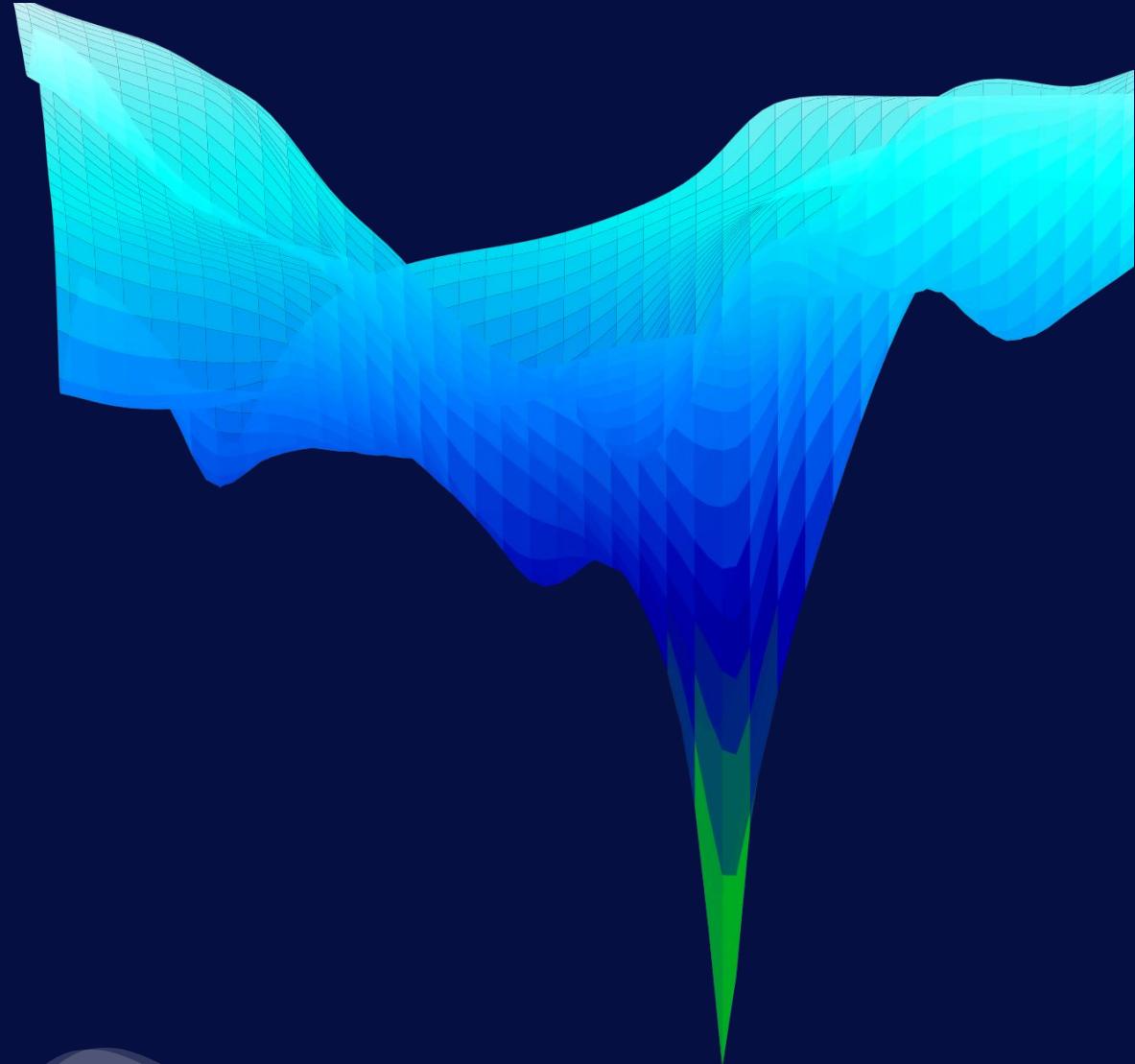


Scientific Machine Learning (SciML) for Solving PDEs

(Case Studies: two-phase flow in porous media)



University of Campinas (Nov. 2024)

A part of INTPART project, supported by NCS2030

- National Centre for Sustainable Subsurface Utilization of the Norwegian Continental Shelf.



NCS 2030
University of Stavanger

National Centre for
Sustainable Subsurface Utilization of the
Norwegian Continental Shelf





JASSEM ABBASI

Scientific Machine Learning & Reservoir Engineering

CURRENT ACTIVITY

Application of Physics-informed Machine Learning for Modelling of Multiphase Flow Processes in Porous Media

EXPERIENCE

ETH Zürich (2024)

ETH AI Center – Visiting Researcher

EQUINOR ASA, Norway (2022) [intern]

Subsurface Geoscience/Reservoir Simulation Engineer

ZODAN SOLUTIONS LTD., UK (2019-2020)

Scientific Software Developer

SHIRAZ UNIVERSITY/PETROAZMA COMPANY (2016-2018)

Reservoir [Simulation] Engineer/Researcher

PETROTIRAZIS OIL COMPANY PTED. (2016) [intern]

Scientific Software Developer (Intern)

EDUCATION

UNIVERSITY OF STAVANGER (2021- Dec. 2024)

Scientific Machine Learning (PhD)

SHIRAZ UNIVERSITY (2014-2016)

Reservoir Engineering (M.Sc.)

PETROLEUM UNIVERSITY OF TECHNOLOGY (2010-2014)

Reservoir Engineering (B.Sc.)

PUBLICATIONS (selected)

[ML4PS @ NeurIPS \(2024\)](#): History-Matching of Imbibition Flow in Multiscale Fractured Porous Media Using Physics-Informed Neural Networks (PINNs)

[SPE Journal \(2024\)](#): Application of Physics-Informed Neural Networks for Estimation of Saturation Functions from Counter current Spontaneous Imbibition Tests →

[Neurocomputing \(2024\)](#): Physical Activation Functions (PAFs): An Approach for More Efficient Induction of Physics into Physics-Informed Neural Networks (PINNs) →

[Energy and Fuels \(2023\)](#): Simulation and Prediction of Spontaneous Imbibition at Early and Late Times Using Physics-Informed Neural Networks →

...

Contents

Day 1

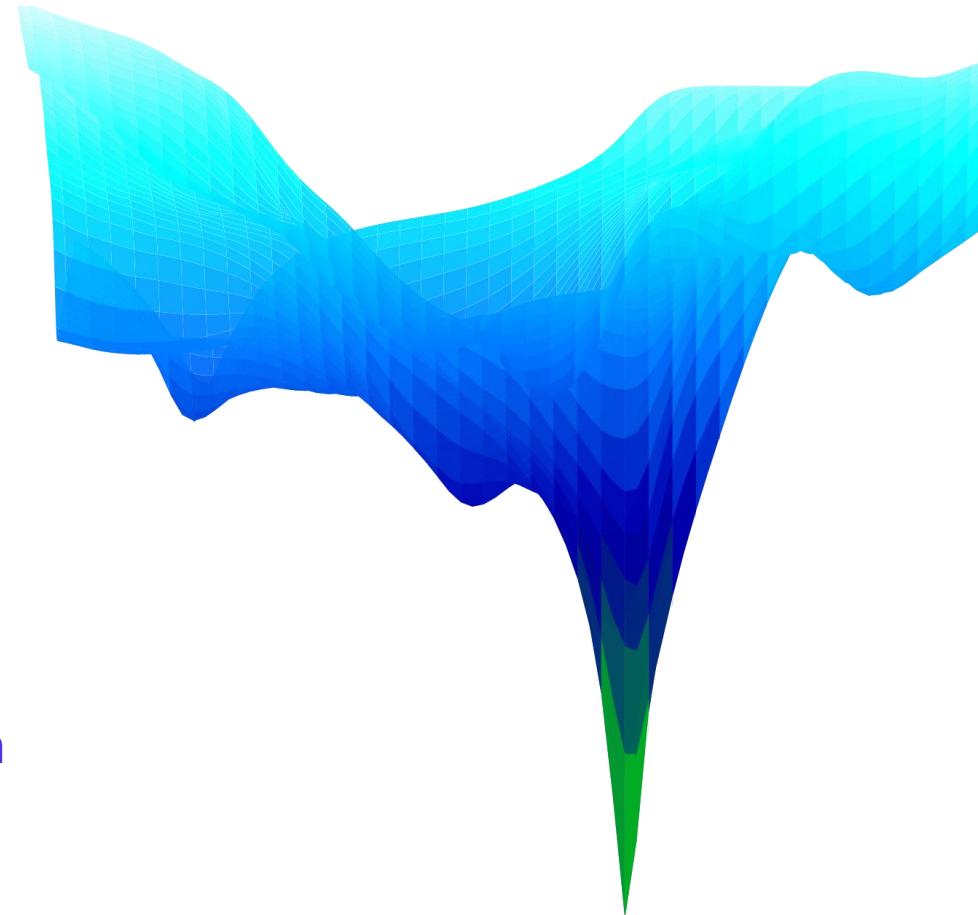
Part 1: Scientific Machine Learning (SciML): Introduction and Recent Advances

Part 2: Physics-Informed Neural Networks (PINNs)

Day 2

Part 3: A Case Study: Inverse Calculations on Spontaneous Imbibition Experiments

Part 4: Hands-on Experience with PINNs and Neural Operators



Key Take-aways

- Understand what **SciML** is?
- Recognize the limitations of traditional numerical methods for PDEs, and why **SciML** can help.
- Identify the unique advantages **SciML** offers in handling complex PDE challenges.
- Limitations and future directions of **SciML** in PDEs
- See real-world examples where **SciML** improved **PDE-solving** outcomes

References

- AI in the Sciences and Engineering (2024), ETH Zurich, CAMLab
<https://camlab.ethz.ch/teaching/ai-in-the-sciences-and-engineering-2024.html>
- Deep Learning for Scientists and Engineers, by George Em Karniadakis, Khemraj Shukla, Summer 2023 at KTH Stockholm
- Steve Brunton YouTube channel. <https://www.youtube.com/@Eigensteve>
- <https://sciml.tamids.tamu.edu/ecen-689-scientific-machine-learning-spring-2024/>
- ...

What is Scientific Machine Learning (SciML)?

- Scientific Machine Learning (SciML) is an interdisciplinary field that combines principles of scientific computing, applied mathematics, data science, and machine learning to model, predict, and analyze complex systems governed by the laws of physics, chemistry, biology, or engineering.
- Main Characteristics: Use Domain Knowledge

#AI4Science

The Nobel Prize in Physics & Chemistry

Trained neural networks using physics:

- John Hopfield (Princeton University)
- Geoffrey Hinton (University of Toronto)

For computational protein design

- David Baker (University of Washington)
- Demis Hassabis (Google DeepMind)
- John M. Jumper (Google DeepMind)



NOBELPRISET I FYSIK 2024
THE NOBEL PRIZE IN PHYSICS 2024



John J. Hopfield

Princeton University, NJ, USA



Geoffrey E. Hinton

University of Toronto, Canada

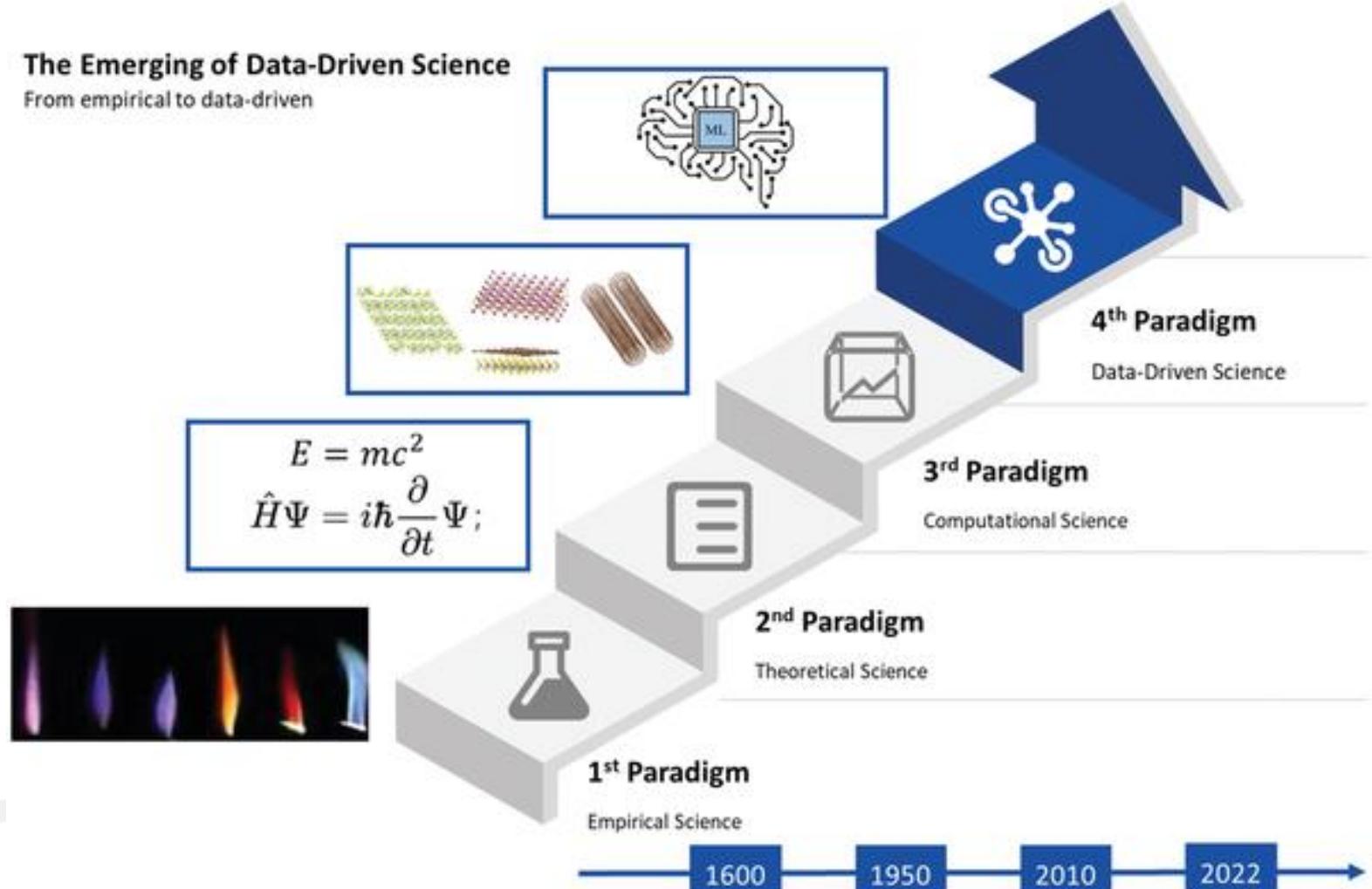
"För grundläggande upptäckter och uppfinningar som möjliggör maskininlärning med artificiella nätverk"

"for foundational discoveries and inventions that enable machine learning with artificial neural networks"



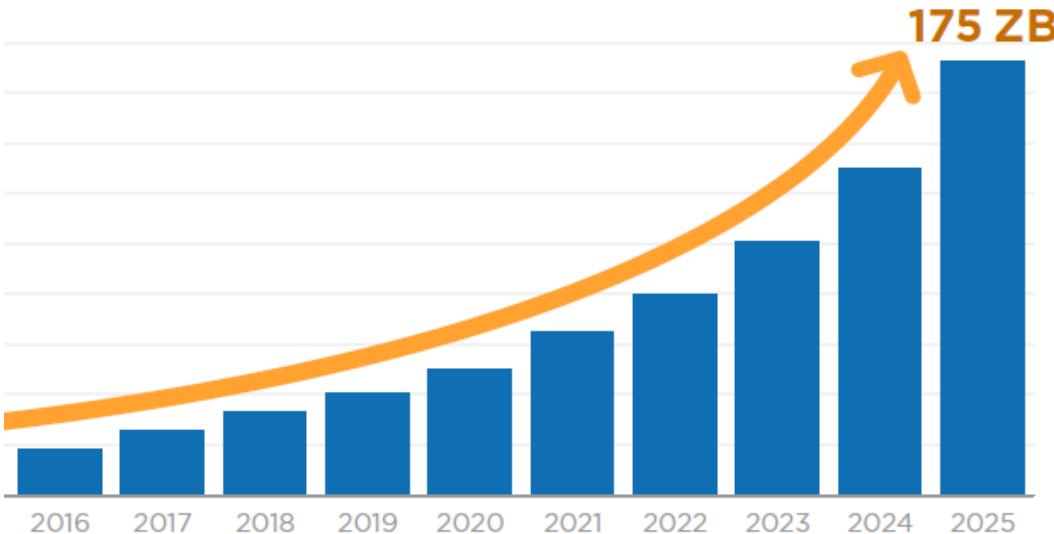
Paradigms of Science

What is happening?



Why now?

Volume of Data Generated Annually



Training Compute



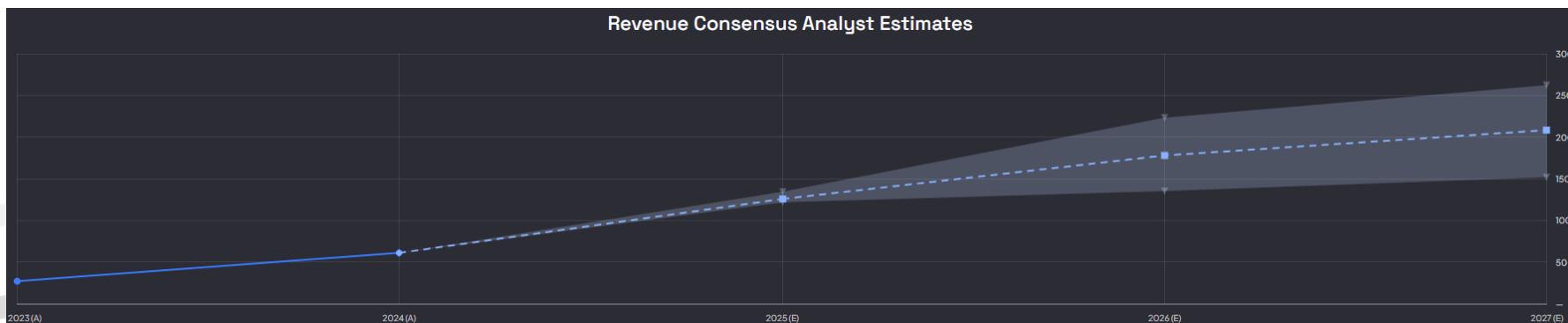
Larger
Datasets

Better
Hardware

Smarter
Algorithms

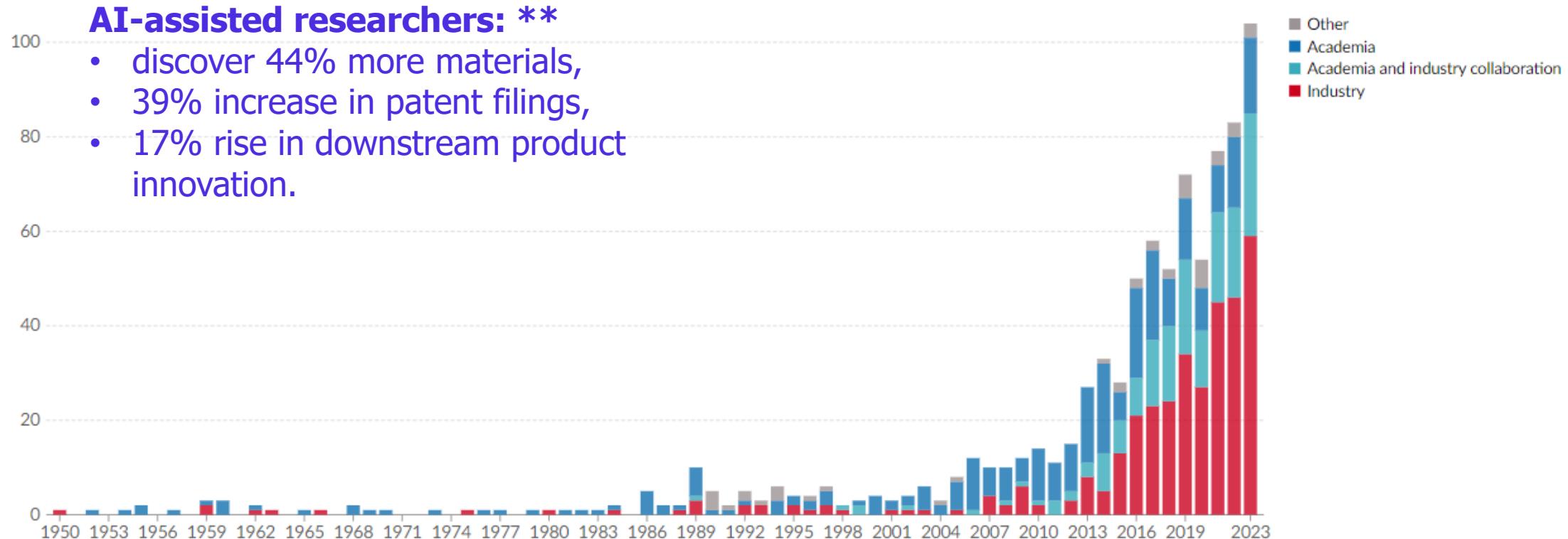
NVIDIA, a new giant!

Rank	Name	Market Cap	Price	Today	Price (30 days)	Country
1	Apple AAPL	\$3.518 T	\$231.41	▲ 0.36%		USA
2	NVIDIA NVDA	\$3.471 T	\$141.54	▲ 0.80%		USA
3	Microsoft MSFT	\$3.183 T	\$428.15	▲ 0.81%		USA
4	Alphabet (Google) GOOG	\$2.013 T	\$166.99	▲ 1.50%		USA
5	Amazon AMZN	\$1.971 T	\$187.83	▲ 0.78%		USA



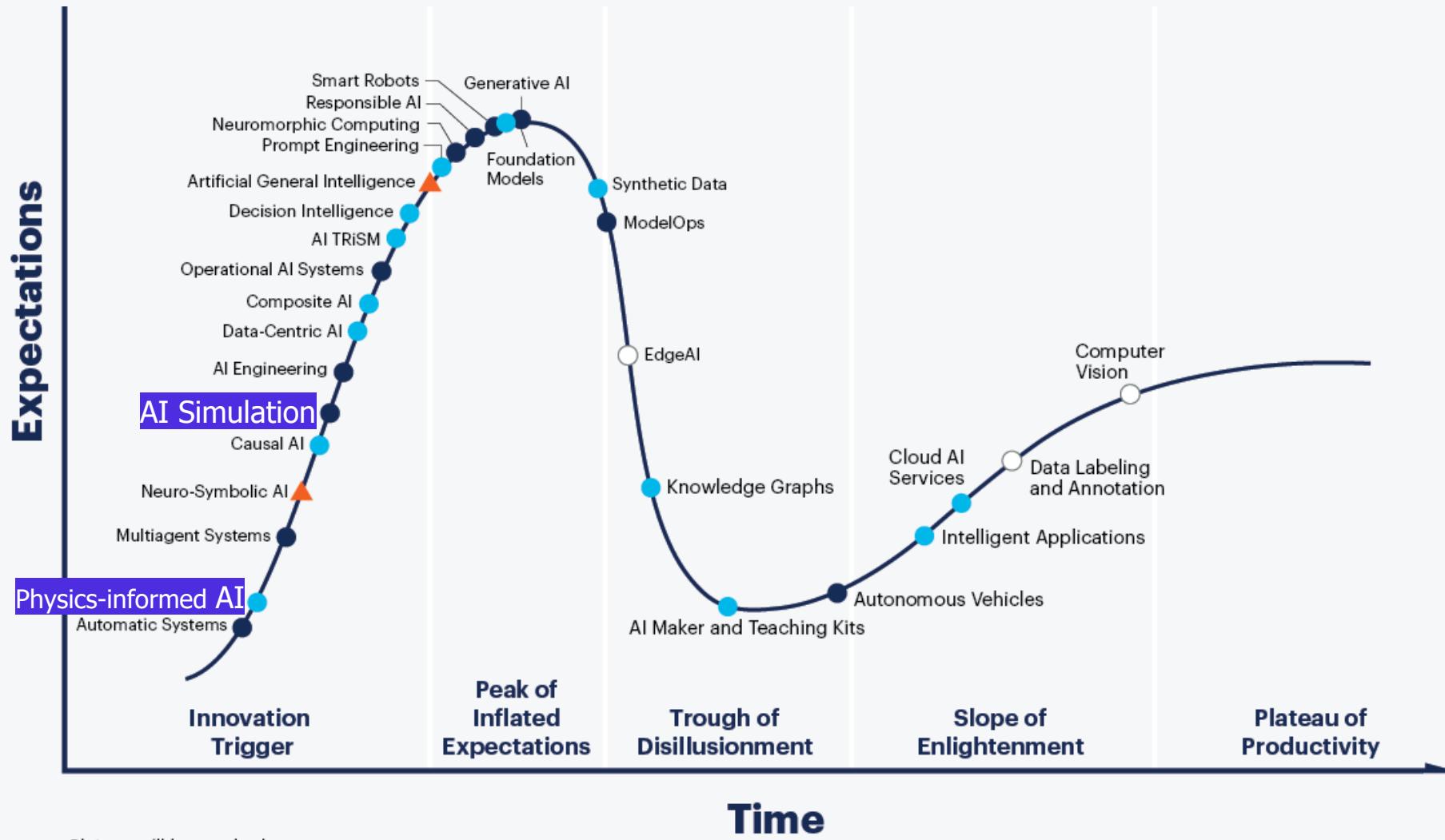
Affiliation of teams building notable AI systems

Growing ...



Artificial Intelligence Hype Cycle (2023)

Just
Beginning
of an Era!



Plateau will be reached:

○ less than 2 years

● 2 to 5 years

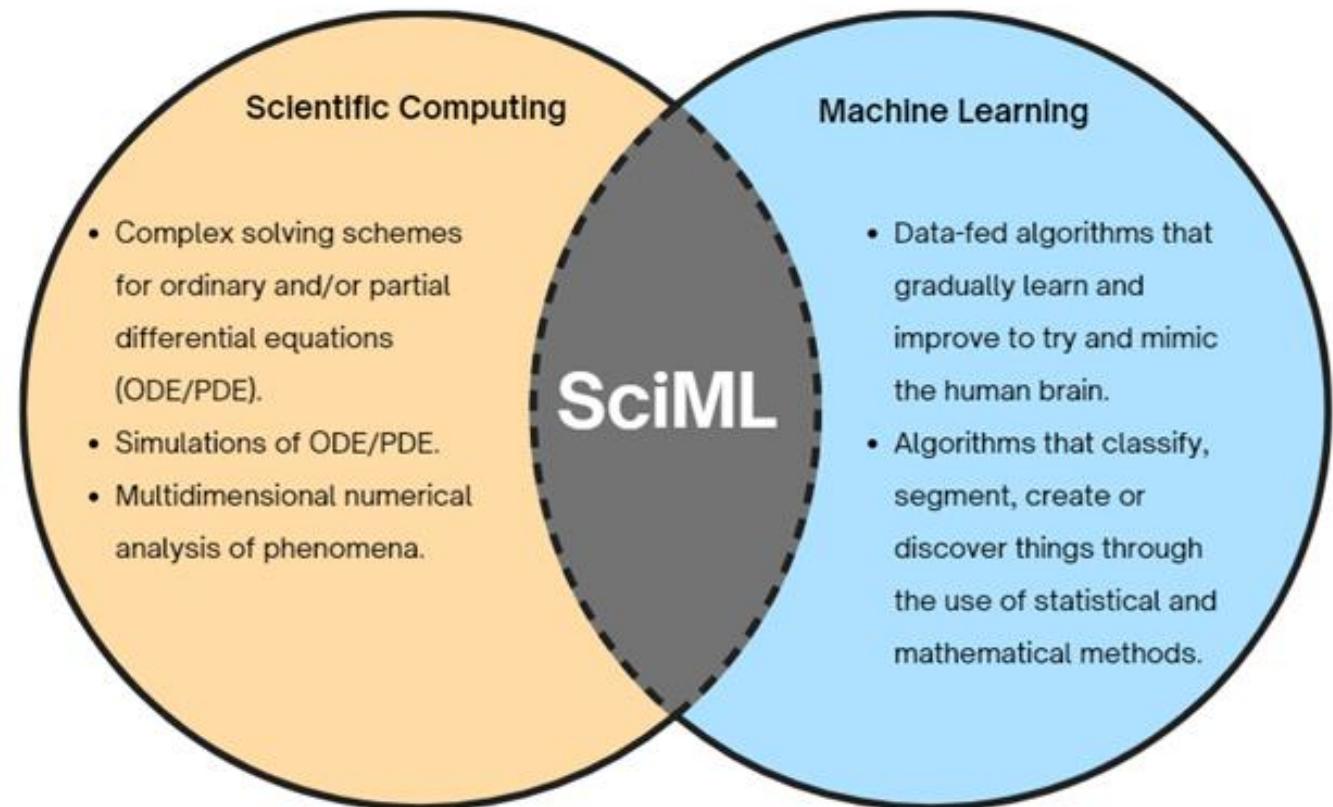
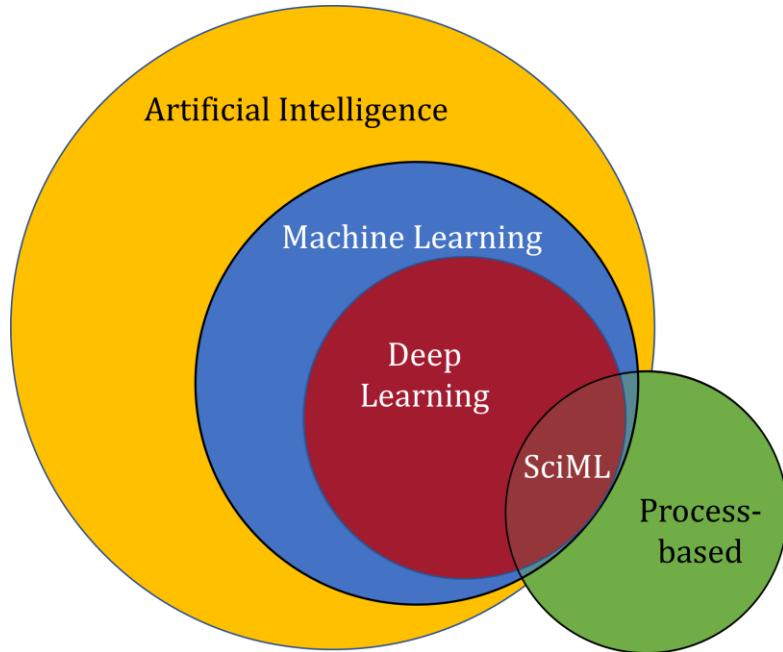
● 5 to 10 years

▲ more than 10 years

✗ obsolete before plateau

As of July 2023

Scientific Computing & Machine Learning for PDEs

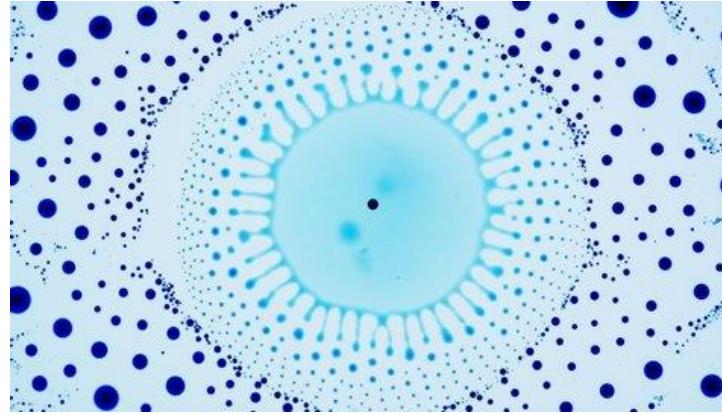


Partial Differential Equations (PDEs)

They are everywhere!



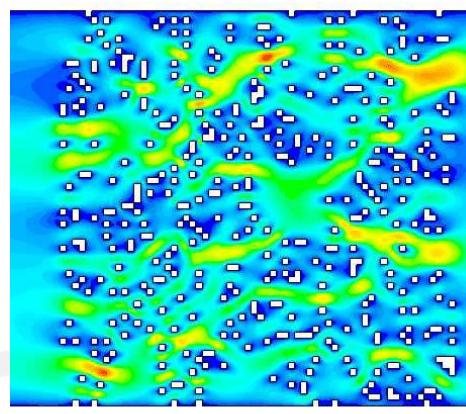
Black-holes



Surface Phenomena



Navier-Stokes Equations



Flow in Porous Media



Cup of Espresso!

Partial Differential Equations (PDEs)

They are everywhere!

Classification of Second-Order PDEs:

1) Elliptic PDEs (e.g., Laplace's equation):

Steady-state problems, no time dependency.

2) Parabolic PDEs (e.g., Heat equation):

Time-dependent problems with diffusion-like behavior.

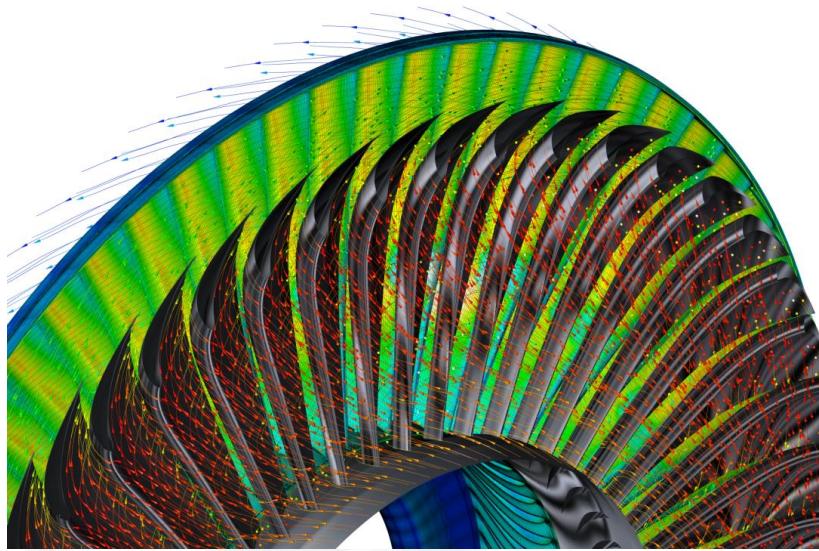
3) Hyperbolic PDEs (e.g., Wave equation):

Time-dependent problems with wave-like behavior.

Key Scientific Tasks

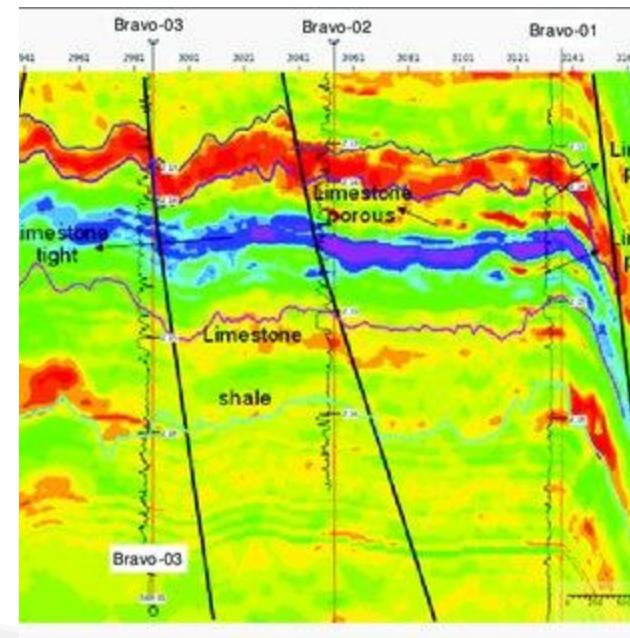
Forward Simulation

$$y = f(x)$$



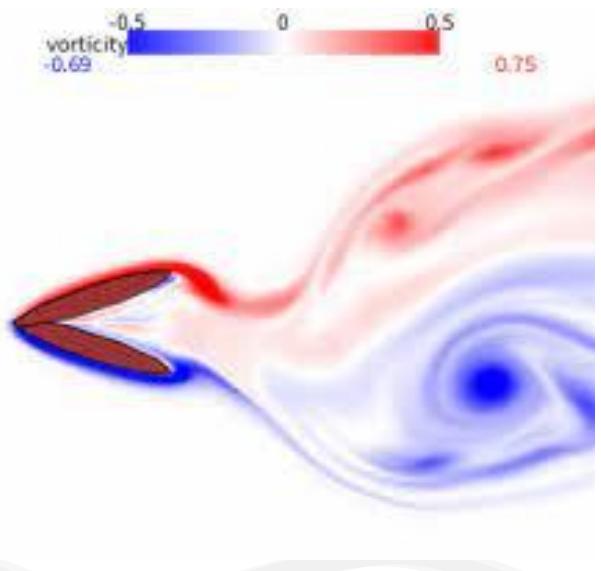
Inverse Simulation

$$y = f(\textcolor{red}{x})$$



Equation Discovery

$$y = \textcolor{red}{f}(x)$$



Why a revolution is needed?

Numerical Methods are very Successful

(issues: high resolution, multiphysics, multiscale)

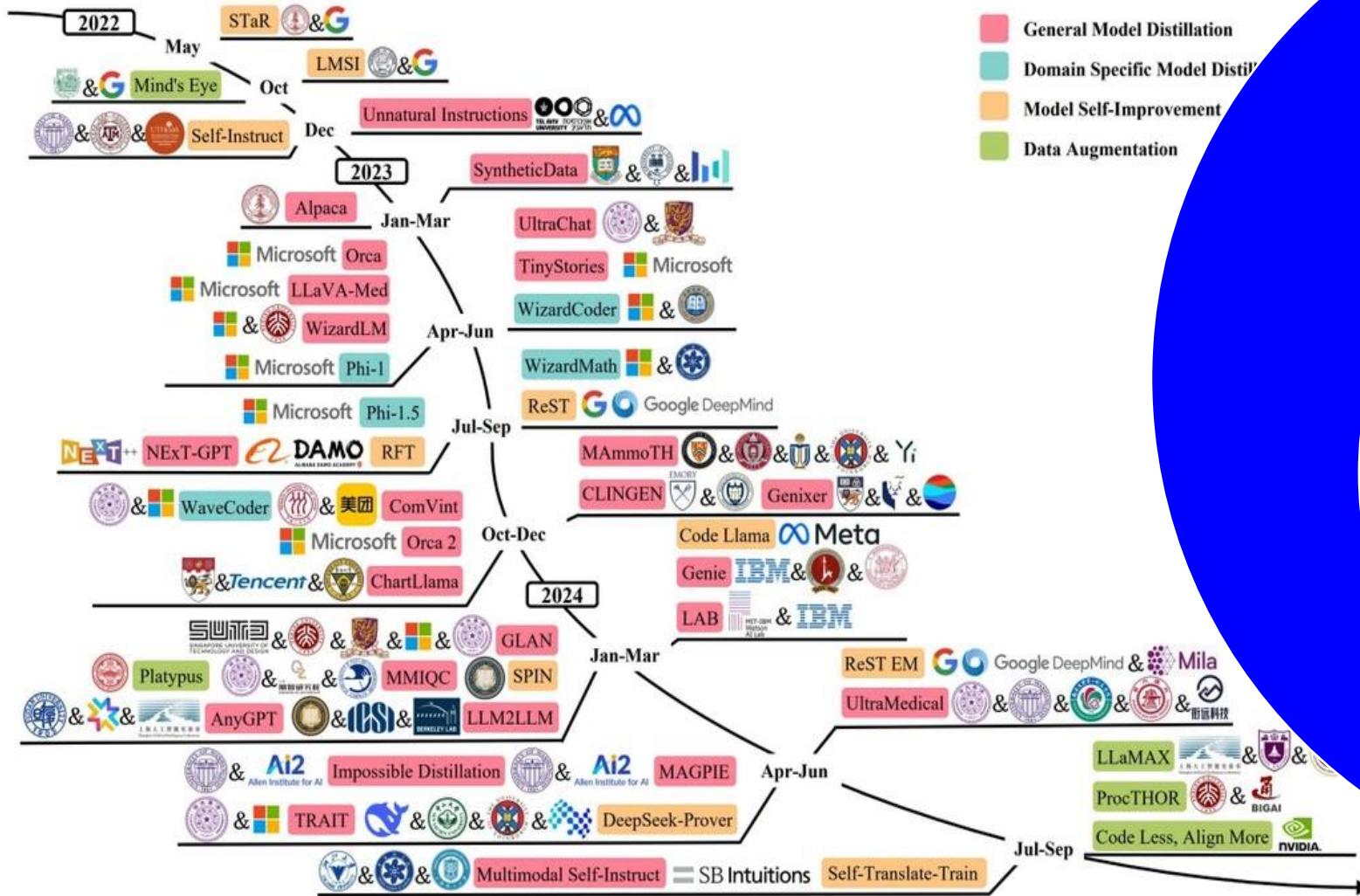
Challenging Tasks:

- Optimal Design
- Inverse Problem
- Uncertainty quantification (UQ)

Deep Learning



Deep Learning



Artificial Intelligence

A program that can sense, reason, act and adapt

Machine Learning

Algorithm whose performance improve as they are exposed to more data over time

Deep Learning

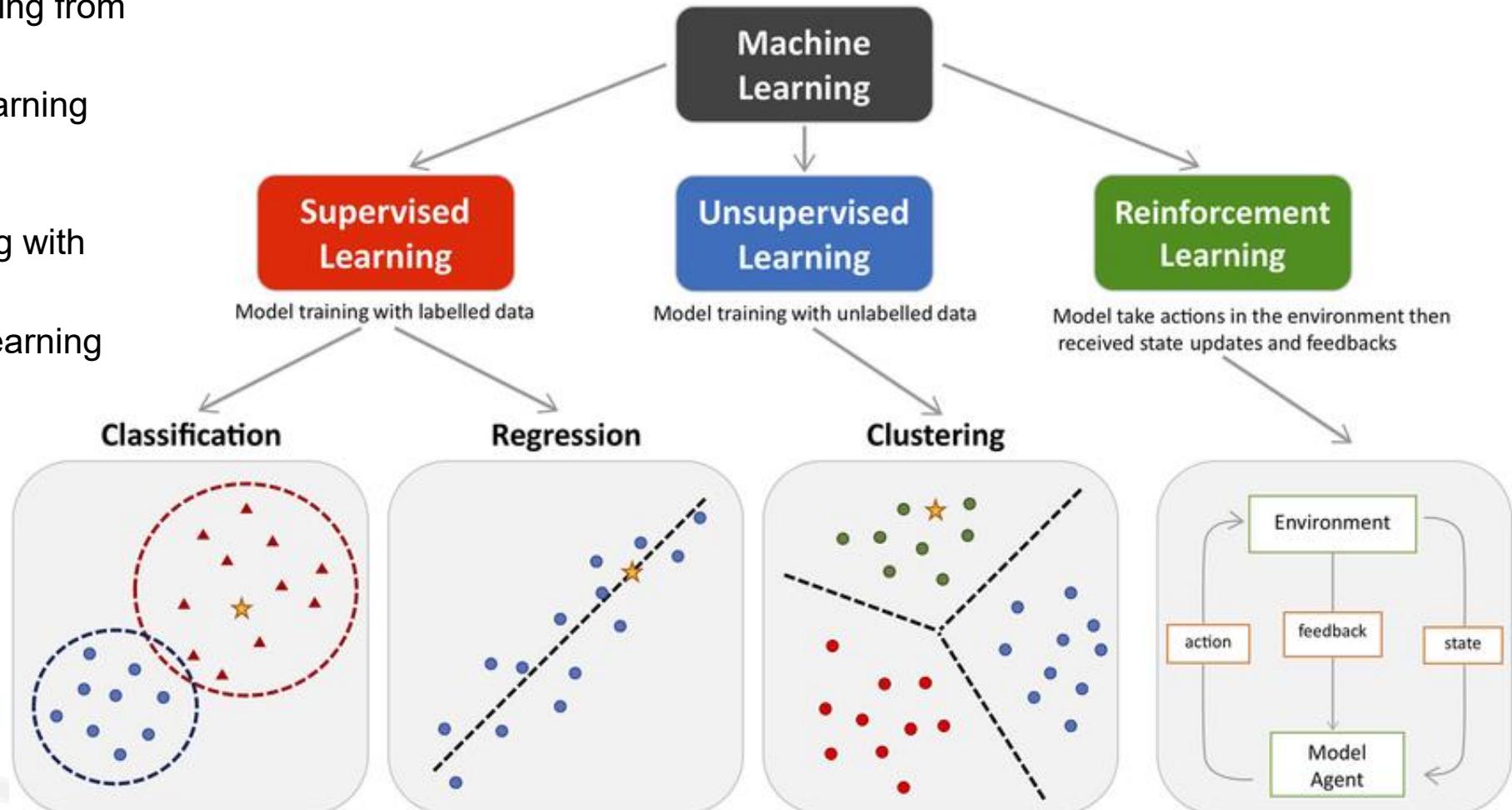
Subset of machine learning in which multilayer neural networks learns from vast amount of data

Deep Learning: Concepts

- **Neural Networks** (also, activation functions, loss function)
- **Model Architectures**
- **Training** and **Optimization** Techniques (also, Transfer Learning, Regularization, Hyperparameter Tuning)
- **Supervised / Unsupervised / Self-supervised** learning
- **Reinforcement Learning (RL)**:
- **Bayesian Neural Networks (BNNs)**
- Emerging Topics: Multimodal Models, **Foundation models**, Generative AI

Types of Learning in Deep Learning

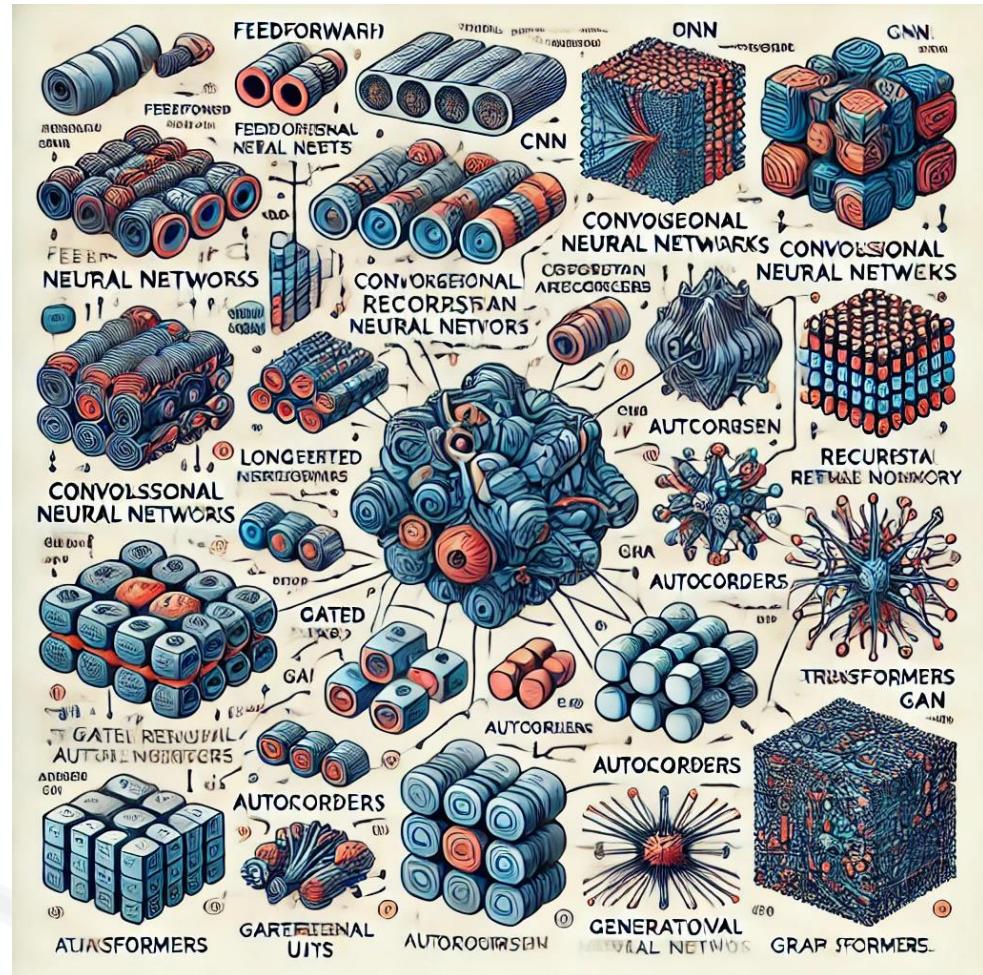
- **Supervised learning:** learning from samples with labels
- **Unsupervised learning:** learning from samples without labels
- **Semi-supervised learning:** augment supervised learning with unlabeled data
- **Reinforcement learning:** learning through the interaction with environment



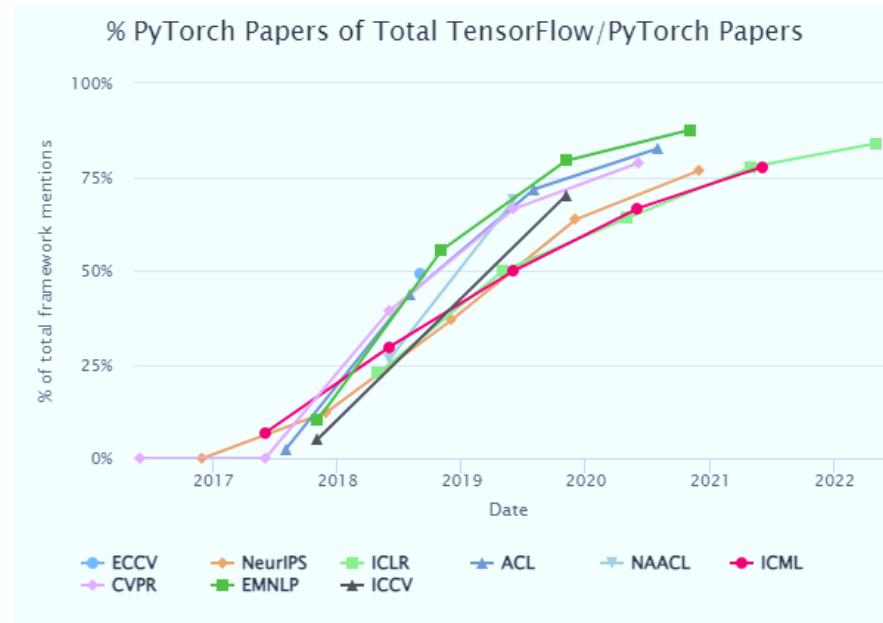
Deep Learning: Architecture

- Feedforward Neural Networks (FNNs)
- Convolutional Neural Networks (CNNs)
- Recurrent Neural Networks (RNNs)
- Long Short-Term Memory Networks (LSTMs)
- Gated Recurrent Units (GRUs)
- Autoencoders
- Variational Autoencoders (VAEs)
- Generative Adversarial Networks (GANs)
- Transformers
- Graph Neural Networks (GNNs)

ChatGPT 4o



Libraries & Frameworks



<https://miguelgfierro.com/blog/2022/an-analysis-of-the-adoption-of-top-deep-learning-frameworks/>

theano

before

Caffe

Microsoft
CNTK

K

TensorFlow

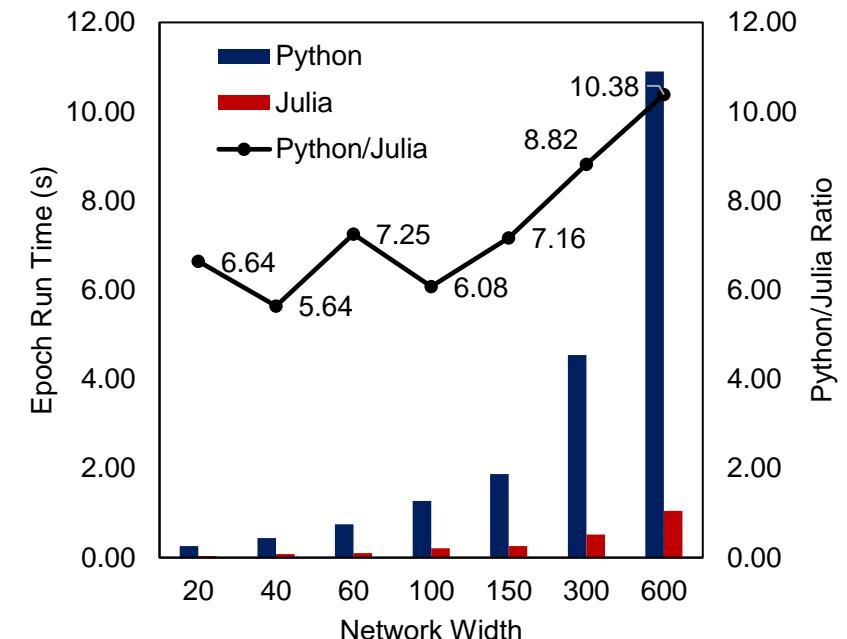
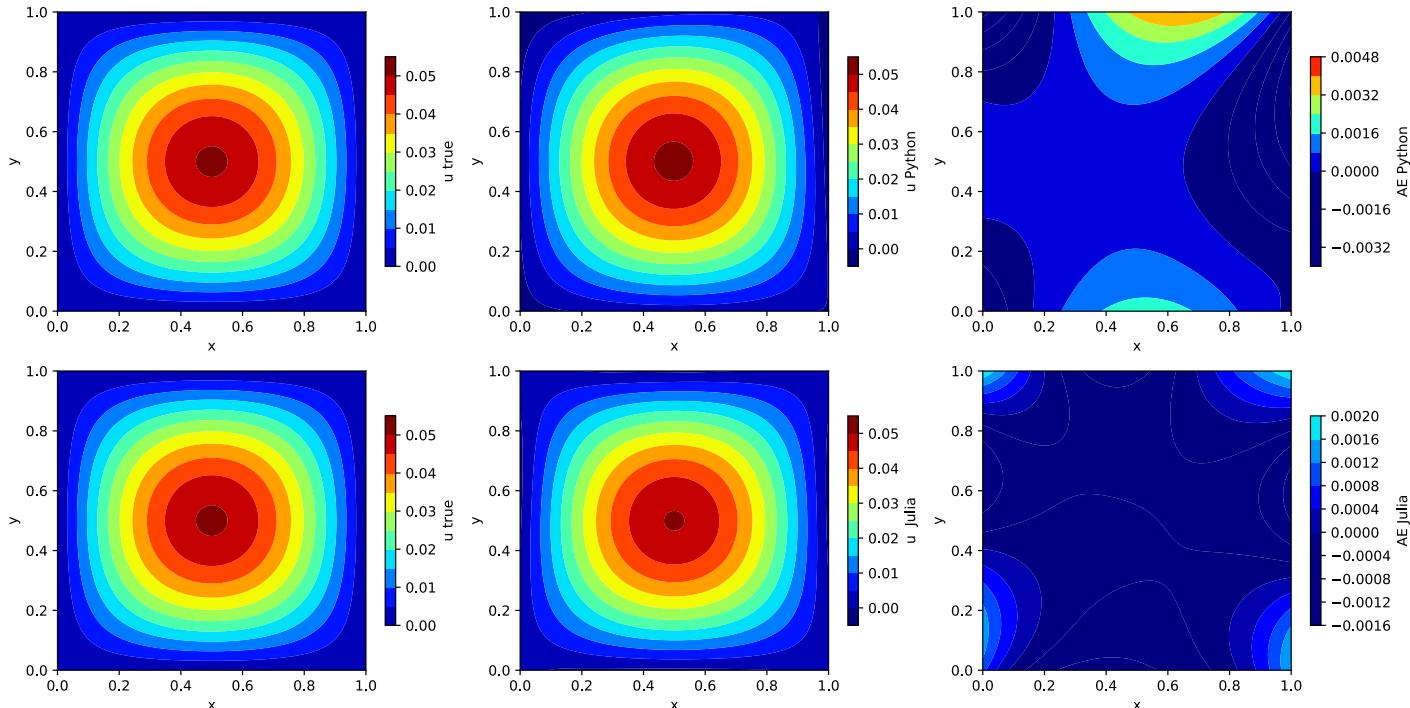
Caffe2

Deep Learning Framework Power Scores 2018

2012 2013 2014 2015 2016 2017

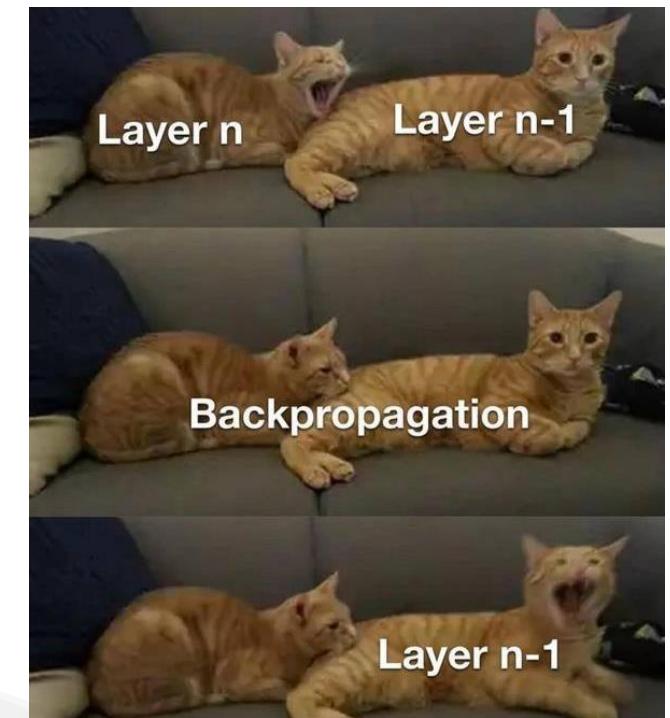
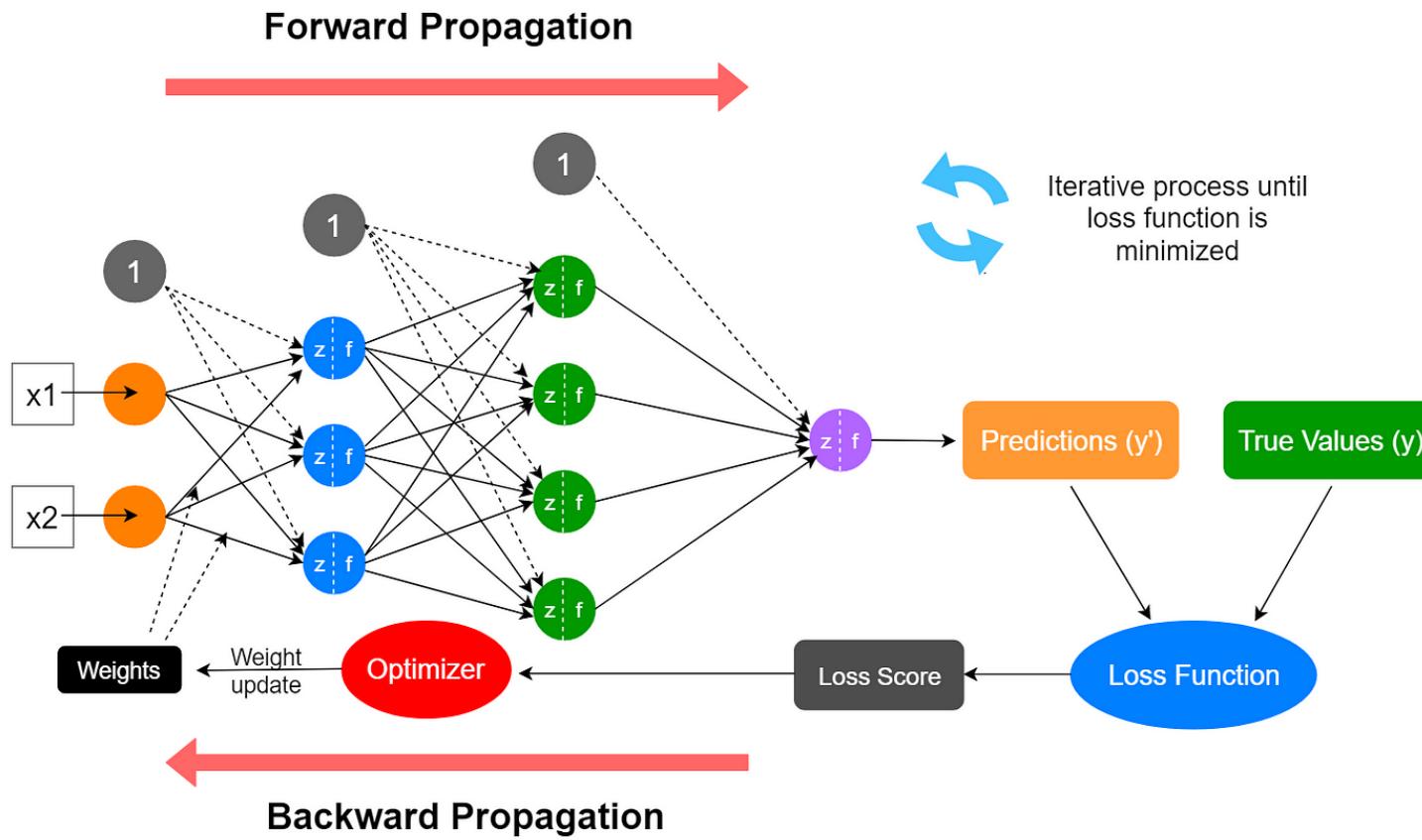
Programming Language also Matters

Python vs. Julia

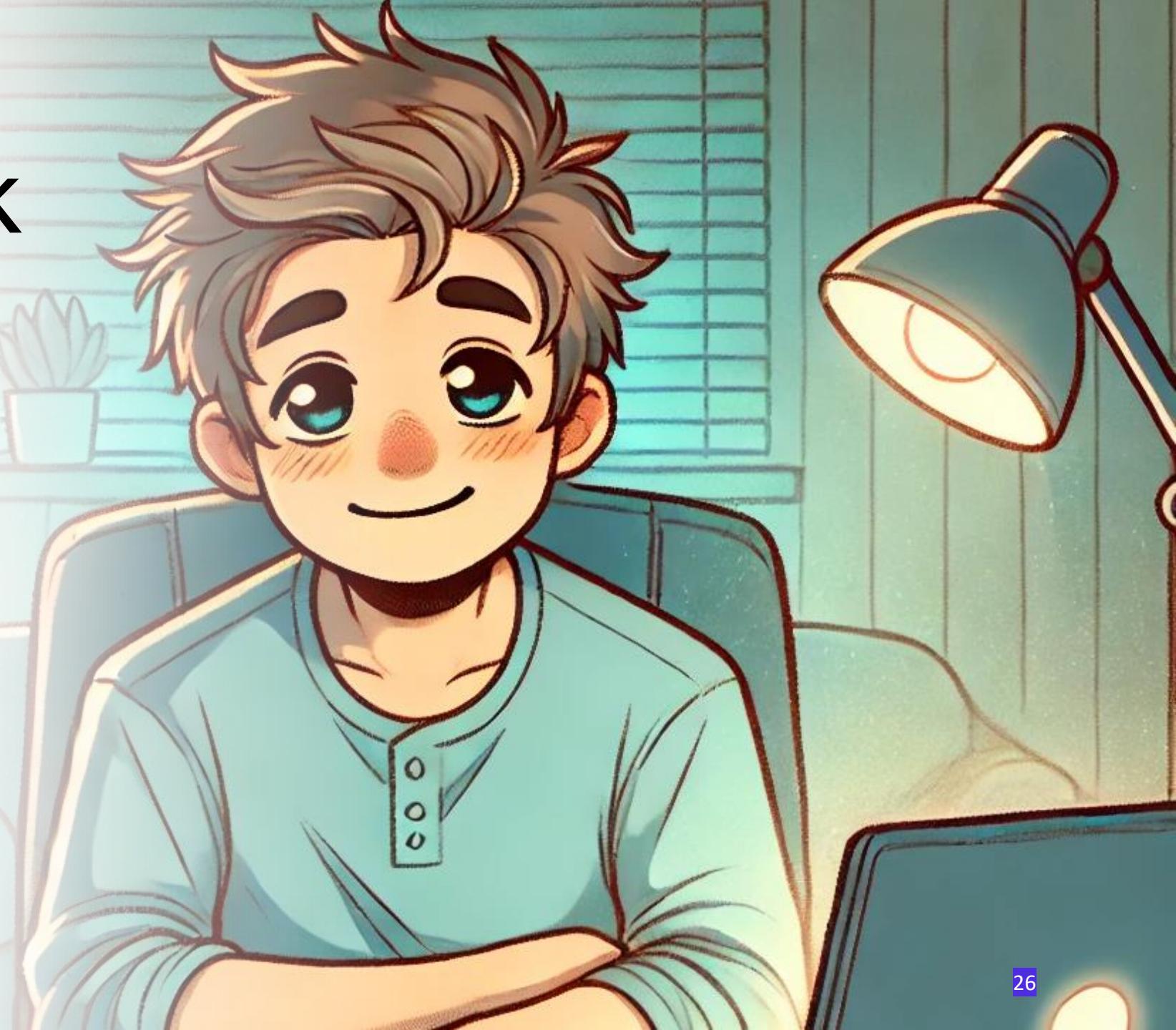


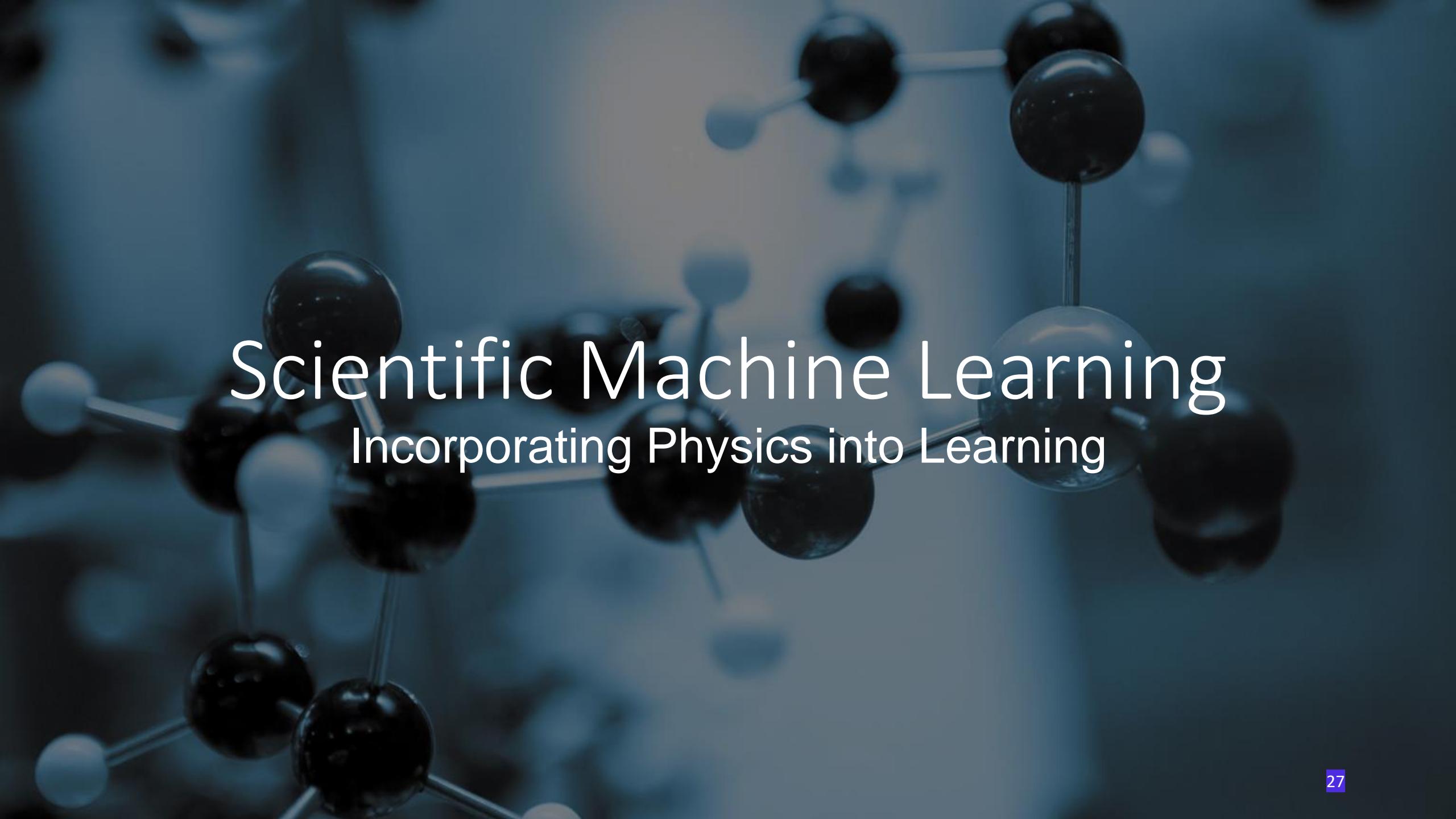
- When Python code is highly optimized with frameworks and GPU acceleration, the performance gap narrows significantly.

Training Process



A short break



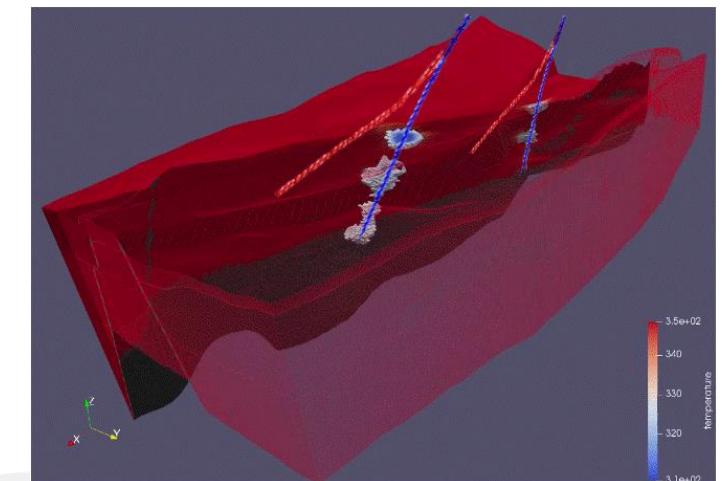
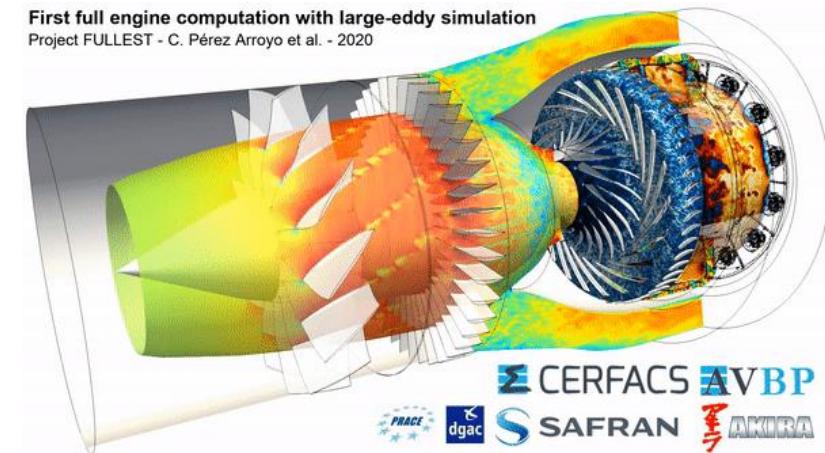


Scientific Machine Learning

Incorporating Physics into Learning

Why Numerical Methods?

- **Overcome Analytical Limitations:** Handles complex geometries and real-world problems where analytical methods fail.
- **Improved Modeling:** Approximate solutions often outperform oversimplified "exact" ones.
- **Flexibility:** Supports parametric studies and diverse scenarios.
- **Simplify Complex Solutions:** Reduces the effort of dealing with intimidating analytical formulas.
- **Enhanced Usability:** Provides efficient computations and visually appealing outputs for interpretation.



DARTS - Delft Advanced Research Terra Simulator

Why NOT Numerical Methods?

Current numerical methods come with several limitations and challenges:

- 1. Computational Complexity:** Solving PDEs numerically can be computationally demanding, particularly for large-scale and real-world problems.
- 2. Independent Computations:** Each instance of the input space needs to be processed independently when using numerical methods (no interaction and mutual computations).
- 3. Exact Physics Knowledge:** Numerical methods heavily rely on a precise understanding of the physics governing the problem.
- 4. Data Agnostic:** Traditional numerical methods are *not designed to* leverage existing datasets for learning or data-driven approaches.

Incorporating Physics into Learning

- **Semi-supervised Learning**

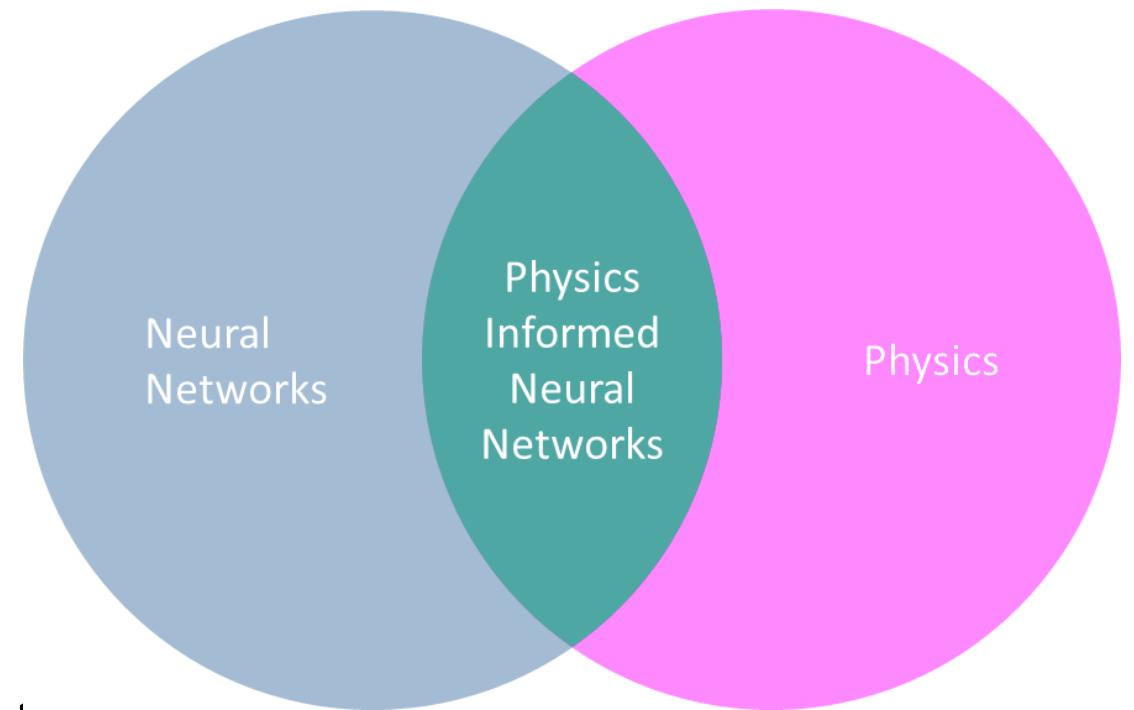
(Physics Informed Learning)

Enforce **physical laws** as hard/soft constraints

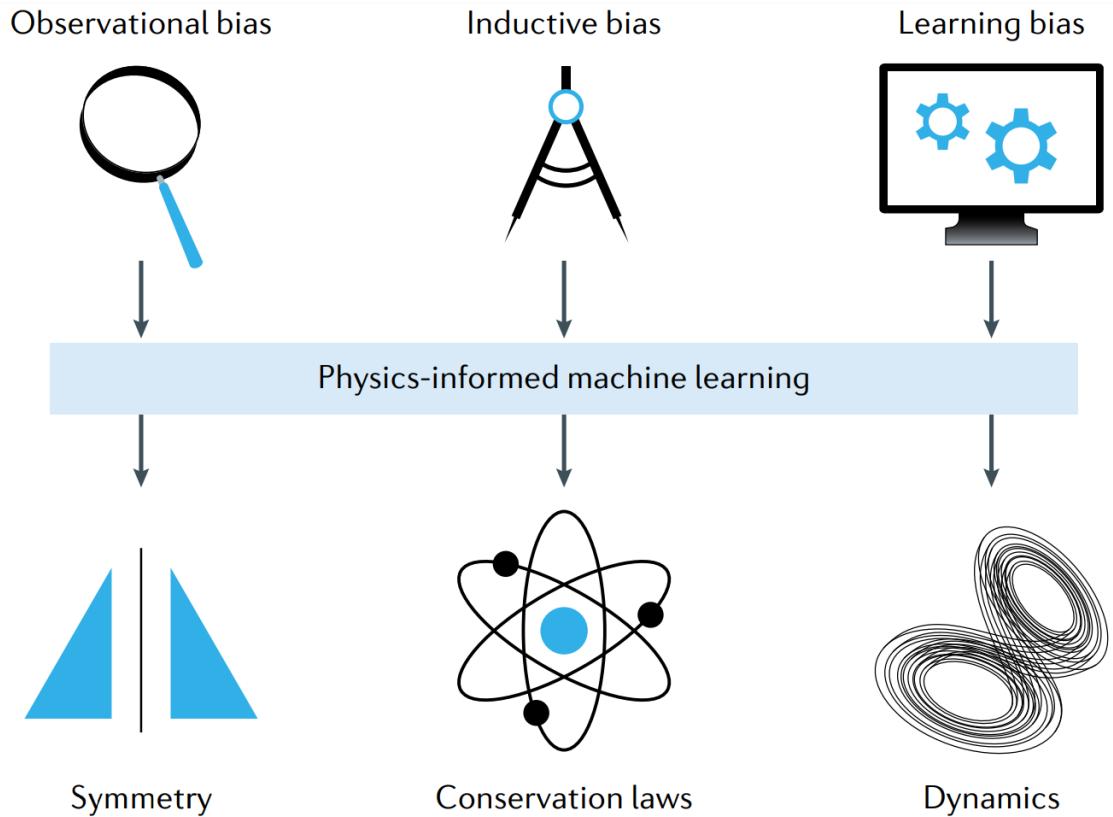
- **Supervised Learning**

(Operator Learning)

Train on **large amount of data** and let the NN learn the physics based operators



Physics Informed Machine Learning



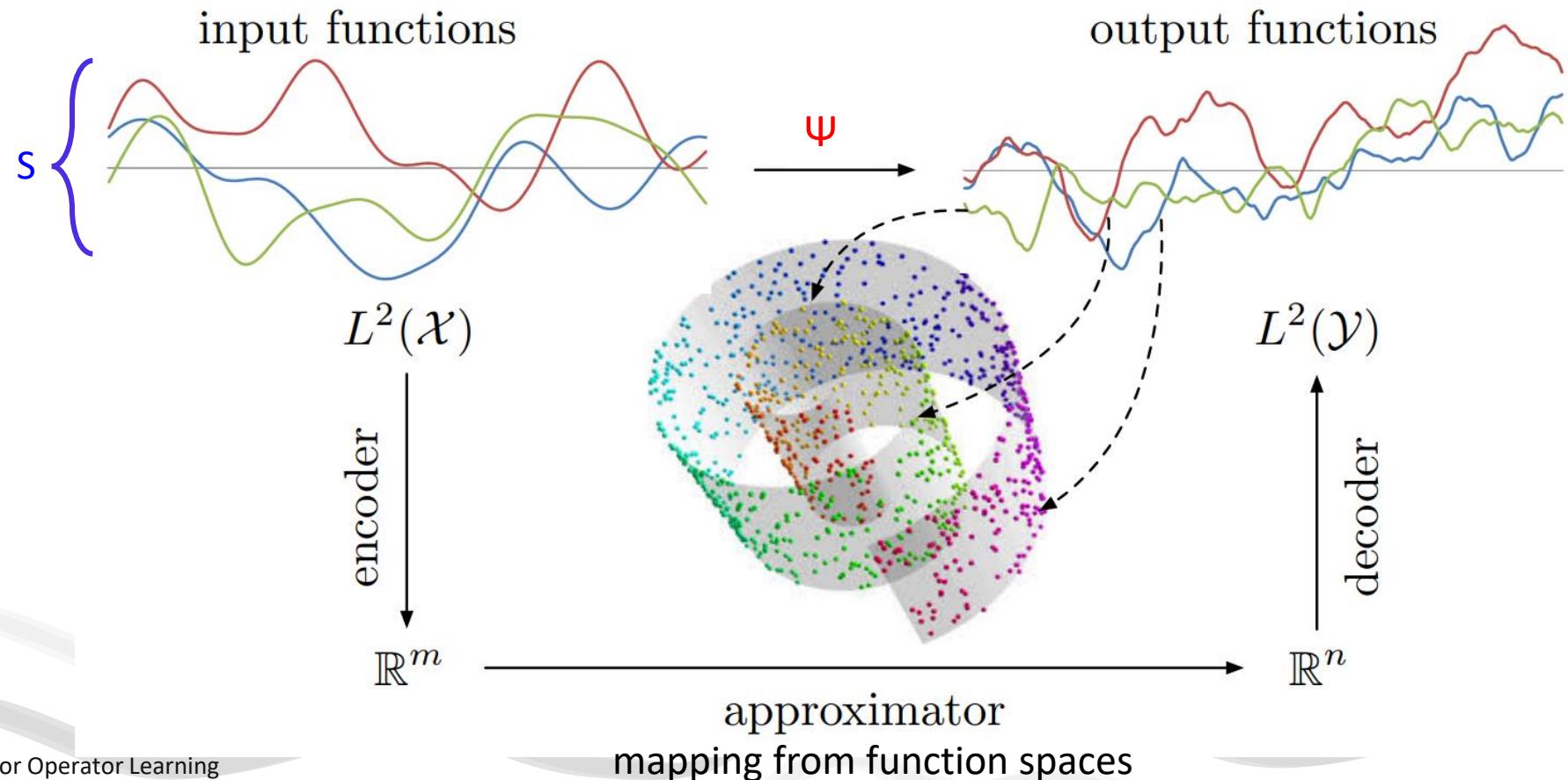
> PINNs: Great for some PDEs, particularly with **low complexity**, and **low training data**. Have several negatives. We need alternatives

Operator Learning ($\Psi : X \rightarrow Y$)

- Goal: Learn Ψ from samples S : Supervised Deep Learning

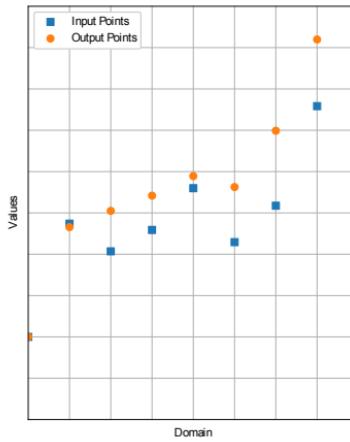
> Train on large amount of data (and hope) that the NN learns the constraints

Task: Find a Surrogate (based on DNNs) from data.

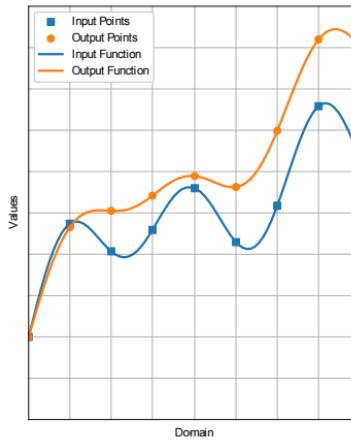


Operator Learning ($\Psi : X \rightarrow Y$)

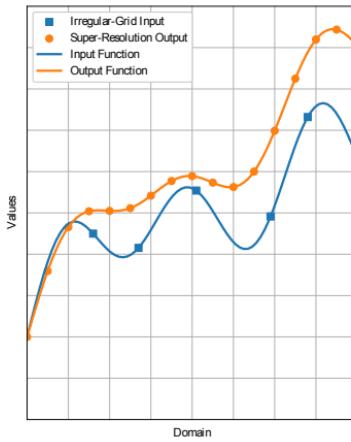
Comparison of neural networks with neural operators



(a) NN learns a mapping between input and output points on a fixed, discrete grid.



(b) NO maps between functions on continuous domains, even when training data is on a fixed grid.

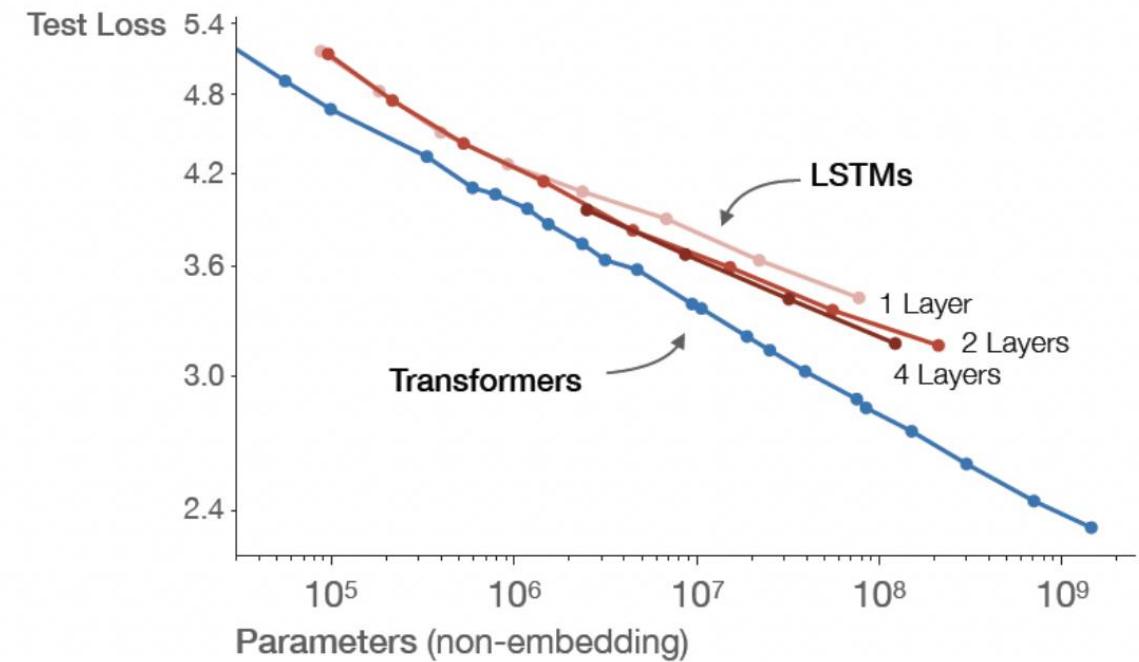


(c) NO maps between functions, so it accepts inputs outside the training grid, and can do super-resolution.

Property \ Model	NNs	DeepONets	Interpolation	Neural Operators
Discretization Invariance	✗	✗	✓	✓
Is the output a function?	✗	✓	✓	✓
Can query the output at any point?	✗	✓	✓	✓
Can take the input at any point?	✗	✗	✓	✓
Universal Approximation	✗	✓	✗	✓

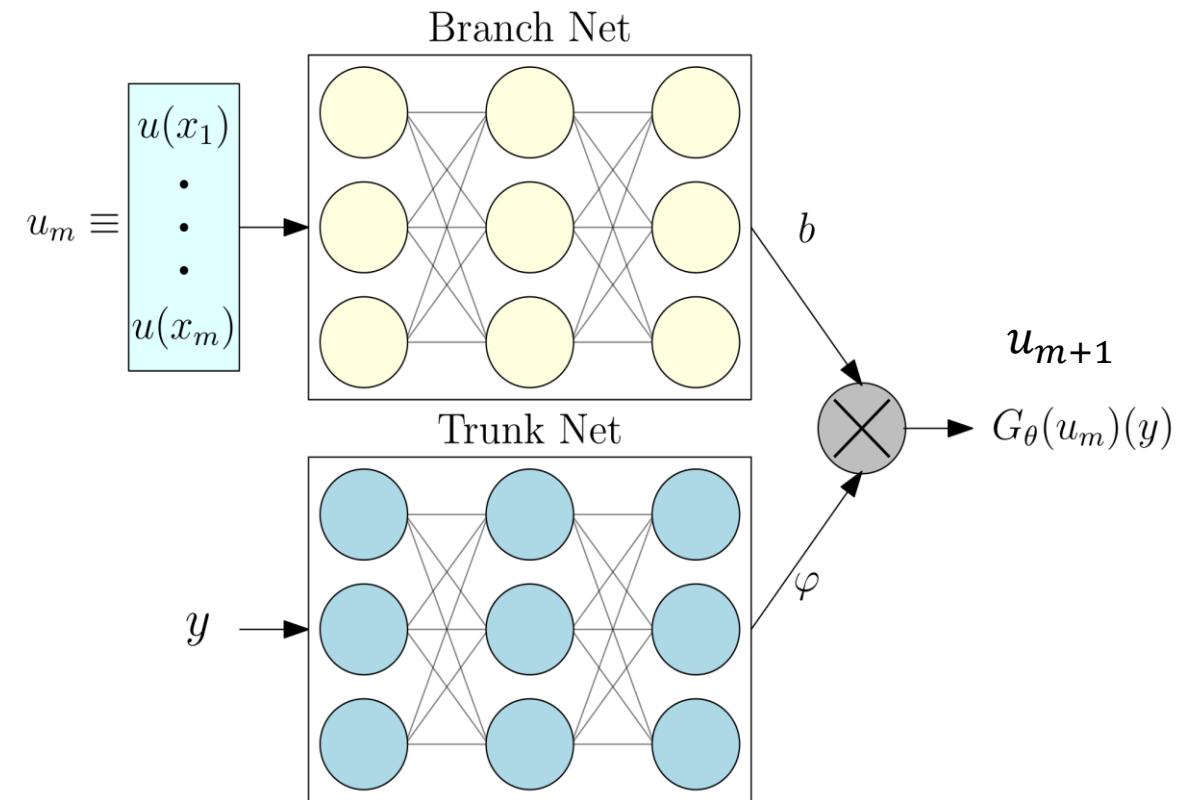
Operator Learning ($\Psi : X \rightarrow Y$)

- DeepONet
- Fourier Neural Operator (FNO)
- Convolutional Neural Operator (CNO)
- Graph Neural Operator (GNO)
- Operator U-Net architecture
- GenCFD
- ...



DeepONet (Deep Operator Network)

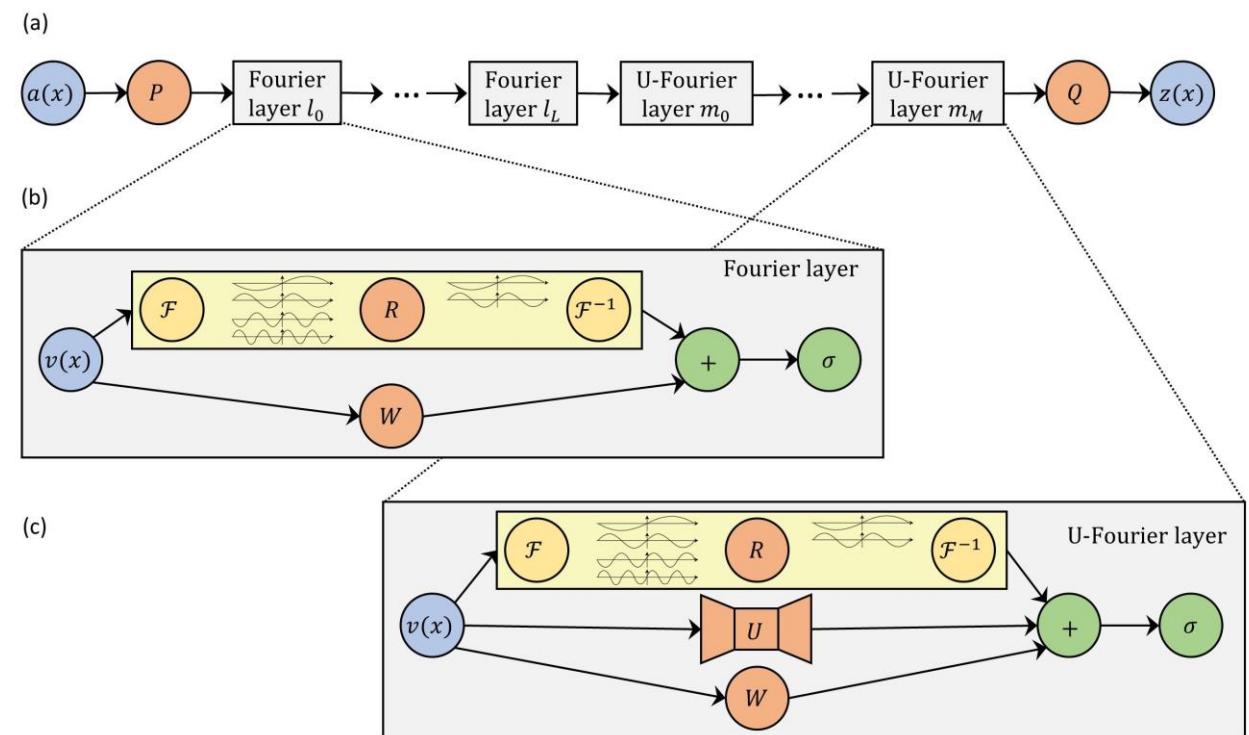
- **Branch Network:** Processes the input function by evaluating it at a set of fixed sensor points. These evaluations are then transformed into a feature representation.
- **Trunk Network:** Takes the coordinates where the output function is to be evaluated and generates corresponding basis functions.



<https://www.mdpi.com/1999-4893/15/9/325>

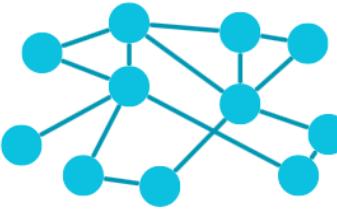
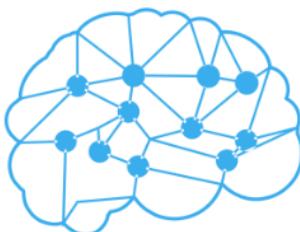
Fourier Neural Operator (FNO) (2020)

- **Architecture:** A series of Fourier transforms, convolutional layers, and Fourier layers to model long-range dependencies and complex spatial patterns.
- **Parameter Count:** Ranges from **millions to tens of millions** of parameters.
- **Application:** Designed to handle high-dimensional PDEs, particularly those involving turbulence or nonlinear dynamics, like the Navier-Stokes equations.
- **Use Case:** Applications in complex fluid dynamics and atmospheric modeling due to FNO's ability to capture intricate spatial structures over larger domains.

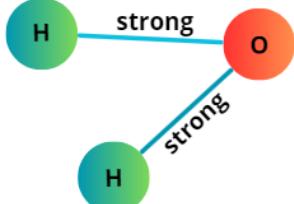
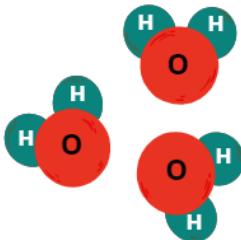


Graph Neural Networks

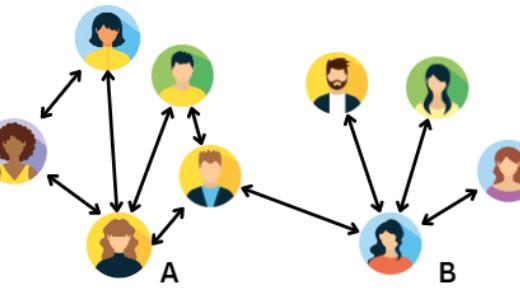
Graphs : Nodes + Edges



Brain networks



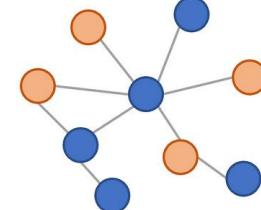
Chemical compounds



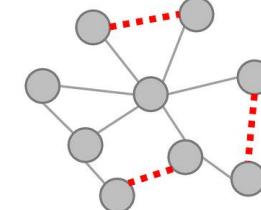
Social networks

Interesting Possibilities

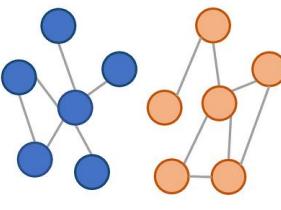
Node Classification



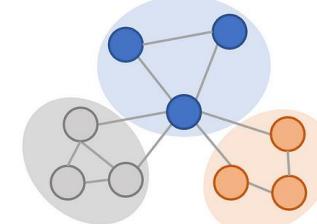
Link Prediction



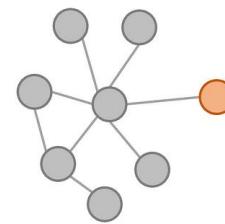
Graph Classification



Community Detection

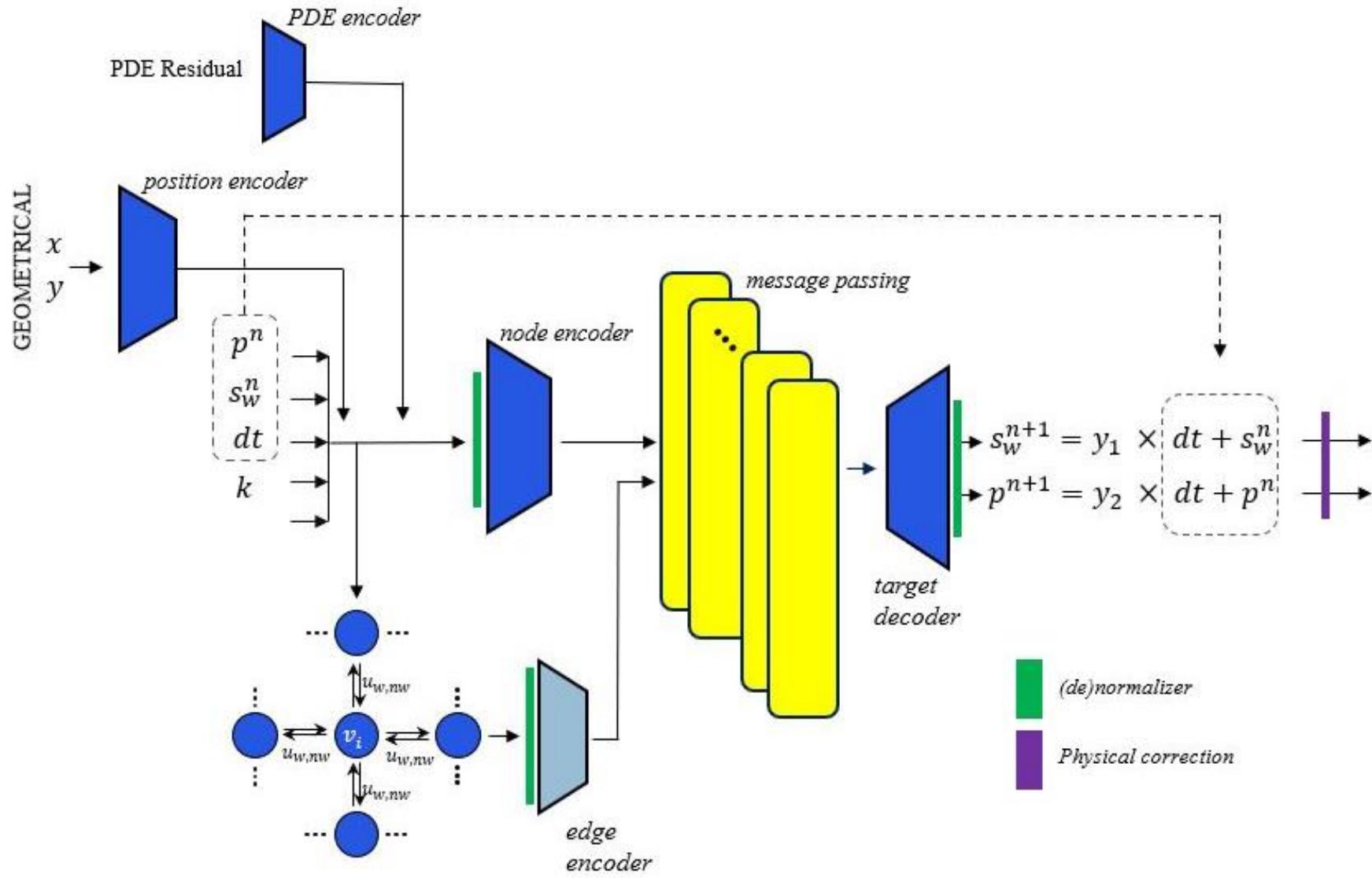


Anomaly Detection



<https://medium.com/@bscarleth.gtz/introduction-to-graph-neural-networks-an-illustrated-guide-c3f19da2ba39>

Graph Neural Networks

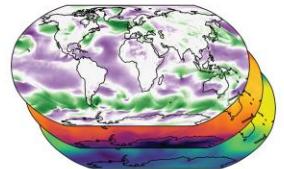


Graph Neural Networks

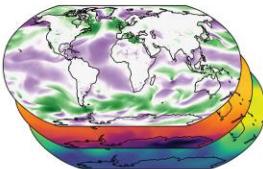


GraphCast

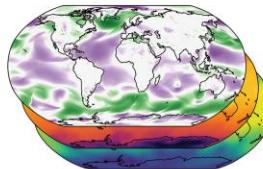
A Input weather state



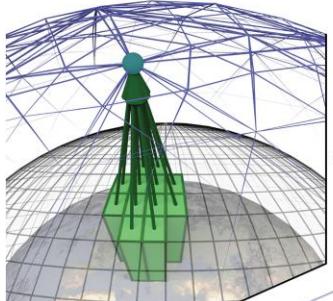
B Predict the next state



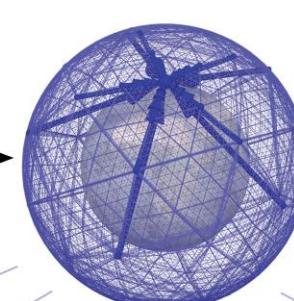
C Roll out a forecast



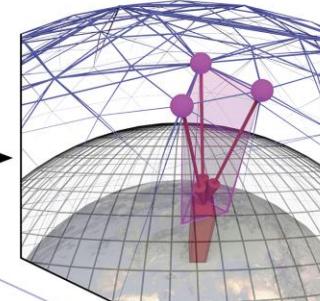
D Encoder



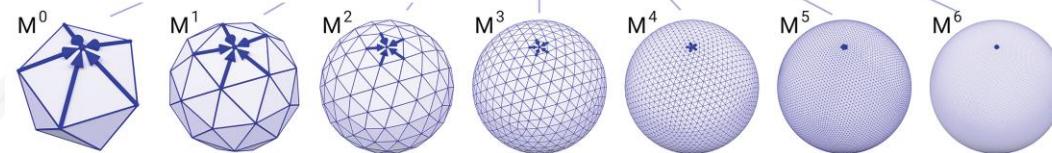
E Processor



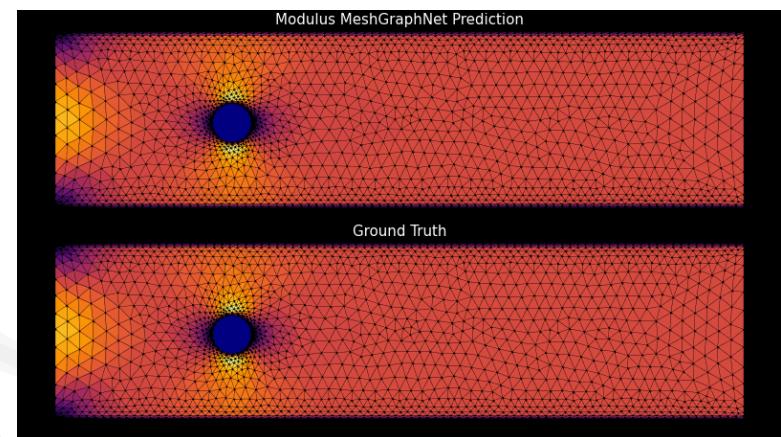
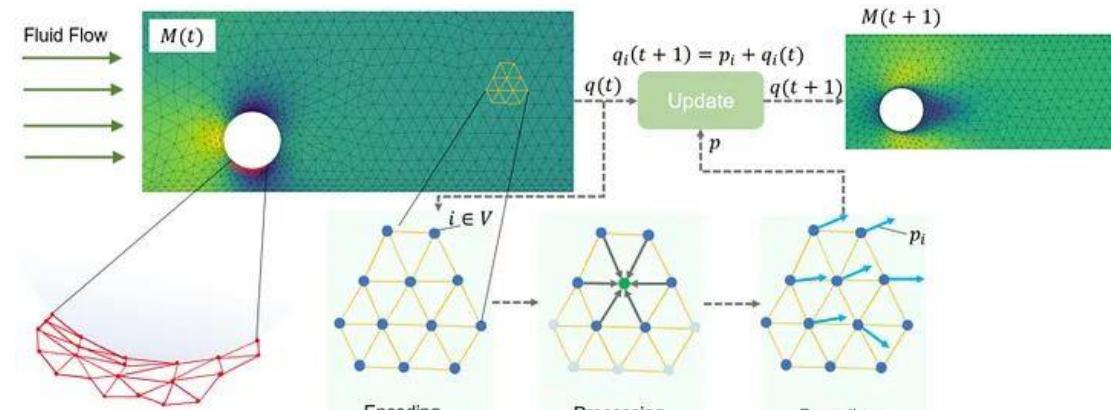
F Decoder



G Simultaneous multi-mesh message-passing



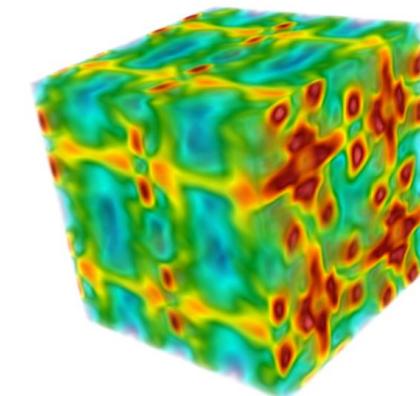
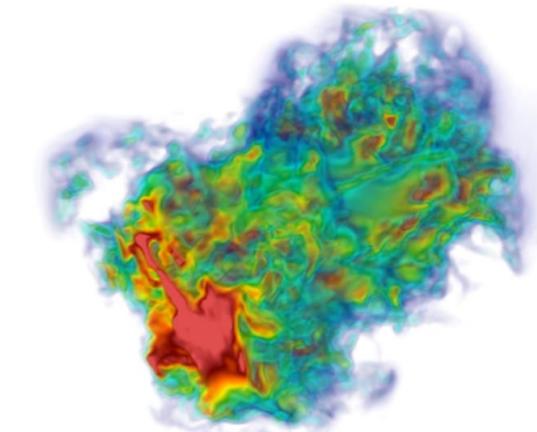
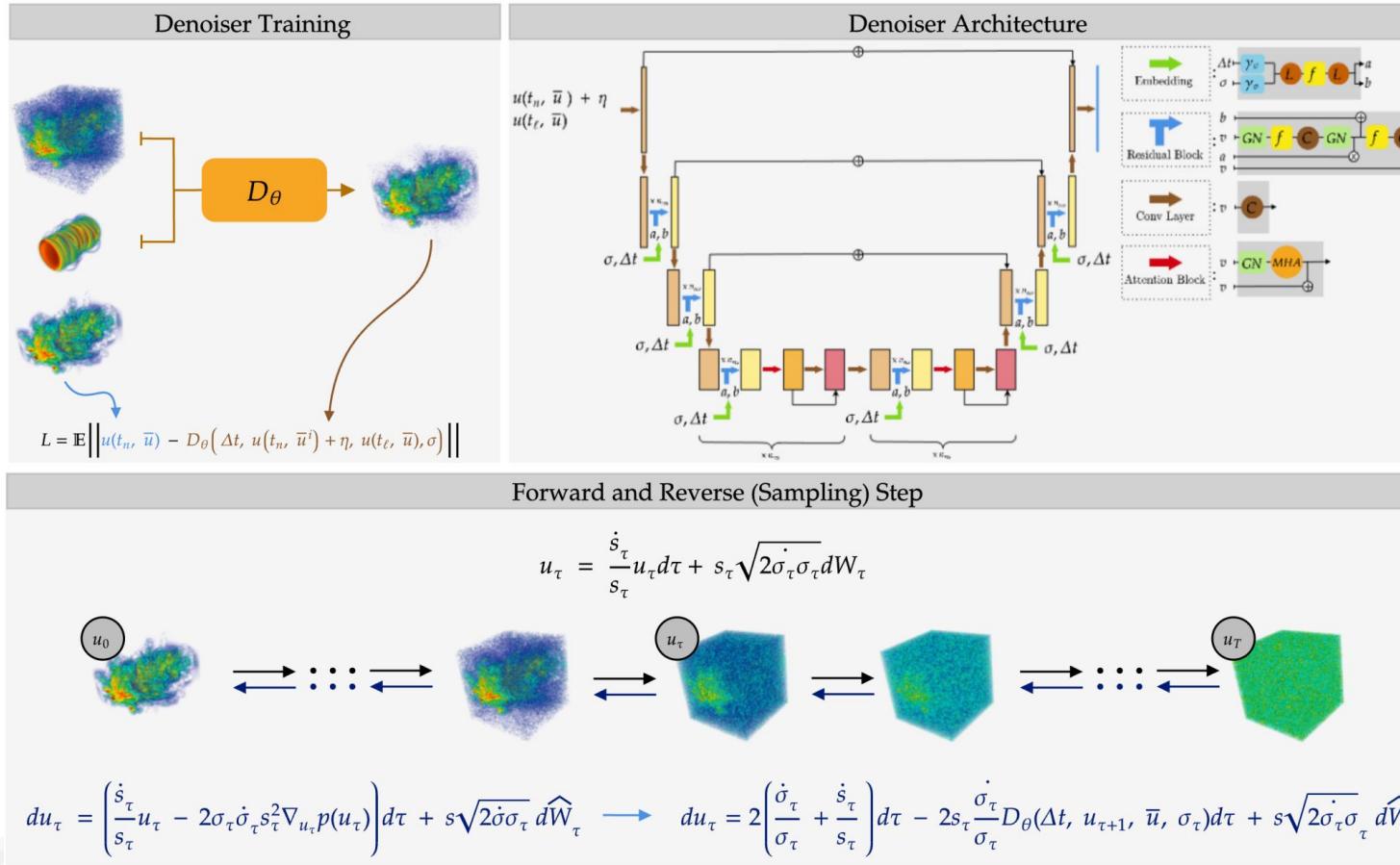
<https://www.science.org/stoken/author-tokens/ST-1550/full>



<https://developer.nvidia.com/blog/develop-physics-informed-machine-learning-models-with-graph-neural-networks/>

GenCFD

Generative AI for Statistical Computation of Fluids



Limitations of Operators

- They need **lots** of training data
- Generalization to **unseen domains**
- Computational cost of training
- Limited Interpretability
- Handling **High-Dimensional Inputs** and Outputs
- Scalability to Complex Systems

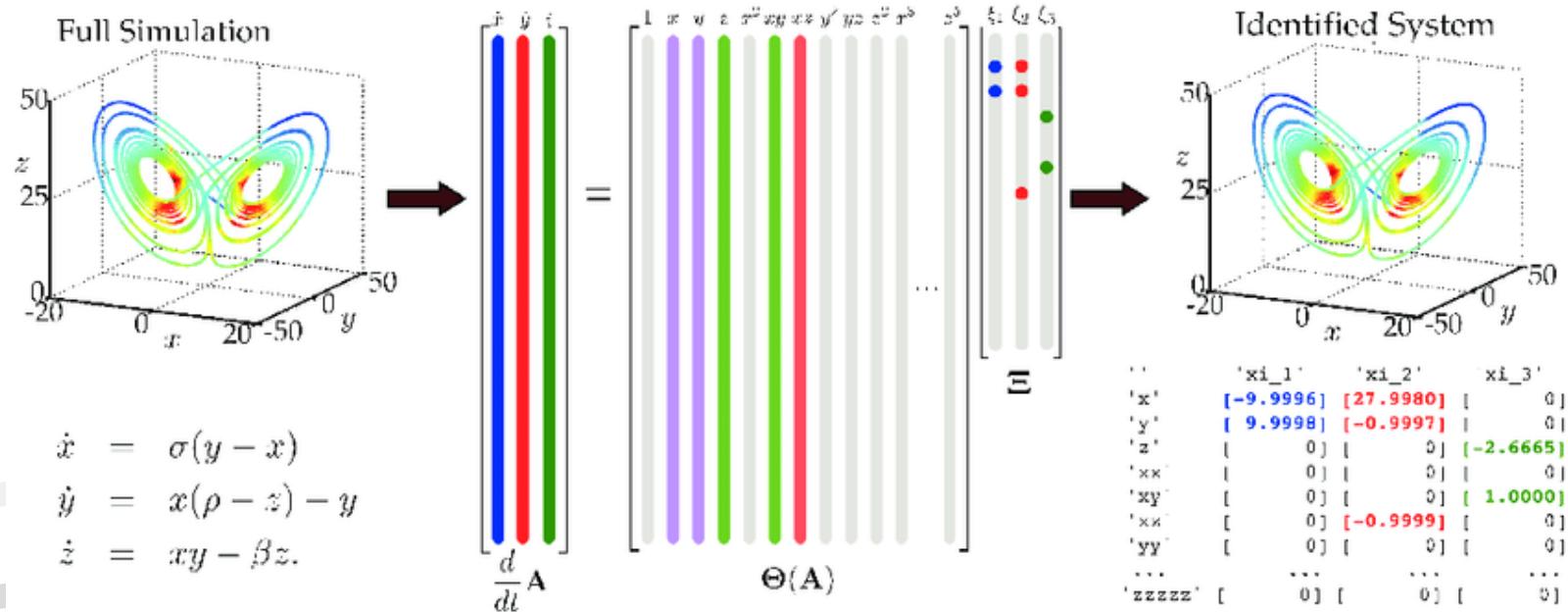
They are still under development. A long way is ahead.

A short break ☺



Sparse Identification of Nonlinear Dynamics (SINDy)

- **Purpose:** SINDy identifies governing equations of a dynamical system directly from data.
- **Key Idea:** It combines sparse regression techniques with a library of candidate functions to discover concise, interpretable models.



Foundation Models

Multi-Operator Learning (MOL)

Data



Gemini

Training

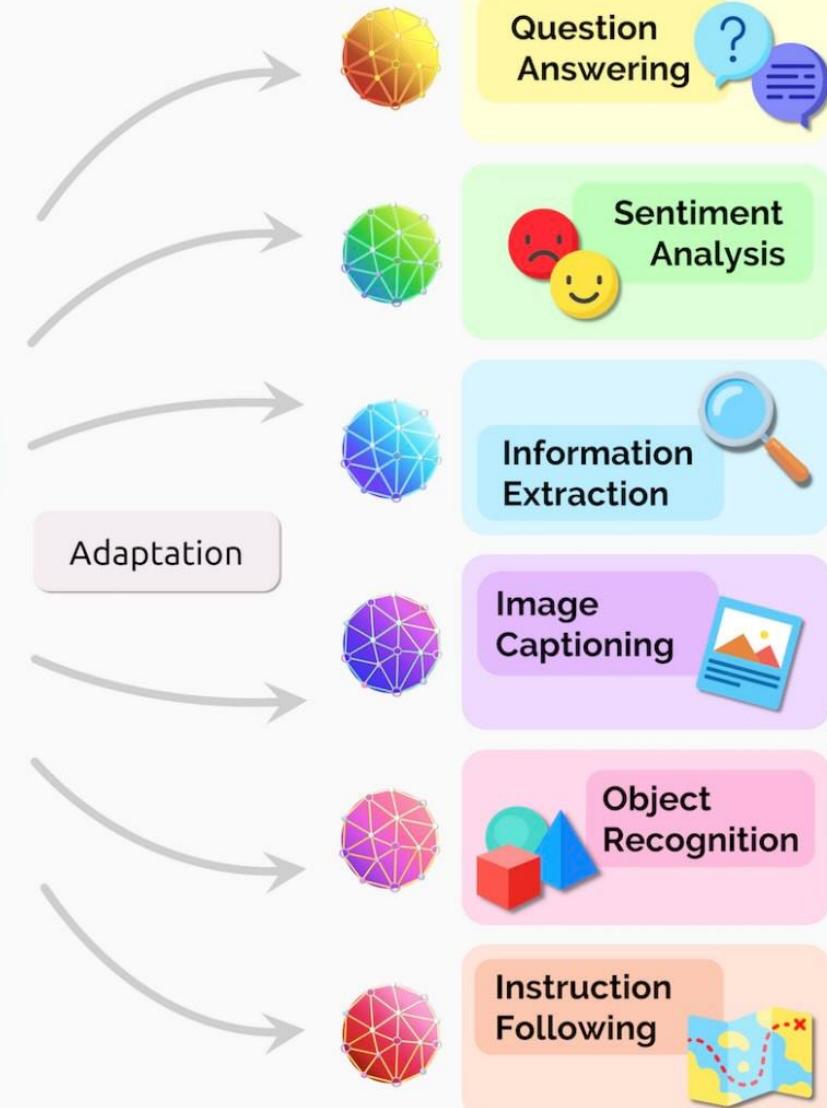
Foundation Model



ChatGPT



perplexity

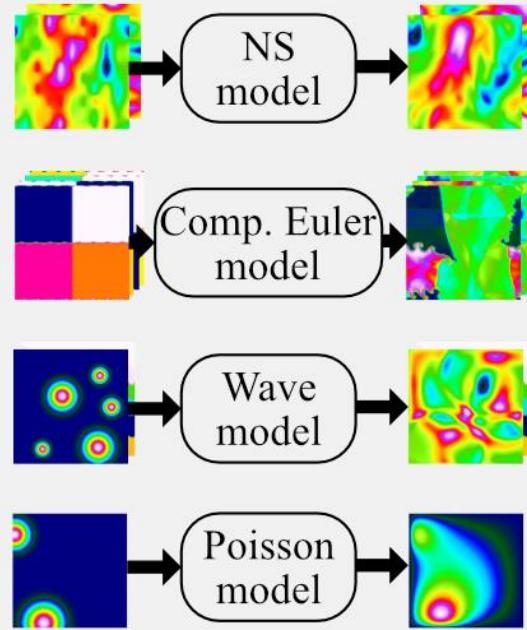


Foundation Models for PDEs

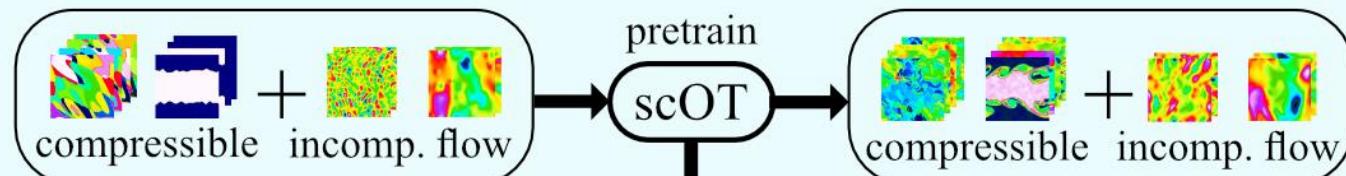
Poseidon: Efficient Foundation Models for PDEs (2024)



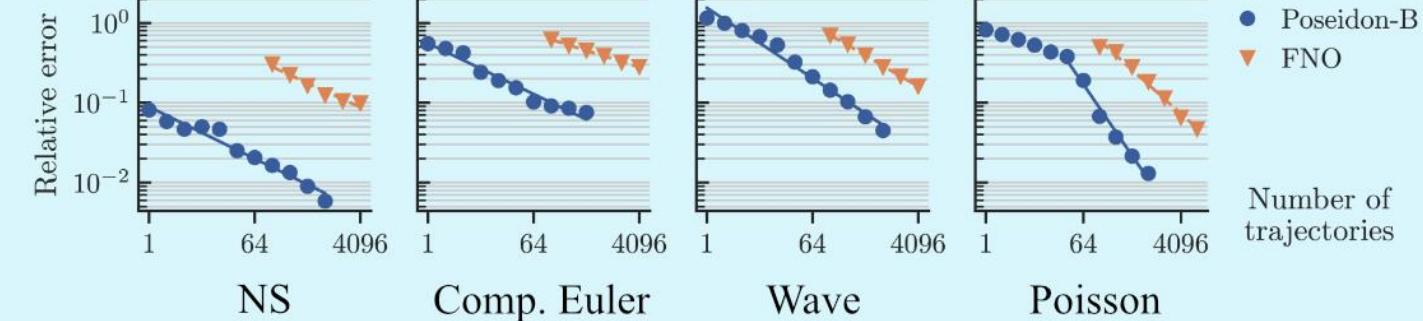
Task-specific
Operator Learning



POSEIDON: Foundation Model for PDEs



finetune on out-of-distribution downstream tasks

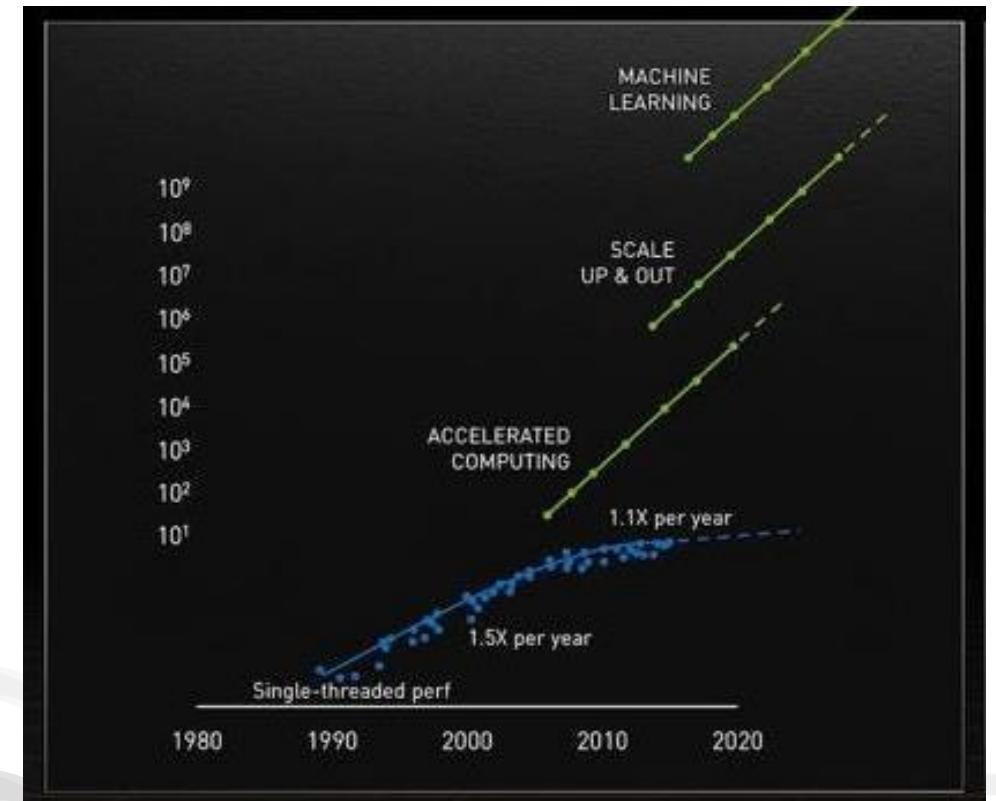
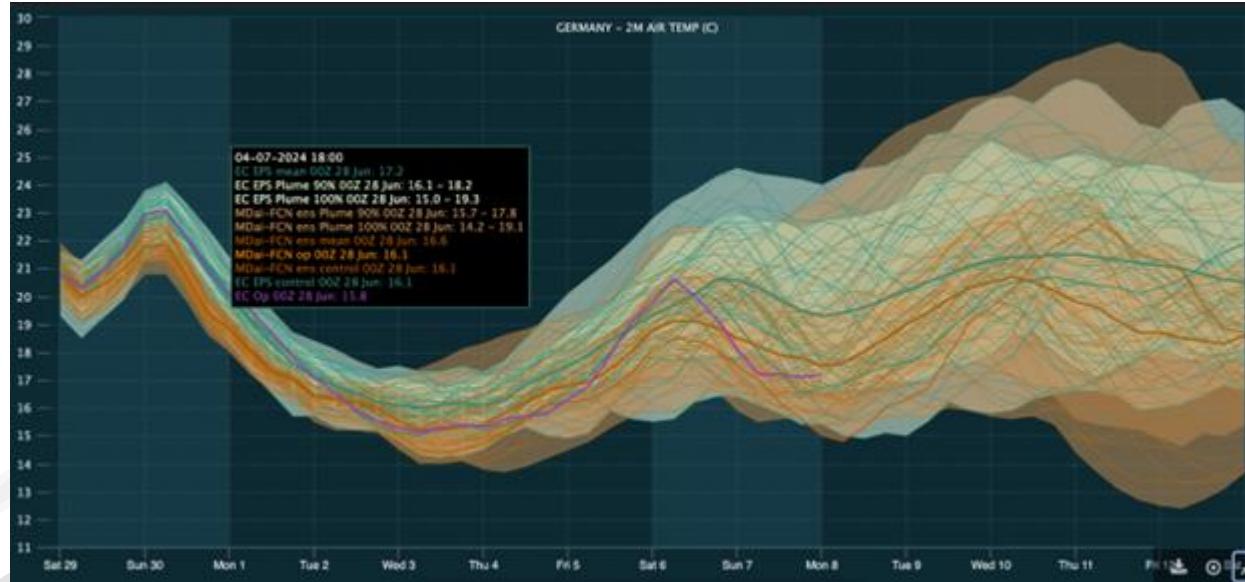


Examples of Real World Applications



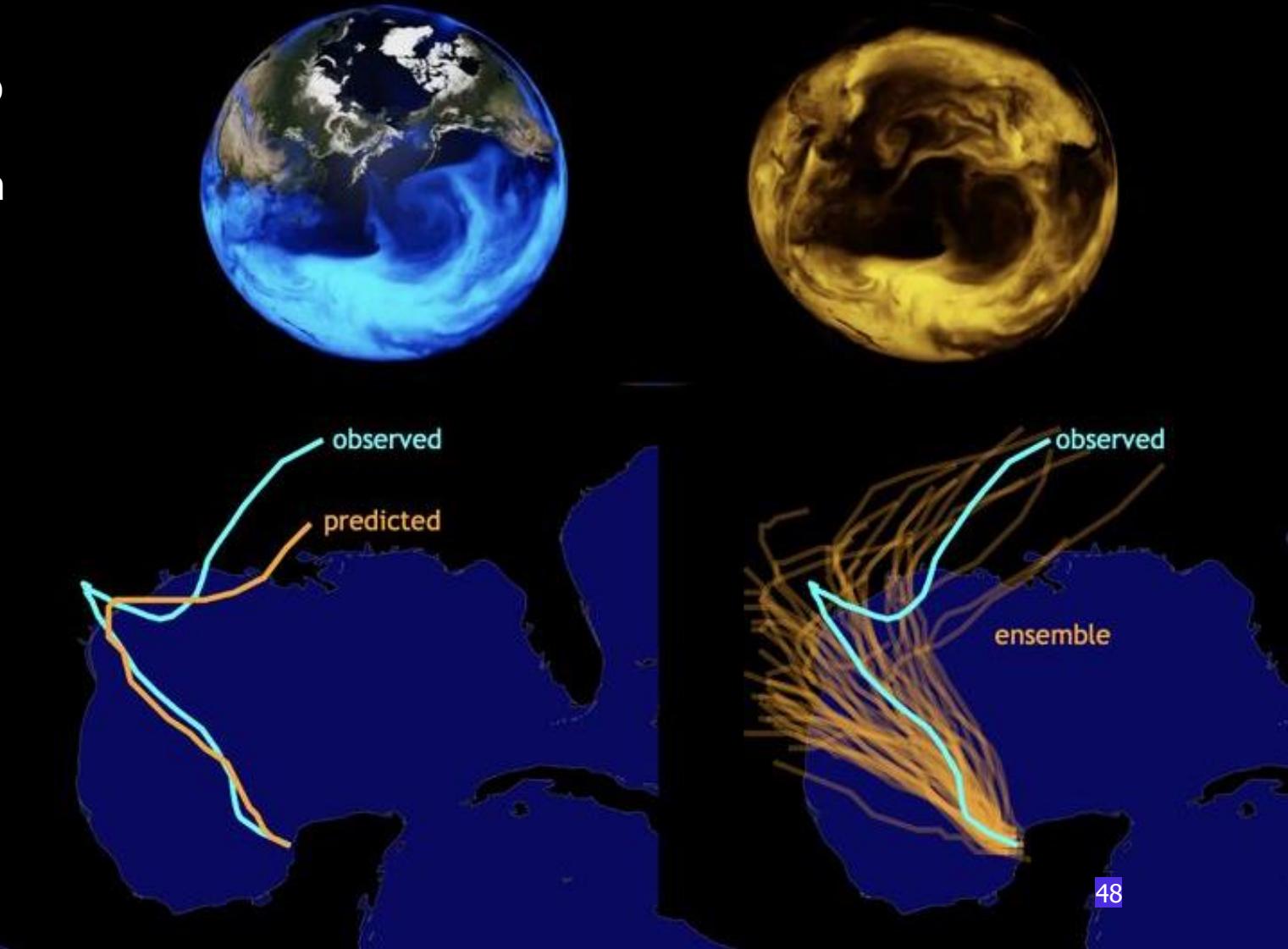
Caltech: Predicting Extreme Weather Predictions

FourCastNet: Fourier ForeCasting Neural Network



Caltech: Predicting Extreme Weather Predictions

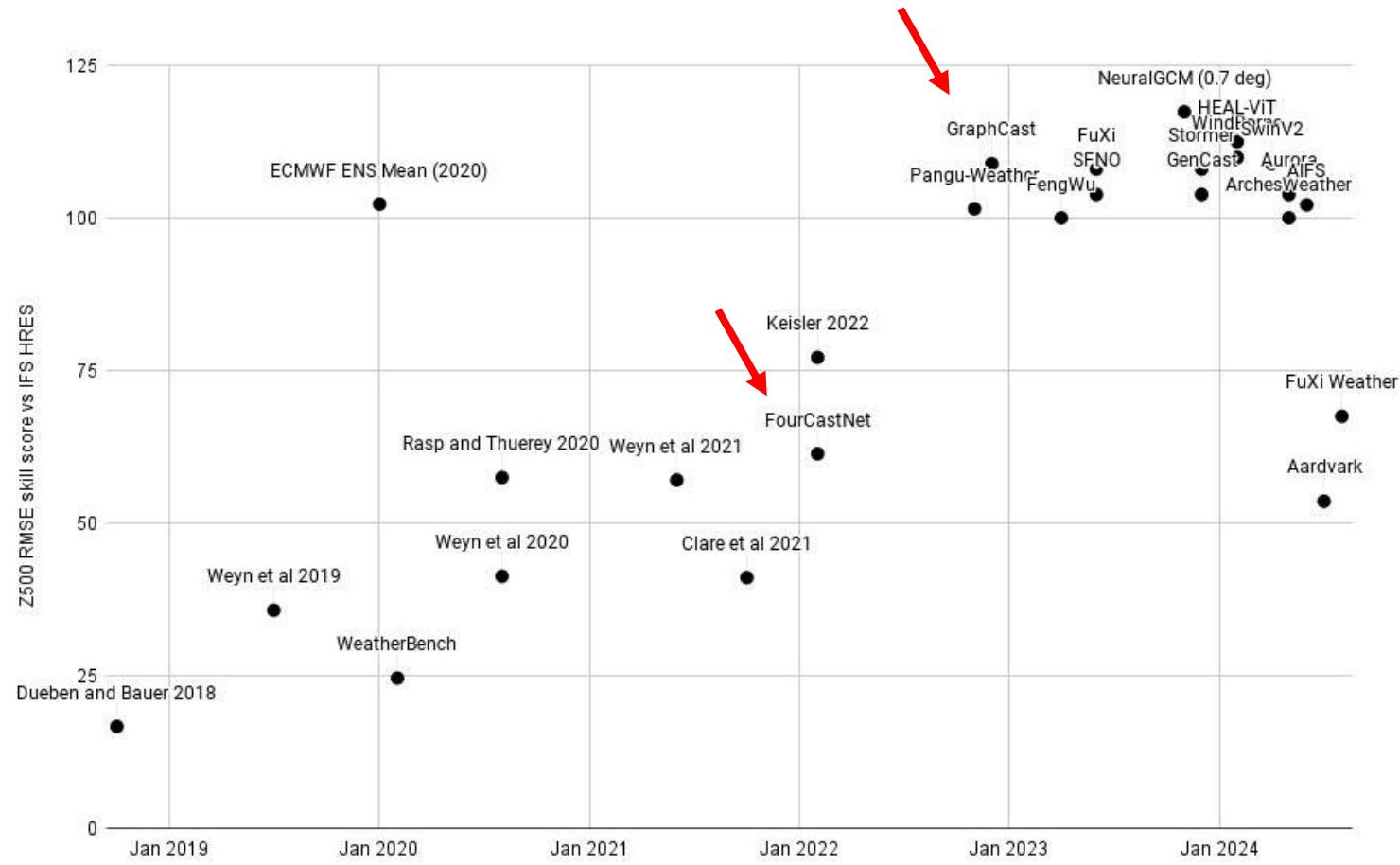
- The speedup allows weather predictions to be obtained in a matter of seconds **vs.** traditional weather models taking hours on a large CPU cluster (**45,000 times faster**).
- What matters is not just a single run of a forecast but rather **a large number of slightly different scenarios** and seeing how the trajectories evolve over time.
- In such cases, deterministic forecasts (**the plot on the left**) are just not sufficient.



Anima Anandkumar, FourCastNet



Progress of AI-weather models over time



https://docs.google.com/spreadsheets/d/1n30zDDjEzlXI5nAGF8uD_dbZWJAamqlmQGCZjfOMuDg/edit?gid=0#gid=0

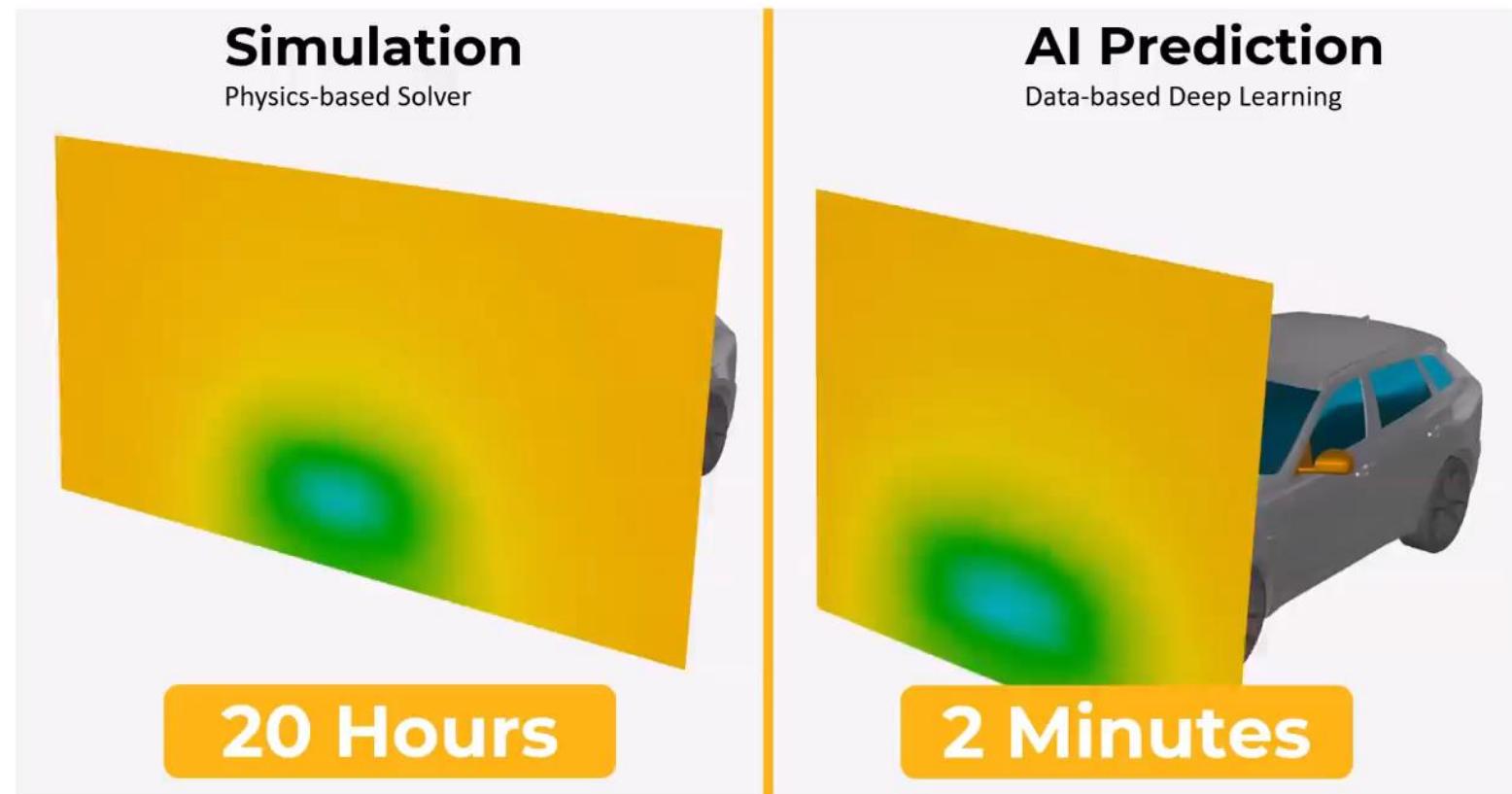
Author: Stephan Rasp (srasp@google.com)

Computational Costs

- FourCastNet's training utilizes 3,072 A100 GPUs
- 40GB PCIe Version: ~ \$7,400.
- 80GB PCIe Version: ~ \$24,300.
- Total: 23-76 M\$
- Training time is 67.4 minutes

Ansys SimAI vs. Fluent

- [Ansys #SimAI](#) Prediction on new SUV geometry takes less than 1 min.
- [SimAI](#) Drag error compared to CFD is less than 0.5% (5 to 10 drag counts) and accurate skin friction field and wake topology prediction.



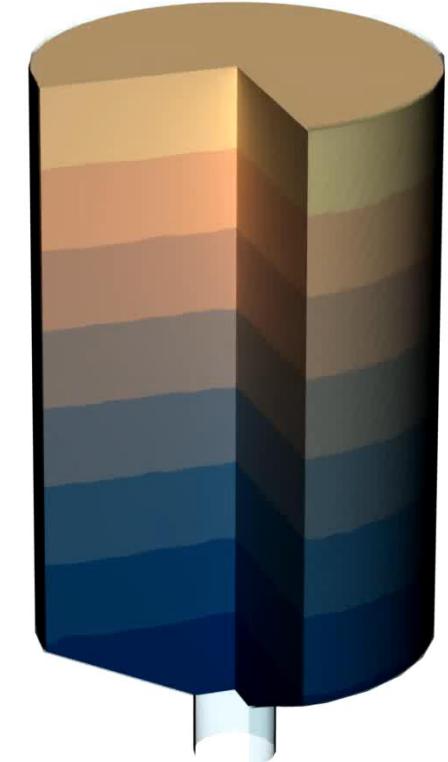
NeuralDEM

Real-time Simulation of Particulate Flows

- NeuralDEM presents an end-to-end approach to replace Discrete Element Method (DEM) routines and coupled multiphysics simulations with deep learning surrogates.



DEM



NeuralDEM

Mass flow

Then, what is PINNs?

- Next Session ☺



Before that,
We need a real break!



Thank You For Your Attention!

* Showing the loss-landscape during
training a PINNs model!