

A futuristic robot head with glowing eyes and a hand to its chin, set against a background of mathematical and scientific formulas. The robot is white and blue, with a glowing orange light in its eye. The background is dark blue with various mathematical and scientific formulas in white and yellow. A large yellow and blue diagonal shape is overlaid on the image.

AI+Science at the University of Chicago

Rebecca Willett

Groundbreaking Discoveries and Translation

- Develop a new understanding of the laws of nature and rules of life
- Accelerate affordable drug development
- Engineer green materials
- Build quantum computers
- Develop sustainable climate policies

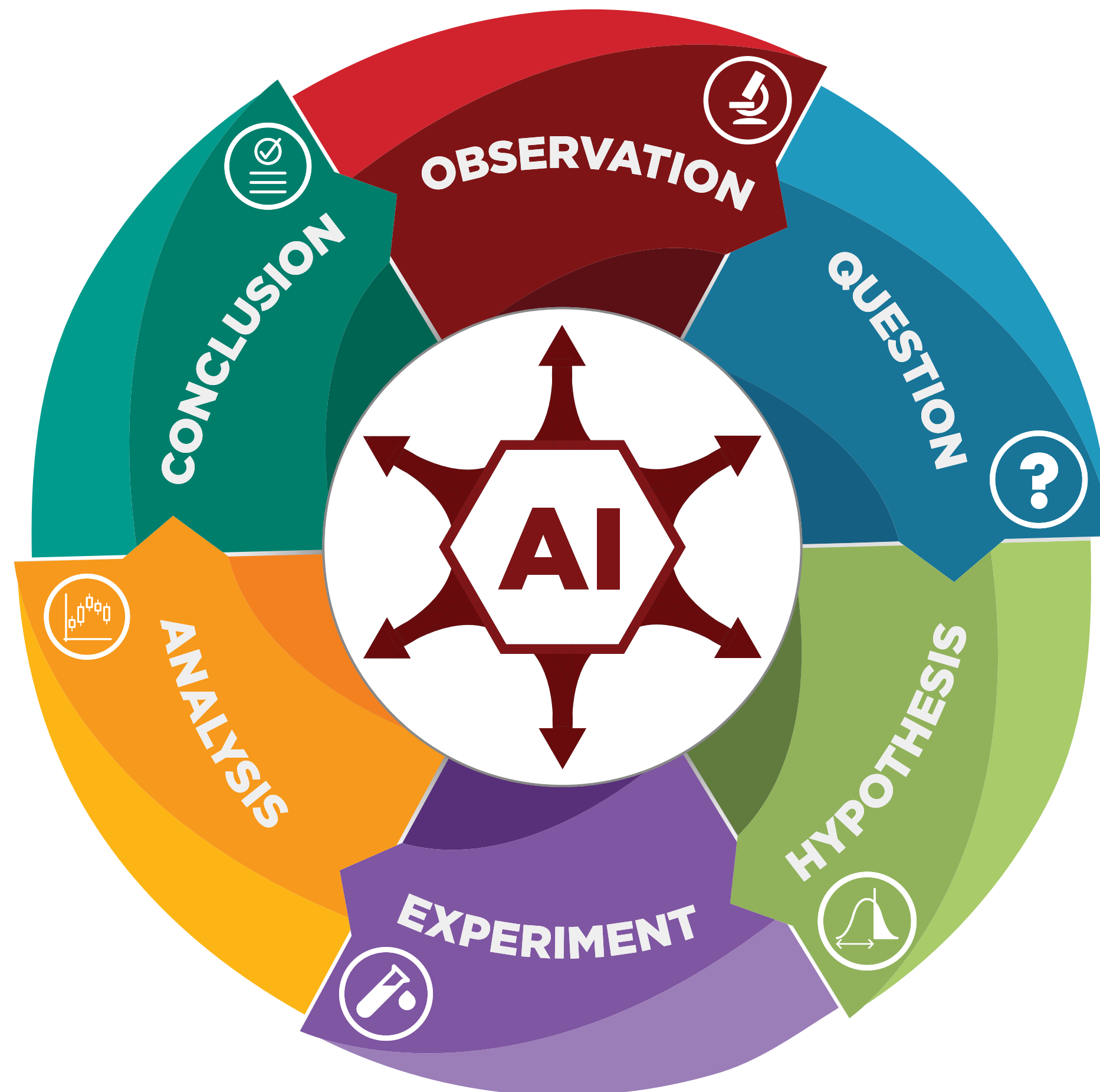


image credit: <https://www.greenbiz.com/article/whats-your-sustainability-moonshot>



THE UNIVERSITY OF CHICAGO

DATA SCIENCE
INSTITUTE



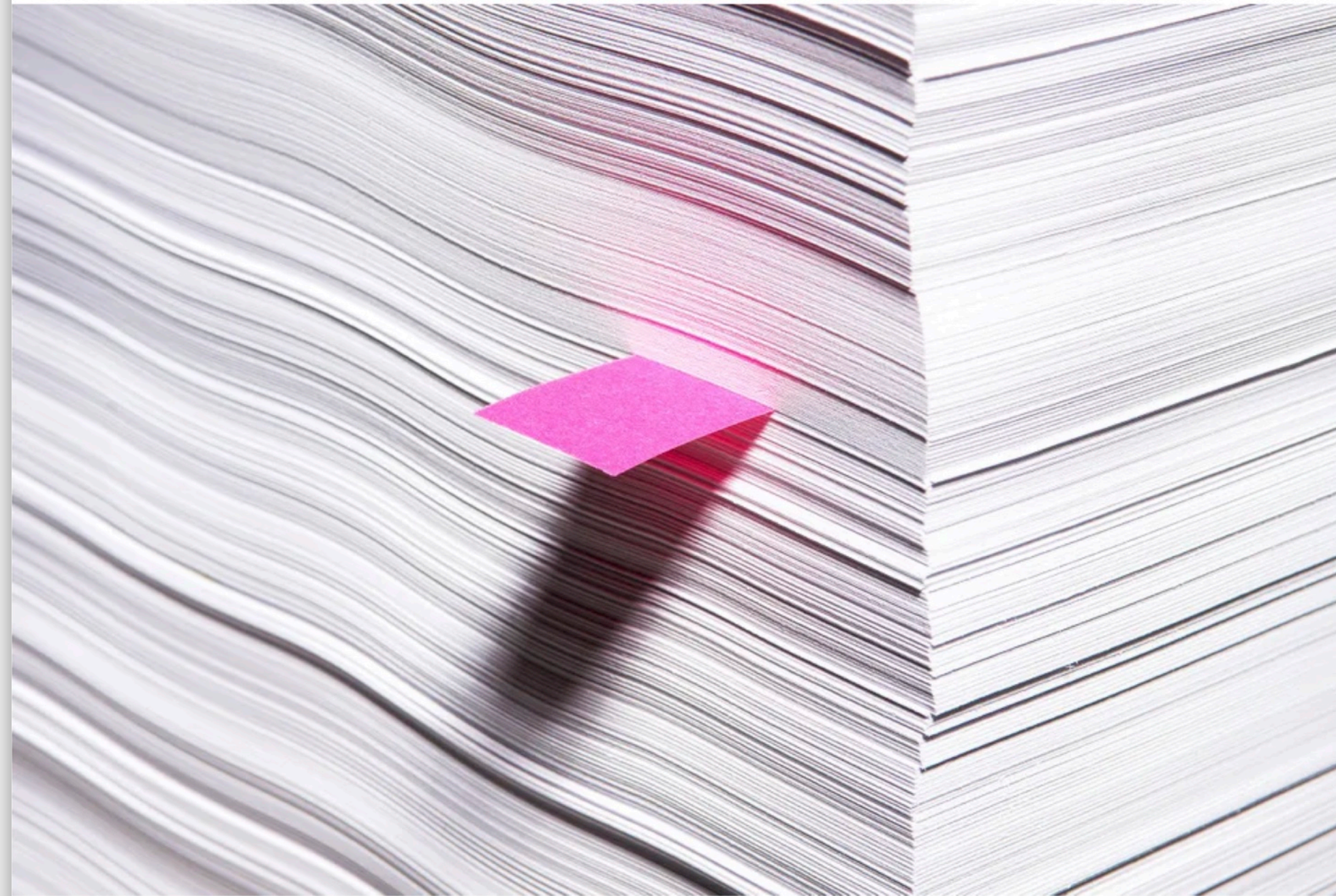
AI will fundamentally change the nature and pace of scientific discovery, influencing data analysis, hypothesis generation, simulation, and experimental design

WIRED

WILL KNIGHT BUSINESS AUG 18, 2022 7:00 AM

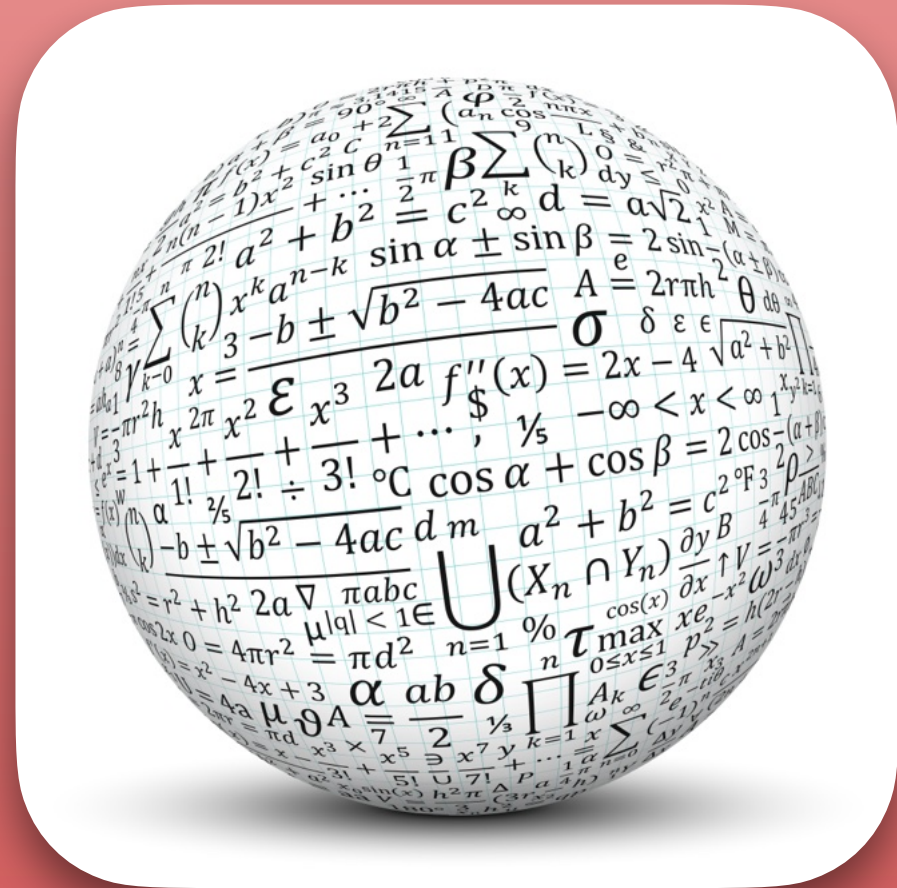
Sloppy Use of Machine Learning Is Causing a 'Reproducibility Crisis' in Science

AI hype has researchers in fields from medicine to sociology rushing to use techniques that they don't always understand—causing a wave of spurious results.



PHOTOGRAPH: PM IMAGES/GETTY IMAGES

Developing **AI4Science** without understanding **AI foundations** is like developing **biotech** without understanding **biology**.



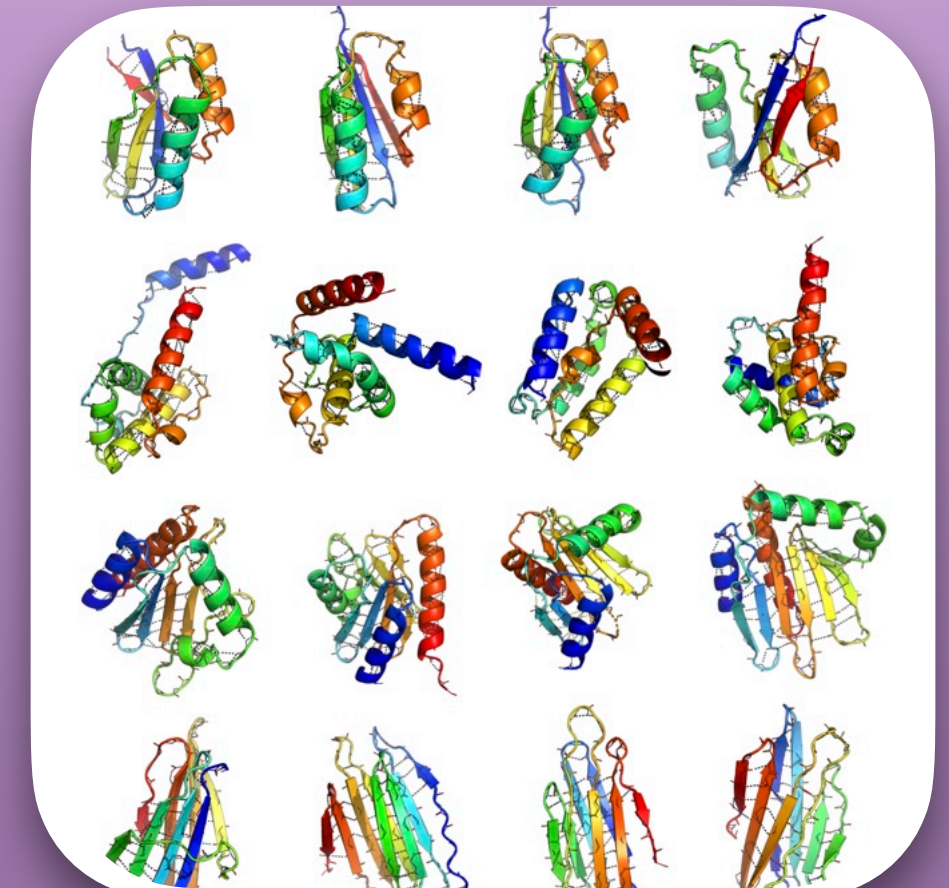
**Uncovering
new laws of
nature**



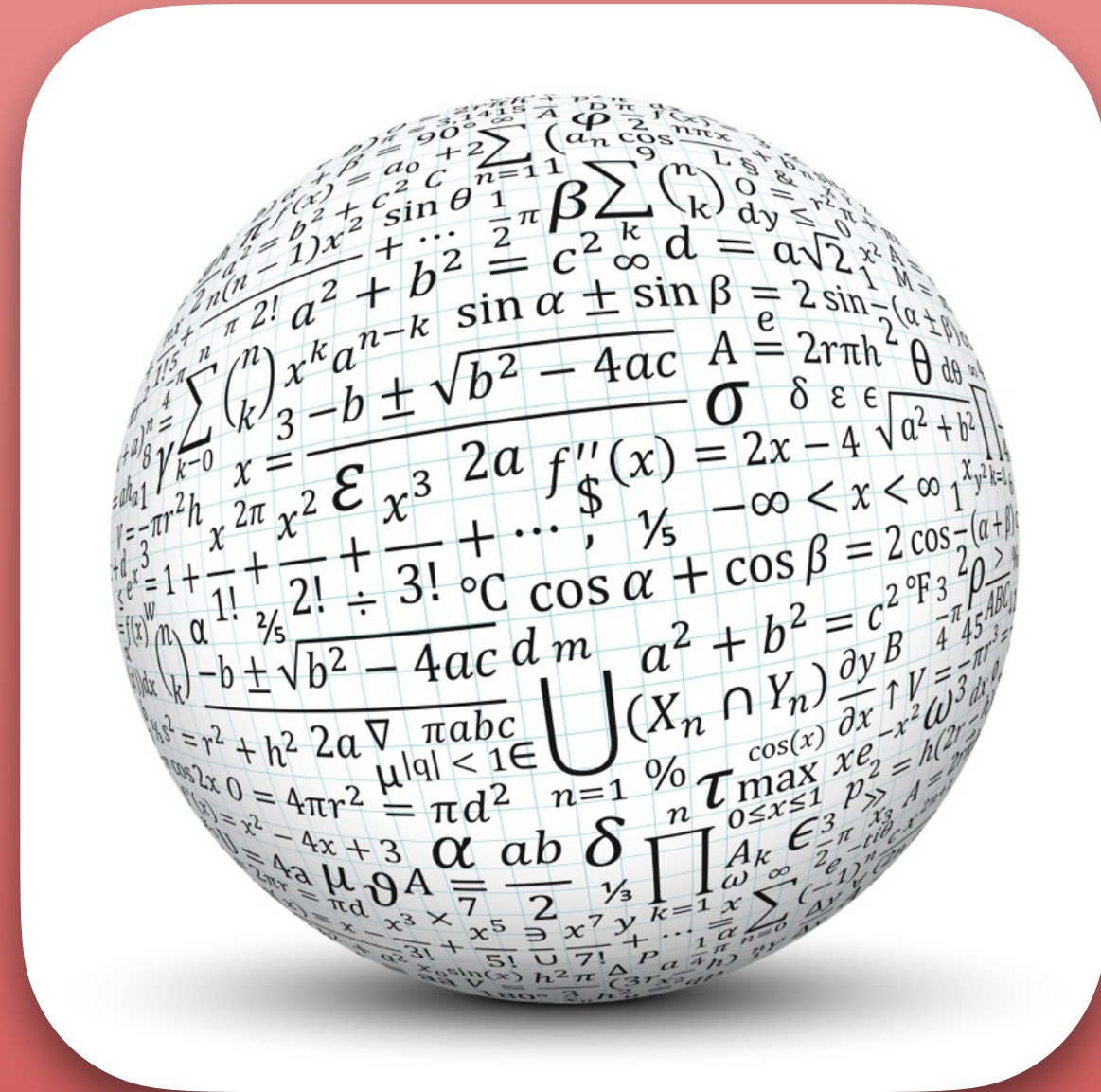
**AI-guided
scientific
measurement**



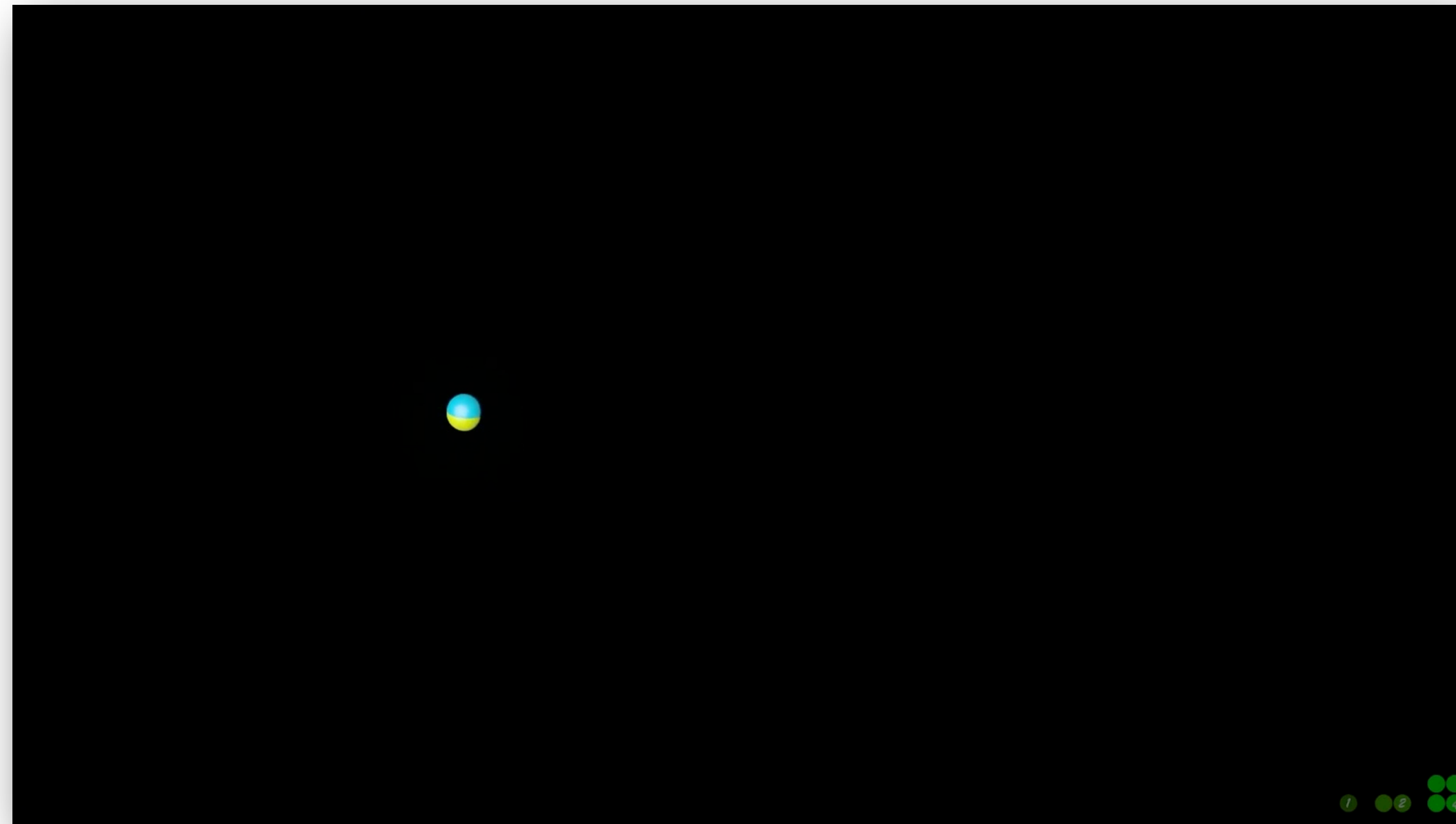
**Physics-
informed
AI**



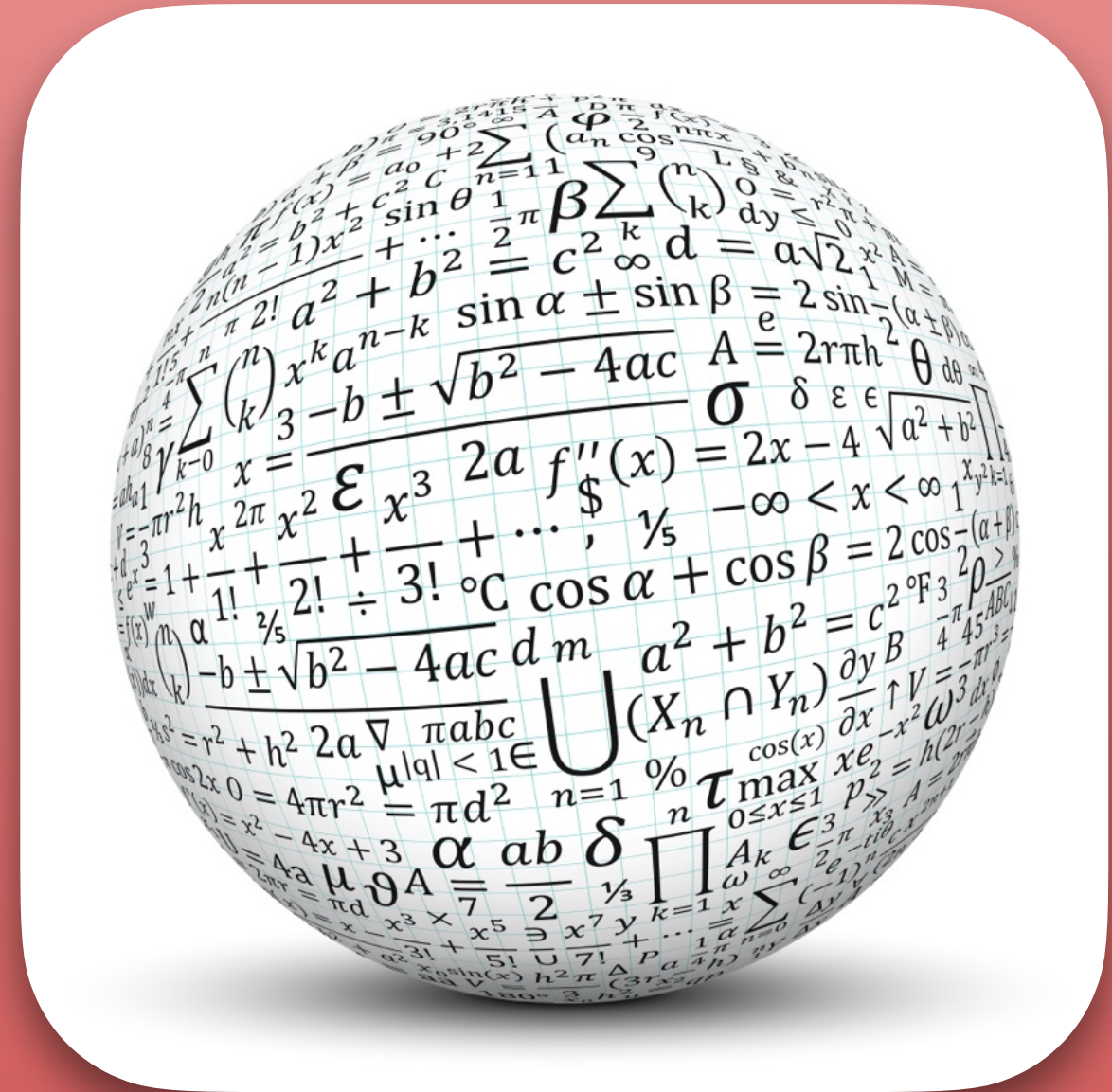
**Generative
AI for
Science**



Given observations
of a system, use AI
to uncover the
governing physical
laws



$$\begin{aligned}\frac{dx}{dt} &= \sigma(y - x) \\ \frac{dy}{dt} &= x(\rho - z) - y \\ \frac{dz}{dt} &= xy - \beta z\end{aligned}$$



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Experiment



ML Prediction



Vincenzo Vitelli



Use AI to design
better
experiments,
simulations, and
sensors



Seppie Kuehn —
adaptive design of
microbial communities

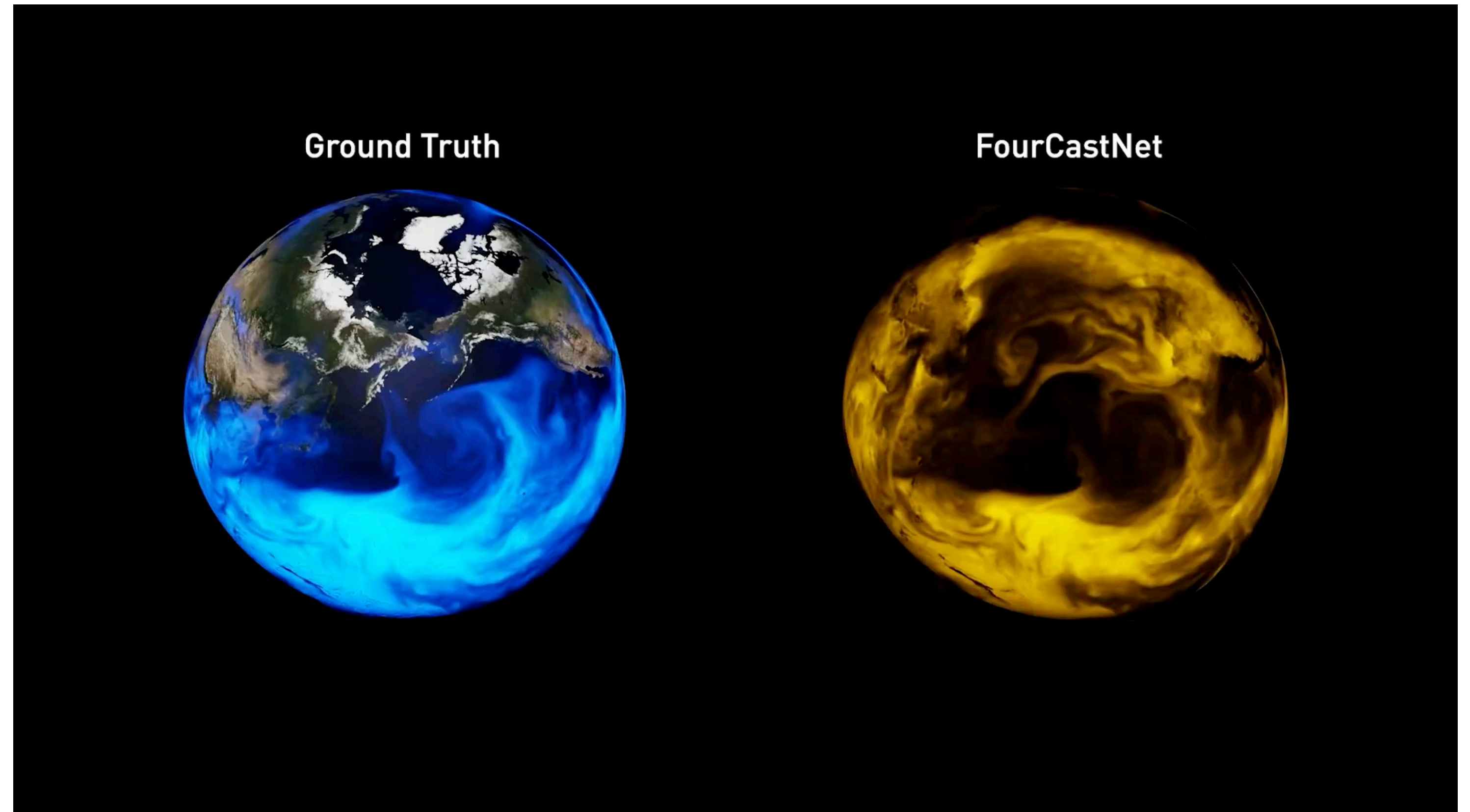
Rina Barber —
uncertainty
quantification
foundations

The screenshot shows the AWS logo at the top left, followed by a navigation menu with links for Products, Solutions, Pricing, Documentation, Learn, Partner Network, AWS Marketplace, and Customer. Below the navigation is a secondary menu with 'AWS Blog Home', 'Topics', and 'Edition'. The main content area features the 'AWS Machine Learning Blog' header, the article title 'Introducing Fortuna: A library for uncertainty quantification', the authors 'by Gianluca Detommaso, Alberto Gasparin, Cedric Archambeau, Michele Donini, Matt and Andrew Gordon Wilson', the date 'on 16 DEC 2022', and the categories 'in Amazon Machine Learning, Artificial Intelligence, Foundational (100)'. There are also links for 'Permalink', 'Comments', and 'Share'. The article text begins with 'Proper estimation of predictive uncertainty is fundamental in applications that involve decisions. Uncertainty can be used to assess the reliability of model predictions, trigger intervention, or decide whether a model can be safely deployed in the wild.'

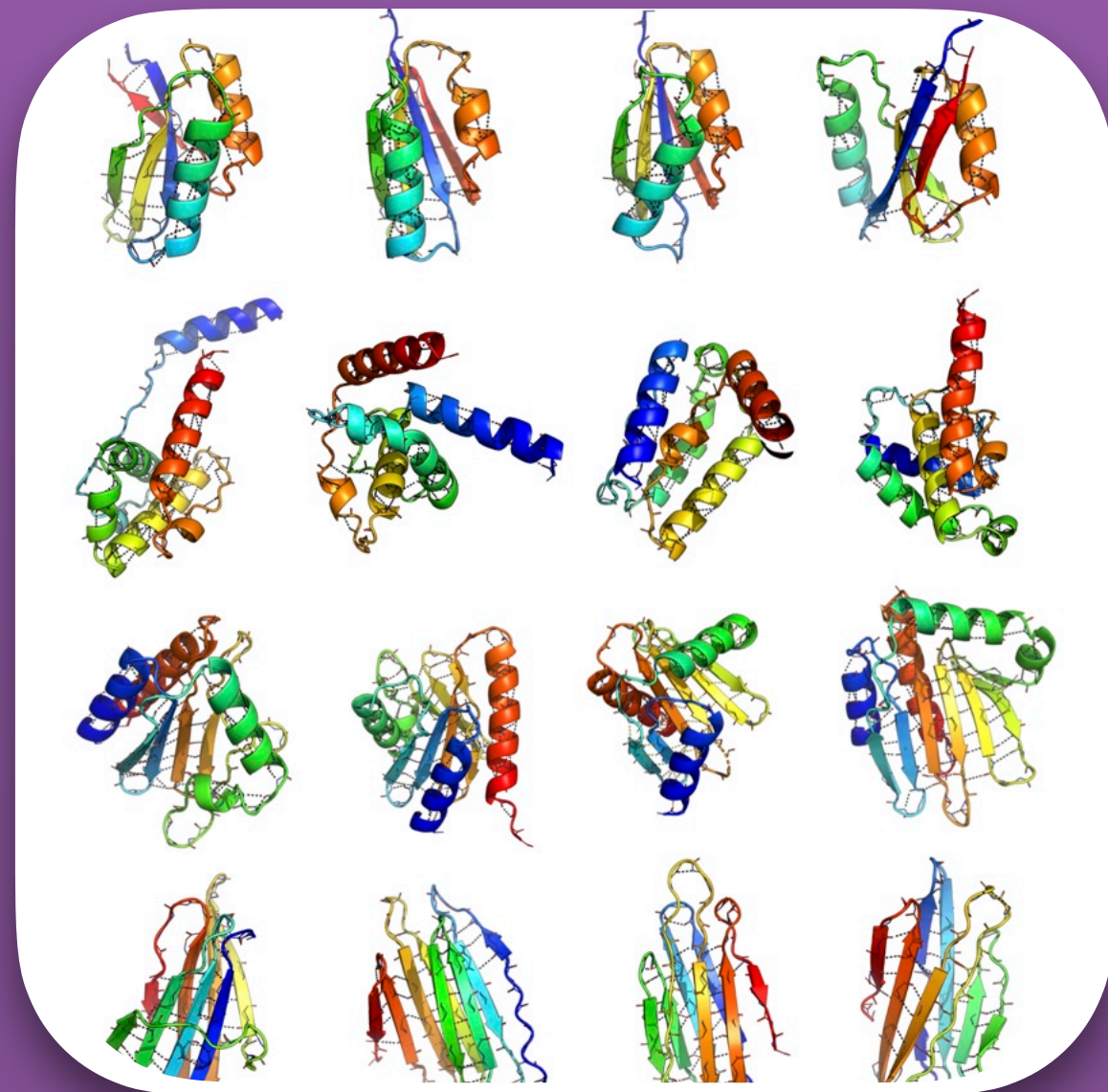


Optimally leverage
physical models
and experimental
or observational
data

Pedram Hassanzadeh —
learned emulators of climate simulations

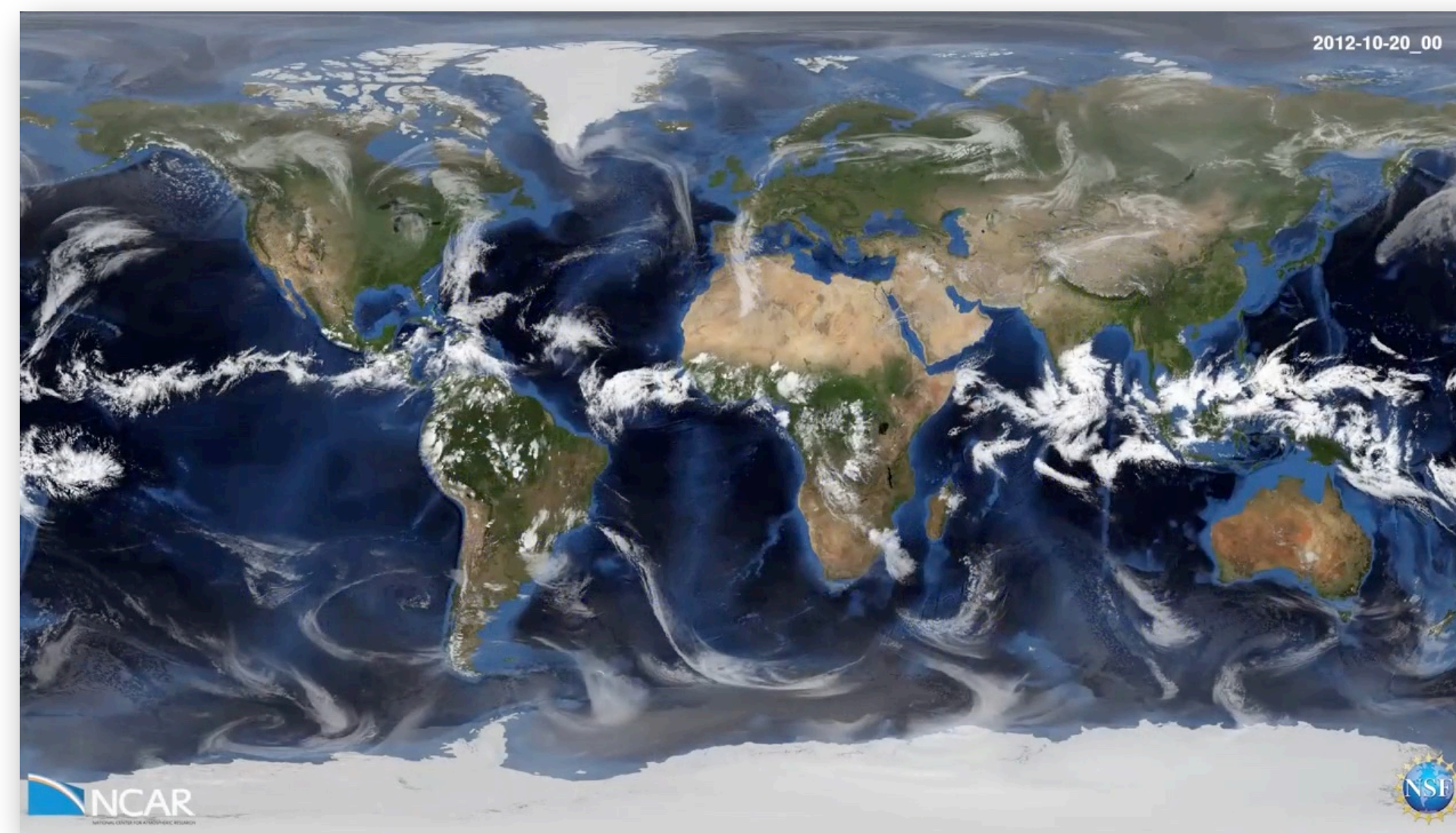


https://www.youtube.com/watch?v=nuT_U1AQz3g



Generate new examples of physical objects or processes to aid discovery

- Chaotic systems exhibit extreme sensitivity to initial conditions
- Emulators trained to give accurate “point” forecasts (e.g. small MSE) are doomed to failure past a short-term horizon

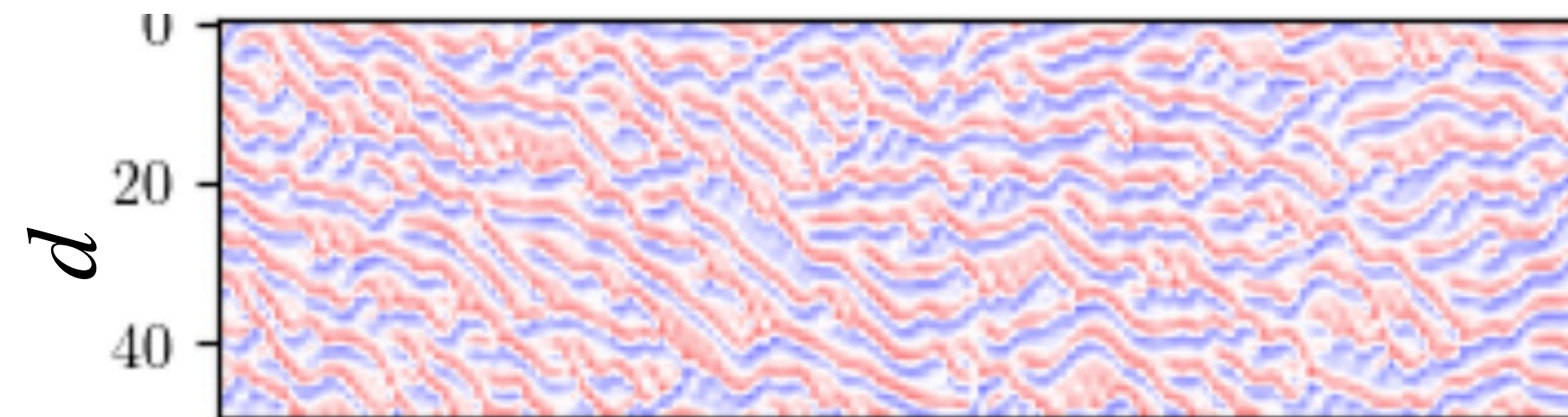


Emulators are important for understanding statistical trends (e.g., hurricane frequency and severity over long time horizons)

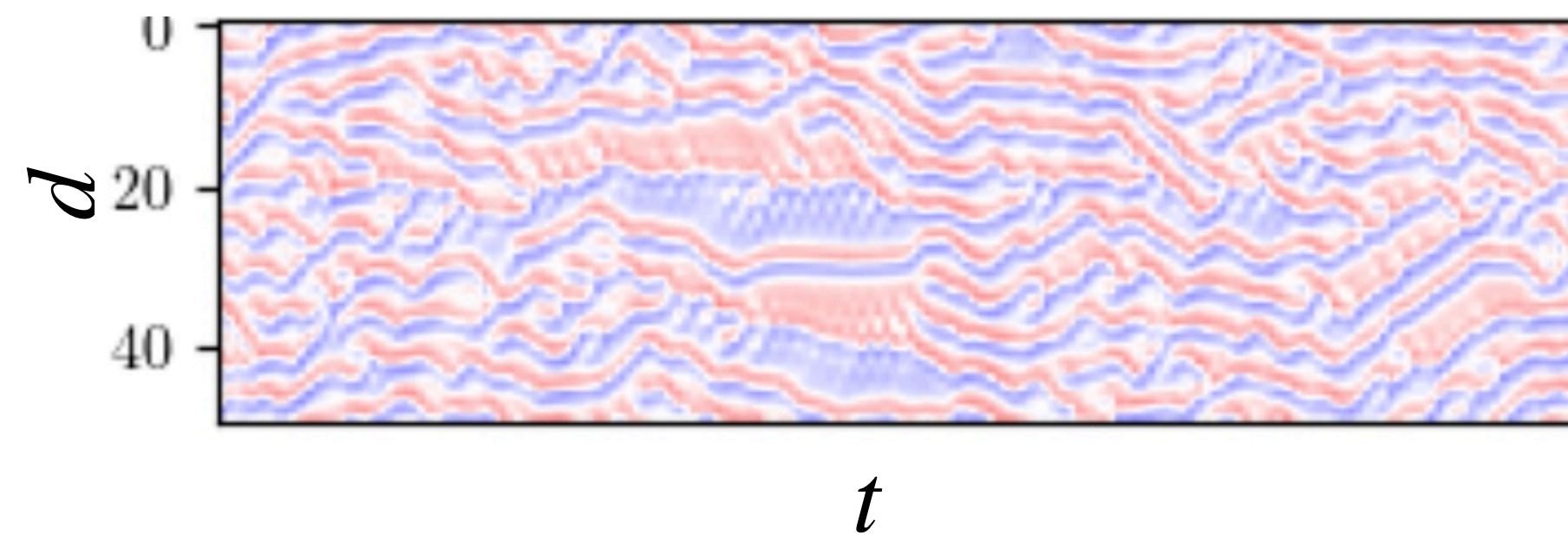
Failure of MSE-minimizing emulators

Kuramoto-Sivashinsky equation

Truth

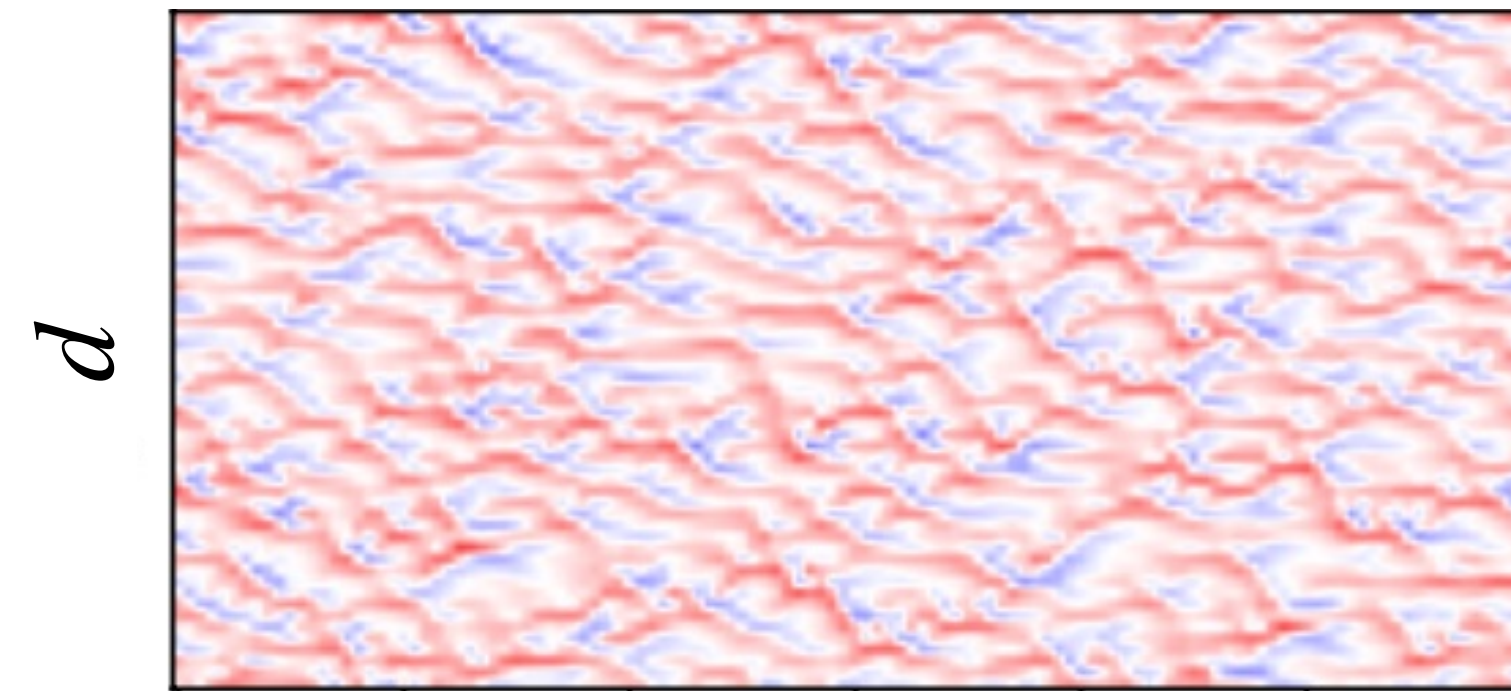


low MSE emulation result

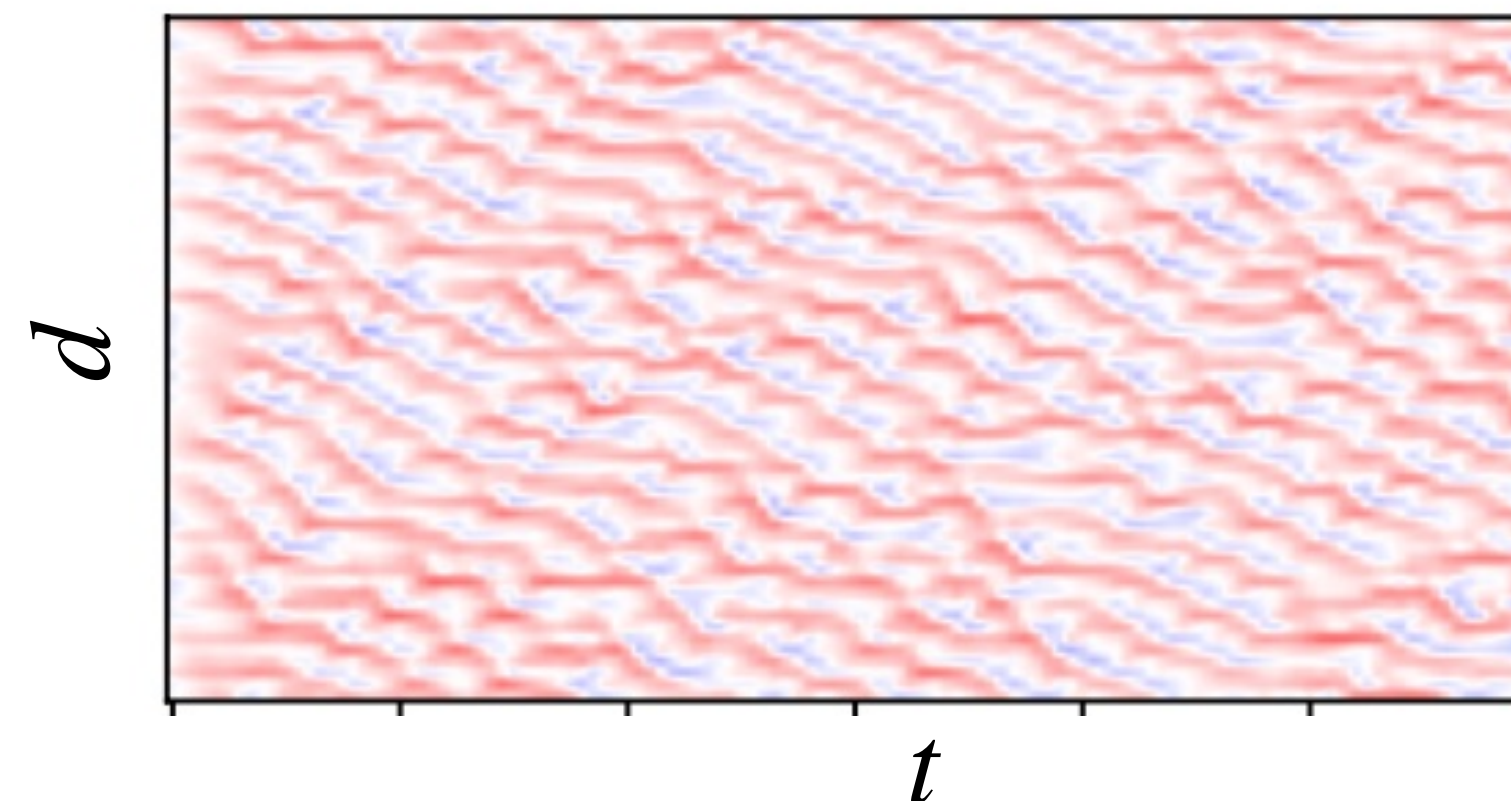


Lorenz 96 ODE

Truth



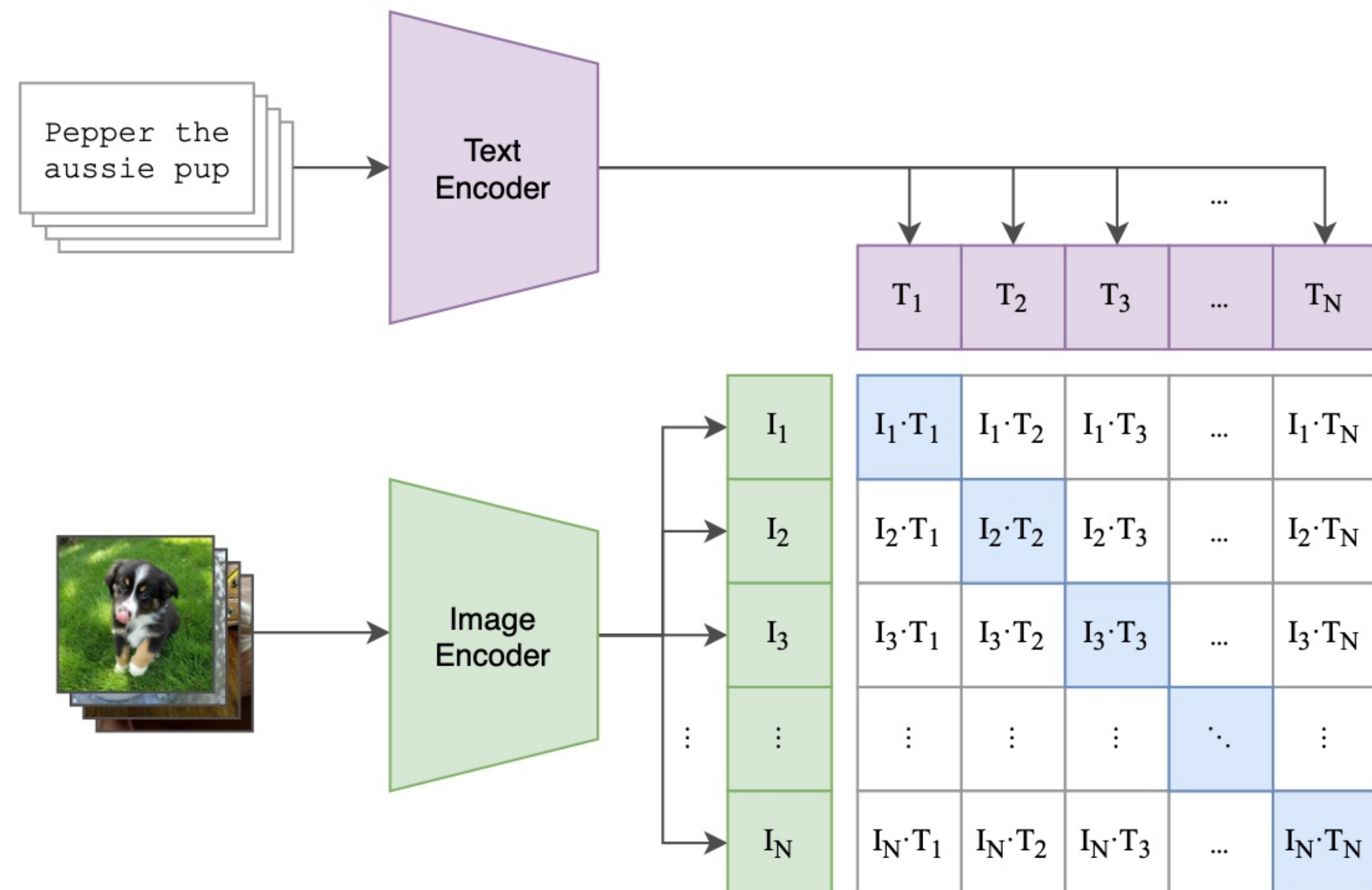
low MSE emulation result



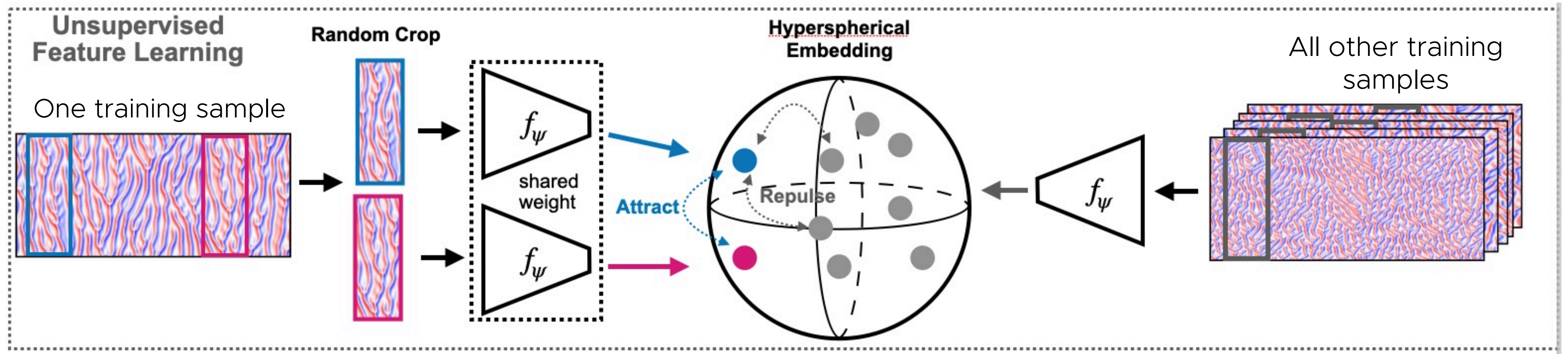
A new hope

- Instead of focusing on small MSE, want emulator to **preserve invariant measures of chaotic attractors** and the corresponding time-invariant statistics
- **Contrastive learning preserves chaotic attractors**

Example: CLIP
(Contrastive Language-
Image Pre-training)



Unsupervised contrastive feature loss (CL)



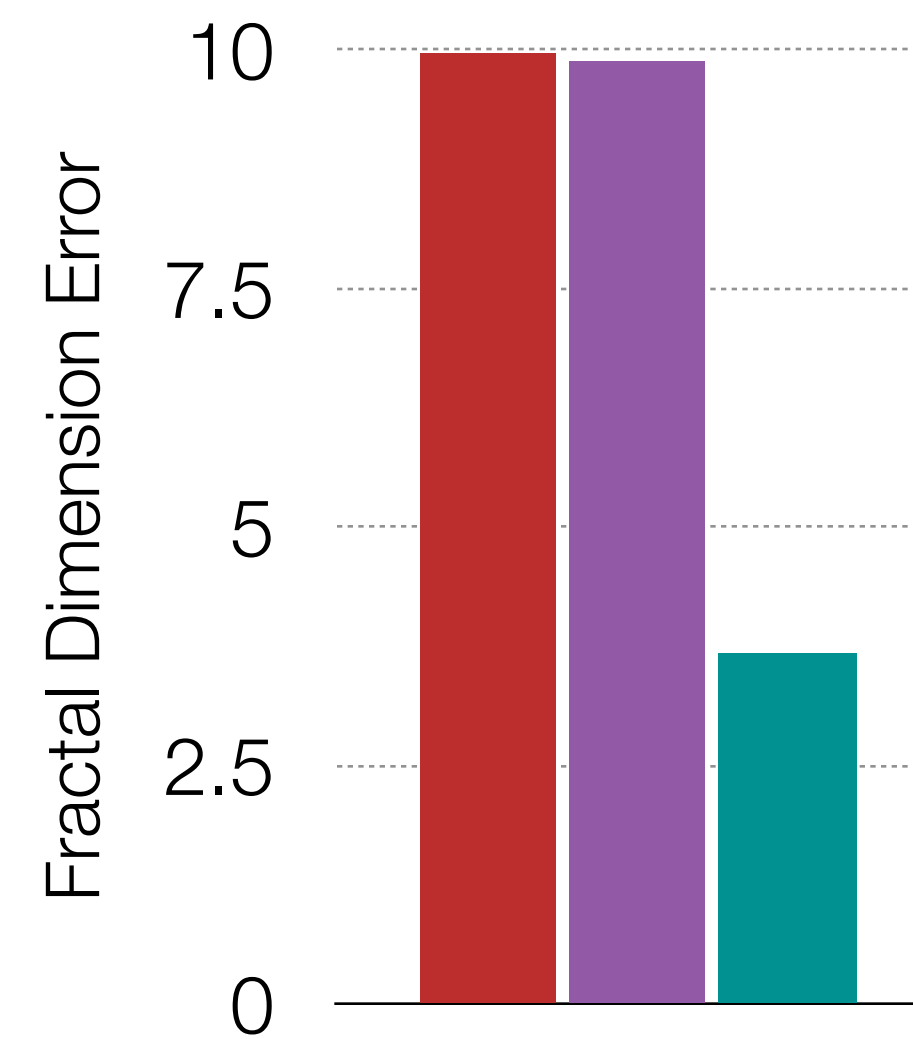
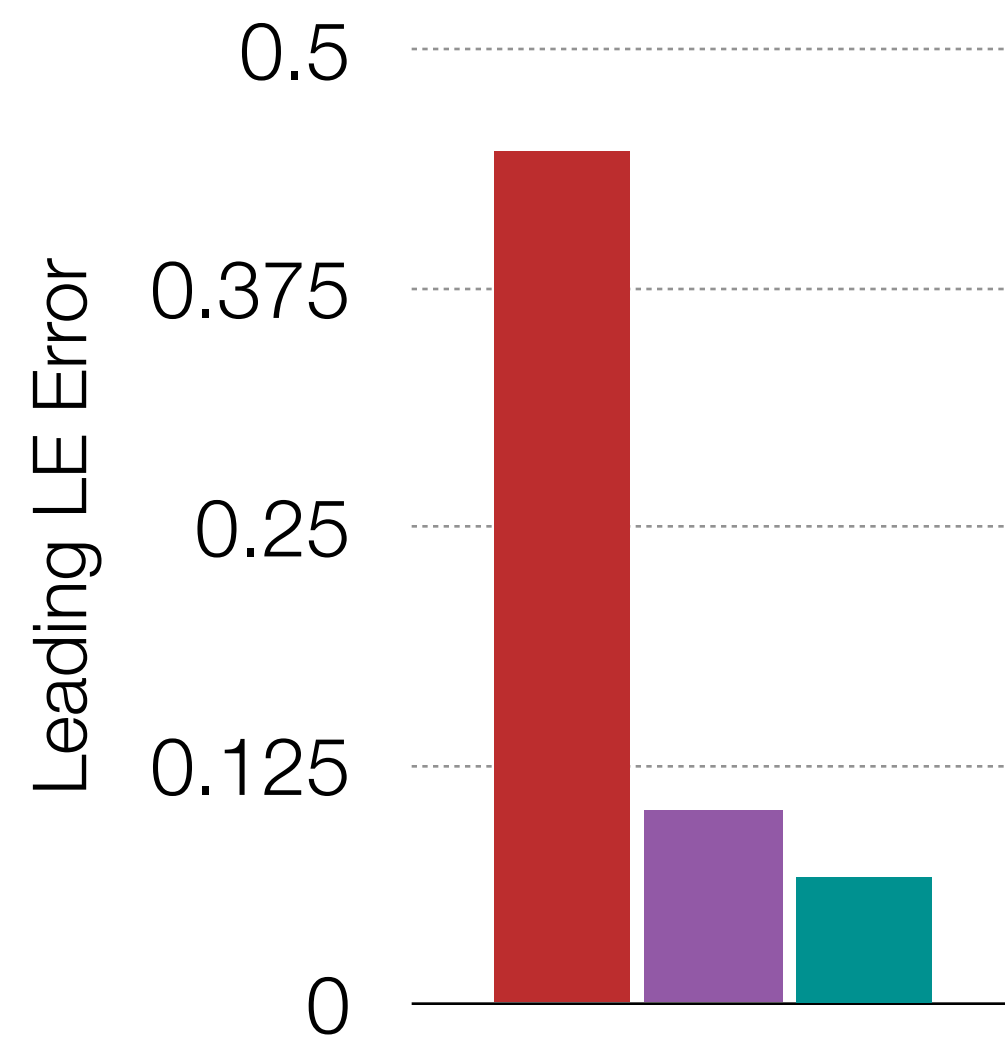
Learn embedding of short time windows so that:

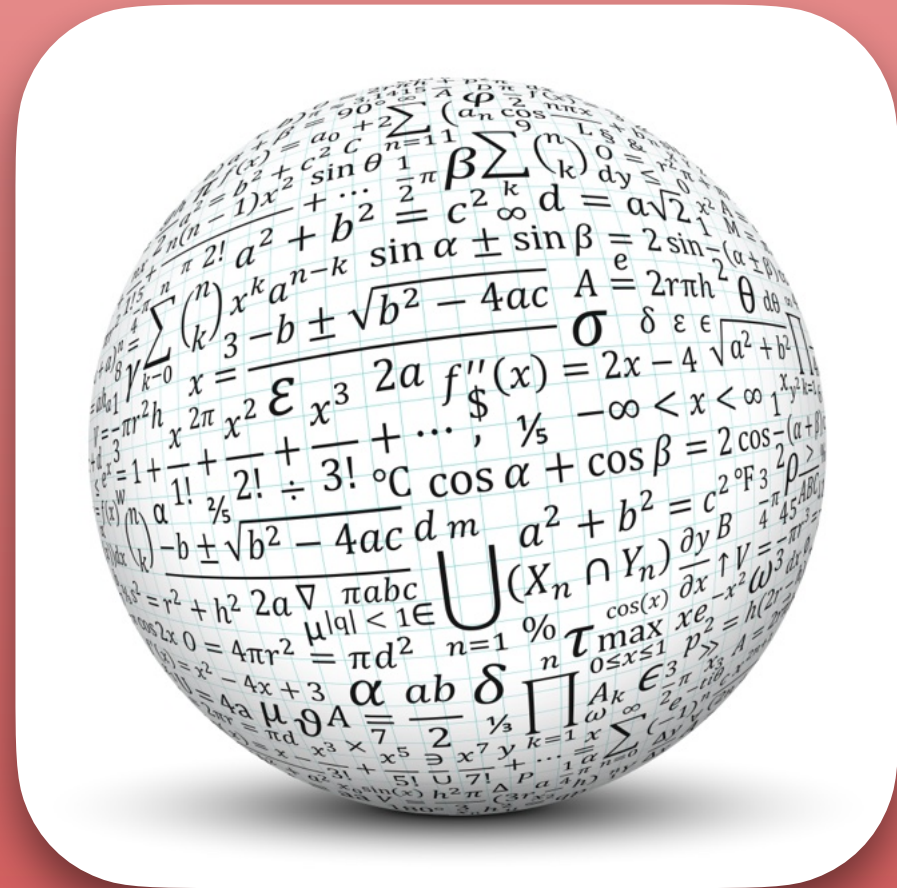
- two time windows from same simulation (i.e. with same chaotic attractors) are nearby in embedding space and
- two time windows from different simulations are far away in embedding space

Lorenz 96 Illustration

(Unknown) governing equation: $\frac{du_i}{dt} = (u_{i+1} - u_{i-2})u_{i-1} - u_i + F$

- MSE loss
- Optimal transport loss (assume extra knowledge)
- Contrastive loss





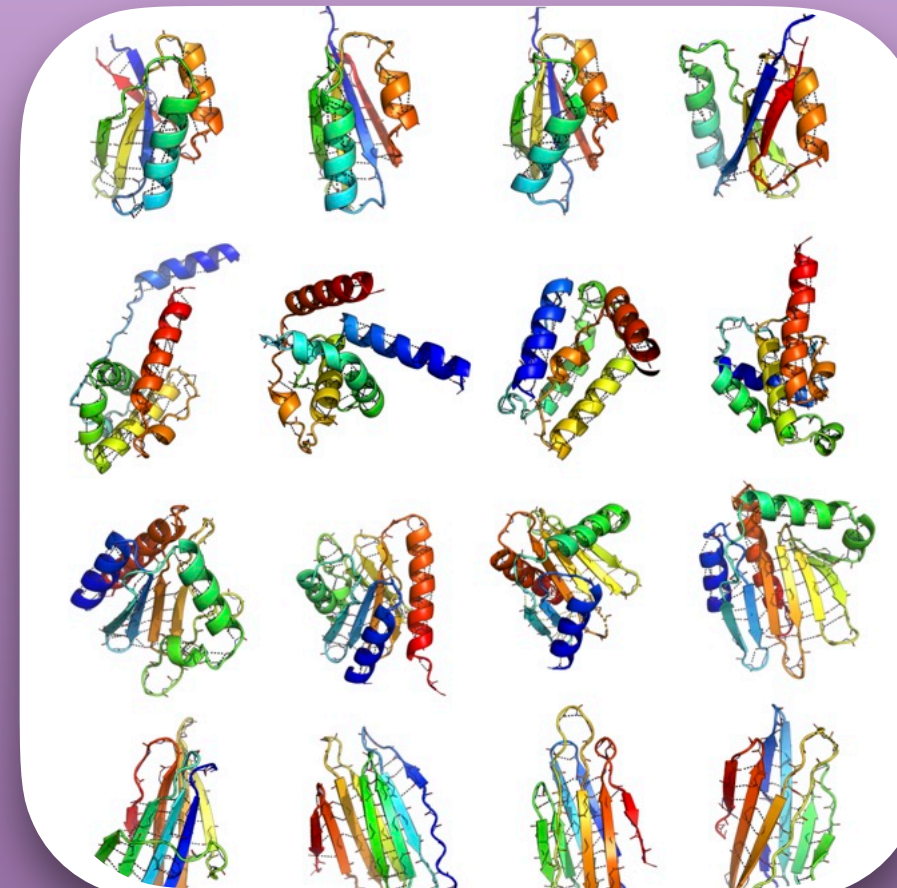
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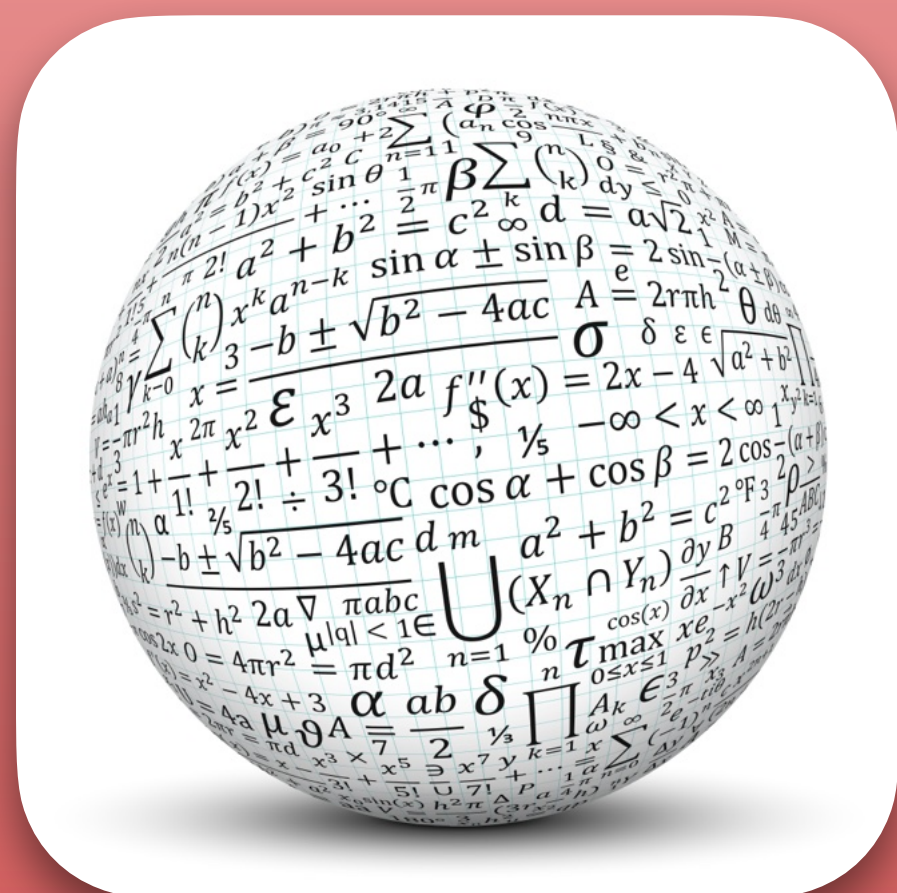
**AI-guided
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**Physics-
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**Generative
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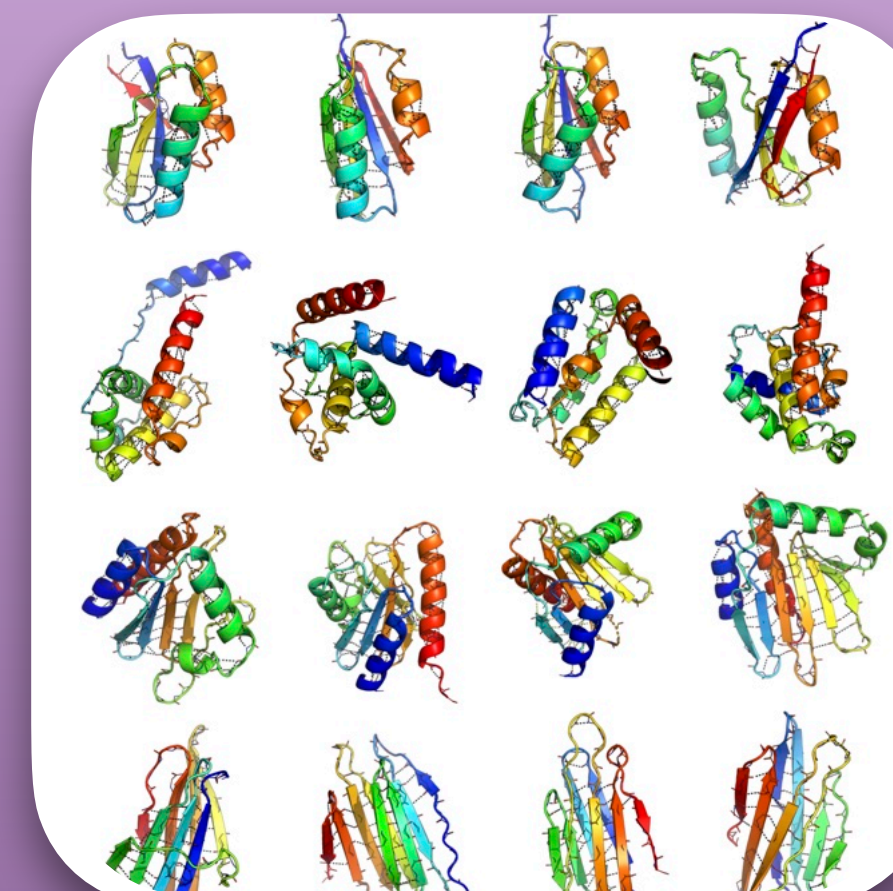
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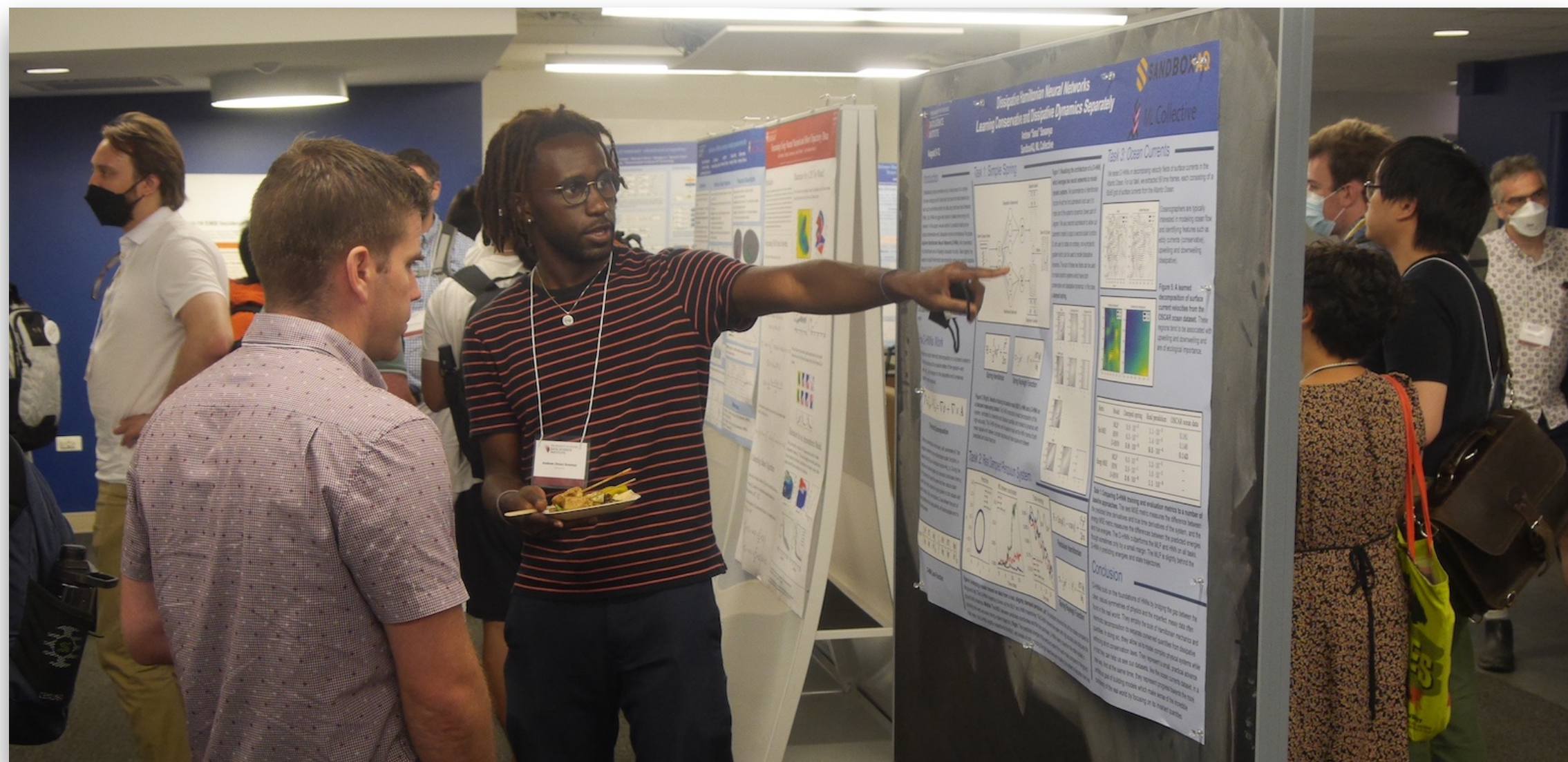


**Physics-
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AI Foundations





Training activities (summer schools, workshops, cross-disciplinary collaborations) **catalyze** ground-breaking research and **accelerate** workforce development



Key Catalysts

- Cross-disciplinary co-mentoring
- “Unseminars”, including free-form Q&A sessions with experts
- Summer schools: 208 trainees from 66 institutions
- Conferences: 4600 views of conference videos
- Annual retreats
 - Communications workshops
 - Carefully designed science brainstorming sessions with cross-disciplinary teams

The Eric and Wendy Schmidt AI in Science Postdoctoral Fellowship



National Institute for Theory
and Mathematics in Biology



SIMONS
FOUNDATION

AI foundations fuel **AI4Science**
like **biology** fuels **biotech**.

Thank you!

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