

Surrogate modeling using INR and uncertainty quantification

ANITI



ISAE
Institut Supérieur de l'Aéronautique et de l'Espace
SUPAERO

HALSED & PhySimAI

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Feb. 2026

Introduction

Main goal of this talk

*How to create an effective surrogate model for CFD applications using **deep network**?*

CFD = Computational Fluid Dynamics
= simulation of fluid flows

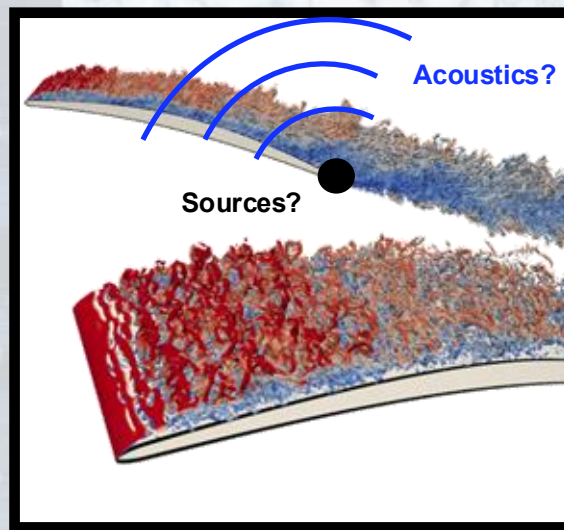
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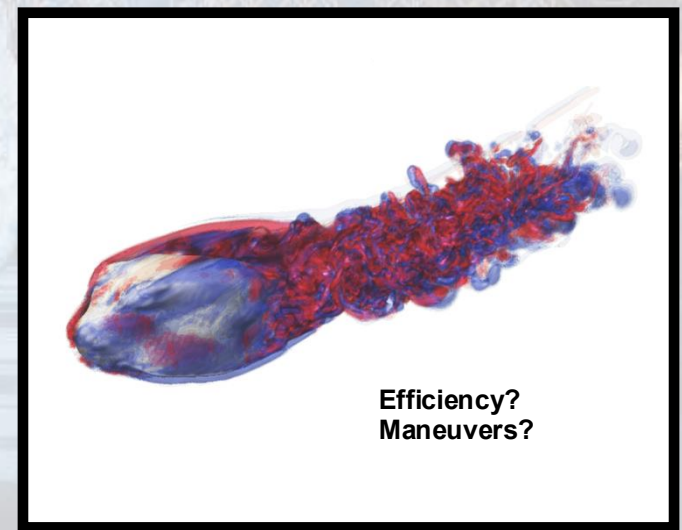
How to create an effective surrogate model for CFD applications using **deep network**?



Combustion in engines



Aerodynamics and acoustics (e.g wing)



Bio-inspiration (e.g boxfish)

BUT fluid flows are challenging:

- ✓ Expensive to compute (10^3 - 10^7 CPUh)
 - ✓ Few data ($10^1 - 10^3$ samples)
- ✓ Unstructured data (mesh = very large graph)
 - ✓ Data is huge (10^7 - 10^9 degree of freedom)
 - ✓ Expensive to store (1-100 Go per data)
 - ✓ Nonlinear (e.g turbulence, shocks etc.)
 - ✓ Multi-scale (large/small $\sim Re^{3/4} \sim 10^3$ - 10^5)

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Deep Learning methods?

- Well adapted to **high dimensional spaces**
- **Non-linear & differentiable** by construction
- Can leverage **large (noisy) datasets**
- **Flexible method** (dynamical systems, videos, unstructured fields, point clouds, distributions, ...)

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Current difficulties?

- What about **limited dataset**?
 - Are they really **accurate** (e.g. on multi-scale problems)?
- } **Sample-Efficiency?**
Accuracy = f(dataset size)

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 - Can we **trust them**?
- } Guarantees & Uncertainties?**
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- **Flexi**
distrib

int clouds,

So is AI really adapted to CFD?

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Presentation outline

1. How can AI represent complex flows?

- *From CNN to Implicit Neural Representation (INR)*

2. Can AI move from flow prediction to flow discovery?

- *Introducing Active Learning and Uncertainties*

3. Research vision and perspectives

- *Hailed & PhiSimAI*

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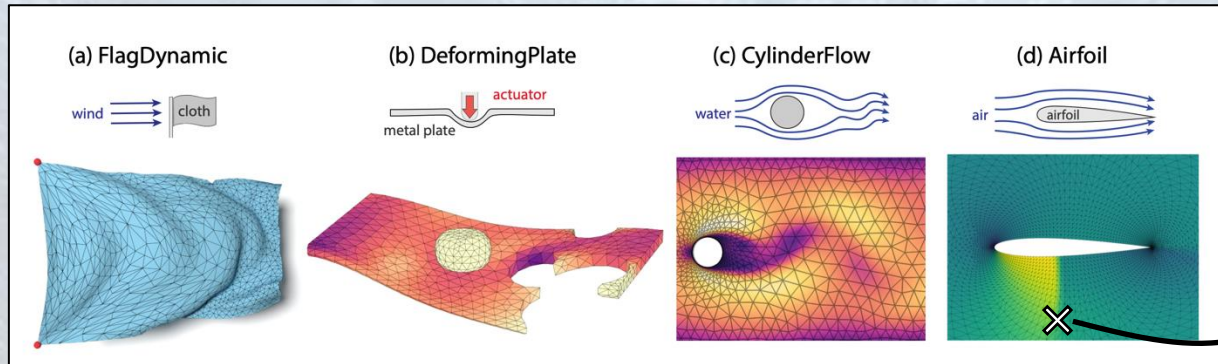
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1. How can AI represent complex flows

*How to learn flow solutions on **meshes** & **manifolds**?*

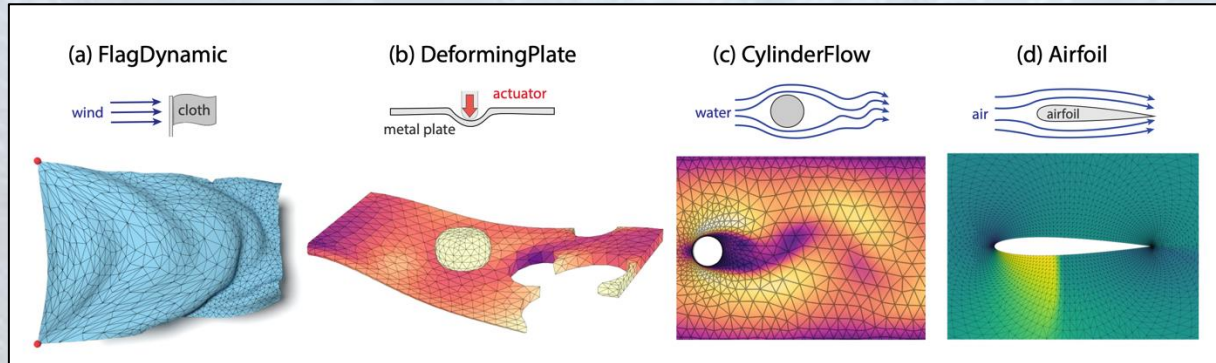


$N_{\text{node}} = 10^6 - 10^8$
Low connectivity
Long-distance interaction

Off-the-shelf AI models were NOT necessary well-adapted to CFD data format and requirements

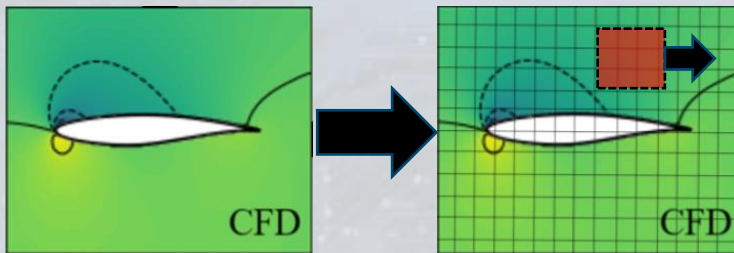
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2017 - 2021

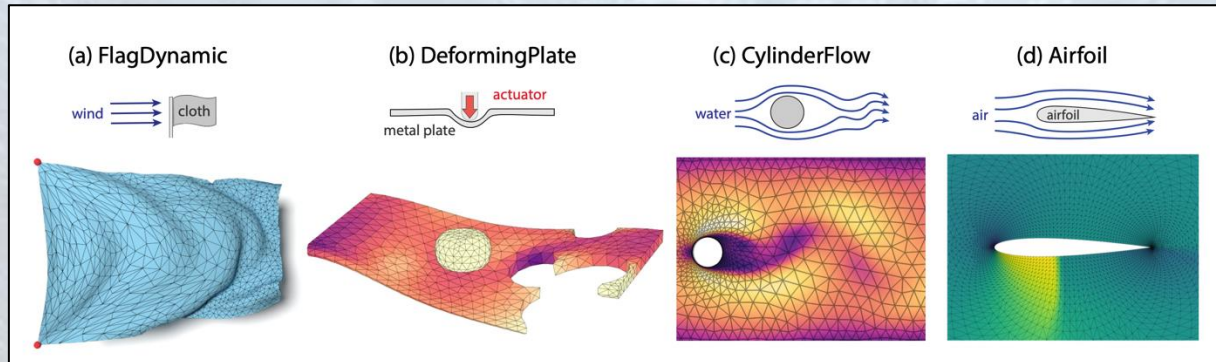
(a) Interpolation + Convolutional network



- Catalani et al., « A comparative study of learning techniques for the compressible aerodynamics over a RAE2822 airfoil », **Computers & Fluids**, 2023

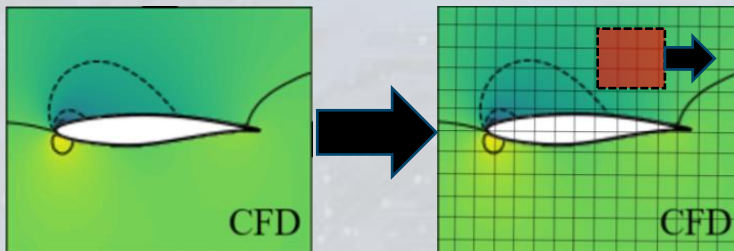
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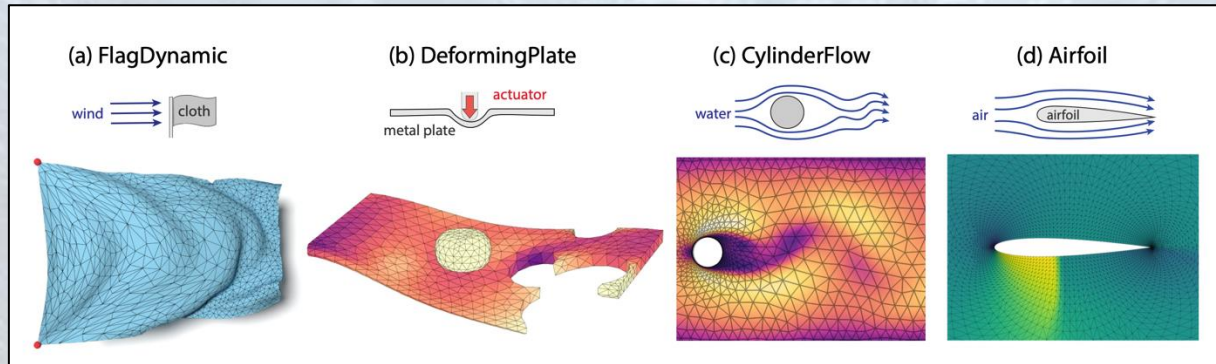


- ✓ Small (weight sharing)
- ✓ Easy to train
- ✓ Local in space (e.g Unet)
- ✗ Interpolation loss
- ✗ Resolution non-invariance

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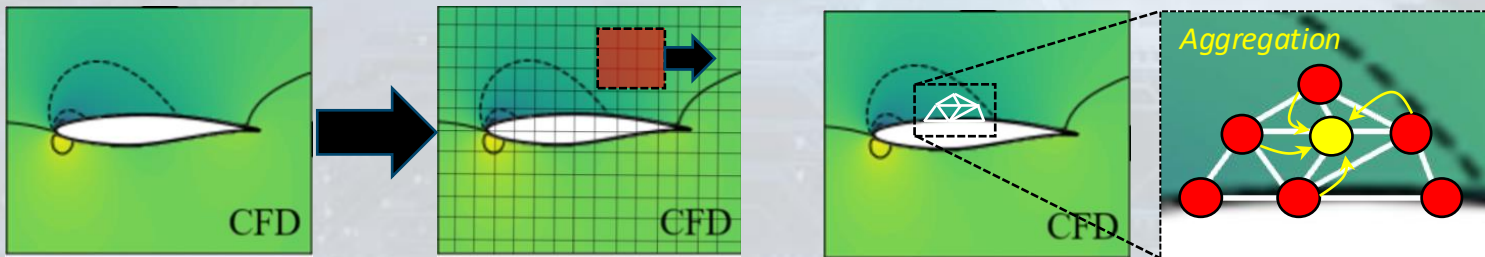


2017 - 2021

2021 – 20xx

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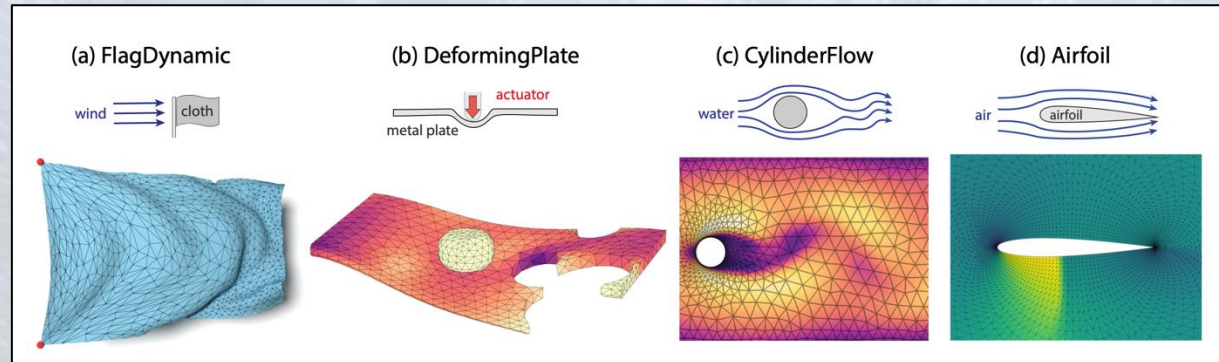
(b) Graph Networks



- Pfaf et al., « Learning mesh-based simulation with graph networks », ICLR, 2021

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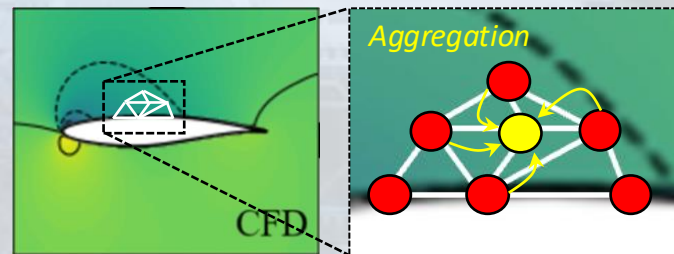


2017 - 2021

2021 – 20xx

- ✓ Adapted to meshes and CFD
- ✗ Resolution non-invariance
- ✗ Local in space
- ✗ Memory expensive

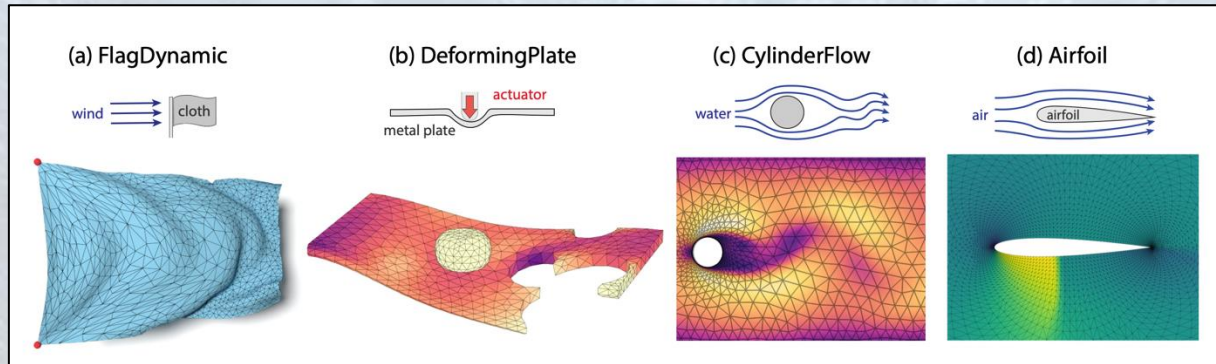
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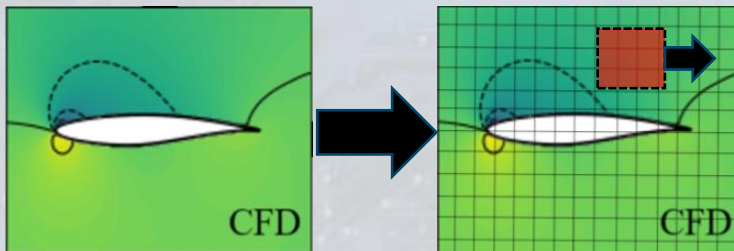


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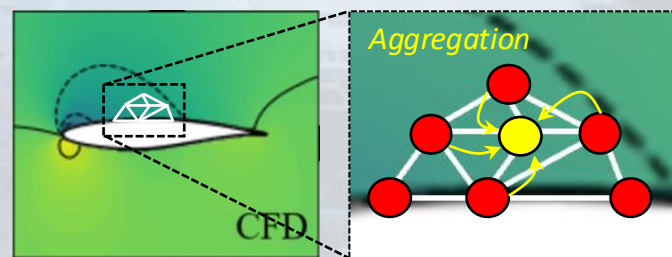
2021 - 20xx

2023 - 20xx

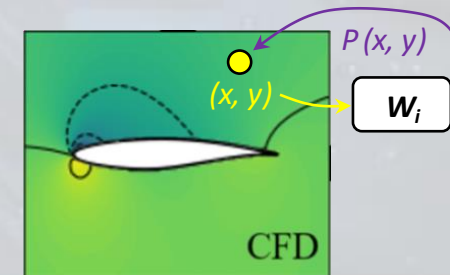
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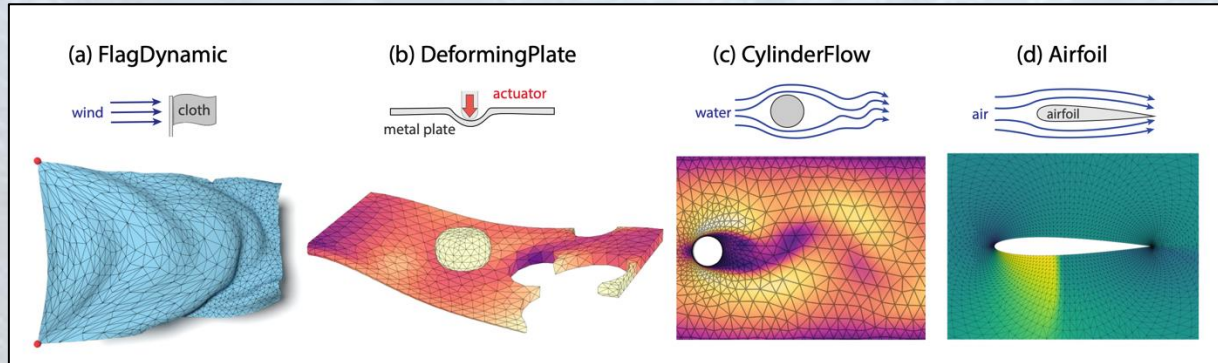


(c) MLP



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**Fourier features
(Tancik et al.)**

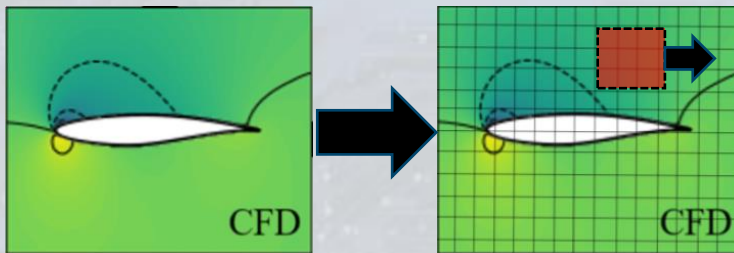


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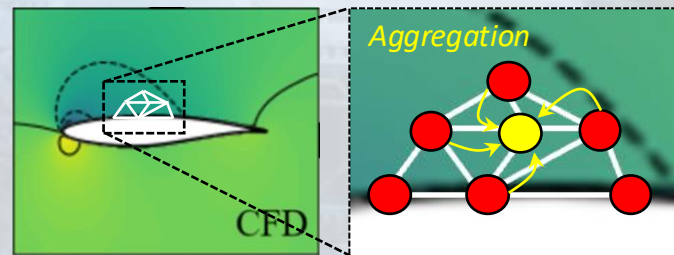
2021 - 20xx

2023 - 20xx

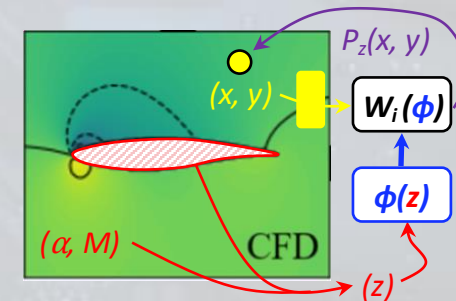
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(c) Implicit Neural Representation (INR)

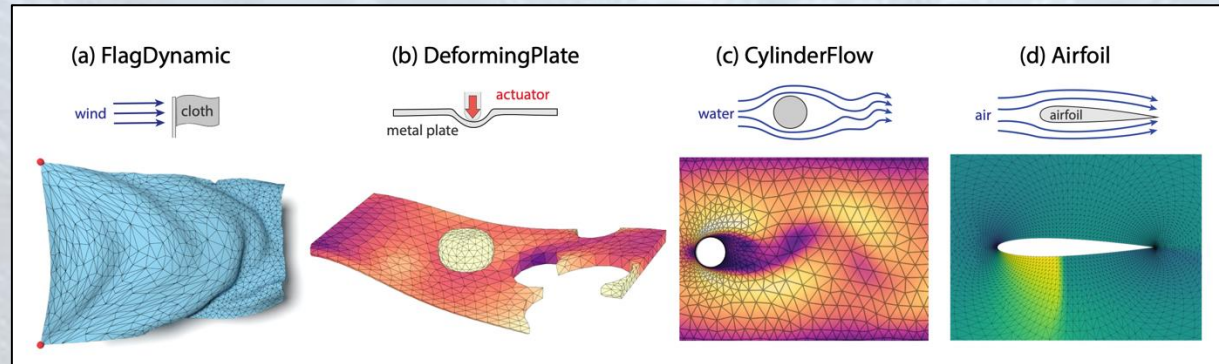


Modulation

- Tancik et al., « Fourier Features Let networks learn high frequency functions in low dimensional space », NeurIPS, 2020
- Catalani et al., « Neural fields for rapid aircraft aerodynamics simulations », **Scientific Report**, 2024

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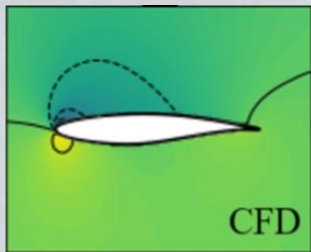


2017 - 2021

2021 - 20xx

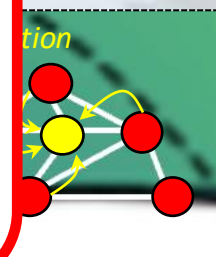
2023 - 20xx

(a) Interp
Convolution

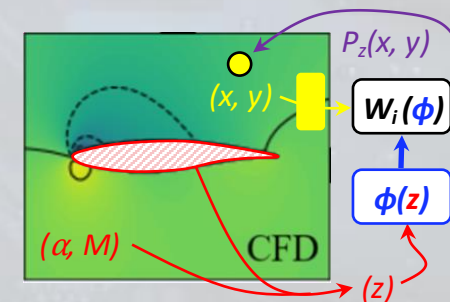


- ✓ Versatile
- ✓ Resolution invariance (continuous)
- ✓ Non-Local in space
- ✓ Memory efficient
- ✓ Easy and flexible to train
- ✗ Not yet fully mature

orks



(c) Implicit Neural Representation (INR)



Modulation

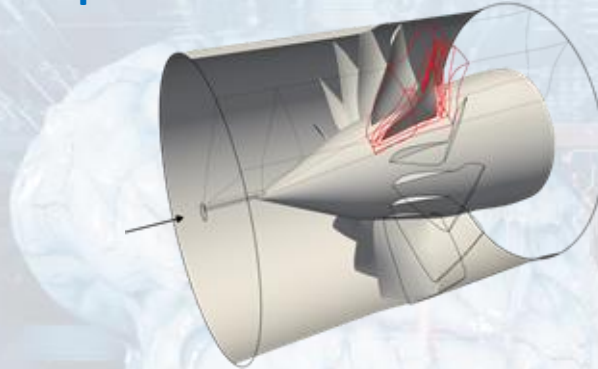
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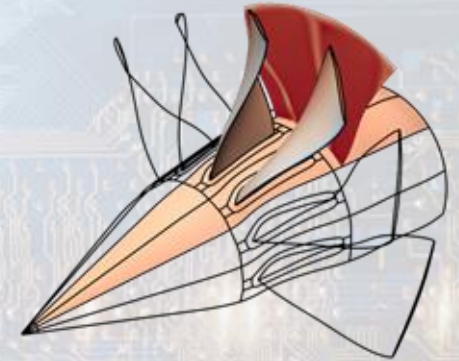
- Fan blade – 3D varying geometries & Operating point (flow separation, shocks)
290 samples over varying shapes



DGEN-380 (Akira)



- *Single geometry [FaNN380]*
- *Various geometries [FaNN]*



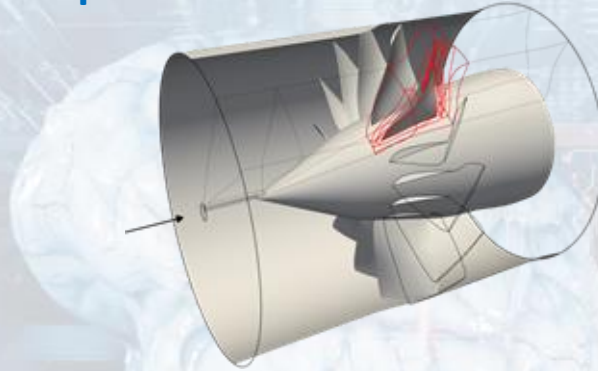
3D CFD dataset
[FaNN380 : 60 ; FaNN : 290]
Mesh : 10^7 nodes

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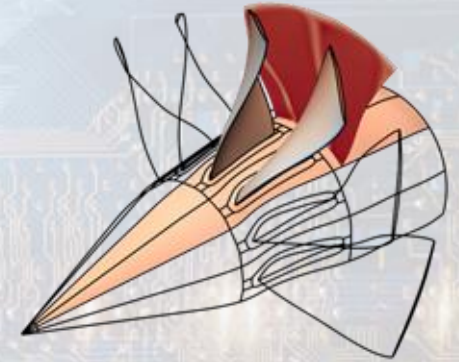
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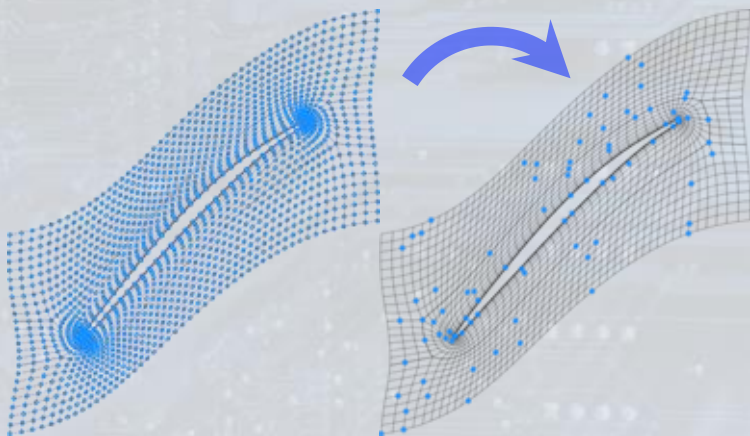
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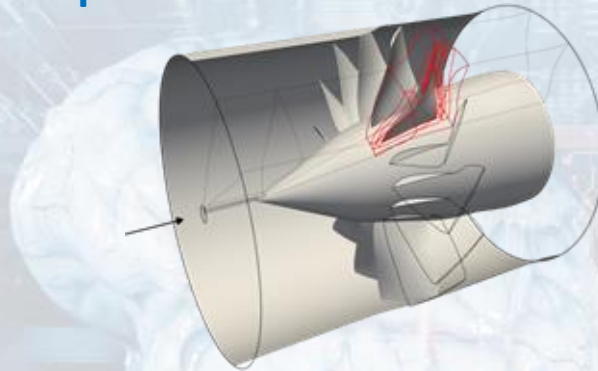
Mesh sampling for fast training

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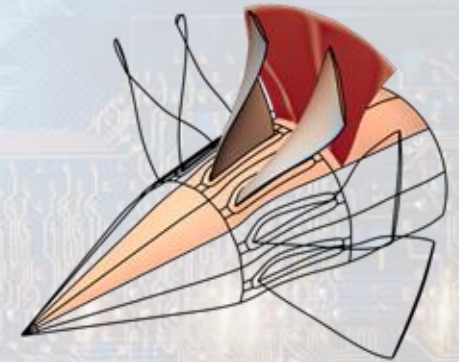
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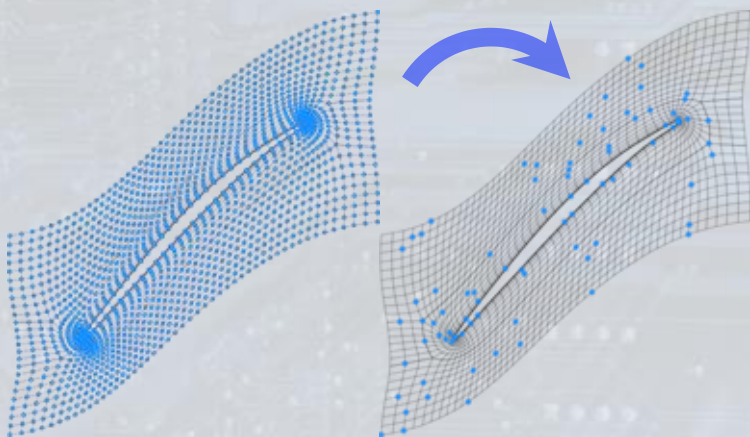
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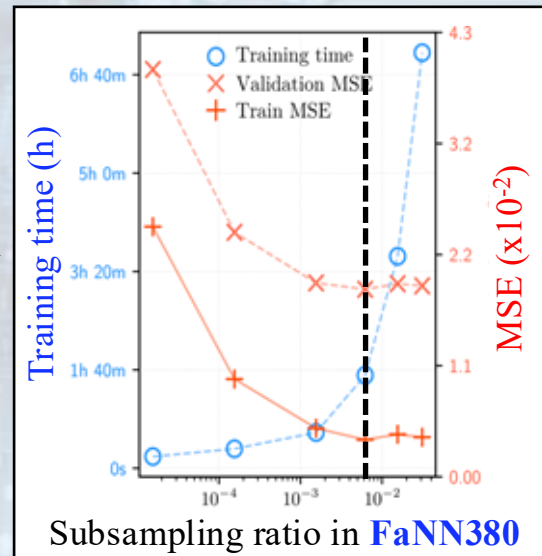
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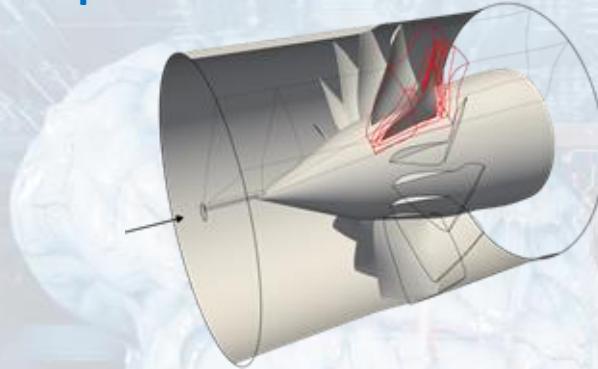


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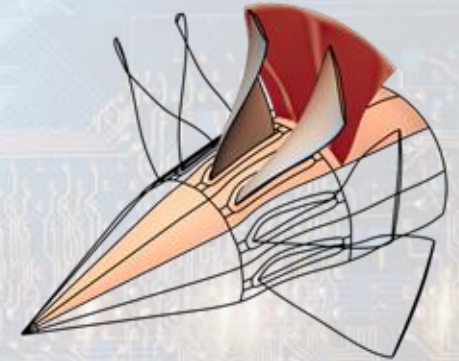
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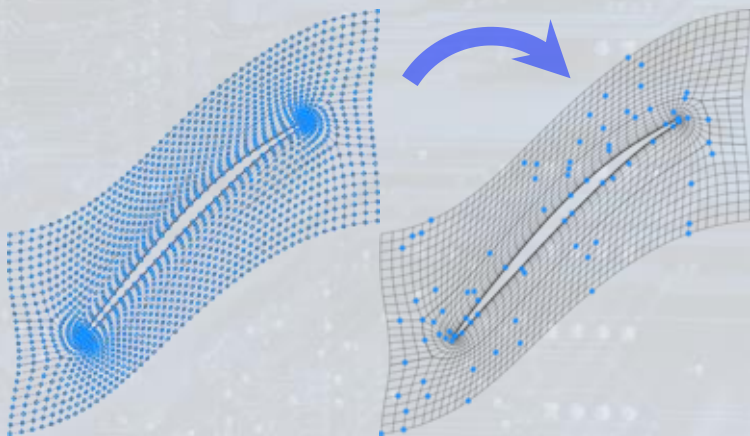
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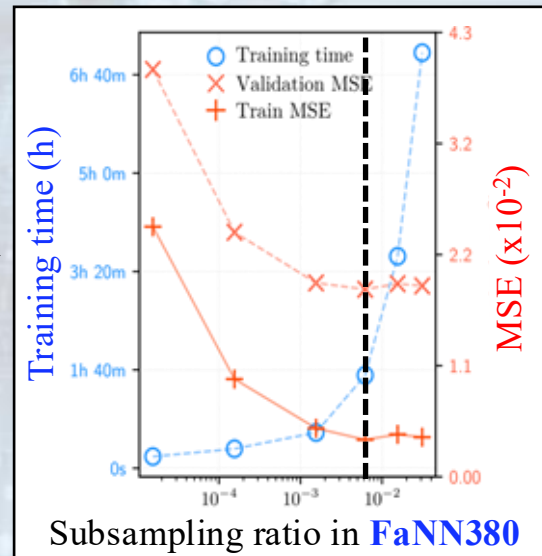
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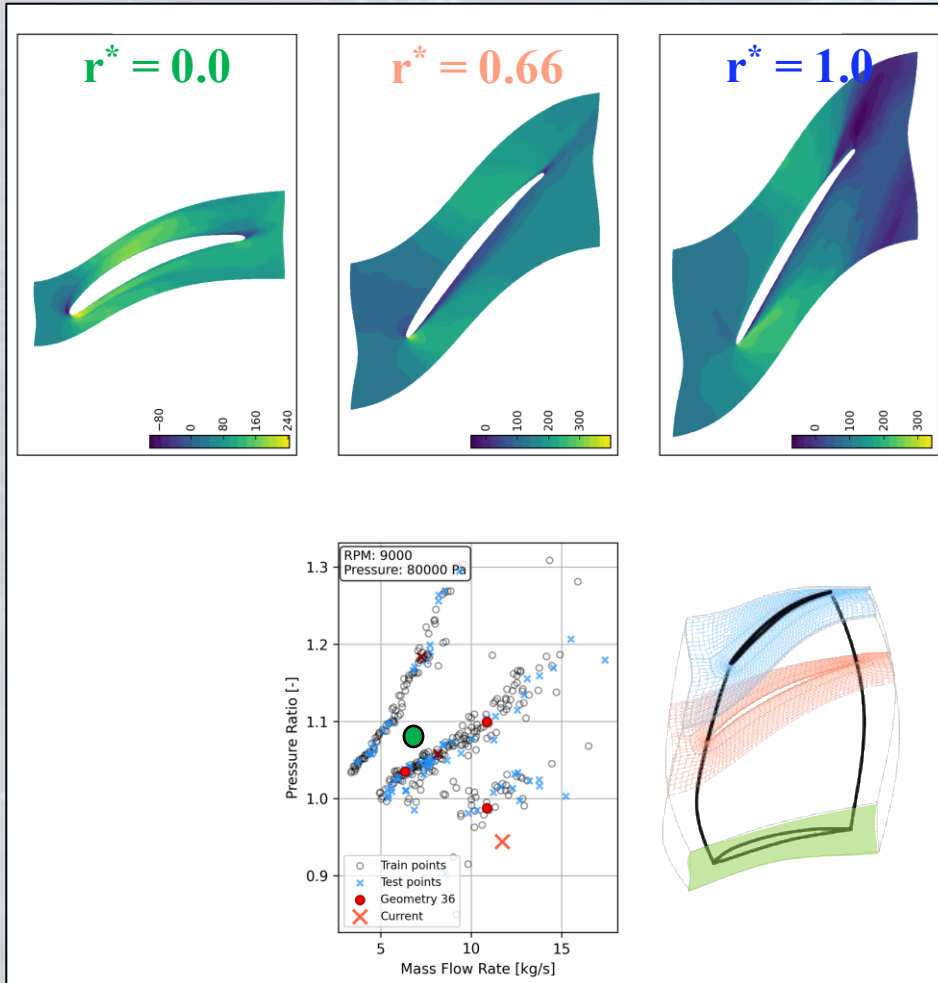
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Case	Time	Samples
FaNN380	1h30	60
FaNN	8h	290

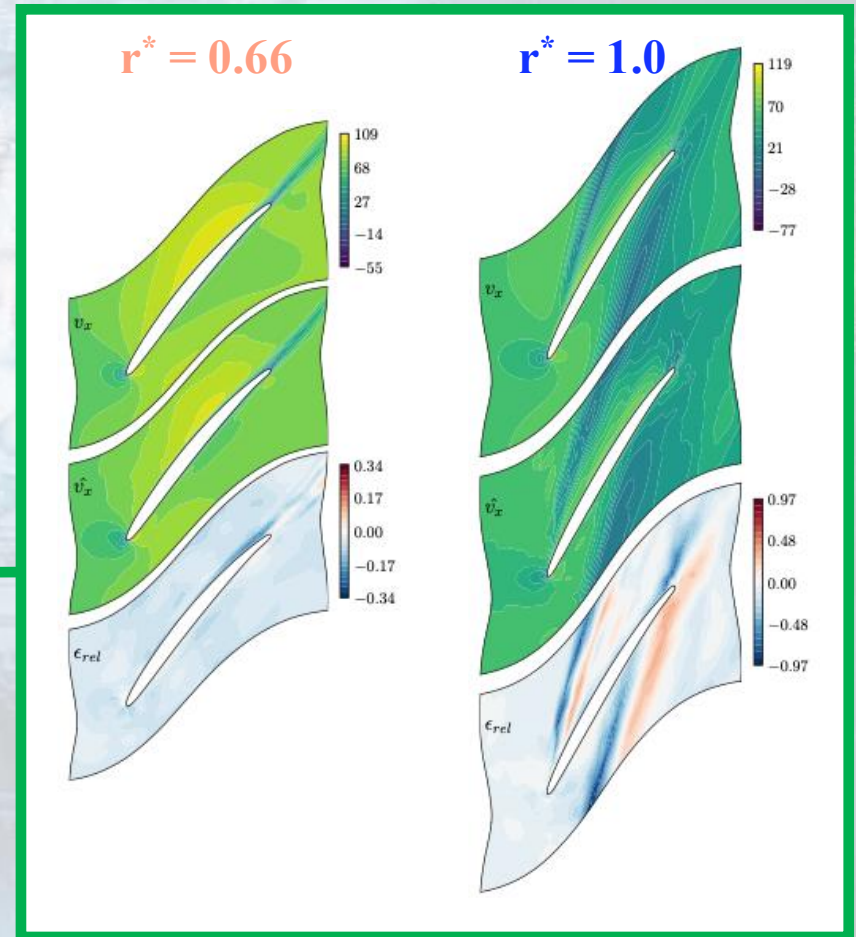
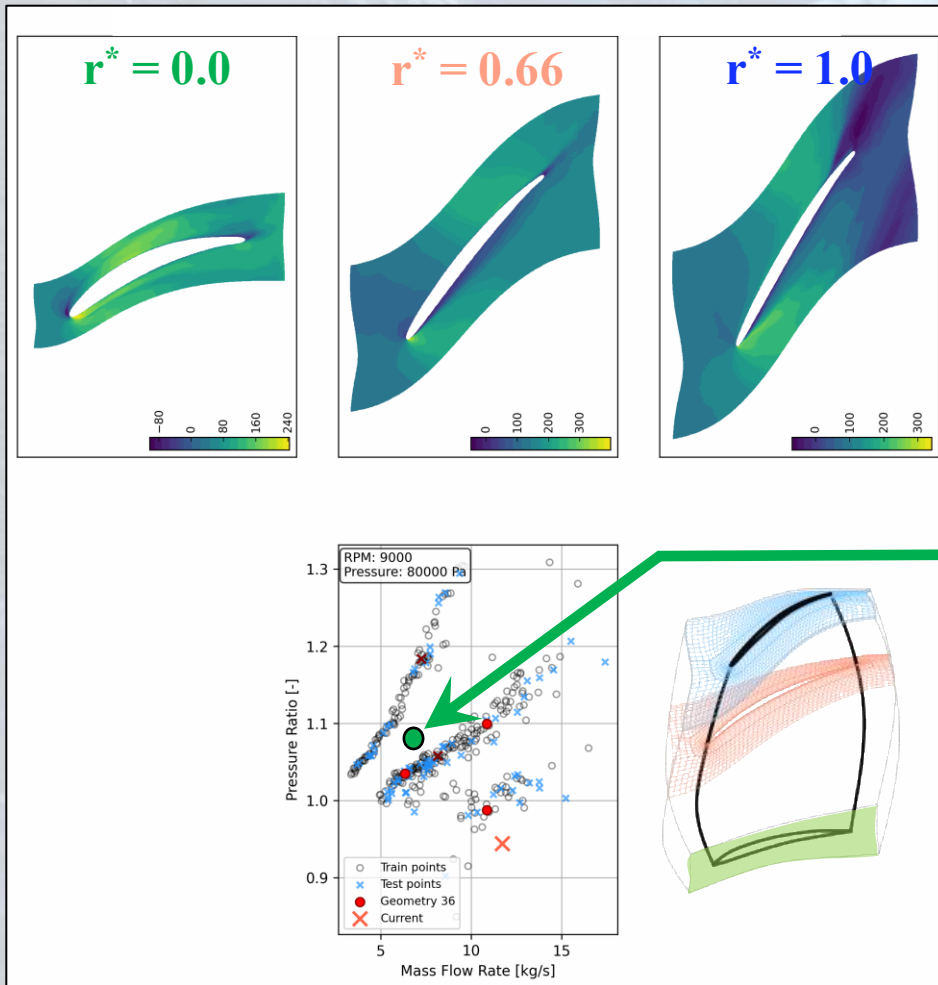
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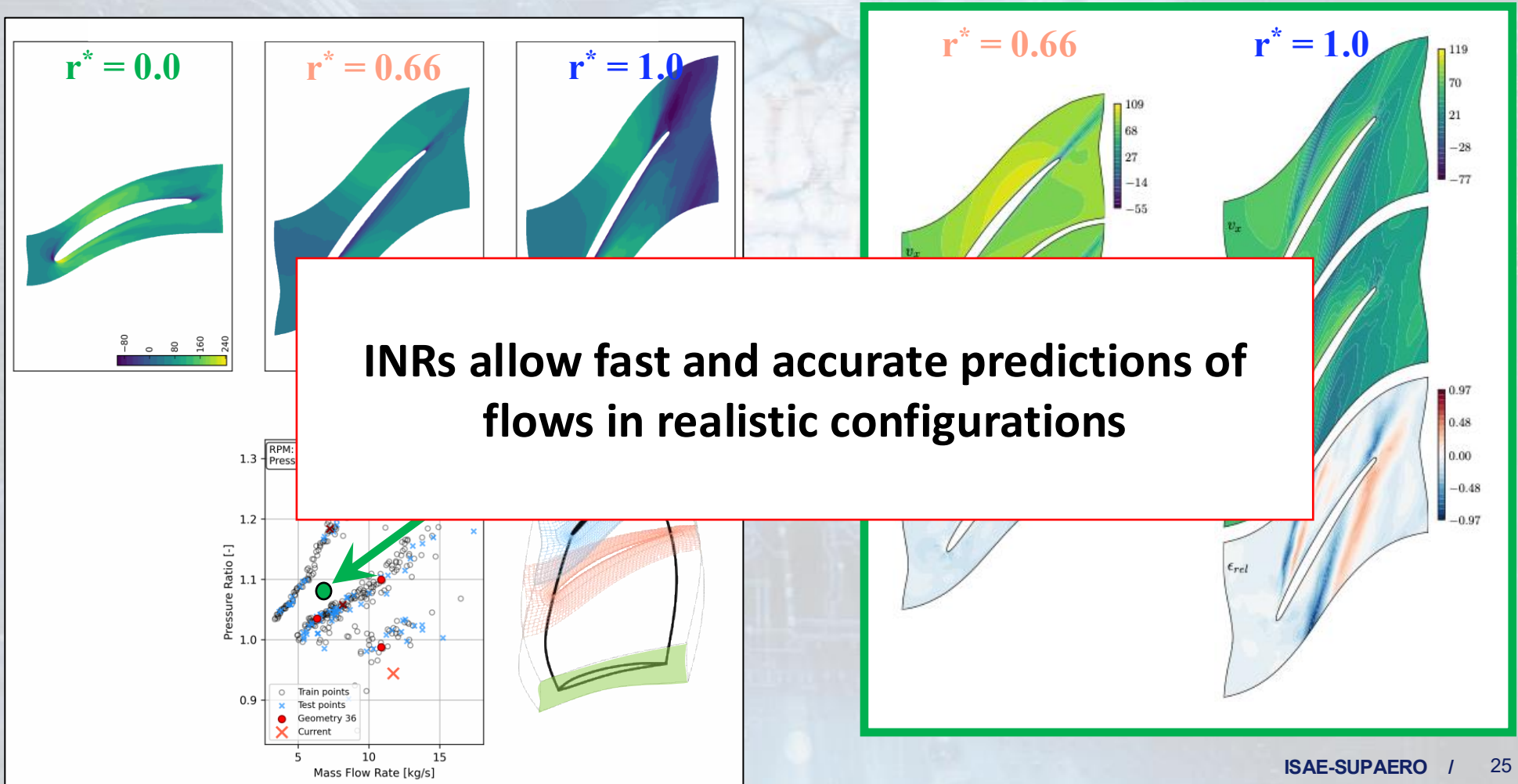
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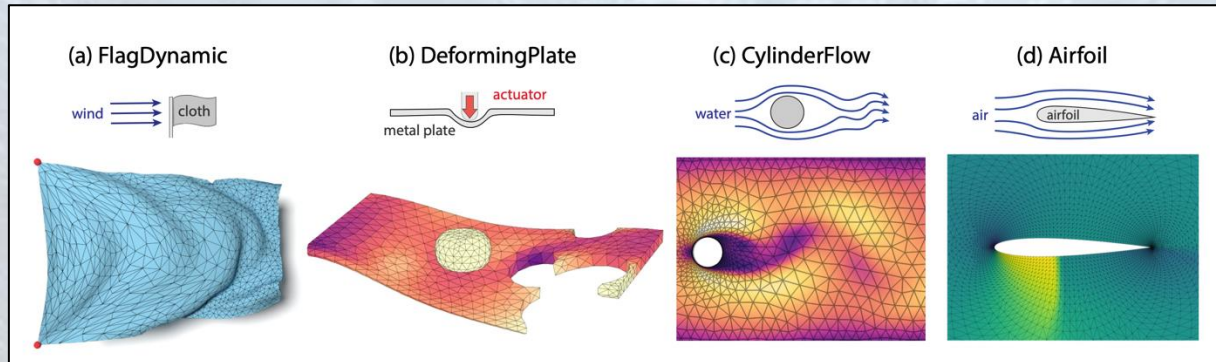
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*How to learn flow solutions on **meshes** & **manifolds**?*



2017 - 2021

2021 – 20xx

2023 – 20xx

2026?

What would be the next generation of AI models?

- **Attention-based models?** e.g. AROMA, ENMA, Equivariant Neural Fields
- **Foundational models?** e.g. FluidZero
- **Novel physics-based AI methodology?** e.g. GLOBE

- A. Kassaï Koupaï et al., « ENMA: tokenwise autoregression for generative Neural PDE operators », **NeurIPS**, 2025
- L. Serrano et al. « AROMA: preserving spatial structure for latent PDE modeling with local neural fields », **NeurIPS**, 2024
- G. Catalani et al., « Geometry aware inference of steady state PDEs using equivariant neural field representations », **NeurIPS workshop**, 2025
- H. Feng et al., « FluidZero: mastering diverse tasks in fluid systems through a single generative model », **not peer reviewed**, 2025
- P. Sharp, « GLOBE: accurate and generalizable PDE surrogates using domain-inspired architectures and equivariance », **arXiv**, 2025

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- *Introducing Active Learning and Uncertainties*

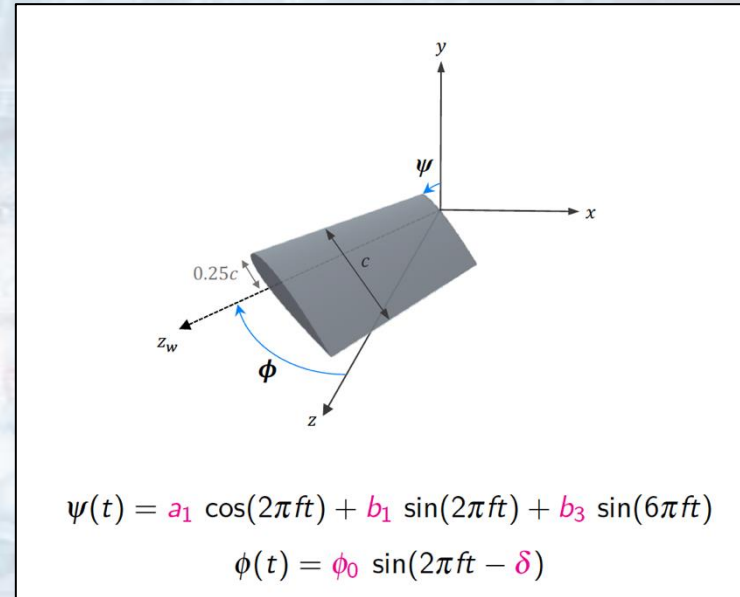
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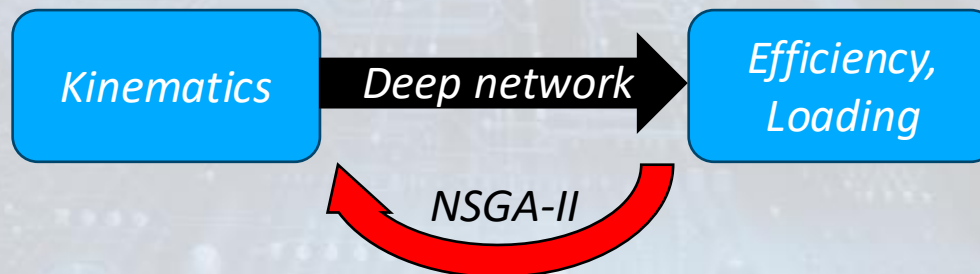
2. Can AI move from prediction to discovery?



Honeybee flapping motion

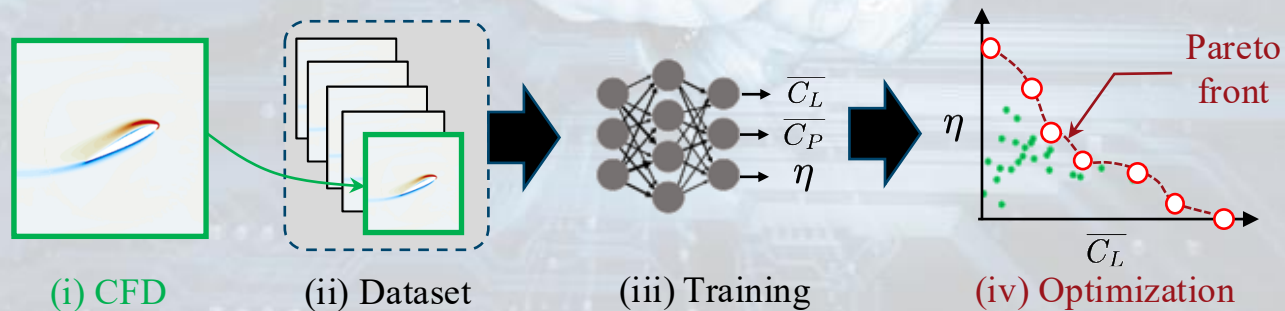
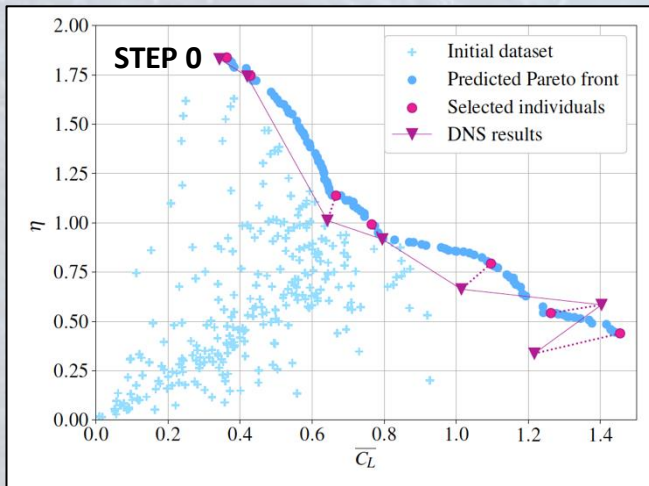


5D Parameterization of the kinematics for DNS



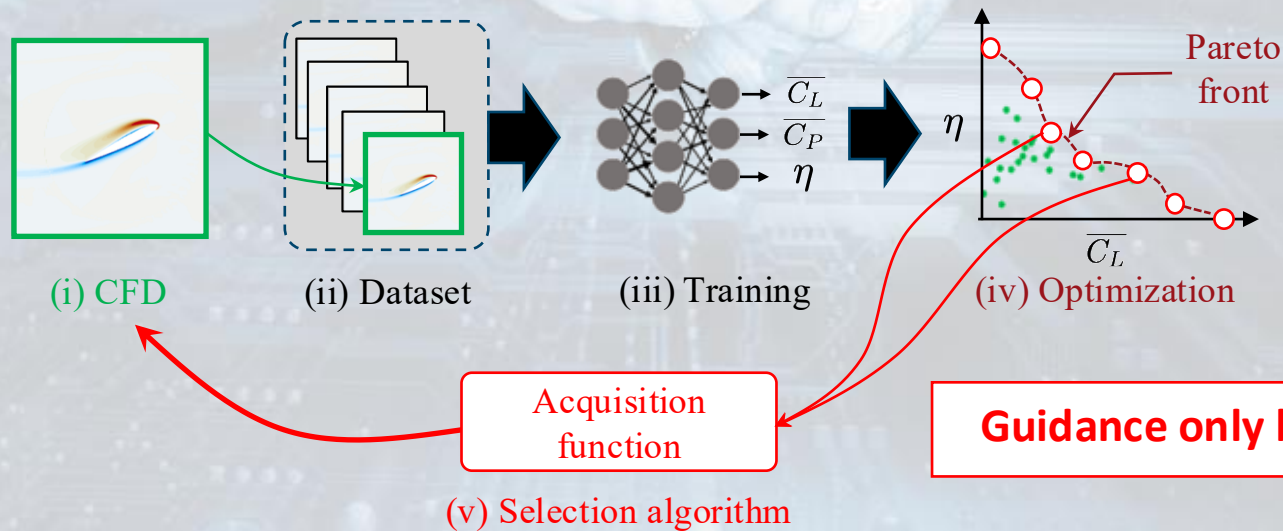
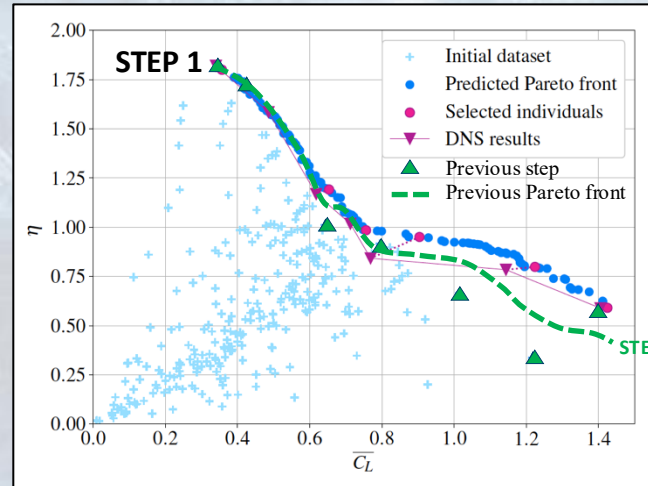
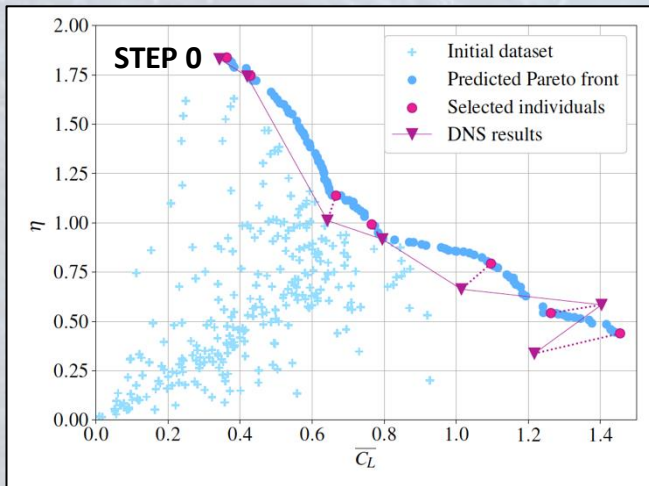
2. Can AI move from prediction to discovery?

Optimisation using DL yields a pareto front



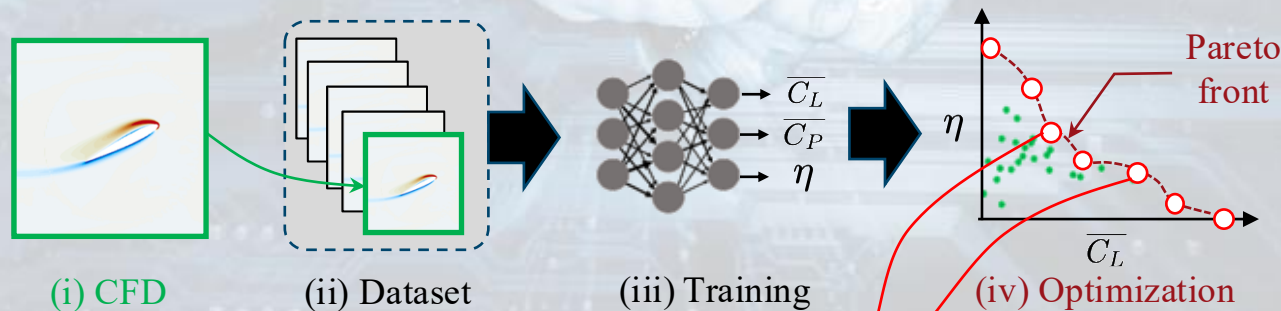
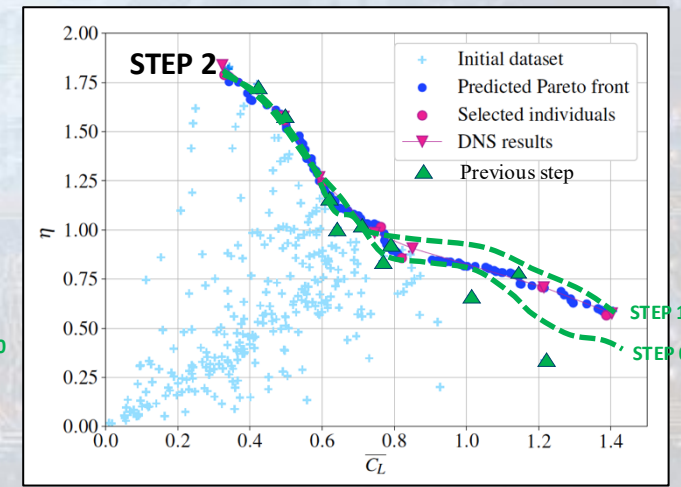
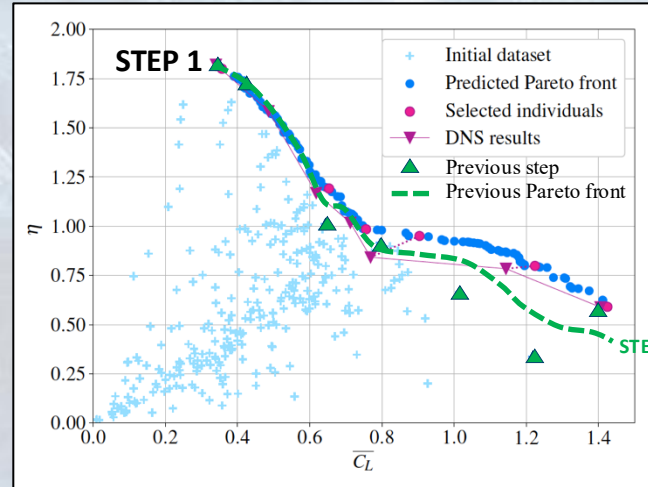
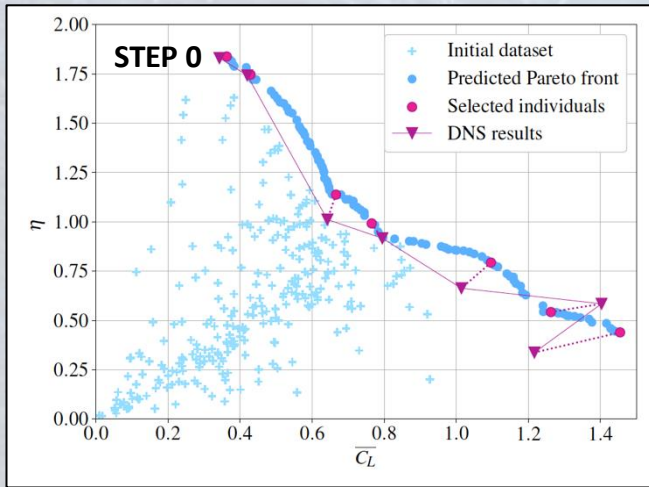
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DL is **unreliable**: iterative process (**active learning**)



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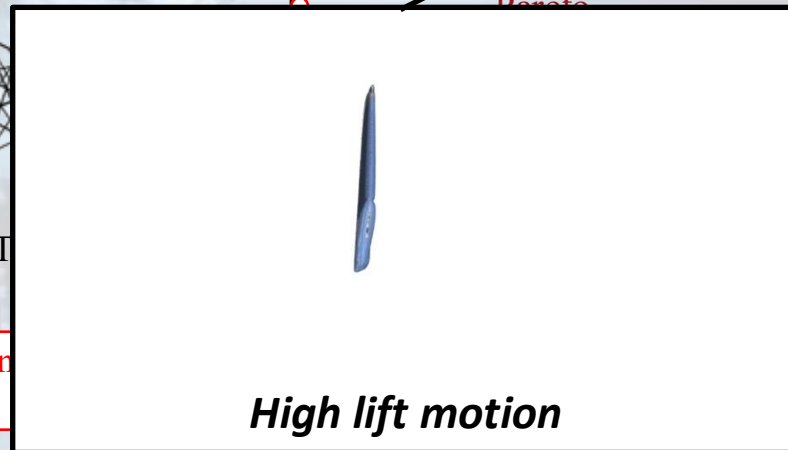
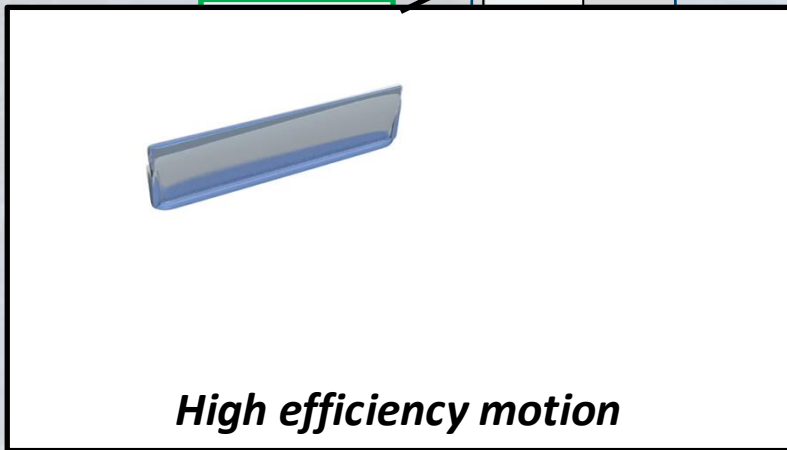
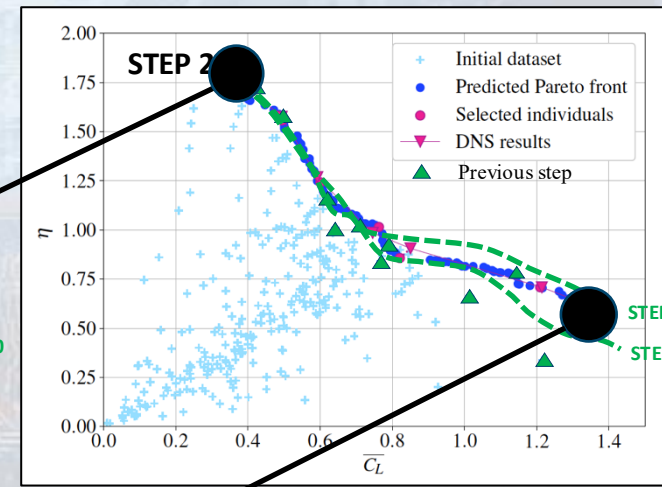
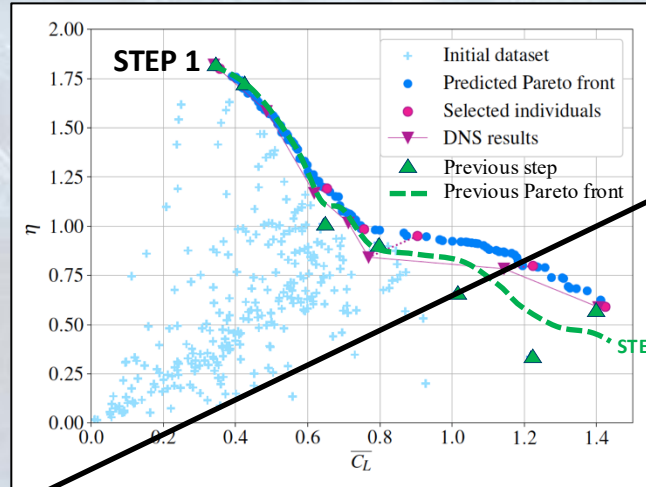
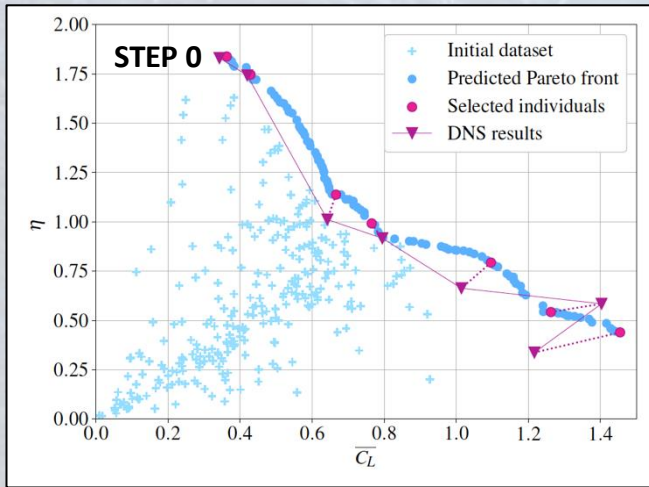
Acquisition function

Guidance only by errors

(v) Selection algorithm

2. Can AI move from prediction to discovery?

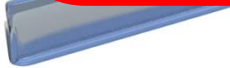
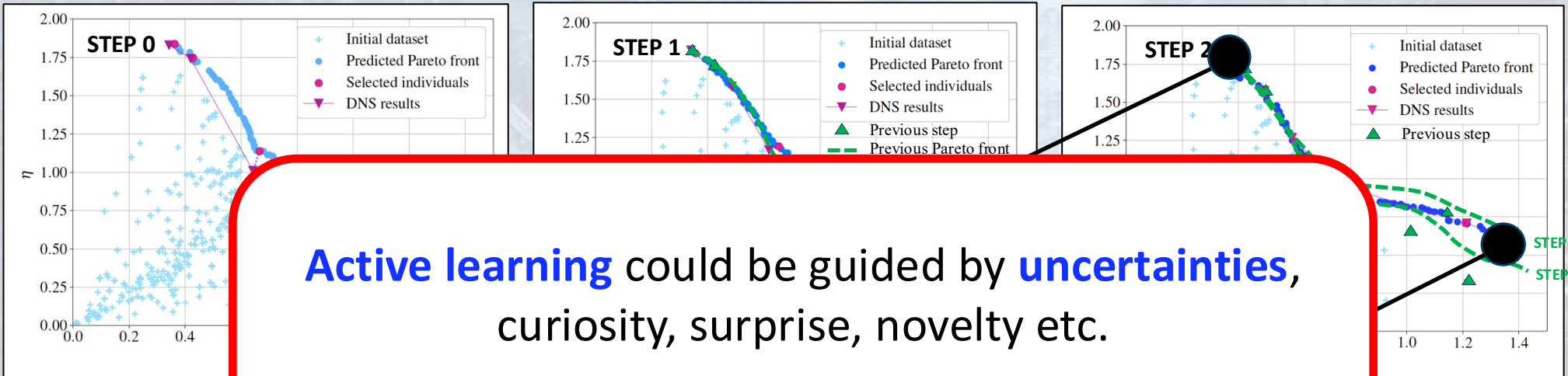
DL is **unreliable**: iterative process (**active learning**)



(v) Selection algorithm

2. Can AI move from prediction to discovery?

DL is **unreliable**: iterative process (**active learning**)



High efficiency motion

(iii) T

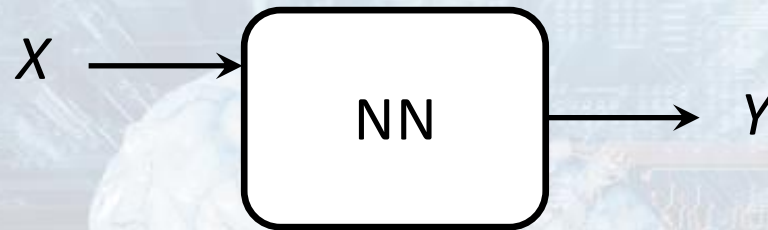
Position
action



High lift motion

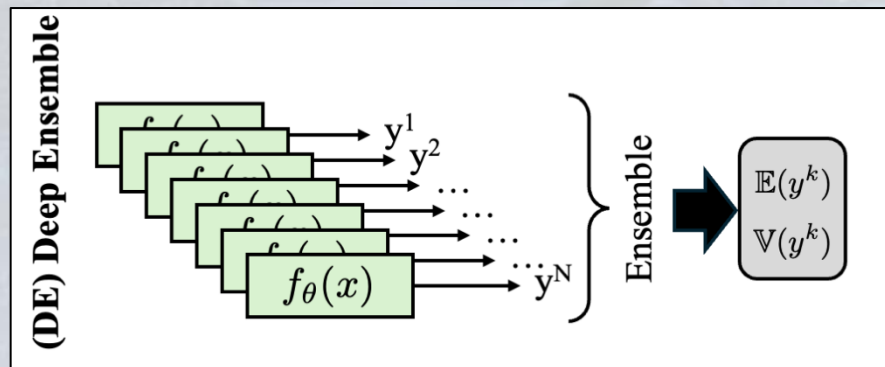
(v) Selection algorithm

2. Can AI move from prediction to discovery?



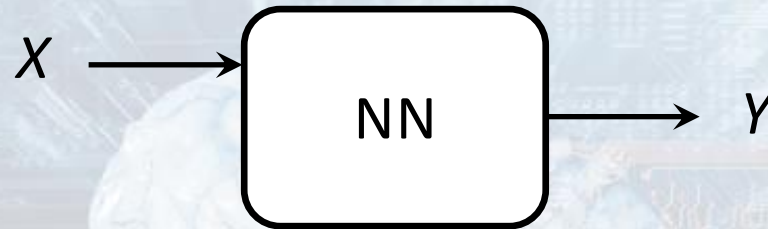
- Deep Ensemble (DE): *multiple uncorrelated* NN: uncertainties as *variance of the models* output

N trainings / N inferences



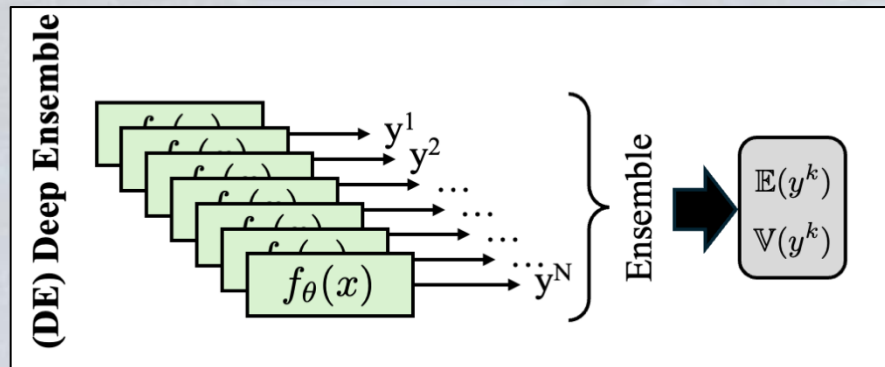
- Lakshminarayanan et al., « Simple and scalable predictive uncertainty estimation using DE », NIPS, 2017

2. Can AI move from prediction to discovery?

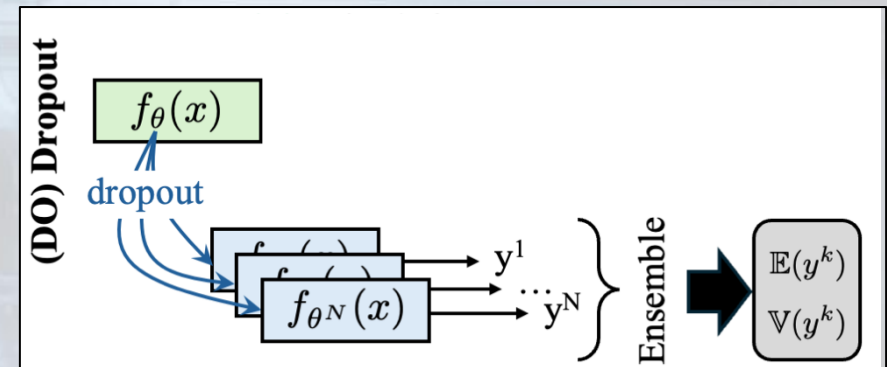


- Deep Ensemble (DE): **multiple uncorrelated** NN: uncertainties as **variance of the models** output
- MC Dropout (DO): **multiple correlated** NN: uncertainties as **variance of the models** output

N trainings / N inferences

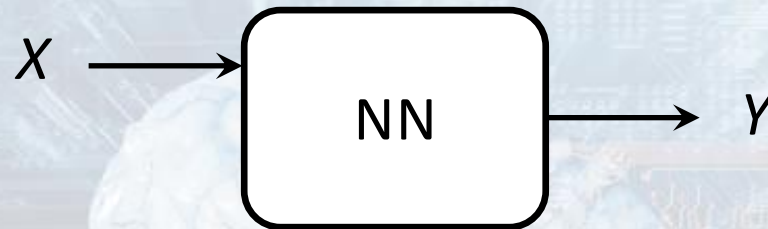


1 trainings / N inferences



- Lakshminarayanan et al., « Simple and scalable predictive uncertainty estimation using DE », NIPS, 2017
- Gal et al., « Dropout as a Bayesian approximation », ICML, 2016

2. Can AI move from prediction to discovery?

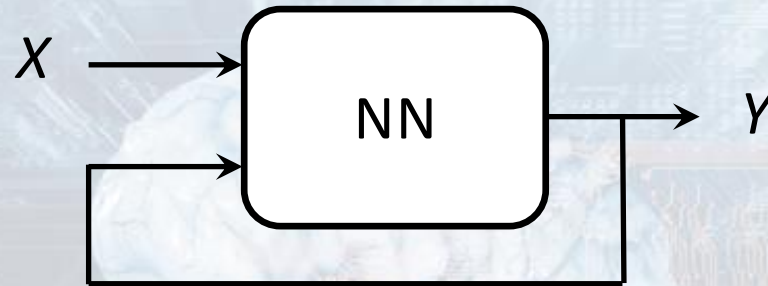


- Deep Ensemble (DE): *multiple uncorrelated* NN: uncertainties as *variance of the models* output
- MC Dropout (DO): *multiple correlated* NN: uncertainties as *variance of the models* output

	« Accuracy »	Cost
DE	Very good	Costly
MCD	So-so	Cheap

- Lakshminarayanan et al., « *Simple and scalable predictive uncertainty estimation using DE* », NIPS, 2017
- Gal et al., « *Dropout as a Bayesian approximation* », ICML, 2016

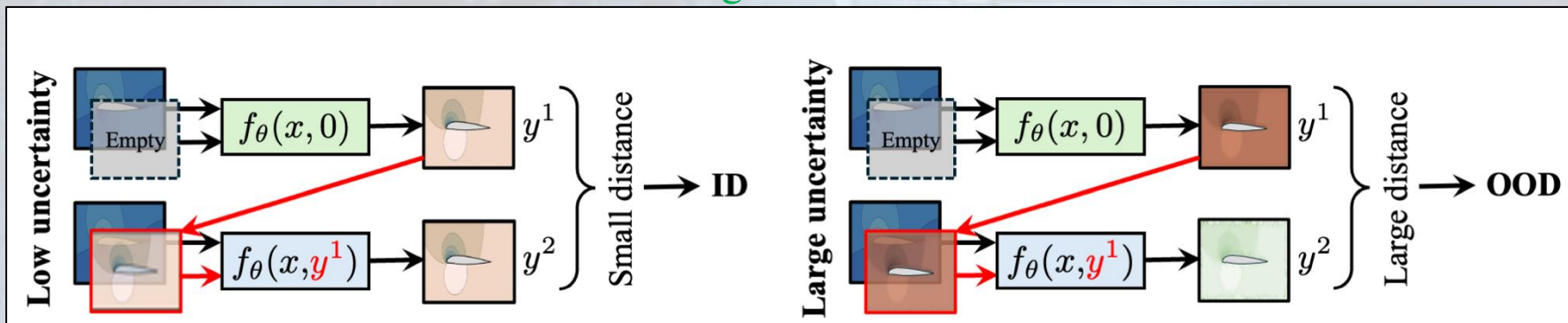
2. Can AI move from prediction to discovery?



- ZigZag [Durasov et al.]: **single** model, but **run twice!**

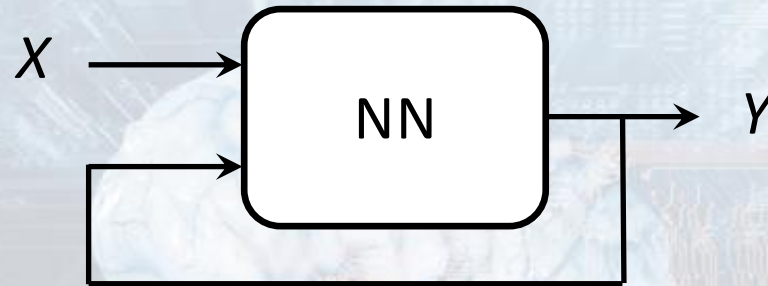
□ Start from $\{X, Y=0\}$ – predict $Y^1 = NN(X, 0)$ – predict $Y^2 = NN(x, NN(x, 0))$

1 trainings / 2 inferences



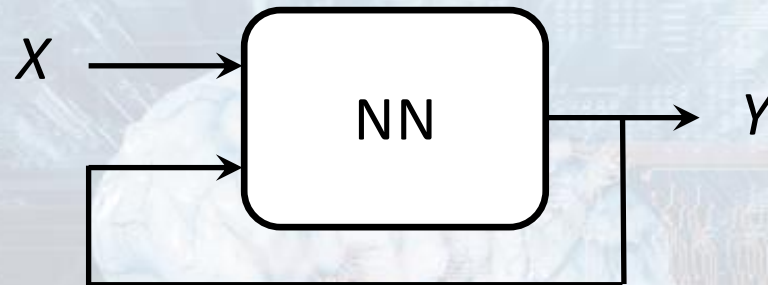
- Durasov et al., « ZigZag: universal sampling-free uncertainty estimation through 2-step inference », ICML, 2024

2. Can AI move from prediction to discovery?



- ZigZag [Durasov et al.]: **single** model, but **run twice!**
 - ❑ Start from $\{X, Y=0\}$ – predict $Y^1 = NN(X, 0)$ – predict $Y^2 = NN(x, NN(x, 0))$
 - ❑ $|Y^1 - Y^2|$ is a measure of the **total uncertainty** [Foglia et al.]

2. Can AI move from prediction to discovery?



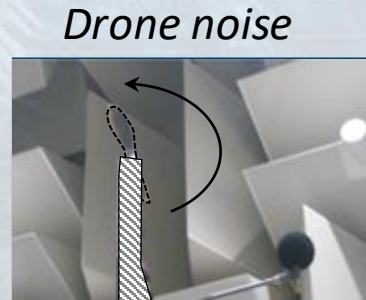
- ZigZag [Durasov et al.]: **single** model, but **run twice!**
 - ❑ Start from $\{X, Y=0\}$ – predict $Y^1 = NN(X, 0)$ – predict $Y^2 = NN(x, NN(x, 0))$
 - ❑ $|Y^1 - Y^2|$ is a measure of the **total uncertainty** [Foglia et al.]
- [Foglia et al.]: If you have **uncorrelated training pairs** $\{X, Y_1, Y_2\}$, then ZigZag can separate **aleatoric** vs. **Epistemic** uncertainties

$$Epistemic = Cov(\hat{Y}_1, \hat{Y}_2)$$

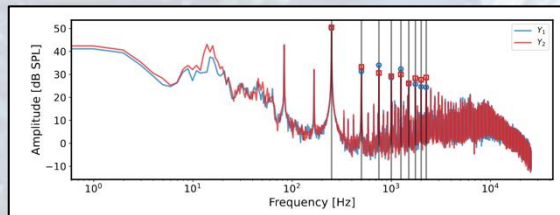
2. Can AI move from prediction to discovery?

- **Experimental tests**

Setup



Outputs



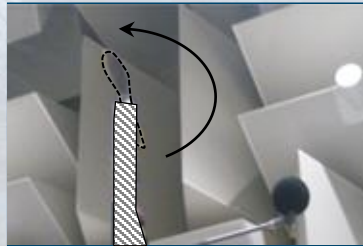
Noise spectrum

2. Can AI move from prediction to discovery?

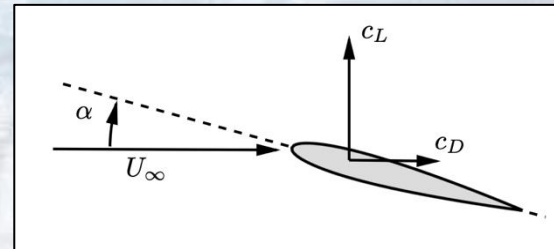
- Experimental tests

Setup

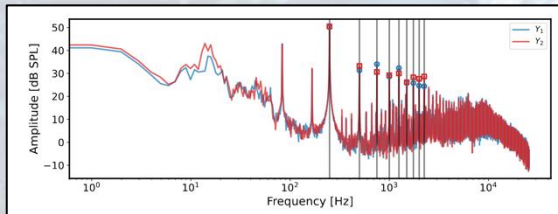
Drone noise



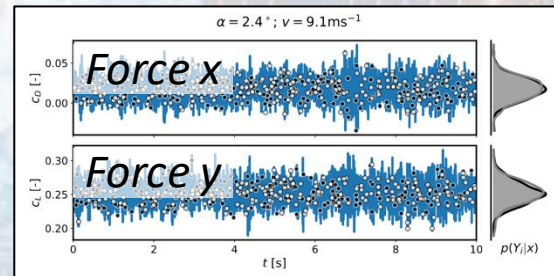
Airfoil aerodynamics



Outputs



Noise spectrum



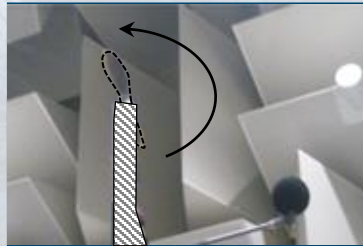
Aerodynamic forces

2. Can AI move from prediction to discovery?

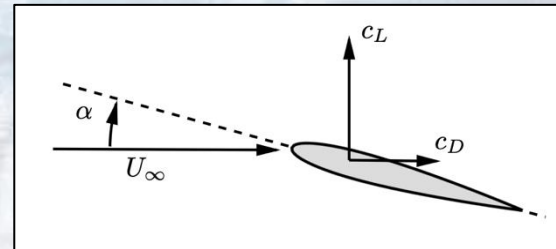
- Experimental tests

Setup

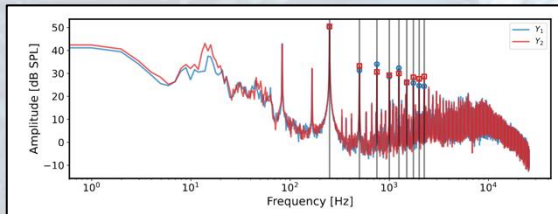
Drone noise



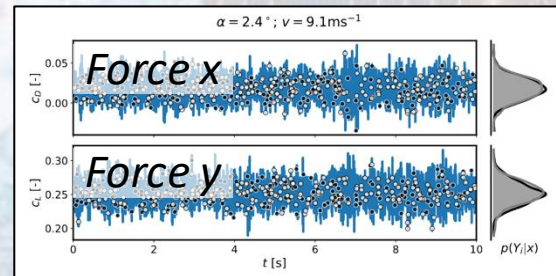
Airfoil aerodynamics



Outputs



Noise spectrum



Results

Model	AUROC		Cost of training
	Drone noise	Airfoil aerodynamics	
Deep Ensembles	0.99±0.01	0.98±0.01	×5
MC Dropout	0.84±0.01	0.49±0.01	×1
Ours	0.88±0.03	0.87±0.02	×1.25

2. Can AI move from prediction to discovery?

- Experimental tests



Outputs

Next step is to **guide active learning using uncertainty** measures in INR-like architectures (on going work)

Results

Model	AUROC		Cost of training
	Drone noise	Airfoil aerodynamics	
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Presentation outline

1. *How can AI represent complex flows?*

- *From CNN to Implicit Neural Representation (INR)*

2. *Can AI move from flow prediction to flow discovery?*

- *Introducing Active Learning and Uncertainties*

3. *Research vision and perspectives*

- *Hailed & PhiSimAI*

3. Research vision and perspectives

AI in CFD is still new! Need to further improve methodologies tailored to its specific challenges



3. Research vision and perspectives

AI in CFD is still new! Need to further improve methodologies tailored to its specific challenges

HAILSED - Hybridizing AI with Large-scale Simulations for Engineering Design

(lead by A. Kopanicakova)

- Improve guarantees by **embedding AI into simulation** approaches
-

3. Research vision and perspectives

AI in CFD is still new! Need to further improve methodologies tailored to its specific challenges

HAISED - Hybridizing AI with Large-scale Simulations for Engineering Design

(lead by A. Kopanicakova)

- Improve guarantees by **embedding AI into simulation** approaches
-

Integrative program – PhySimAI

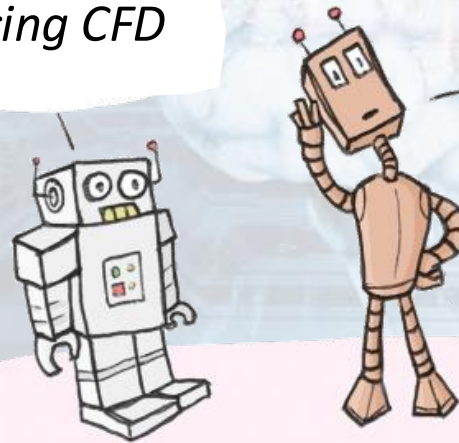
(lead by P. Novello)

- Create an **open-source toolbox** with state-of-the-art models **tailored to the specific challenges** of large engineering problems
- Develop **hybrid** and **uncertainty** approaches towards **trustworthy models**
- Benchmarks this on **realistic industrial** « demonstrators »

Conclusion

*Actually, we are still
far from replacing CFD*

*If I had feelings,
I would be very
disappointed*



@vismktg
pour @sparklane_fr

Thank you!