



# Scientific Machine Learning

CSU/IMU Oct'2023

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# Plan

1. Introduction and Motivation—it's all about data.
2. What is Scientific Machine Learning?
3. How can SciML contribute to CSE?



# Think out of the box!

the world has changed....



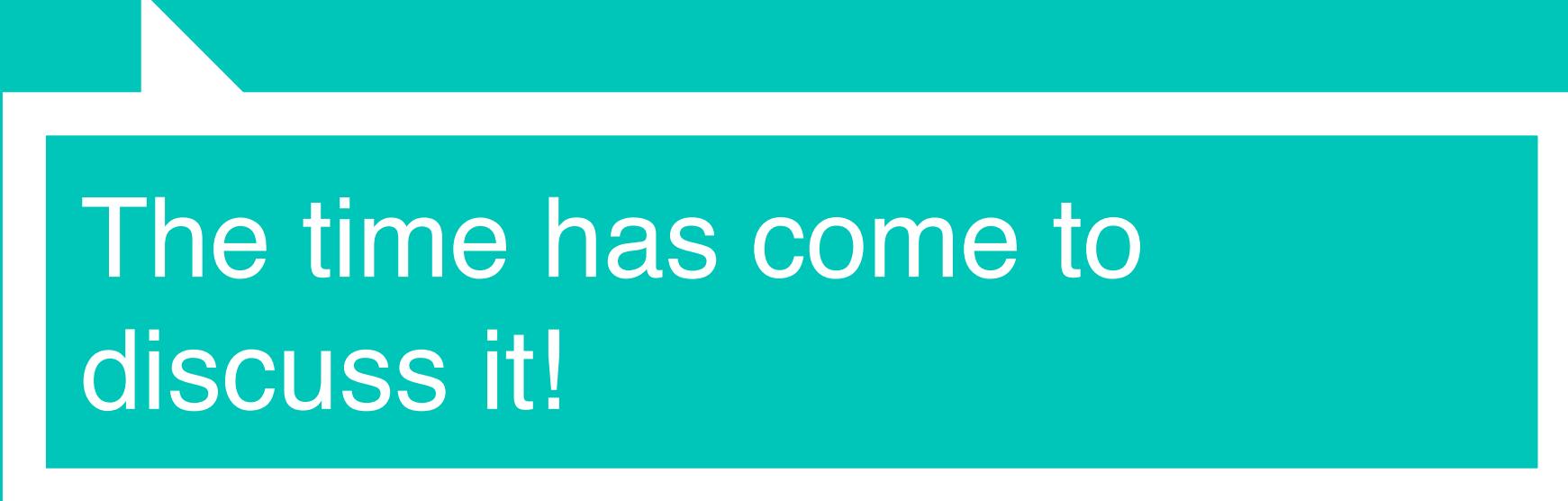
# Questions, questions, questions

HOW? (Analyse)

WHY? (Understand)

WHAT IF? (Predict)

# 1. A new approach to computational science ?



The time has come to  
discuss it!

# The Fourth Paradigm (2009)

1. Experiment



From antiquity, till now.

2. Theory

From middle ages, till now.

3. Simulation

20th Century (1980's), till now.

4. Data, data, data

21st Century (2010–), NOW!

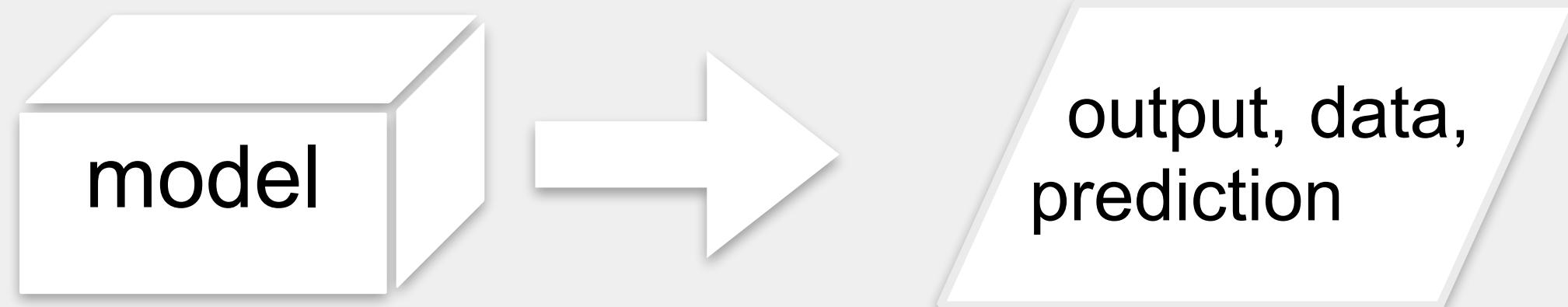


# Machine Learning

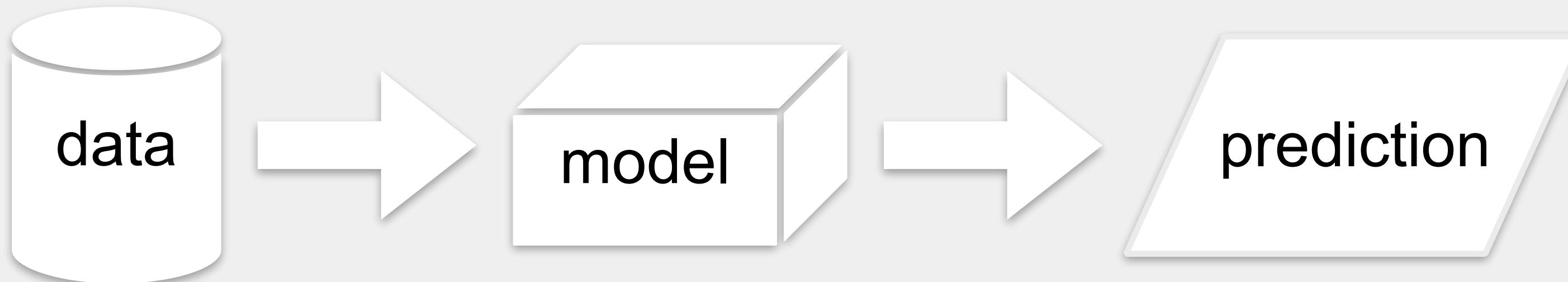
Turning our world (CSE) inside-out...

## Two, diametrically opposite approaches?

- CSE: from models to data (predictions)



- ML/AI: from data to models to predictions ("Let the data talk")





# African proverb

"If you want to go quickly, go alone. If you want to go far, go together."

“

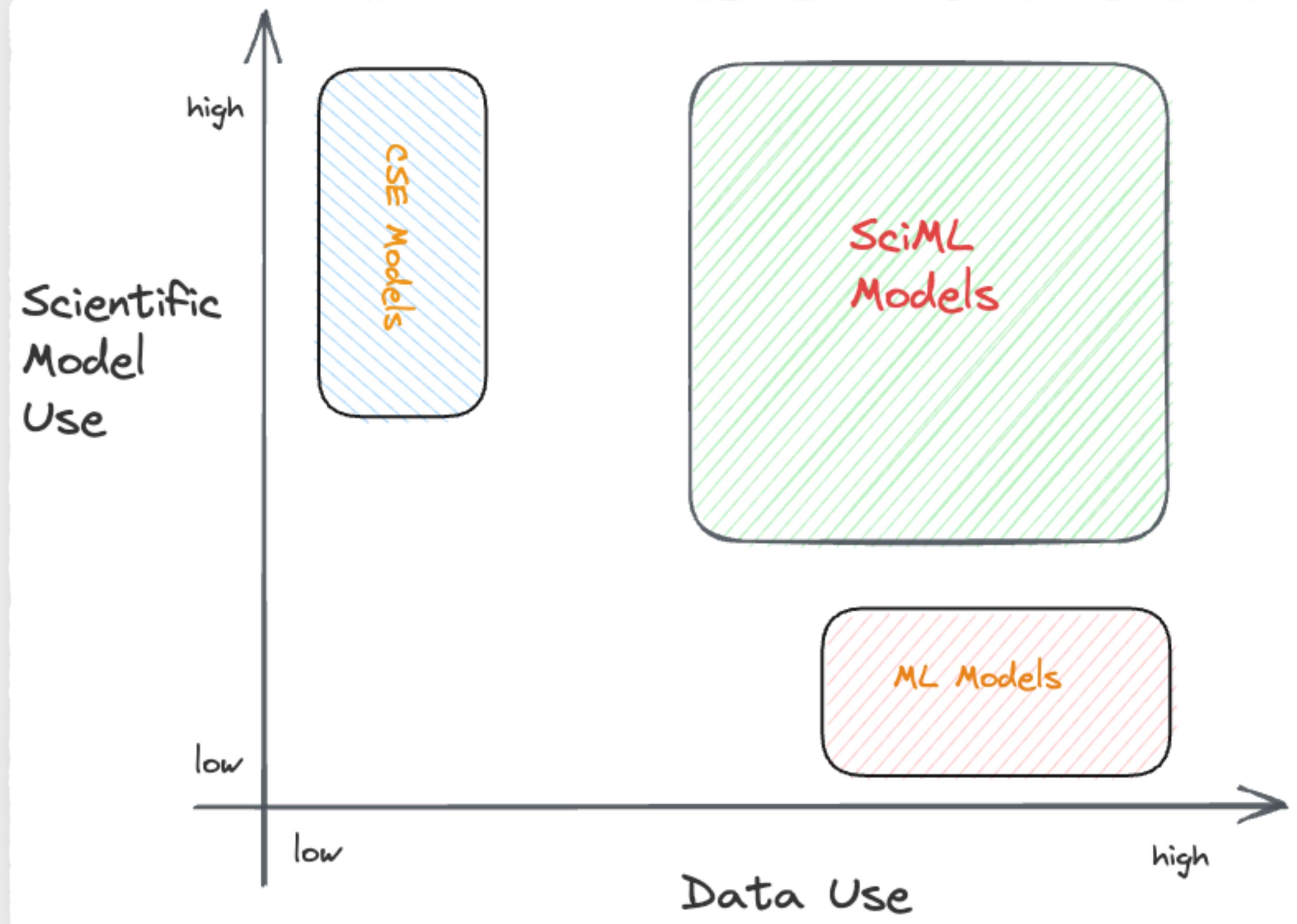
**Scientific Machine Learning** (SciML) is a field of research that *combines* traditional scientific modeling with machine learning techniques. It aims to develop new methods and tools for solving scientific problems that are more accurate, efficient, and generalizable than traditional methods.

SciML is still a young field, but it has the potential to make a *major impact* on a wide range of scientific disciplines..

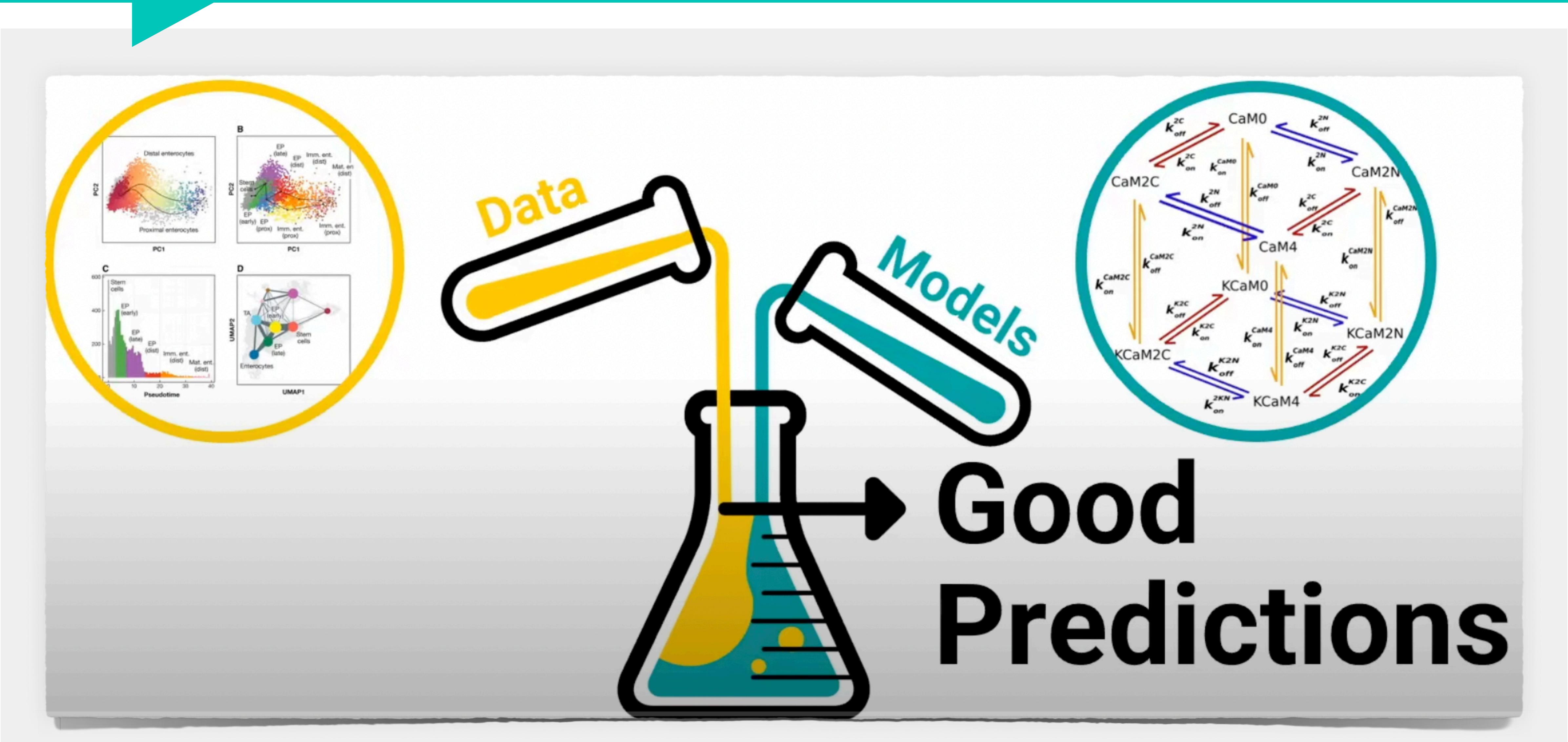
Credit: Bard...

# It's a question of balance...

- How much is data-driven?
- How much is scientific knowledge-driven?
- Multi-objective optimization problem

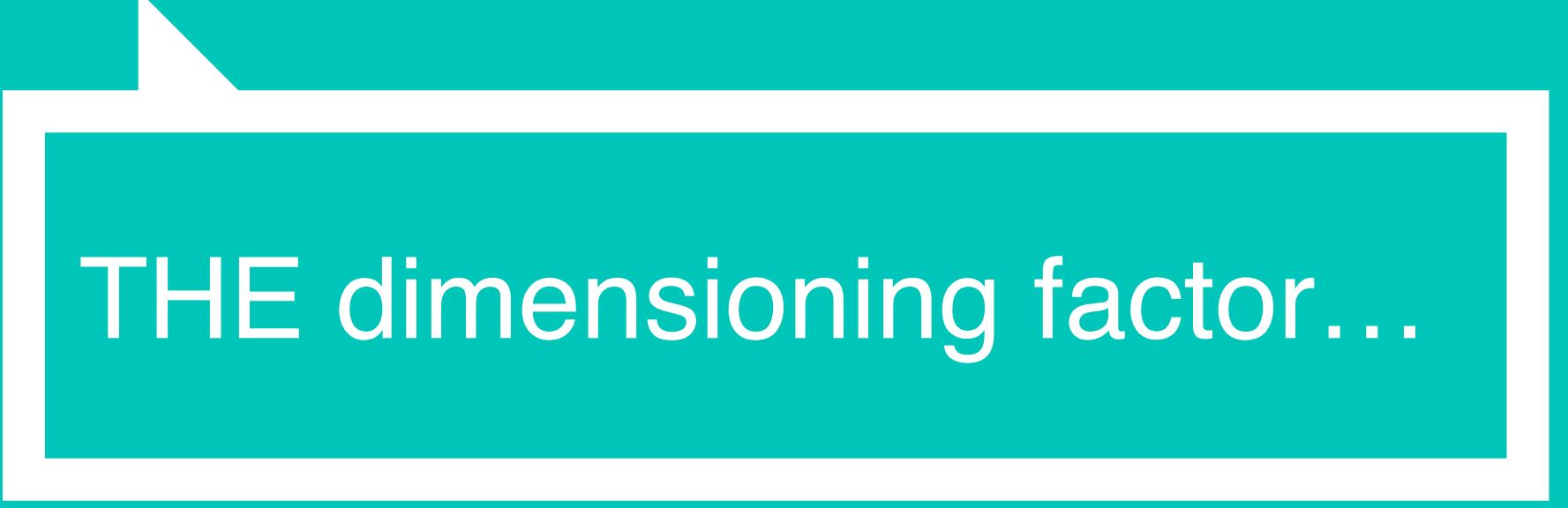


It's a question of balance...



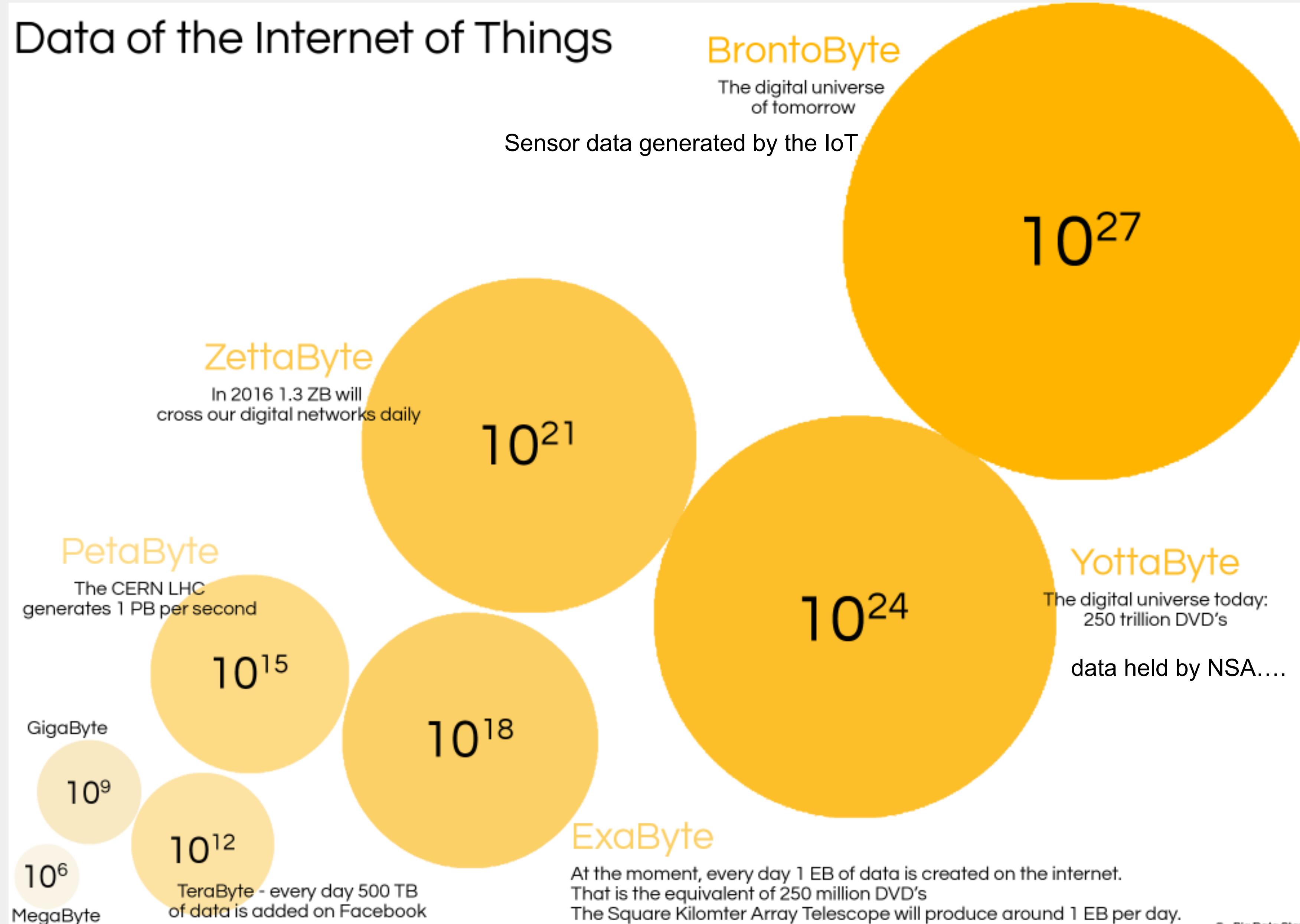
Credit: C. Rackauckas

## 2. Data, data, data



THE dimensioning factor...

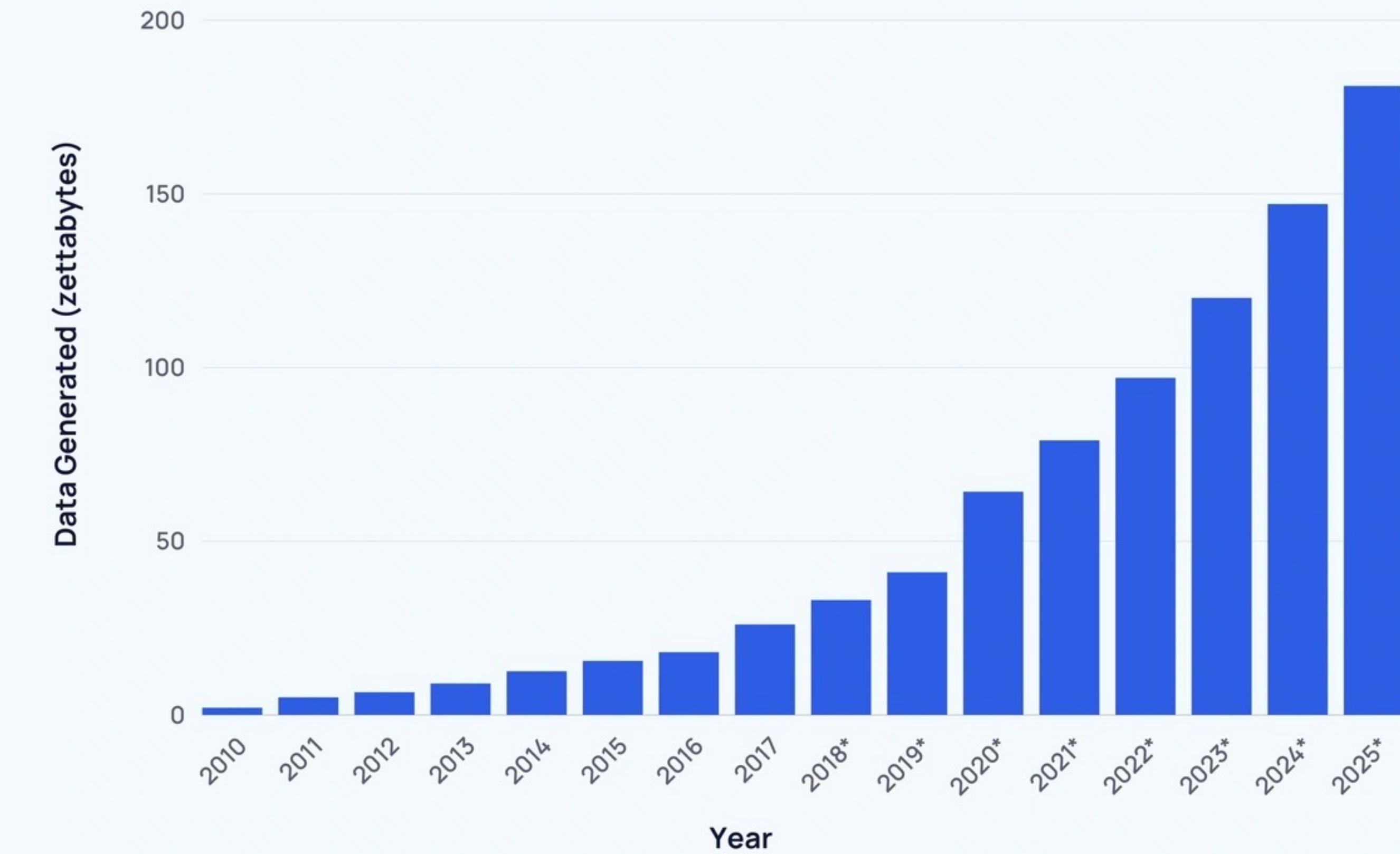
# Data of the Internet of Things



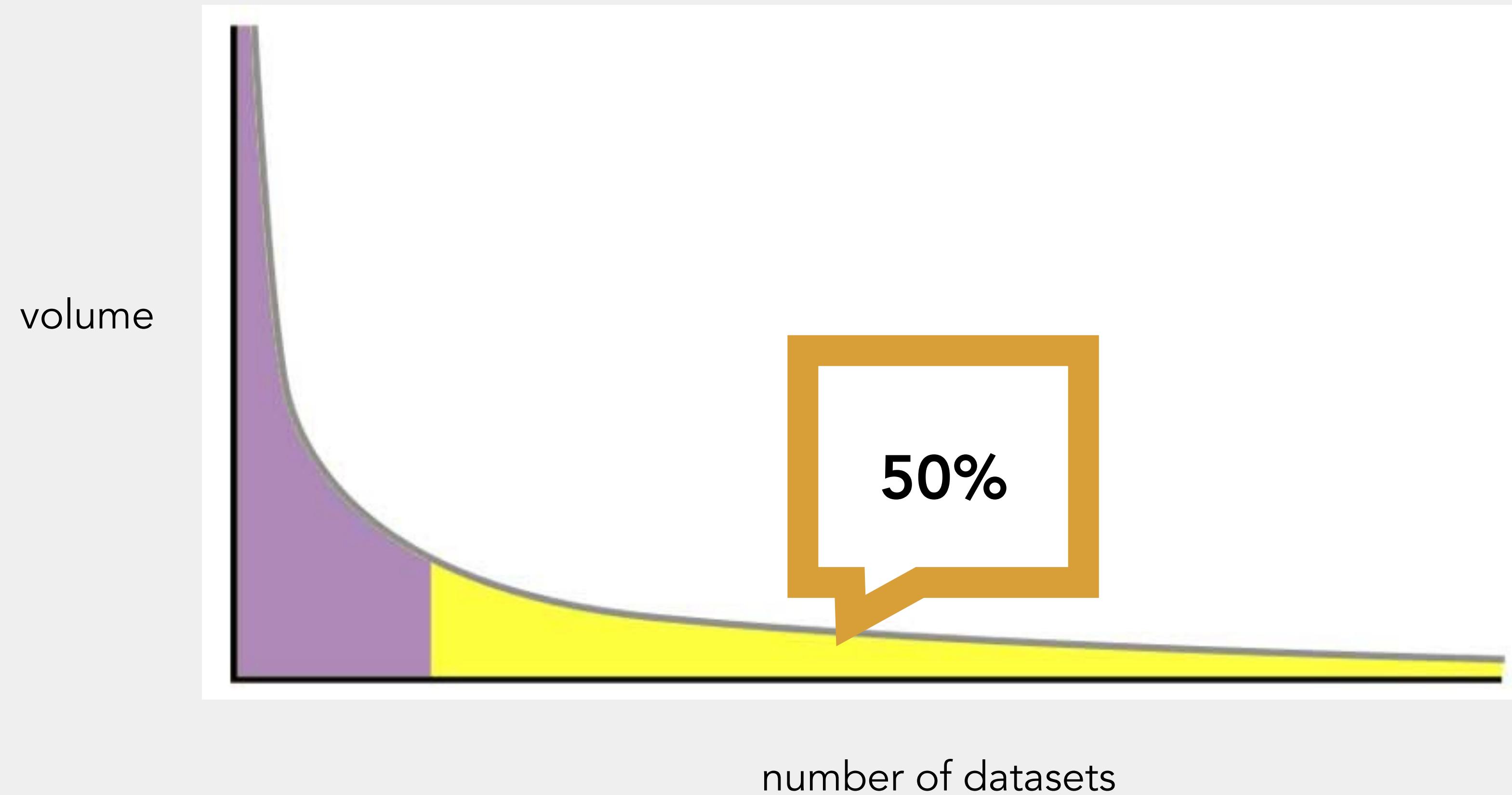
# How much data is generated (daily, annually)?

**Daily volume:**  
328 Exabytes

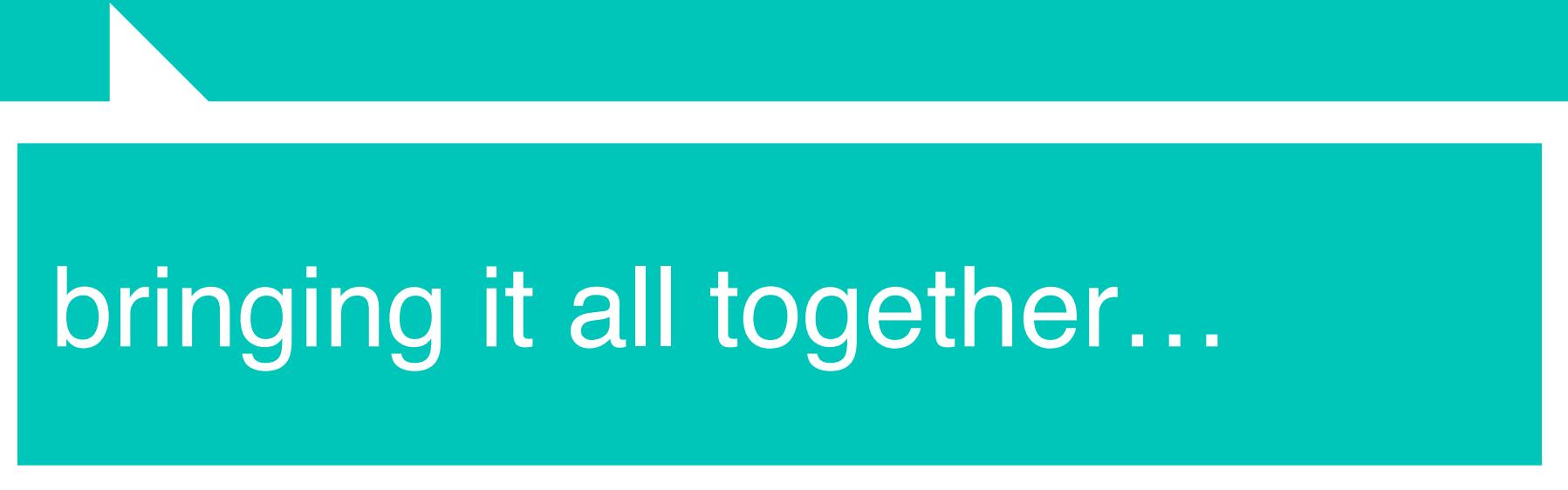
## Global Data Generated Annually



# The Long Tail of Research Data



### 3. SciML



bringing it all together...

# What's it all about?

1. Balancing CSE and ML.

⋮



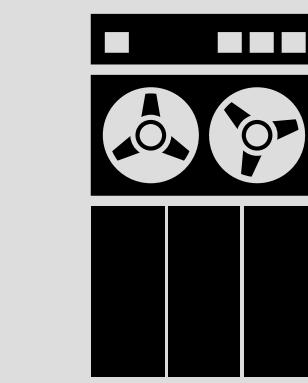
2. Advancing science for society.



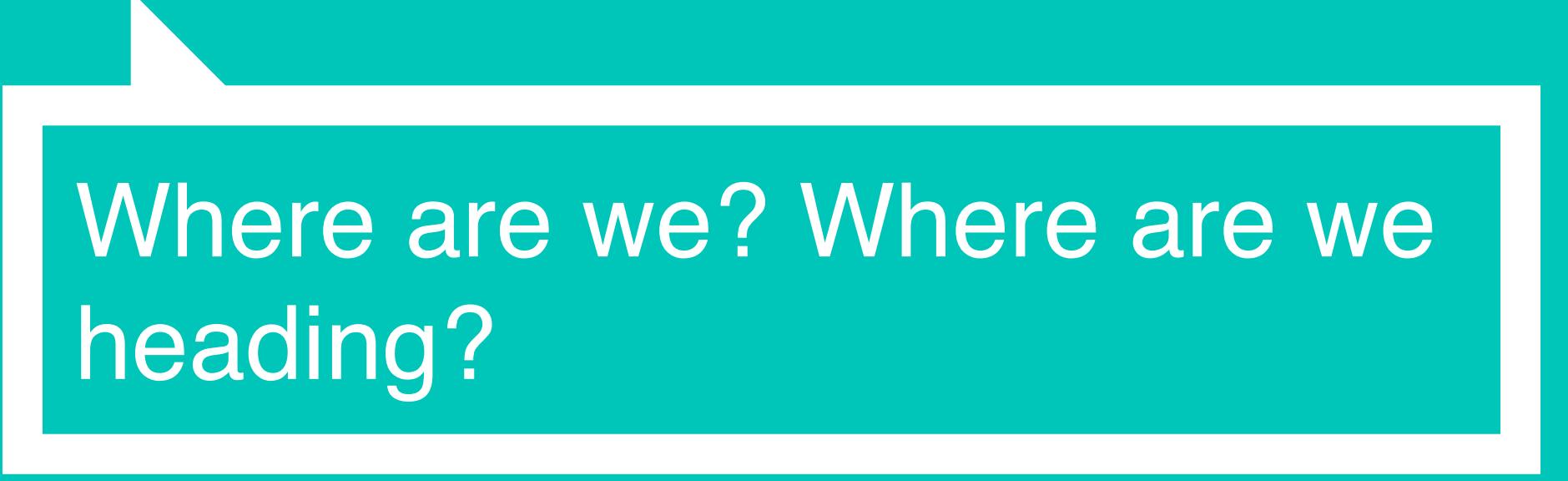
3. Budgets: cost vs. speed.



4. Needs computing capacity.



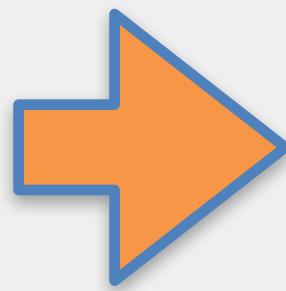
# 4. SciML - Promise and Reality



Where are we? Where are we heading?

# SciML promise

- For solving **real-world**, PDE-based problems, direct and inverse, using ML
- It's moving very, very fast!



10 000X speedup!

- **NVIDIA** (FourCastNet) claims similar performance.

Science, July 7, 2023.



New AI techniques could help better predict cyclones such as 2018's Typhoon Yutu, which intensified rapidly before hitting Tinian and Saipan.

## METEOROLOGY

### Artificial intelligence forecasts the weather in a flash

A model using artificial intelligence (AI) forecasts global weather as accurately, and more than 10,000 times faster, than the best system in use, researchers report. The conventional tool, run by the European Centre for Medium-Range Weather Forecasts, is computationally intensive, requiring hours of supercomputer calculations to produce a 10-day forecast. The new AI-based model—named Pangu-Weather and developed by Huawei, the Chinese

tech giant—improves on previous AI-powered models by simulating weather at different altitudes and forecasting tropical cyclones, with results reliable out to 10 days, researchers say. The research team trained the model on 39 years of historical weather data; the system is untested yet using real-time observational data. Another AI-based weather model, GraphCast, described by Google DeepMind in a December 2022 preprint, also outperformed the European system.

# SciML reality

- For solving **real-world**, PDE-based problems, direct and inverse, using ML
- It's moving very, very fast!
- But...

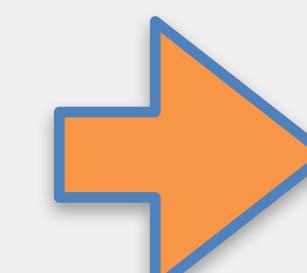
The banner features the FAU logo and text: "Friedrich-Alexander-Universität Research Center for Mathematics of Data | MoD". Below the logo is "FAU MoD Lecture Series". A circular portrait of George Karniadakis, a man with glasses, is centered over a background of white hexagonal patterns. To the right of the portrait, his name "George Karniadakis" is written in orange, with "Brown University, MIT, PNNL" listed below it. The main title of the lecture is "From Physics-Informed Machine Learning to Physics-Informed Machine Intelligence: QUO VADIMUS?". The date "Tue. May 30, 2023 • 14:00H" and the website "www.mod.fau.eu" are at the bottom.

**George Karniadakis**  
Brown University,  
MIT, PNNL

**From Physics-Informed Machine Learning  
to Physics-Informed Machine Intelligence: QUO VADIMUS?**

Tue. May 30, 2023 • 14:00H

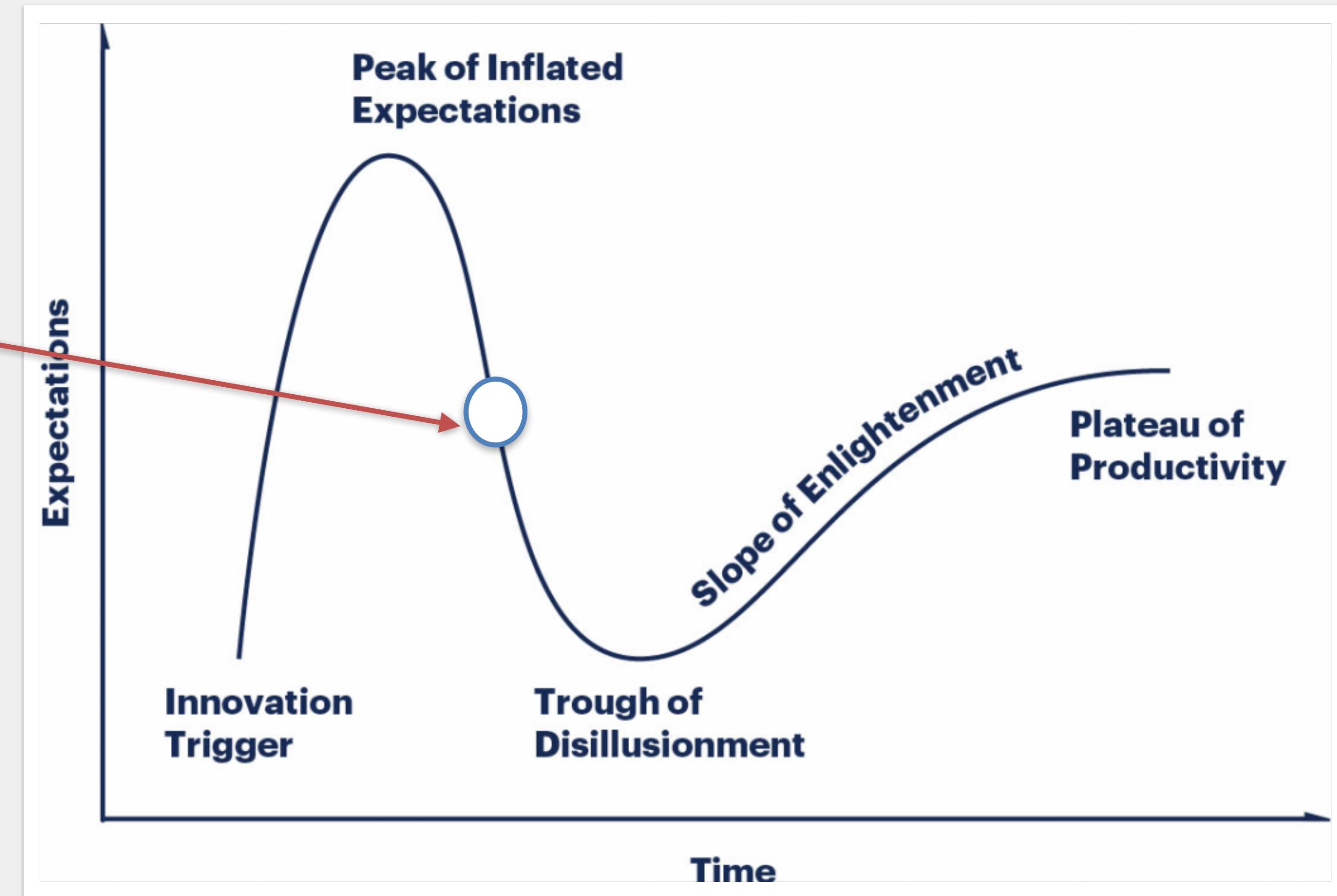
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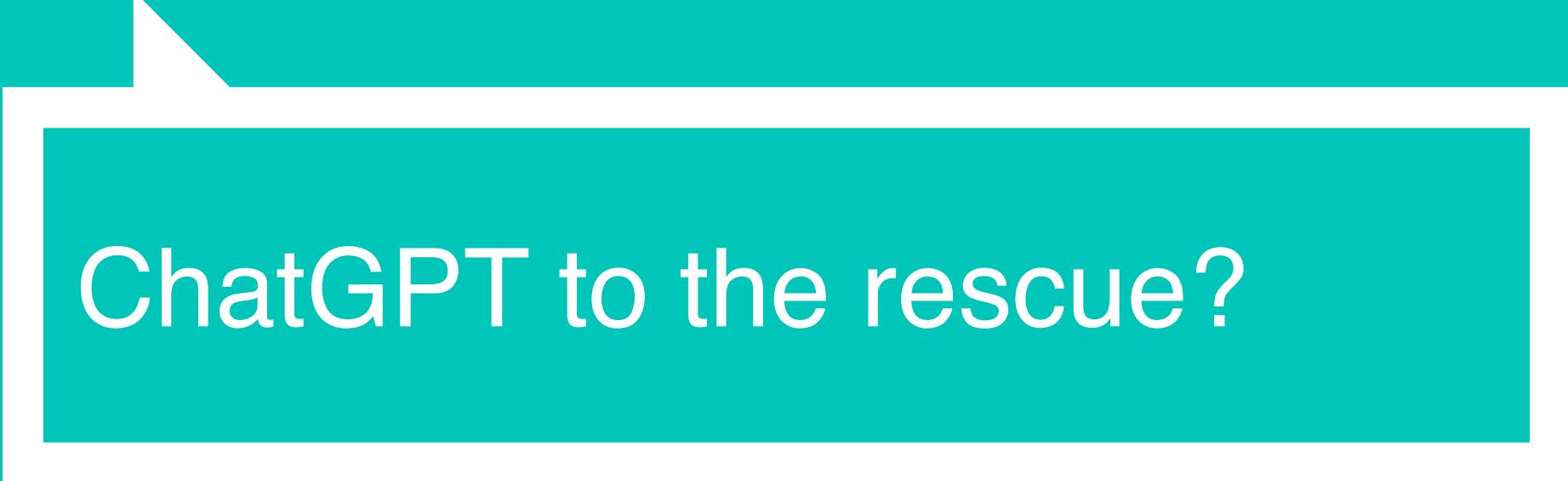
"Our group has developed the original concepts of neural PDEs (PINNs) and neural operators (DeepOnet), but **significant problems** remain related to **generalisation, efficiency** and **excessive computational cost**."

# SciML hype cycle

- For solving **real-world**, PDE-based problems, direct and inverse, using ML, we are somewhere here
- It's moving very, very fast!



# 5. SciML - Foreseeable future...



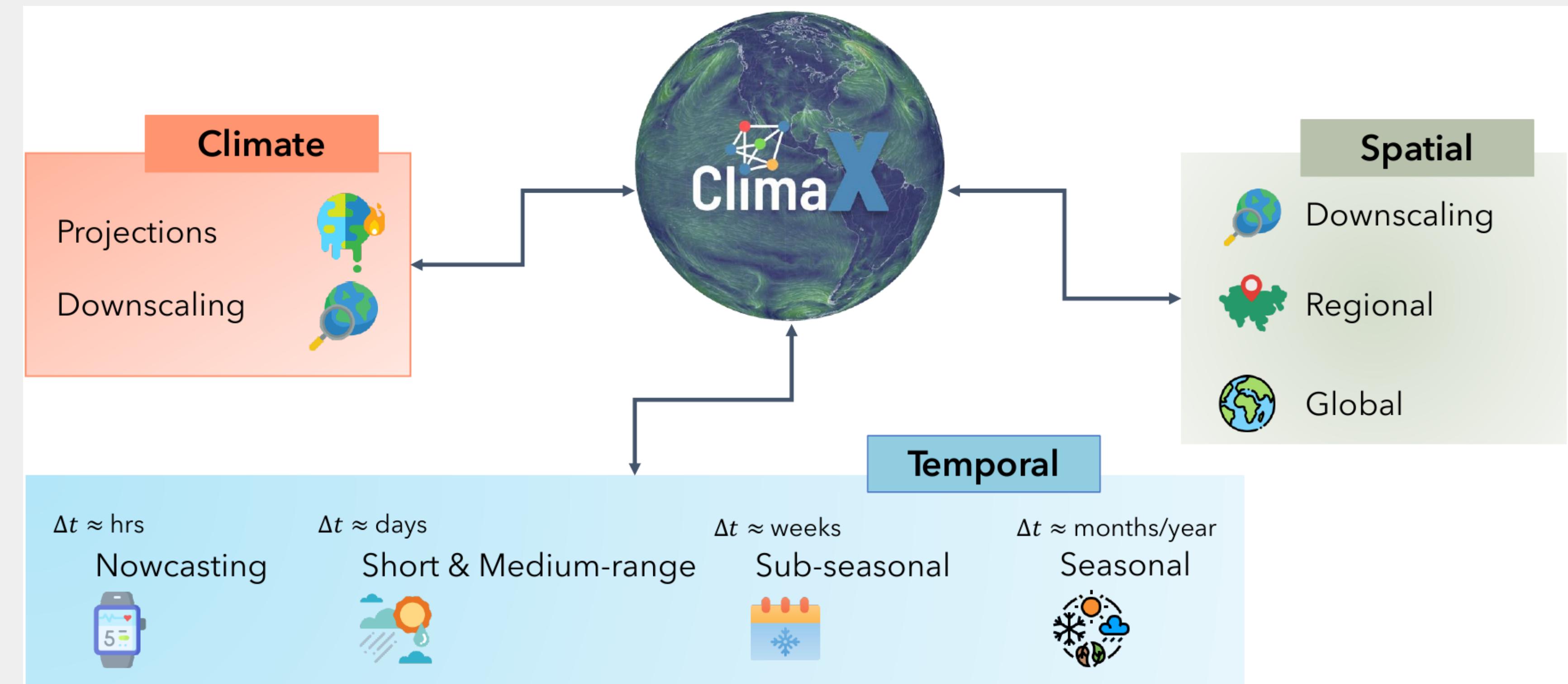
ChatGPT to the rescue?

# Transformers and SSL to the rescue?

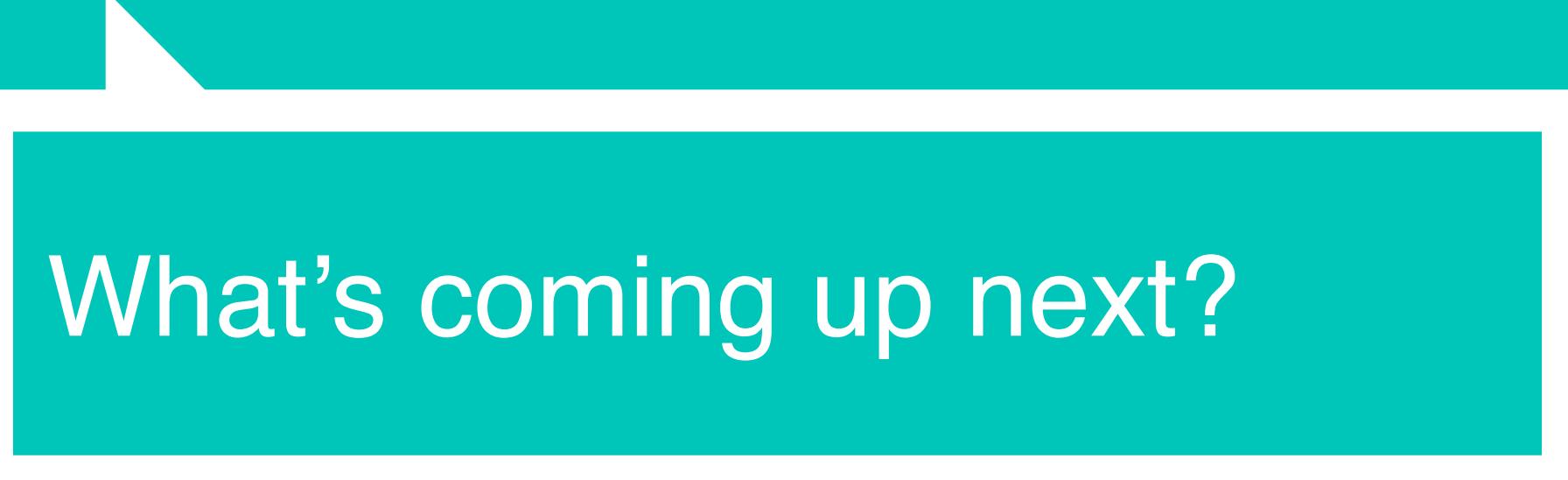
(ICIAM, August 2023): use **transformers** and **self-supervised learning**, based on tokenisation and aggregation.

ClimaX (Microsoft Research)  
“a flexible and generalizable  
deep learning model for  
weather and climate science”

- trained on **Petascale data**,
- uses a “ChatGPT”  
approach—fill-in the gaps  
(based on Markov chains)



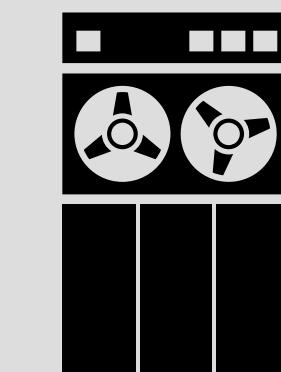
# 6. SciML Course Outline

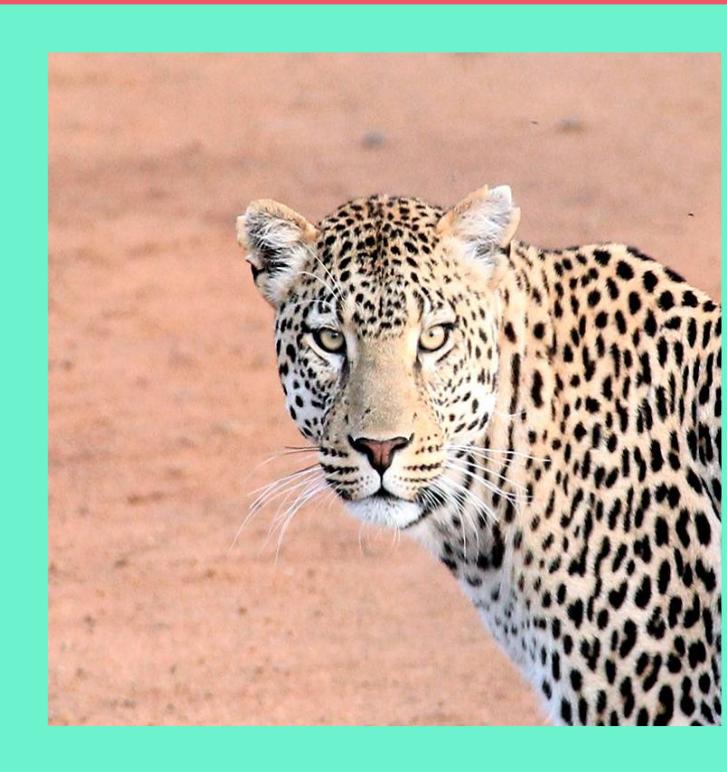


What's coming up next?

# Outline of SciML course

1. Gradients, adjoints and optimization.
2. Differentiable programming.
3. ML methodologies.
4. Direct and Inverse Problems. DA.
5. Physics Constrained approaches.
6. SUMO and other approaches.
7. Strengths and weaknesses.





Thank you!  
Questions/Discussion?

You can find me at:

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## Credits

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