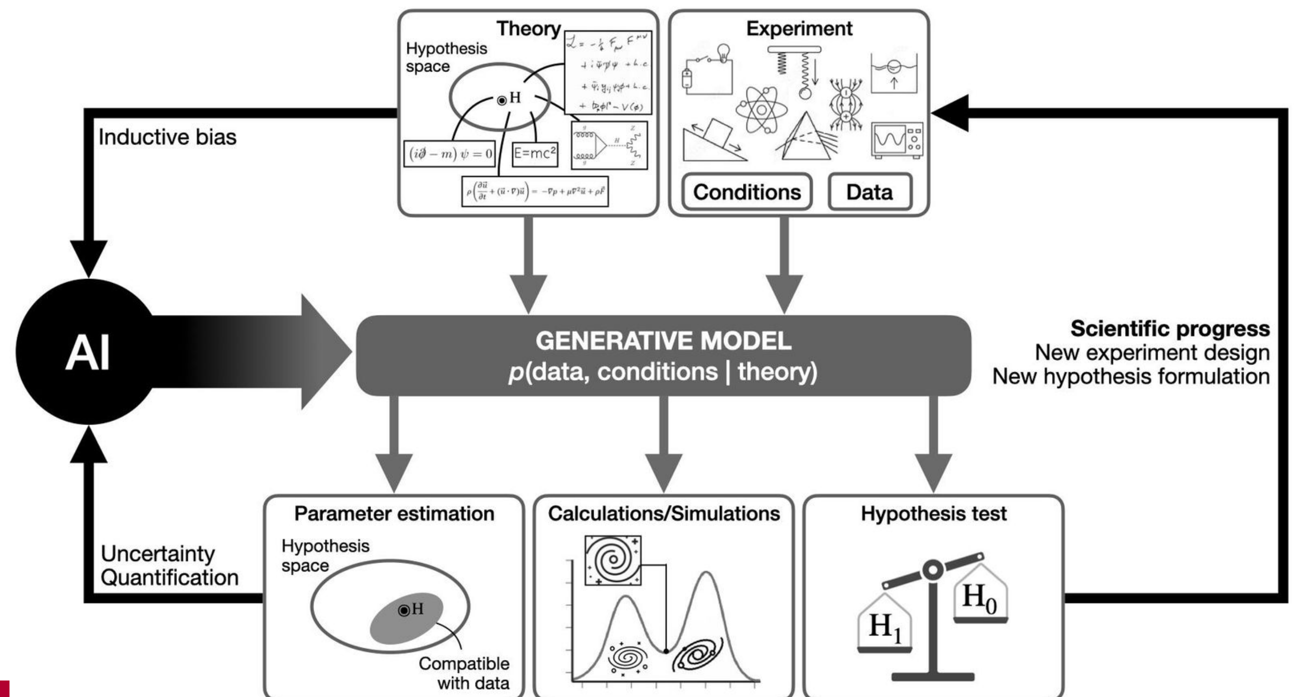
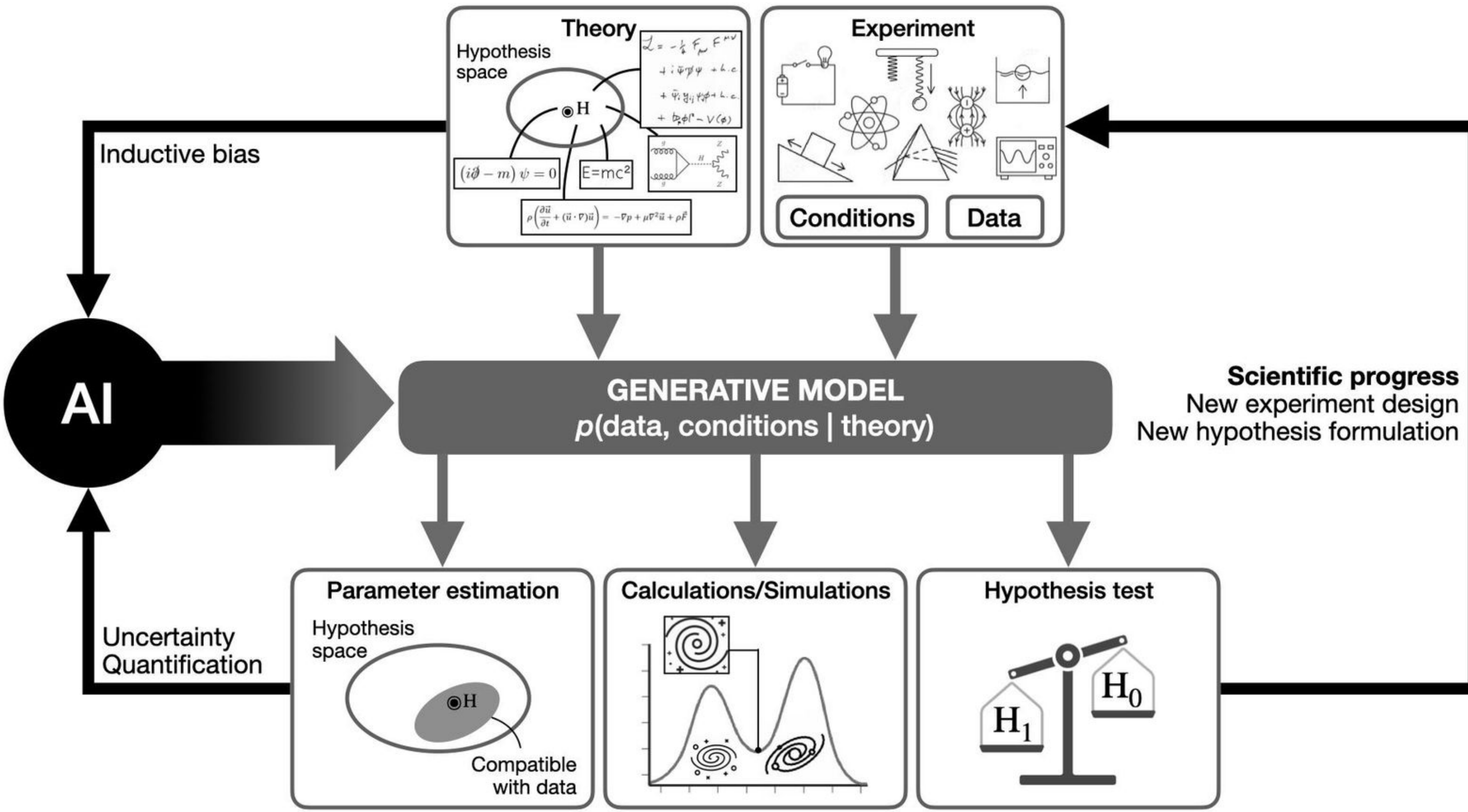
Gen AI and Physics

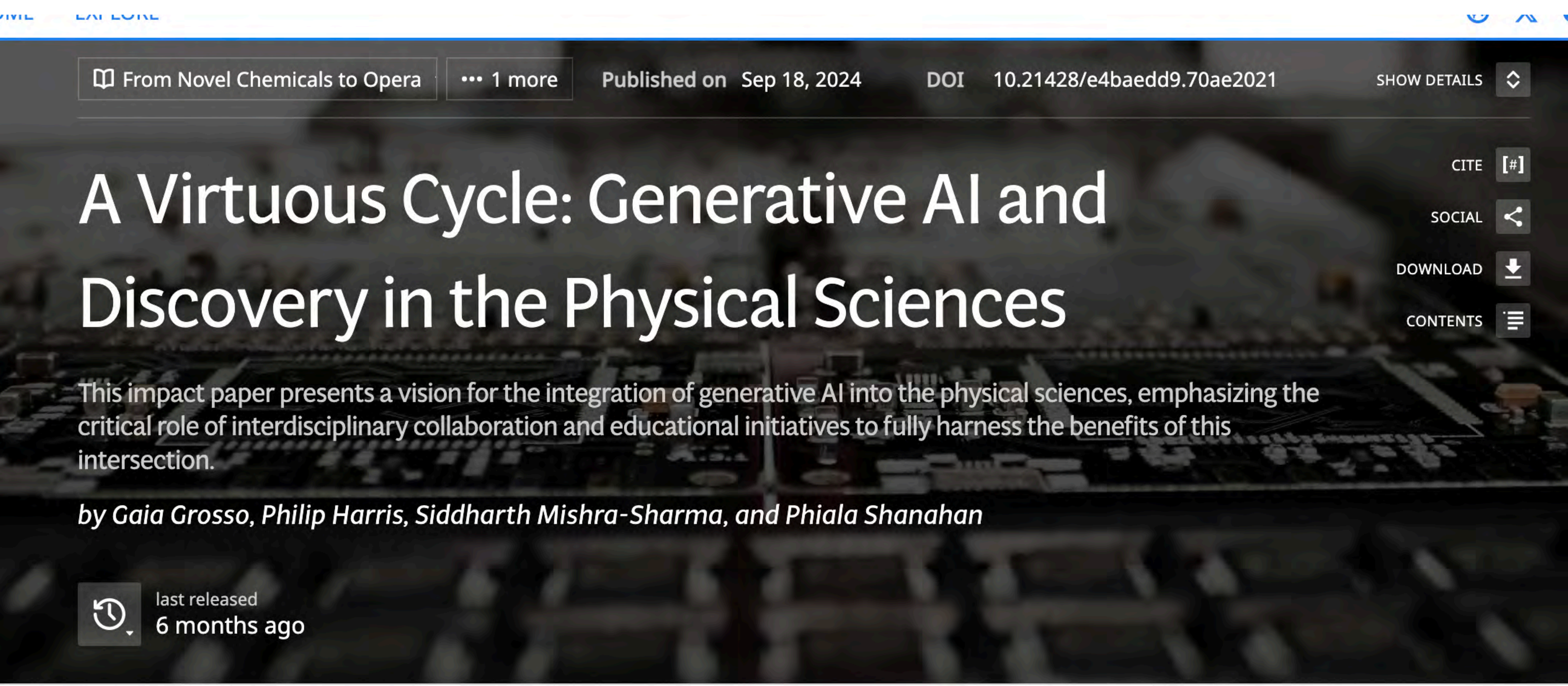


Phil Harris

MIT


Theory
Hypothesis space
H
$(i\partial\!\!\!/ - m)\psi = 0$
E=mc²
Experiment
Conditions
Data
Inductive bias
AI
GENERATIVE MODEL
p(data, conditions | theory)
Scientific progress
New experiment design
New hypothesis formulation
Uncertainty Quantification
Parameter estimation
Hypothesis space
H
Compatible with data
Calculations/Simulations
Hypothesis test
H1
H0

Generative Models Physics



This talk is a summary of this GenAI paper

https://mit-genai.pubpub.org/pub/ewp5ckmf/release/2

It is a summary of this workshop

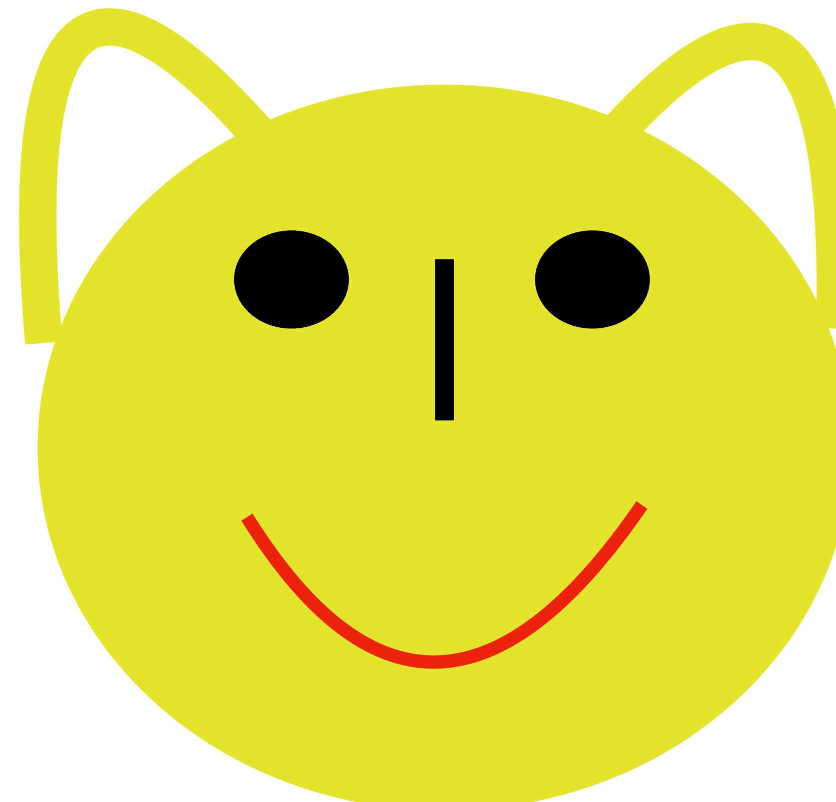
https://iaifi.org/generative-ai-workshop.html#speakers

What Is the Potential Impact of Generative AI in the Physical Sciences?

A simplified example built on some recent research of mine

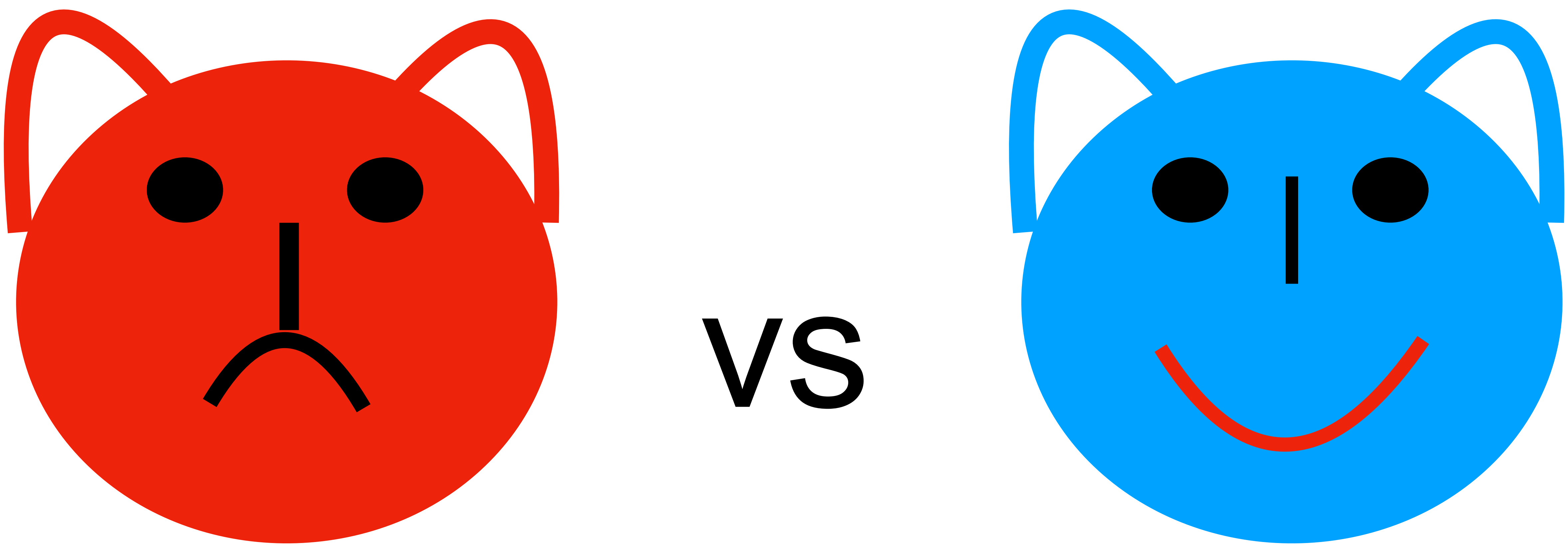
Lets illustrate a tagger

vs

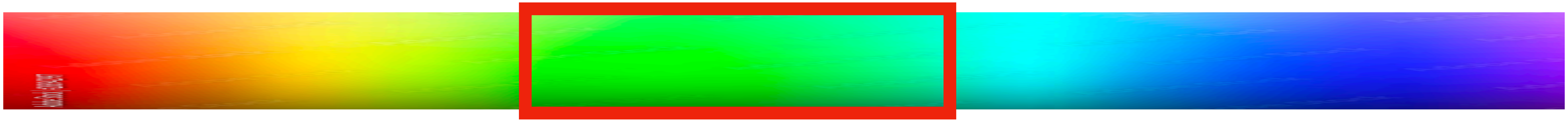


- We are going to discriminate a happy face form a sad

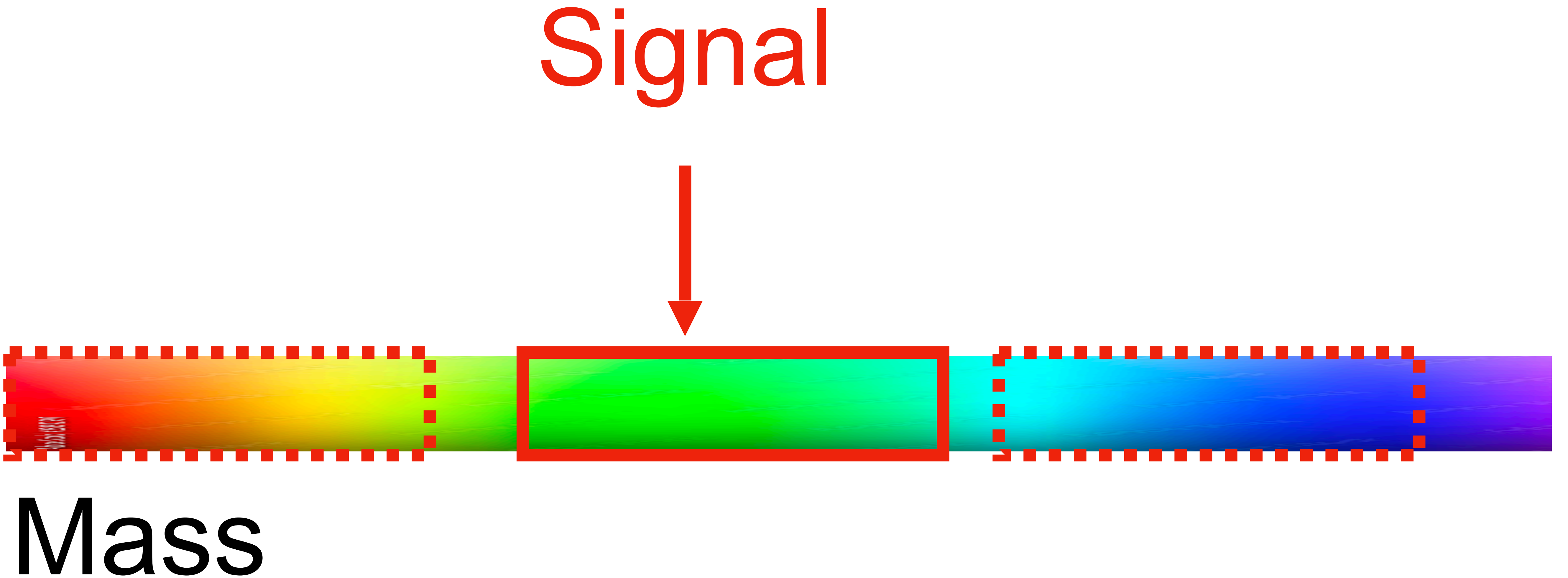
Lets illustrate a tagger



- We are going to discriminate a happy face form a sad
- They will vary in color, signal will be in center of spectrum



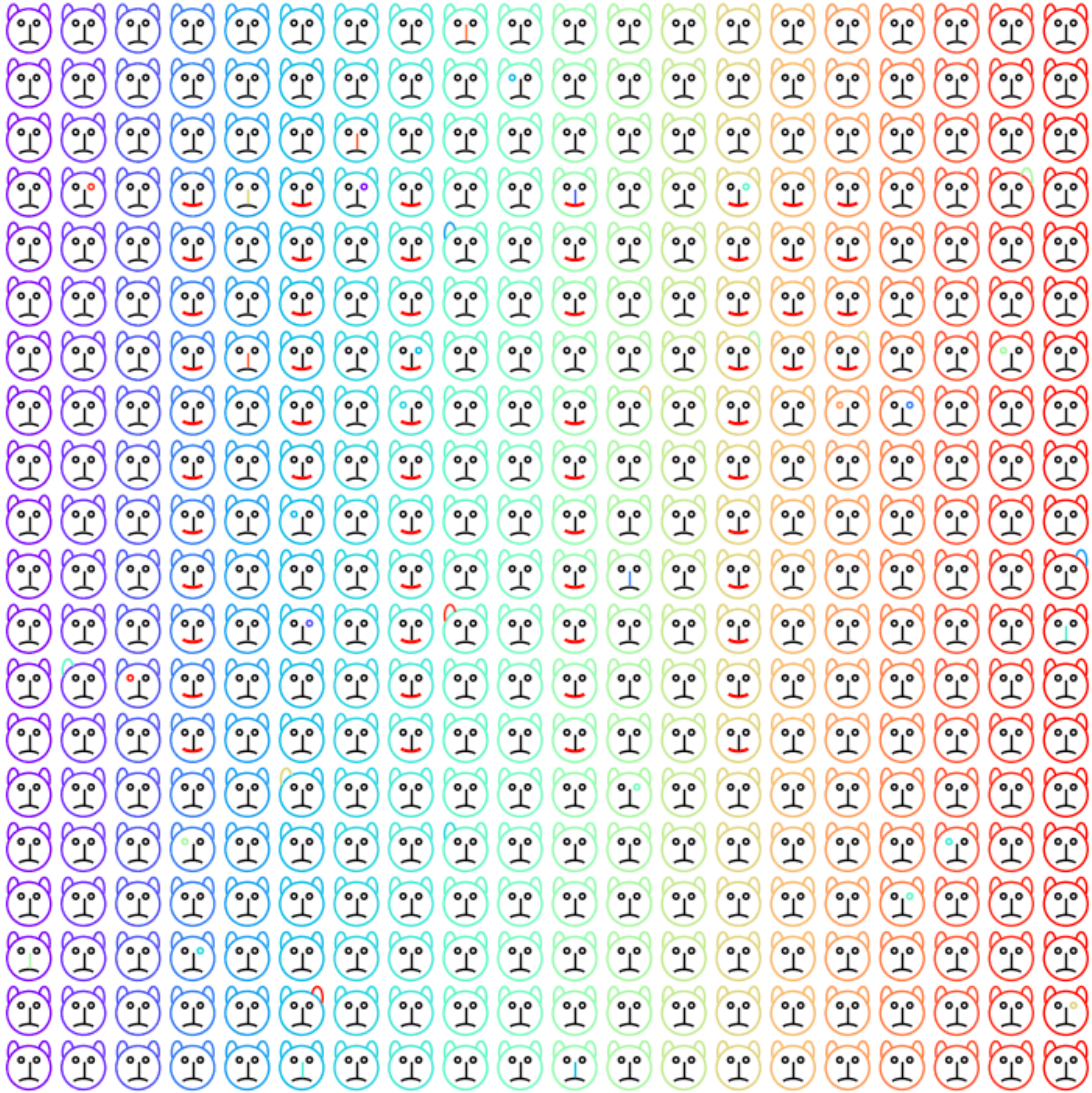
Signal

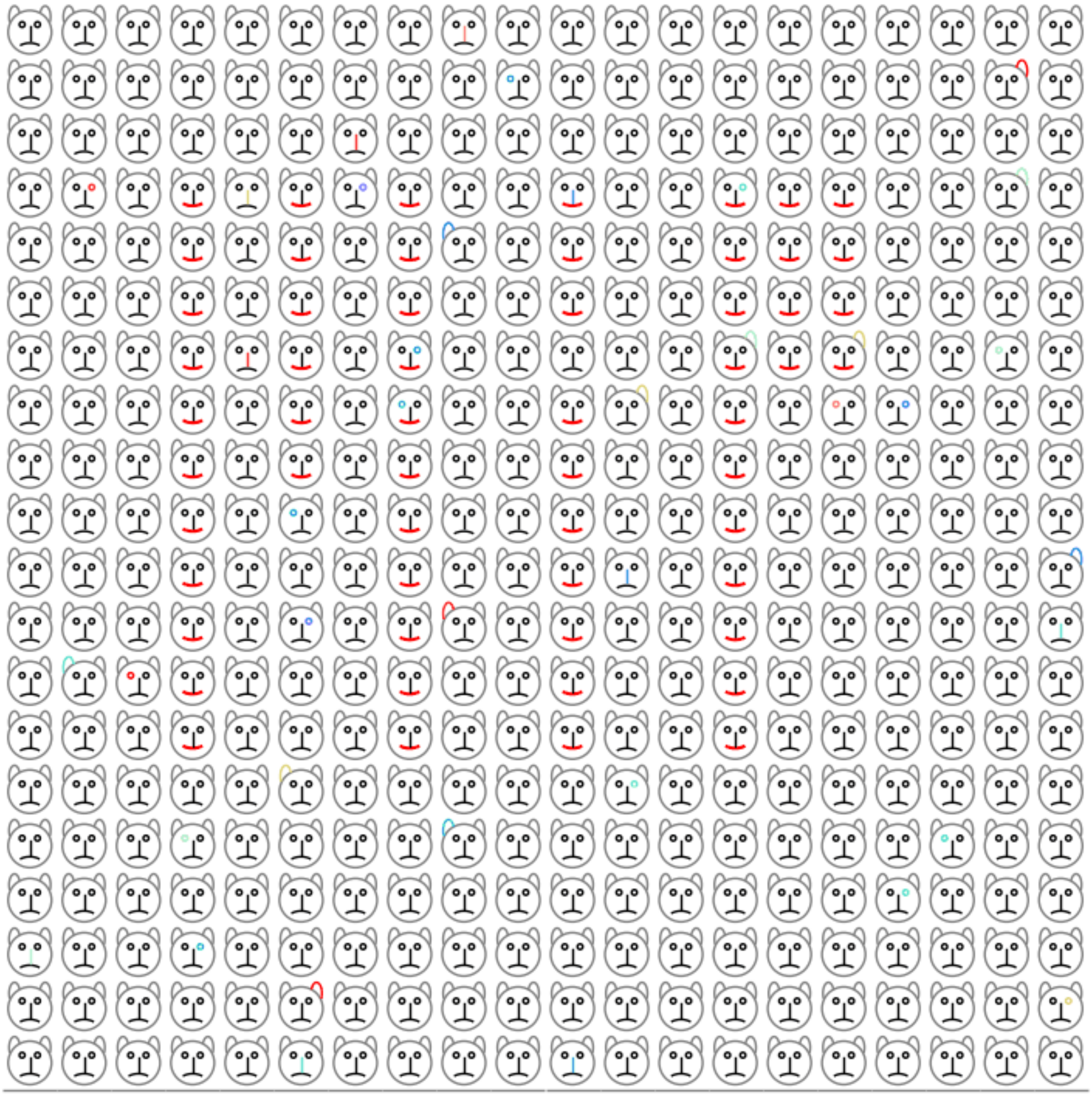


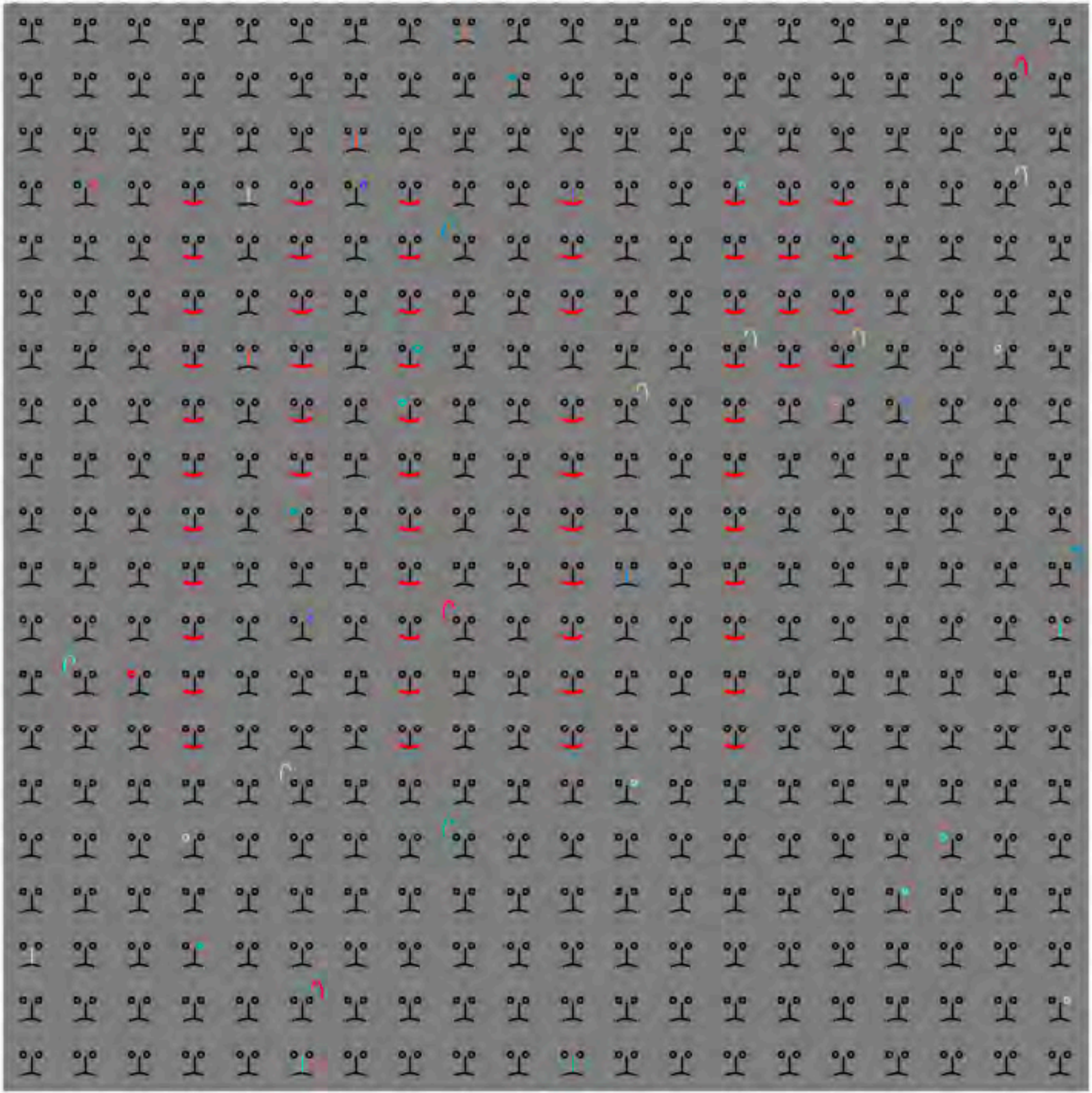
We don’t know where it will be

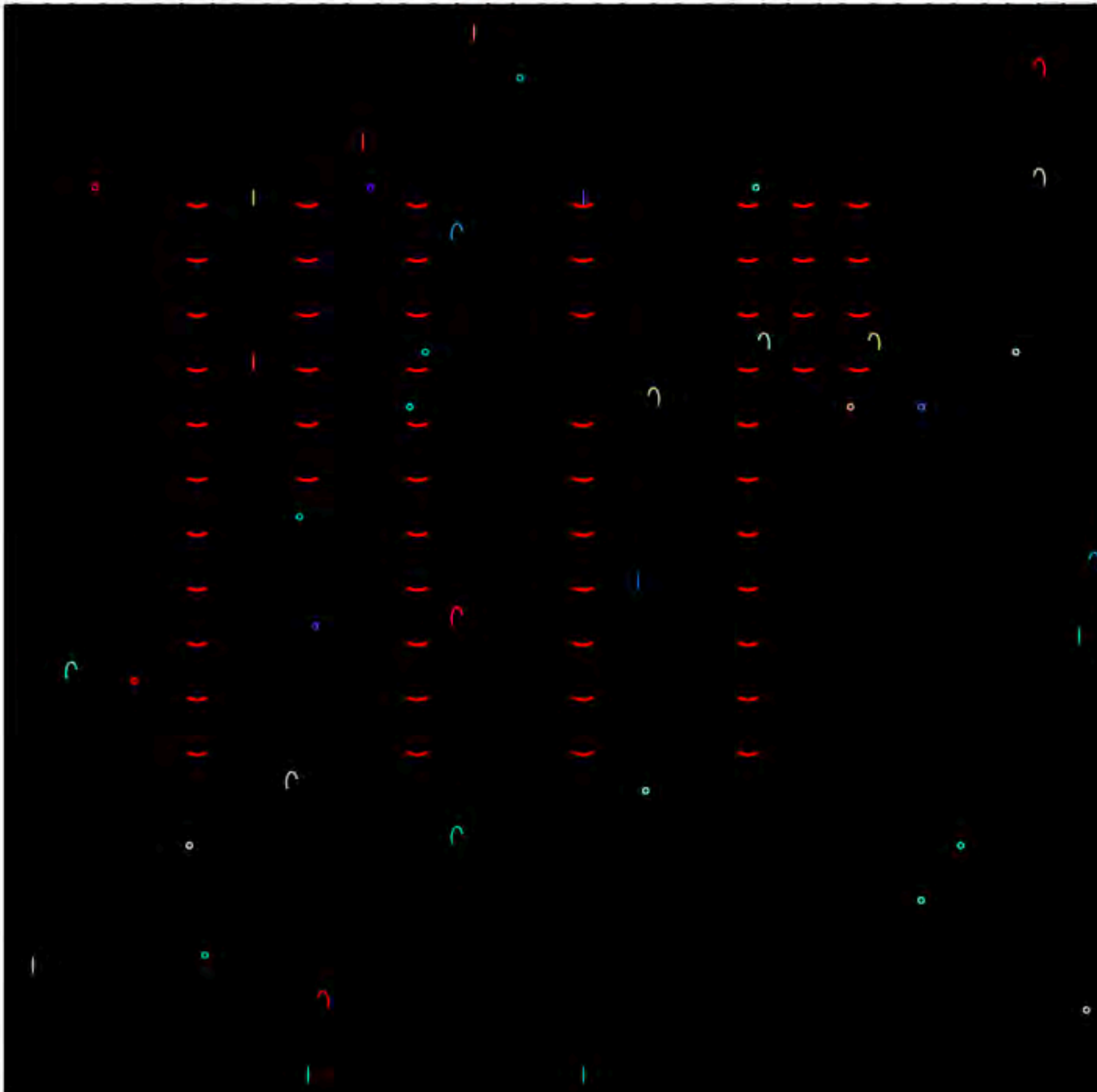
Color blinding is the key

Telling an NN to be blind is hard

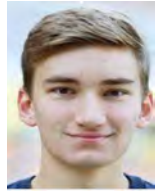




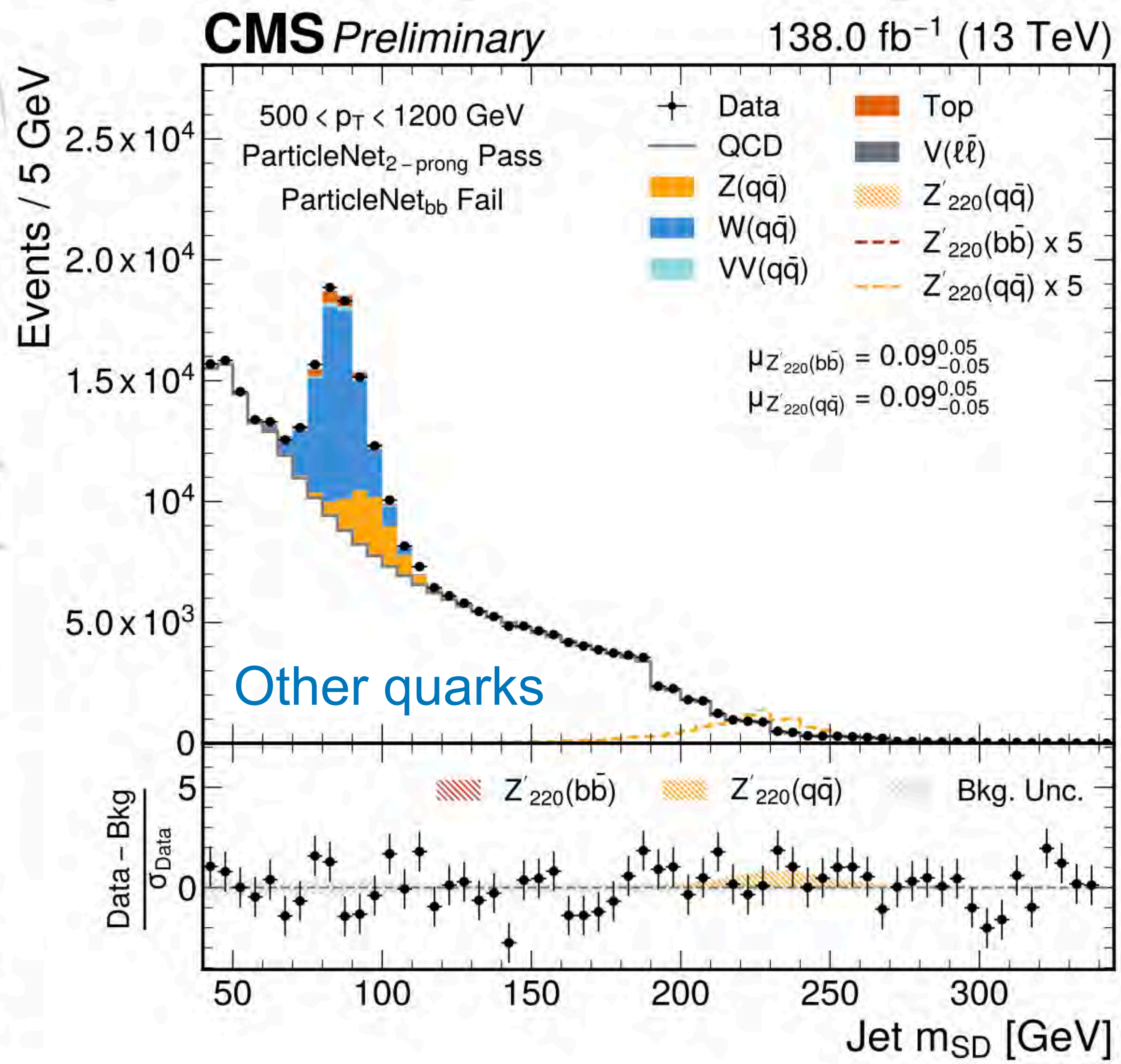


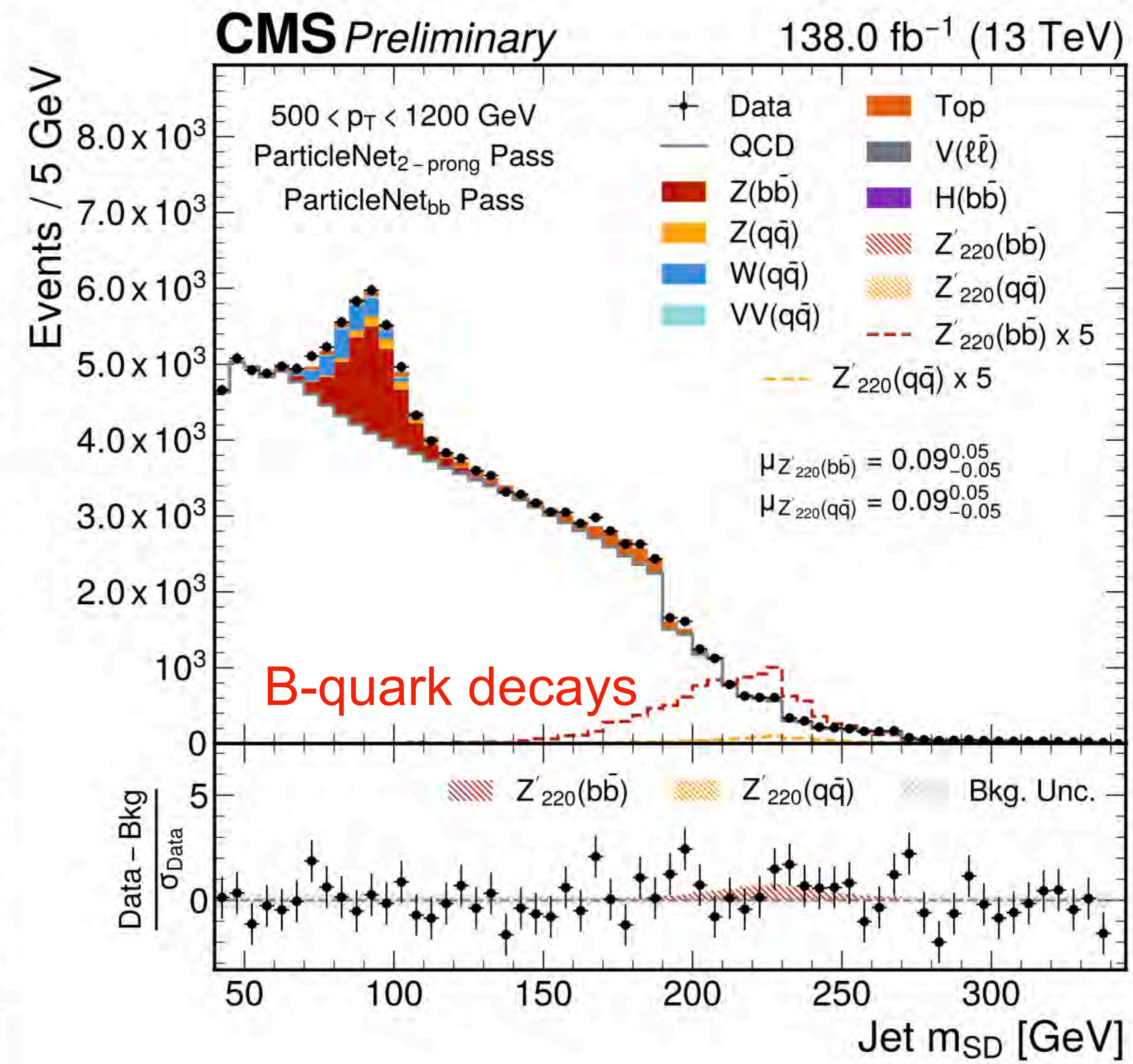


CMS-EXO-24-007



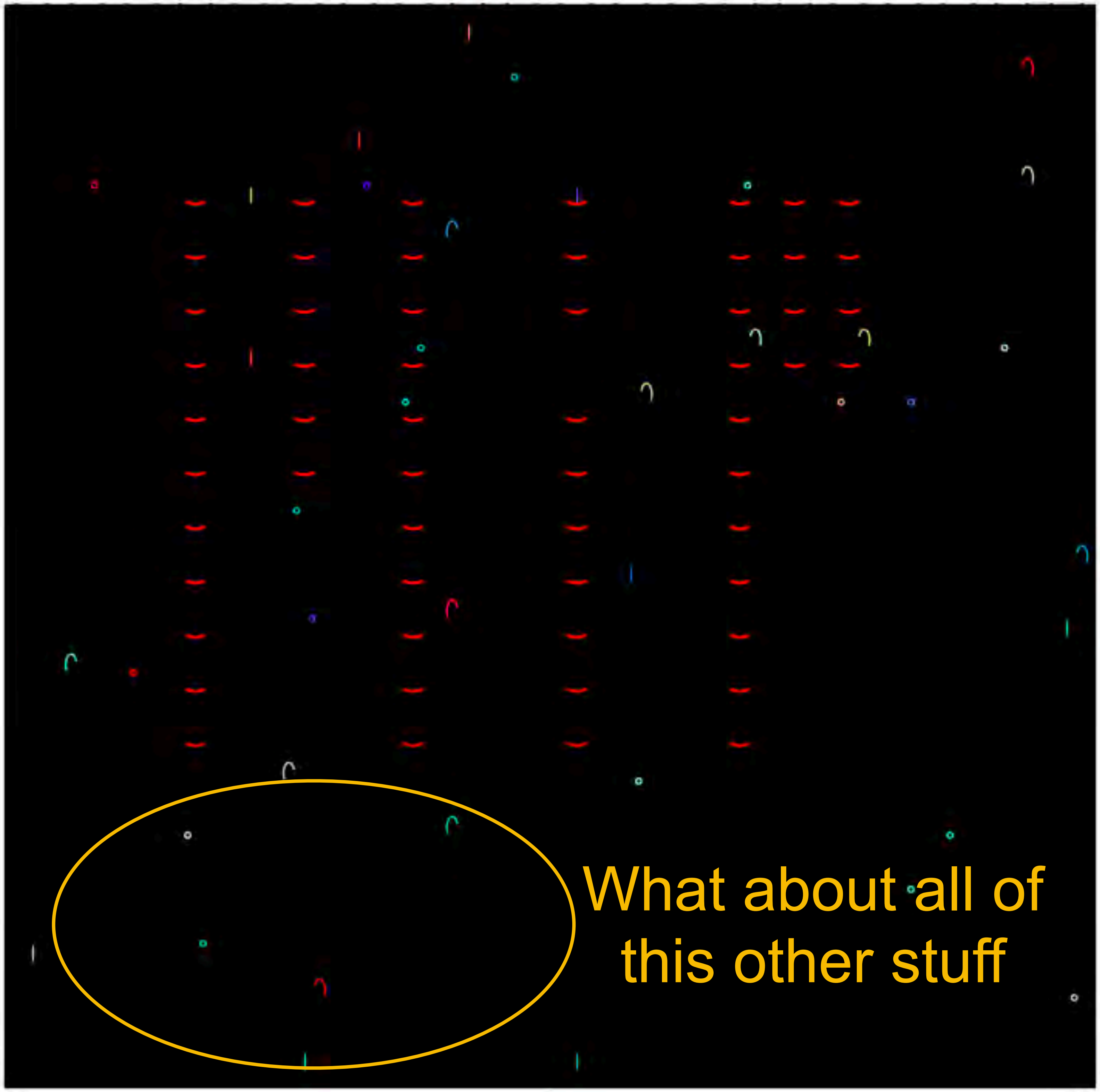
Physics Results





- By making sure our network was mass neutral
  - We could suddenly extract processes that were not possible

Anomaly detection



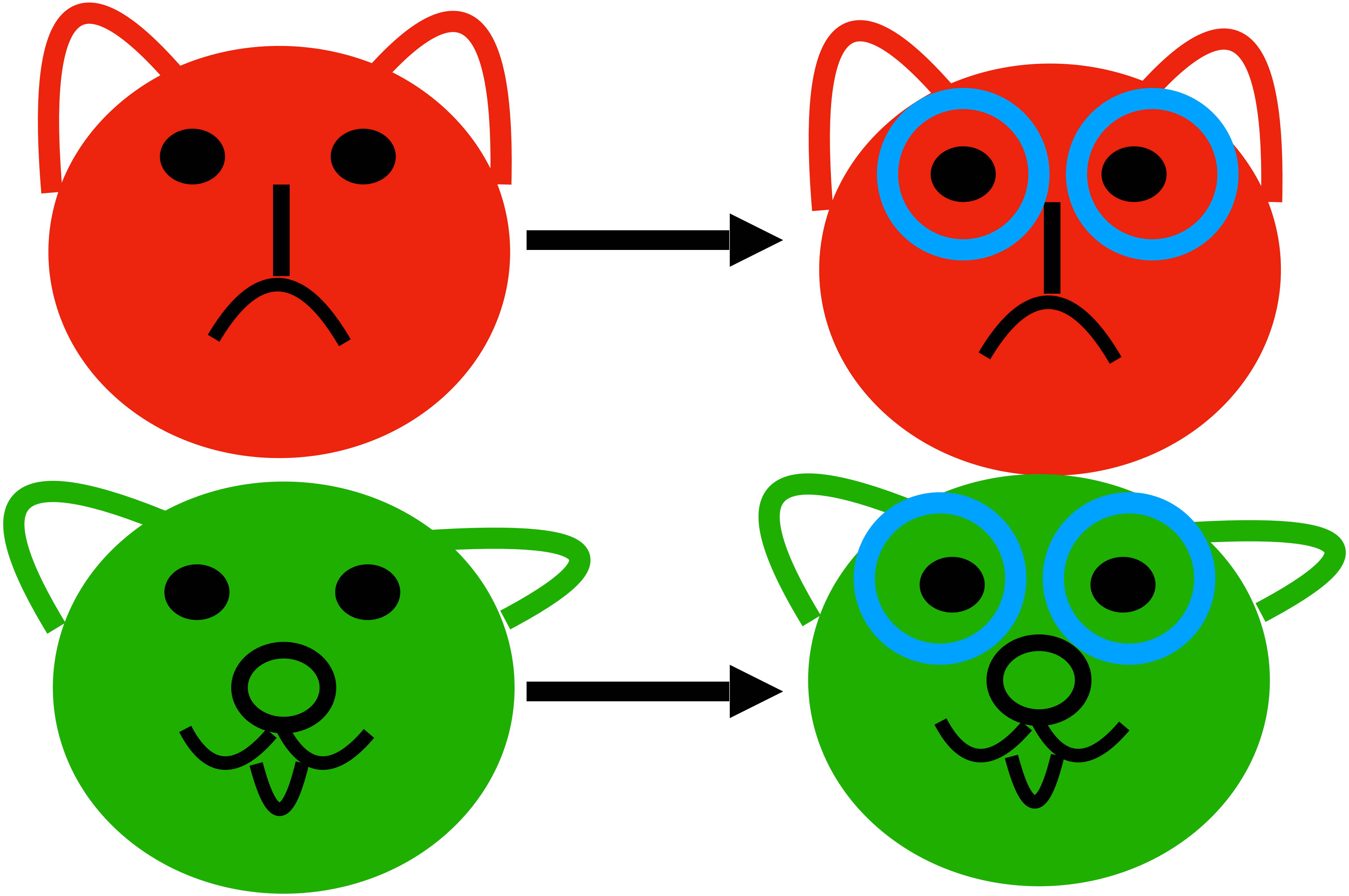
Can we generalize this?

Image

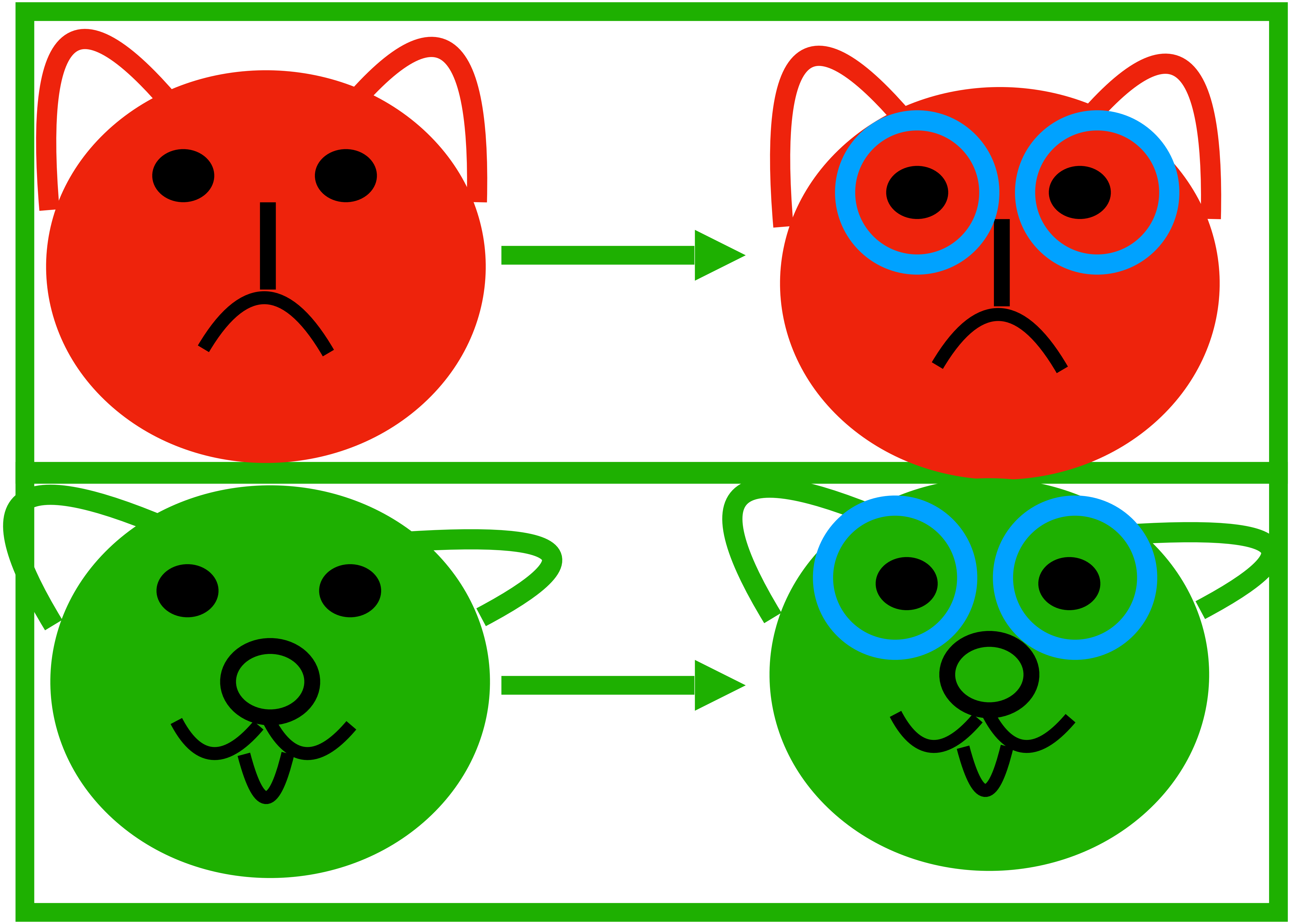
Augmented Image

Take Objects & Modify slightly

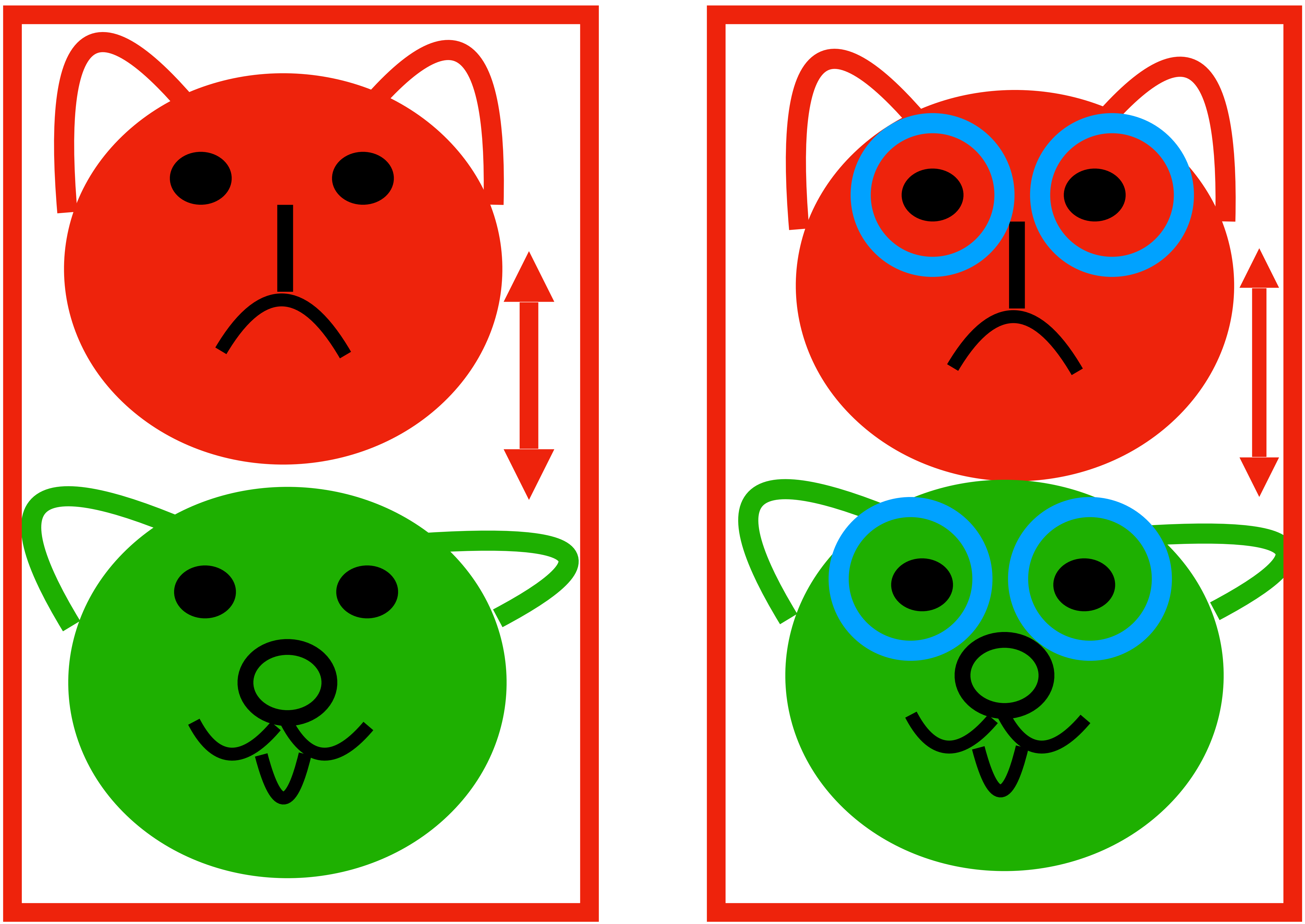
Take Objects & Modify slightly



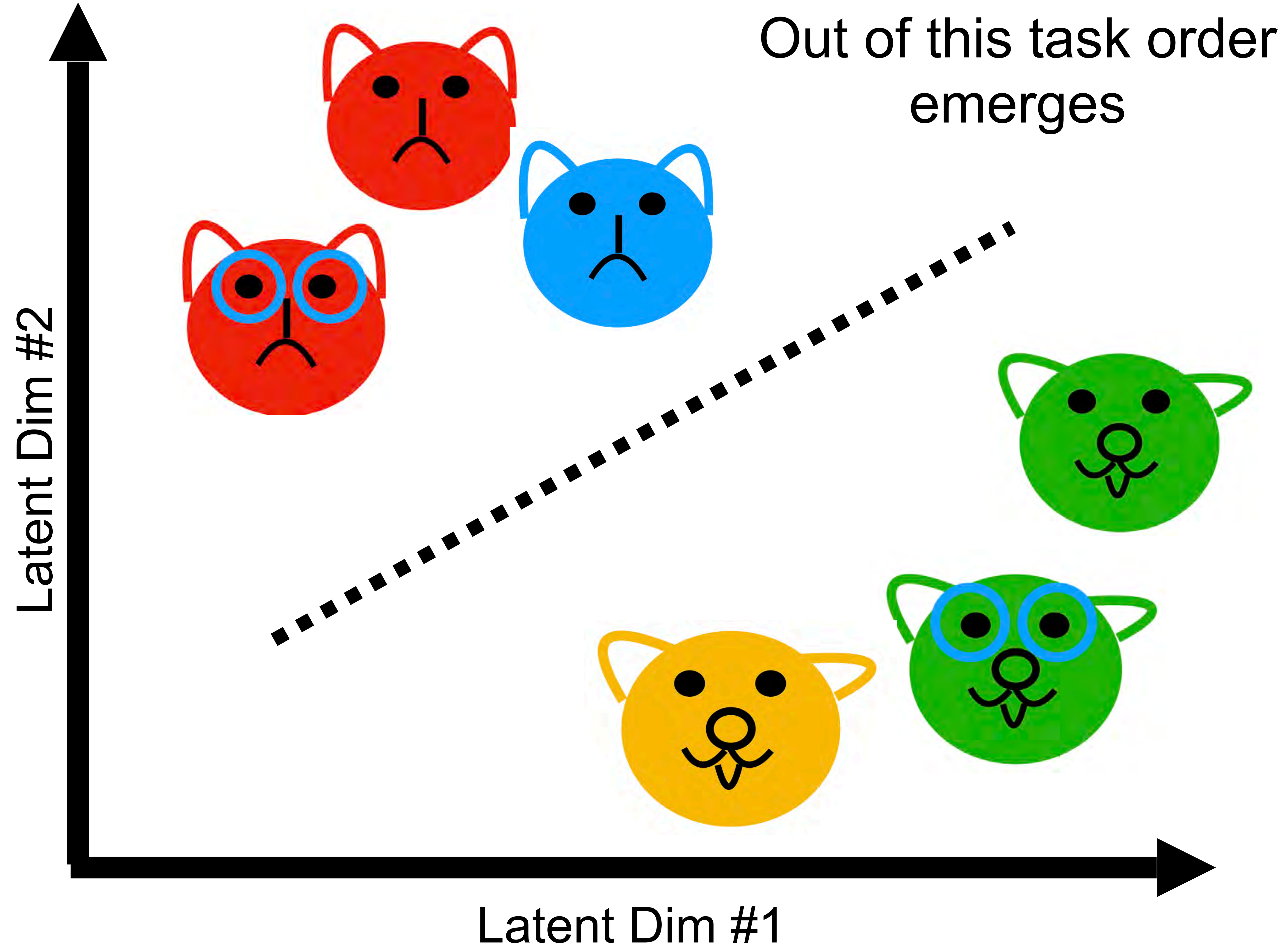
Minimize



Maximize

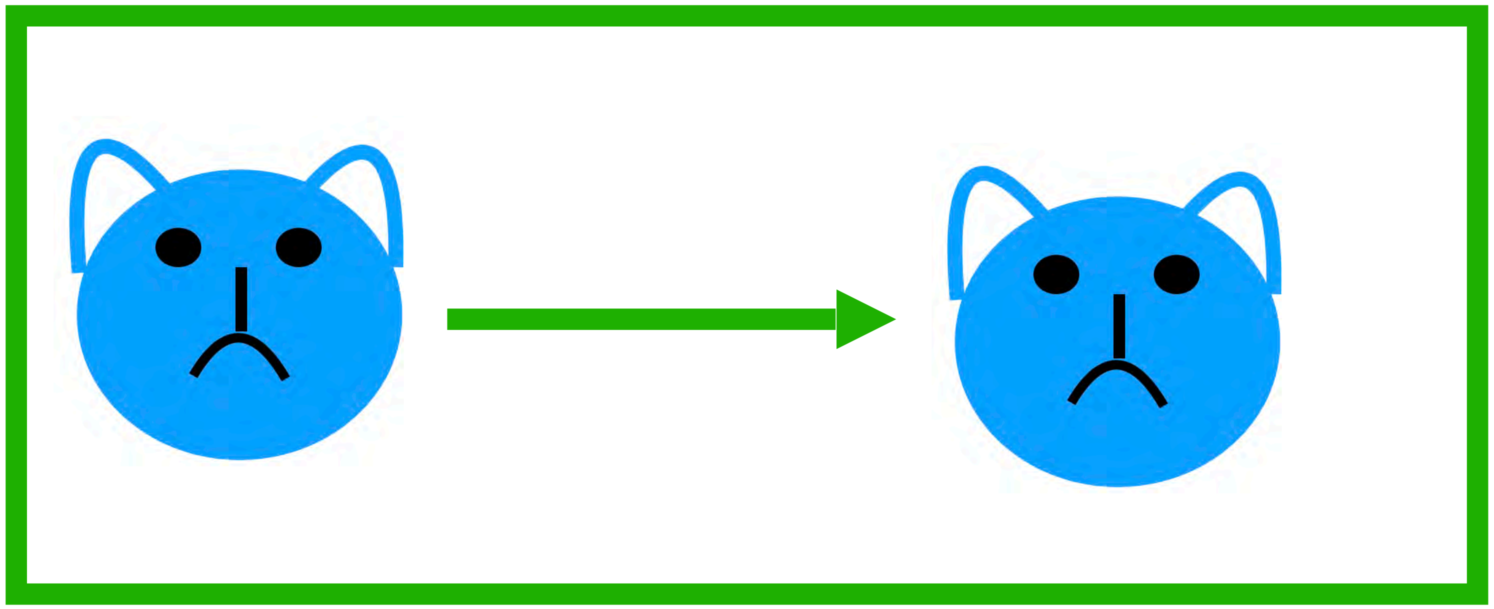


A space



Whats the right augmentation?

Shift in X or Y direction
In our Original Space

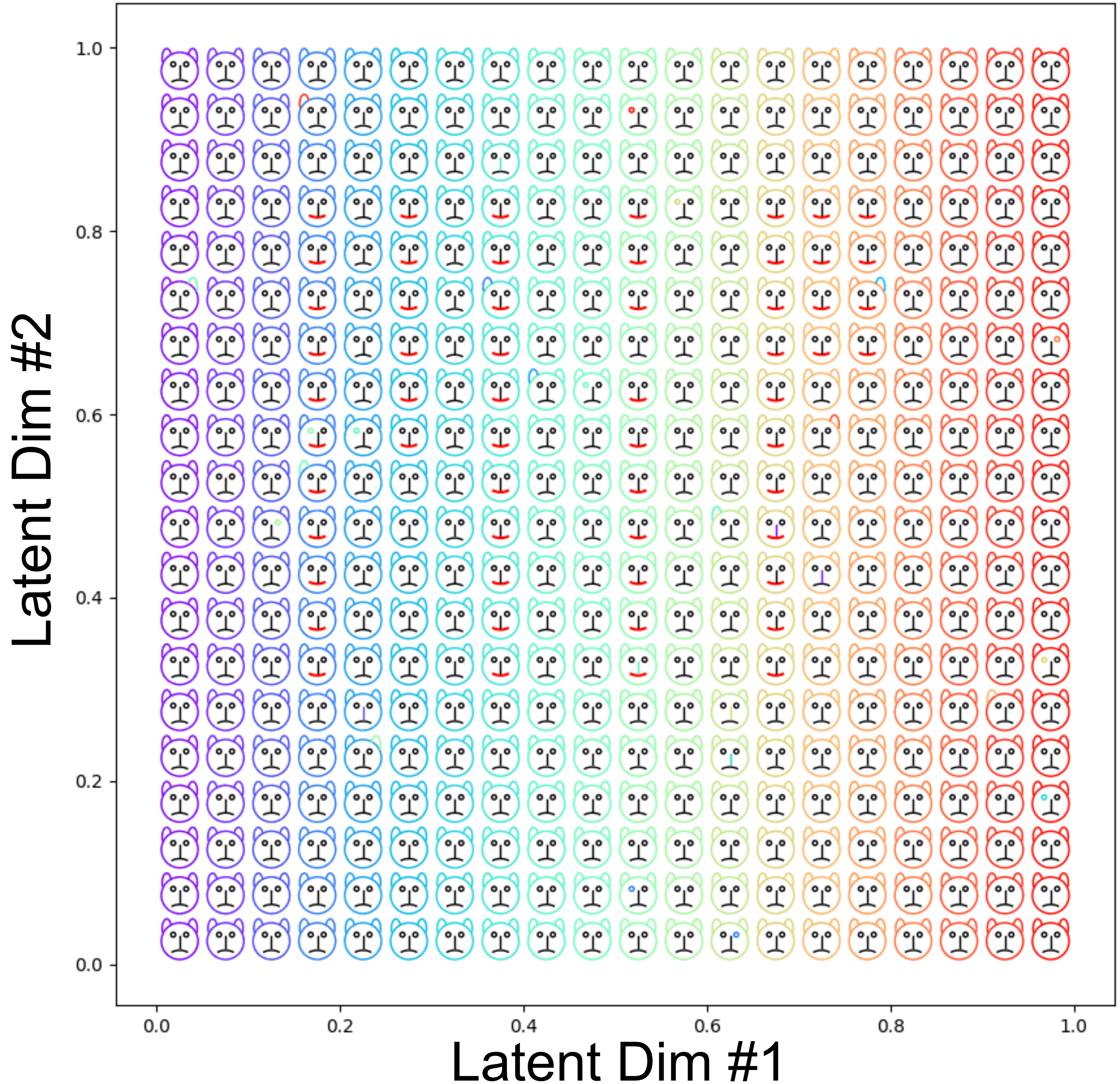


Should give same result

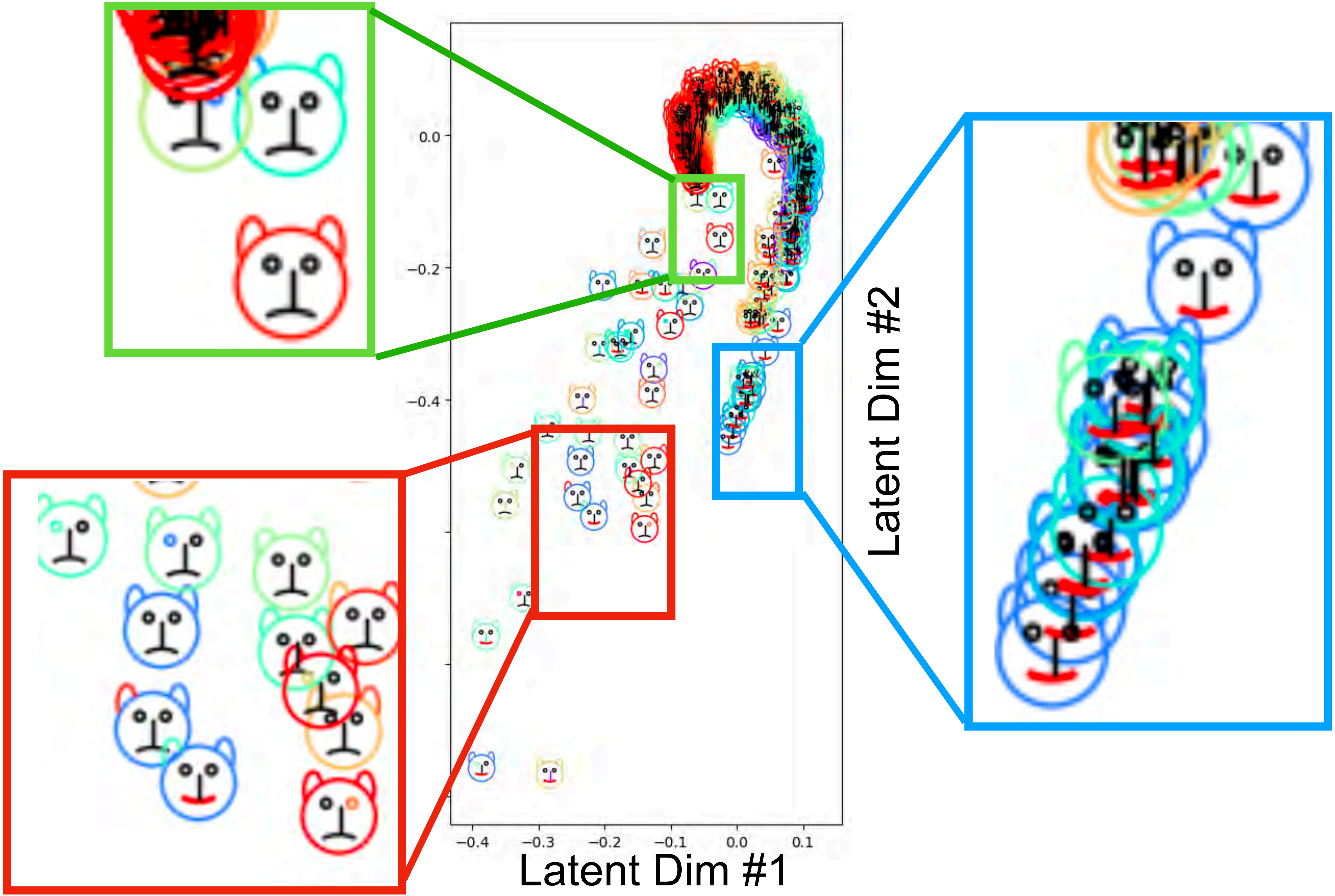
Noether's theorem

Embedding translation **symmetry invariance**
as a learning strategy
This also makes us colorblind

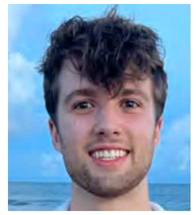
In Action



In Action



Arxiv:2403.07066

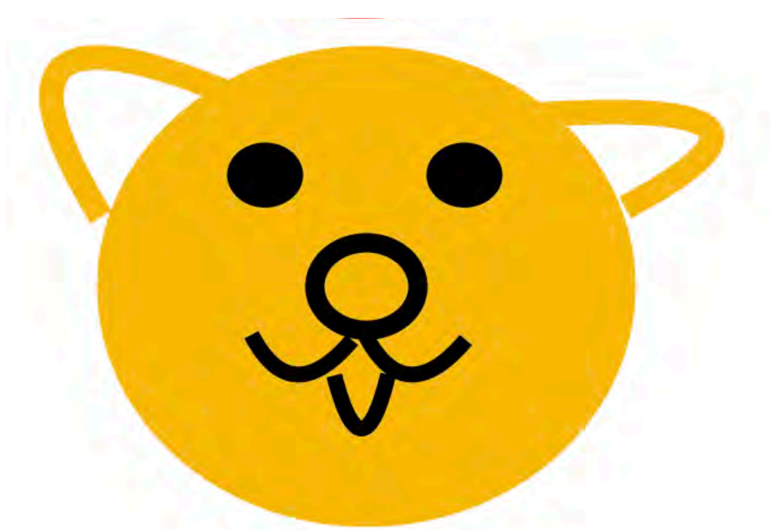


Re-simulation

Cats

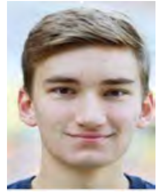
Higgs

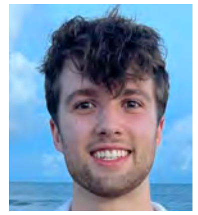
Dogs



Quarks and Gluons

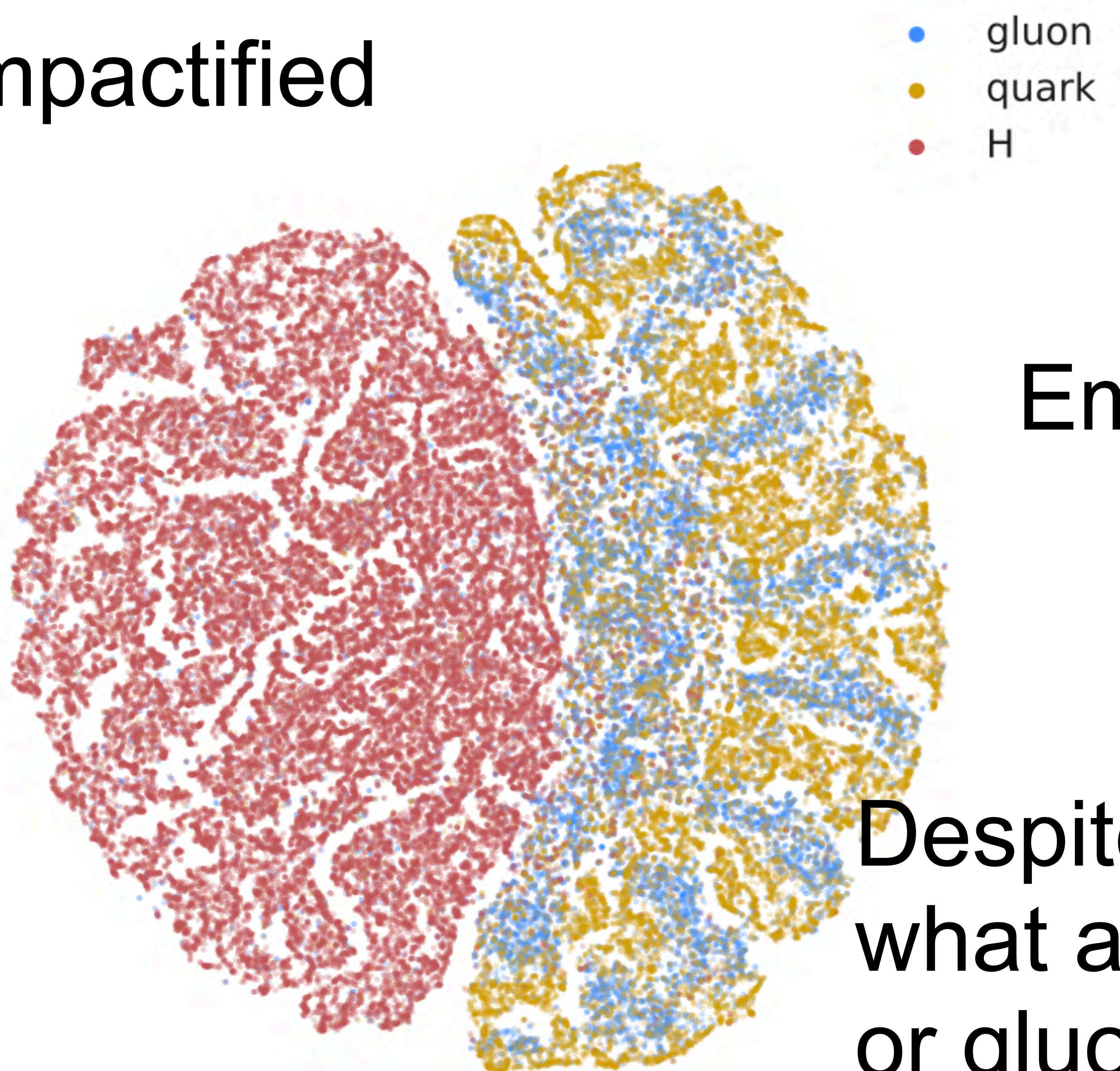
Arxiv:2403.07066





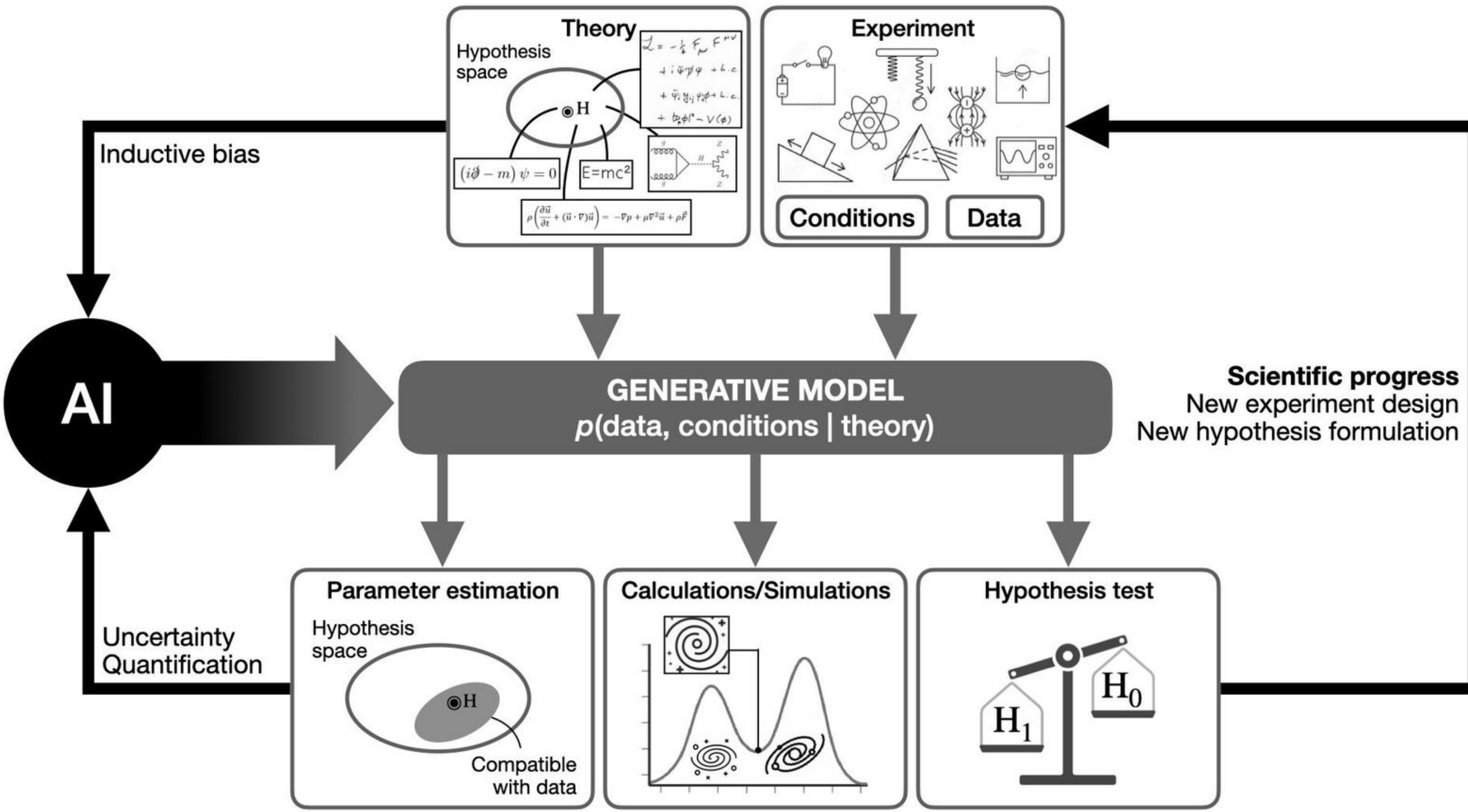
Embedded Space

Compactified



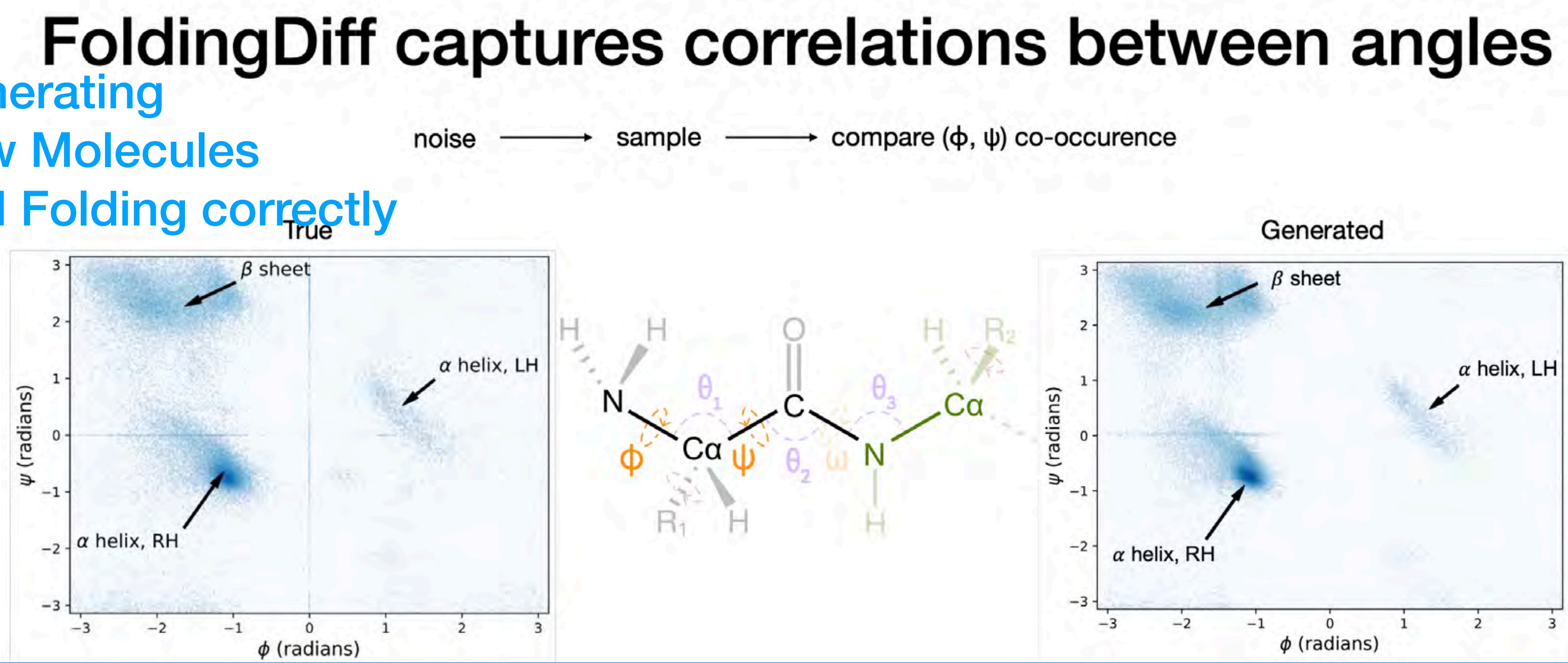
Embed in 8D

Despite Not knowing what a Higgs quark or gluon is
We build a space

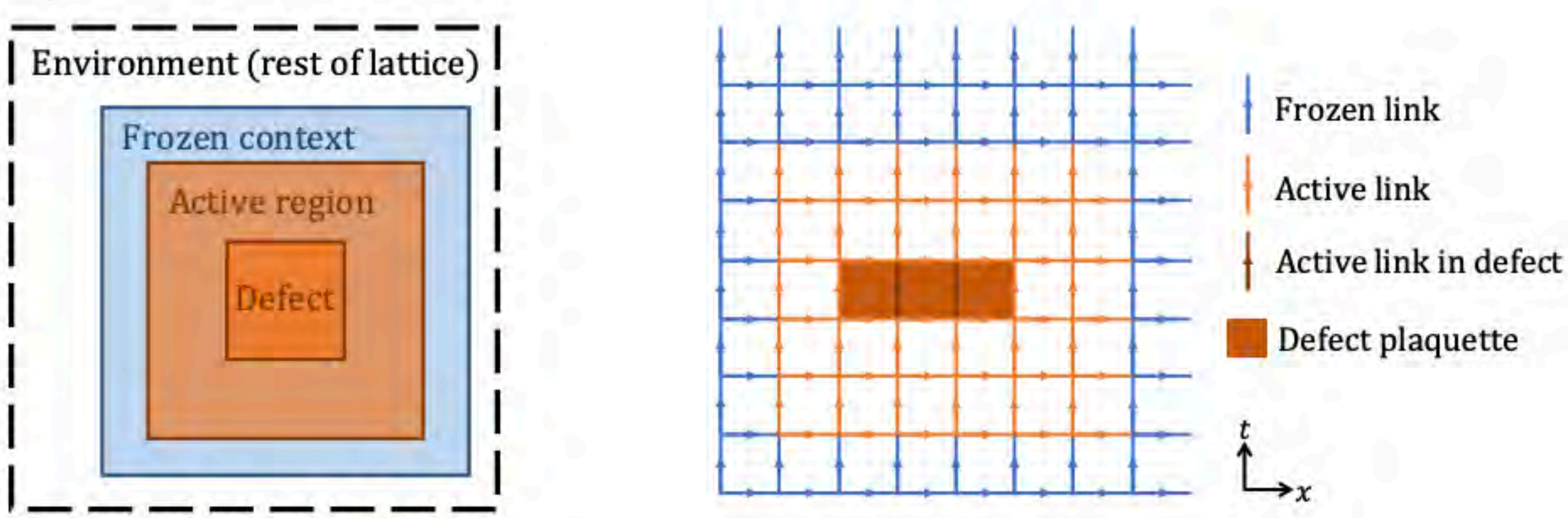

Theory
Hypothesis space
H
$(i\partial\!\!\!/ - m)\,\psi = 0$
E=mc²
Experiment
Conditions
Data
Inductive bias
AI
GENERATIVE MODEL
p(data, conditions | theory)
Scientific progress
New experiment design
New hypothesis formulation
Uncertainty Quantification
Parameter estimation
Hypothesis space
H
Compatible with data
Calculations/Simulations
Hypothesis test
H1
H0

Accelerating and Leveraging Simulations and Calculations for Scientific Discovery

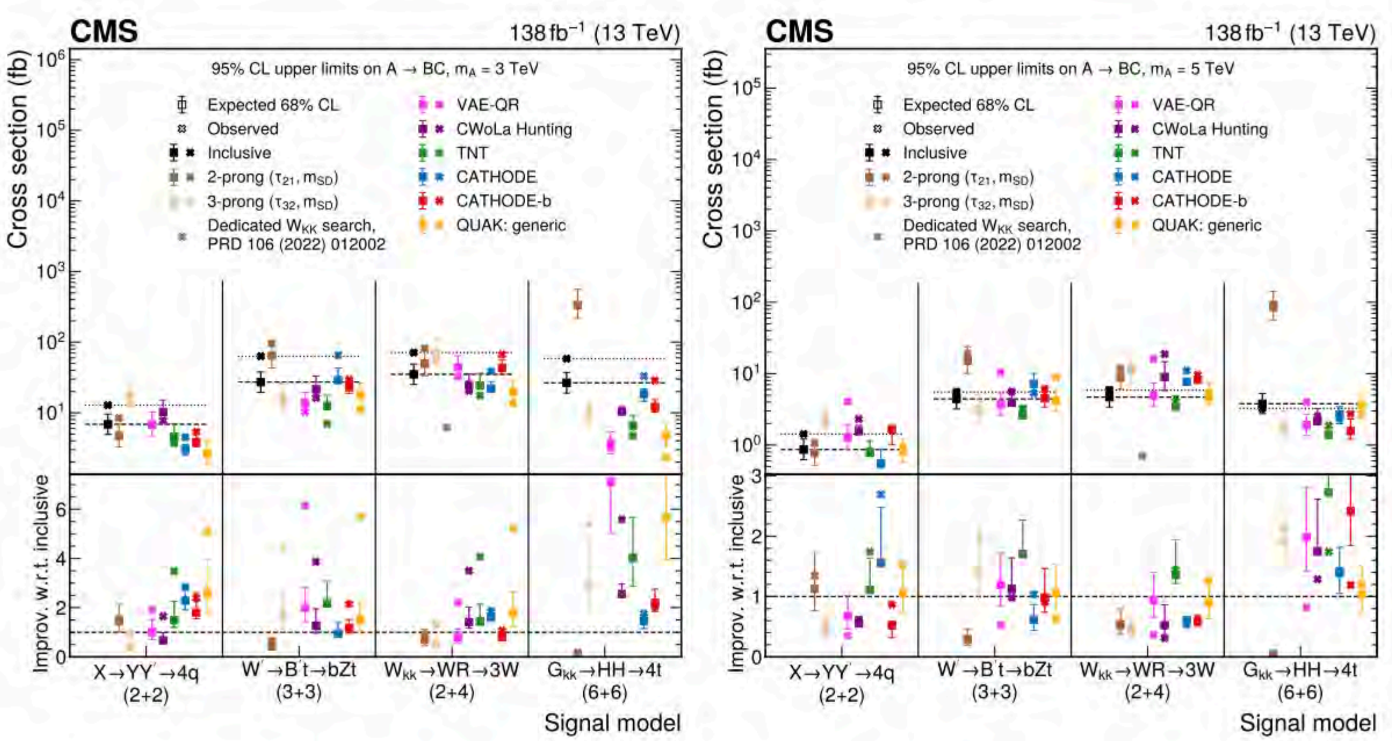
Generating New Molecules And Folding correctly



Lattice QCD Calculations

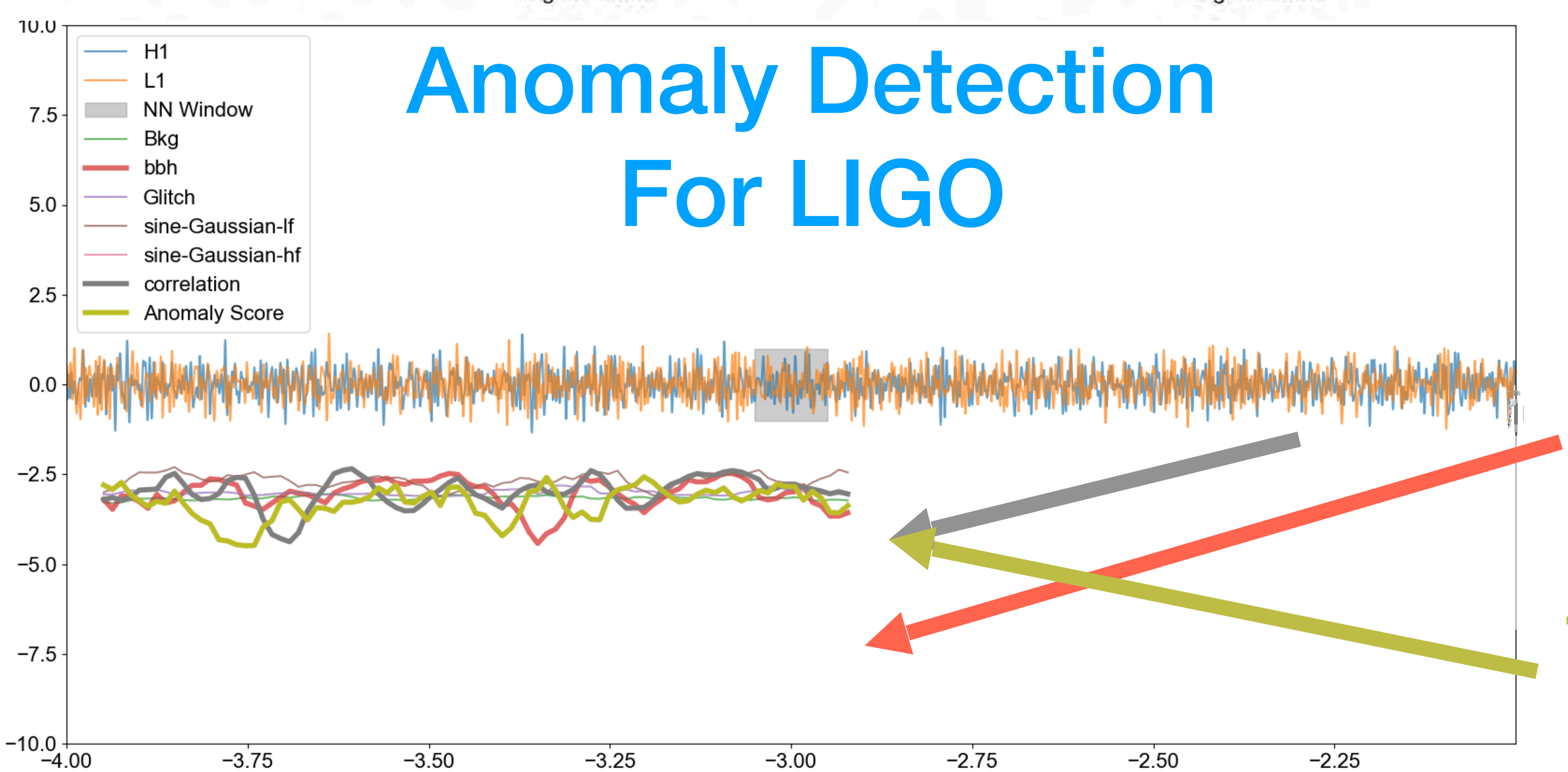


Enhancing Anomaly Detection and the Search for New Physics



Many Models All in One Go

Automating physics searches by imposing all the rules of physics and searching for any type of devaition



Key Insights

11D space

Correlation

BBH Prob

Others

Total Score

AI-Assisted Theory Discovery

Prospect of LLMs is making it possible to perform many theoretical calculations

Problem Statement: A photon with the energy E scatters on an electron at rest at angle θ in the electron's reference frame. Find the angular frequency ω of the scattered photon.
Answer Requirements: Provide the answer in the form of a python function with the following signature:

```
#let c be the speed of light, m_e - electron mass, h_bar - reduced Planck constant
def omega_scattered(E: float, m_e:float, theta:float, c:float, h_bar:float) -> float:
    pass
```

Model Answer:

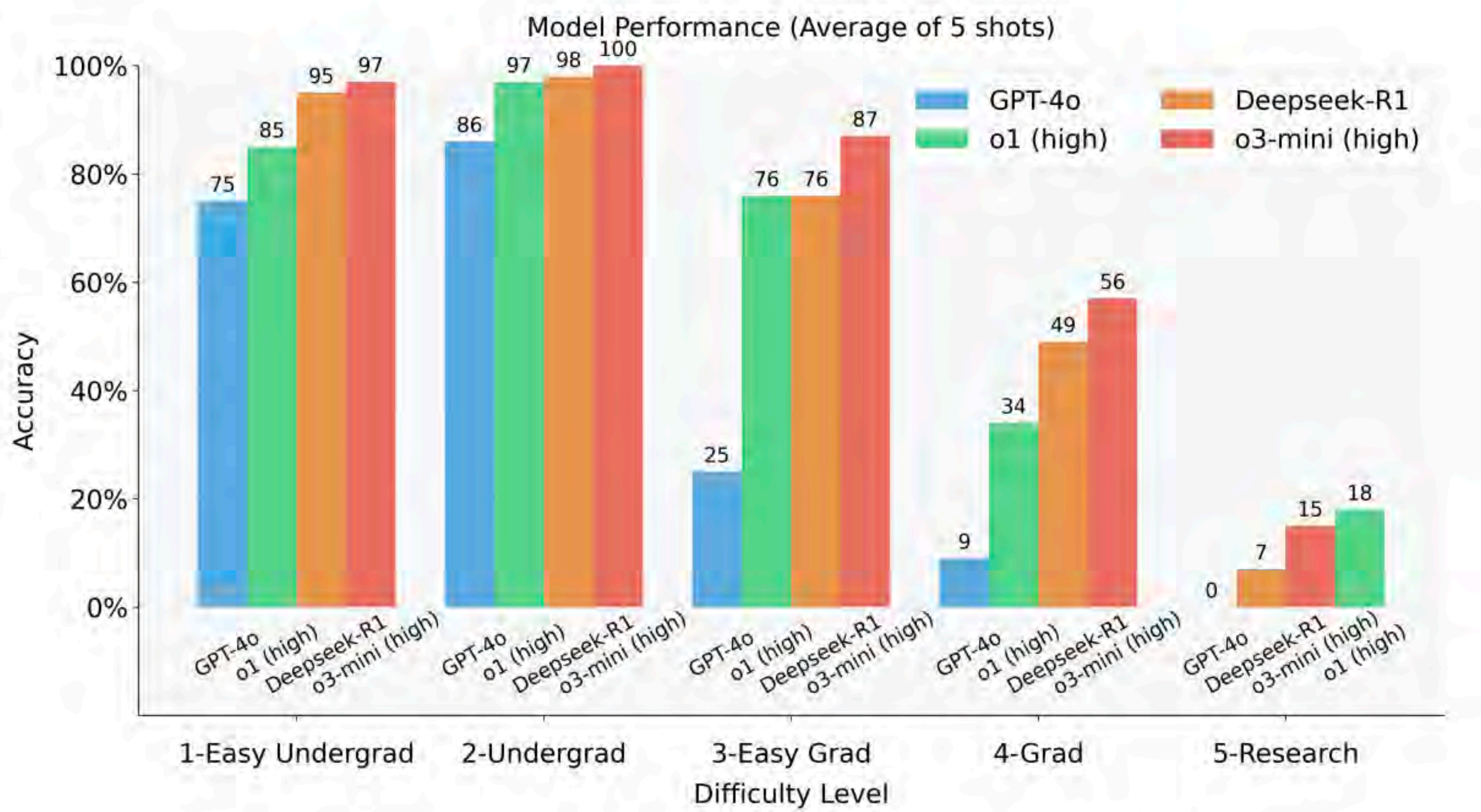
$$\omega = \frac{1}{\frac{\hbar}{E} + \frac{\hbar}{mc^2}(1 - \cos\theta)}$$

```
import math
def omega_scattered(E: float, m_e:float, theta:float, c:float, h_bar:float) -> float:
    return 1/(h_bar/E + h_bar/(m_e*c**2)*(1-math.cos(theta)))
```

https://arxiv.org/pdf/2502.15815

AI-Assisted Theory Discovery

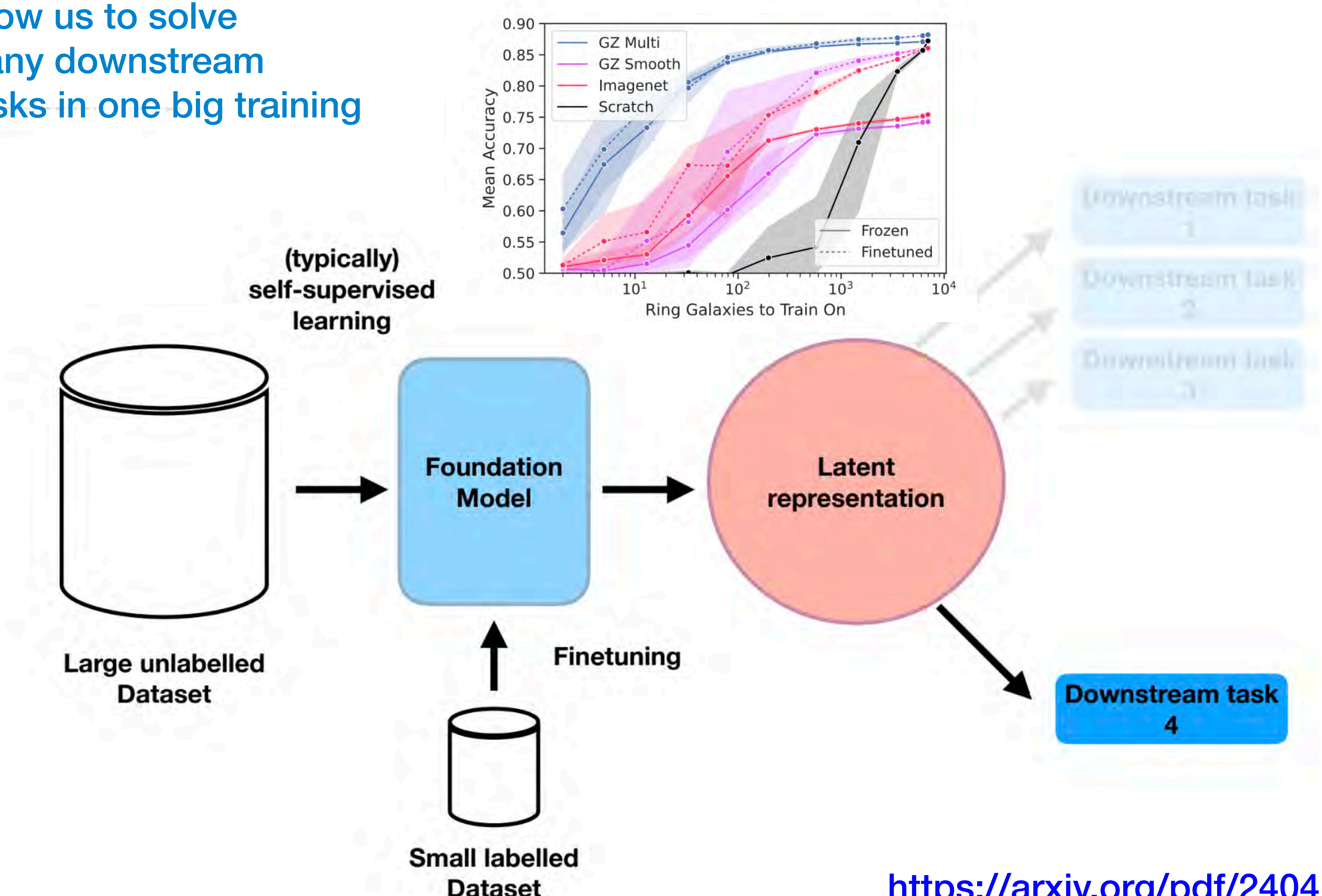
Prospect of LLMs is making it possible to perform many theoretical calculations



https://arxiv.org/pdf/2502.15815

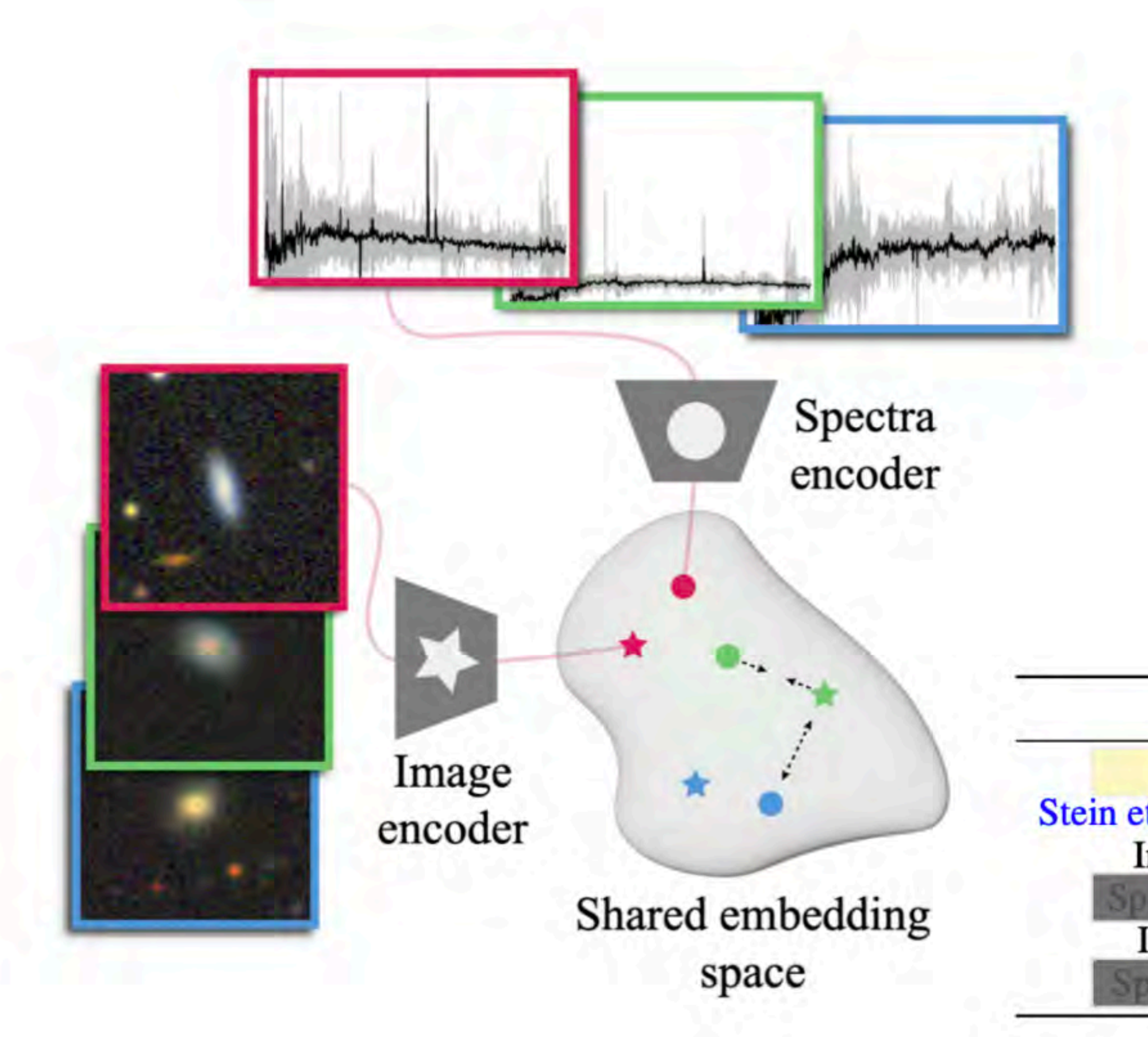
Foundation Models for the (Physical) Sciences

New structures
Allow us to solve
Many downstream
Tasks in one big training



https://arxiv.org/pdf/2404.02973

Foundation Models for the (Physical) Sciences



Sharing of different types of data formats can be embedded in one network

Regression method	Redshift R^2	Stellar Mass R^2
(r, g, z) Photometry + MLP	0.69	0.65
Stein et al. (2021b) Image Embedding + MLP	0.39	0.45
Image Embedding + k-NN (**ours**)	0.71	0.66
Spectrum Embedding + k-NN (ours)	0.97	0.86
Image Embedding + MLP (**ours**)	0.63	0.57
Spectrum Embedding + MLP (ours)	0.99	0.86

https://arxiv.org/abs/2310.03024

Substantial Improvements
Are present from this

What Are the Pathways for Contribution from the Physical Sciences to Influence Generative AI?

Neural networks and physical systems with emergent collective computational abilities

(associative memory/parallel processing/categorization/content-addressable memory/fail-soft devices)

J. J. Hopfield

Division of Chemistry and Biology, California Institute of Technology, Pasadena, California 91125; and Bell Laboratories, Murray Hill, New Jersey 07974

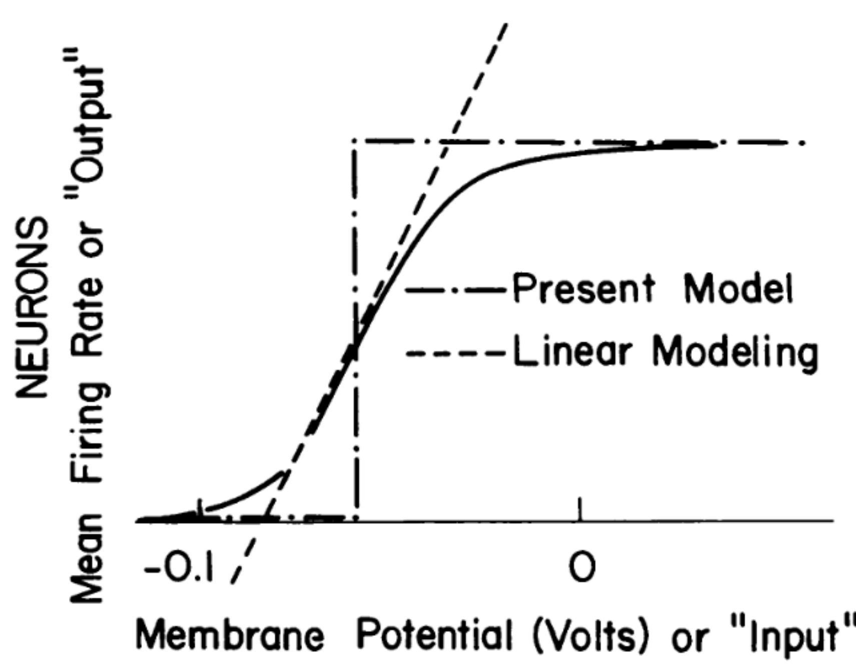


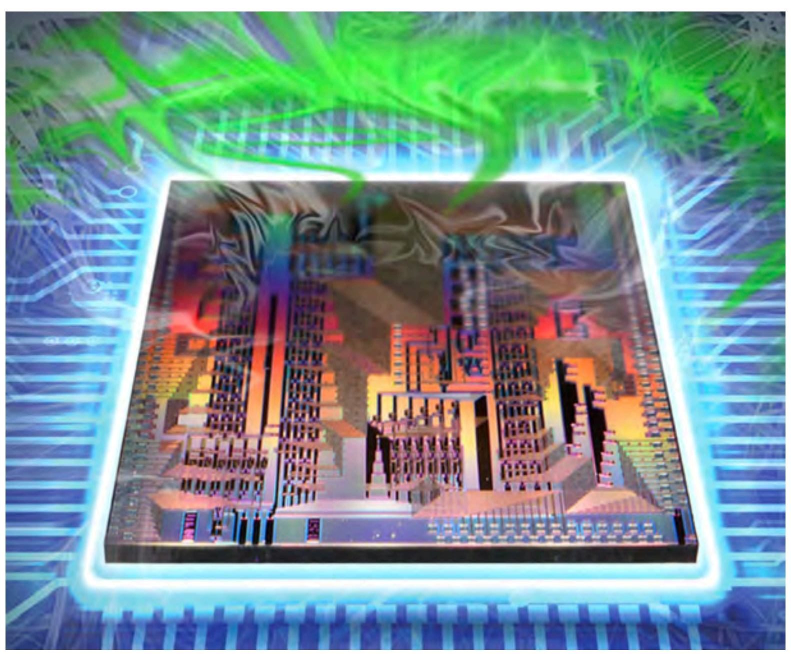
Fig. 1. Firing rate versus membrane voltage for a typical neuron (solid line), dropping to 0 for large negative potentials and saturating for positive potentials. The broken lines show approximations used in modeling.

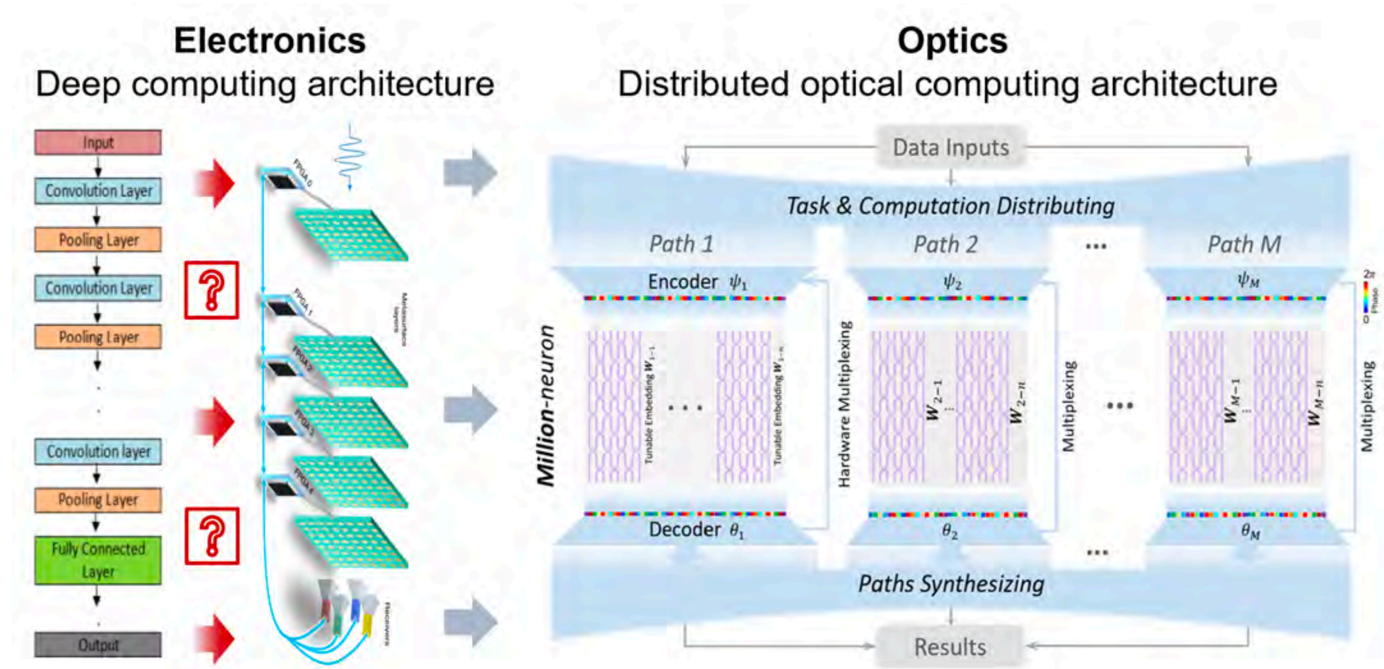
Revival of Neural Networks started when Hopfield used a Spin-Glass model to learn

Physics-Inspired Hardware for Generative AI

MIT News
ON CAMPUS AND AROUND THE WORLD

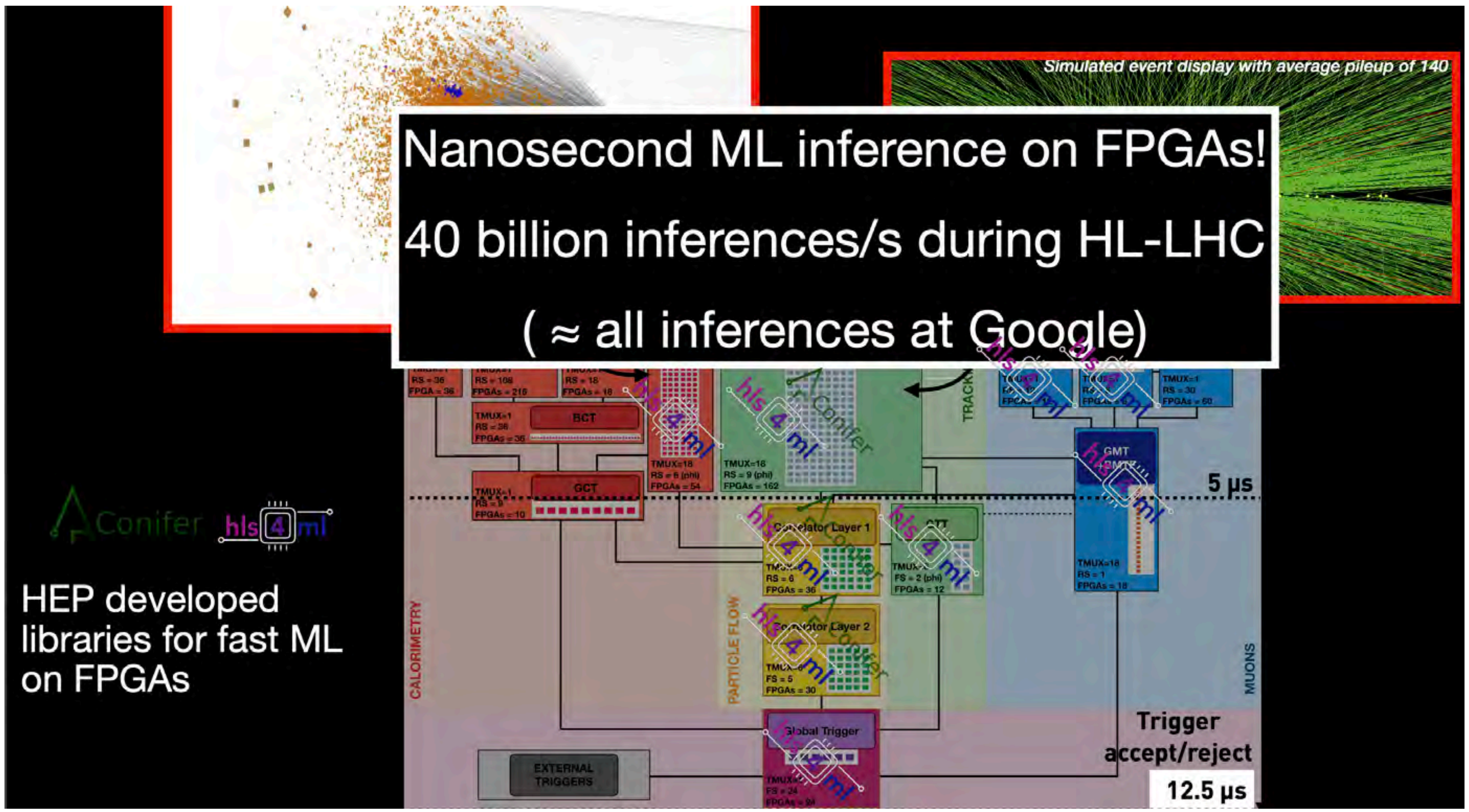
Photonic processor could enable ultrafast AI computations with extreme energy efficiency

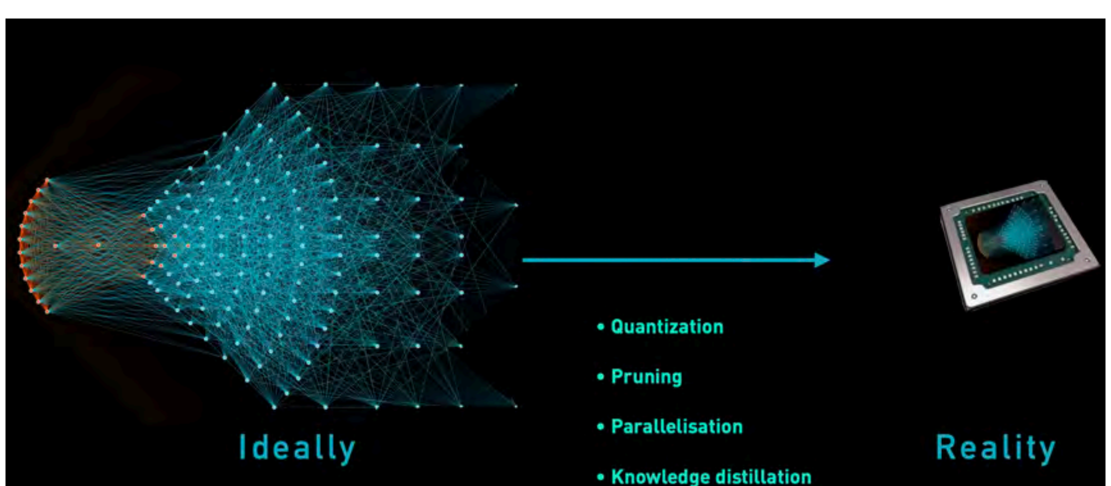




Photonics processing can lead to very significant speedups in ML processing through the use of Light to perform ML infernece

Physics-Inspired Hardware for Generative AI



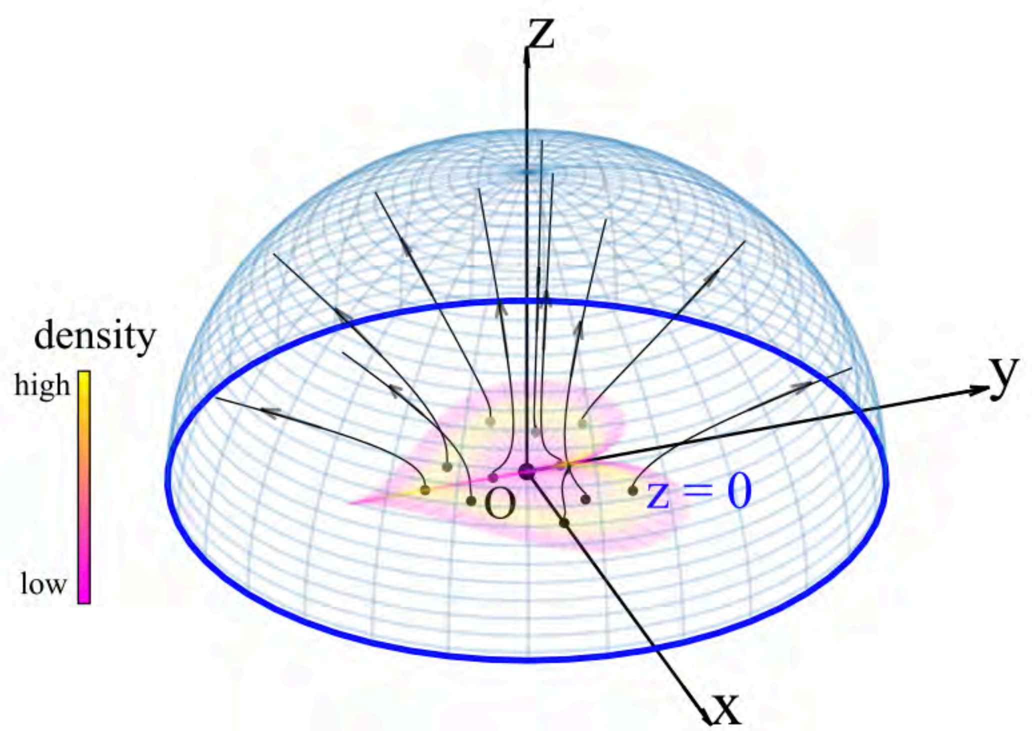


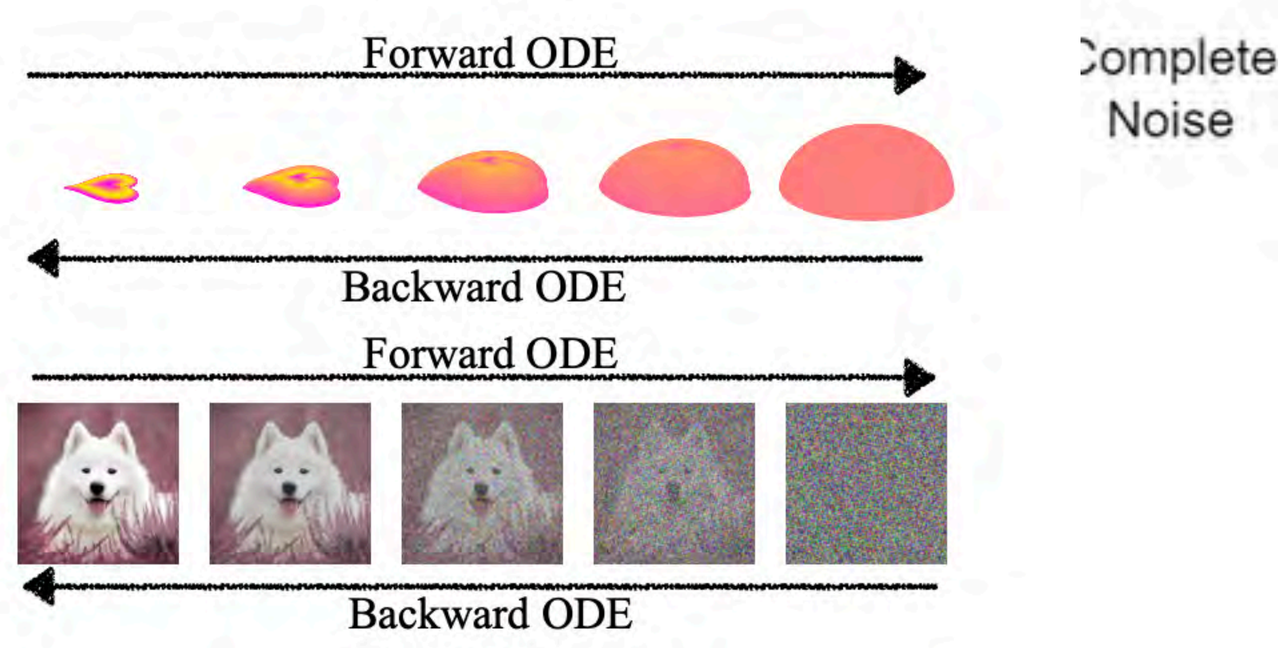
Computing demands at the LHC has led to a new software to program optimized, ultrafast NNs on Chip

Physics-Inspired Algorithms for Generative AI

The Forward Process

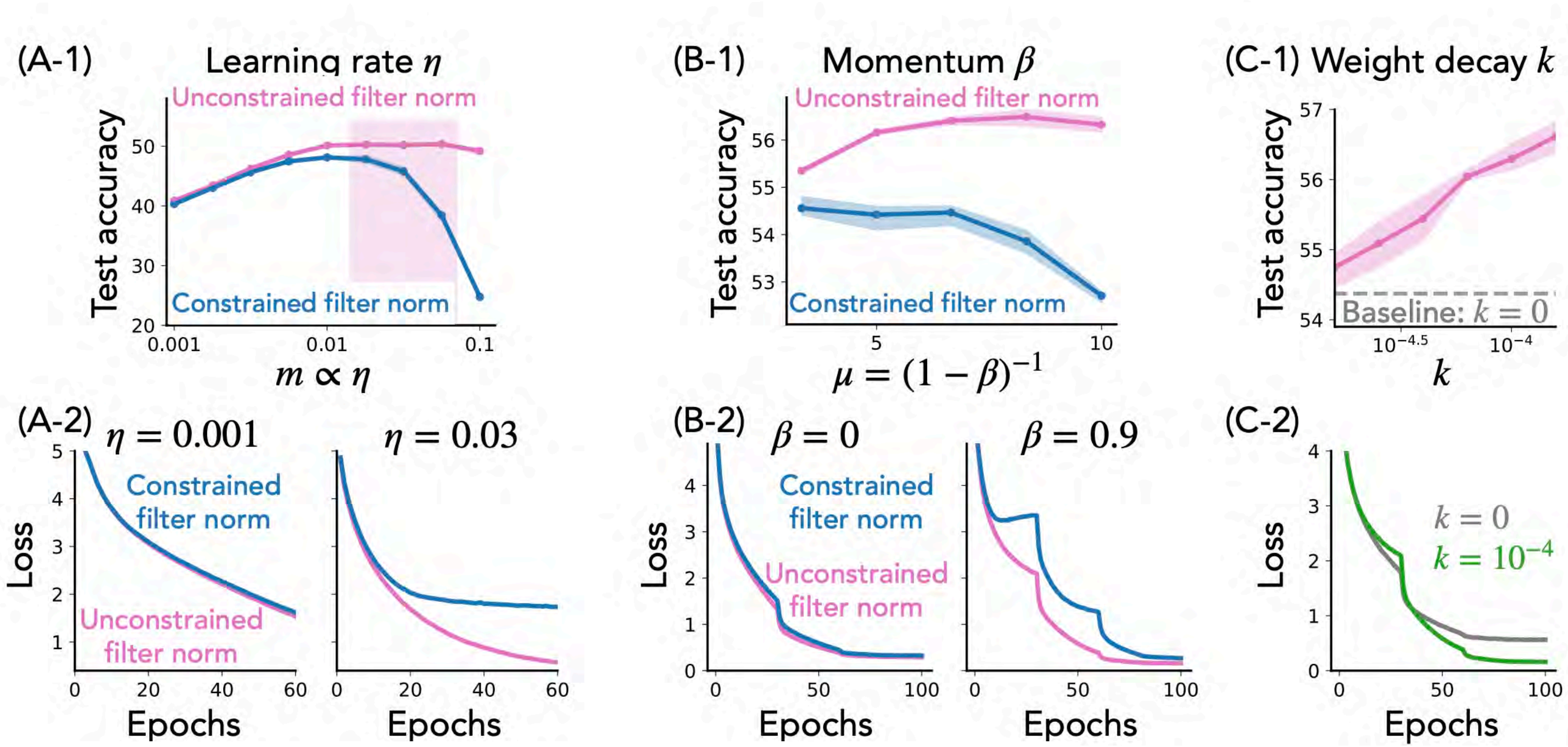
$$x_0 \rightarrow x_1 \rightarrow \cdots \rightarrow x_T$$





A more modern example comes from diffusion, which came straight out of physics

Theoretical Foundations of AI through the Lens of Physics

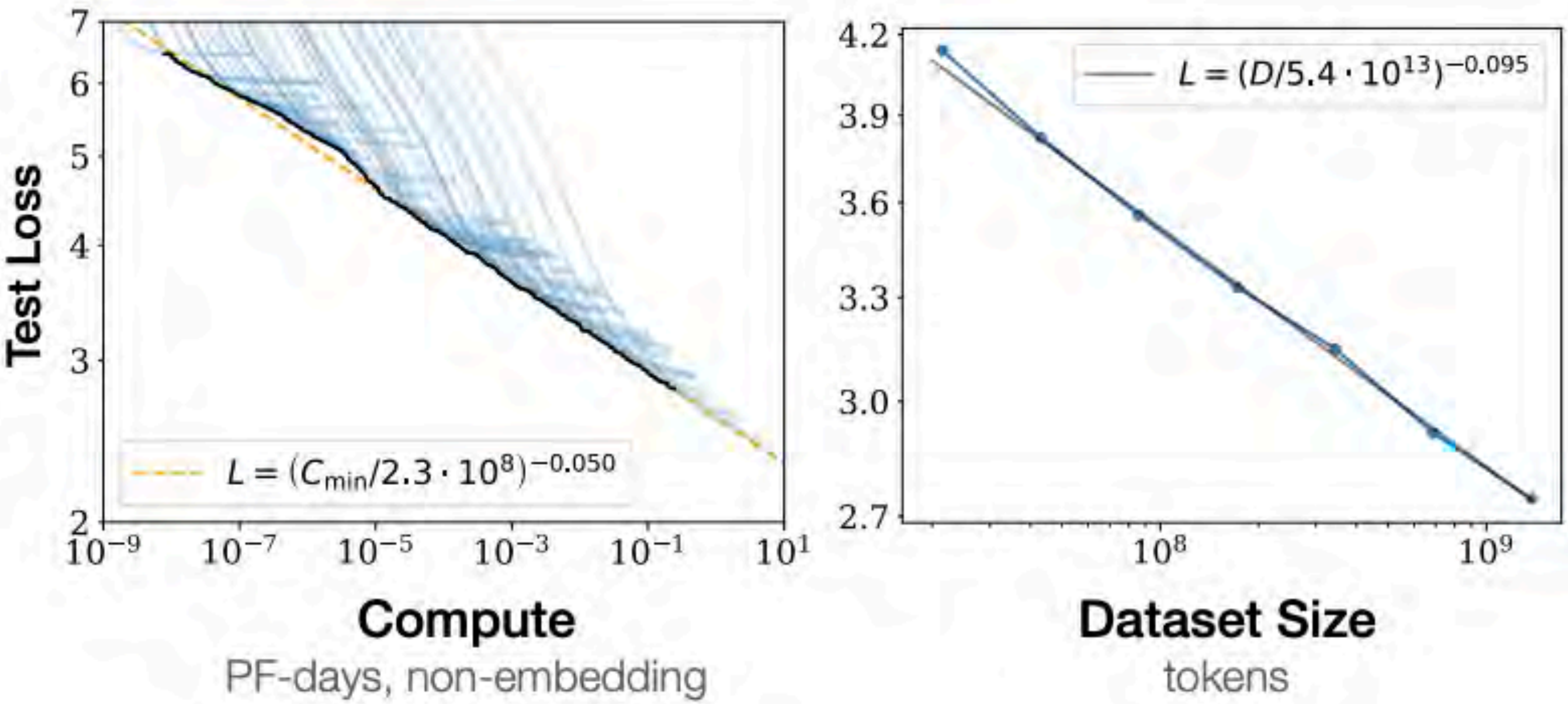


$$\mathcal{L}_c = e^{\frac{\mu}{m}t}\left[\frac{m}{2}\dot{r}^2 + \left(\frac{m}{2}\left|\dot{\hat{q}}\right|^2 - \frac{k}{2}\right)r^2 - f(\hat{q})\right] + \lambda(t)\left(|\hat{q}|^2 - 1\right)$$

https://arxiv.org/pdf/2105.02716

Using Physics symmetries to improve minimization strategies
And Ensure minimal convergence of models

Theoretical Foundations of AI through the Lens of Physics

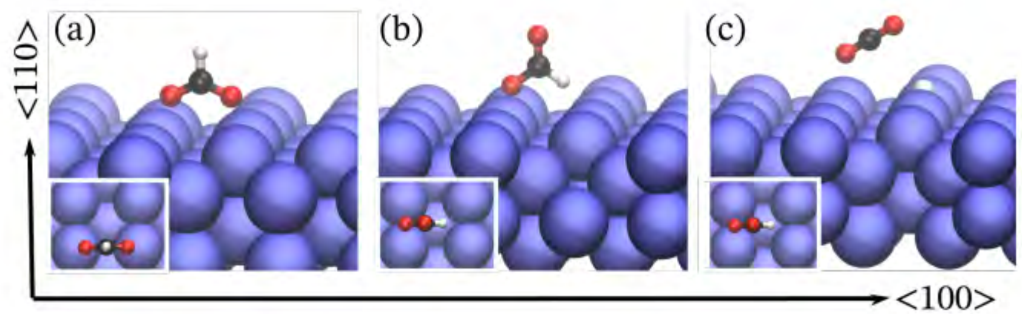


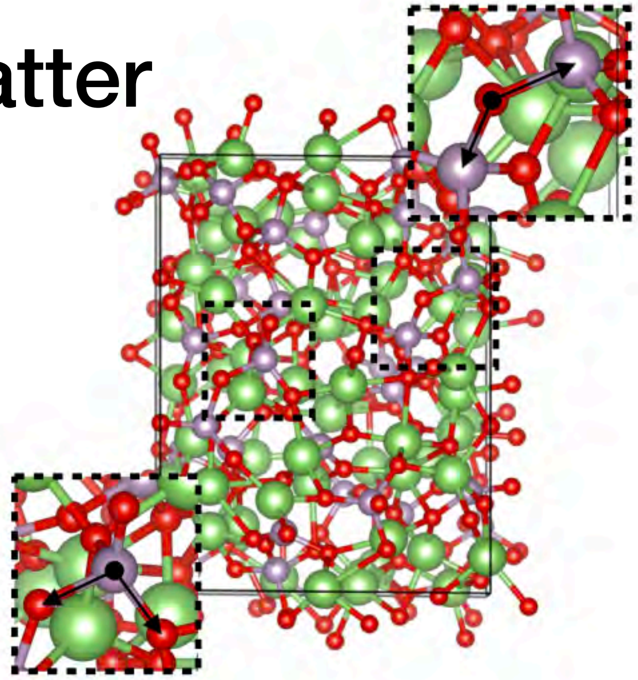
https://arxiv.org/pdf/2001.08361

Considering scaling laws as a model for information complexity
Understanding thermodynamic properties/Scaling behavior

Algorithmic Developments Driven by Physics Applications

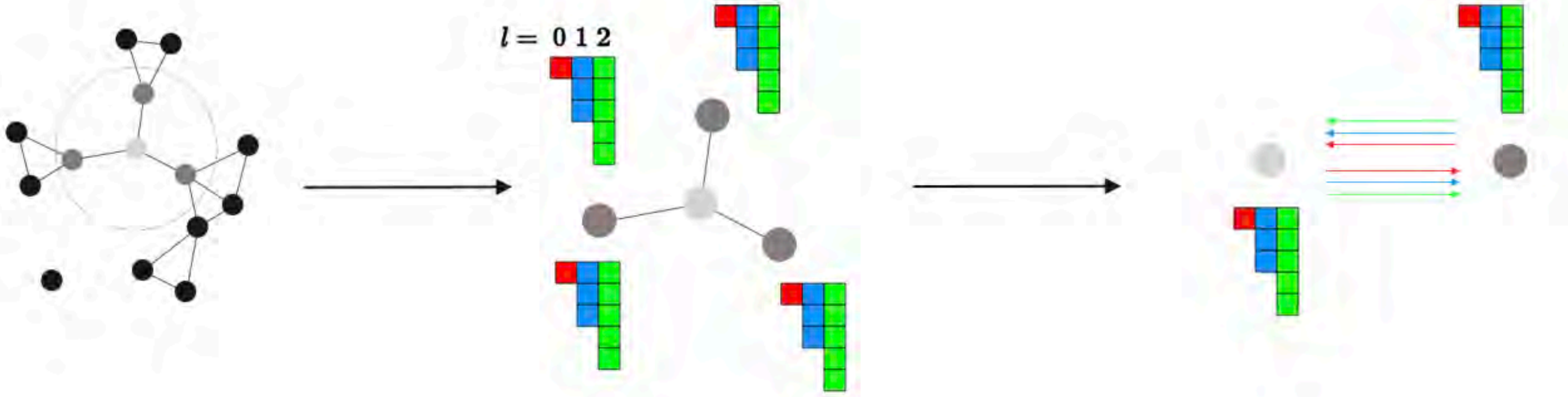
Modeling of Complex stats of matter





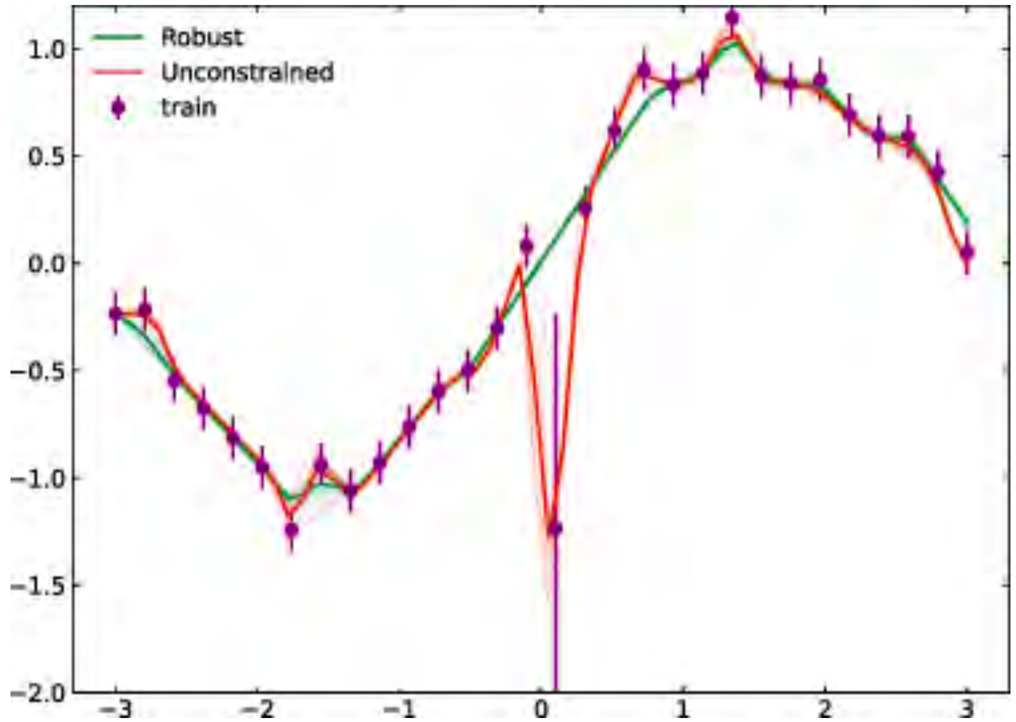
https://arxiv.org/pdf/2101.03164

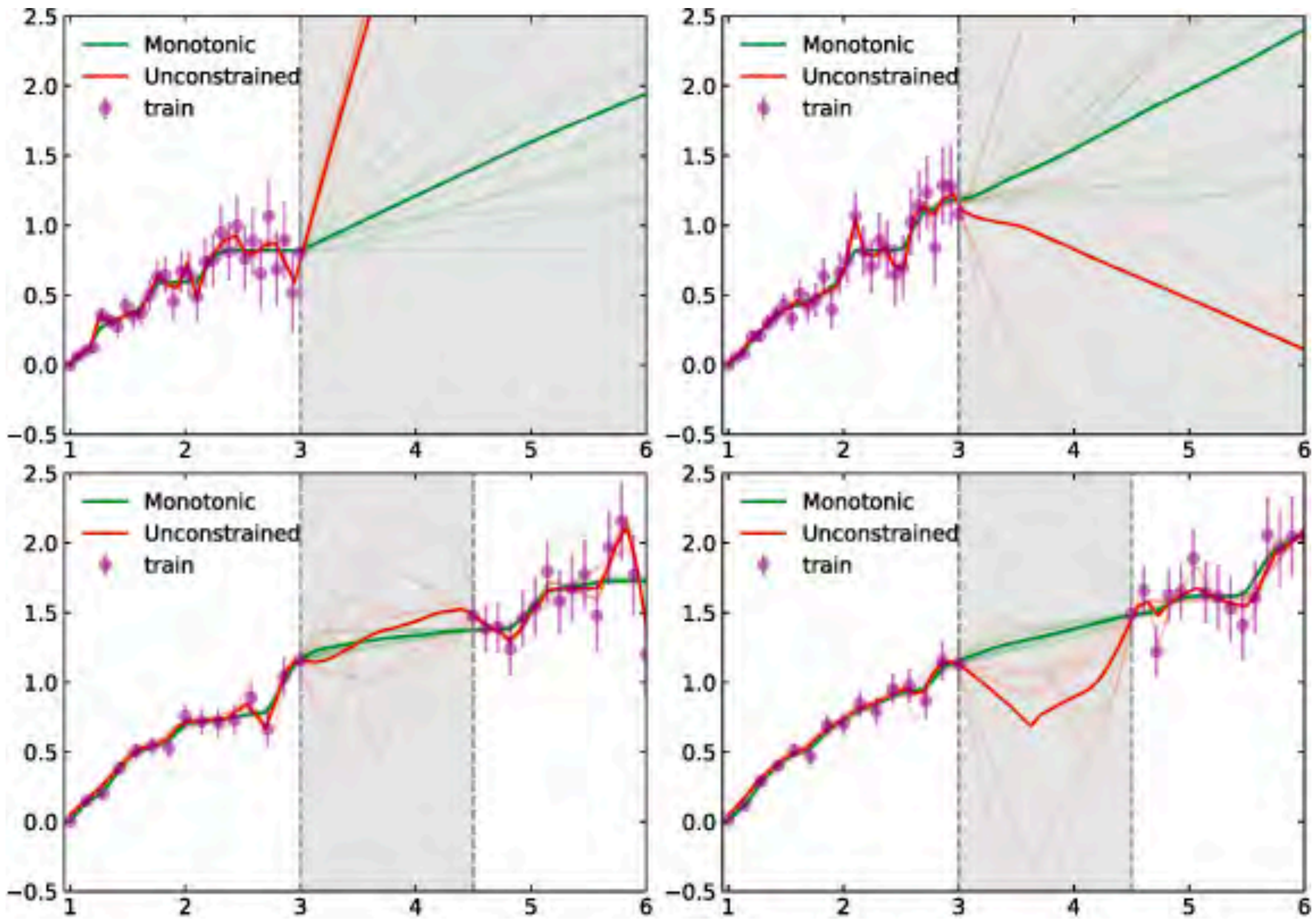
Rotational Equivariance



Modelling of complex matter states (crystals other molecules) led to a need for NNs that respect rotational equivariance

Algorithmic Developments Driven by Physics Applications





Lipshitz continuous neural networks

Smooth functional forms, and positive turn-on curves for extrapolating physics behavior needed for LHC algorithms

https://iopscience.iop.org/article/10.1088/2632-2153/aced80

What Is Needed from a Community Perspective to Achieve These Impacts?

Creating Viable Career Pathways for Interdisciplinary Researchers

IAIFI Fellows

https://iaifi.org/fellows.html

IAIFI

Call for Applications for 2025-2028 IAIFI Fellows

Schmidt Sciences

The Eric and Wendy Schmidt AI in Science Postdoctoral Fellowship

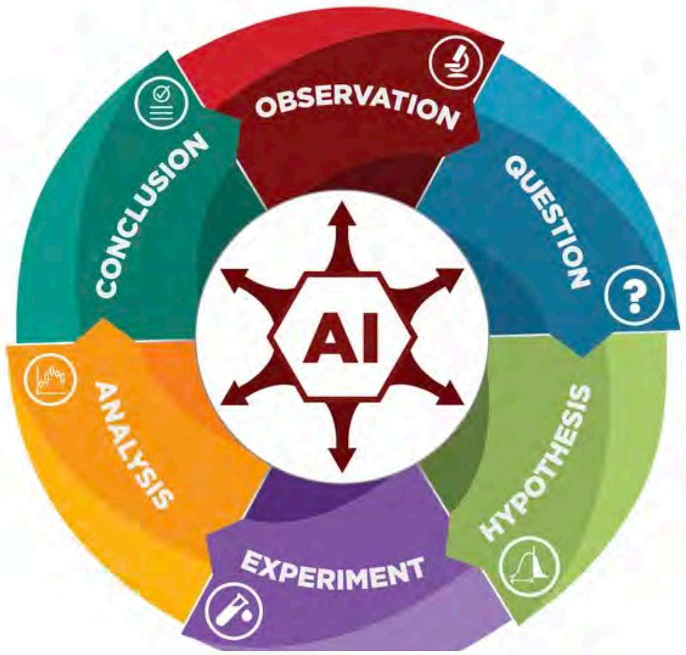
https://www.schmidtsciences.org/schmidt-ai-in-science-postdocs/

A3D3 Postbaccalaureate Fellowship Program

The A3D3 Postbaccalaureate Fellowship Program is a one-year research opportunity in neuroscience, high energy physics, astronomy, computer science, and/or electrical engineering, for recent graduates with a bachelor's degree.

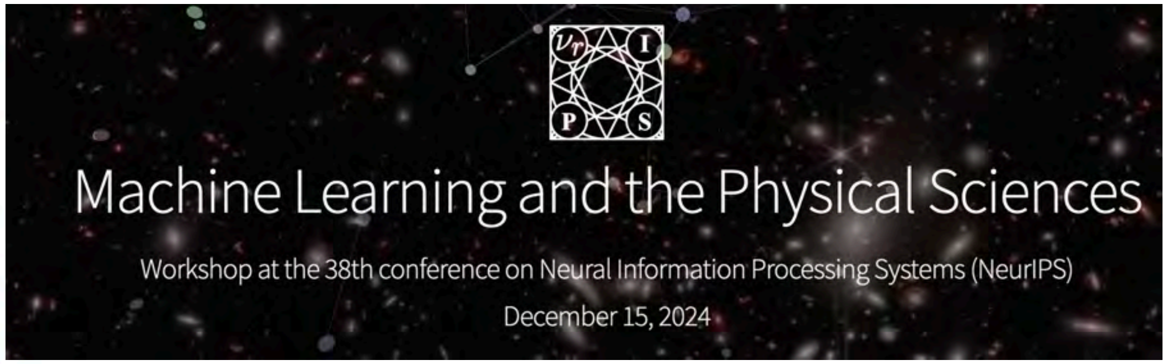
Creating New Spaces for Interdisciplinary Work and Collaboration

https://aiscienceconference.caltech.edu/



Caltech

THE UNIVERSITY OF CHICAGO



https://ml4physicalsciences.github.io/2024/

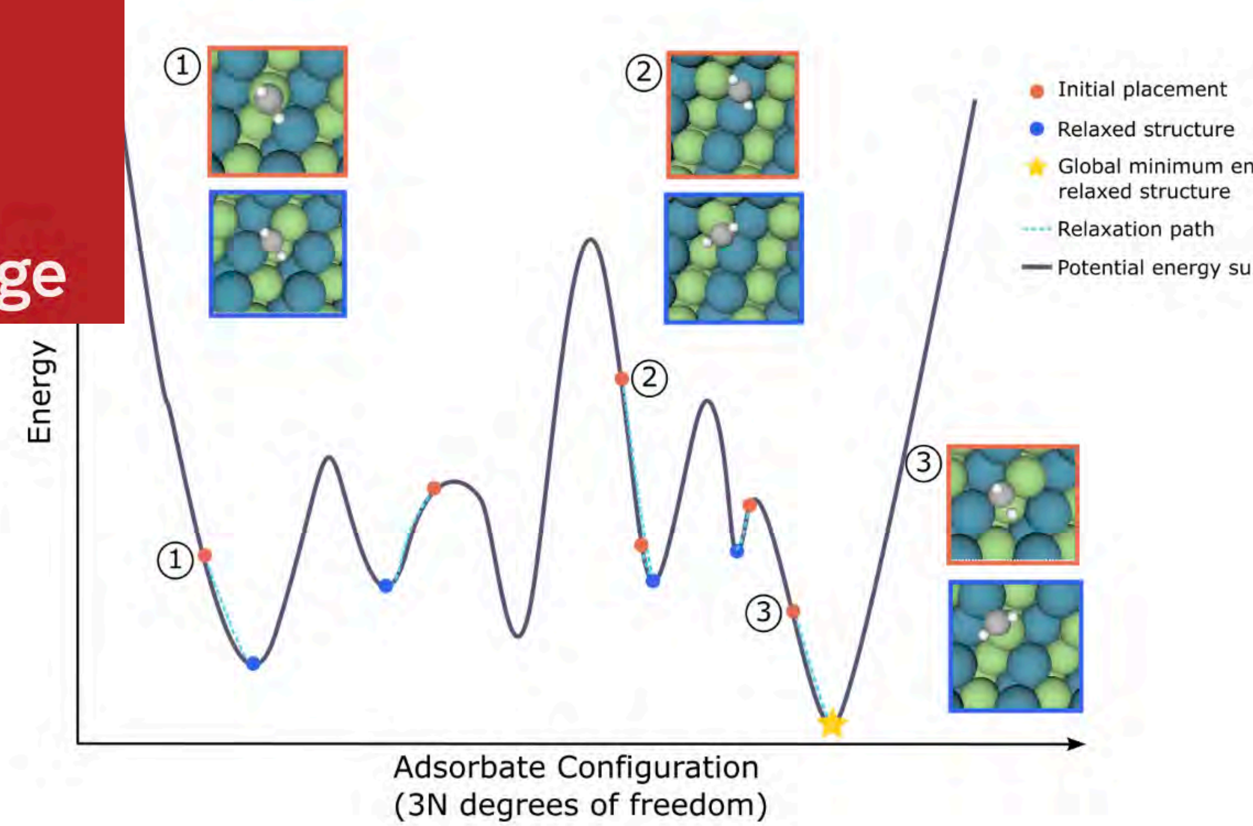
https://www.nsfhdr.org/mlchallenge

https://fair-universe.lbl.gov/

iHARP

NSF HDR ML Challenge

Developing New Models for Academia–Industry Partnership



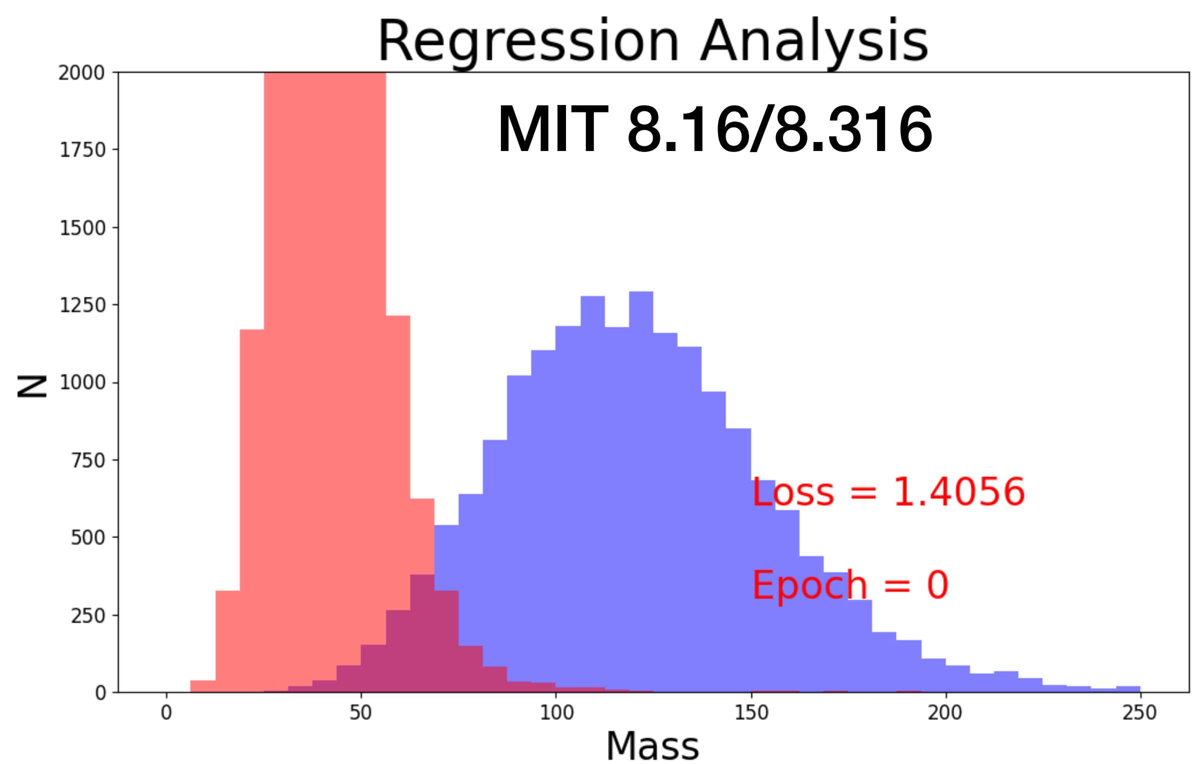
ML Commons

Joint Industry/Academic ML Challenges

Consortiums like MLCommons serve as a forum for unbiased communication

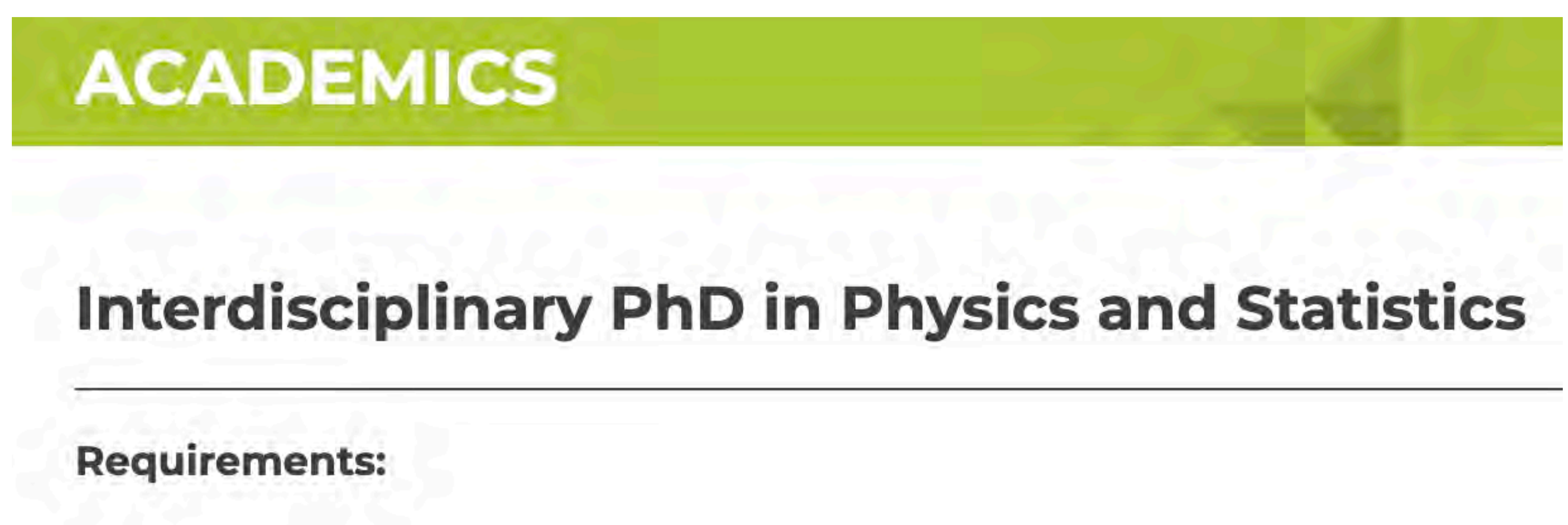
The Role of Education in Fostering Interdisciplinary Research

There is a need for interdisciplinary classes targetting the joint skills needed for research



Computational Data Science in Physics

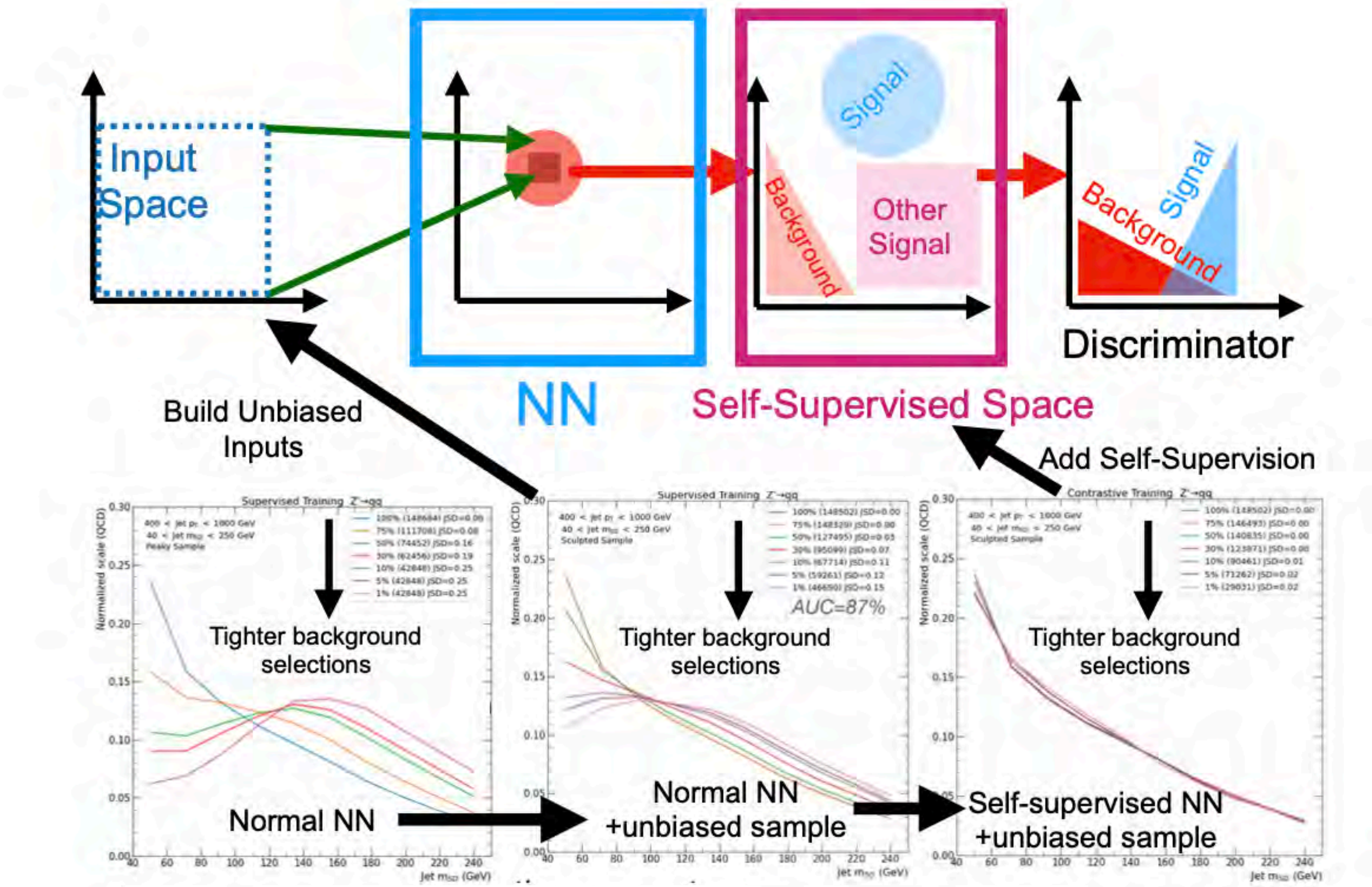
Joint degrees that provide the skillsets and qualifications for interdisciplinary work


ACADEMICS

Interdisciplinary PhD in Physics and Statistics

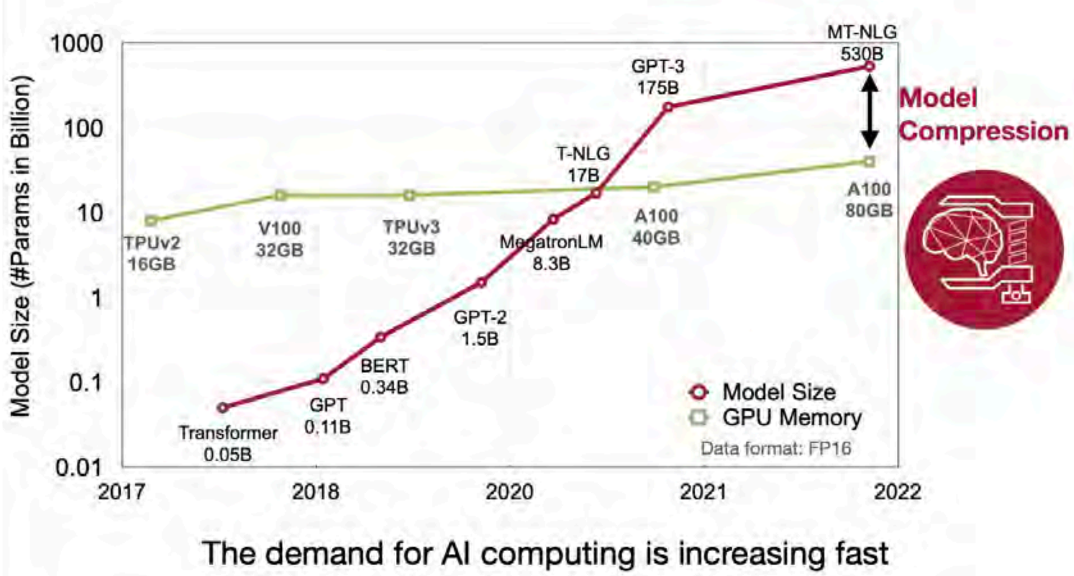
Requirements:

Ethical Considerations



Removing Bias in ML for physics is often objective Leads to robust results

The same cannot be said for other domains



Larger and growing power consumption from larger AI

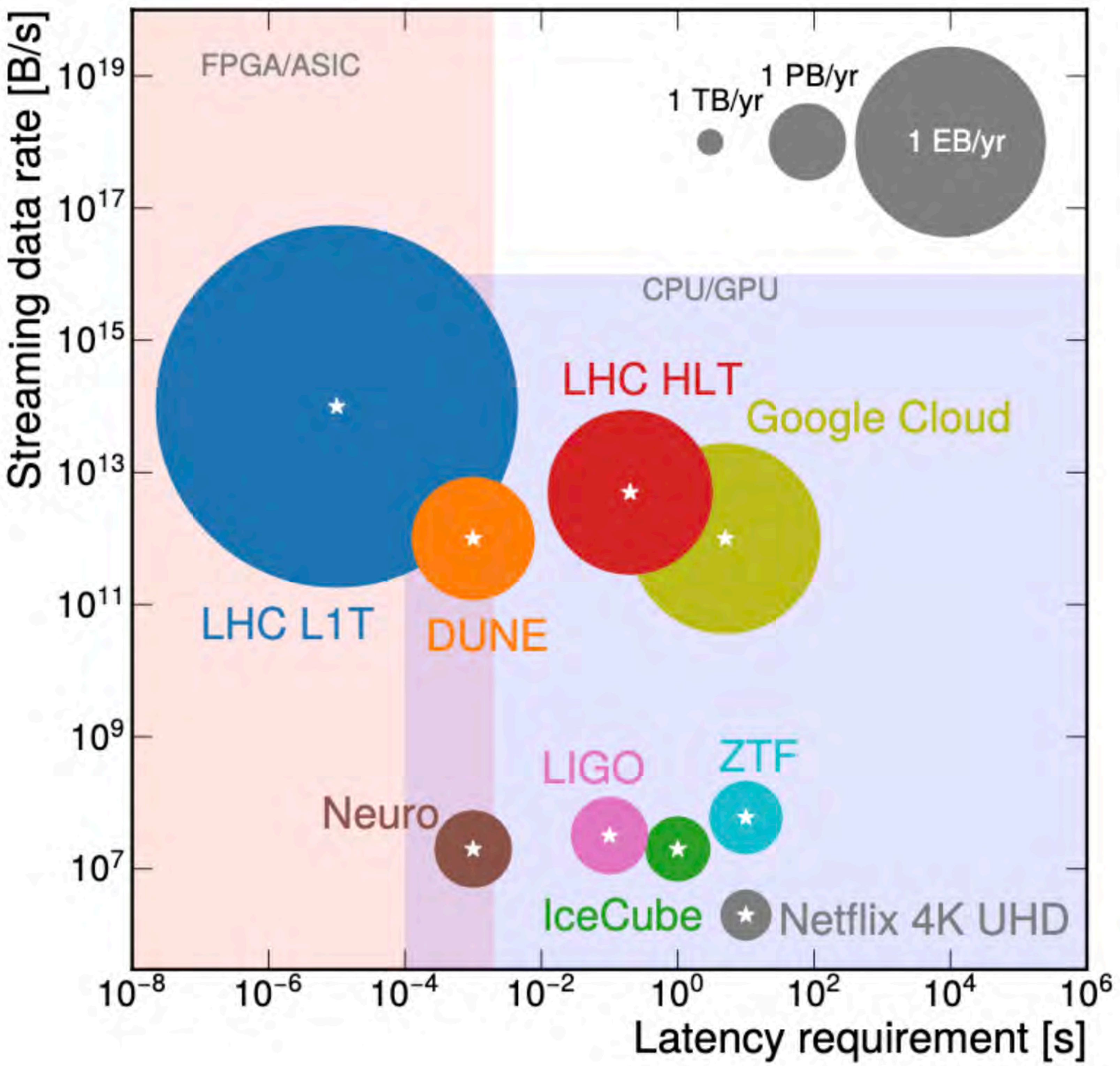
Conclusions

- Facilitating scientific discovery in physics
  - Generative AI offers a powerful set of tools
  - Physics provides a rich set of abstractions and methods for new AI
- Realizing the full potential of generative AI in physics requires
  - Addressing the unique challenges posed by physics
  - Robustness, precision, and interpretability needs bespoke algos
  - An opportunity for the physics community to drive AI
- Unique computational challenges historically pushed developments
- Viable long-term career pathways at intersection of AI and physics
  - May involve rethinking traditional structures and tenure processes

Conclusions

- Fostering collaboration across disciplines is crucial
  - Revisions to departmental structure/interdisciplinary venues
- Education is a critical component in preparing future researchers
  - Interdisciplinary AI and Physics educational programs
- New models for partnership between academia and industry
  - Ensure advances in gen-AI for physics propagate and vice-versa
  - Partnerships can facilitate knowledge-sharing & resource access
- Articulating a clear and compelling vision for future of AI in physics

Thanks!


Streaming data rate [B/s]
Latency requirement [s]
FPGA/ASIC
CPU/GPU
1 TB/yr
1 PB/yr
1 EB/yr
LHC L1T
DUNE
LHC HLT
Google Cloud
Neuro
LIGO
ZTF
IceCube
Netflix 4K UHD