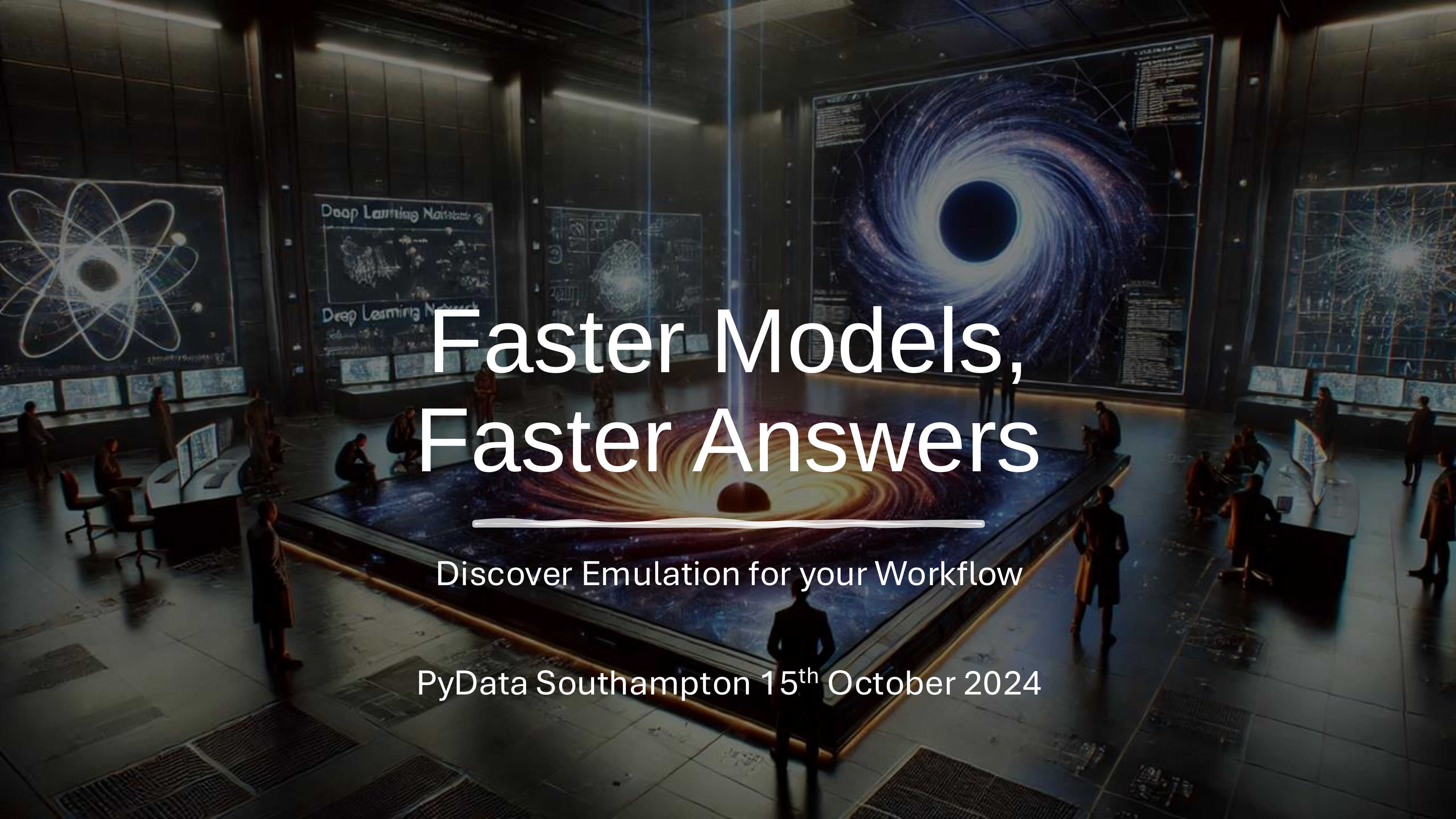
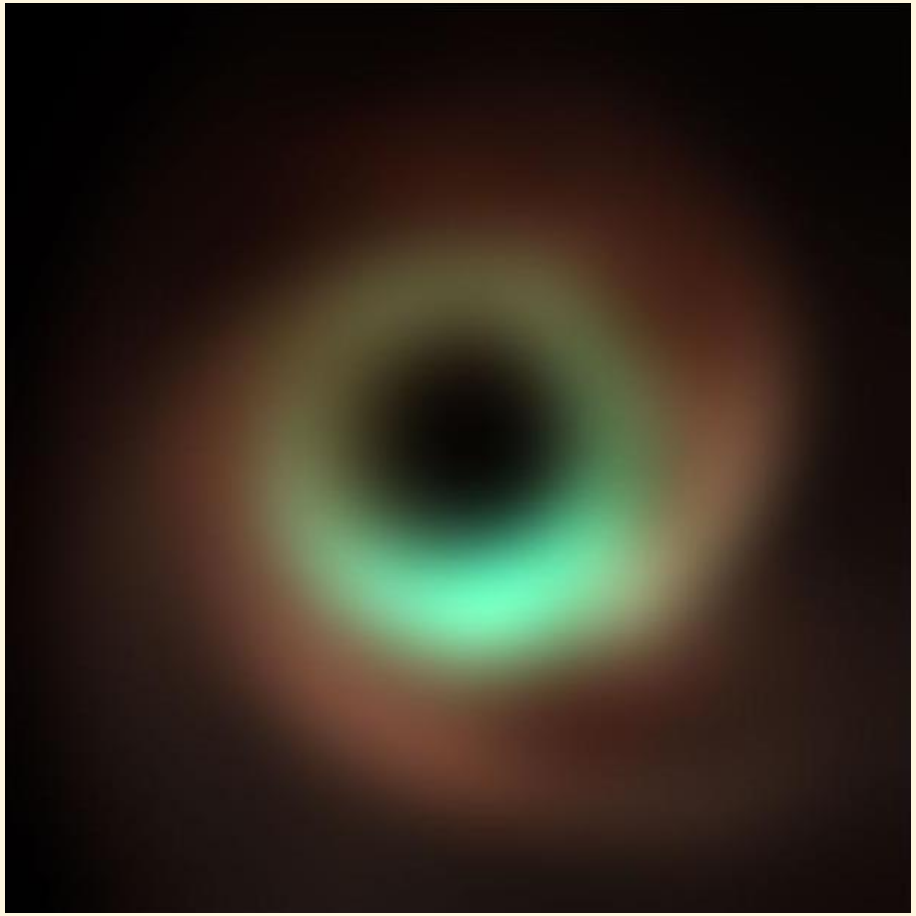


Faster Models, Faster Answers

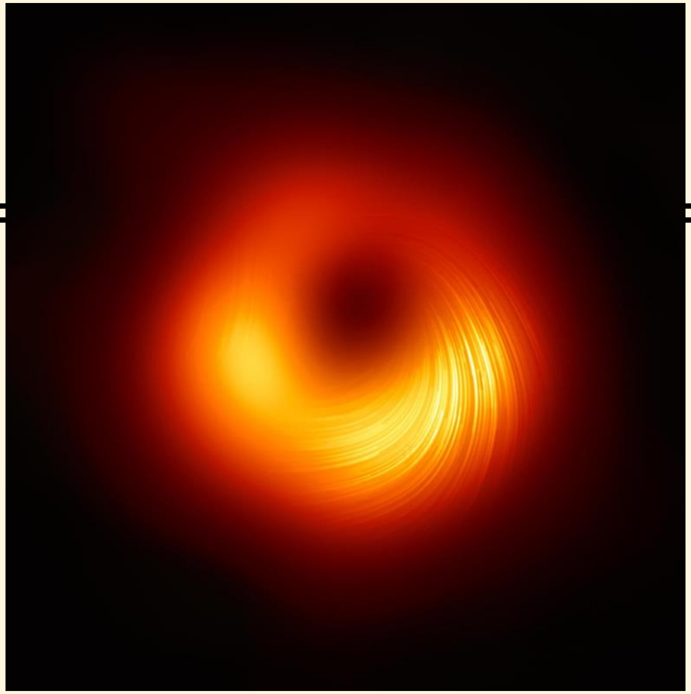
Discover Emulation for your Workflow

PyData Southampton 15th October 2024

Astronomy

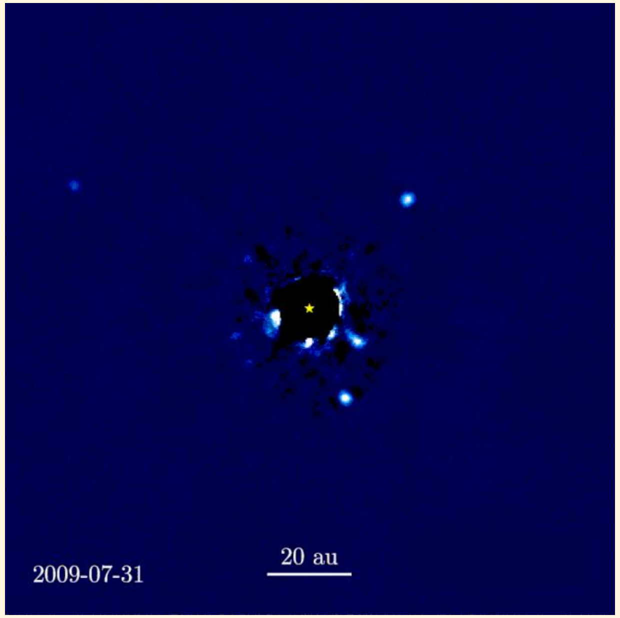


Colour Composite of Sagittarius A* and M87



Sagittarius A*

The Antennae Galaxies



Exoplanet – Artistic Impression

Accretion Wind Modelling

Blackhole

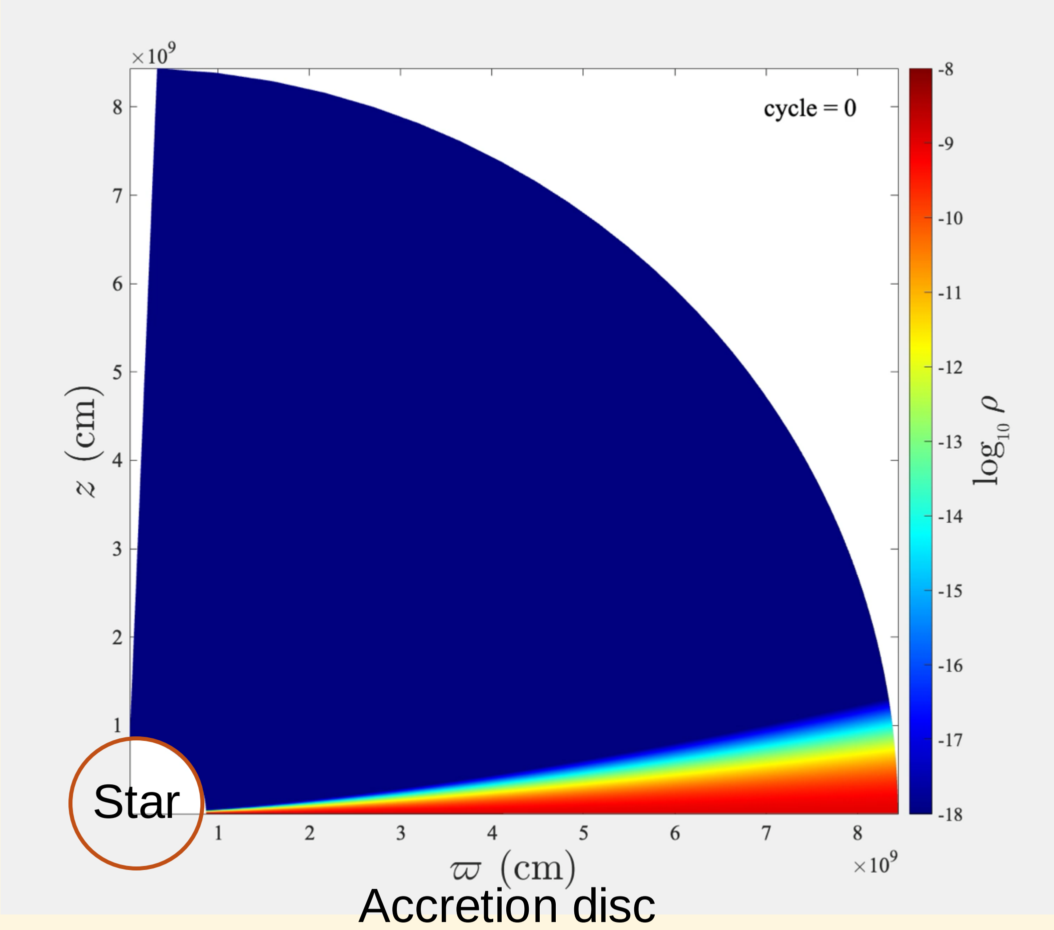
White Dwarf Star

Donor Star

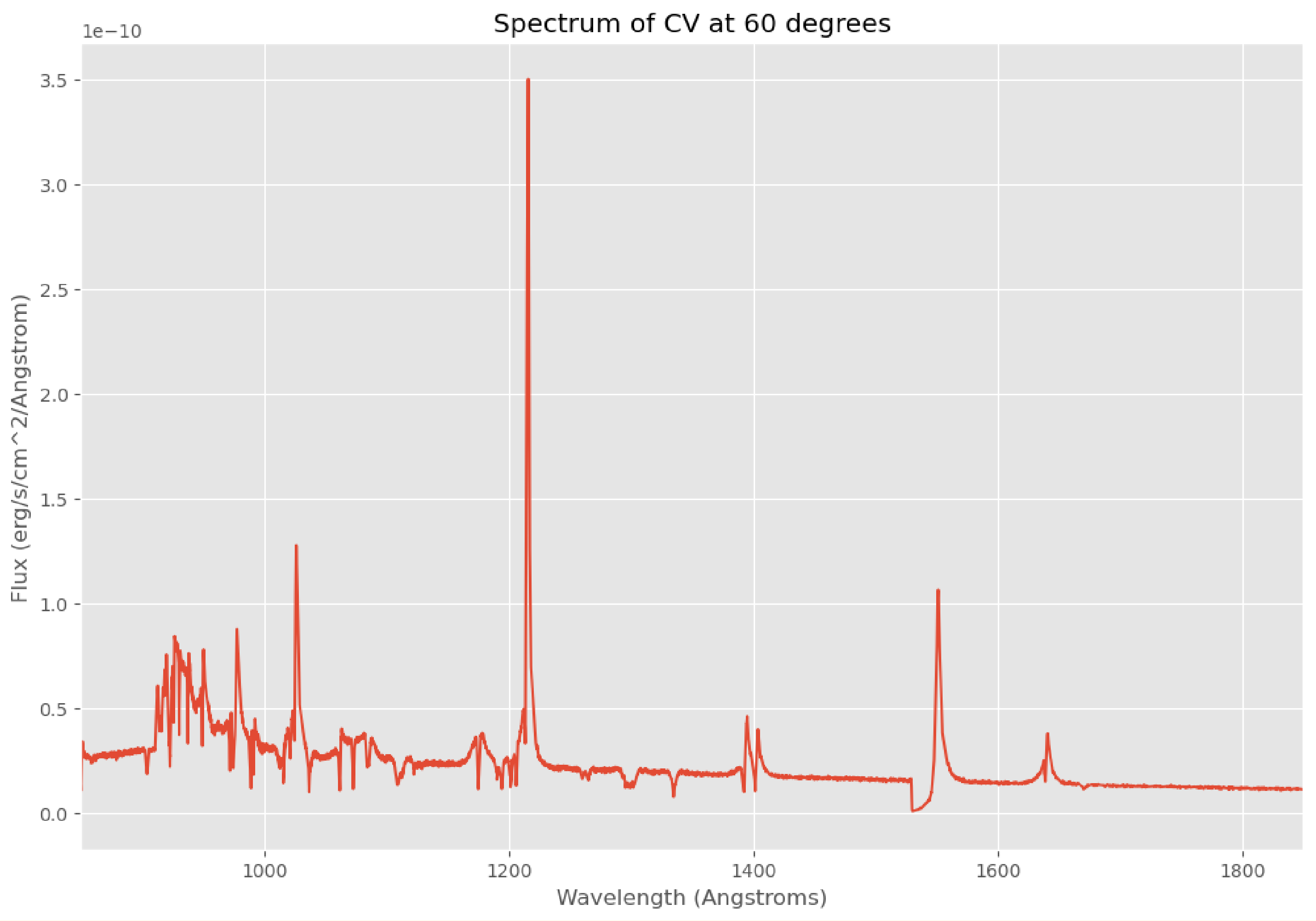
Accretion Discs

Scientific Modelling

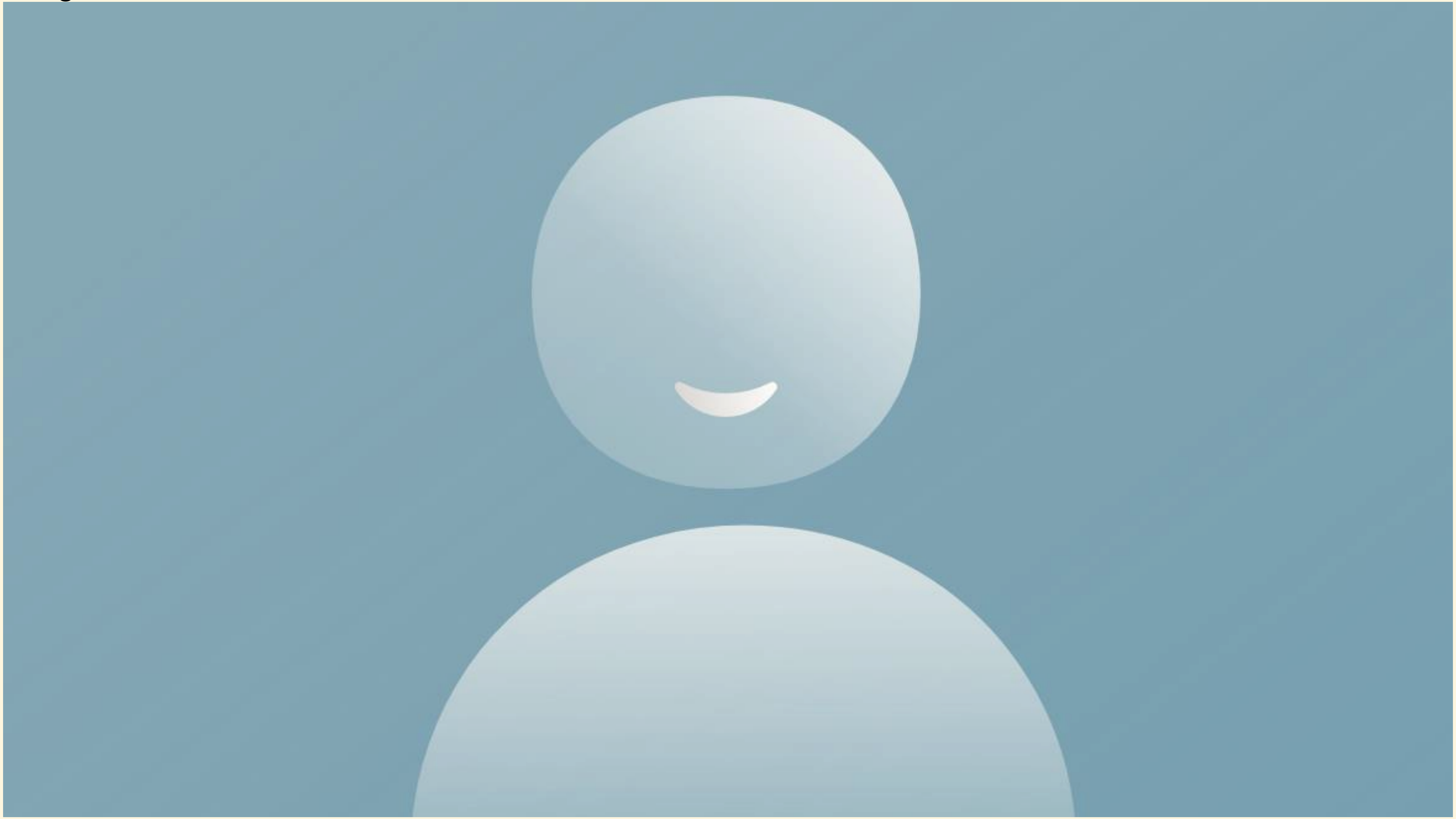
MHD 2D Wind Quadrant Slice



Monte-Carlo Simulations



Running a Simulation…



Faster Simulations w/ Emulation

Emulation /ˌem.jəˈleɪ.ʃən/ *(n)*

> *A machine learning method designed to approximate the behaviour of a more complex and expensive system.*

Key Benefits:

- Much faster computation times
- Simulations can be used for real-time applications
- Can perform inference with high-dimensional simulations

The Simplest Emulator

A linear interpolator … Emulators in their simplest forms can be reduced to basic interpolators

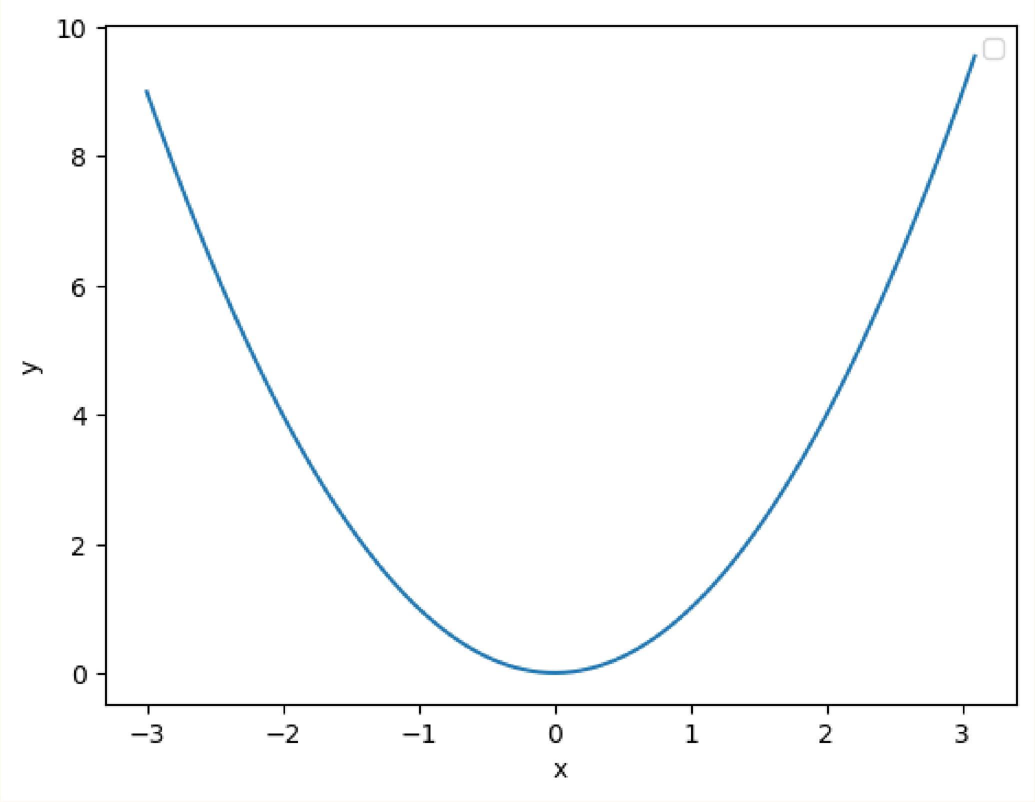
Input parameter

Physics Simulator

Output

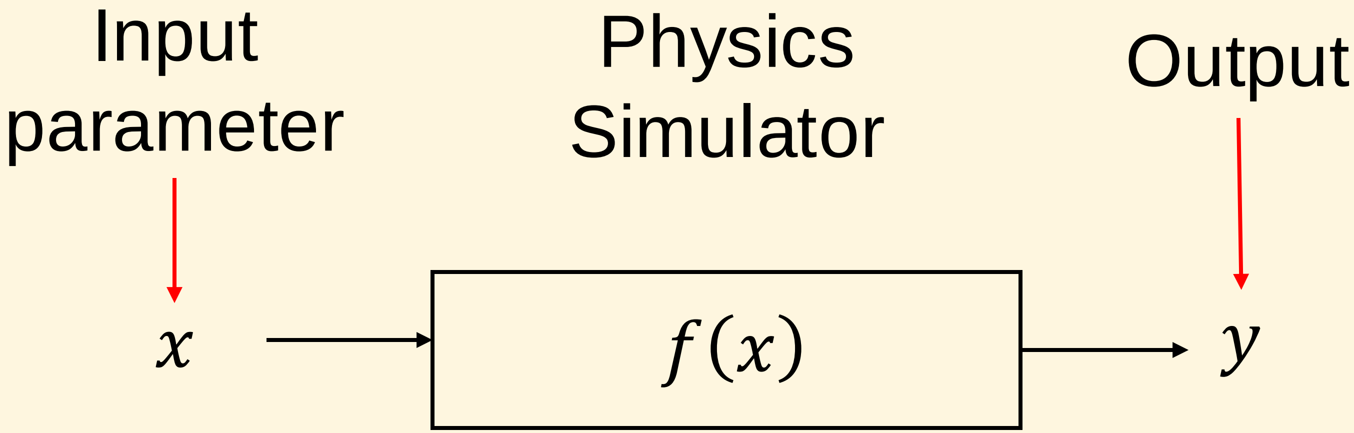
$$x \longrightarrow \boxed{f(x) = x^2} \longrightarrow y$$

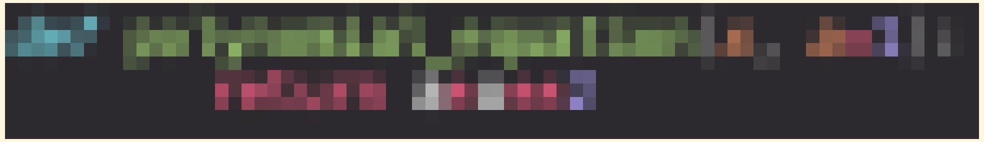
```
def quadratic_equation(x, a=1):
    return a*x**2
```

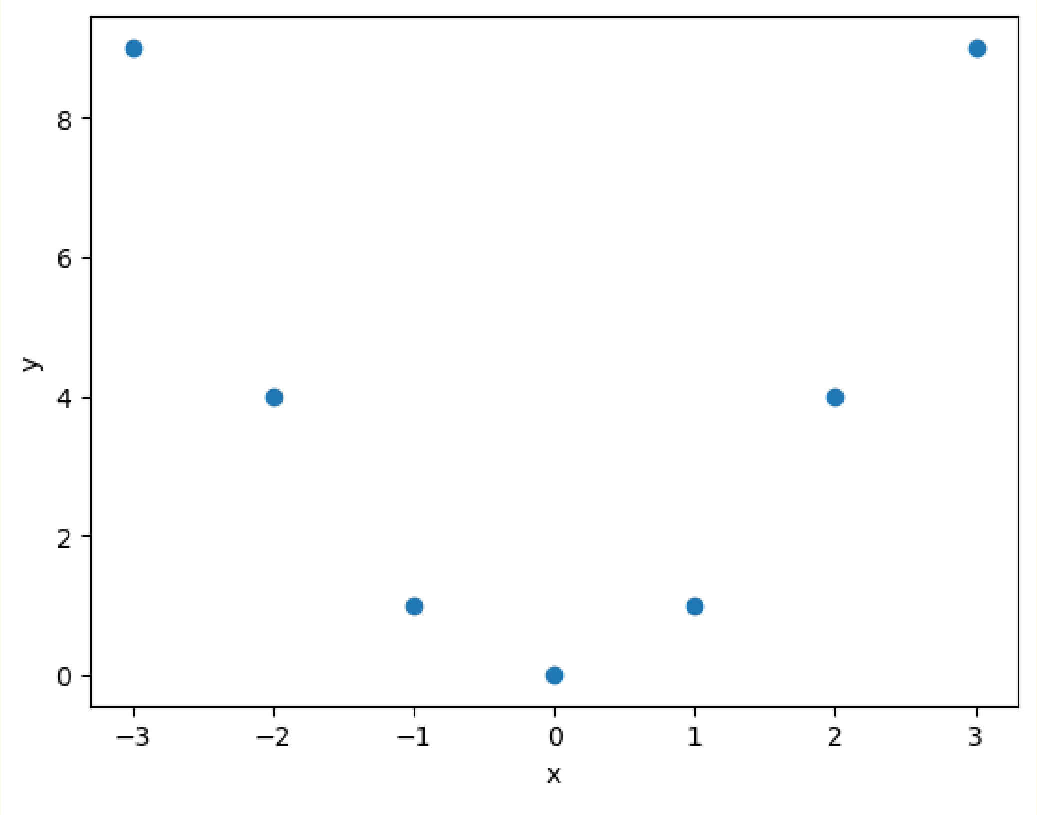


The Simplest Emulator

A linear interpolator … Emulators in their simplest forms can be reduced to basic interpolators







The Simplest Astro Emulator

A linear interpolator … Emulators in their simplest forms can be reduced to basic interpolators

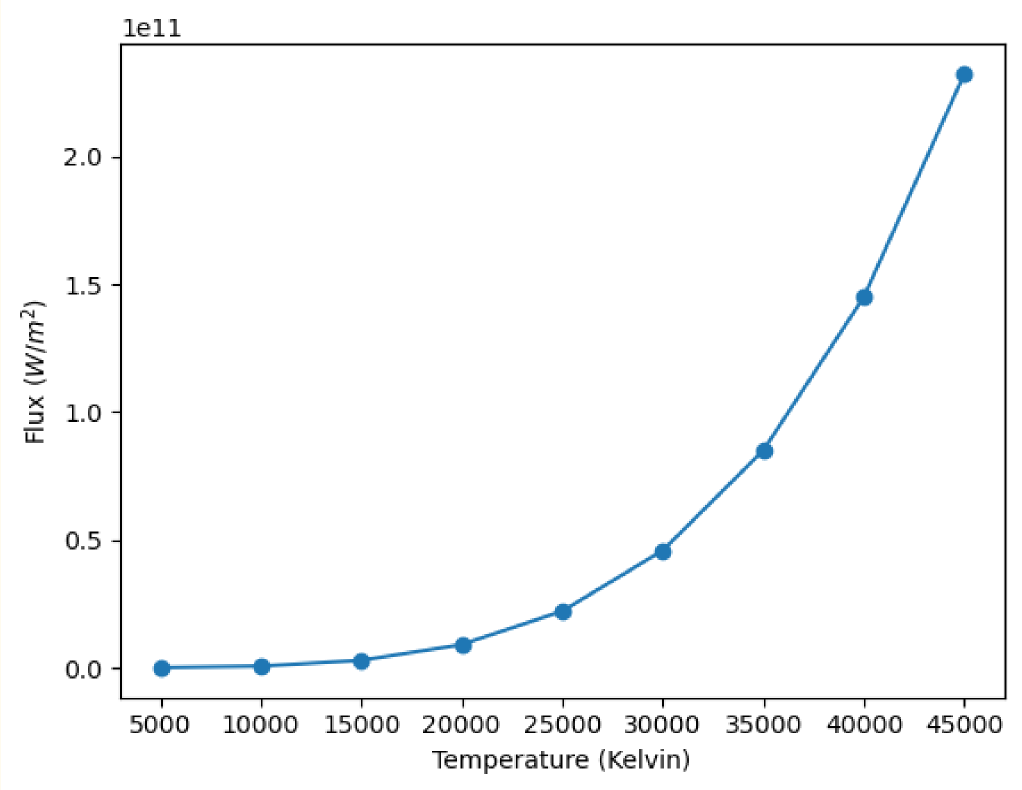
Input parameter

Physics Simulator

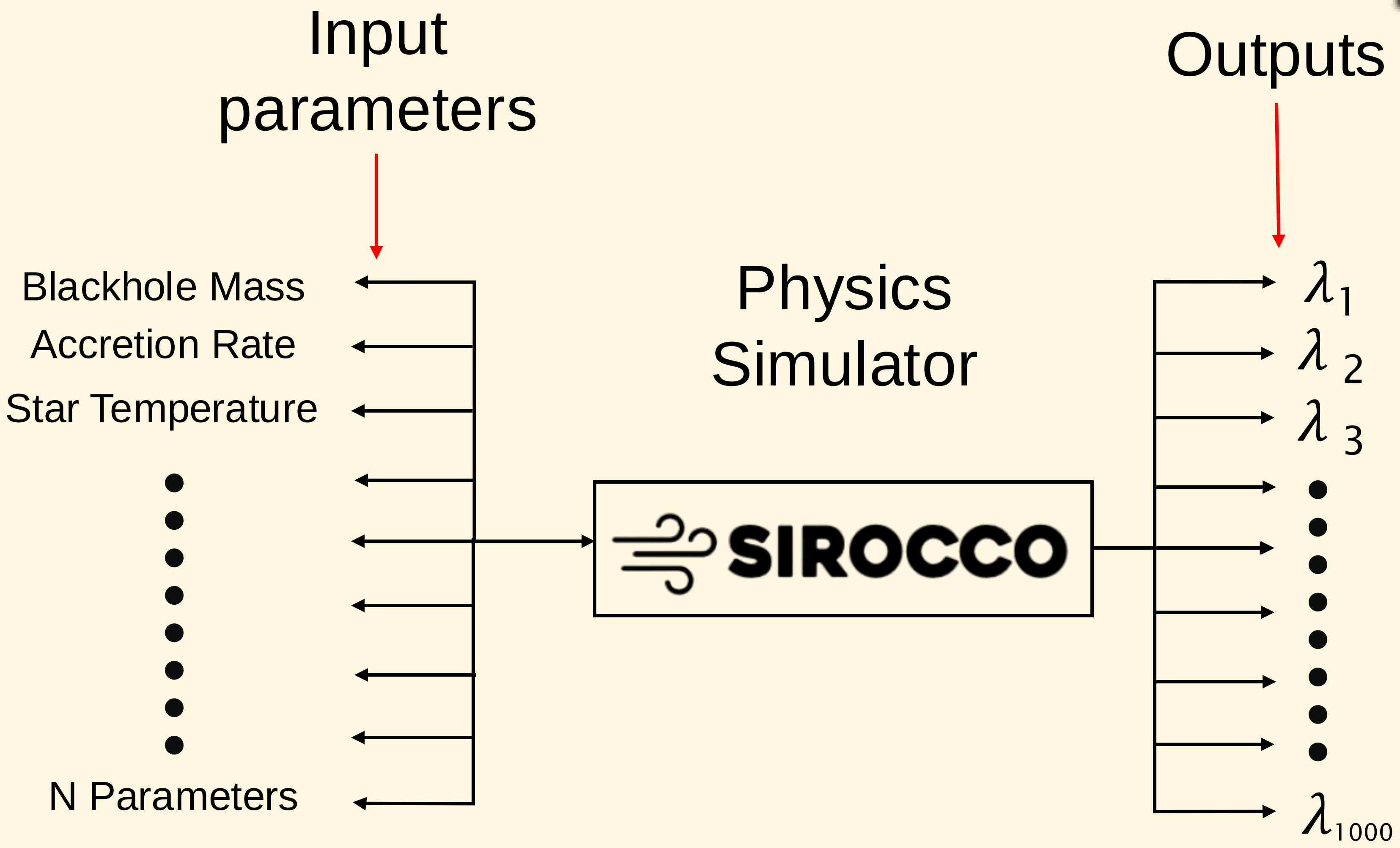
Output

$$x \longrightarrow \boxed{Flux = \sigma_{SB} T^4} \longrightarrow y$$

```
def star_flux(temperature_K):
sb_constant = 5.67e-8 # W/m^2/K^4
return sb_constant * temperature_K**4
```



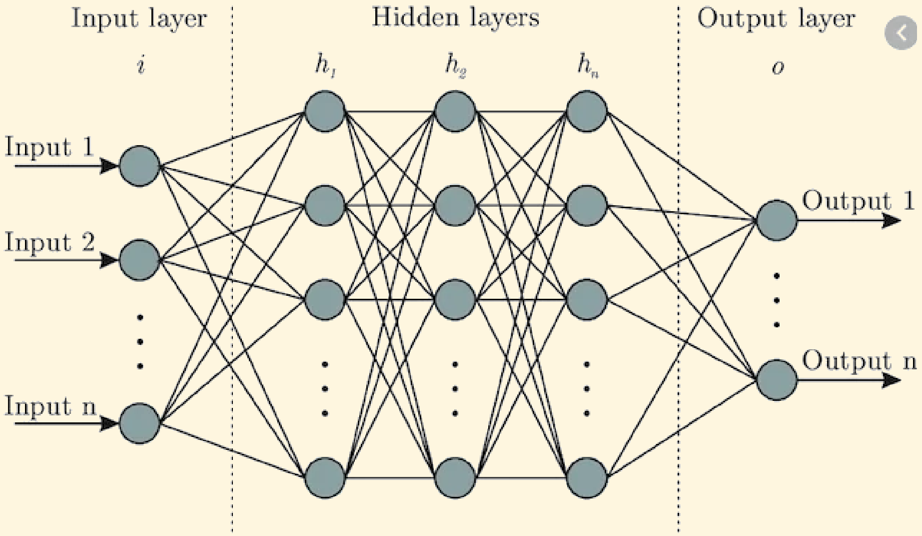
A Complex Astro Emulator



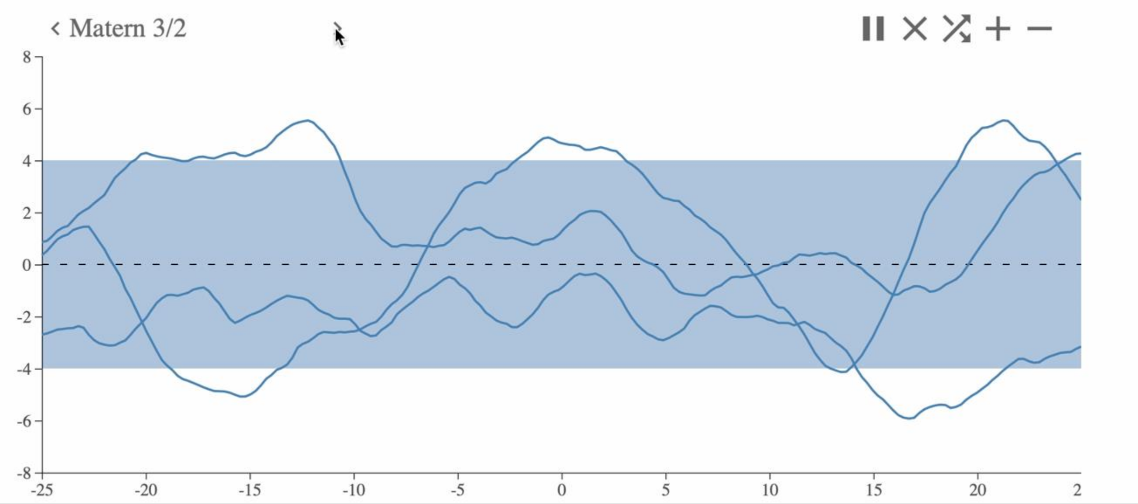
Two Main Emulator Types

Emulators are commonly fancy interpolators using machine learning methods…

Neural Networks



Gaussian Processes



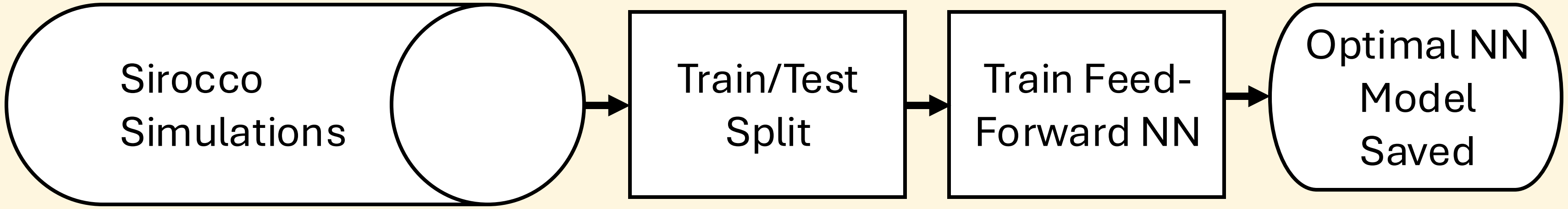
Great for:

- Fast-Real Time Use
- Less expensive Simulations

- Uncertainty Quantification
- Limited training Data

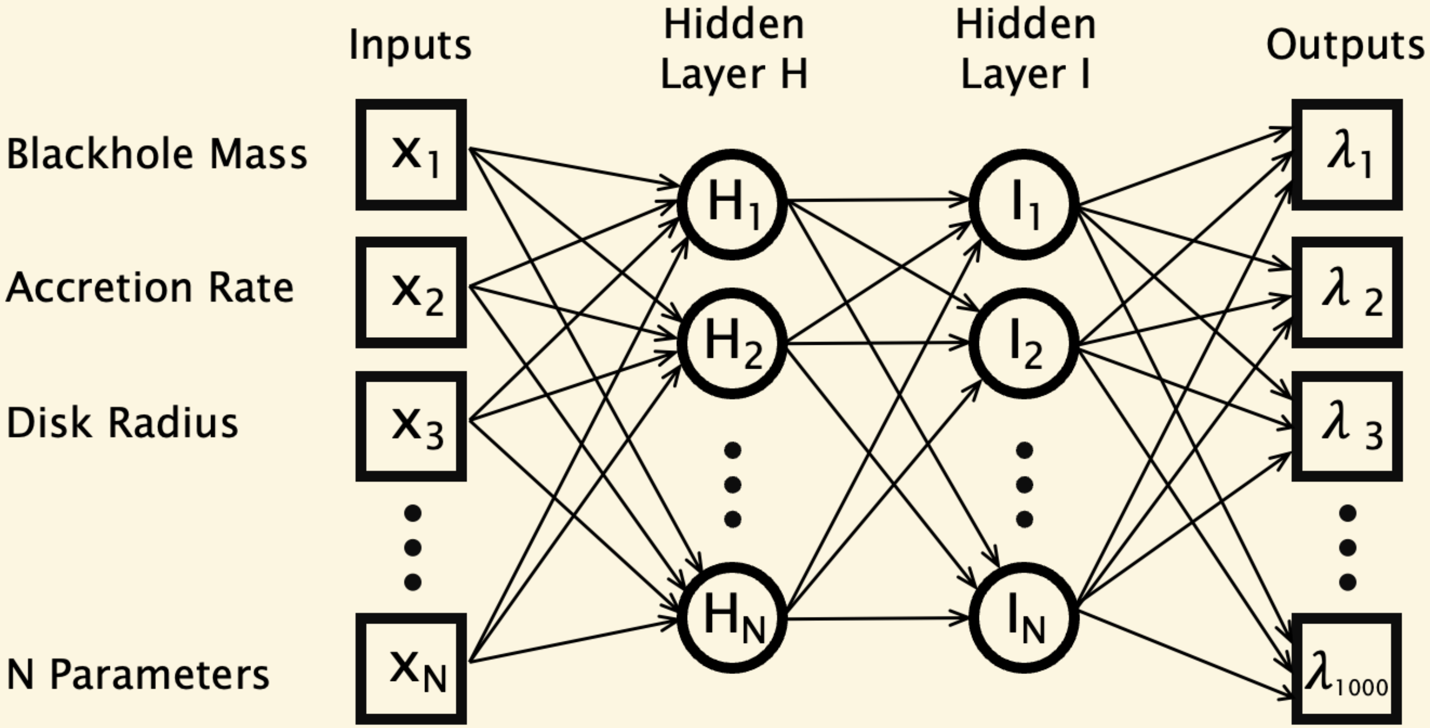
Neural Network Emulators

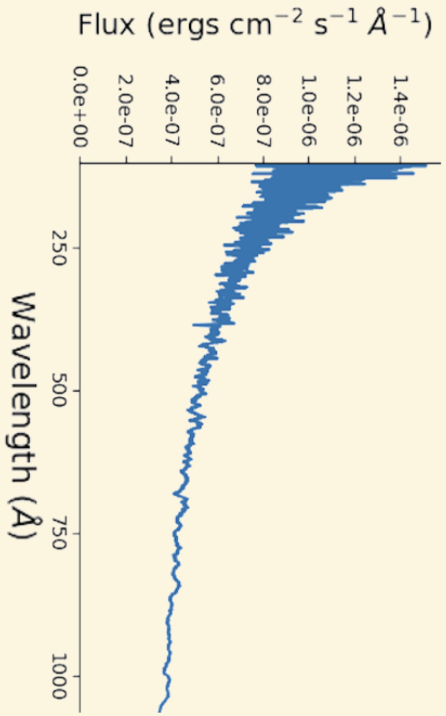
Simple Training Emulator Workflow:



However,

we can do better…





NN Hyperparameter Selection

Optuna is a hyperparameter optimisation framework,
Let's you vary parameters such as:

- The activation functions *(Relu, LeakyRelu etc)*
- The number of network layers *(Deep networks)*
- The number of neurons per layer *(Wide networks)*
- The optimiser *(Adam, AdamW etc)*
- The weight decay *(Regularisation)*
- Batching size

Parameter Selection

Sirocco contains upwards of 30 physical parameters, 3 values for each means a regular grid size of 2×10^{14} combinations!

Improvements:

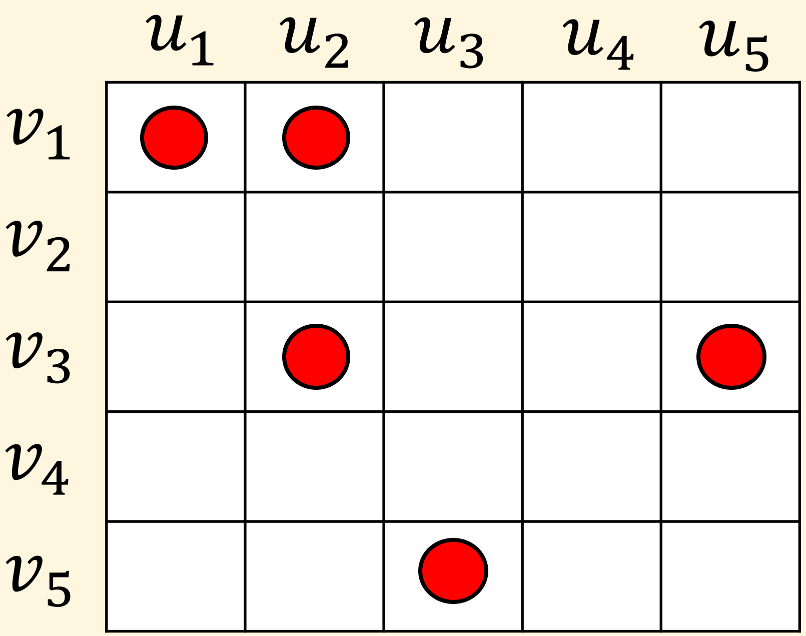
- ***Intuition:*** Restrict to only known important physical parameters.

- Run smaller subsets of parameters and feature select through random forests/gradient boosting to identify weak parameters.

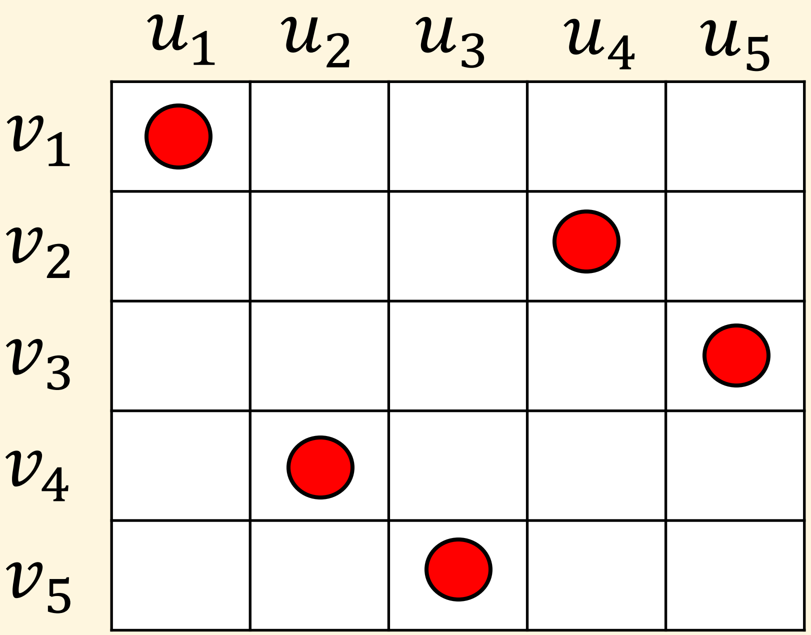
The Latin Hypercube

Sample the grid space to further reduce training simulations.

Random Sampling



Latin Hypercube Sampling



2D Example

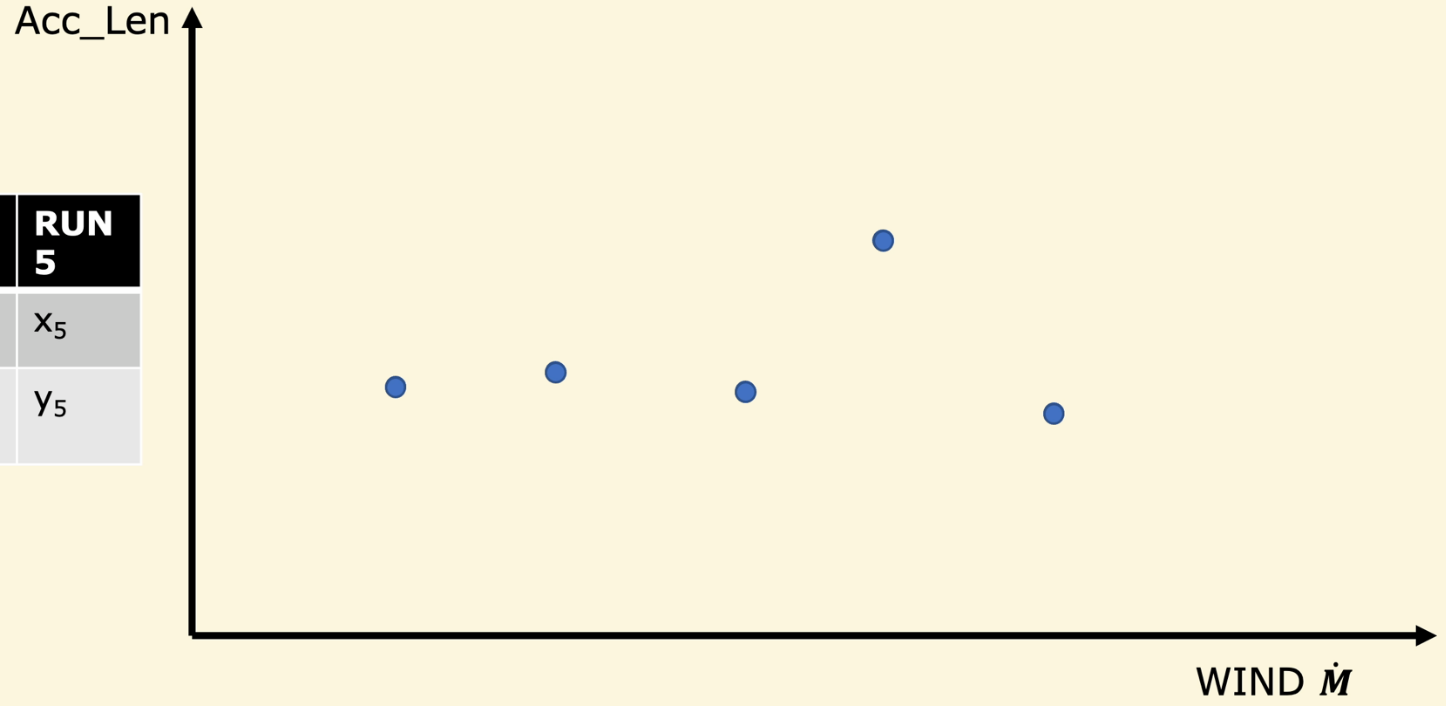
The Latent Space - PCA

You can reduce the number of dimensions
in both inputs and outputs

Create an emulator grid space from Principal Component Analysis with Scikit-learn decomposition methods.

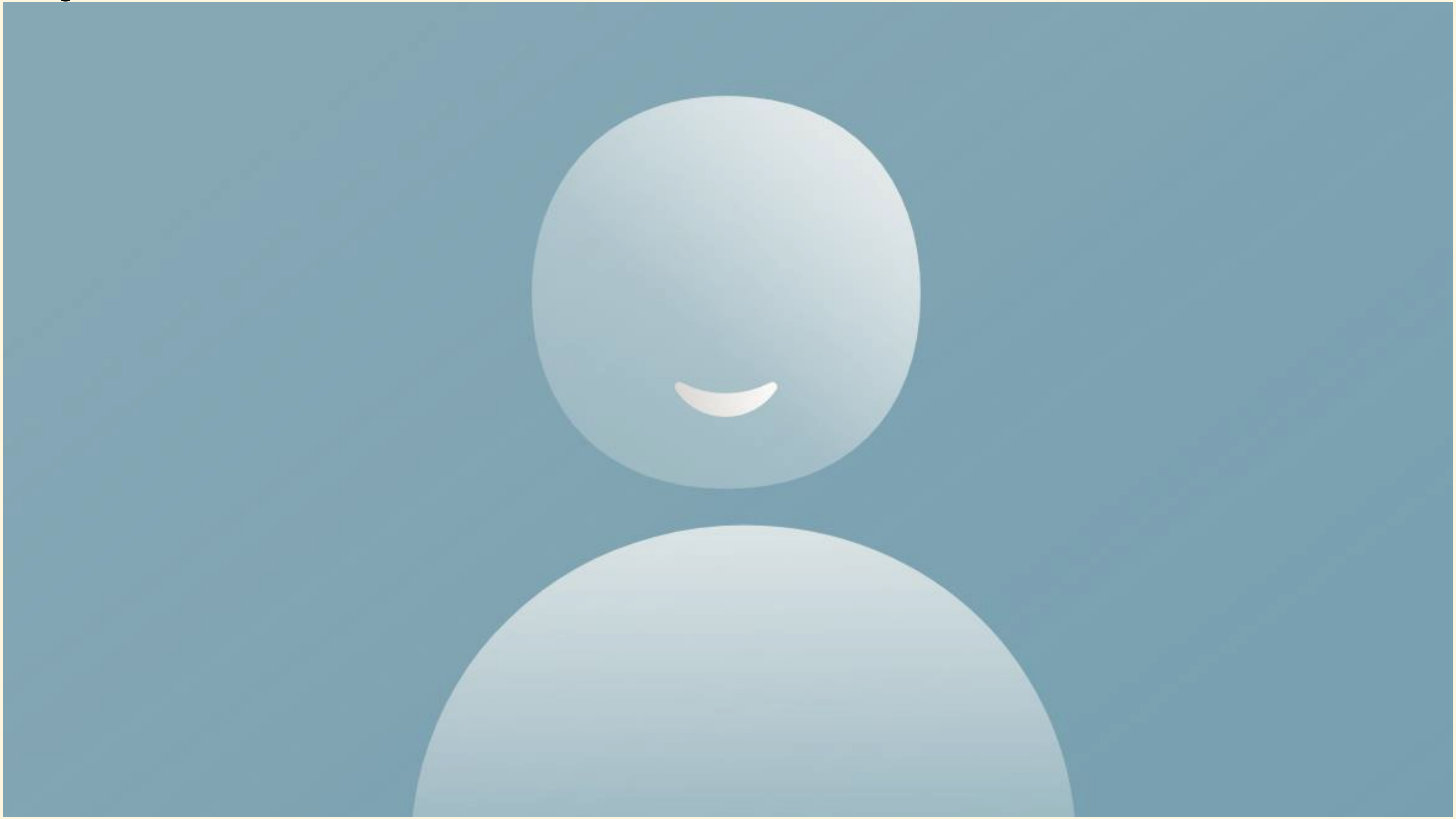
Two Variable Example

Sirocco	RUN 1	RUN 2	RUN 3	RUN 4	RUN 5
WIND $\dot{M}$	x_1	x_2	x_3	x_4	x_5
Acceleration Length	y_1	y_2	y_3	y_4	y_5



Illustrative; not to scale

Running a Emulation…



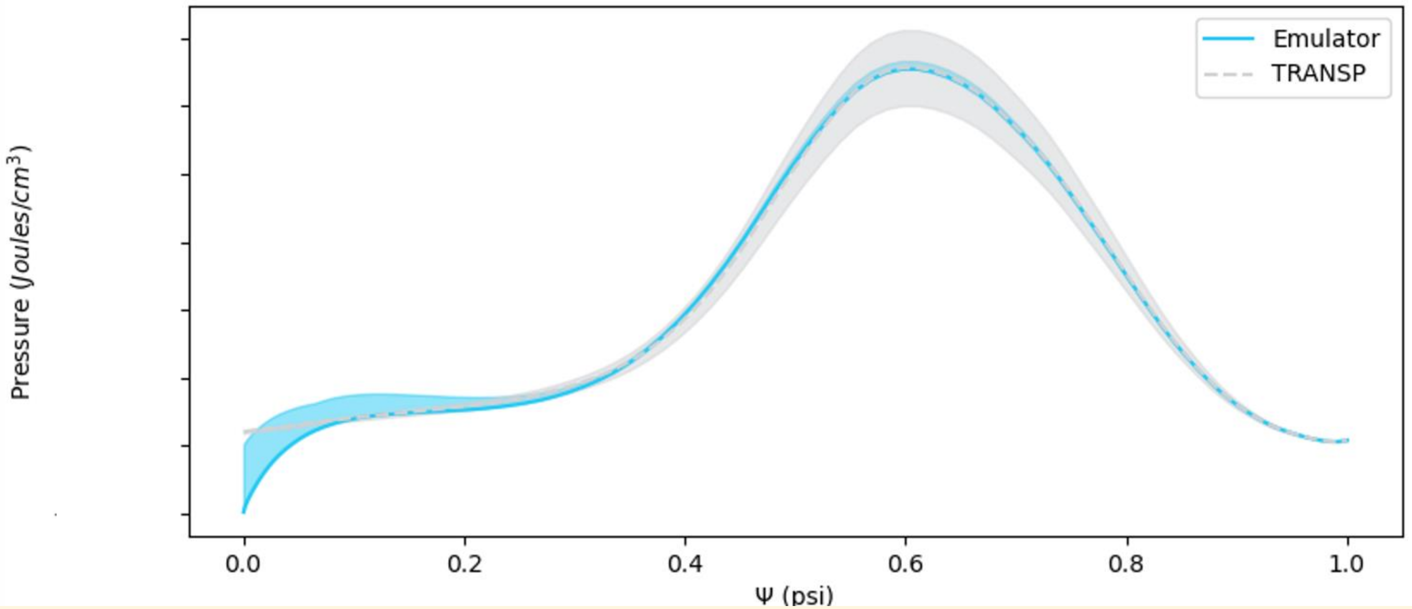
Case Study: Fusion Energy

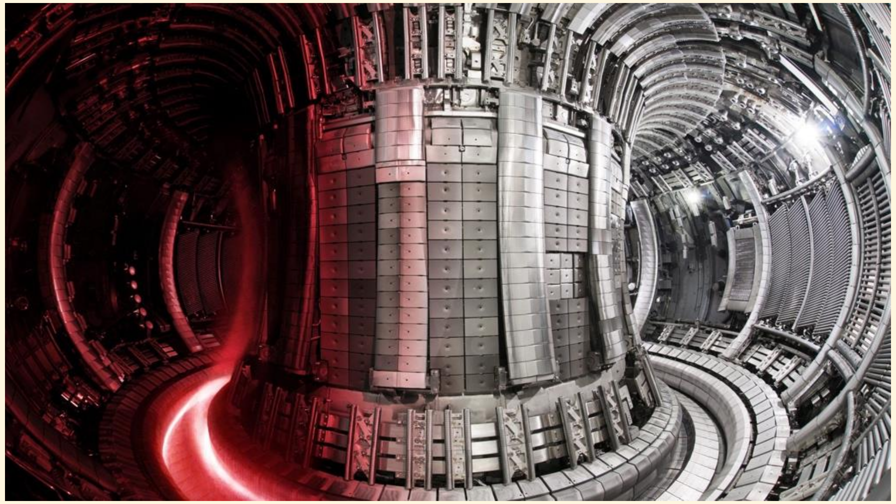
Google DeepMind

UK Atomic Energy Authority

Emulators are being adopted universally

Plasma pressure profiles:





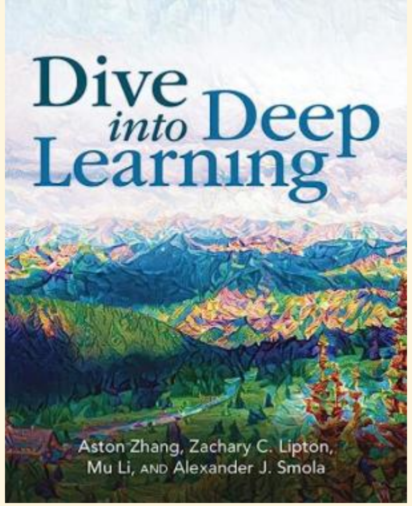
Open-Source Example:

TORAX *(Google Deepmind)*

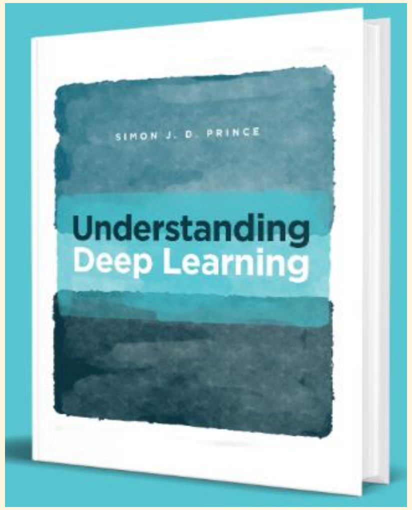
Deep Learning Books

*Both **FREE** books with supplementary material…*

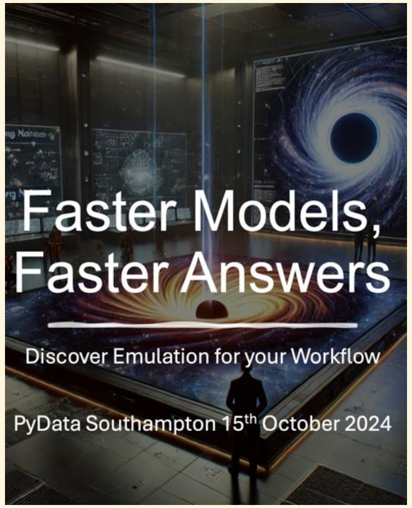
Dive into Deep Learning *(1089 pages)*



Understanding Deep Learning *(527 pages)*



Presentation Resources



A human (me)

You’ve gone too far … how did you get here!

Title:

Faster Models, Faster Answers: Discover Emulation for Your Workflow

Abstract:

AI this and AI that, the world in the past couple of years has become overrun with news of Generative AI and the ever-improving odds of a takeover from our new robot overlord, ChatGPT. However, have you ever heard about Generative Modelling? This research field is no longer just about creating pretty pictures and making funky tunes about your favourite branded baked beans. No, step with me into the world of Emulation! We'll probe how simple generative deep-learning models can improve complex physics simulations to not only be rapid but quick as a flash. So, fasten your seat belts as I take you on an ultra-fast whistle-stop tour exploring the universe of surrogate modelling, neural networks and the latent space. As I showcase the raw power of emulators, we'll uncover how faster models unlock new answers (and questions) in both Astrophysics and fusion energy. Also, we'll examine introductory examples of how you can build your own emulator from scratch.

For an evening event, you don't want to miss, I look forward to seeing you there … and bring a fire extinguisher; my GPU will be on fire 🔥!

Topic keywords: Machine/Deep learning, Generative Modelling, Emulation, Neural Networks, Gaussian Processes, Astrophysics, Fusion Energy, Simulations, Data-processing, Inference (☞⌐■͜ʖ■)☞