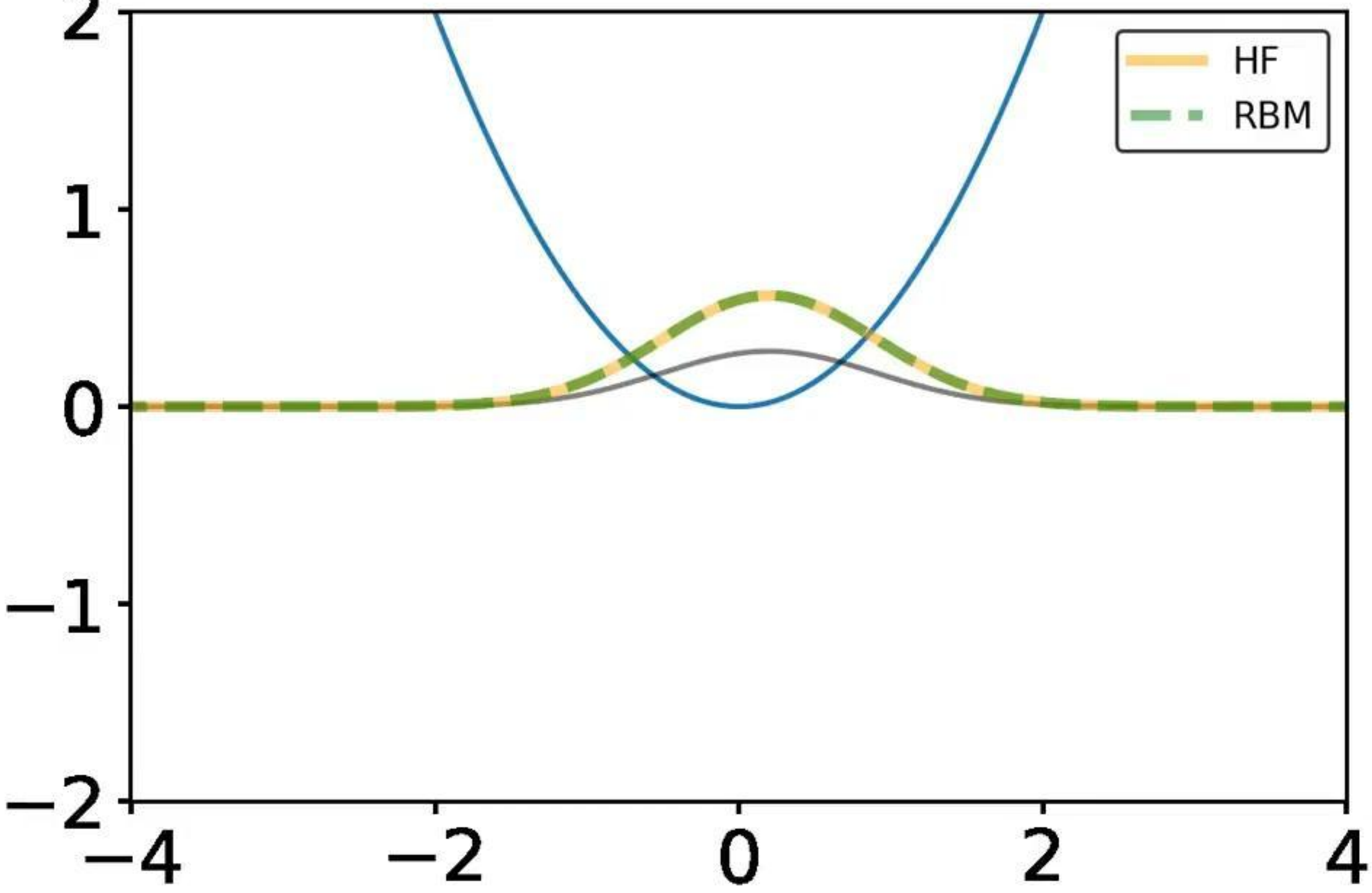
TDRBM Examples - Particle in a HO Trap



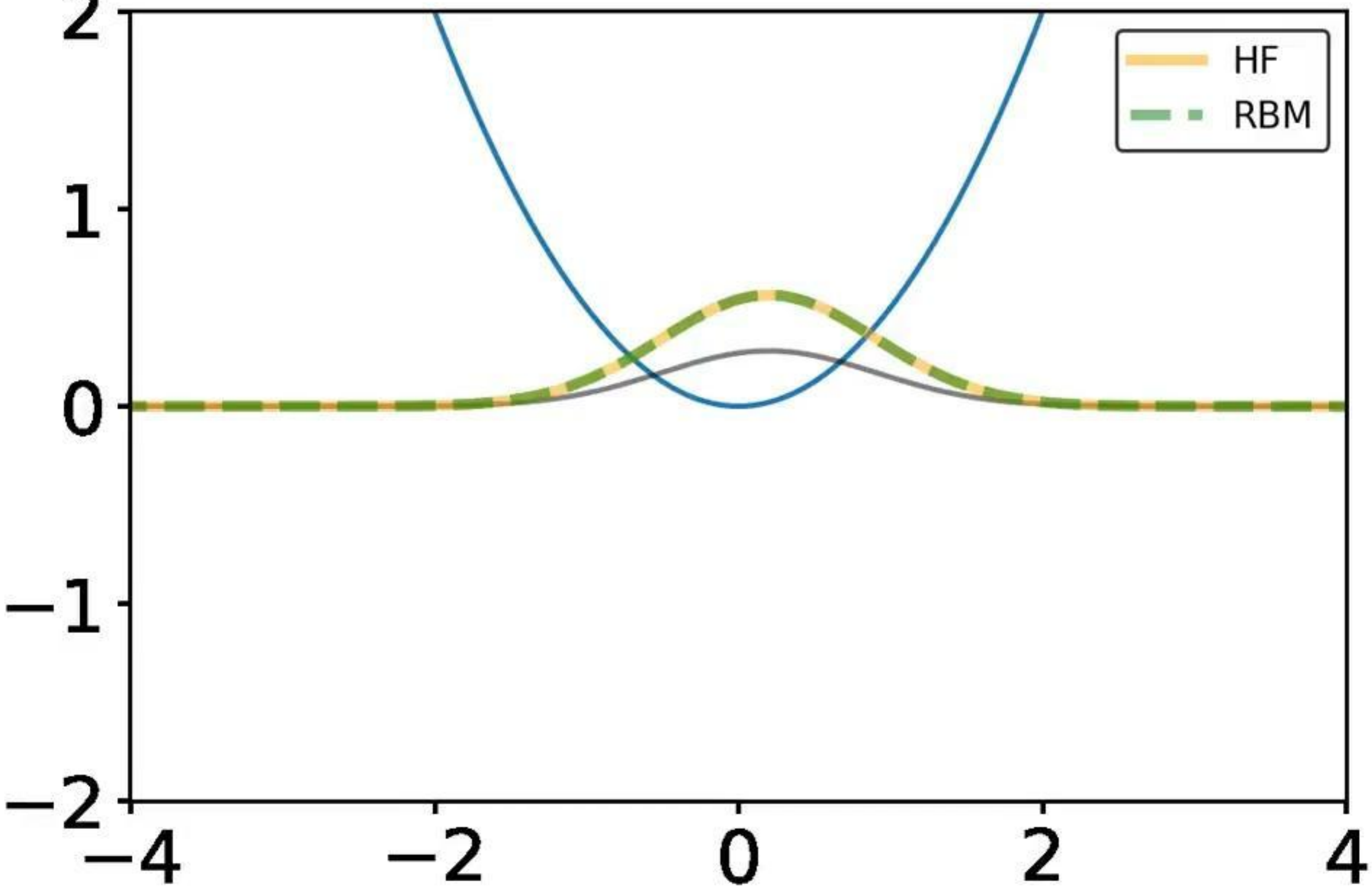
TDRBM Examples - Adding Nonlinearity



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

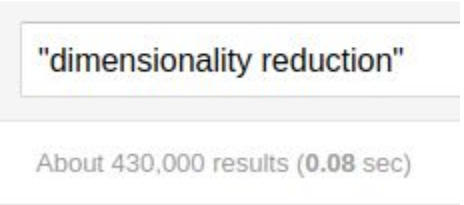
Data-driven:

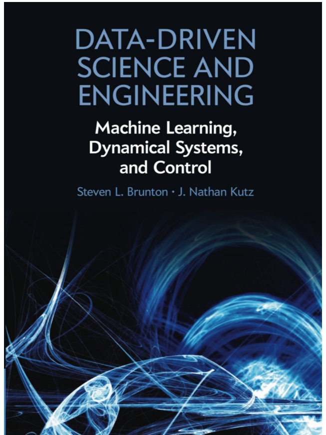
Dynamic Mode Decomposition (DMD)

Fourier Neural Operators

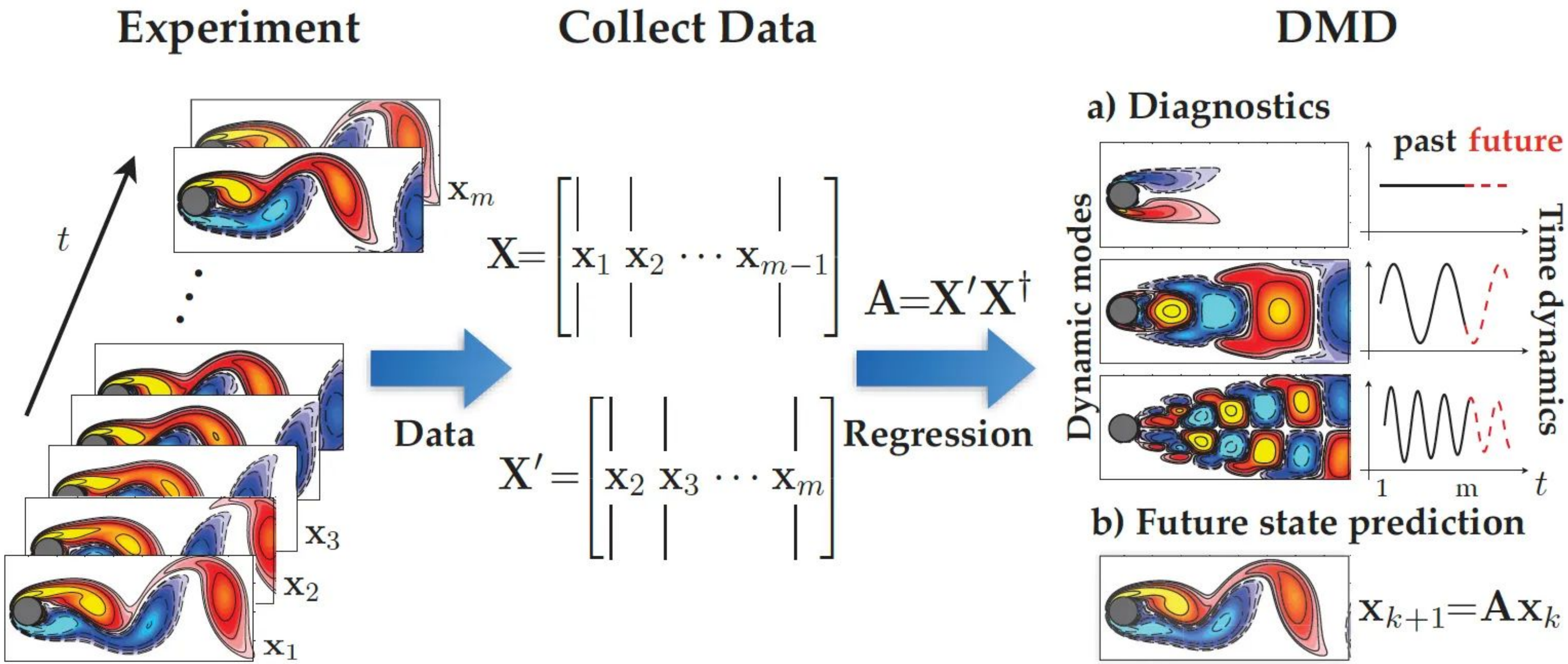
Neural Implicit Flow (NIF)

+ a whole zoo...



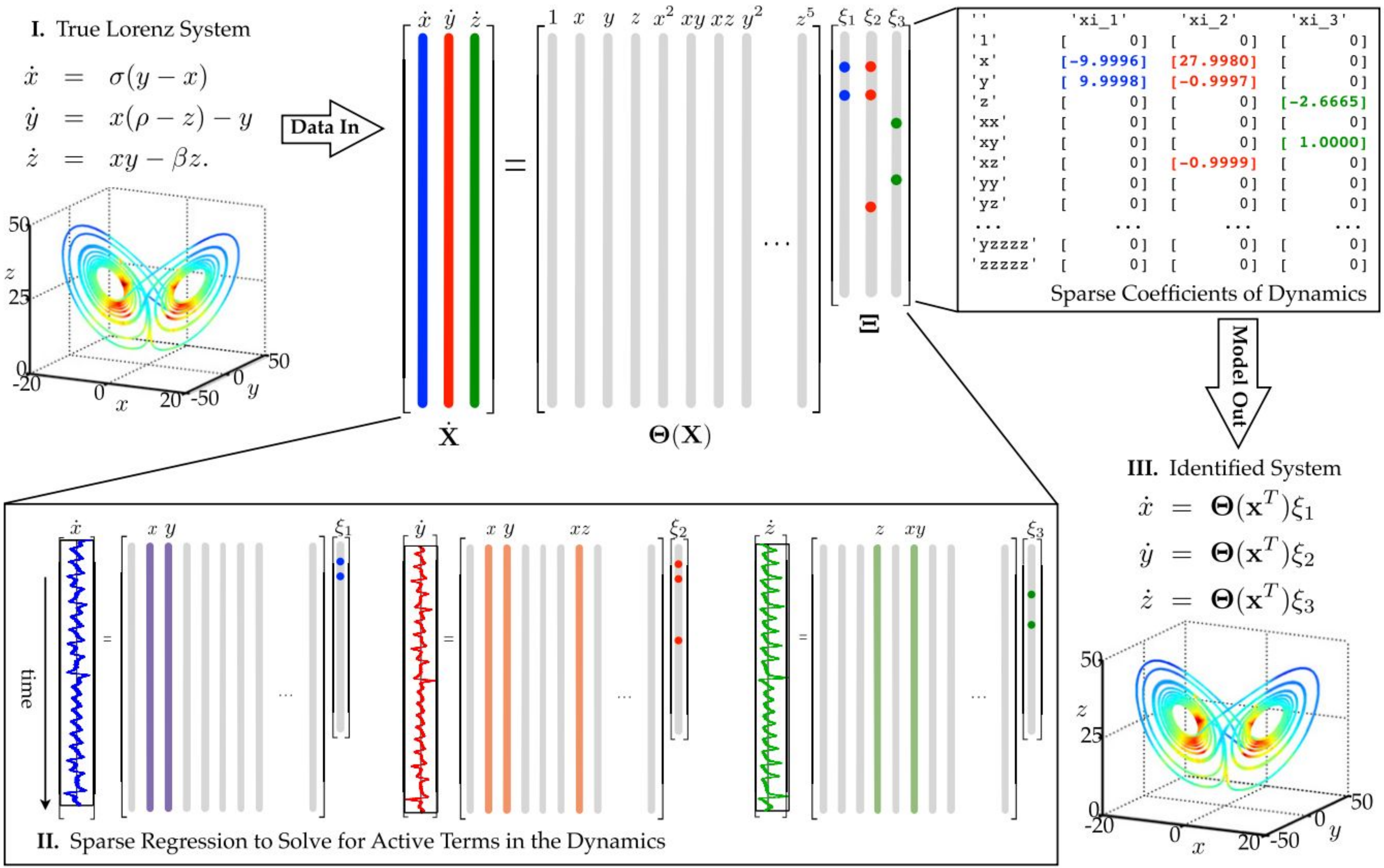


Dynamic Mode Decomposition



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
$\dot{\mathbf{X}} = \mathbf{\Theta}(\mathbf{X})\,\mathbf{\Xi}$
$1 \;\; x \;\; y \;\; z \;\; x^2 \;\; xy \;\; xz \;\; y^2 \;\cdots\; z^5$
$\xi_1 \;\; \xi_2 \;\; \xi_3$
'' '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

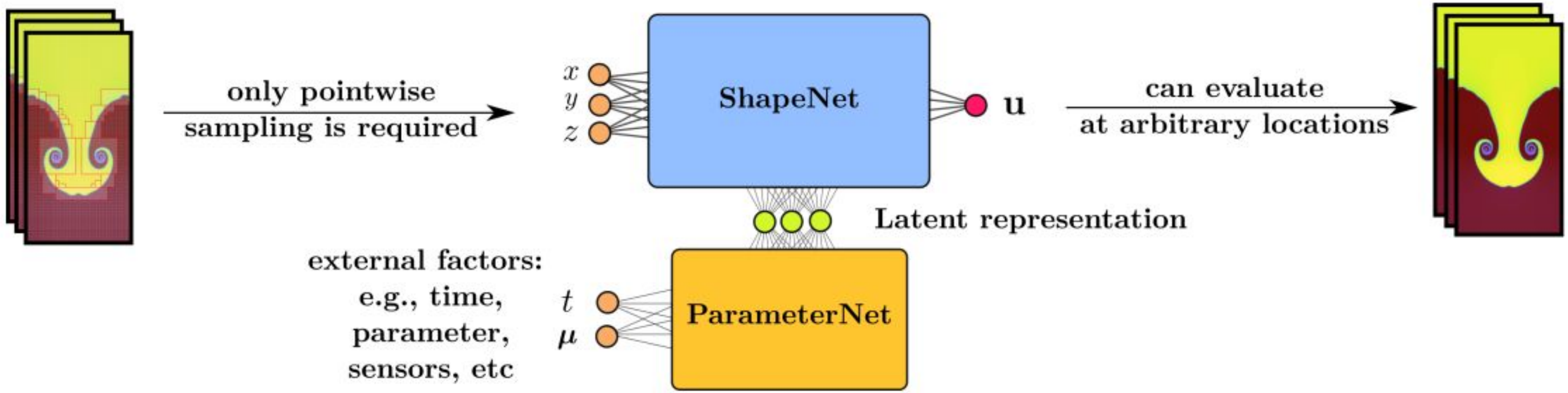
Sparse Identification of Nonlinear Dynamics

Also good candidate for model discovery even beyond time dynamics!

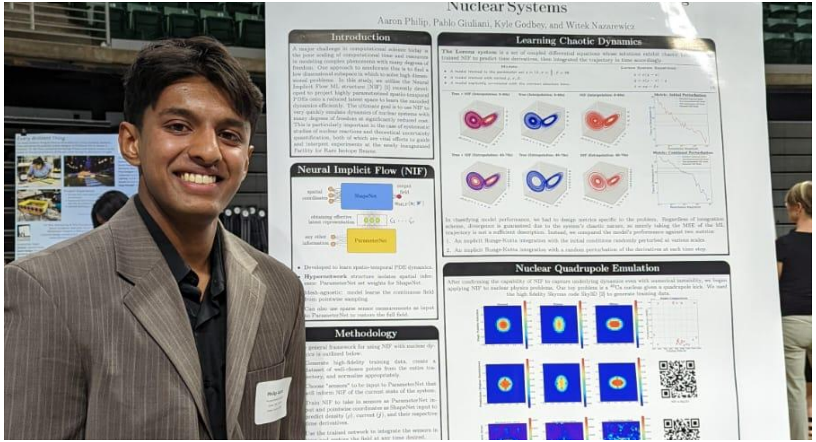
Neural Implicit Flow

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

Neural Implicit Flow



Neural Implicit Flow



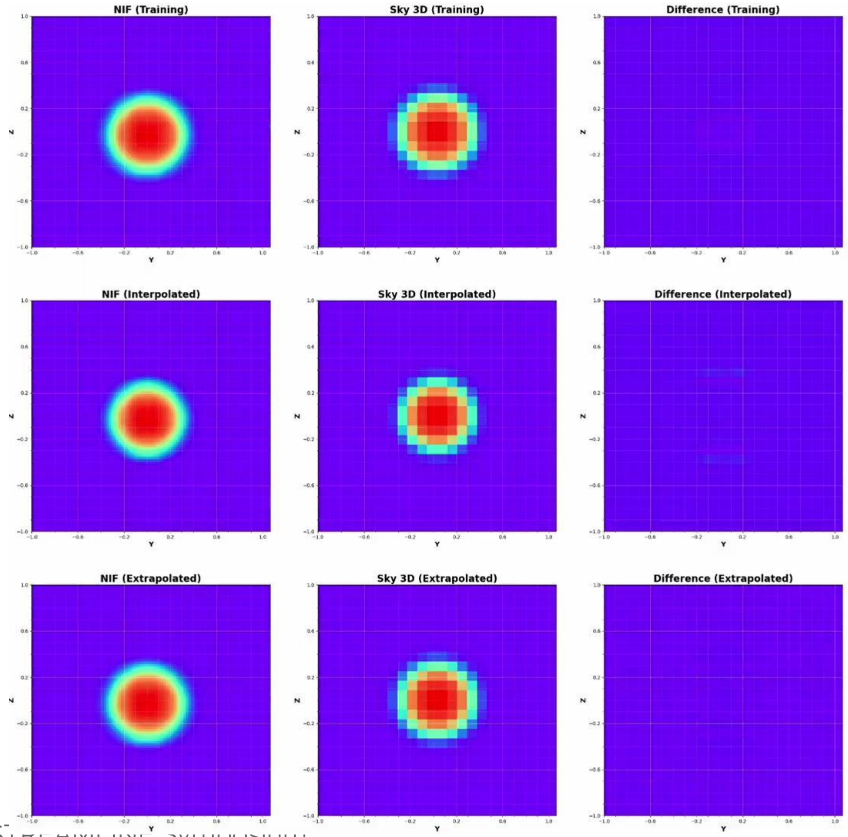
Student Aaron Philip making good headway for applications to TDDFT! First phase is wrapping up now.

Neural Implicit Flow

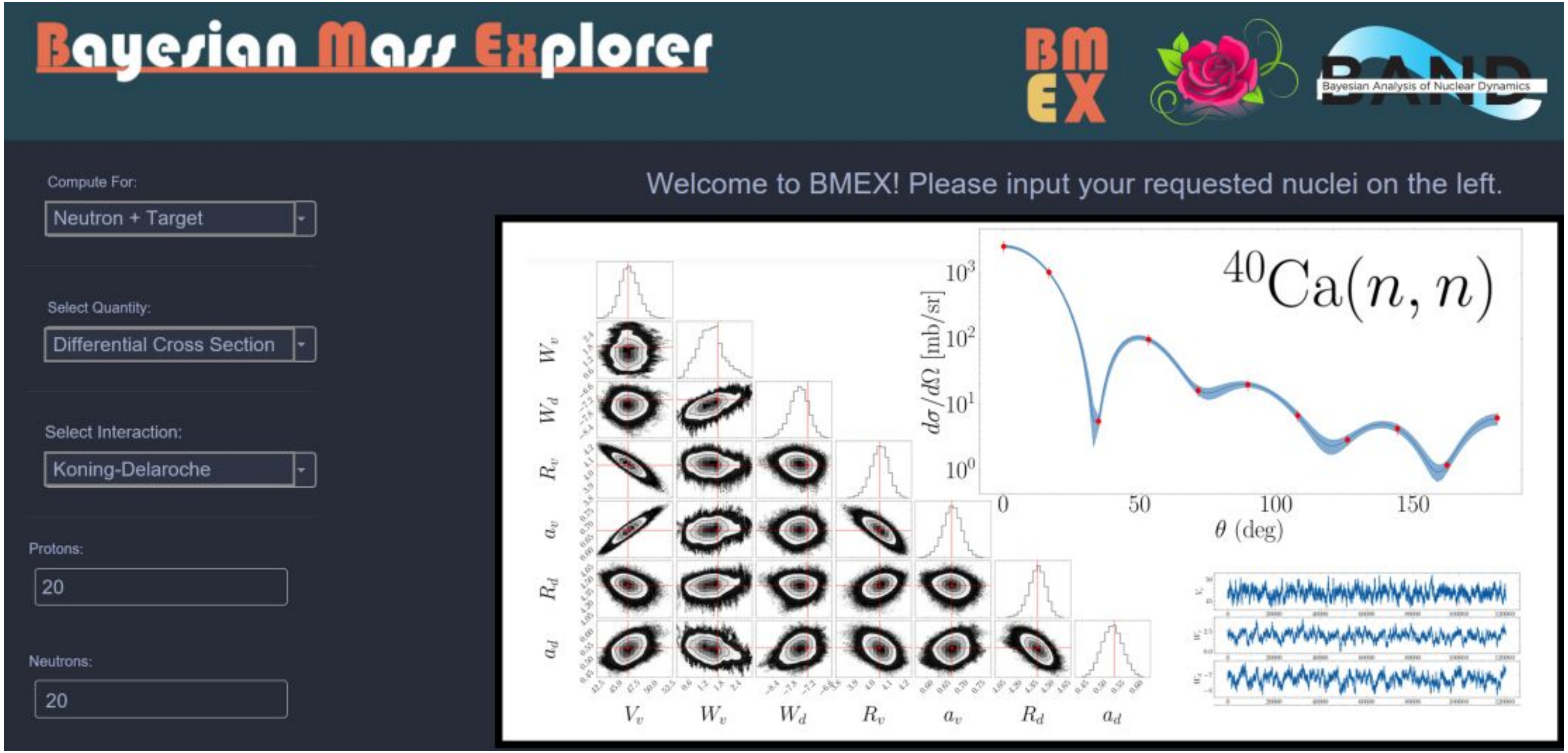
UURAF 2023 Award Winner

Goldwater Scholarship 2024

Neural Implicit Flow (as an interpolator)

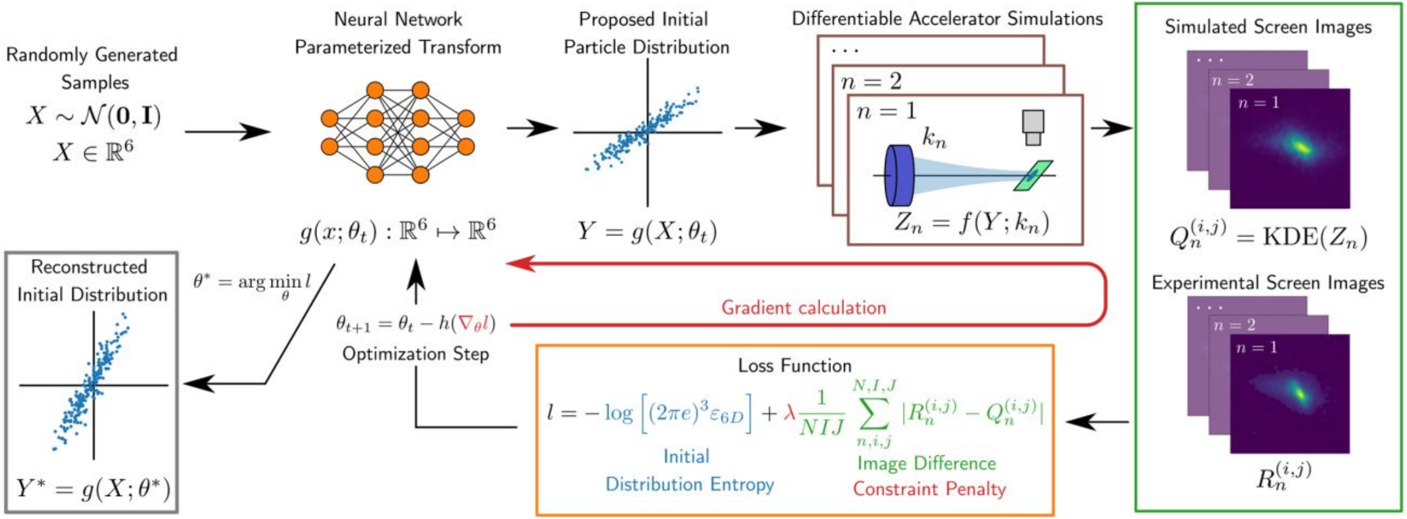


Deployable Emulators



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 appropriate solutions

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

https://dr.ascsn.net

https://forum.ascsn.net