Machine Learning for physical simulation in industry. Application to airfoil design

TER Project, Msc AI/DS of UPSaclay. 2024/2025

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A collective TER proposal

General information

- **Number of students in this TER:** 6 students

- **Prerequisites:** Basics in deep learning and Python. Basics in physical simulation can be an asset but are not necessary.

- **Deliverables:** Those required by the Msc program (short report and presentation). Students are strongly encouraged to open-source their solutions on platforms like GitHub.

- **Team Structure:** A group of 6 students, with typically 2 focused on the machine learning component, 2 on the simulation component, and 2 on the use case component.

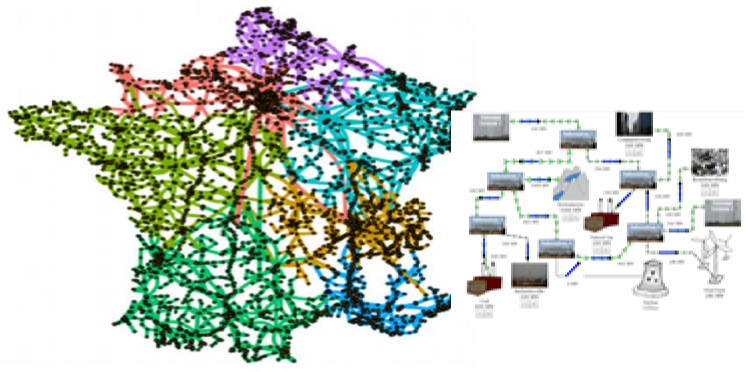
- **Meeting Schedule:** Regular meetings of 30 minutes to 1 hour will be scheduled with the students. Meetings will take place either at Université Paris-Saclay or remotely on Teams/Zoom.
- **Calendar:** As defined by the TER schedule in the MSc program.

Motivation: Some physical problems in Industry

Related to the design and supervision of complex (physical) systems

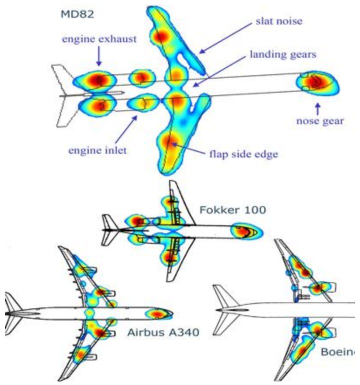
- Covering various fields in physics (mechanics, fluid dynamics, aerodynamics, electromagnetism …)
- In a wide variety of Applications in industry, in particular in numerical **simulation**

Electricity (power grids)



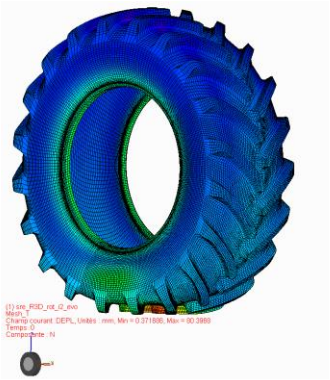
Picture from Marot, A., et al. (2018).

Aerodynamics



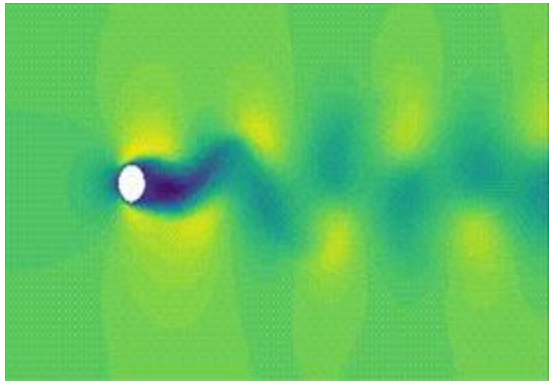
Merino-Martínez *et al. CEAS Aeronautical* Journal (2019).

Solid Mechanics pneumatics



Project HSA – SystemX

Fluid Flows/Dynamics



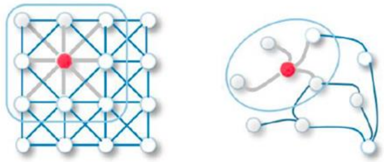
E. Menier (PhD, LSIN/SystemX, 2024)

Domain Challenges : Physical systems that are (eg. , in Computational Fluid Dynamics – CFD, Turbulance, Flows)

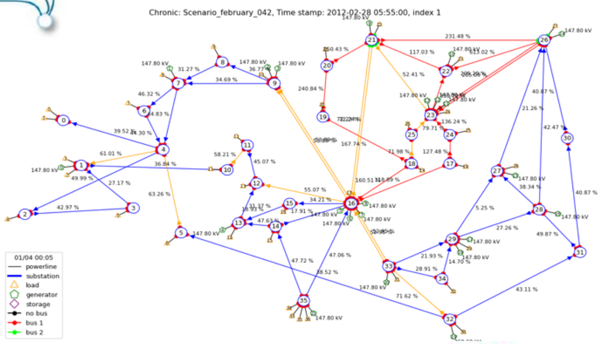
- Complex to model/solve analytically

- Compuationally expensive to solve numerically

Physics and Machine Learning



Power Grid
Substations and lines



- Physics knowledge to guide learning

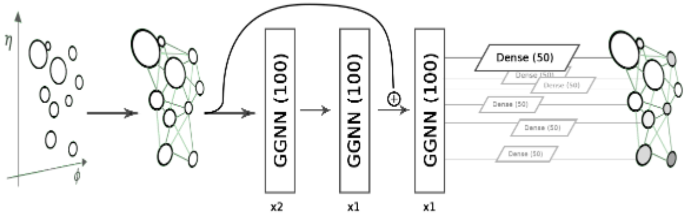
Integrating geometric priors in learned representations (Bronstein 2017)
Geometric deep learning, **GNN** and neural passing message (Arjona Martínez 2019)

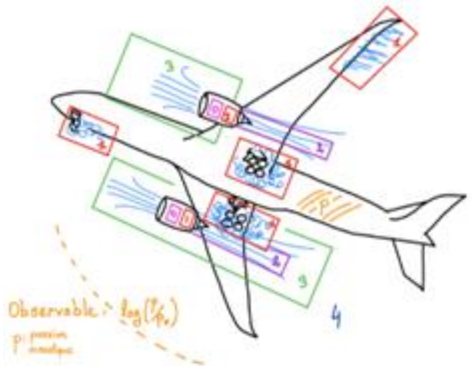
- **D**ifferential **e**quations to improve deep learning

Neural differential equations, diffusion models, …

- Deep learning to solve differential equations

Hypersolvers, hybrid solvers, neural operators,
PINNs - Physics-Informed NNetworks, … (Raissi 2019)





⇒ **Promising for engineering**, it allows :
- the integration of analytic knowledge from physical laws governing the engineering systems, to augment statistical knowledge learned from data (eg. by deep learning)
- reducing the high cost of physical simulation in industry

Scientific Challenges

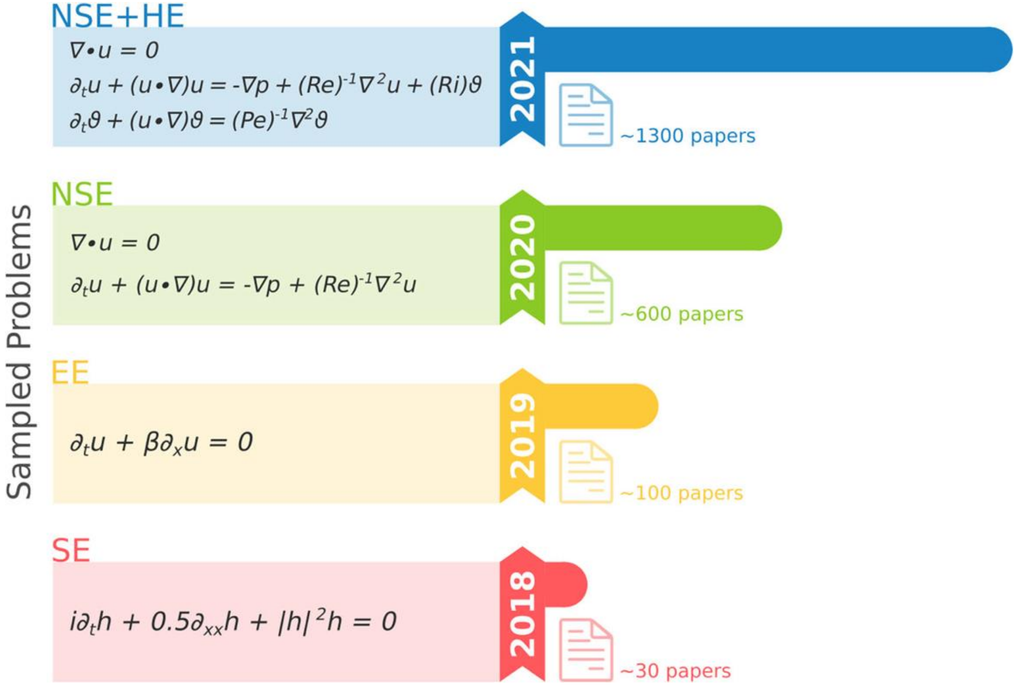
- Problems highly-nonlinear, high-dimensional, with complex structures (eg. organized in graphs…)
- Need for adapted NN architectures: GNNs, Deep AEs ..

Physics-Informed Machine Learning: combining ML and Physics

- ➔ Enables prior scientific knowledge based on physics to be taken into account in data-driven machine learning methods

  e.g including PINNs - Physics-Informed Neural Nets (Raissi's paper in 2019)

- ➔ Has been *successfully and increasingly* applied to solve a wide variety of linear and nonlinear problems in physics, covering various fields like mechanics, fluid dynamics, thermodynamics, electromagnetism, including :

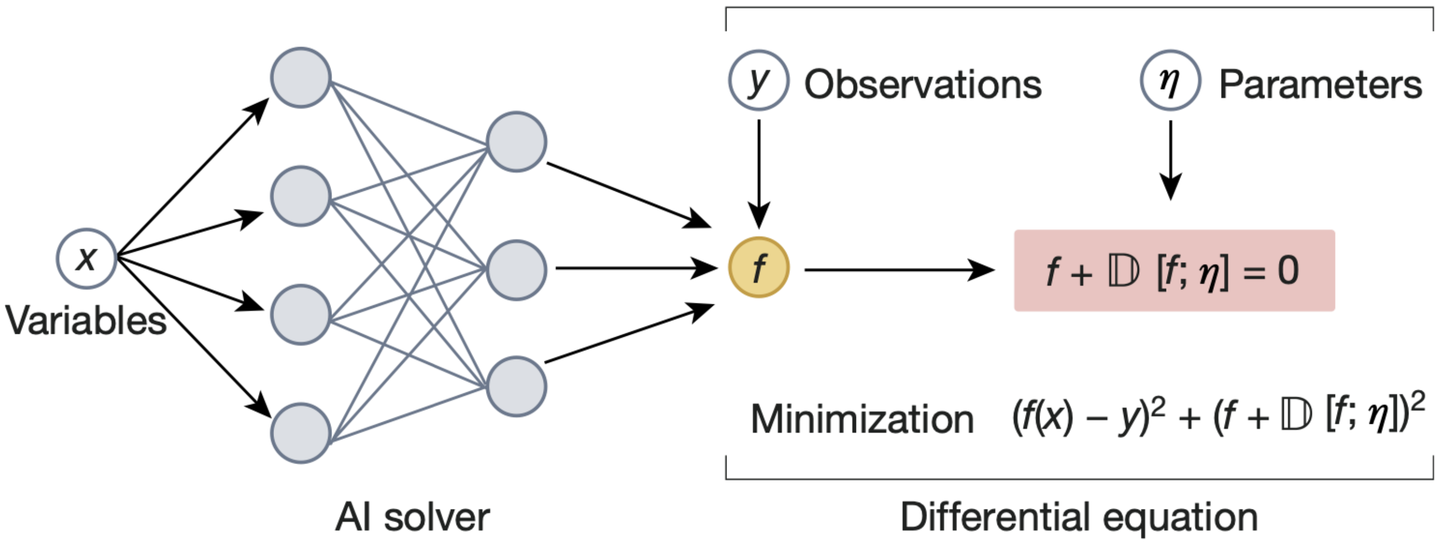


- Solving Navier–Stokes equations coupled with the corresponding temperature equation for analyzing heat flow convection (NSE+HE). Cai et al, 2021
- Solving incompressible Navier–Stokes equations (NSE). Jin et al., 2020.
- Solving Euler equations (EE) that model high-speed aerodynamic flows. Mao et al, 2019
- Solving the nonlinear Shrödinger Equation (SE).

Raissi, M et al. (2019) Physics-Informed Neural Networks: A Deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear Partial Differential Equations. Journal of Computational Physics. 378. Online

Cuomo, S., et al., (2022). Scientific machine learning through physics–informed neural networks: Where we are and what's next. *Journal of Scientific Computing*, *92*(3), 88. Read Online

Hybrid ML modeling for solving Partial Differential Equations



A neural framework for solving PDEs, where

- the AI solver is a PINN trained to estimate target function ***f***.
- The derivative of ***x*** is calculated by automatically differentiating the NN's outputs.
- When the differential equation parametrized by **(η)** is unknown, it can be estimated by solving a loss that optimizes both the functional form of the equation and its fit to observ ***y***.

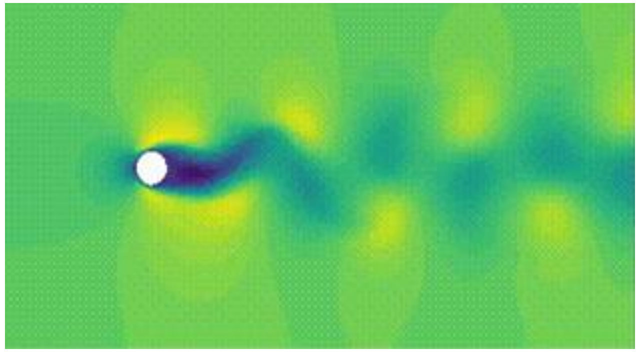
Wang & al. (2023). Scientific discovery in the age of artificial intelligence. Nature, 620. Read Online

- Eg. Learning Computational Fluid Dynamics

- Navier-Stokes Equations: fundamental partial differentials equations (**PDE**) that describe the flow of incompressible fluids.

C.L. M. H. Navier, Memoire sur les Lois du Mouvements des Fluides, Mem. de l'Acad. d. Sci.,6, 398 (1822)
C.G. Stokes, On the Theories of the Internal Friction of Fluids in Motion, Trans. Cambridge Phys. Soc., 8, (1845)

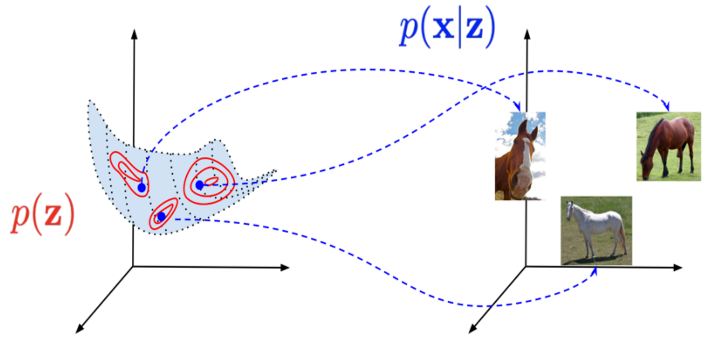
- Challenge: **High-Dimensional non-linear** Physical Equations



Eg. 1000 equations: Menier, PhD LISN/SystemX

Deep NNets for unsupervised representation Learning

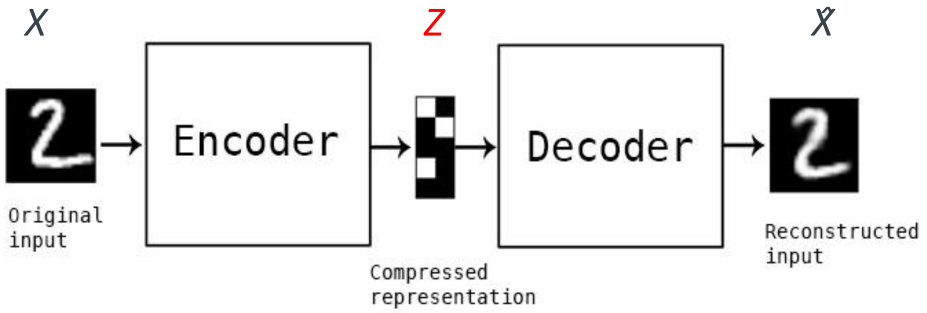
Latent Variable Models: A family of probabilistic models capable of inferring the intrinsic latent structure (of reduced dimension) of the data



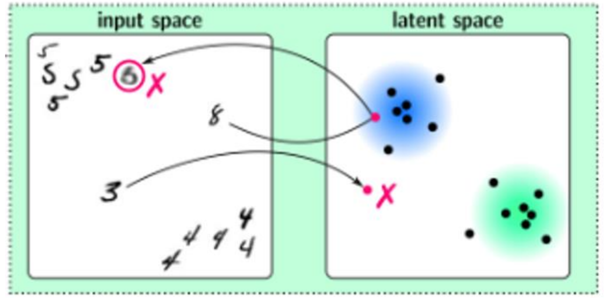
Z: Latent variables of reduced dimension

X: Observations Of high-dimnsion

- **Auto-Encoders - AE** (LeCun 1987): The **encoder** projects the input ***X*** (of high-dimension dimension) in a compressed latent representation ***Z*** (the **code**) to reconstruct it using the **decoder** with outpu $\hat{X}$
- ➔ Learning by minimizing the reconstruction error between $\hat{X}$ and **X**. The smaller the error, the better the compressed representation ***Z***.



- **Variational Auto-encoders - VAE** (Kingma & Welling 2014) improve the representational capabilities of AEs by regularizing the latent space with a Gaussian prior, coupled with a **variational learning**
- **=>** can learn complex distributions.

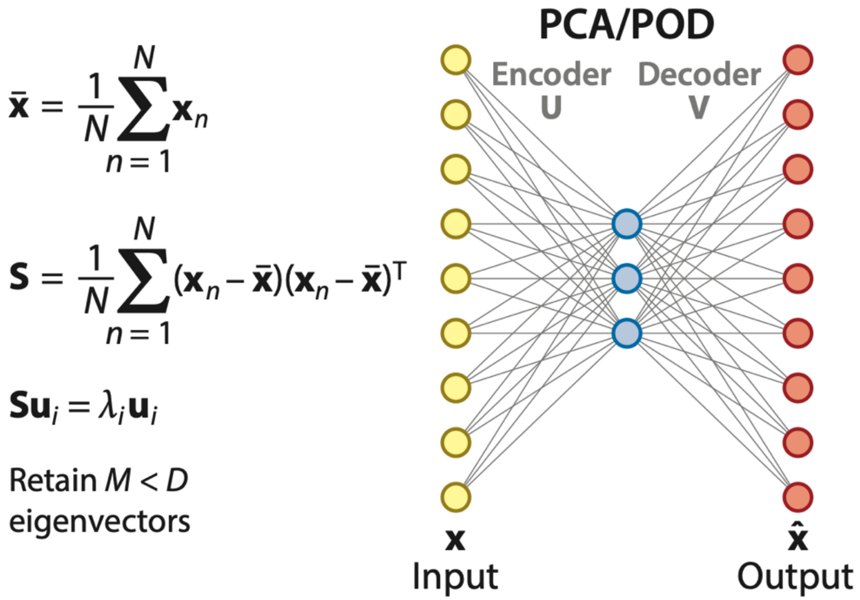


➔ **Deep NNets** are excellent candidates

Deep NNets for unsupervised representation Learning

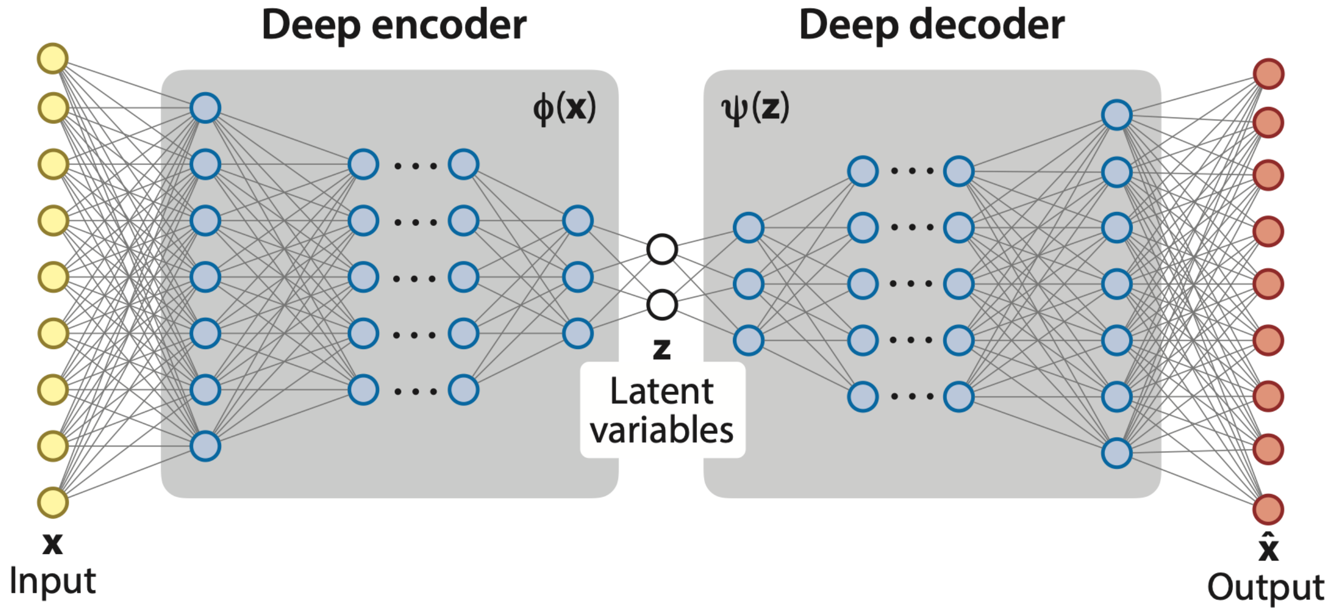
- Nnets are capable to recover highly non-linear relationships in the data
- Adapted architectures that work in a low-dimensional (latent) space

Shallow / Linear



POD: proper orthogonal decomposition
PCA: principal component analysis

Deep / Non-Linear



Auto-Encoding Deep Nets

Brunton, S. L., Noack, B. R., & Koumoutsakos, P. (2020). Machine learning for fluid mechanics. *Annual review of fluid mechanics*, *52*, 477-508. Read Online

TER challenge: How to exploit knowledge of physical (scientific) nature in data-driven learning models.

- Numerical simulation for solving physical problems is at the core of many engineering systems in industry, notably for the design of critical systems (e.g. airfoil design in aeronautics [1,5], tire design in automotive [2], rail design in railways) as well as for the management and monitoring of such systems (e.g. management of electricity or gas distribution networks [3,4], simulation of fluid flow in a nuclear power plant…).

- Current physical solvers, however, have certain limitations, such as the highly expensive computations required to perform such physical simulations, especially in 3D

- The use of machine learning techniques to learn how to solve complex physical problems from their numerical simulations (surrogate [2] or hybrid techniques [6–11]) is increasingly recognized as a promising approach to accelerate simulations. For example, graph neural networks are used for mesh-based simulations [2], or more generally, physics-informed neural networks (PINNs) [6–11].

- However, this hybridization can come at the expense of the accuracy of the solutions obtained, and there is a need to evaluate these hybrid approaches prior to industrial use.

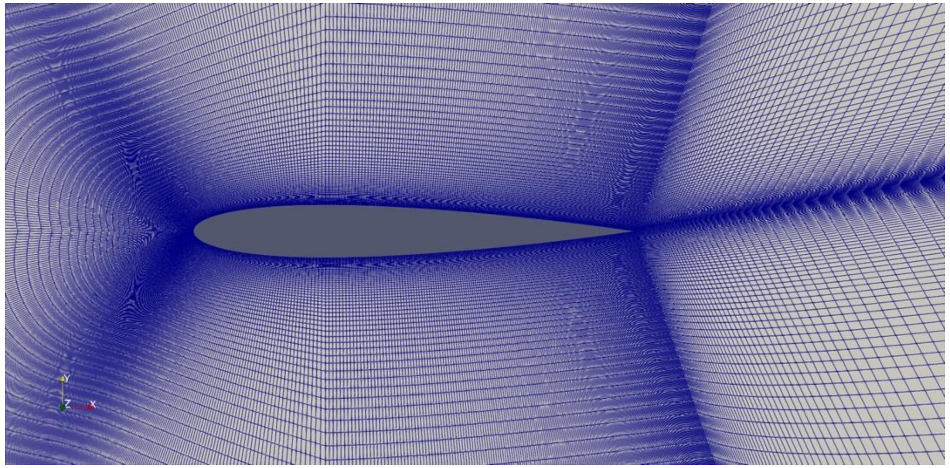
Airfoil design use case

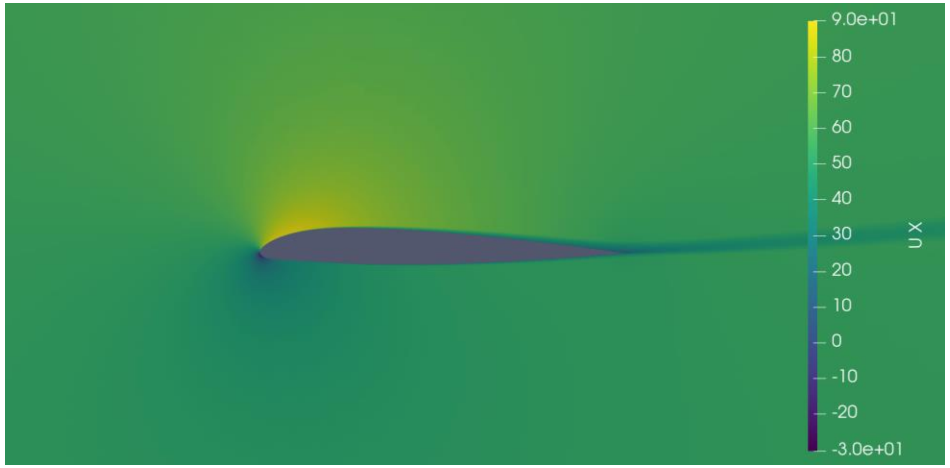
- Apply learning techniques to an industrial physics application using the AirFoil use case, based on AirfRANS data

- The AirfRANS dataset [1, 13] (AIRFRANS: High Fidelity Computational Fluid Dynamics Dataset for Approximating Reynolds-Averaged-Navier-Stokes Solutions; NeurIPS 2022) consists of 1000 computational fluid dynamics (CFD) simulations of steady-state aerodynamics over two dimensions (2D) airfoils in a subsonic flight regime, splitted in different tasks.

- It contains numerical resolutions of the incompressible Reynolds-Averaged Navier–Stokes (RANS) equations over the NACA 4 and 5 digits series of airfoils and in a subsonic flight regime setup [1, 13]..

- More details on the Airfoil design DataSet : AirfRANS paper





How you can evaluate your model ?

The LIPS platform [12, see figure] - “Learning industrial physical simulations” [12] offers an answer to this question by providing **metrics for assessing the quality of the solutions** obtained, based on several aspects, in particular

- Statistical accuracy of models (performance)

- Computing cost

- Level of respect for the physical laws underlying the physical system (physical compliance

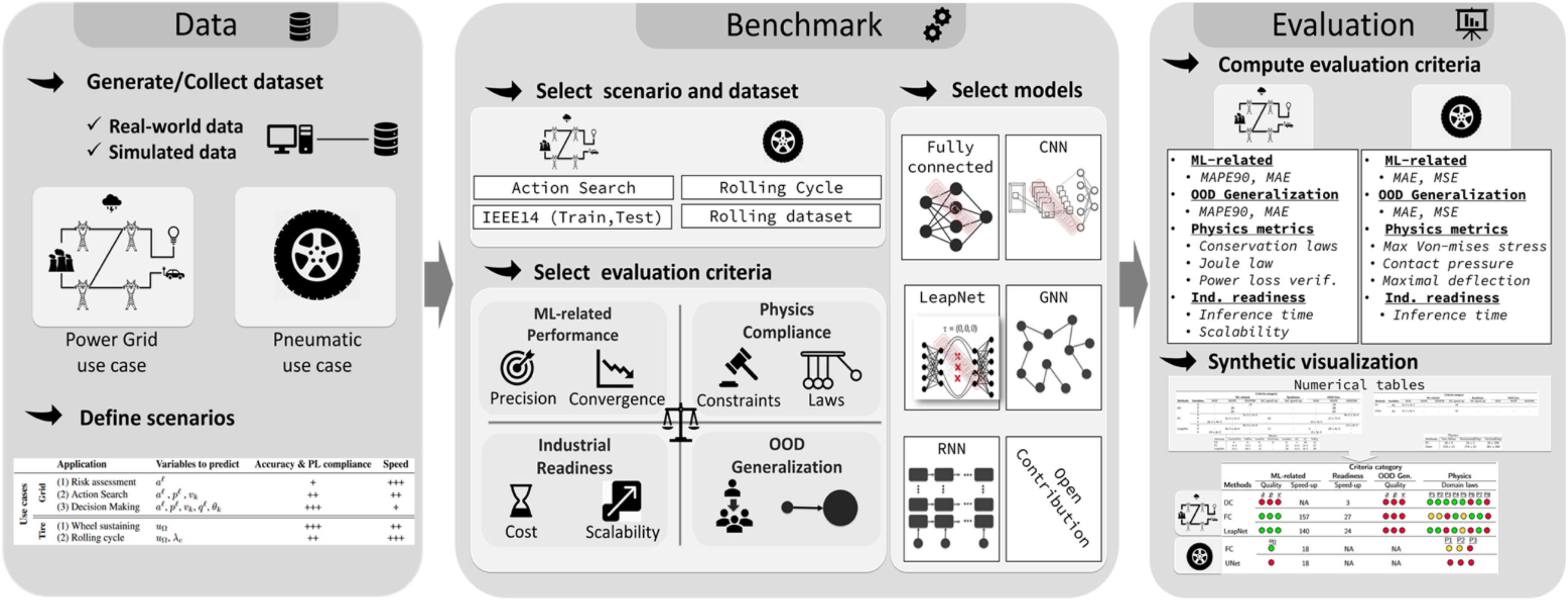
- Generalizability (i.e. their ability to be generalized to different use cases)

- etc,

to ensure the industrialization potential of the models evaluated.

Validation of hybrid physical-ML systems: LIPS Platform

- **How you can validate your hybrid (with physics) ML approach** ?
  - Several evaluation criteria are required (statistical performance, physical compliance, generalization, etc)
  - Comparison of # ML methods on several specific physical problems => need for a common evaluation framework
- LIPS "Learning Industrial Physical Simulation" benchmark suite https://github.com/IRT-SystemX/LIPS
  - Open-source framework for the evaluation of physical simulators augmented by machine learning
  - 7 use cases integrated
- More details on LIPS : **LIPS paper**
- LIPS : **Github repository**



TER objectives and calendar

Objectives

By the end of the project, the students should have acquired the following skills related to :

1. The study the state of the art of a family of machine learning techniques hybridized with physics,
2. The practice chosen learning techniques in the context of an industrial physiccal application through the AirFoil use case: simulation of airfoil design, using the AirfRANS dataset [1, 13]
3. The rvaluation of the solutions obtained by the models used (eg. via the LIPS platform) on the basis of different criteria to ensure a computationally efficient/accurate compromise: model accuracy, computation time, and respect for physical principles.

Calendar:

- Period 1: Familiarization with the subject of AI for physics
- Period 2: Familiarization with the AirFoil use case and the evaluation metrics (eg. LIPS platform)
- Period 3: Application and evaluation of selected state-of-the-art AI algorithms on the use

Notebooks to familiarize with the subject: https://github.com/IRT-SystemX/NeurIPS2024-ML4CFD-competition-Starting-Kit

Some references

1. Yagoubi et al. 2023 : Mouadh Yagoubi, Milad Leyli-Abadi, David Danan, Jean-Patrick Brunet, Jocelyn Ahmed Mazari, Florent Bonnet, Asma Farjallah, Marc Schoenauer, Patrick Gallinari : ML4PhySim : Machine Learning for Physical Simulations Challenge (The airfoil design). Read online: https://arxiv.org/pdf/2403.01623. Read online (website): https://www.codabench.org/competitions/1534/
2. Deep Graph Neural Networks for Numerical Simulation of PDEs. PhD of W. Liu. 2023 (LISN, Inria/SystemX). Read Online
3. Marot, A., et al. (2018). Guided machine learning for power grid segmentation. In *2018 IEEE PES Innovative Smart Grid Technologies Conference Europe (ISGT-Europe)* (pp. 1-6).
4. Mouadh Yagoubi, Milad Leyli-Abadi, Jean-Patrick Brunet, Maroua Gmati, Antoine Marot, Jérôme Picault, Asma Farjallah, Marc Schoenauer : 2024 Machine Learning for Physical Simulations Challenge (The power grid): Read online: https://ml-for-physical-simulation-challenge.irt-systemx.fr/powergrid-challenge/
5. Yagoubi et al. 2024 : Mouadh Yagoubi, David Danan, Milad Leyli-abadi, Jean-Patrick Brunet, Jocelyn Ahmed Mazari, Florent Bonnet, maroua gmati, Asma Farjallah, Paola Cinnella, Patrick Gallinari, Marc Schoenauer: NeurIPS 2024 ML4CFD Competition: Harnessing Machine Learning for Computational Fluid Dynamics in Airfoil Design
6. Raissi, M et al. (2019) Physics-Informed Neural Networks: A Deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear Partial Differential Equations. Journal of Computational Physics. 378. Online
7. Brunton, S. L., Noack, B. R., & Koumoutsakos, P. (2020). Machine learning for fluid mechanics. *Annual review of fluid mechanics*, *52*, 477-508. Read Online
8. Cuomo, S., et al., (2022). Scientific machine learning through physics–informed neural networks: Where we are and what's next. *Journal of Scientific Computing*, *92*(3), 88. Read Online
9. Hao Z. el al. (2022). Physics-informed machine learning: A survey on problems, methods and applications. Read Online
10. Wang & al. (2023). Scientific discovery in the age of artificial intelligence. Nature, 620. Read Online
11. E. Menier et al., 2023. CD-ROM: Complementary Deep-Reduced Order Model. *Computer Methods in Applied Mechanics and Engineering* 410. Read Online. Thèse Emmanuel Menier : https://theses.hal.science/tel-04616516v1/document
12. Milad Leyli-Abadi, David Danan, Mouadh Yagoubi, Seif-Eddine Attoui, Antoine Marot, et al. **LIPS** - Learning Industrial Physical Simulation benchmark suite. NeurIPS - Data & Benchmark Track, Nov 2022, New Orleans, United States. <hal-03780816>. Read online
13. Florent Bonnet, Jocelyn Ahmed Mazari, Paola Cinnella, and patrick gallinari. AirfRANS: High fidelity com- putational fluid dynamics dataset for approximating reynolds-averaged navier–stokes solutions. In Thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track, 2022. Read online

- Marot, A., et al. (2018). Guided machine learning for power grid segmentation. In *2018 IEEE PES Innovative Smart Grid Technologies Conference Europe (ISGT-Europe)* (pp. 1-6).
- Merino-Martínez *et al. CEAS Aeronautical* Journal (2019).
- Raissi, M et al. (2019) Physics-Informed Neural Networks: A Deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear Partial Differential Equations. Journal of Computational Physics. 378. Online
- Cuomo, S., et al., (2022). Scientific machine learning through physics–informed neural networks: Where we are and what's next. *Journal of Scientific Computing*, *92*(3), 88. Read Online
- C.L. M. H. Navier, Memoire sur les Lois du Mouvements des Fluides, Mem. de l'Acad. d. Sci.,6, 398 (1822)
- C.G. Stokes, On the Theories of the Internal Friction of Fluids in Motion, Trans. Cambridge Phys. Soc., 8, (1845)
- Wang & al. (2023). Scientific discovery in the age of artificial intelligence. Nature, 620. Read Online
- Brunton, S. L., Noack, B. R., & Koumoutsakos, P. (2020). Machine learning for fluid mechanics. *Annual review of fluid mechanics*, *52*, 477-508. Read Online
- Donon, B., et al. (2020). Deep statistical solvers. *Advances in Neural Information Processing Systems*, *33*, 7910-7921. Read Online
- Donon, B. (2022). *Deep statistical solvers & power systems applications* (Doctoral dissertation, Université Paris-Saclay). Read Online
- E. Menier et al., 2023. CD-ROM: Complementary Deep-Reduced Order Model. *Computer Methods in Applied Mechanics and Engineering* 410. Read Online
- Deep Graph Neural Networks for Numerical Simulation of PDEs. PhD of W. Liu. 2023 (LISN, Inria/SystemX). Read Online
- D. Shu et al., 2023. A physics-informed diffusion model for high-fidelity flow field reconstruction, Journal of Computational Physics, 478, 2023. Read Online

- D. Shu et al., 2023. A physics-informed diffusion model for high-fidelity flow field reconstruction, Journal of Computational Physics, 478, 2023. Read Online

THANK YOU FOR YOUR ATTENTION !