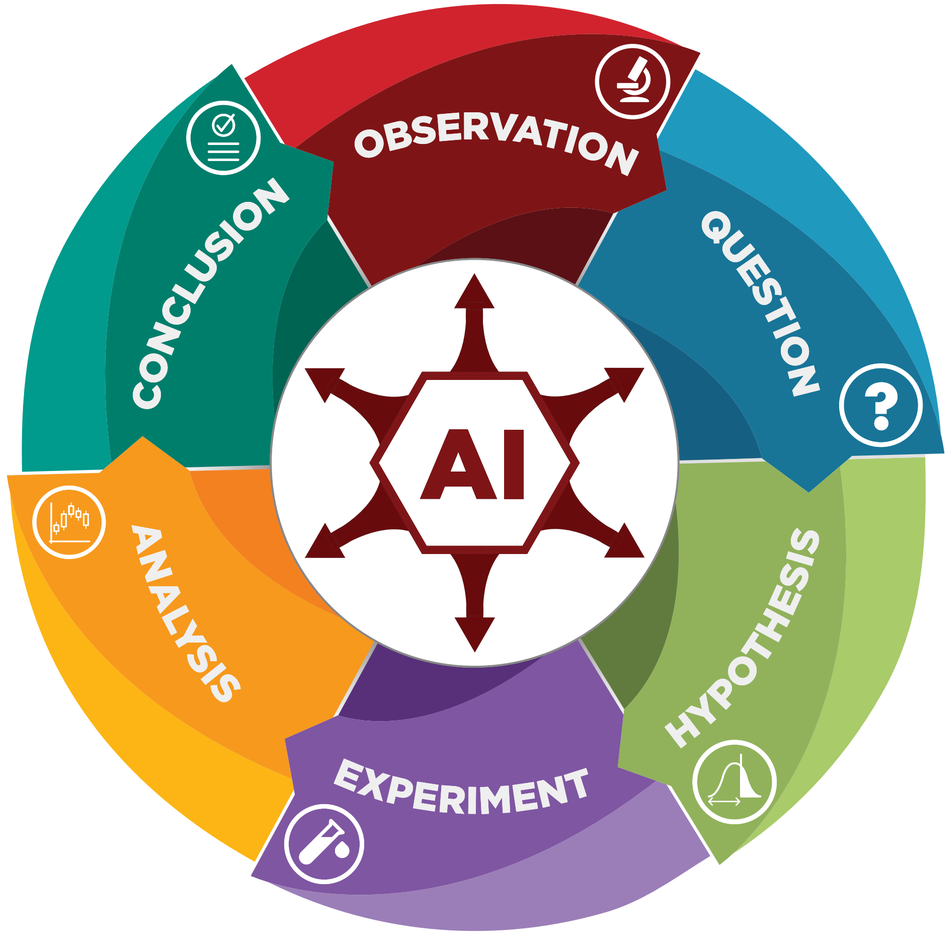
AI+Science at the University of Chicago

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

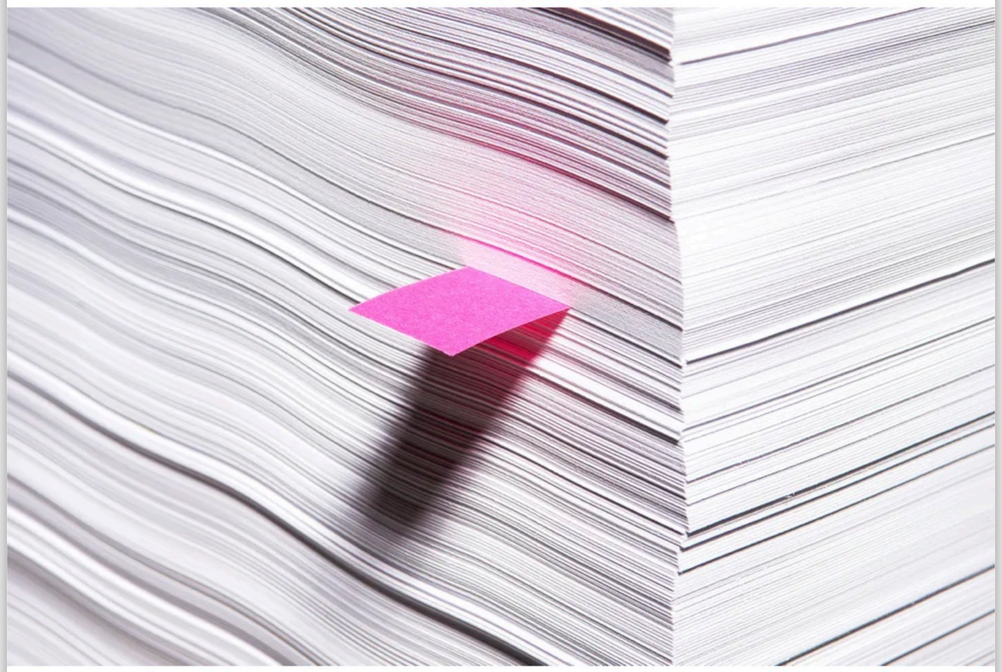
AI will fundamentally change the nature and pace of scientific discovery, influencing data analysis, hypothesis generation, simulation, and experimental design

WIRED

WILL KNIGHT BUSINESS AUG 10, 2022 7:00 AM

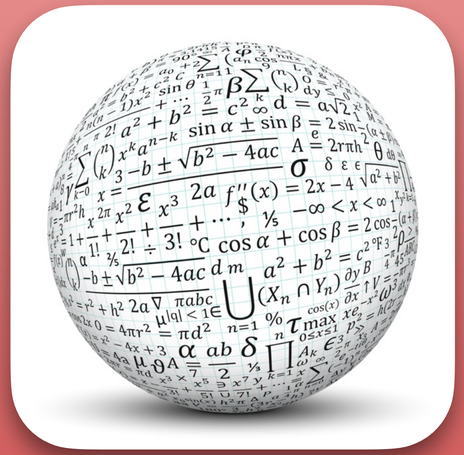
Sloppy Use of Machine Learning Is Causing a 'Reproducibility Crisis' in Science

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

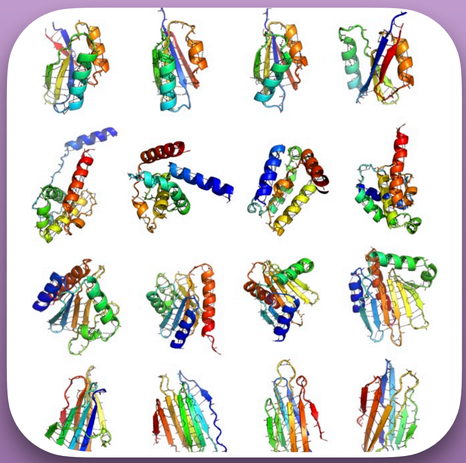
Developing **AI4Science** without understanding **AI foundations** is like developing **biotech** without understanding **biology**.



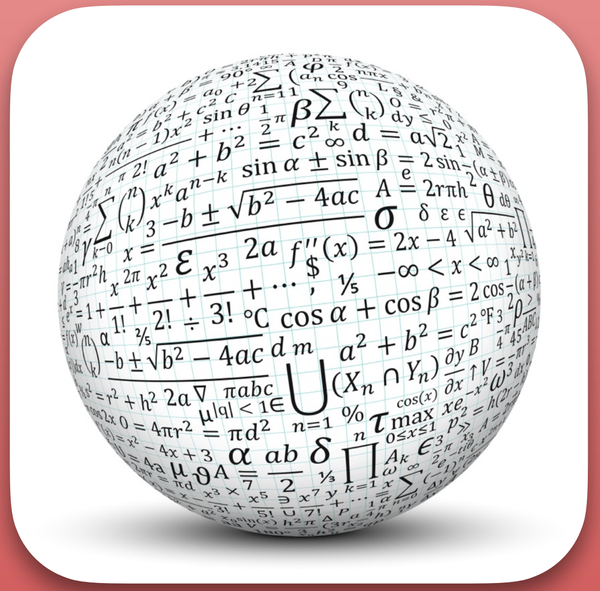
Uncovering new laws of nature

AI-guided scientific measurement

Physics-informed AI



Generative AI for Science



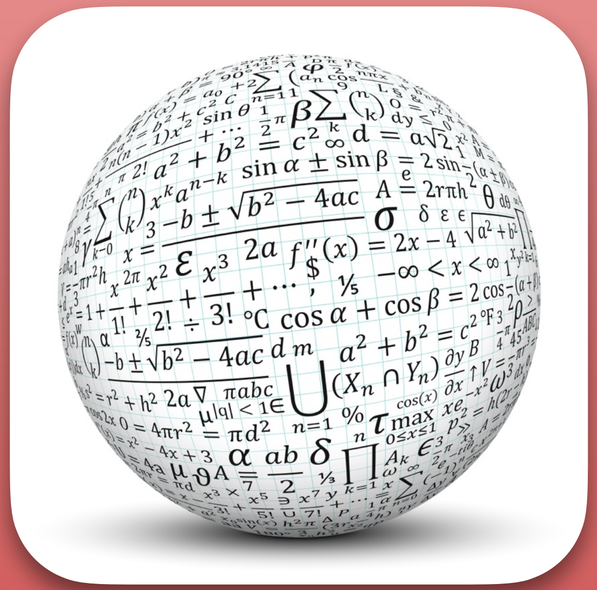
Given observations of a system, use AI to uncover the governing physical laws

$$\frac{dx}{dt} = \sigma(y - x)$$

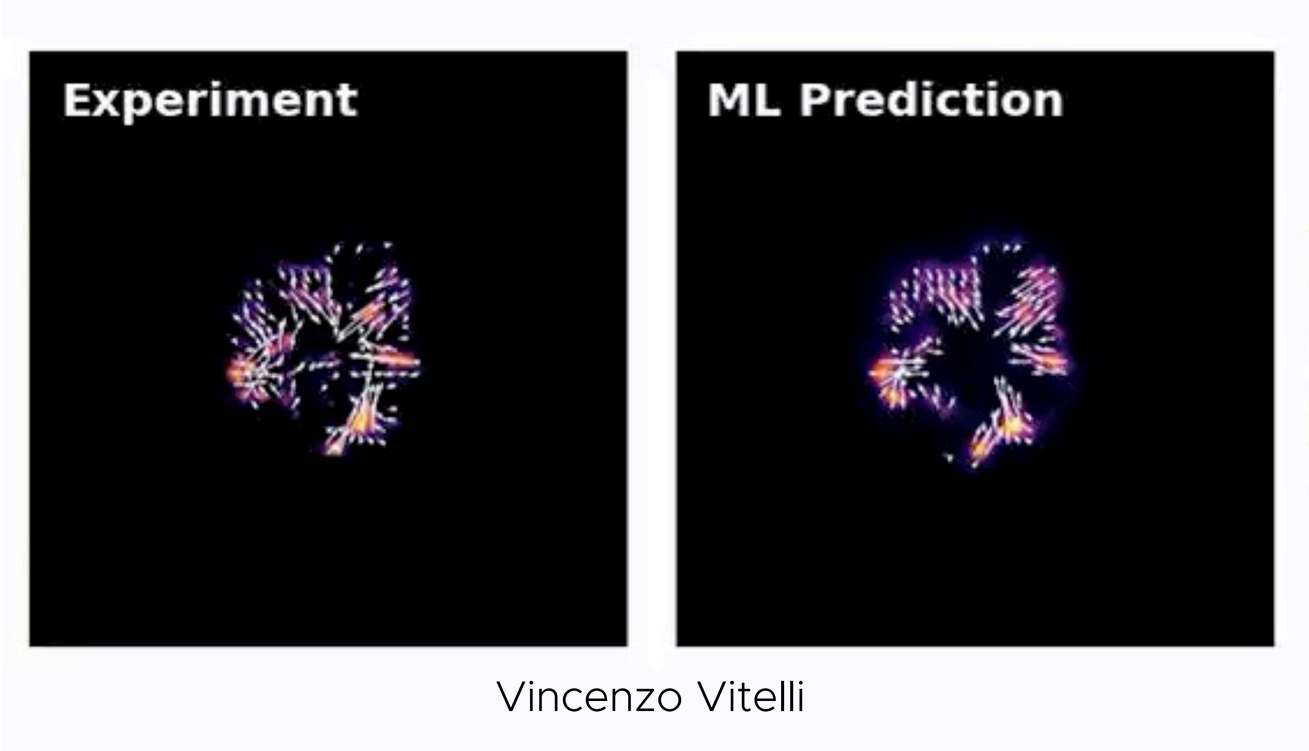
$$\frac{dy}{dt} = x(\rho - z) - y$$

$$\frac{dz}{dt} = xy - \beta z$$

https://www.youtube.com/watch?v=q3kNHomvU0k



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

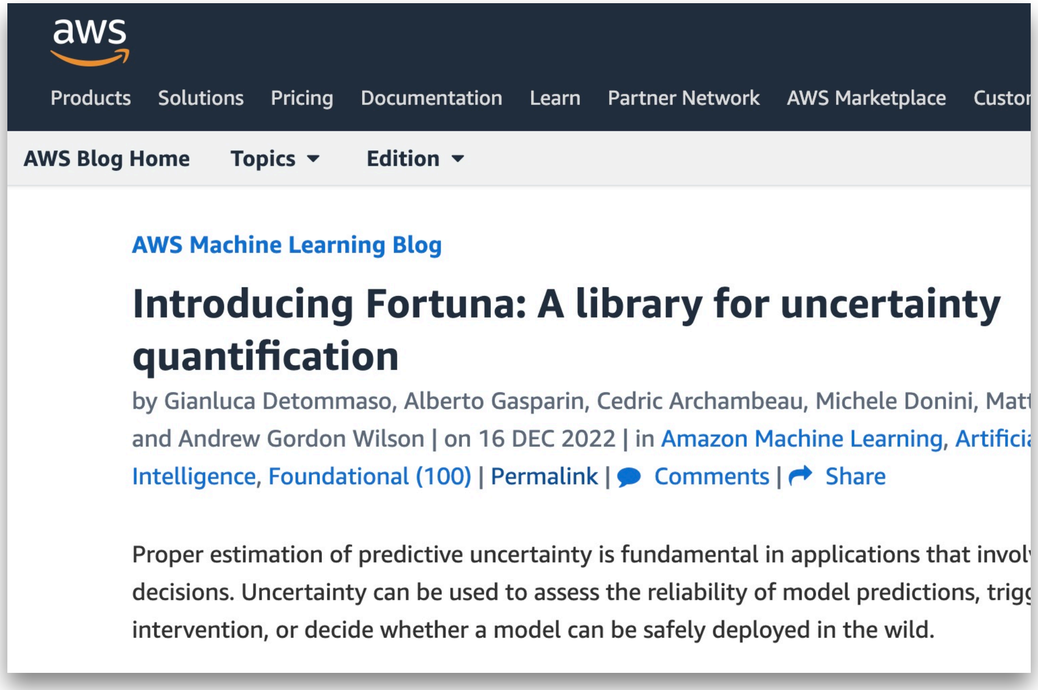


Vincenzo Vitelli

Use AI to design better experiments, simulations, and sensors

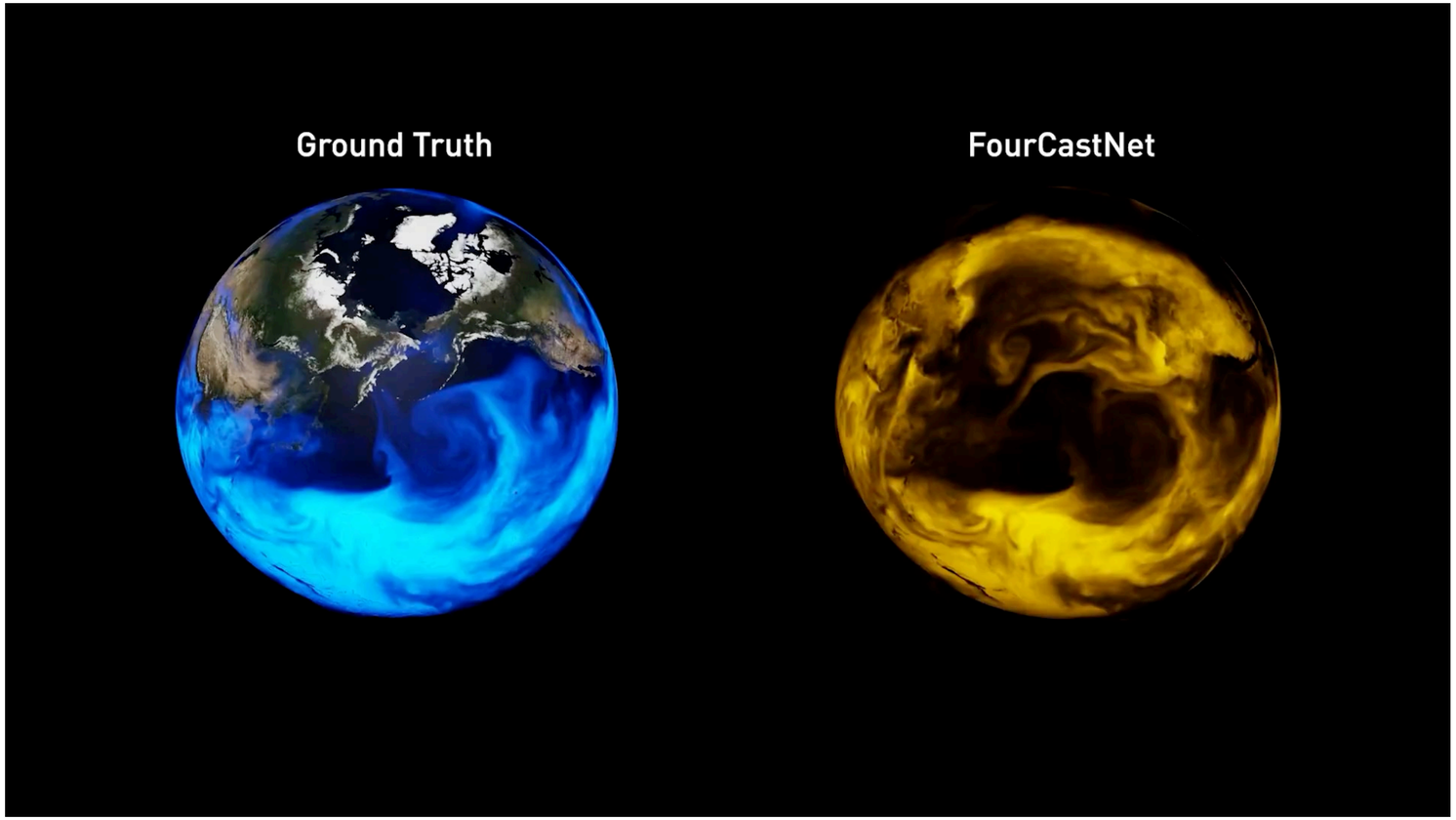
Seppe Kuehn — adaptive design of microbial communities

Rina Barber — uncertainty quantification foundations



Optimally leverage physical models and experimental or observational data

Pedram Hassanzadeh —
learned emulators of climate simulations



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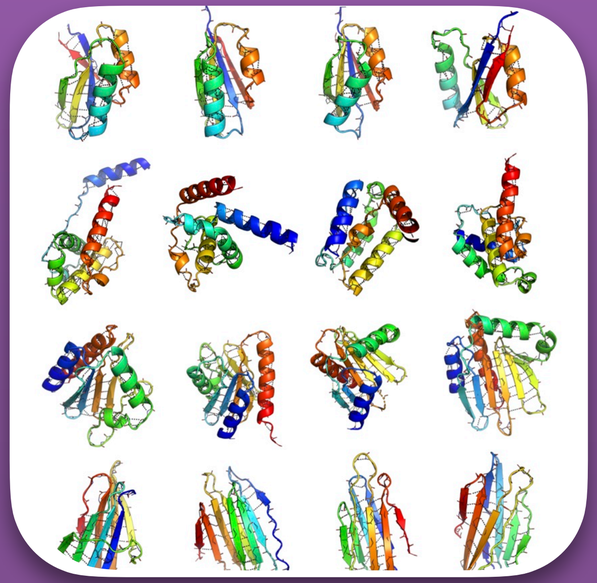
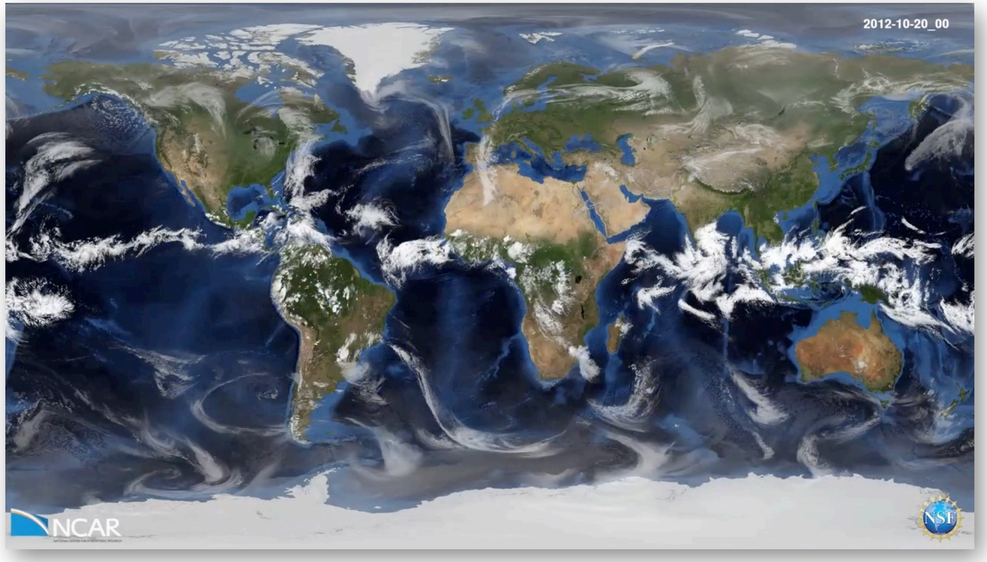


Generate new examples of physical objects or processes to aid discovery

- Chaotic systems exhibit extreme sensitivity to initial conditions

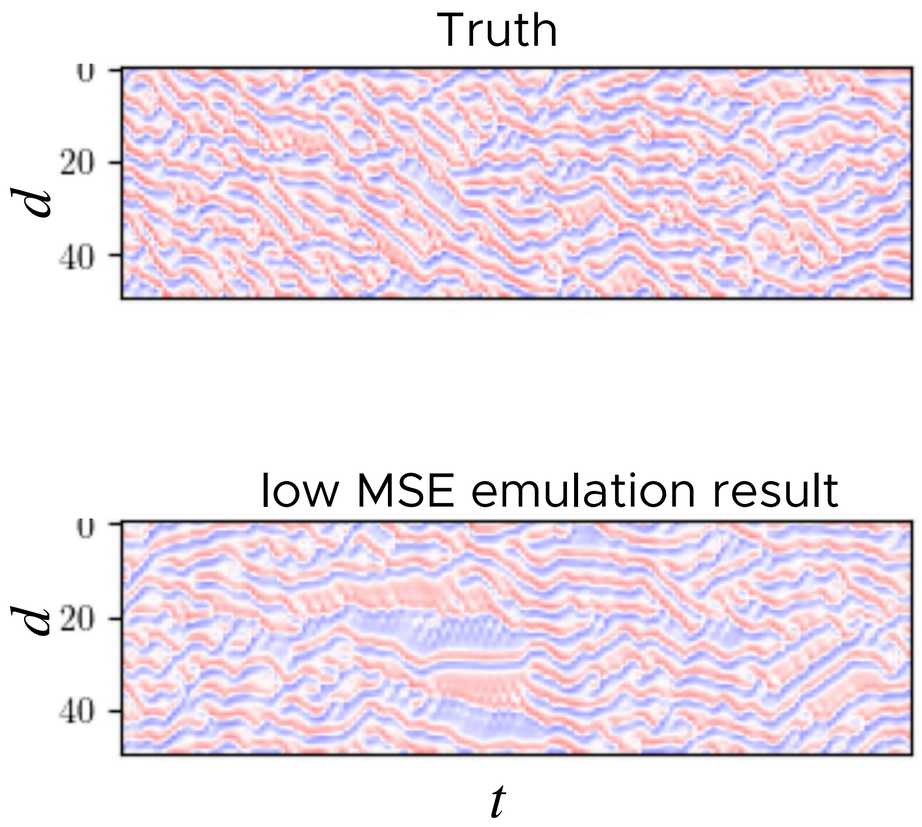
- Emulators trained to give accurate “point” forecasts (e.g. small MSE) are doomed to failure past a short-term horizon



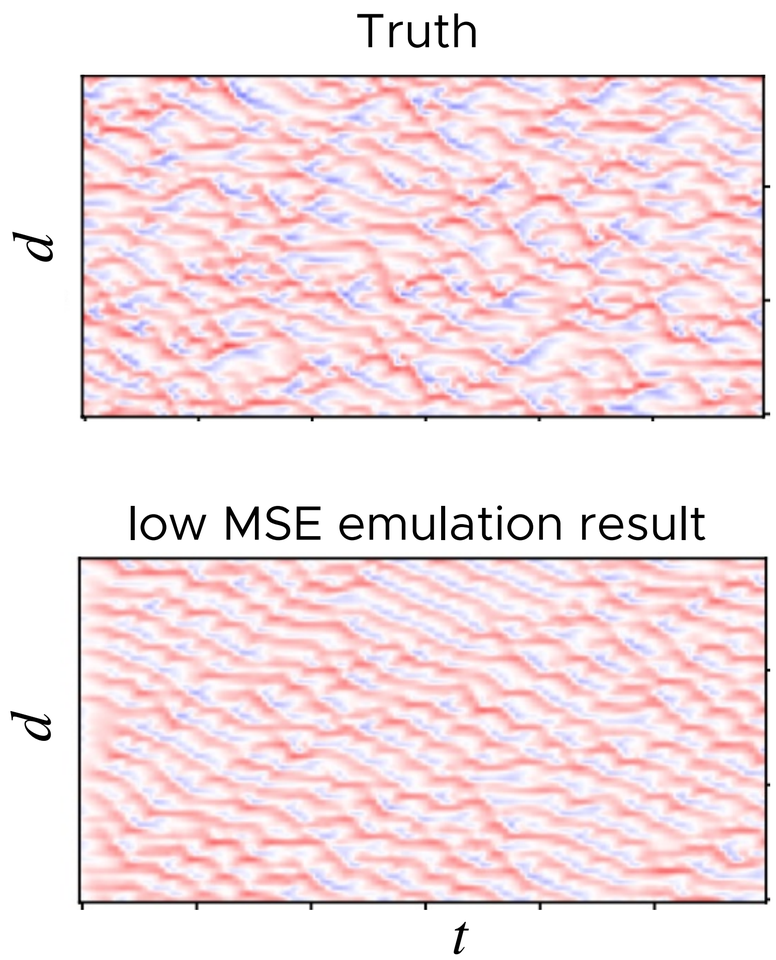
Emulators are important for understanding statistical trends (e.g., hurricane frequency and severity over long time horizons)

Failure of MSE-minimizing emulators

Kuramoto-Sivashinsky equation



Lorenz 96 ODE

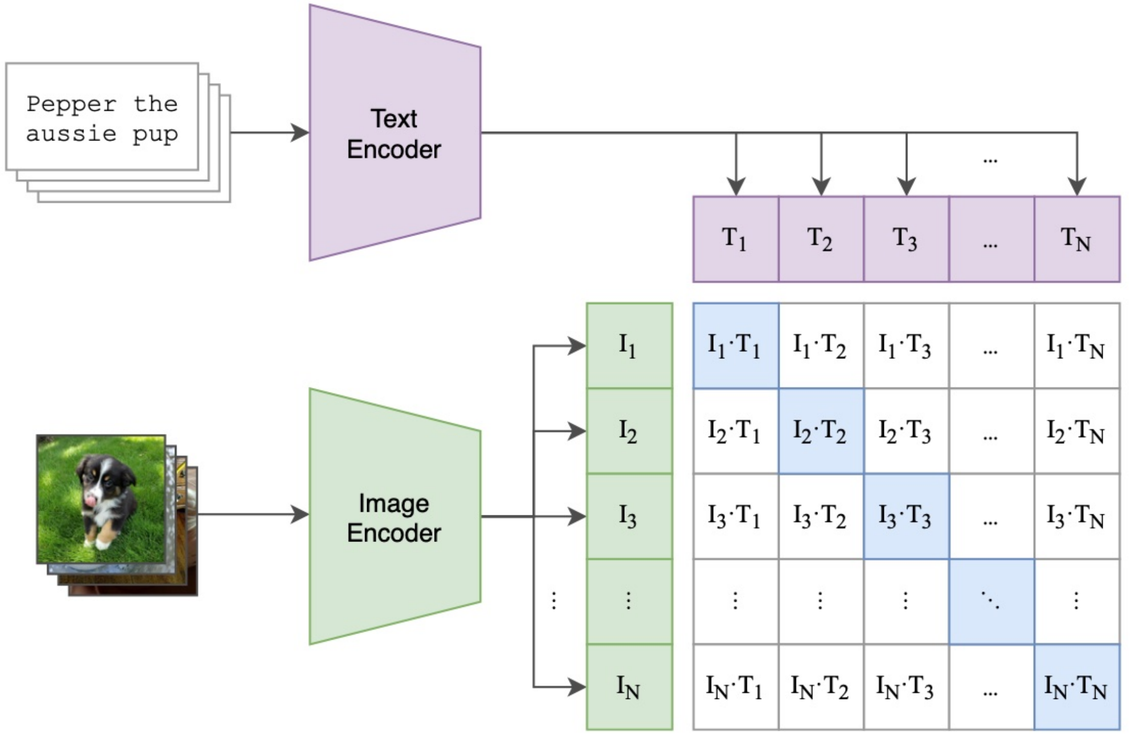


A new hope

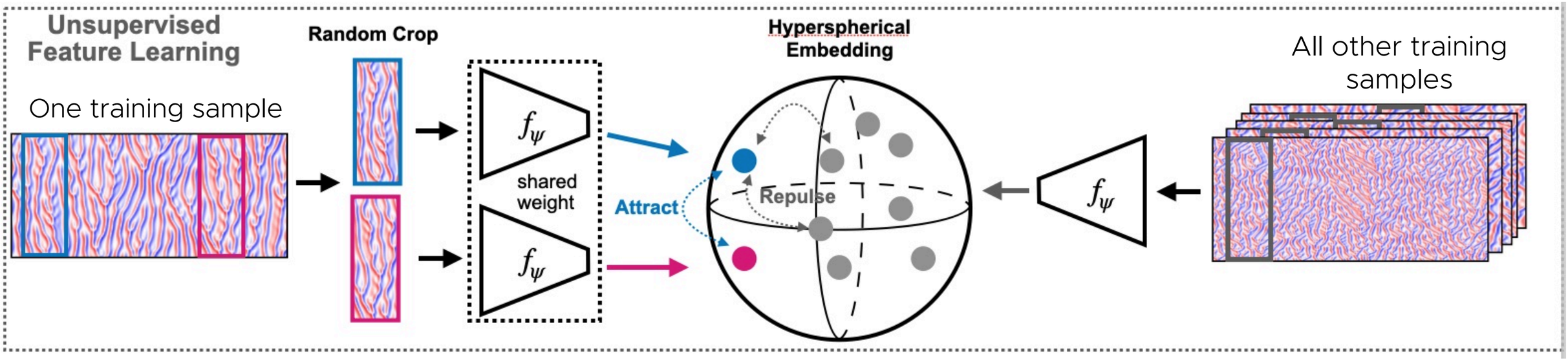
- Instead of focusing on small MSE, want emulator to **preserve invariant measures of chaotic attractors** and the corresponding time-invariant statistics

- **Contrastive learning preserves chaotic attractors**

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



Unsupervised contrastive feature loss (CL)



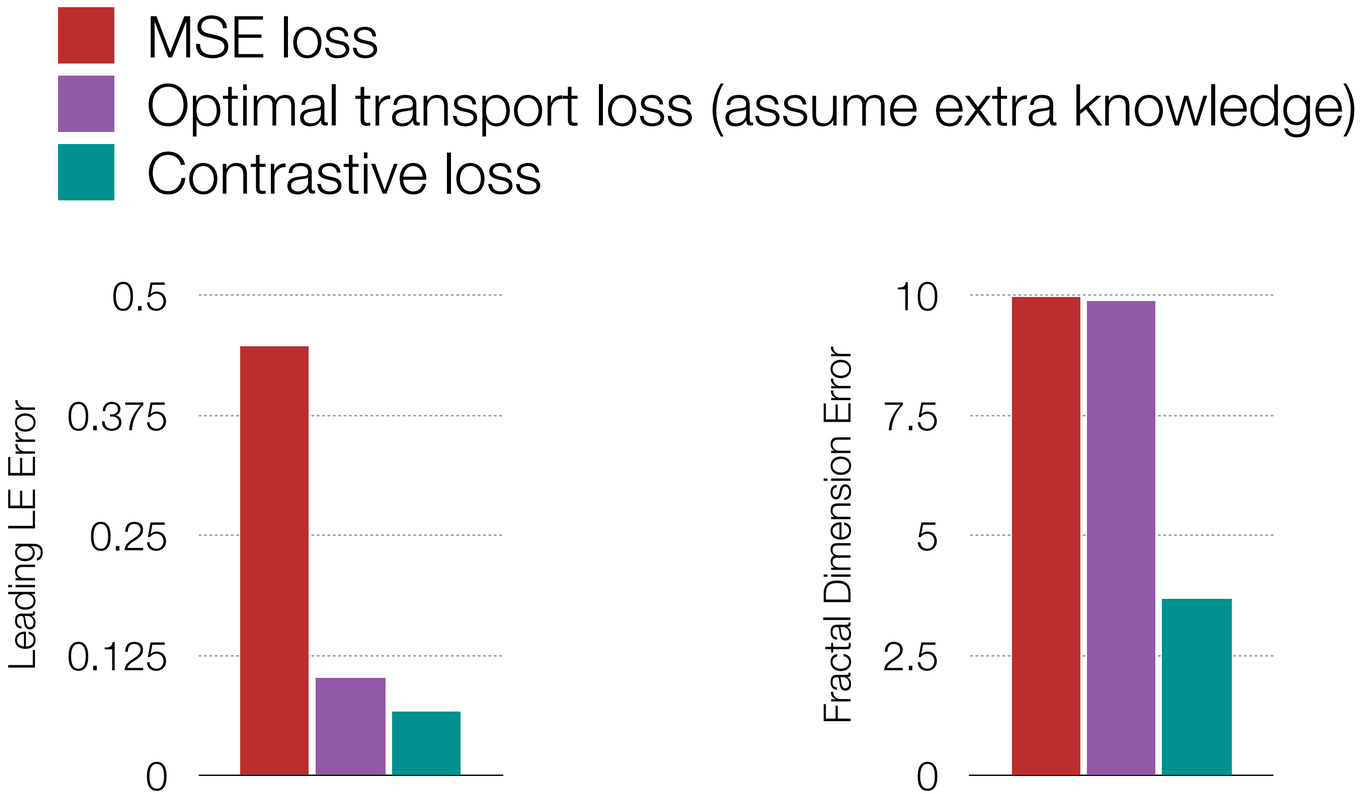
Learn embedding of short time windows so that:

- 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

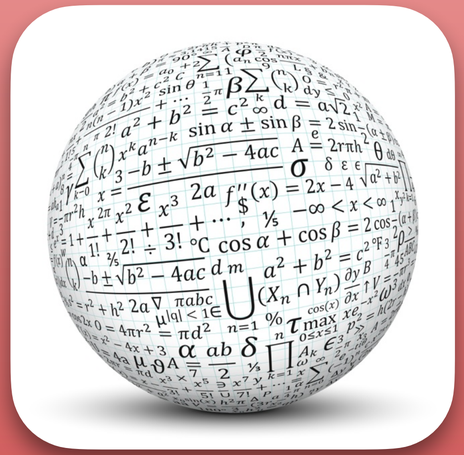
Jiang, Lu, Orlova, and Willett 2023

Lorenz 96 Illustration

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



Jiang, Lu, Orlova, and Willett 2023



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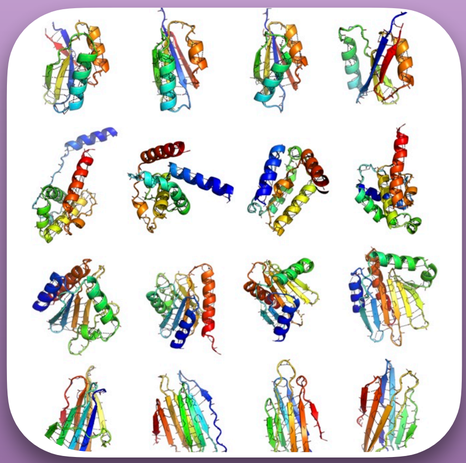

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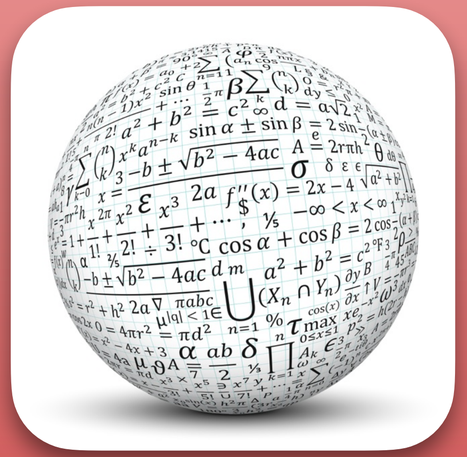

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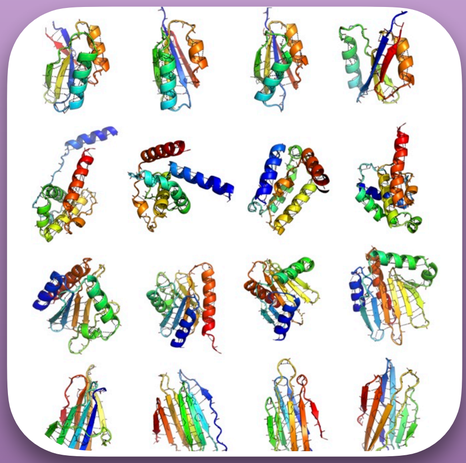
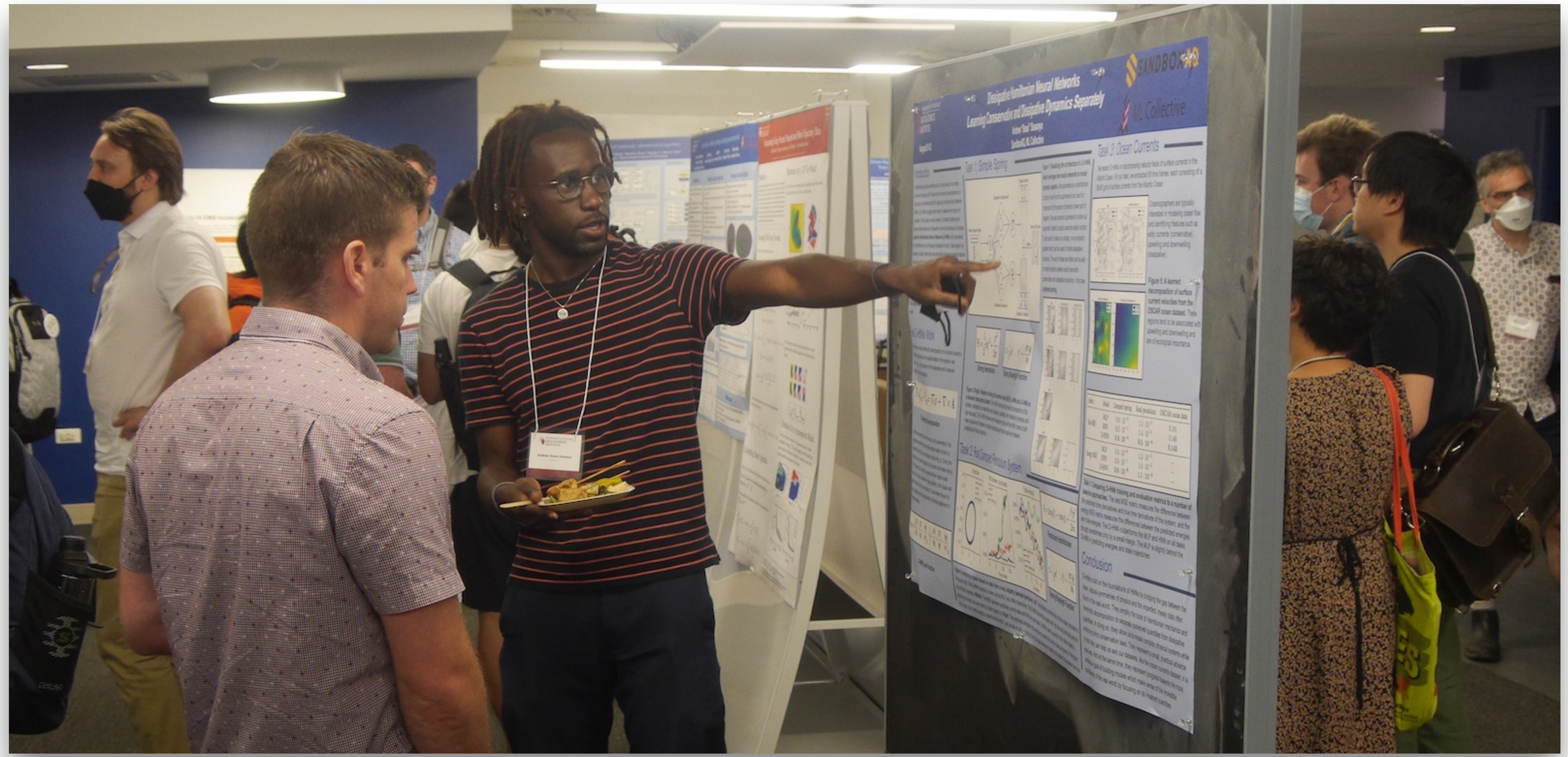


Generative AI for Science

AI Foundations




The University of Chicago and Caltech Conference on AI +Science
Sponsored by the Margot and Tom Pritzker Foundation

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

SCHMIDT FUTURES

National Institute for Theory and Mathematics in Biology

NSF

SIMONS FOUNDATION

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

Thank you!

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SCHMIDT FUTURES