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Deep Learning for Science and Engineering Teaching Kit

# Deep Learning for Scientists and Engineers

Lecture 1: Introduction to Deep Learning

Instructors: George Em Karniadakis, Khemraj Shukla, Lu Lu

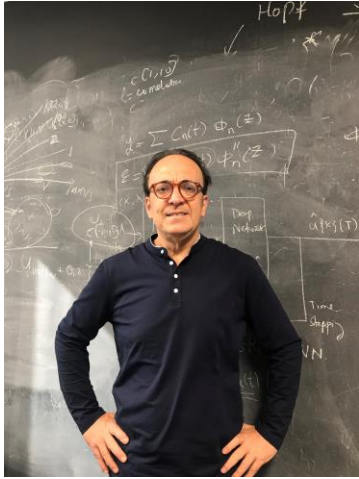
Teaching Assistants: Vivek Oommen and Aniruddha Bora





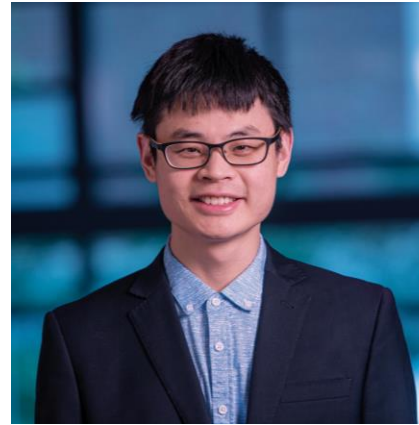
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# Instructors and Teaching Assistants



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# Course Roadmap

## Module-1 (Basics)

- Lecture 1: Introduction
- Lecture 2: A primer on Python, NumPy, SciPy and *jupyter* notebooks
- Lecture 3: Deep Learning Networks
- Lecture 4: A primer on TensorFlow and PyTorch
- Lecture 5: Training and Optimization
- Lecture 6: Neural Network Architectures

## Module-3 (Codes & Scalability)

- Lecture 13: DeepXDE Library
- Lecture 14: MODULUS Library
- Lecture 15: Multi-GPU Scientific Machine Learning

## Module-2 (PDEs and Operators)

- Lecture 7: Machine Learning using Multi-Fidelity Data
- Lecture 8: Data-Driven Dynamical Systems
- Lecture 9: Physics-Informed Neural Networks (PINNs)
- Lecture 10: PINN Extensions
- Lecture 11: Neural Operators
- Lecture 12: Uncertainty Quantification(UQ) in Scientific Machine Learning

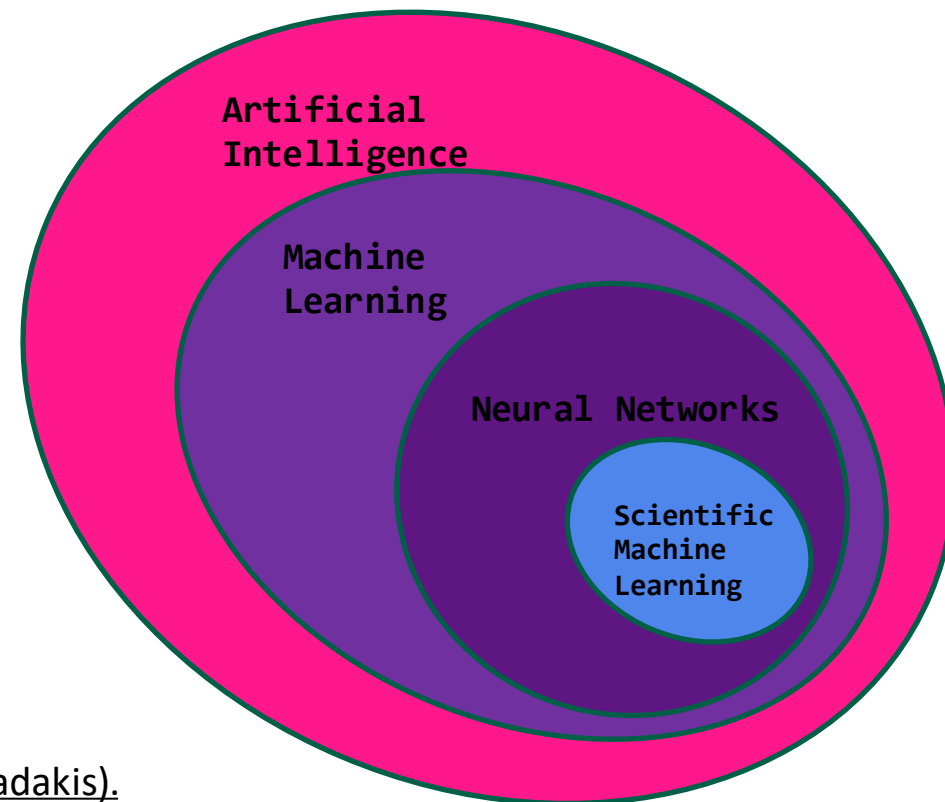
## Course Projects

- Biomedicine
- Dynamical Systems
- Engine Dynamics
- Fluid Mechanics
- Geophysics
- Heat Transfer
- Materials

# Contents

- ☐ History of deep learning
- ☐ Scientific machine learning
- ☐ Rosenblatt's perceptron
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- ☐ Building neural networks
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- ☐ PINNs: data + physical laws
- ☐ Example: non-destructive evaluation of materials
- ☐ Example: Heat transfer
- ☐ Example: Hidden fluid mechanics
- ☐ Example: Rheology of shampoo
- ☐ Example: Reinforcement learning in fluids
- ☐ Different types of deep learning
- ☐ Course roadmap
- ☐ The four pillars of scientific methods
- ☐ References

- ❑ Artificial intelligence (AI) > Machine Learning (ML) > Deep Learning > Scientific Machine Learning (SciML).
- ❑ The expression “Deep Learning” was (probably) first used by Igor Aizenberg and colleagues around 2000.
- ❑ 1960s: Shallow Neural Networks.
- ❑ 1982: Hopfield Network – A Recurrent NN.
- ❑ 1988-89: Learning by backpropagation, Rumelhart, Hinton & Williams; hand-written text, LeCun.
- ❑ 1993 NVIDIA was founded; GeForce is the first GPU.
- ❑ 1990s Unsupervised Deep Learning.
- ❑ 1993: A Recurrent NN with 1,000 layers (Jürgen Schmidhuber)
- ❑ 1994: NN for solving PDEs, Dissanayake & Phan-Thien
- ❑ 1998: Gradient-based learning, LeCun.
- ❑ 1998: ANN for solving ODEs&PDEs, Lagaris, Likas & Fotiadis
- ❑ 1990-2000: Supervised Deep Learning.
- ❑ 2006: A fast learning algorithm for deep belief nets, Hinton.
- ❑ 2006-present: Modern Deep Learning.
- ❑ 2009: ImageNet: A large-scale hierarchical image database (Fei-Fei).
- ❑ 2010: GPUs are only up to 14 times faster than CPUs (Intel).
- ❑ 2010: Tackling the vanishing/exploding gradients: Glorot & Bengio.
- ❑ 2011: AlexNet – Convolutional NN (CNN) - Alex Krizhevsky.
- ❑ 2014: Generative Adversarial Networks (GANs) – Ian Goodfellow.
- ❑ 2015: Batch normalization, Ioffe & Szegedy.
- ❑ 2017: PINNs: Physics-Informed Neural Networks (Raissi, Perdikaris, Karniadakis).
- ❑ 2019: Scientific Machine Learning (ICERM workshop Jan. 2019; DOE report, Feb 2019).
- ❑ 2019: DeepONet – Operator regression (Lu, Jin, Karniadakis).



# Basic Research Needs Workshop for **Scientific Machine Learning**

## Core Technologies for Artificial Intelligence, DOE ASCR Report, Feb 2019

❑ Scientific machine learning (**SciML**) is a core component of artificial intelligence (AI) and a computational technology that can be trained, with scientific data, to augment or automate human skills.

### SciML Foundations

### Machine Learning for Advanced Scientific Computing Research

#### Domain-aware

leveraging & respecting  
scientific domain knowledge

physical principles & symmetries  
physics-informed priors  
structure-exploiting models  
⋮

#### Interpretable

explainable & understandable results

model selection  
exploiting structure in high-dim data  
uncertainty quantification + ML  
⋮

#### Robust

stable, well-posed &  
reliable formulations

probabilistic modeling in ML  
quantifying well-posedness  
reliable hyperparameter estimation  
⋮

❑ SciML must achieve the same level of scientific rigor expected of established methods deployed in science and applied mathematics. Basic requirements include validation and limits on inputs and context implicit in such validations, as well as verification of the basic algorithms to ensure they are capable of delivering known prototypical solutions.

❑ Can SciML achieve Robustness?

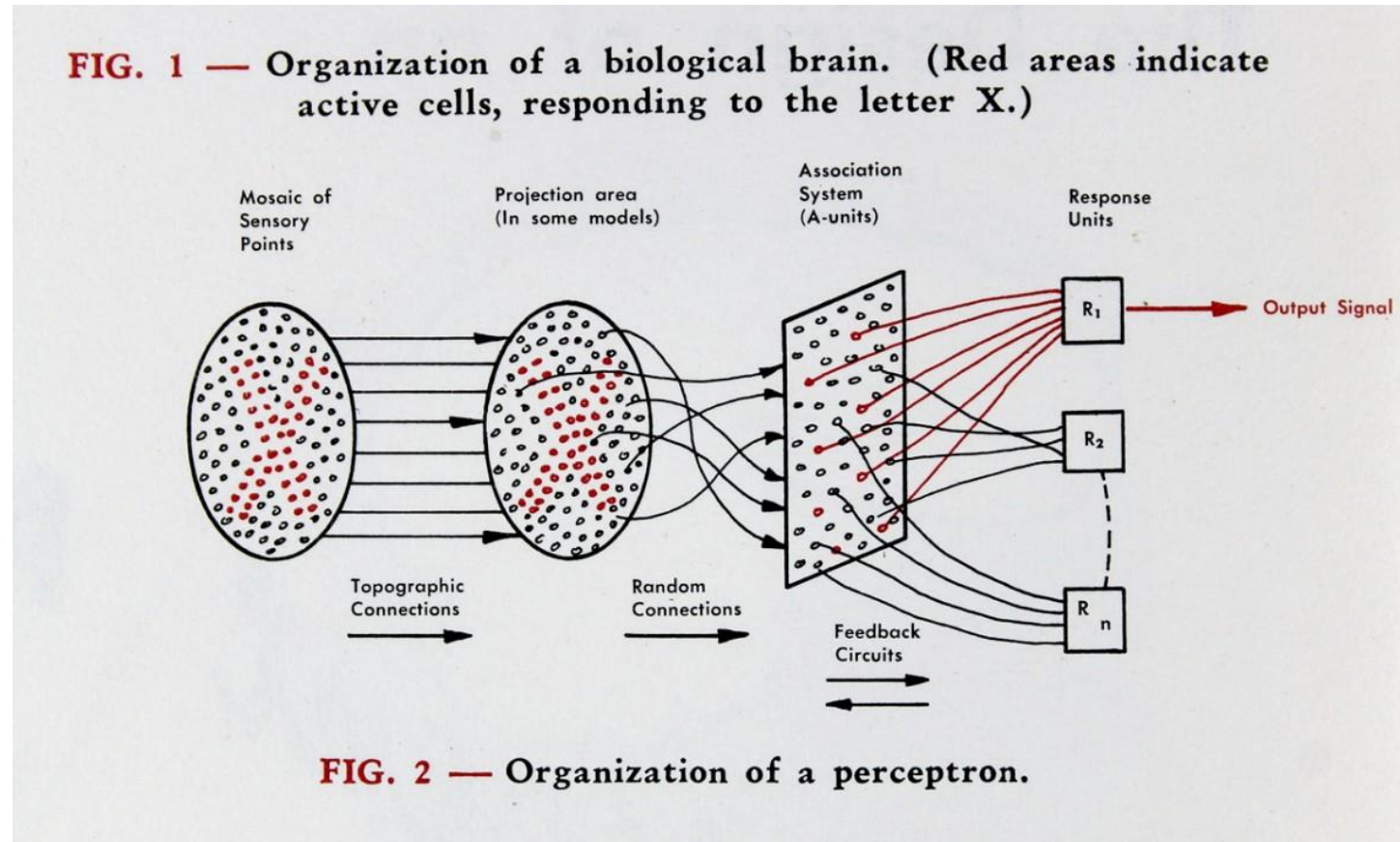


# 1958 @ Cornell – Rosenblatt's Perceptron

➤ Professor Frank Rosenblatt's perceptron paved the way for AI – 60 years too soon!

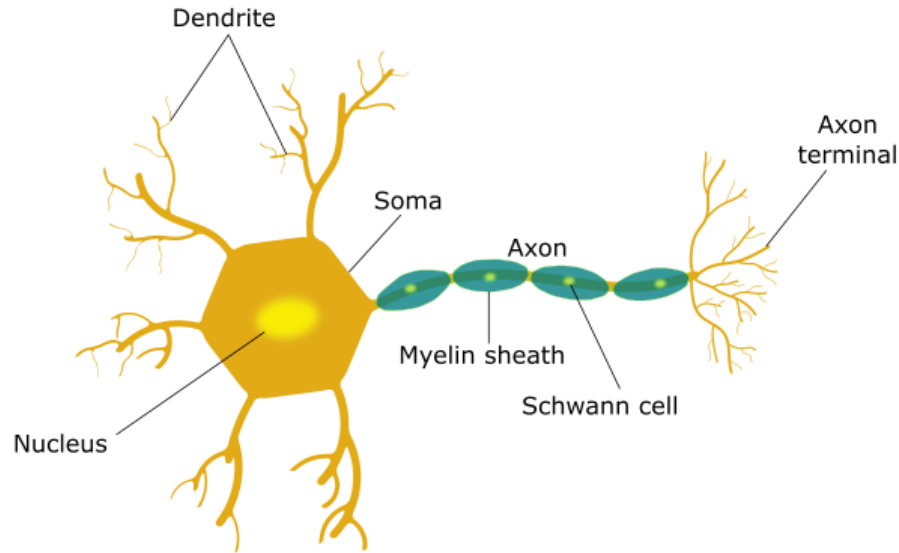
❑ An IBM 704 – a 5-ton computer the size of a room – was fed a series of punch cards. After 50 trials, the computer taught itself to distinguish cards marked on the left from cards marked on the right.

■ An image of the perceptron from Rosenblatt's "The Design of an Intelligent Automaton," Summer 1958.





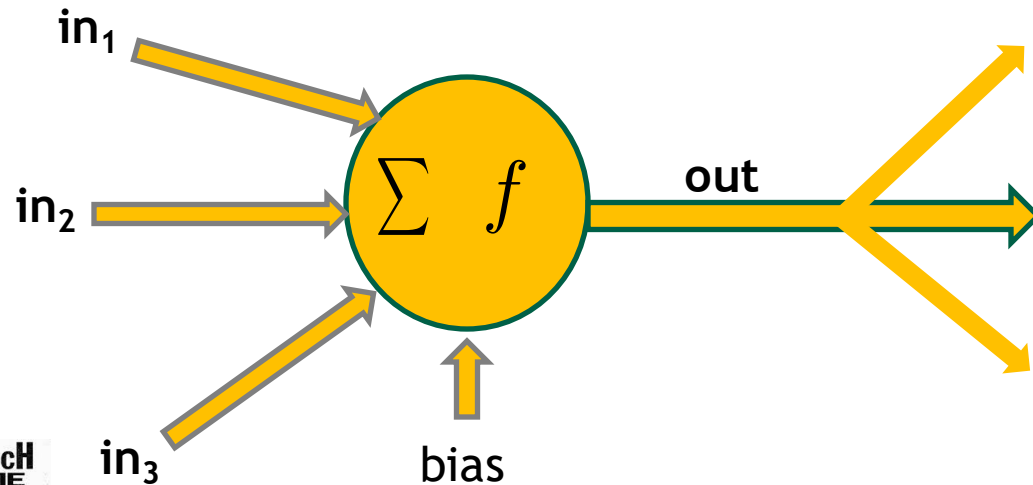
# Differences between Artificial and Biological Neural Networks



❑ **Size:** our brain contains about 86 billion neurons and more than 100-1000 trillion synapses. GPT3 has 175 billion parameters, and the Chinese Wu Dao has 1.75 trillion parameters.

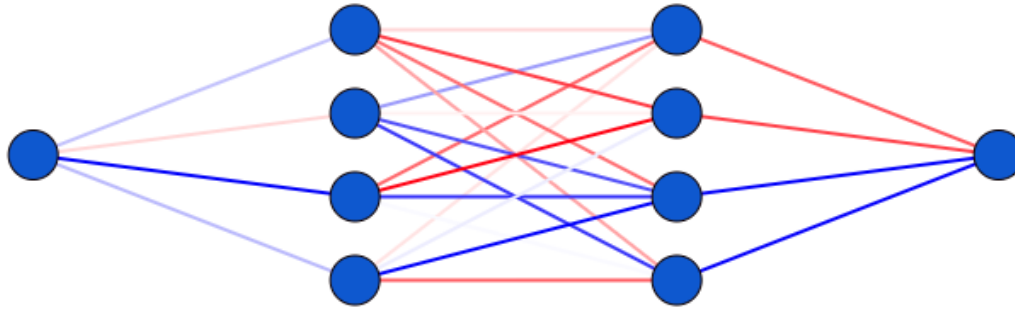
## ❑ Major Differences (in addition to size)

- Topology
- Speed
- Fault-tolerance
- Power consumption
- Signals
- Learning



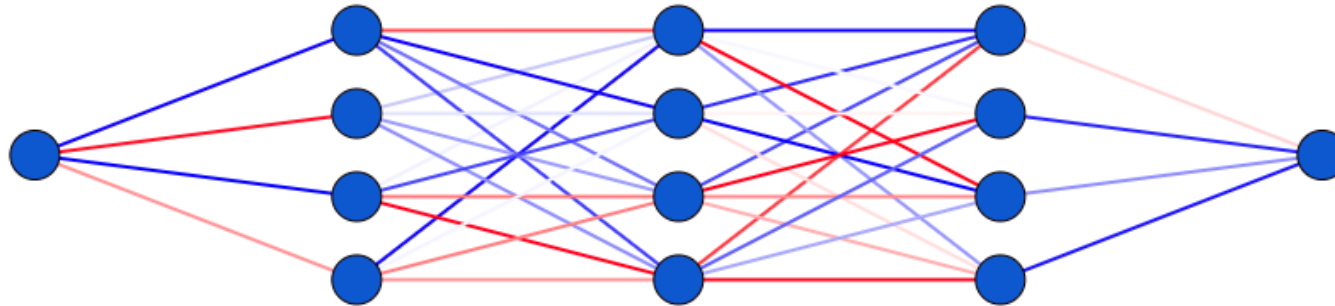
<https://towardsdatascience.com/the-differences-between-artificial-and-biological-neural-networks-a8b46db828b7>

```
net = feed_forward(input_dim=1, output_dim=1, num_neurons=4, num_hidden_layers=2)
```



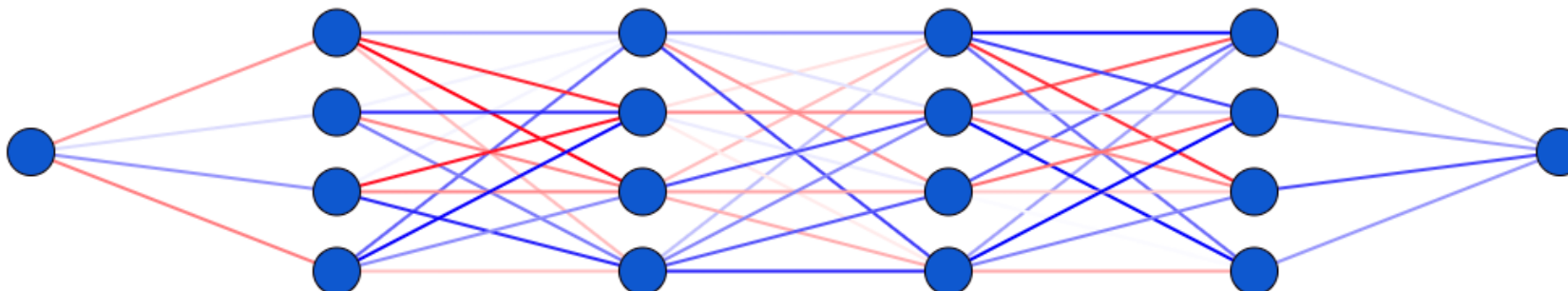
Depth=2

```
net = feed_forward(input_dim=1, output_dim=1, num_neurons=4, num_hidden_layers=3)
```



Depth=3

```
net = feed_forward(input_dim=1, output_dim=1, num_neurons=4, num_hidden_layers=4)
```

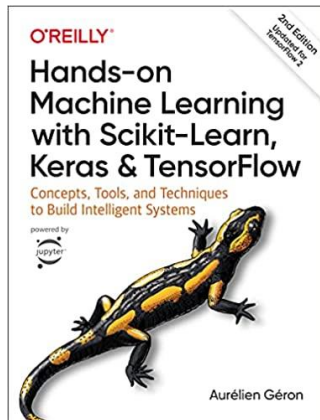
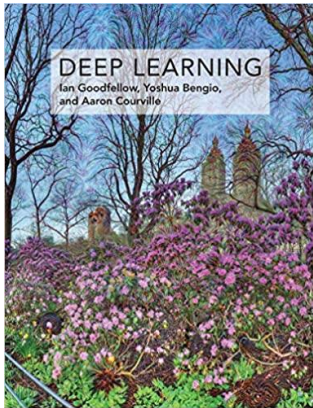


Depth=4

# Course Objectives

At the end of the course participants will be able to:

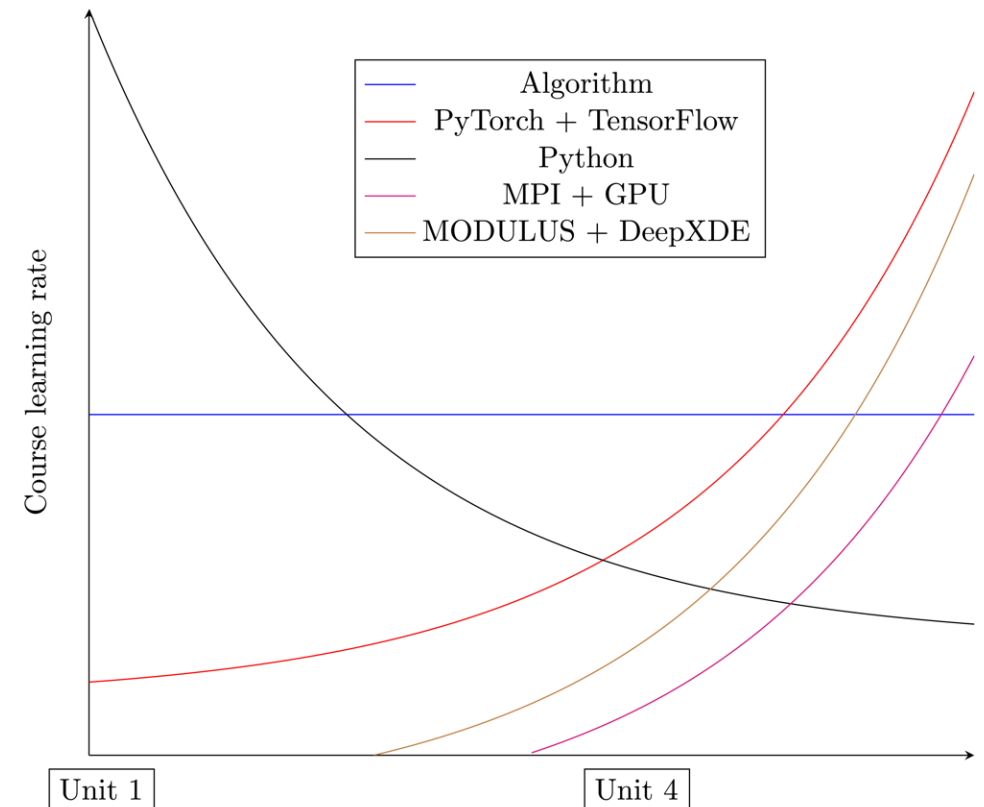
- ☐ Understand the underlying theory and mathematics of deep learning.
- ☐ Analyze and synthesize data in order to model physical, chemical, biological, and engineering systems.
- ☐ Apply physics-informed neural networks (PINNs) and neural operators to model and simulate multiphysics systems in science and engineering.
- ☐ Be fluent in python, Tensorflow, and PyTorch.
- ☐ Be fluent in multi-GPU computing.



1. Goodfellow et al: Prerequisites: Ch. 2-3-4 <https://www.deeplearningbook.org/>

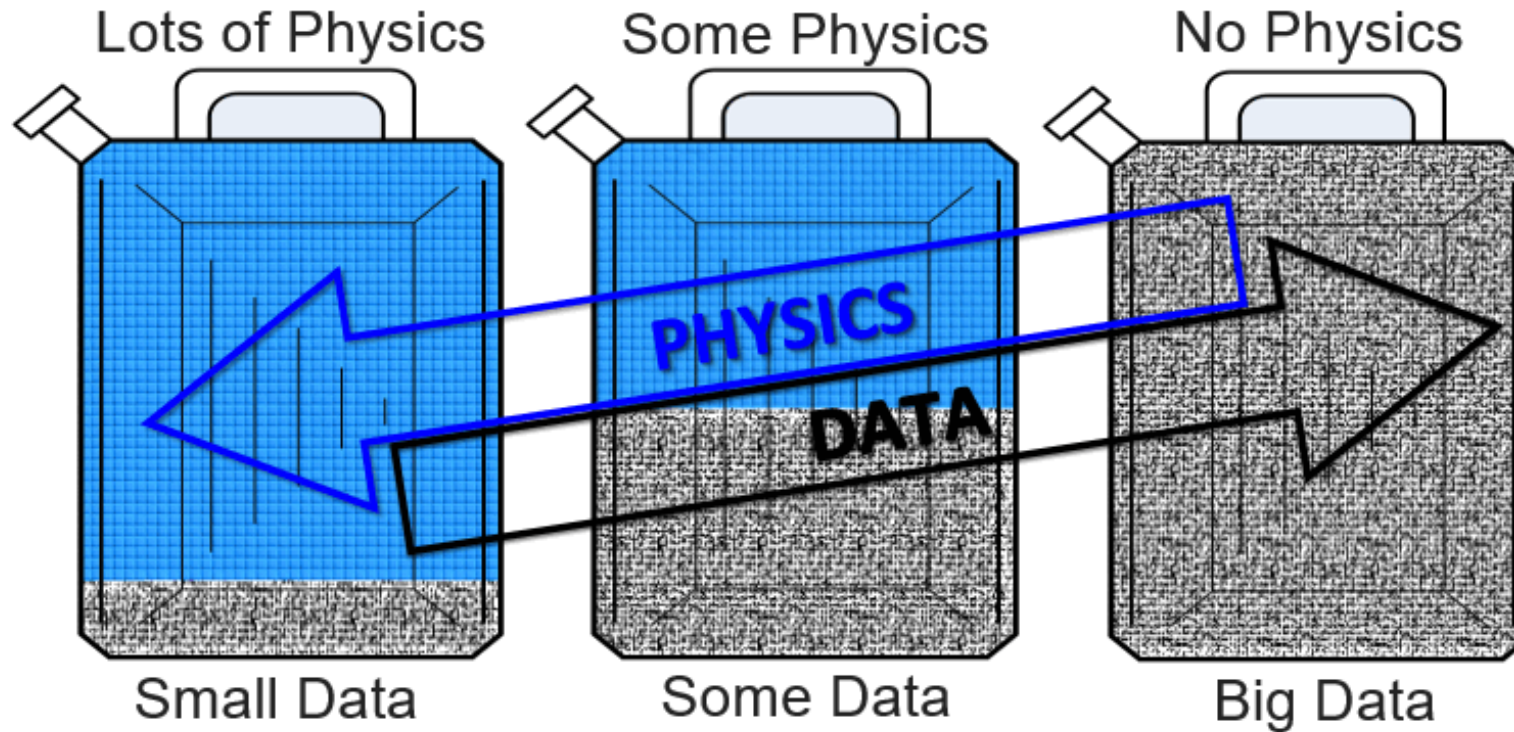
2. A. Geron: Ch. 4 & 11, O'Reilly (2019).

## Course Teaching/Learning Rates



# Data + Physical Laws

## Three scenarios of Physics-Informed Learning Machines



❑ The 5D Law:  
Dinky, Dirty, Dynamic, Deceptive Data

### PINN

- DeepXDE
- Modulus

### DeepONet

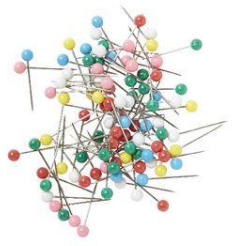
- DeepXDE

### FNO

- Molulus



# PINNs: Physics-Informed Neural Networks



<https://www.youtube.com/watch?v=69nEEpdEJzU>

AI FOR SCIENCE

“... All of the **knowledge** are led to **physics equations** and now **embedded into the neural networks**. And it gives a gigantic head start, **physics informed neural networks...**”

Design Space Exploration ICF + MERLIN – Fusion

Inverse Problems LIGO – Gravitational Waves

Faster Prediction ANI + MD – Chemistry

Real-time Steering ITER – Fusion Energy

EXPERIMENTAL DATA

Real-time Steering

NEURAL ESTIMATION

Fast Approximation

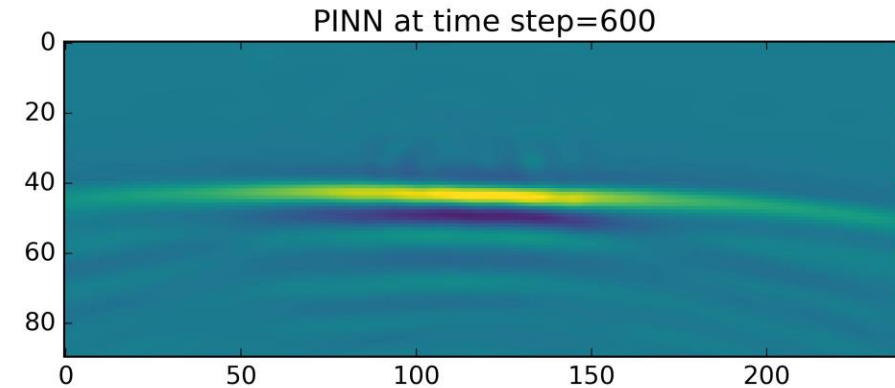
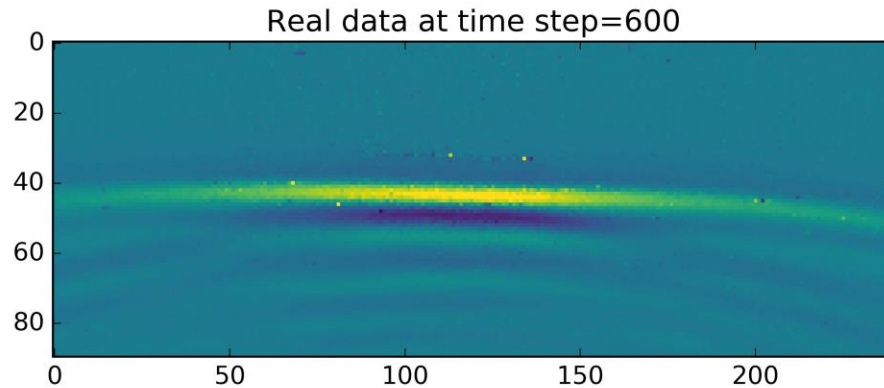
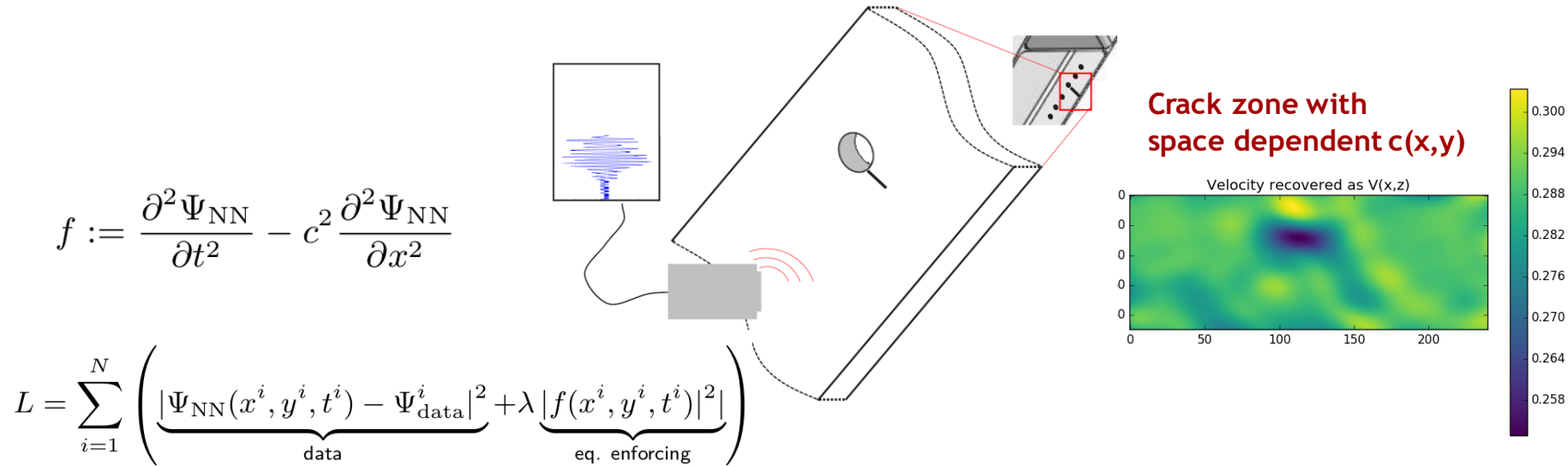
SIMULATION

DATA

NVIDIA CEO J. Huang at SC19, the annual supercomputing conference, Nov 19

[Reference: Raissi, Perdikaris & Karniadakis, arXiv 2017; patent 2020](#)

# Ultra-Sound Testing of Materials (WPAFB Real Data)



□ Shukla K, Di Leoni PC, Blackshire J, Sparkman D, Karniadakis GE. Physics-informed neural network for ultrasound nondestructive quantification of surface breaking cracks. Journal of Nondestructive Evaluation. 2020 Sep;39(3):1-20.



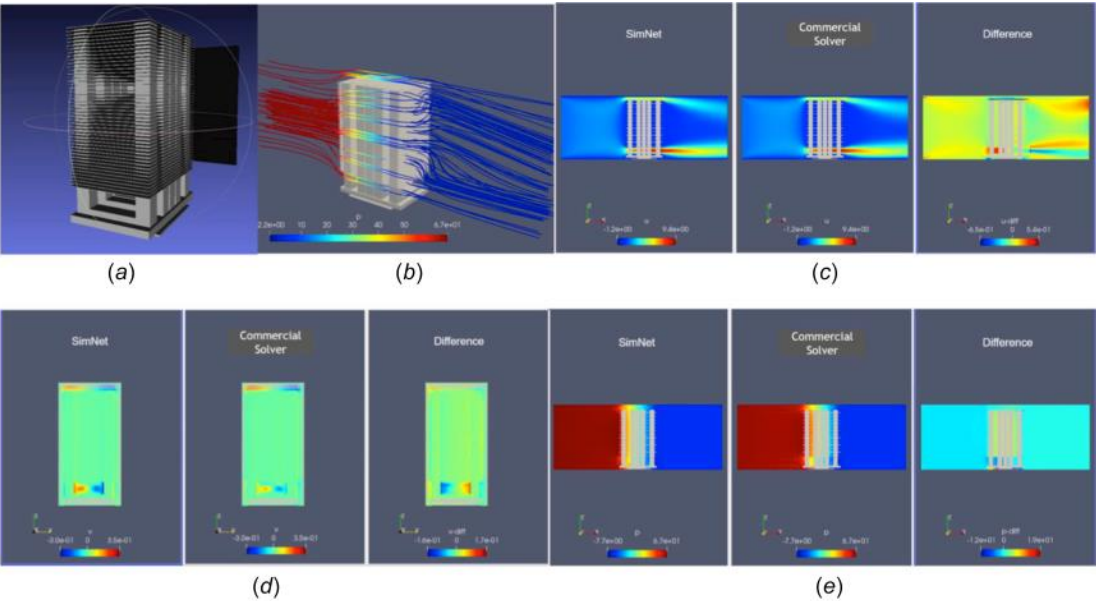
# Physics-Informed Neural Networks for Heat Transfer Problems

J. Heat Transfer. 2021;143(6). doi:10.1115/1.4050542



Date of download: 8/24/2021

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Turbulent Flow (Re=20,687)			Computational Times (10 parameters, 3 values per parameter)	
	Temperature	Pressure Drop	SimNet	
SimNet - Fourier Network	43.1 °C	3.56		1000 V100 GPU hrs.
Commercial Solver	43.5 °C	3.6		
OpenFOAM	41.6 °C	4.58	Traditional Solver (OpenFOAM) 59,049 separate runs (26 wall hours on 12 CPU cores)	18.4M CPU core hrs.

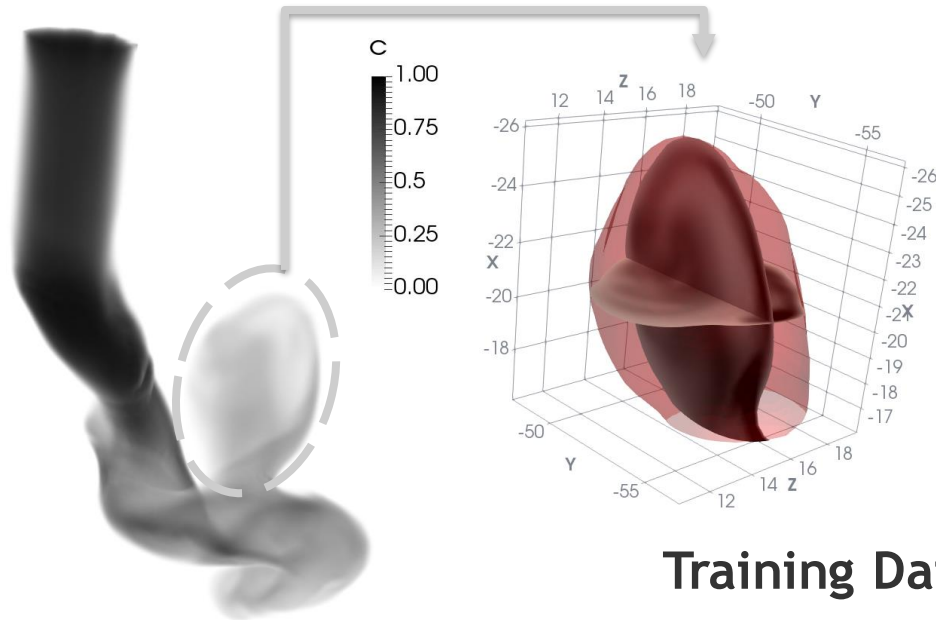
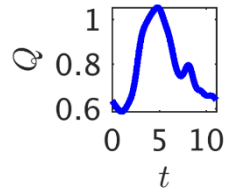
❑ **Solution of conjugate heat transfer problem on a complex parameterized geometry of a heat sink for NVSwitch in DGX-A100 (SimNet Simulation; now known as Modulus).**

- (a) Geometry for a heat sink with fins and heat pipes to dissipate heat from GPU.
- (b) Pressure color-coded flow streamlines and result comparisons between SimNet and CFD commercial code for (c) U-velocity,
- (d) V-velocity, and (e) pressure. (Courtesy of the Nvidia team).

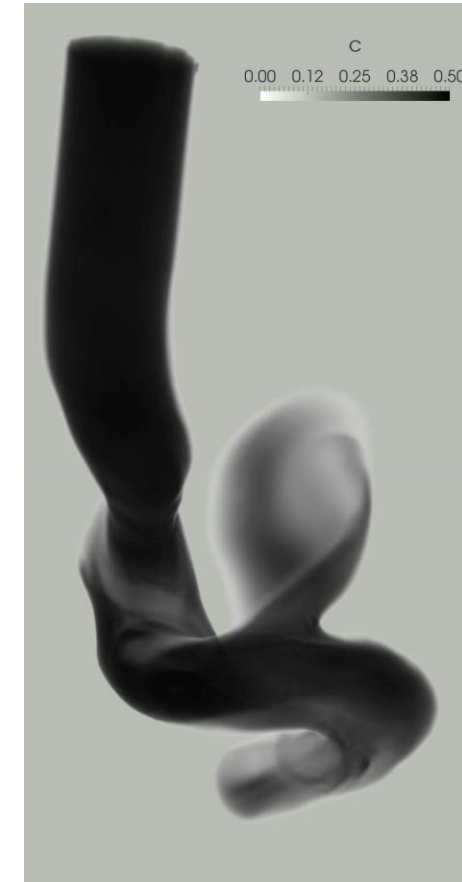
# Hidden Fluid Mechanics: Flow dynamics in an intracranial aneurysm



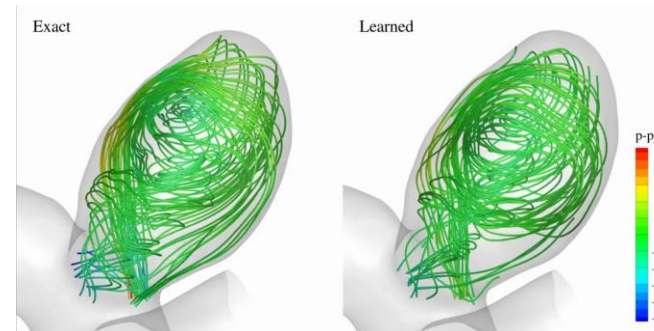
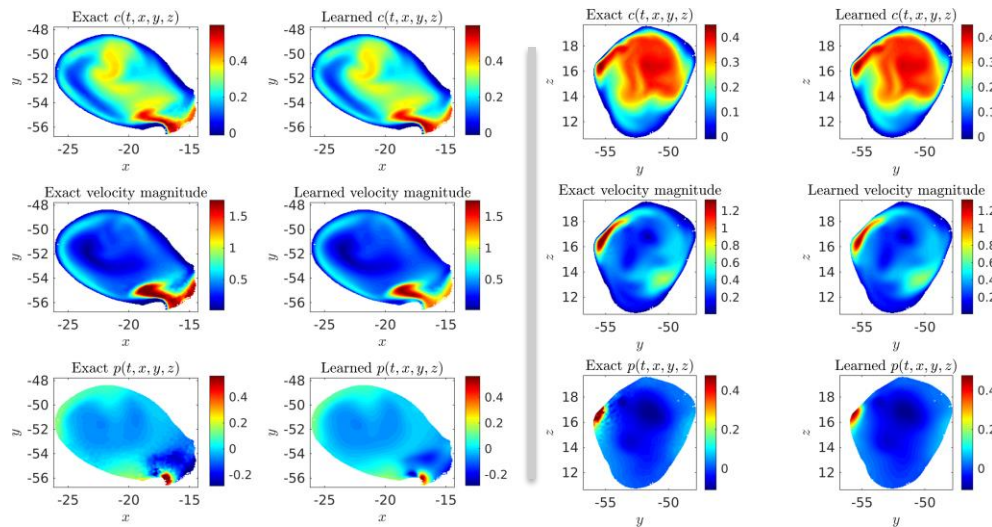
[Science. 2020 Feb 28;367\(6481\):1026-30.](#)



Training Data



Inferred Hidden Physics



# Consumer Product Design Challenge: Rheology of a multicomponent complex fluid

## P&G product (head & shoulders shampoo) design:

### Components:

- A background fluid/solvent (often water)
- Different colloidal particles
- Aromatic additives
- Different oils
- Surfactants for stabilization
- Different polymers
- Salt for pH level / salinity adjustment



"Data-driven physics-informed constitutive metamodeling of complex fluids: a multifidelity neural network (MFNN) framework." *Journal of Rheology* 65.2 (2021): 179-198.

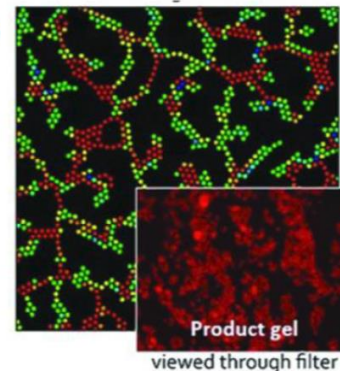
### Challenge:

- No consistent constitutive model available
- No predictions are possible for aging behavior
- New formulation requires extensive testing
- Characterization
- Actual aging of samples

### Expectations:

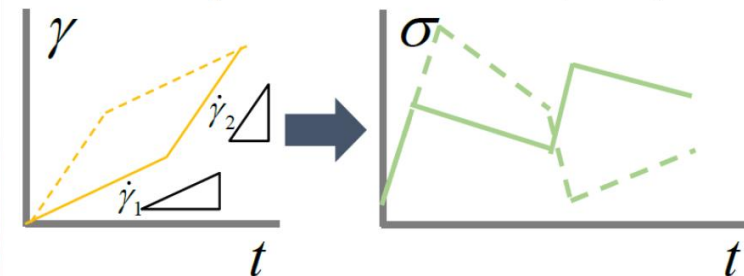
- A range for yield stress
  - To resist phase separation of larger particles
  - To easily flow out of the bottle for use
- Long shelf-life
- A given viscosity upon application
  - Rate-dependent viscosity
- Ease of processing

Typical microstructure



Mechanical response

Thixotropic Elasto-Visco Plastic (TEVP)



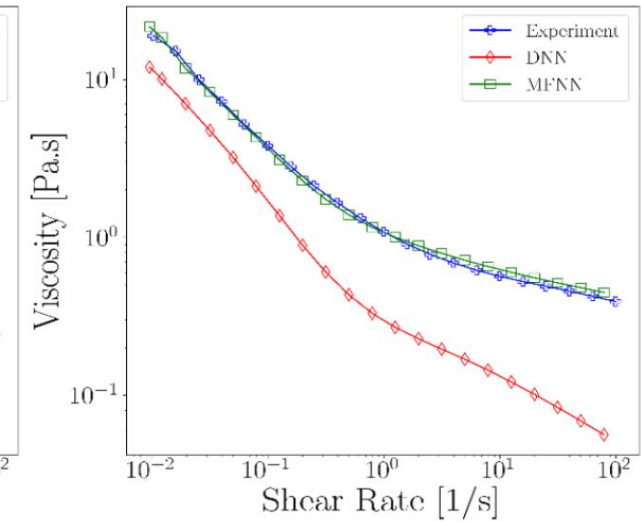
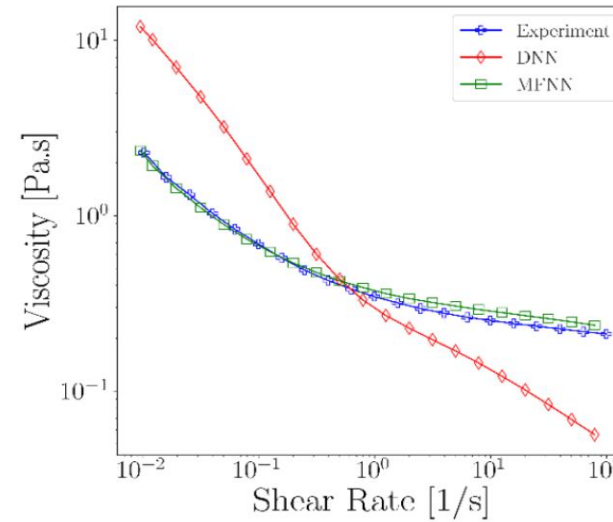


# Rheology of a multicomponent complex fluid: Combining data and physics

"Data-driven physics-informed constitutive metamodeling of complex fluids: a multifidelity neural network (MFNN) framework." *Journal of Rheology* 65.2 (2021): 179-198.

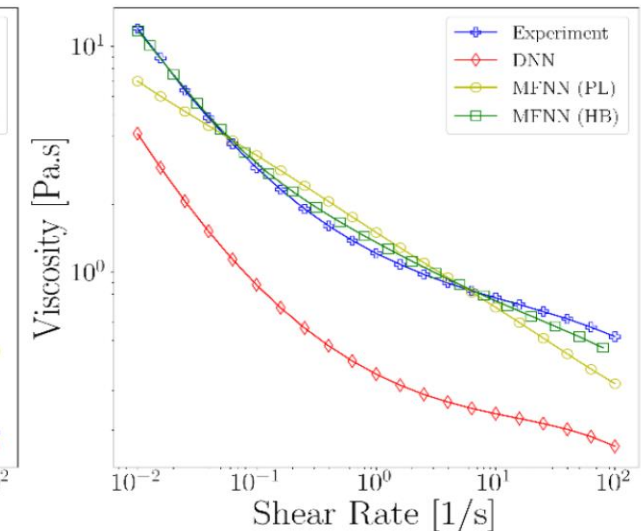
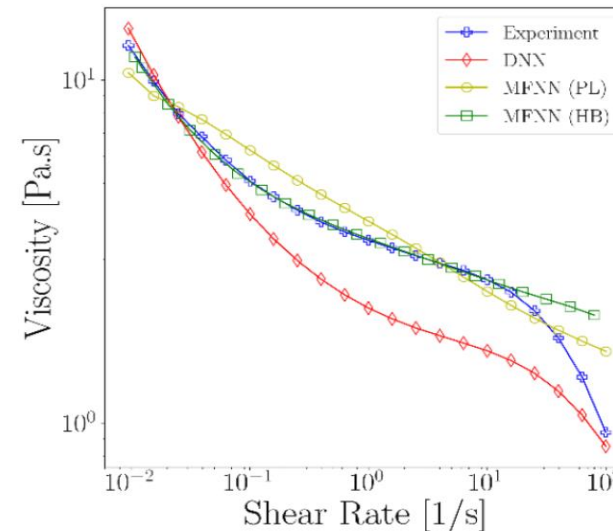
## Capturing the rate dependent rheology:

- Two step shear-thinning
- Yield stress
- Different plateau values



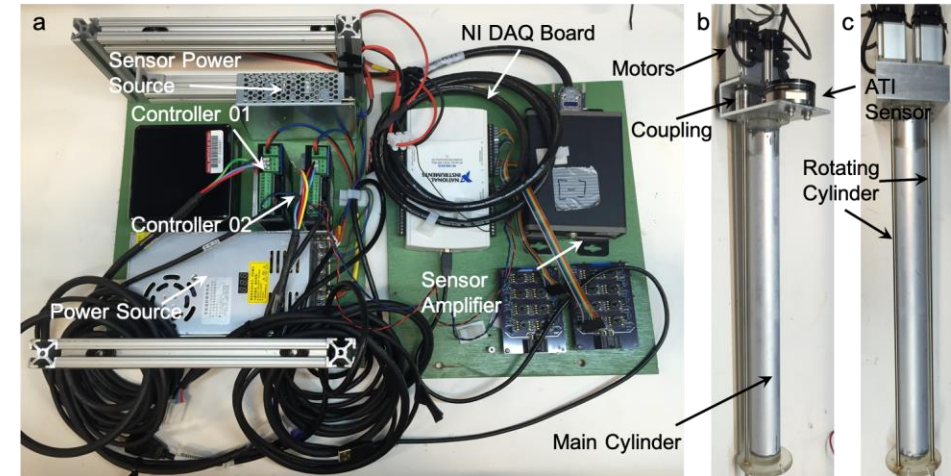
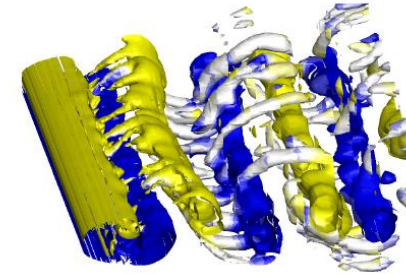
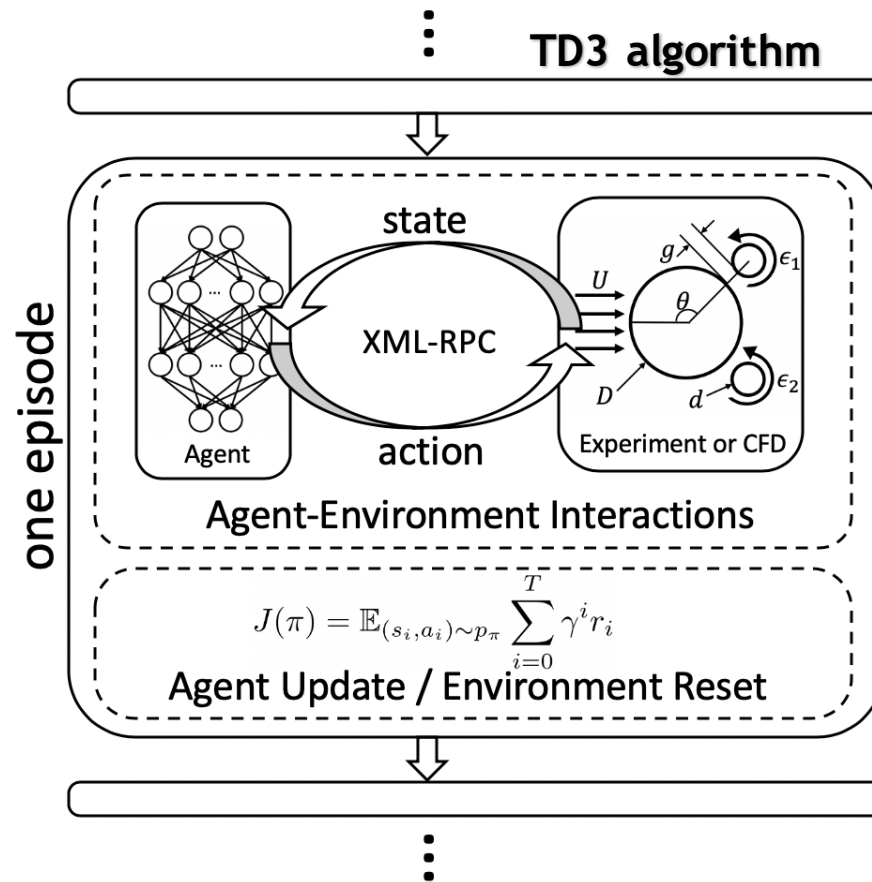
## Role of physics intuition:

- Two parameter "power-law"
- Three parameter "Herschel-Bulkly"
  - Simplest physical model improves the predictions over DNN significantly
  - Commonly known general rheological models now provide predictive ability



# Accelerate Scientific Discovery: Reinforcement Learning for Flow Control in Experiments

Fan D, Yang L, Wang Z, Triantafyllou MS, Karniadakis GE. Reinforcement learning for bluff body active flow control in experiments and simulations. Proceedings of the National Academy of Sciences. 2020 Oct 20;117(42):26091-8.

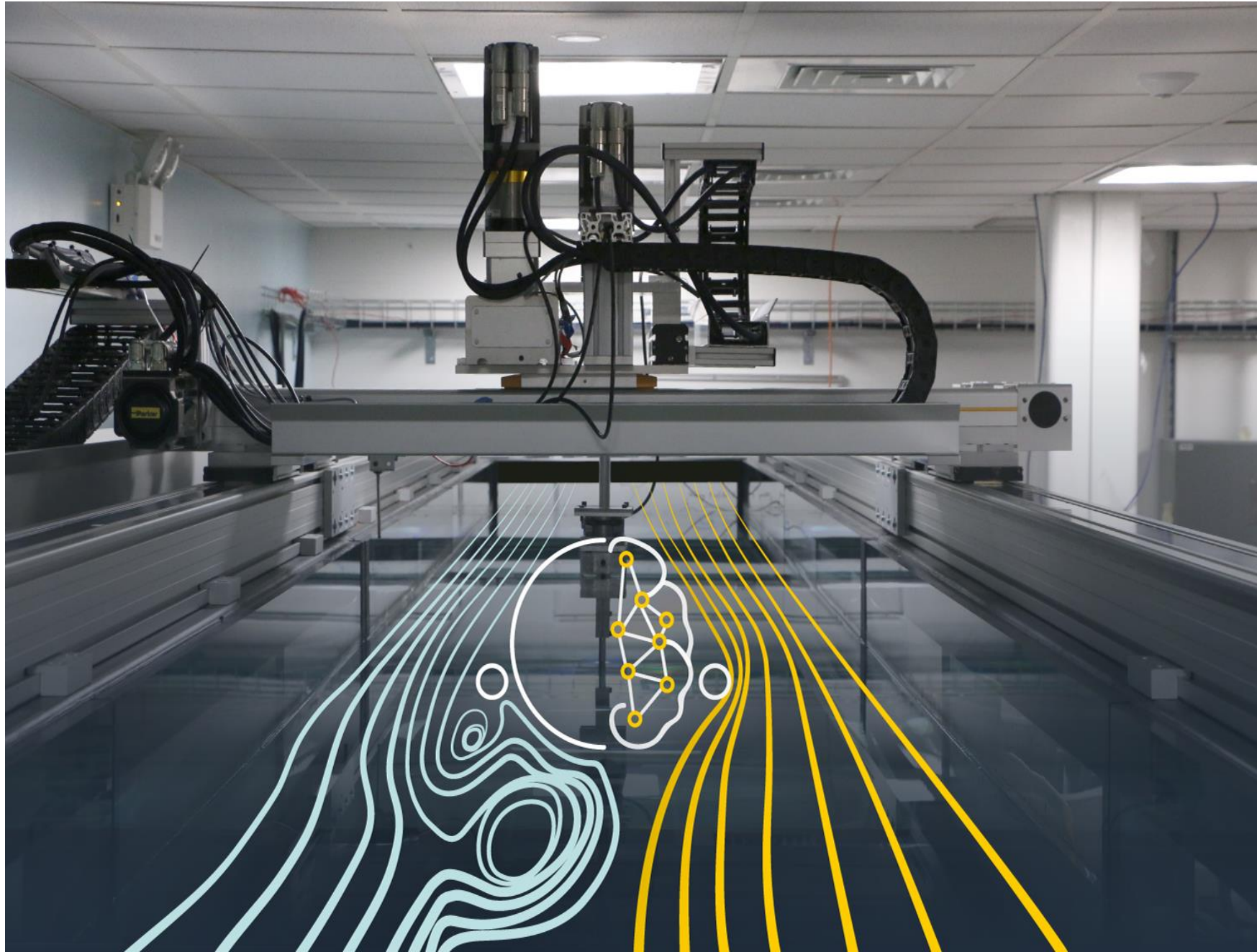


- ❑ We demonstrate, for first time, the effectiveness of RL in experimental fluid mechanics by applying it to reduce the drag of circular cylinders in turbulent flow. Although physics-agnostic, RL managed to reduce the drag by 30% very quickly.



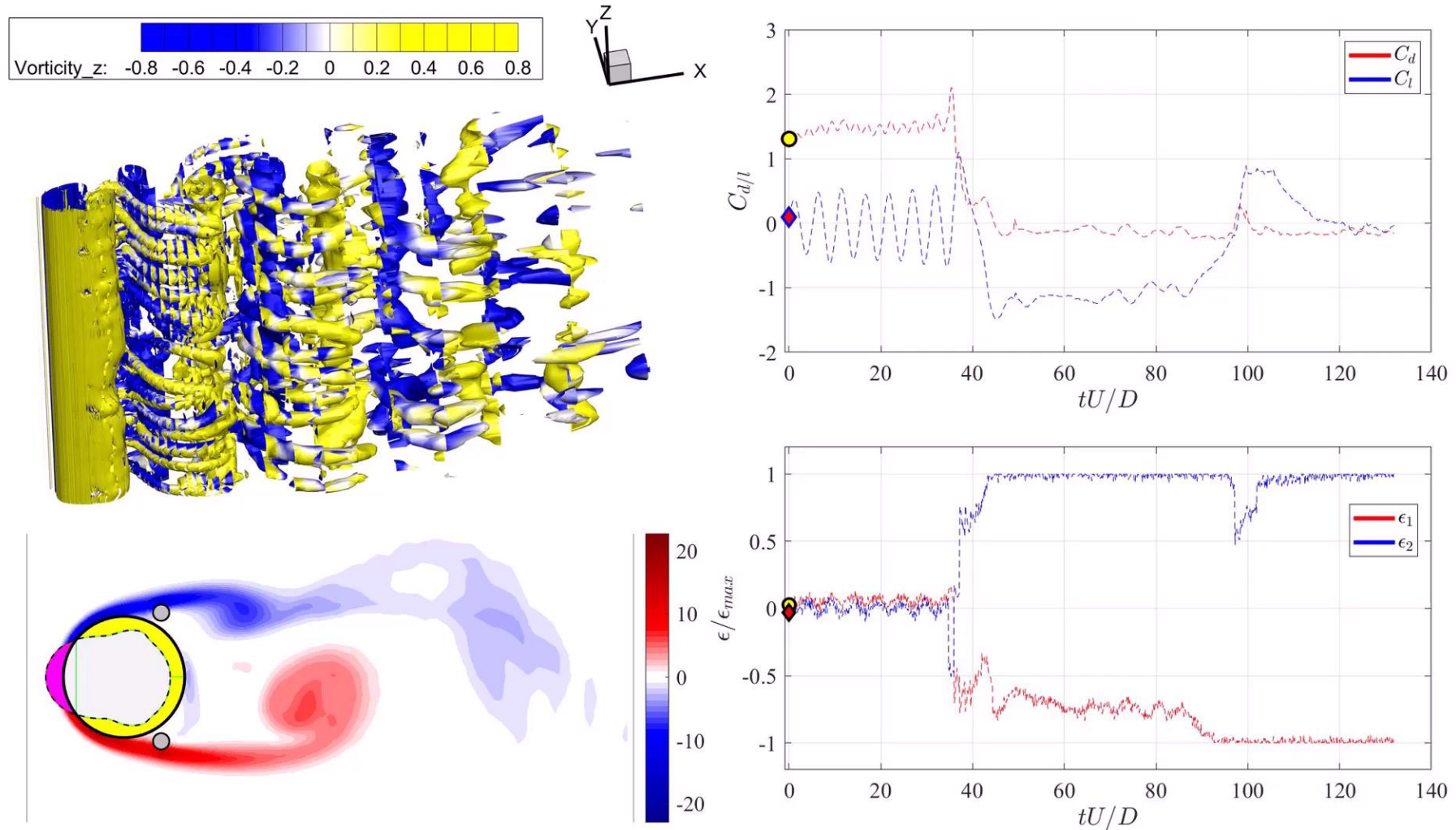
# MIT Intelligent Towing Tank

- Fan, Dixia, et al. "A robotic intelligent towing tank for learning complex fluid-structure dynamics." *Science Robotics* 4.36 (2019).

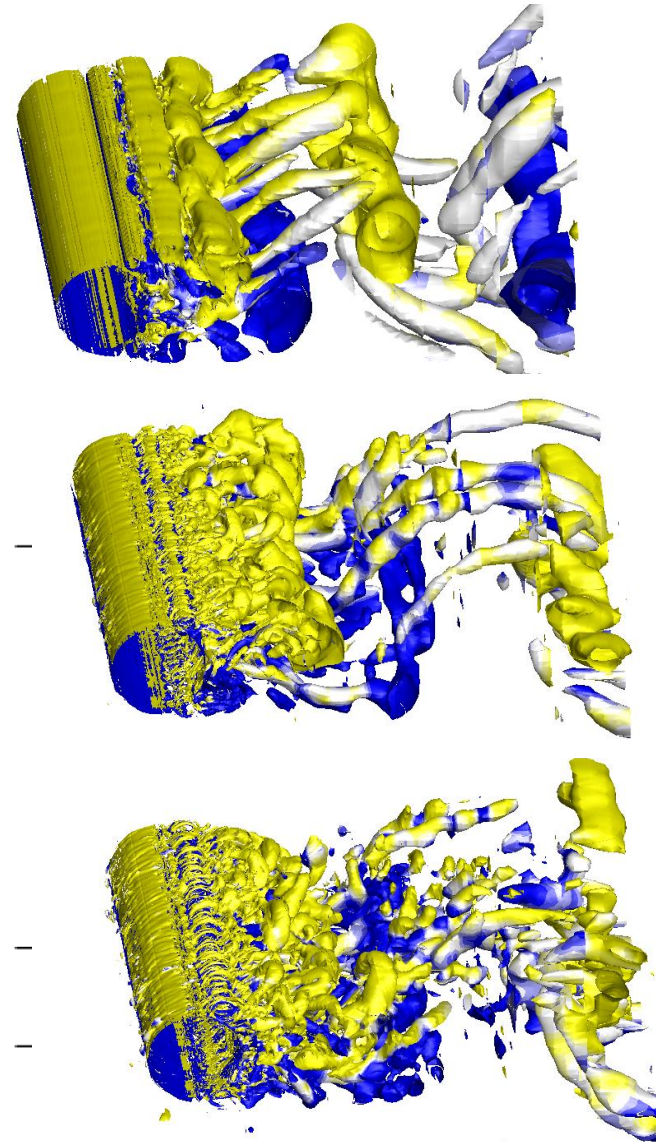
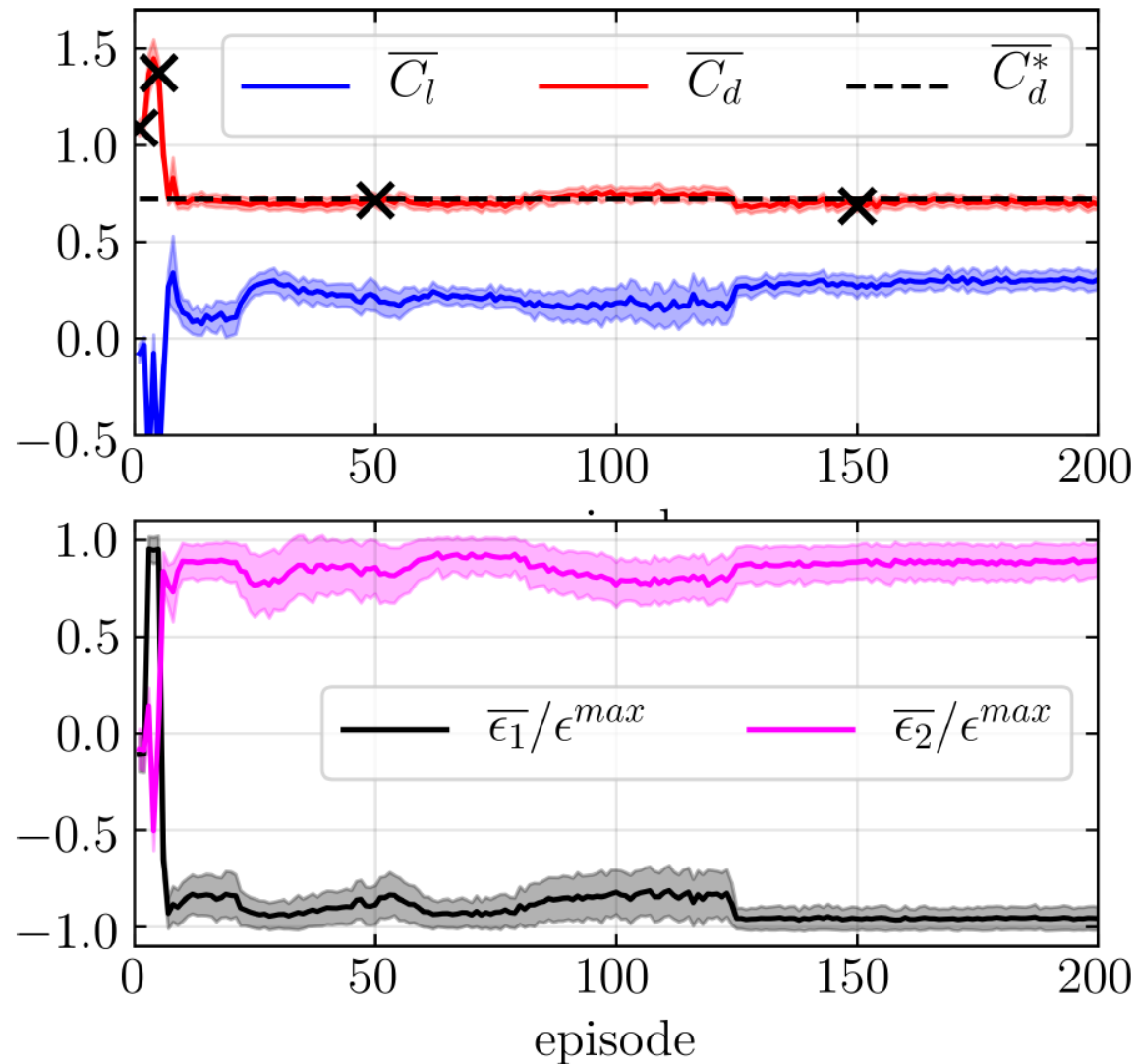




# Reinforcement Learning for Cylinder Flow Control



Case I:  $r = -\text{sgn}(C_d)C_d^2 - 0.1C_l^2$  with KF; **PNAS, (2020)**

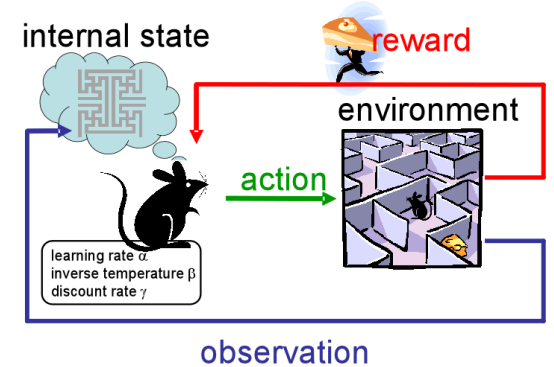


# Supervised Learning Needs Big Data

- ❑ Supervised learning is the process of training a model by feeding it input data as well as corresponding output data. This input/output set is referred to as **labeled data**. It models the relationship between a set of descriptive features and target outcome(s). The model is a neural network that approximates implicitly the function that maps the input to the output in order to solve either classification or regression problems.
- ❑ In **Operator or Functional regression** the inputs are functions and the outputs are corresponding known functions for training, and unknown output functions for prediction.
- ❑ **Training - Where is the Big Data?**
  - Example: UCI Repository: <https://archive.ics.uci.edu/ml/index>.
  - Heart Disease (4 databases: Cleveland, Hungary, Switzerland, and the VA Long Beach): <https://archive-beta.ics.uci.edu/ml/datasets/45>
  - Airfoil Self-Noise: <https://archive-beta.ics.uci.edu/ml/datasets/291>: NASA wind tunnel data set based on aerodynamic and acoustic tests of 2D and 3D airfoil blade sections.
  - Challenger USA Space Shuttle O-Ring: <https://archive-beta.ics.uci.edu/ml/datasets/92>: Predict the number of O-rings that experience thermal distress on a flight at 31 degrees F given data on the previous 23 shuttle flights.

**Unsupervised Learning:** There are no predefined labels, i.e., no known set of outcomes. For example, solving ODEs based on initial conditions is unsupervised learning. Clustering, density estimation or looking for hidden patterns in the data are all examples of unsupervised learning.

**Reinforcement Learning:** Learning through delayed feedback by interacting with the environment. Reinforcement Learning deals with exploitation or exploration, Markov's decision processes, policy learning, and value learning. It is useful for flow control problems (e.g., drag force control in flow past a cylinder; navigation/autonomy, etc.



## Summary

- ❑ Supervised Learning predicts based on a class type; it maps labelled data to known output; immediate feedback.
- ❑ Unsupervised Learning discovers underlying patterns; it explores patterns to predict the output; no feedback.
- ❑ Reinforcement Learning follows a trial-and-error approach; the learning agent works as a reward and action system; delayed feedback.



# 14 Different Types of Learning in Machine Learning

by Jason Brownlee on November 11, 2019 in Start Machine Learning

**Self-Supervised Learning:** It looks like unsupervised learning, where some of the data provides the supervision. Supervised learning algorithms are used to solve an alternate or pretext task, the result of which is a model or representation that can be used in the solution of the original modeling problem.

- ❑ **Autoencoders** is a general example of self-supervised learning algorithms. These are neural networks that are used to create a compressed representation of an input sample. They achieve this via a model that has an encoder and a decoder element separated by a bottleneck that represents the internal compact representation of the input. They are trained using a supervised learning method, but they solve an unsupervised learning problem; they are a projection method for reducing the dimensionality of input data.
- ❑ **Generative Adversarial Networks (GANs)** is another example of self-supervised learning. These are generative models that are inspired by game-theoretic approaches and were originally used for creating synthetic photographs using only a collection of unlabeled examples from the target domain. We will use GANs to obtain informative priors and solve stochastic differential equations in high dimensions.

# Course Roadmap

## Module-1 (Basics)

- Lecture 1: Introduction
- Lecture 2: A primer on Python, NumPy, SciPy and *jupyter* notebooks
- Lecture 3: Deep Learning Networks
- Lecture 4: A primer on TensorFlow and PyTorch
- Lecture 5: Training and Optimization
- Lecture 6: Neural Network Architectures

## Module-3 (Codes & Scalability)

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- Dynamical Systems
- Engine Dynamics
- Fluid Mechanics
- Geophysics
- Heat Transfer
- Materials



# The Four Pillars of Scientific Methods

“Data science (AI+HPC) is the fastest growing field of computer science today. Because of several different factors, it has become the fourth pillar of the scientific method.”



Jensen Huang, NVIDIA

Experiments



Theory



Simulation



Data Science



# References

- Cai S, Wang Z, Wang S, Perdikaris P, Karniadakis GE. Physics-informed neural networks for heat transfer problems. Journal of Heat Transfer. 2021 Jun 1;143(6).
- Fan D, Yang L, Wang Z, Triantafyllou MS, Karniadakis GE. Reinforcement learning for bluff body active flow control in experiments and simulations. Proceedings of the National Academy of Sciences. 2020 Oct 20;117(42):26091-8.
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