Confluences Mathématiques

Le machine learning au pays des équations

Rencontres chercheur·euse·s et ingénieur·e·s - 6ème édition

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Scientific machine learning for fluid flow modeling and design

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Overview

- A very brief introduction to Fluid Mechanics
- Scientific machine learning in Fluid Mechanics
  - Requirements, challenges and opportunities
  - Examples
  - Toward more generalizable data-driven models
- Conclusions and outlook

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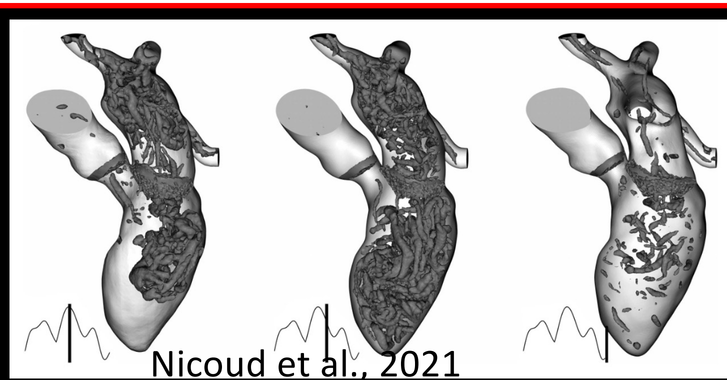
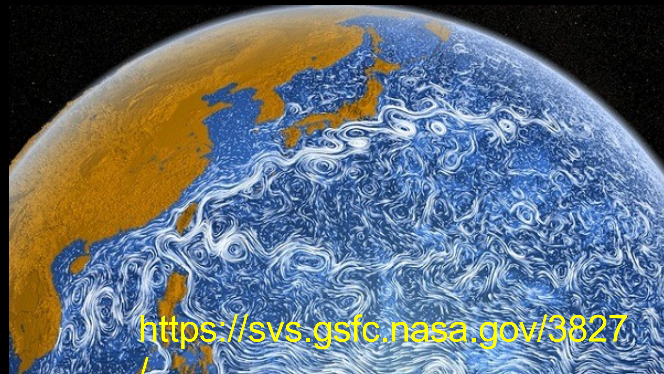
Fluid Mechanics

- Fluids play a fundamental role for life
  - Human body contains 60% water
  - 2/3 earth's surface covered by water
  - Atmosphere extends for 17km above earth's surface
- Fluid mechanics is part of our history
  - Geomorphology
  - Human migrations and birth of civilizations
  - Modern scientific and mathematical theories
- Key to many problems in science and engineering
  - Turbulence, geosciences, biology, astrophysics
  - Weather and climate
  - Aerospace, Energy, Industrial processes, health

Fluid mechanics is in <u>almost every daily event</u>


Nicoud et al., 2021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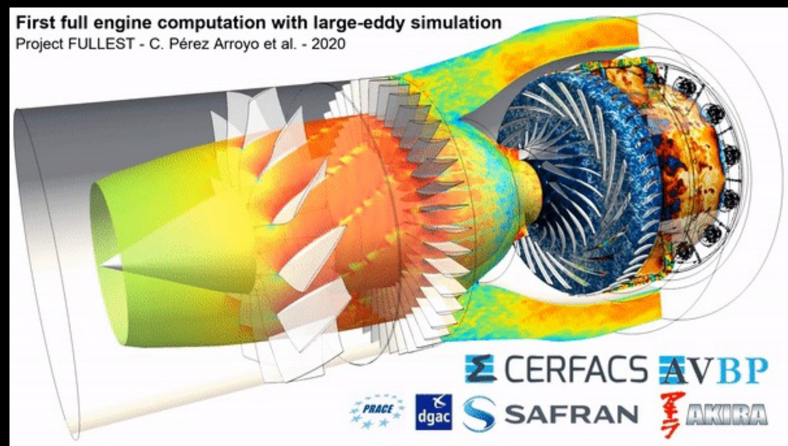
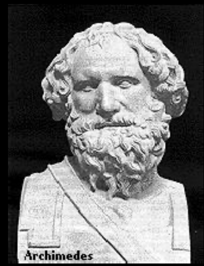
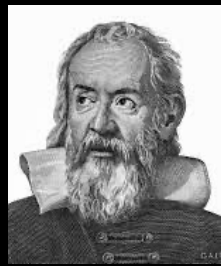


Investigating fluids

1. Experimental Fluid Mechanics
2. Theoretical Fluid Mechanics
3. Computational Fluid Dynamics
4. High-Performance computing
5. **Data-driven Fluid Mechanics**?



Archimede
(C. 287-212 AC)



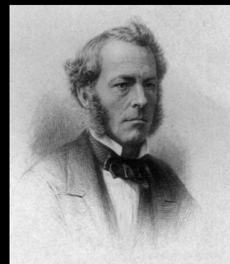
Galileo
(C. 287-212 AC)

Reynolds
(1842-1912)

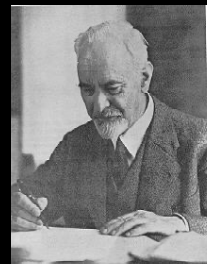
Bernoulli
(1667-1748)

Euler
(1707-1783)

Navier
(1785-1836)

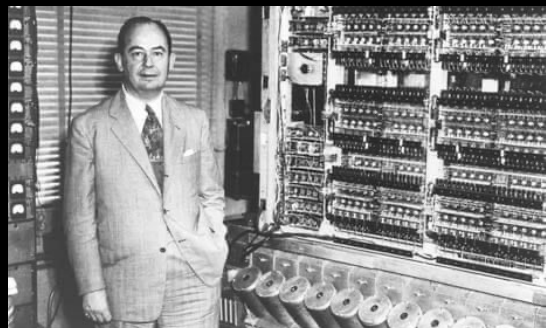


Stokes
(1819-1903)



Prandtl
(1875-1953)

Taylor
(1886-1975)

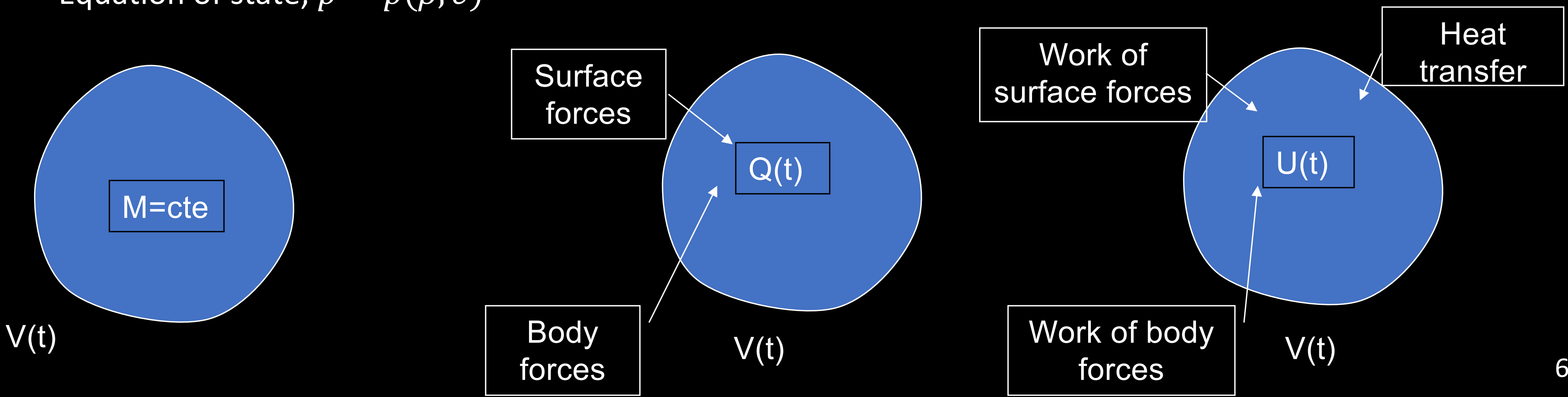


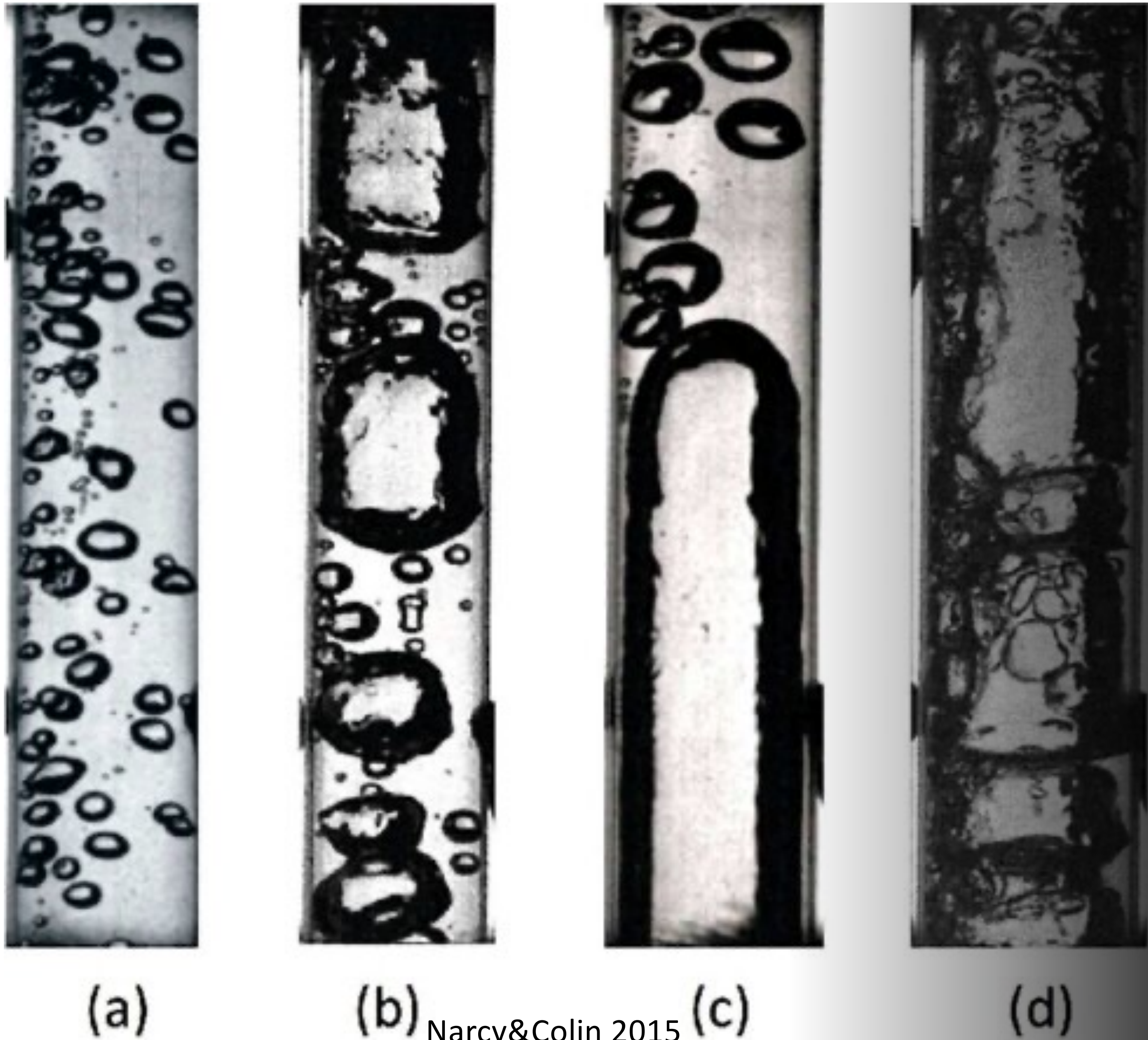
Von Neumann (1903-1957)

Harlow (1928-2016)

Governing equations (continuum limit)

- Conservation of mass : $\frac{D\rho}{Dt} = -\rho\nabla \cdot \mathbf{v}$
- Conservation of momentum : $\rho\frac{D\mathbf{v}}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{\tau}_v + \rho\mathbf{f}$
- Conservation of energy : $\rho\frac{DE}{Dt} = -\nabla \cdot (p\mathbf{v}) + \nabla \cdot (\mathbf{v} \cdot \boldsymbol{\tau}_v) + \rho\mathbf{f} \cdot \mathbf{v} - \nabla \cdot \mathbf{q}$
- Constitutive equations :
  - Rheology models : e.g. Newtonian fluid $\boldsymbol{\tau}_\mathbf{v} = 2\mu\mathbf{S} + \lambda tr(\mathbf{S})I$
  - Heat flux : $\mathbf{q} = -\kappa\nabla T$
  - Equation of state, $p = p(\rho, e)$





Narcy&Colin 2015

Multi-fluid equations…

- Mass, momentum (and energy) conservation for each fluid k

$$\frac{\partial(\rho_k\alpha_k)}{\partial t} + \nabla\cdot(\rho_k\alpha_k\mathbf{v}) = \boldsymbol{\alpha_k}M_k$$

$$\frac{\partial(\rho_k\alpha_k\mathbf{v}_k)}{\partial t} + \nabla\cdot(\rho_k\alpha_k\mathbf{v}_k\mathbf{v}_k) = -\boldsymbol{\alpha_k}\nabla p + \nabla\cdot(\boldsymbol{\alpha_k}\boldsymbol{\tau}_v) + \rho_k\alpha_k\mathbf{f} + \mathbf{I}_k$$

$$\frac{\partial(\rho_k\alpha_k T_k)}{\partial t} + \nabla\cdot(\rho_k\alpha_k\mathbf{v}_k T_k) = \dot{W}_{p,k} + \dot{W}_{\tau,k} + \dot{W}_{f,k} + \dot{W}_{I,k} + \dot{Q}_k$$

- Supplementary models for:
  - Rheology, thermophysical properties, mass-echange terms, interfacial forces, heat fluxes…

The “simple” case

- Navier-Stokes equations for a single-phase, single-species, incompressible, constant-property Newtonian fluid :

$$\nabla \cdot \mathbf{v} = 0$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v}$$

- Buckingham theorem → nondimensional form

$$\nabla \cdot \mathbf{v} = 0$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \frac{1}{\mathrm{Re}} \nabla^2 \mathbf{v}$$

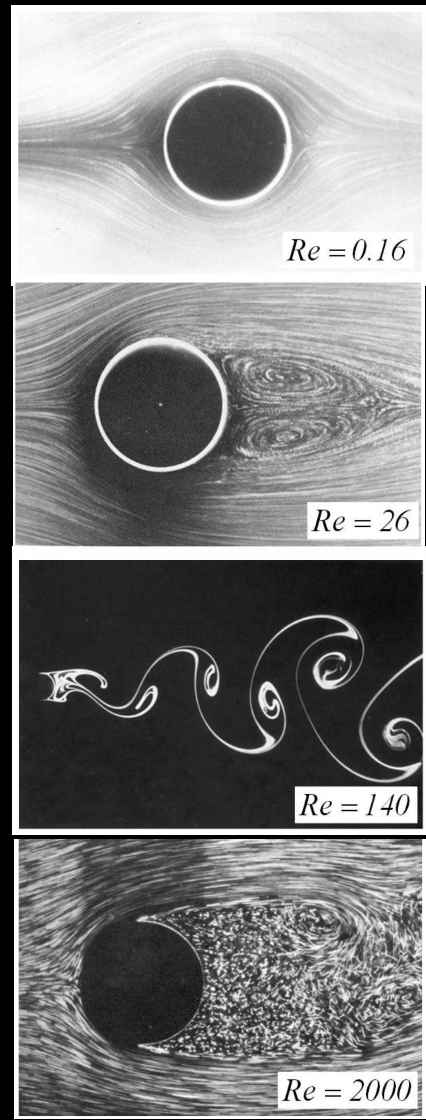
- Reynolds number : $\mathrm{Re} = \frac{V_{ref} L_{ref}}{\nu}$
  - Ratio of inertia to viscous forces ⇔ ratio of diffusion to convection time scales
  - Ratio of nonlinear to linear terms!

Stokes flow

Laminar flow

Turbulent flow

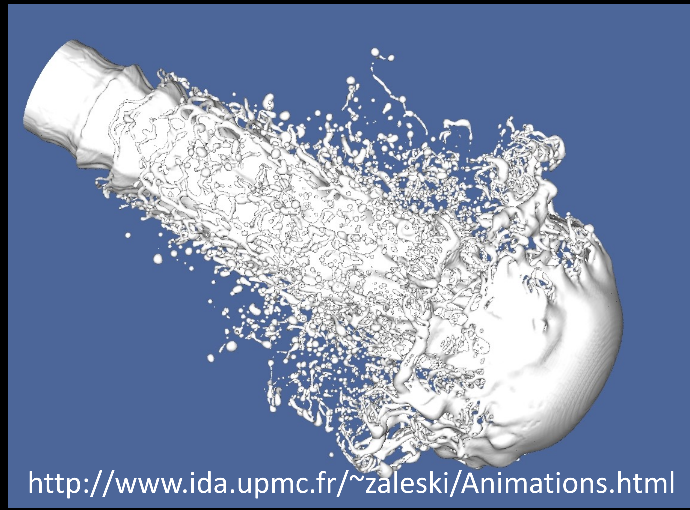
Re

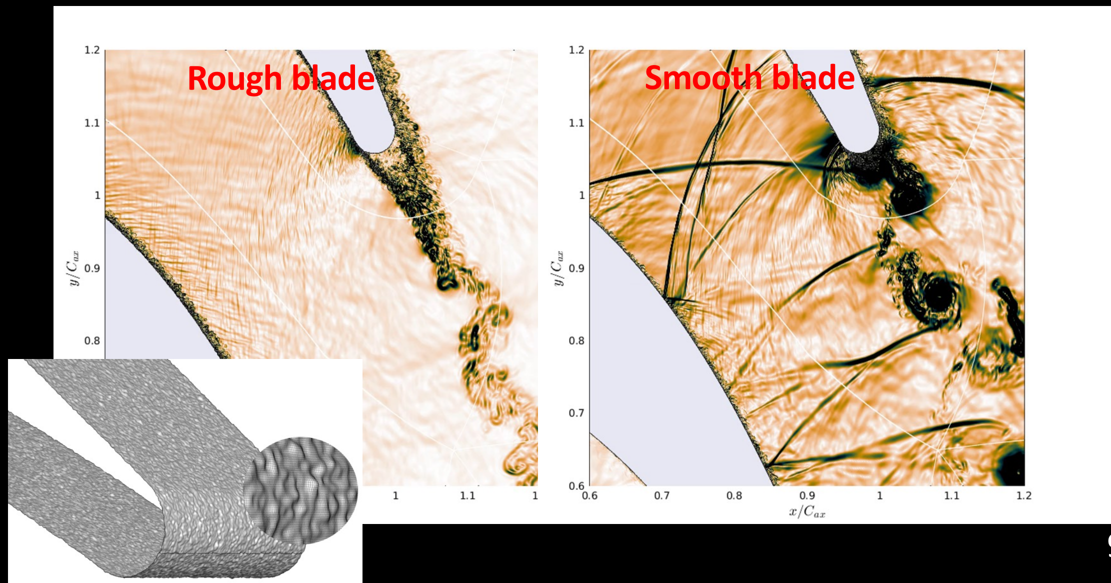


Van Dyke, 1982

Multiples scales

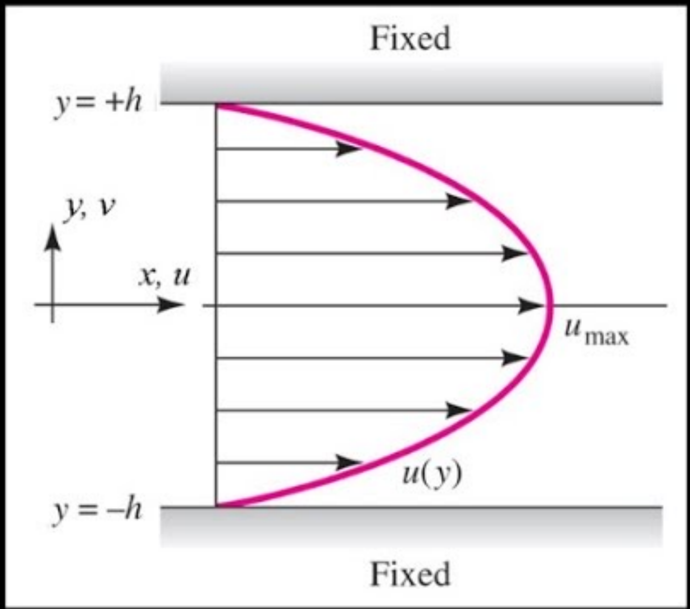
https://svs.gsfc.nasa.gov/3820

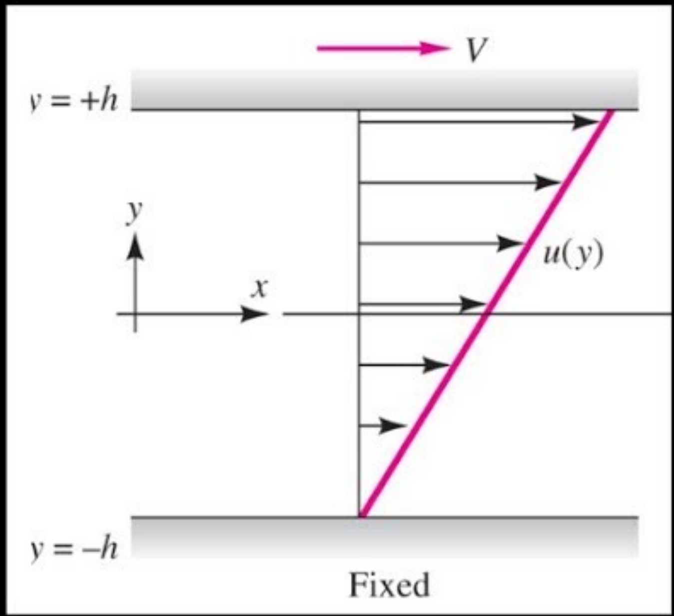




Challenges

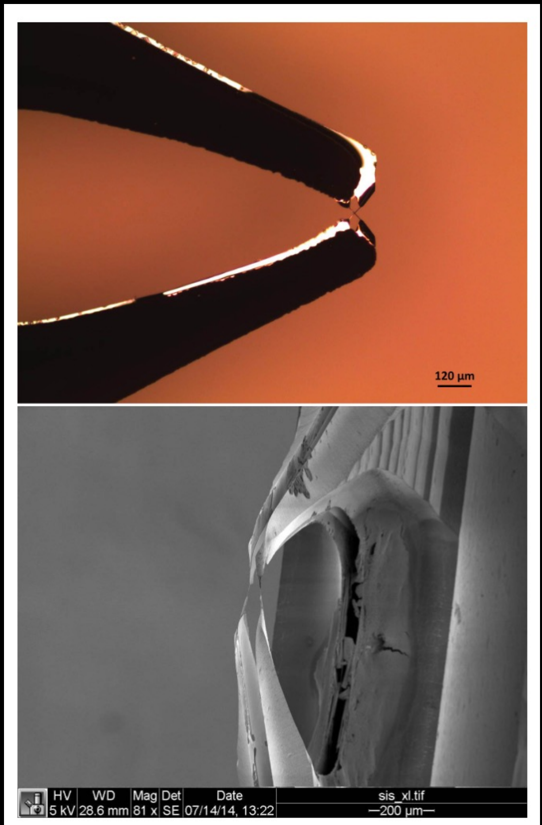
- Analytical solutions possible for a limited range of simple flow cases
- Asymptotic expansions, linearization techniques…
  - Simplifying assumptions
  - But **parcimonious and interpretable** models! Generalizable to some extent…



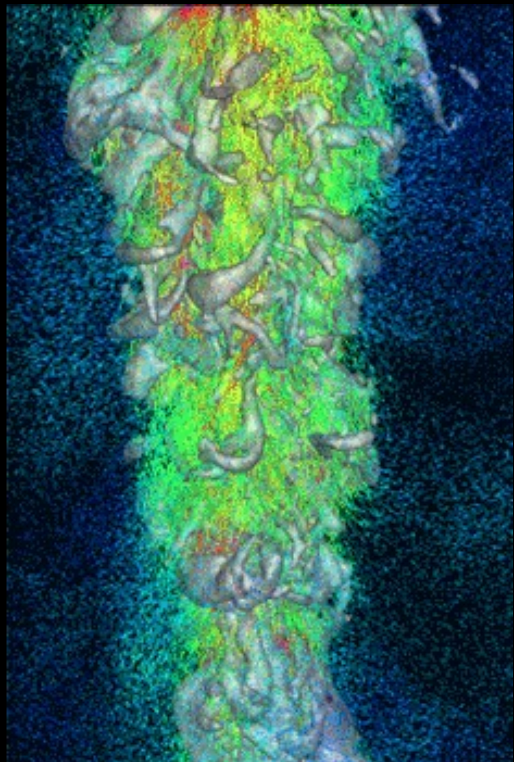


Challenges

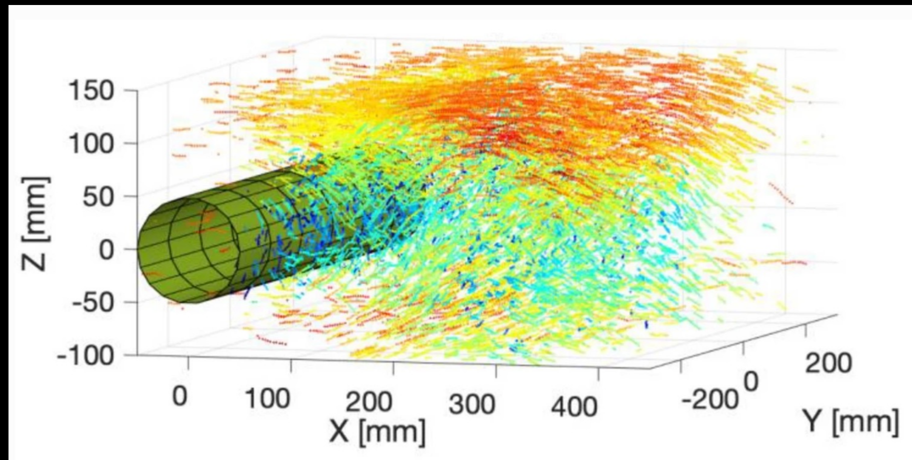
- Experimental investigation costly and time consuming
- Incomplete/noisy (inaccessible regions, scale cutoff, reconstruction errors, unobservable quantities)
- One-shot! Interpretable? Uncertainties?



Smits&Hultmark, 2014



https://www.lavision.de/fr/applications/fluid-mechanics/time-resolved-3d-particle-tracking/i



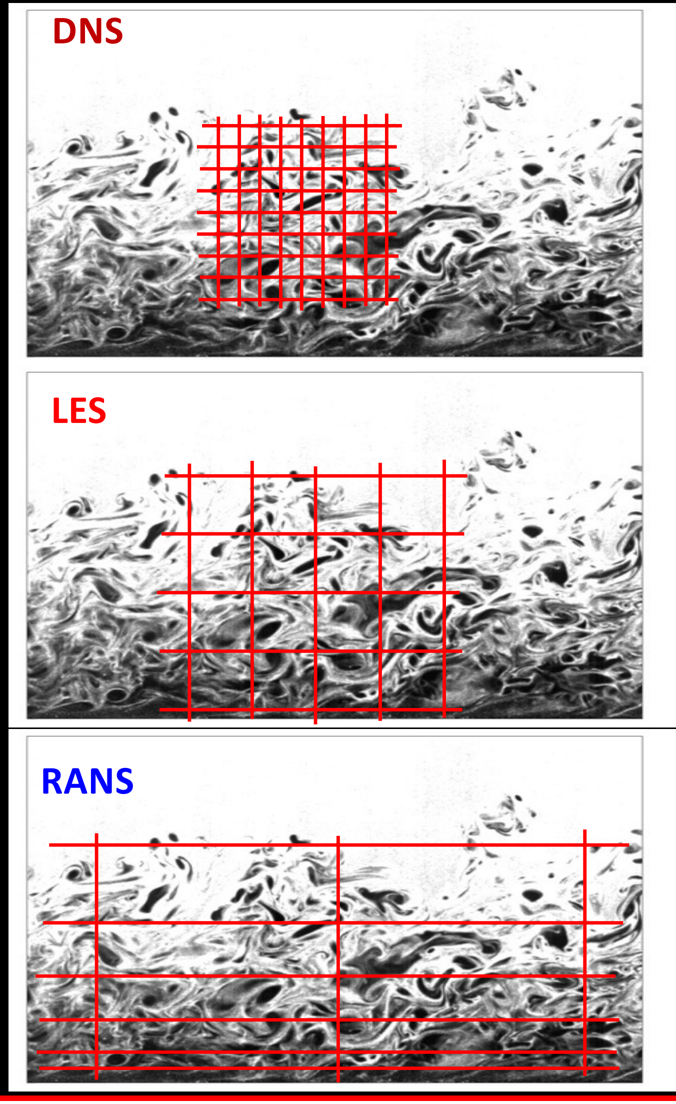
Time-resolved tomographic PIV of incompressible flow past a cylinder at Re_D=27000 (Scarano et al., 2022)

Challenges

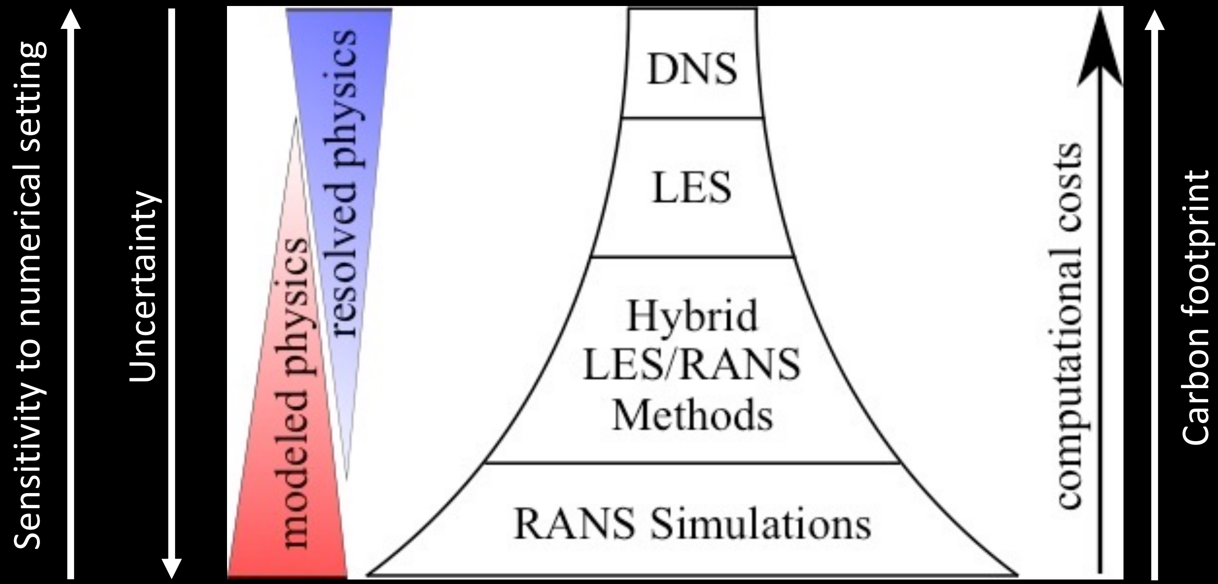
Solving all scales generally unfeasible → coarse-grained approaches

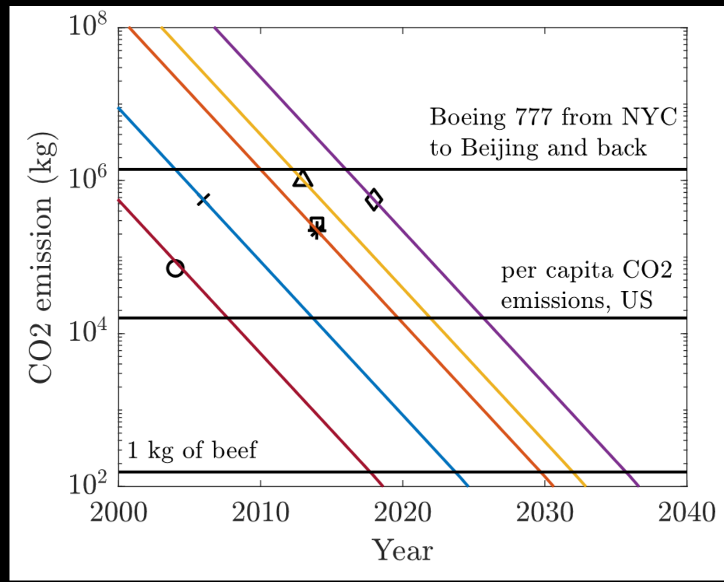
- **DNS**
  - Number of cells required for solving all scales
    $\approx \left(\frac{L}{\eta}\right)^3 = Re^{9/4}$
  - Cost$\approx Re^{11/4}$ (number of cells x number of time iterations)
- **Large Eddy Simulation**
  - Free-shear flow: $\approx Re^{0,4}$; cost $\approx Re^{0,5}$
  - Wall-bounded flows (Wall-Resolved LES, WRLES) : $\approx Re^{1,8}$; cost $\approx Re^{2,4}$

  → **quasi-DNS resolution**
- **RANS**
  - Drastic reduction of computation time
  - Models are less universal and suffer from **uncertainties**



Multiple modeling fidelities





Estimates of carbon footprint for channel flow DNS [Yang et al., 2024]

- **High carbon footprint of large simulations**
- Hi-Fi CFD (DNS, Wall-Resolved LES) limited to low/moderate-Reynolds numbers
- Mid-Fi CFD Wall-Modelled LES, WMLES, and hybrid RANS/LES are attractive alternatives but do not solve all of the problems

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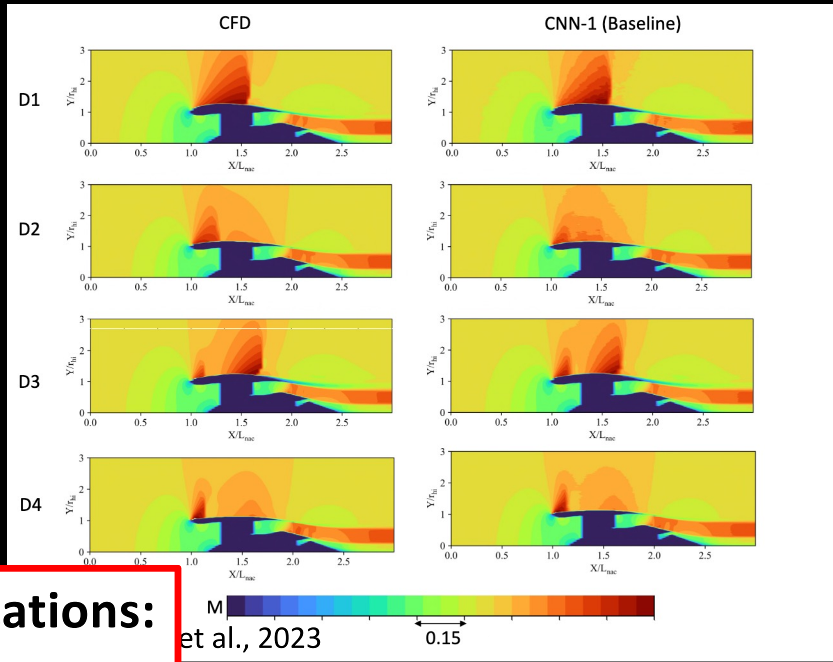
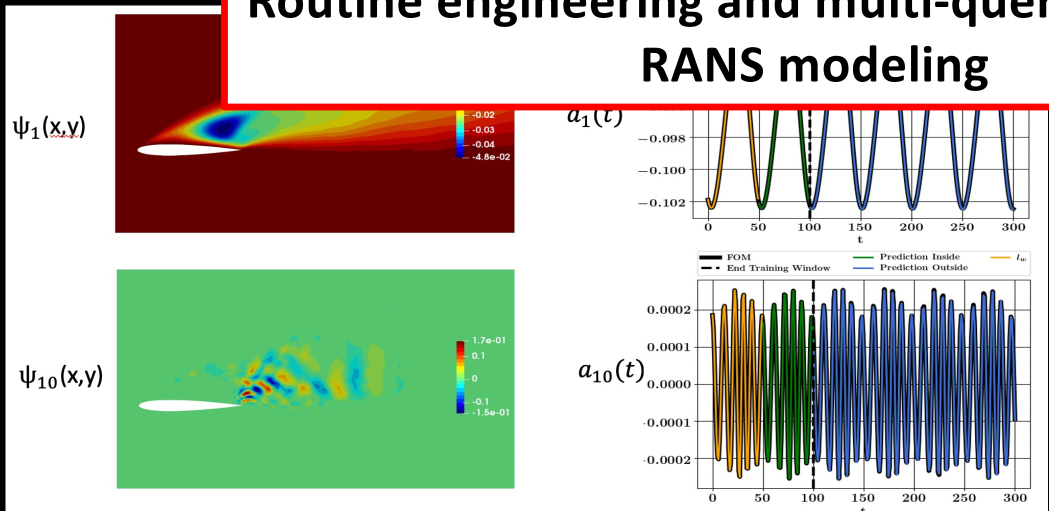
HiFi-quality CFD at the cost of LoFi (or less!)

- Automated design and optimization
- Uncertainty quantification
- Digital Twins and real-time simulation

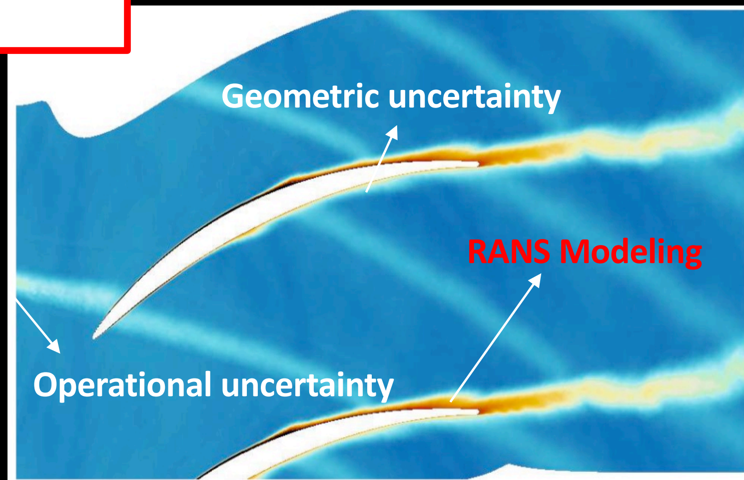


et al., 2023

Routine engineering and multi-query applications: RANS modeling



Sayadi et al., 2020

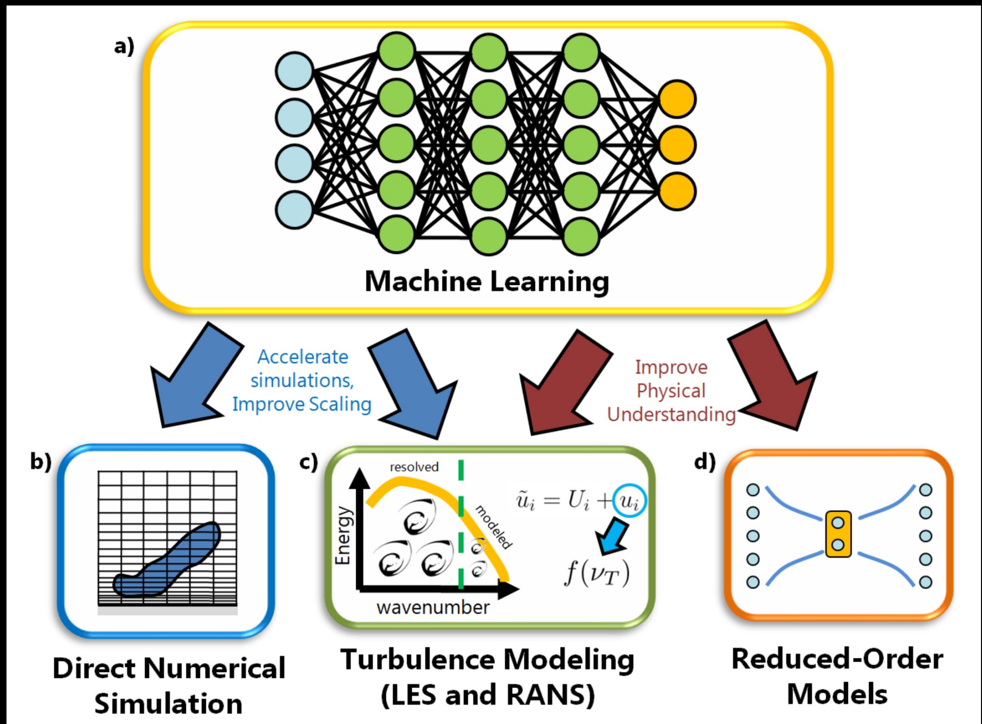


De Zordo Banliat et al., 2020

The promises of Machine Learning

Potentially disruptive impact of artificial intelligence/**machine learning (ML)** techniques:

- Abundant HiFi databases → super-resolution, feature extraction, model augmentation, digital twins, control, surrogate modeling, clustering, classification…



Vinuesa & Brunton, 2022

Can ML enable fast HiFi-quality for scientific discovery and engineering?

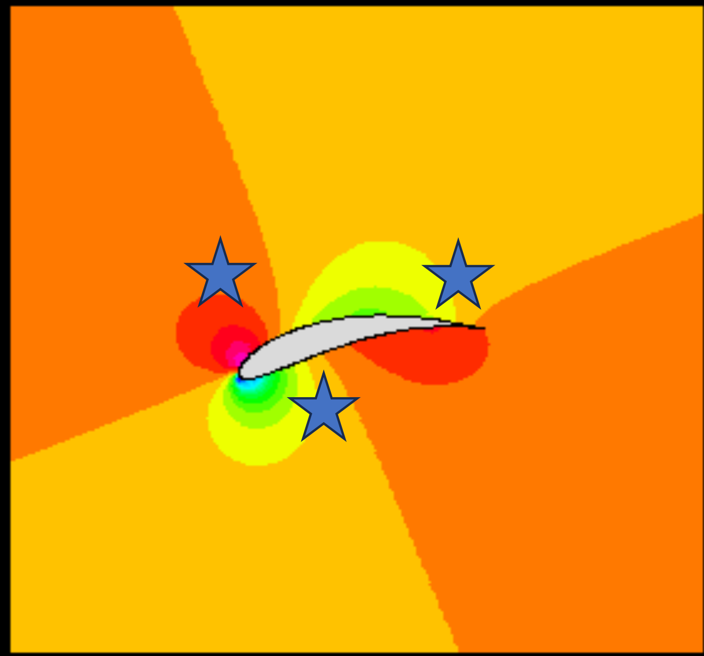
Requirements

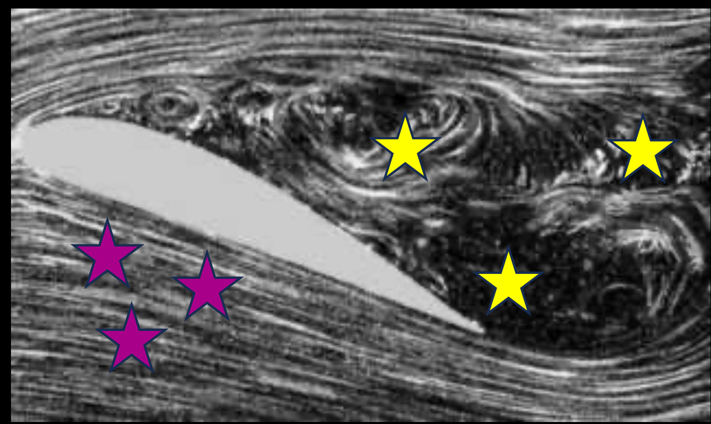
- Interpretable and generalizable models
  - As simple as possible, but not simpler (parcimony principle)
    - Example

$$\nabla^2\phi = 0, \frac{\partial \phi}{\partial n} = 0 \quad \text{and} \quad \frac{p}{\rho} + \frac{1}{2}|\nabla\phi|^2 = cte$$

- Uncertainty control
  - Tell something about model reliability, especially in unseen environments

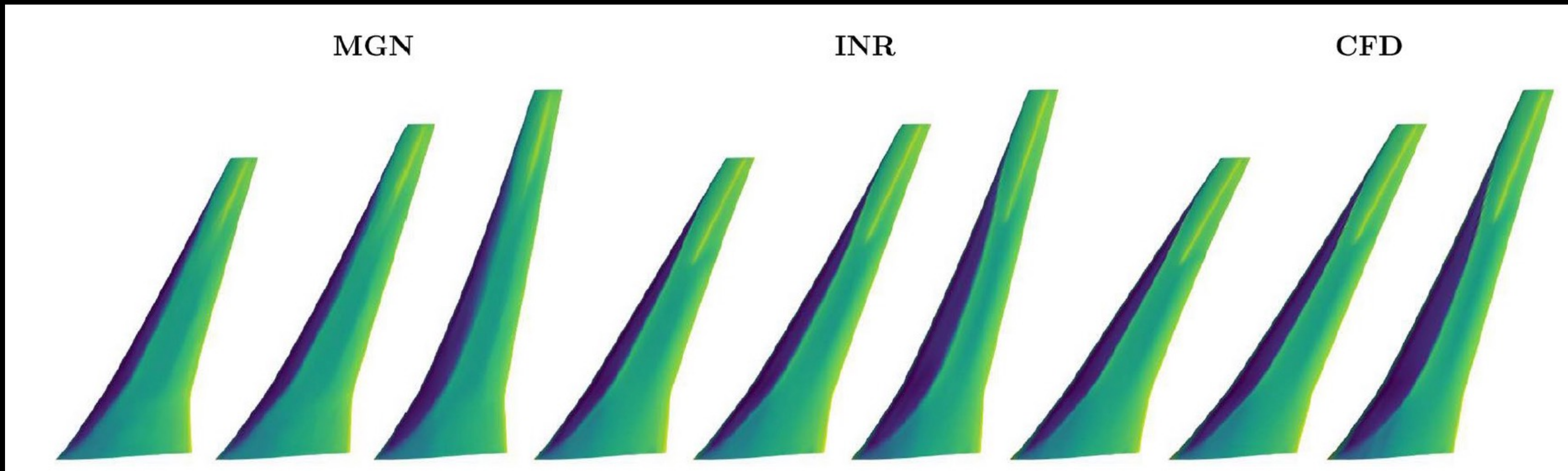
- Deal with sparse/noisy data
  - Very partial sampling from some unknown distribution





Application 1: Reduced-order/surrogate models/neural operators

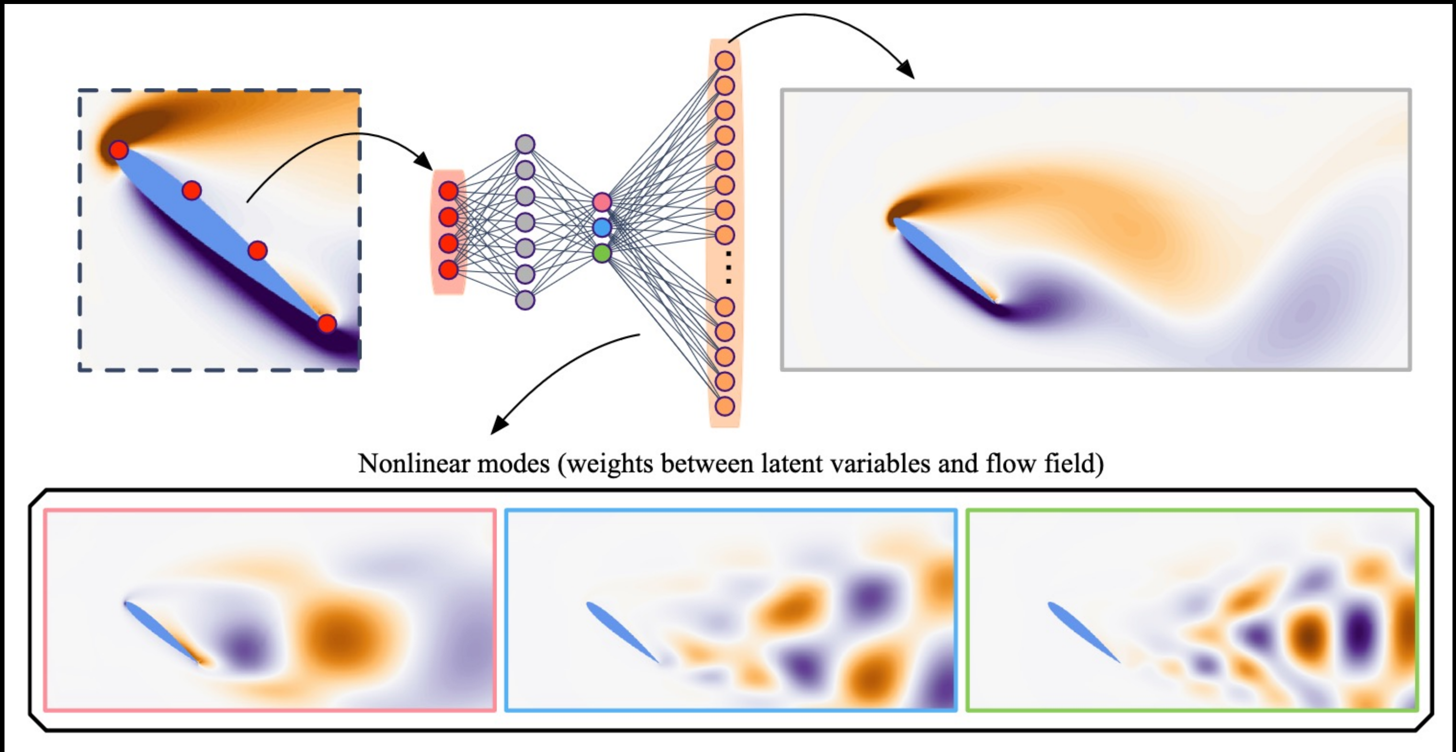
- The response of a costly model to some parameters is reproduced by a cheap ML model (surrogate model or metamodel)
  - Inclusion of physical constraints in the loss function
- Useful for optimization, uncertainty quantification, parameter estimation, control tasks
- Surrogate quality control?
- Amount of required data vs range of configurations potentially covered?



Catalani et al., 2024, Multiscale Implicit Neural Representation (INR)

Application 1: Reduced-order/surrogate models/neural operators

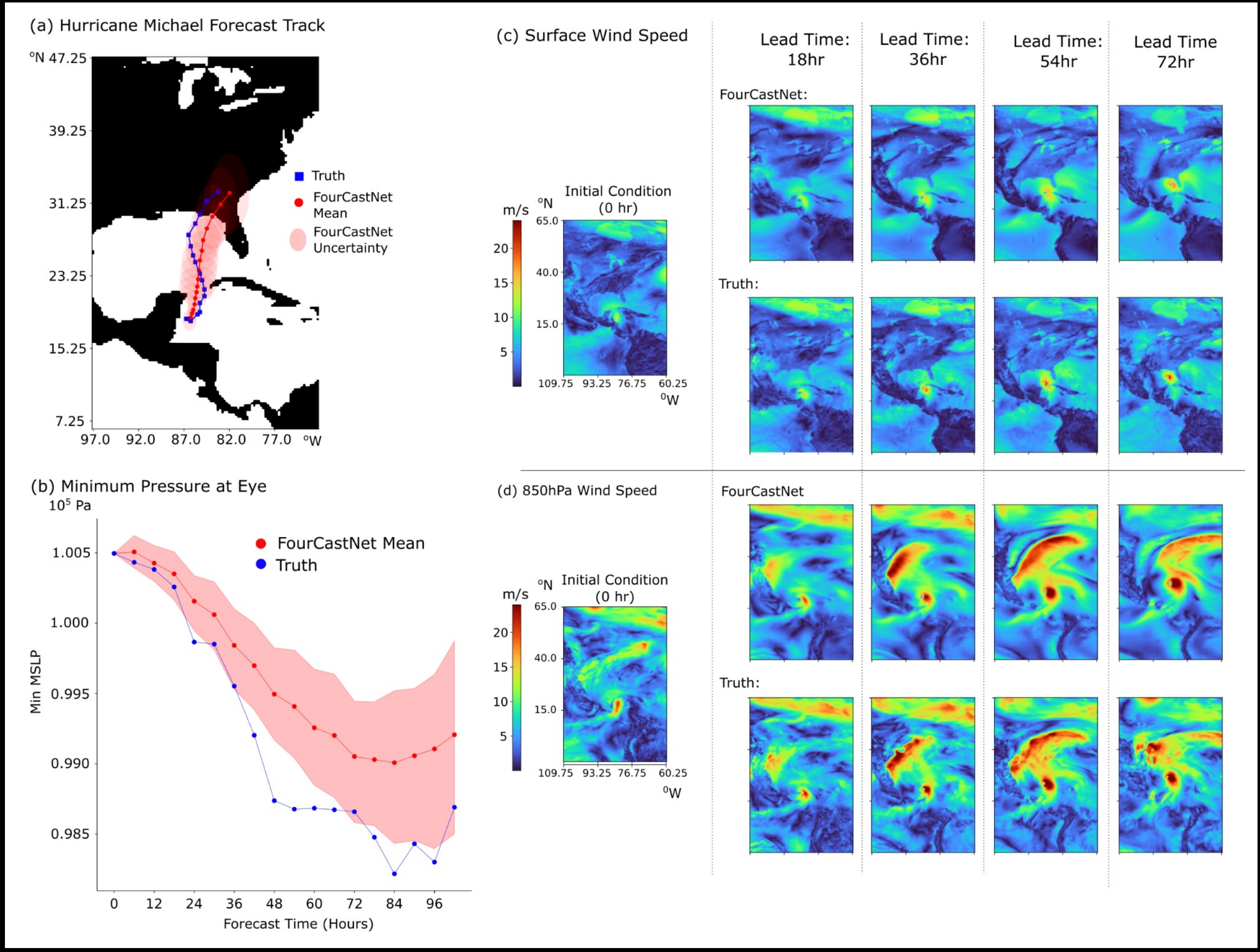
- Nonlinear reduction of flow dynamics, pattern extraction, causality effects
- Single flow, spectral bias (small structures ill-captured)



Fukami et al. 2023

Application 1: Replace costly simulators

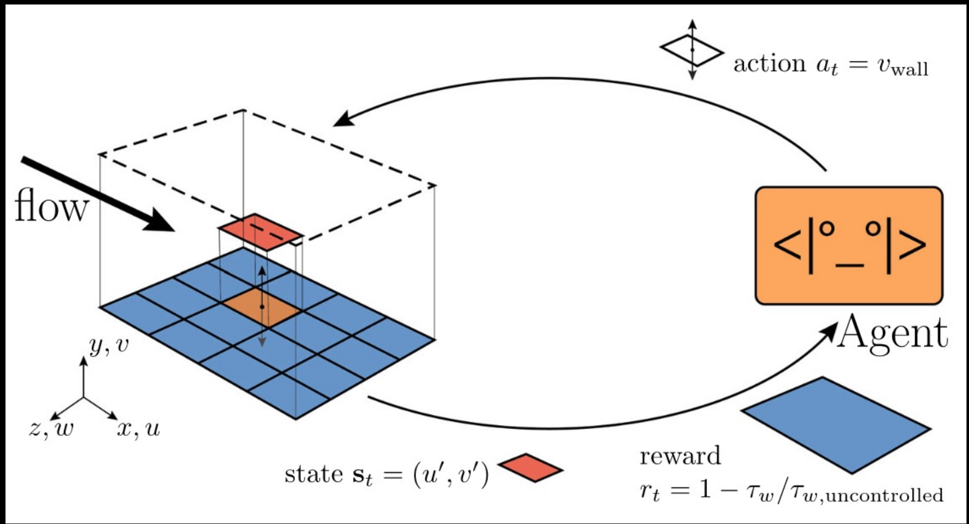
- **Neural operators** learn the solution operator
- FourCastNet (NVIDIA), short for Fourier ForeCasting Neural Network
- Global data-driven weather forecasting model
- Accurate short to medium-range global predictions at 0.25◦ resolution.
- Dramatic reduction of CPU cost
- Ensemble forecasting

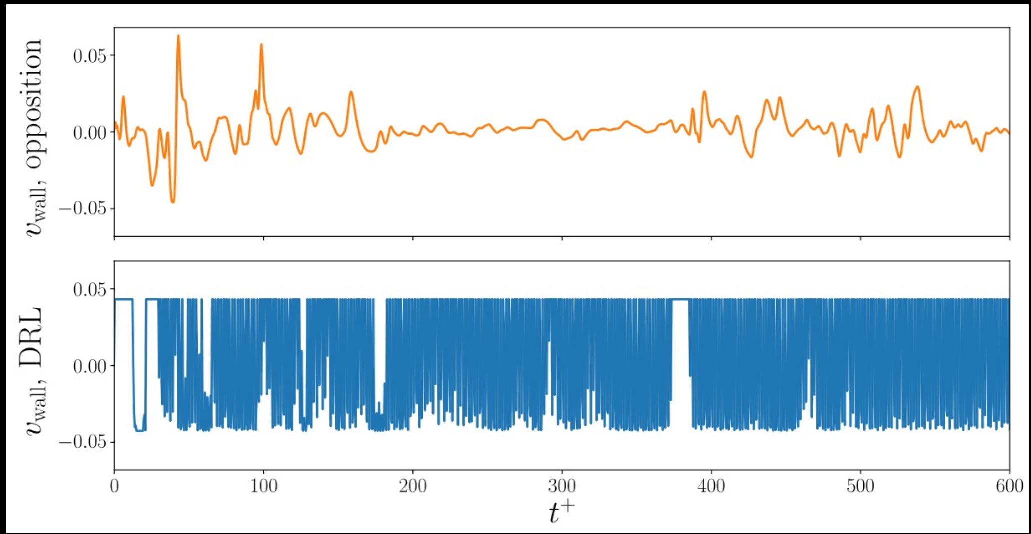


Application 2: Flow control

- Drag reduction via Deep Reinforcement Learning
- Discovery of new control strategies
- Detection of sensitive flow structures

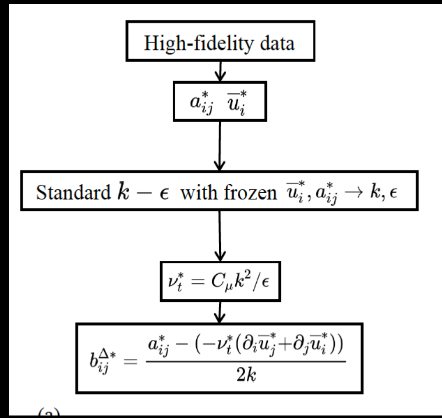
Guastoni et al., 2022

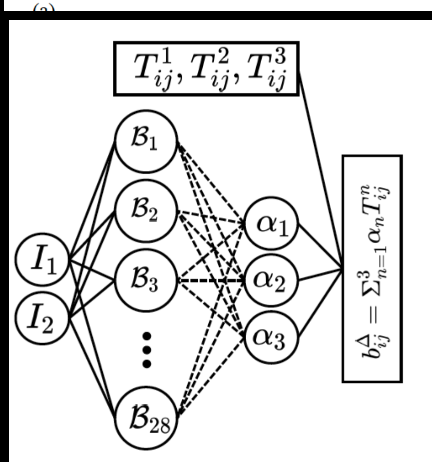


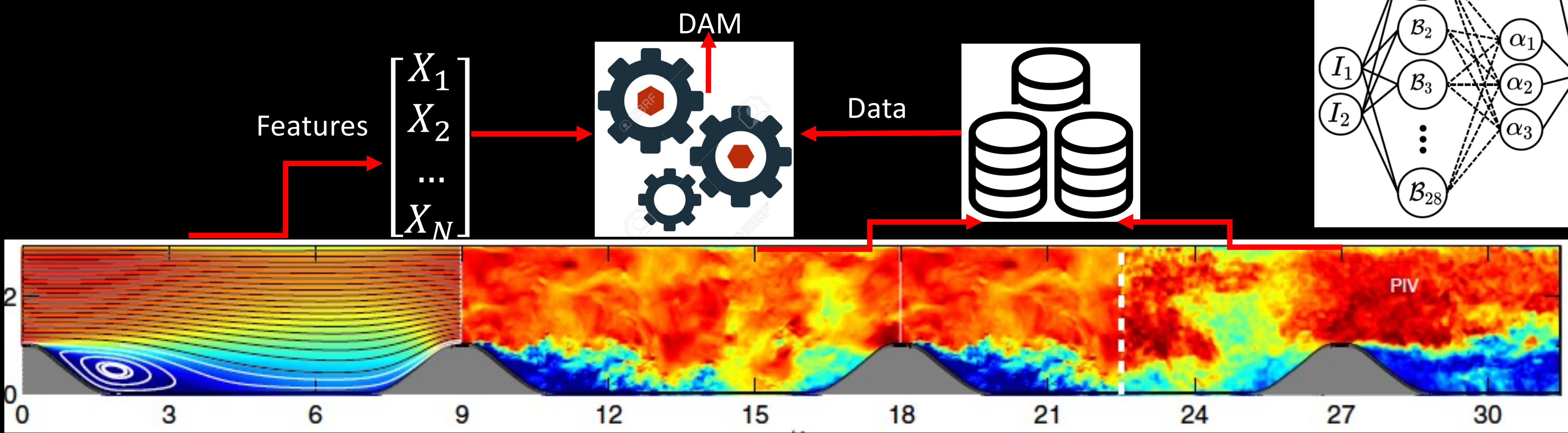


Application 3: Discovery/augmentation of models

- Learn data-driven coarse-grained models
- Symbolic regression, neural networks, random forests, Gaussian processes, …







Low–fidelity CFD (RANS) High-fidelity CFD High-fidelity experiment

Open-box ML for the discovery of turbulence models

[Schmelzer et al., 2020]

SpaRTA = Sparse Regression of Turbulent-stress Anisotropy

- Start with linear eddy viscosity model (here, Menter's $k-\omega$ SST)

$$\tau_{ij} = 2k\left(b_{ij} + \frac{1}{3}\delta_{ij}\right); \quad b_{ij} = -\frac{\nu_t}{k}S_{ij}; \;\; \nu_t = f(k,\omega)$$

+ transport equations for k and ω

- Internal additive corrections of Reynolds stress anisotropy (b_{ij}^{Δ}) and turbulent transport equations (R):

$$b_{ij} = -\frac{\nu_t}{k}S_{ij} + b_{ij}^{\Delta} \qquad \frac{Dk}{Dt} = P + P^{\Delta} + D + T + R \qquad \frac{D\omega}{Dt} = P_{\omega} + P_{\omega,\Delta} + P_{\omega,R} + D + T$$

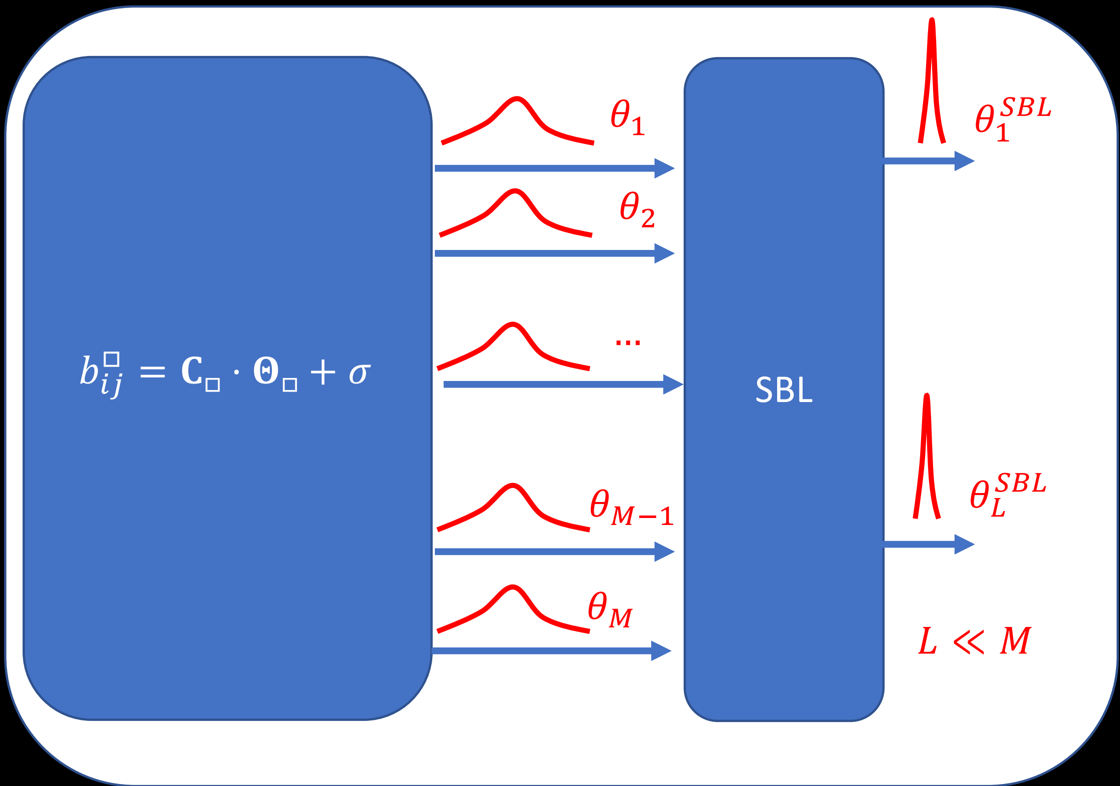
- **Learn b_{ij}^{Δ} and R from high-fidelity data**

SPARSE SYMBOLIC IDENTIFICATION

Open-box learning from a dictionary of explicit operators

Bayesian learning : SBL-SpaRTA [Cherroud et al., 2022]

- Find $p\left(\boldsymbol{\Theta}_{\square}, \alpha, \sigma^2 \middle| b_{ij}^{\square}\right)$ using the efficient Sparse Bayesian Learning (SBL) algorithm (Tipping 2001)
  - Solves a generalized linear regression problem
  - Recursively **select** features in $\mathbf{C}_{\square}$ dictionary and infer parameter posteriors



SBL-SpaRTA : discovered models

- Training data

Case	Data
CHAN	DNS of turbulent channel flow, $180 \leq Re_\tau \leq 590$
ANSJ	PIV of near sonic axisymmetric jet
SEP	LES of Periodic Hills (PH) at Re=10595 DNS of Converging-Diverging (CD) channel at Re=13600 LES of Curved Backward Facing Step (CBFS) at Re = 13700

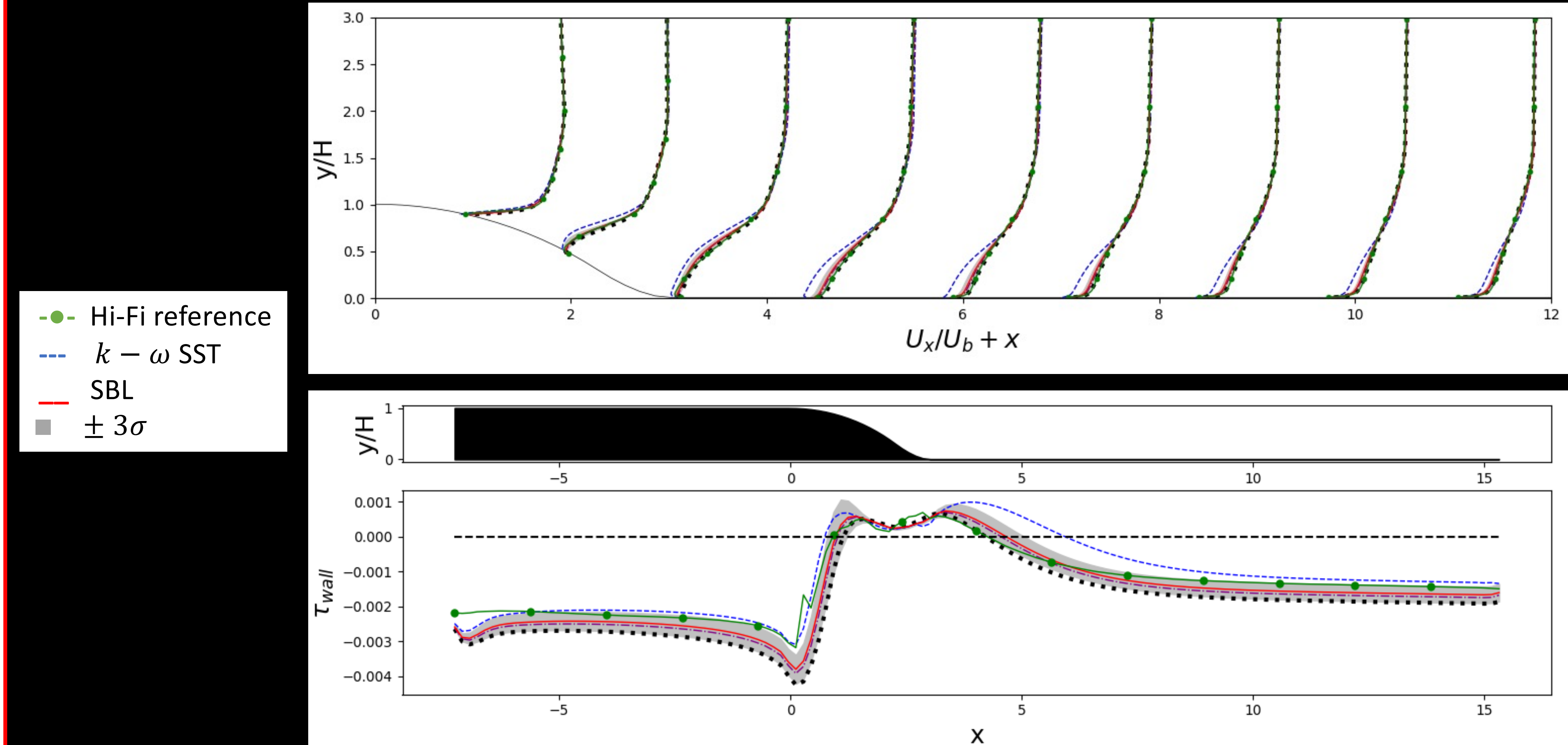
Training case	Model	Interpretation
CHAN	$\begin{cases} \mathbf{M}_{\mathbf{b}\Delta}^{(CHAN)} = [0] \pm 0.0914 \\ \mathbf{M}_{\mathbf{b}^R}^{(CHAN)} = [0] \pm 4.61 \times 10^{-3} \end{cases}$	$P_k^{(CHAN)} = 2\nu_t S^2$ (baseline $k-\omega$ SST)
ANSJ	$\begin{cases} \mathbf{M}_{\mathbf{b}\Delta}^{(ANSJ)} = [(\mathbf{0.33} \pm 0.0189)]\mathbf{T}^{(1)} \pm 0.00622 \\ \mathbf{M}_{\mathbf{b}^R}^{(ANSJ)} = [0] \pm 3.45 \times 10^{-3} \end{cases}$	$(P_k)^{(ANSJ)} = 2\nu_t(1-\mathbf{0.33})S^2 = 0.67 P_k^{(CHAN)}$
SEP	$\begin{cases} \mathbf{M}_{\mathbf{b}\Delta}^{(SEP)} = [(5.21 \pm 0.0173)]\mathbf{T}^{(2)} \pm 0.0348 \\ \mathbf{M}_{\mathbf{b}^R}^{(SEP)} = [(\mathbf{0.681} \pm 0.02)]\mathbf{T}^{(1)} \pm 0.0318 \end{cases}$	$(P_k)^{(SEP)} = 2\nu_t(1+\mathbf{0.681})S^2 = 1.681 P_k^{(CHAN)}$

$E[\theta]$ $std[\theta]$ σ

Channel flow : the discovered model correction is 0!

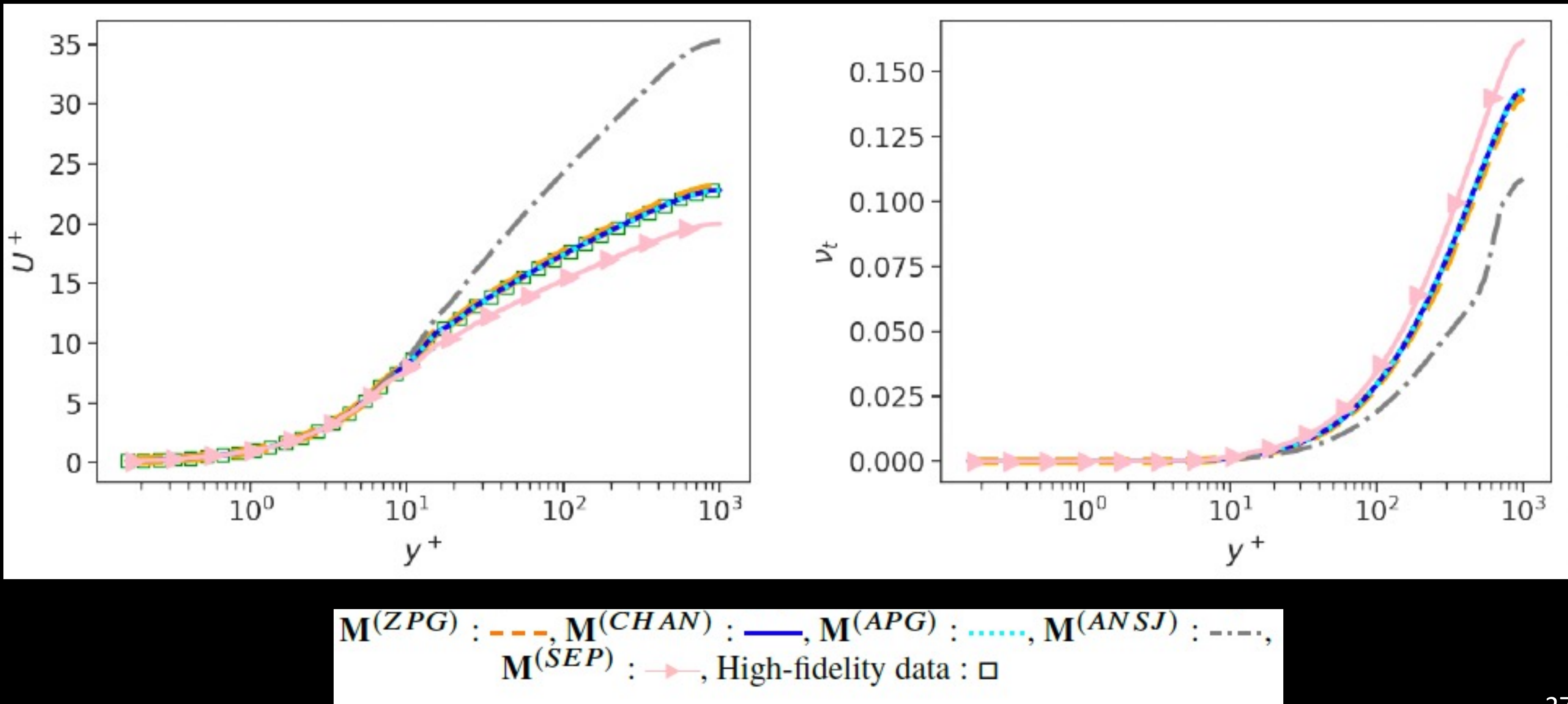
SBL-SpaRTA

- Curved backward-facing step flow at Re=13700



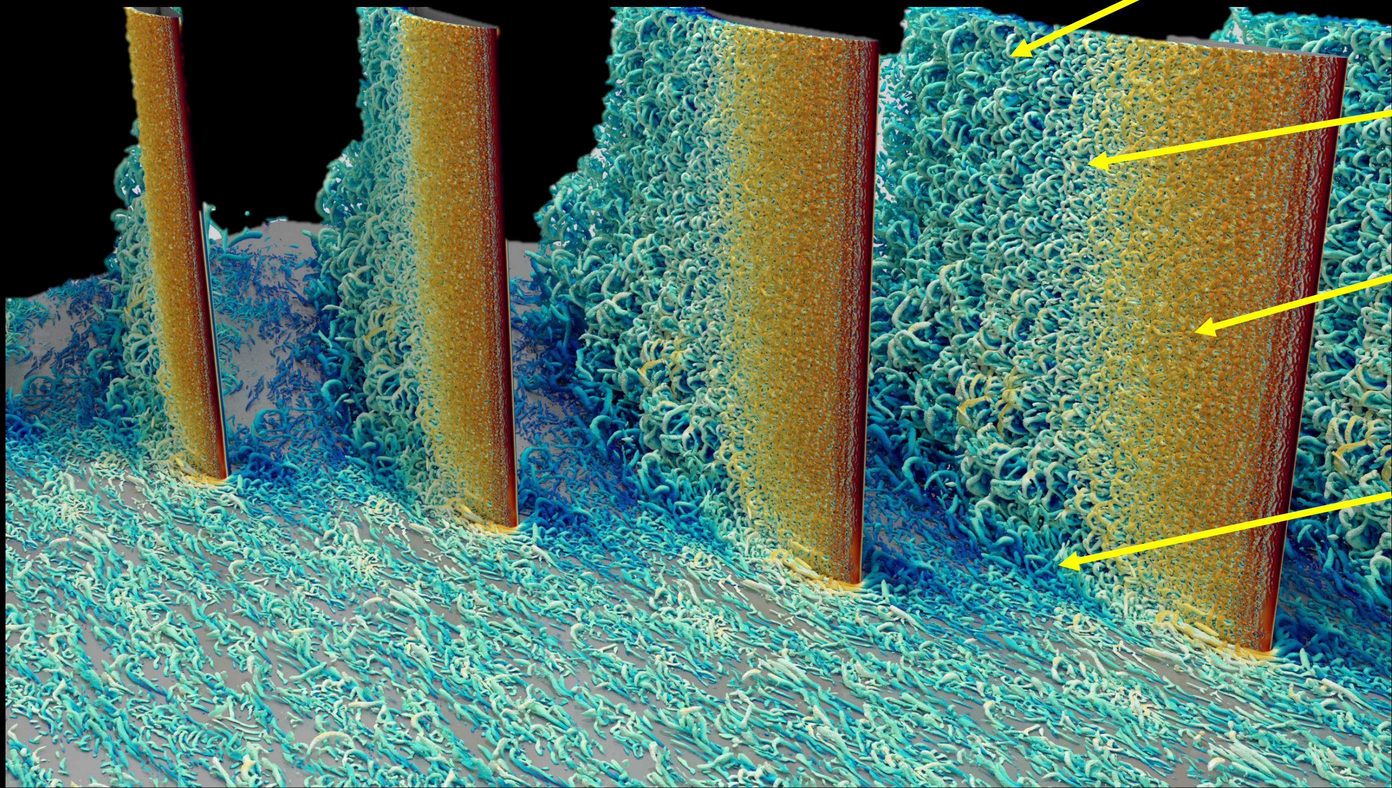
Generalization

- Customized models may generate large errors when applied outside their application range



Quest for the “universal” model

- Some degree of generality needed
- Hand-set “zonal” models not acceptable for industry

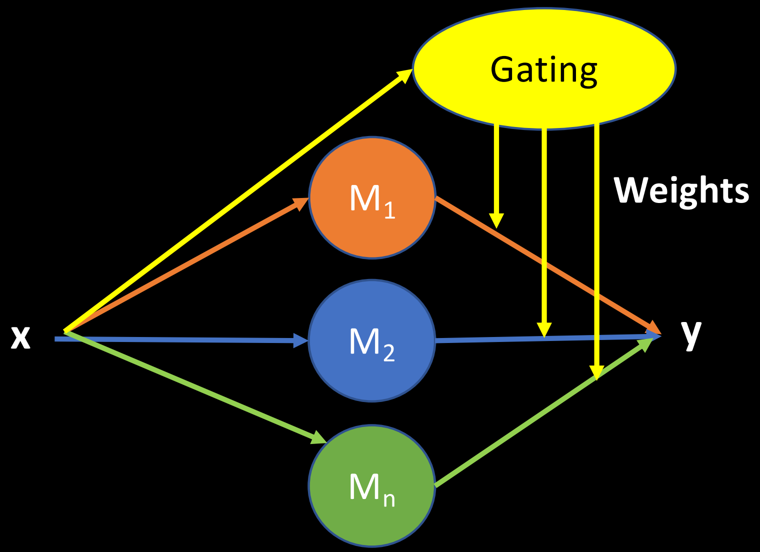


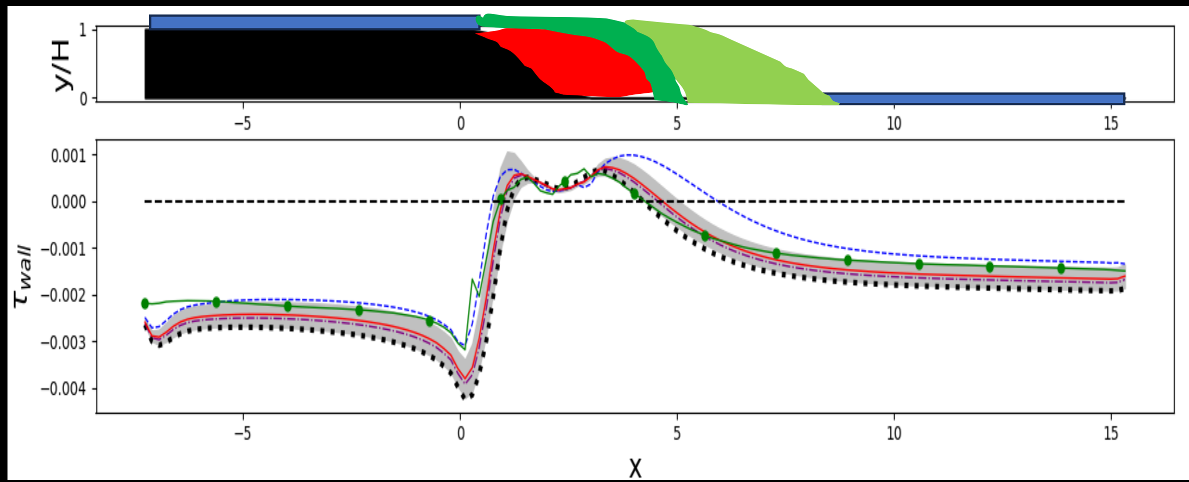
LES data and figure by D.Papadogiannis

Towards more generalizable ML models

- **Model Mixtures**
  - Large data sets: combining models trained on subsets better than single model trained over all data
  - Out of distribution predictions: uncertainty on which model (among those at hand) is better
  - Generate hypermodels by combining component models

Mixture of Experts





Spatial model aggregation (XMA) of turbulence models [de Zordo et al., 2021]

- Consider a set of K competing models $\mathcal{M} = \{\boldsymbol{M_1}, \boldsymbol{M_2}, \dots, \boldsymbol{M_K}\}$

- « Hypermodel »: $M_{hyp}(\mathbf{x}, \boldsymbol{\theta}) = \sum_{k=1}^{K} w_k M_K(\mathbf{x}; \boldsymbol{\theta})$, with

$$w_k = w_k(\mathbf{x}) = w_k(\boldsymbol{\eta}(\mathbf{x}))$$

- Regress $w_k(\boldsymbol{\eta}(\mathbf{x})|\mathbf{Y})$ from data as a function of features → **Random Forests, Gaussian Processes, ANN…**
  - Features from Ling&Templeton (2015)
  - Predict local model weights for a new case $w_k(\boldsymbol{\eta}(\mathbf{x})|\mathbf{Y})$ and use them to aggregate individual model predictions

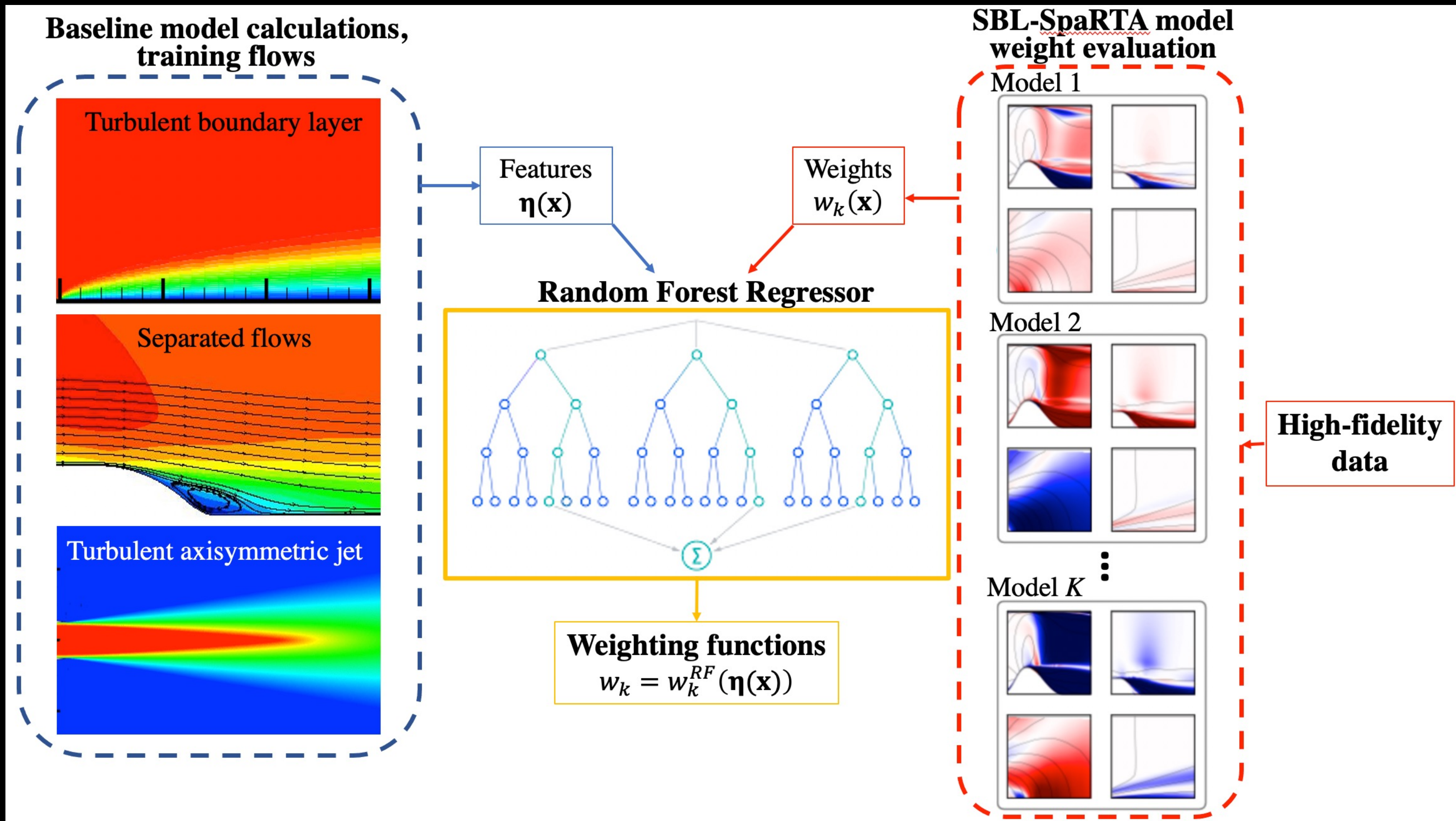
- Uncertainty estimates can be obtained by aggregating the **component variances**

$$Var[M_{hyp}(\mathbf{x}, \boldsymbol{\theta})] = \sum_{k=1}^{K} w_k^2 Var[M_K(\mathbf{x}; \boldsymbol{\theta})]$$

XMA : offline training

[Cherroud et al., 2023]

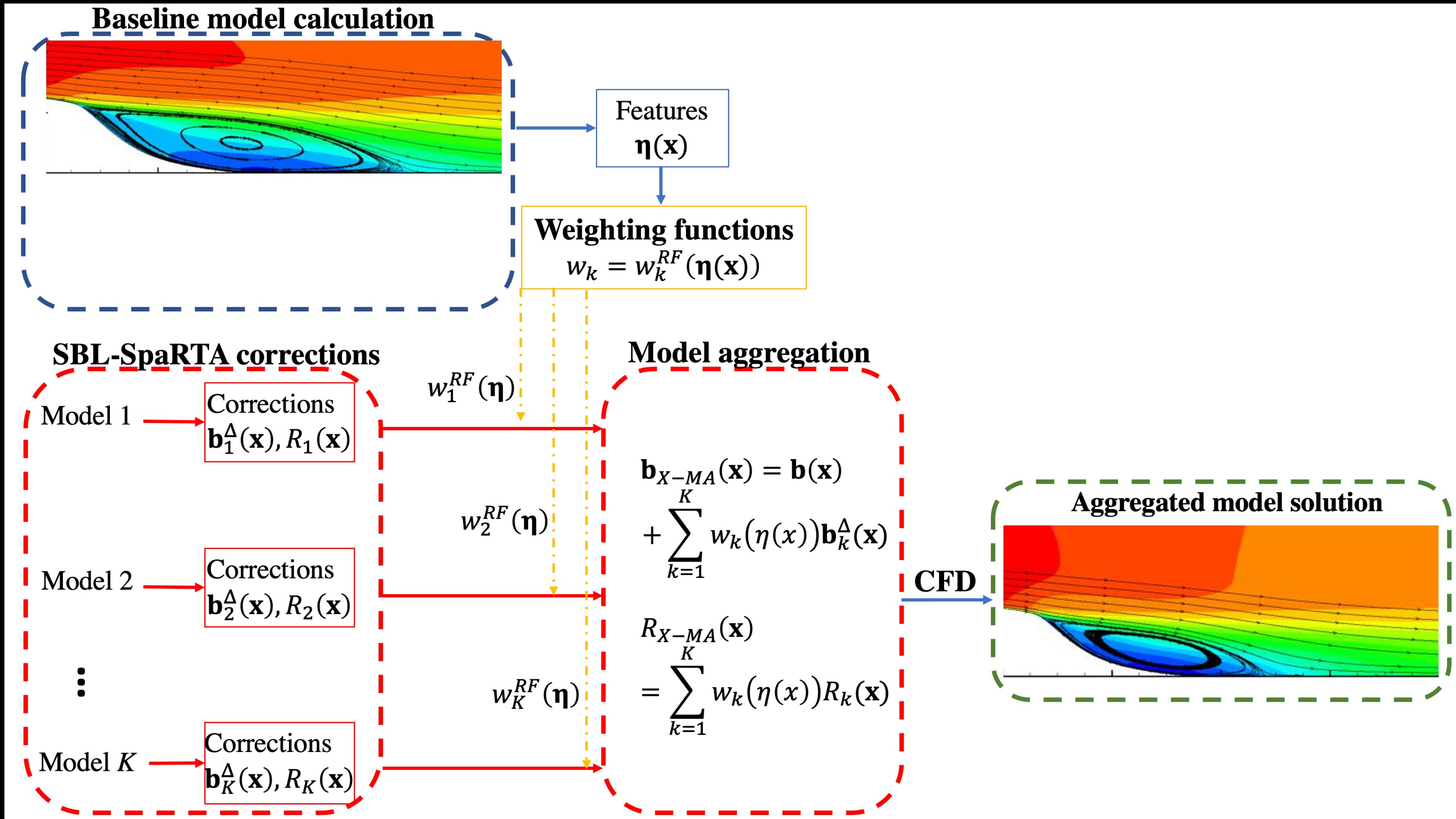
XMA Training Workflow



XMA prediction: model blending

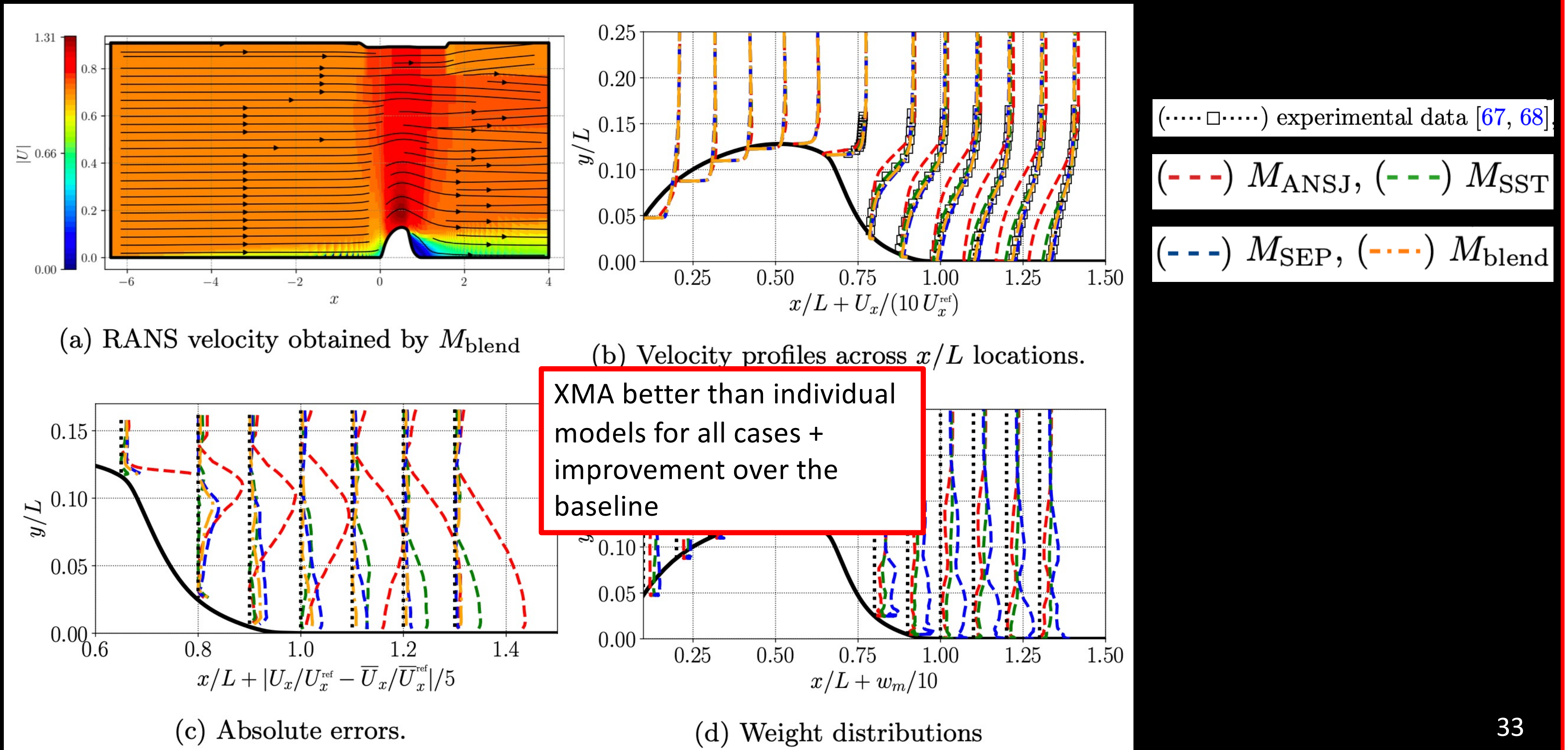
Oulghelou et al., 2024: https://arxiv.org/abs/2410.14431

Intrusive X-MA Prediction Workflow



NASA Turbulence Modeling Testing Challenge

- Application to Test Case 4 2DWMH: 2D NASA Wall-Mounted Hump Separated Flow Validation Case



(a) RANS velocity obtained by M_{blend}

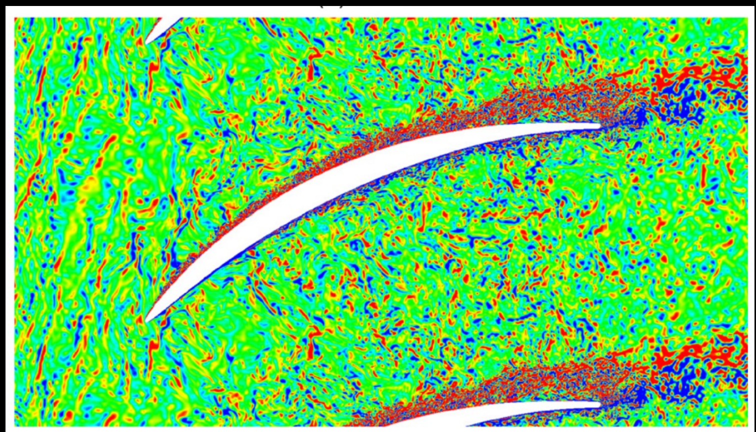
(b) Velocity profiles across x/L locations.

(c) Absolute errors.

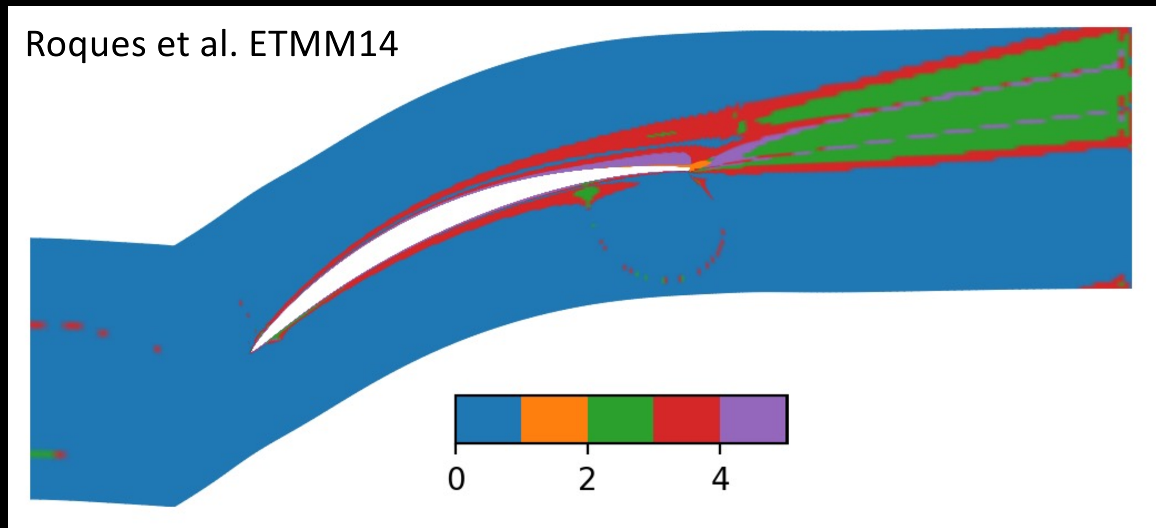
(d) Weight distributions

Training from clustered data

- Training flows contain several physical processes at once
  - Equilibrium BL, non-equilibrium BL, separation, wakes, corner flows, vortices, shocks…
  - Training algorithms tend to find a compromise among such processes
- Is it possible to find a better training strategy?
  - IDEA: Train by clusters, then aggregate



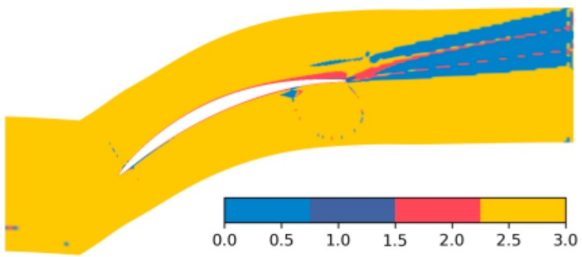
Leggett et al. ASME J Turbo, 2016



Clustered model aggregation [Roques et al., ETMM14]

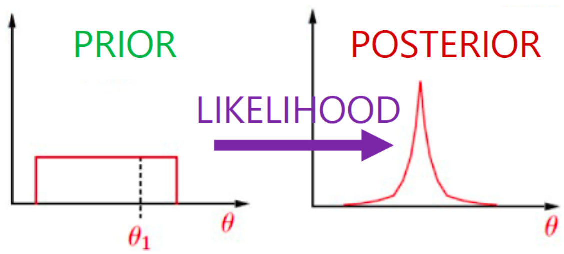
Offline training

Clustering



Identify the dominant physical processes*

Bayesian learning



$$p(\theta|D) \propto p(D|\theta)p(\theta)$$

For each cluster *k*

Within-cluster weights

Based on local score of model *I* in cluster *k*

$$p(M_i|\mathbf{Y_k}) = \frac{p(\mathbf{Y_k}|M_i)p(M_i)}{\sum_{j=1}^{I} p(\mathbf{Y_k}|M_j)p(M_j)}$$

Online prediction

Cluster probability → Within-cluster weighting → Reconstruction

$$\Delta = \sum_k \sum_i p(C_k) w_{ik} \Delta(M_i)$$

*Inspired from Callaham et al. 2021

Overview

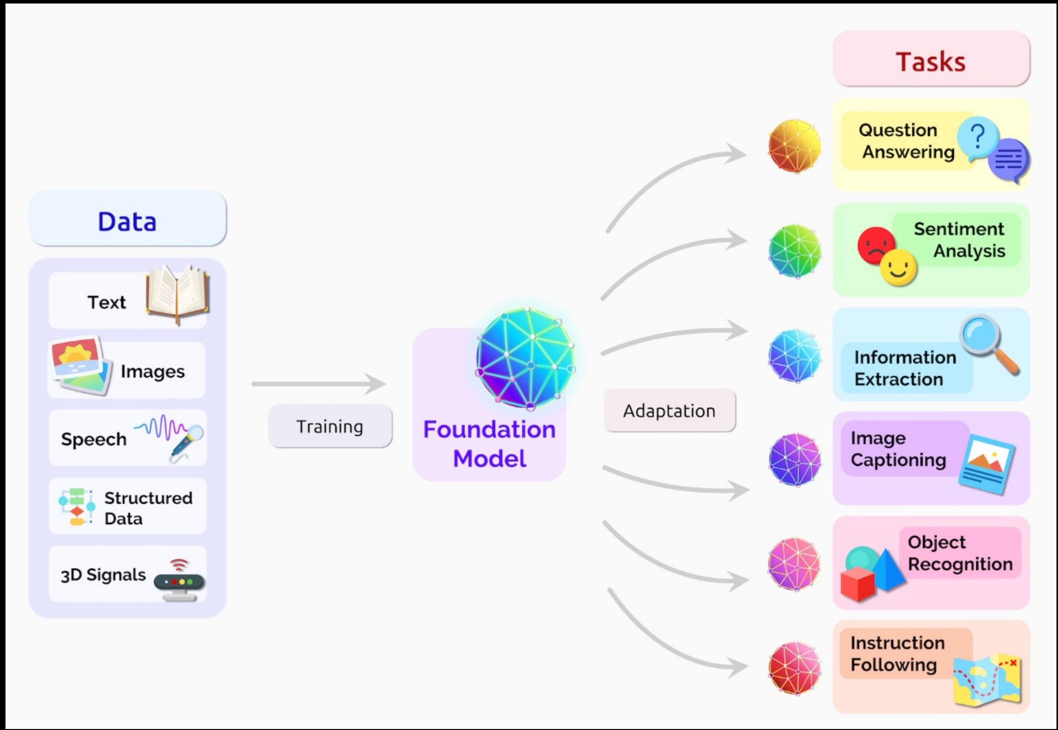
- A very brief introduction to Fluid Mechanics
- Scientific machine learning in Fluid Mechanics
  - Requirements, challenges and opportunities
  - Examples
  - Toward more generalizable data-driven models
- **Conclusions and outlook**

Conclusions

- Artificial intelligence and physics are changing one another
  - Physical modeling , simulation, and experiments can successfully merge with ML to mine large datasets or to solve complex problems
  - ML can be analysed under the lens of physics/mathematics
- Fluid Mechanics complex multiscale and highly nonlinear flow problems are difficult and costly to represent with standard modeling technique and may hugely benefit from AI
- High standards of scientific discovery (interpretability, uncertainties, …) call for more generalizable ML
  - Enforcement of hard constraints, inductive biases, novel definitions of loss functions…
- Massive amount of HF data are becoming available BUT
  - Mostly limited to “simple” configurations and low Reynolds numbers
  - A relatively small number of well-detailed configurations is available
  - Use of **experimental data** is essential for reaching more complex, high-Reynolds configurations
- Likely, we will NEVER have enough data to cover all possible fluid flow processes BUT

Outlook

- "Smart" training instead of "brute-force" training → **learn the "language of fluids"**
  - Identify and extract features and "building blocks" representative of dominant physical processes
  - Recursively encode and combine blocks for prediction based on **context**
  - Use uncertainty estimates to **update** the model



Bommasani et al., 2022

- **Foundation models**: train from heterogeneous data and for multiple tasks, fine-tune
  - Translate into simpler, **explicit models** (AI-Feynman, pySR) for specific end use