Boosting
digital transformation

On some research and innovation challenges in AI*

Faïcel Chamroukhi, October 25, 2024.

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The University of Dublin

Outline

Challenges and industrial applications in

- Hybrid AI: How to exploit industry knowledge of physical (scientific) and symbolic (semantic) nature in data-driven learning models.
- Trustworthy AI: Towards integrating AI into critical system engineering
- Generative AI for industry: How to evaluate and advance specialized generative AI models for industrial applications

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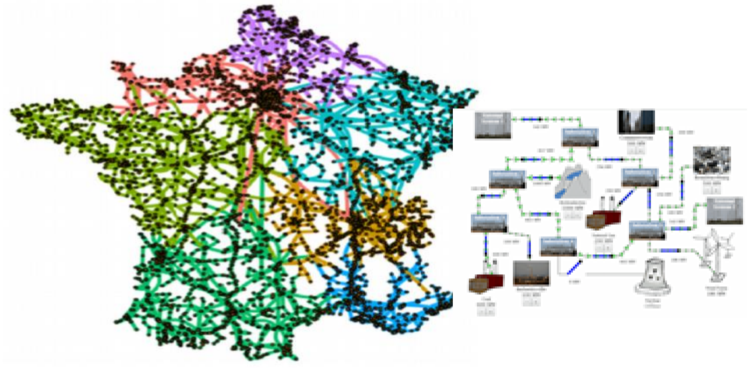
Motivation: Some physical problems in Industry

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

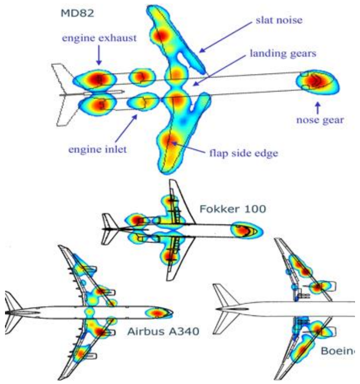
- Covering various fields in physics (mechanics, fluid dynamics, aerodynamics, electromagnetism …)
- In a wide variety of Applications in industry, in particular in numerical **simulation**

Electricity (power grids)



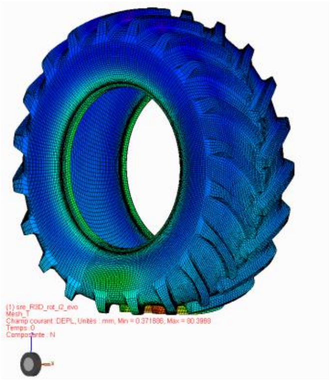
Picture from **Marot**, A., et al. (2018).

Aerodynamics



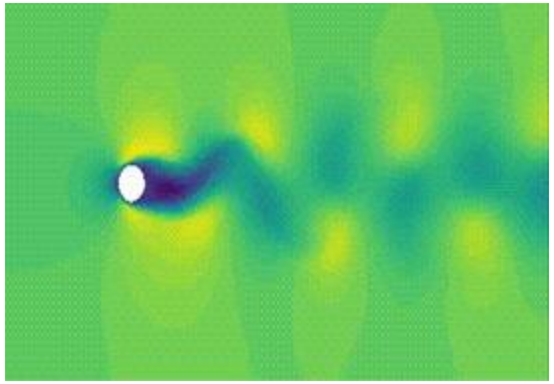
Picture form Merino-Martínez *et al. CEAS Aeronautical* Journal (2019).

Solid Mechanics pneumatics



From HSA – SystemX

Fluid Flows/Dynamics



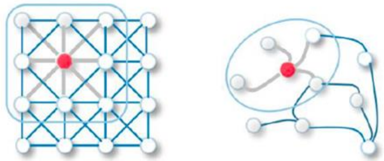
from Emmanuel Menier (PhD, LSIN/SystemX, 2024)

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

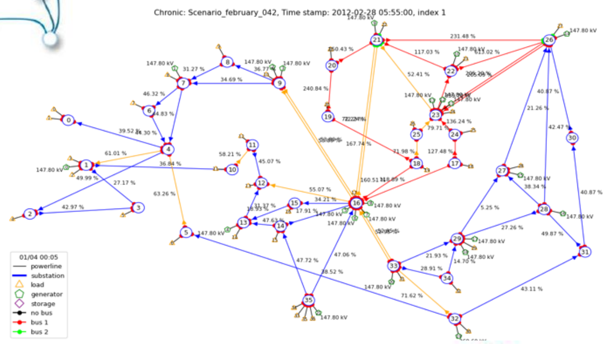
- Complex to model/solve analytically

- Compuationally expensive to solve numerically

Physics and Machine Learning



Power Grid (HSA Project)
Substations and lines



- Physics knowledge to guide learning

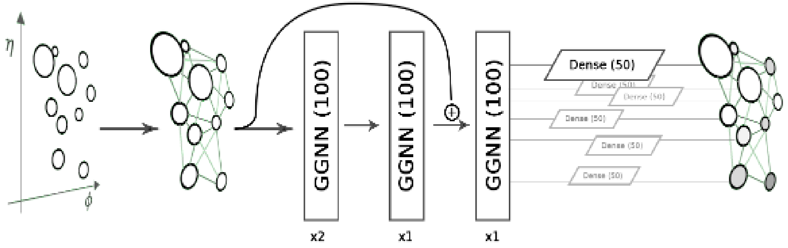
Integrating geometric priors in learned representations (Bronstein 2017)
Geometric deep learning, **GNN** and neural passing message (Arjona Martínez 2019)

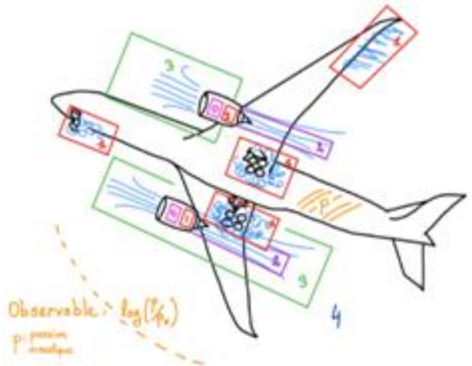
- **D**ifferential **e**quations to improve deep learning

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 particular in industry

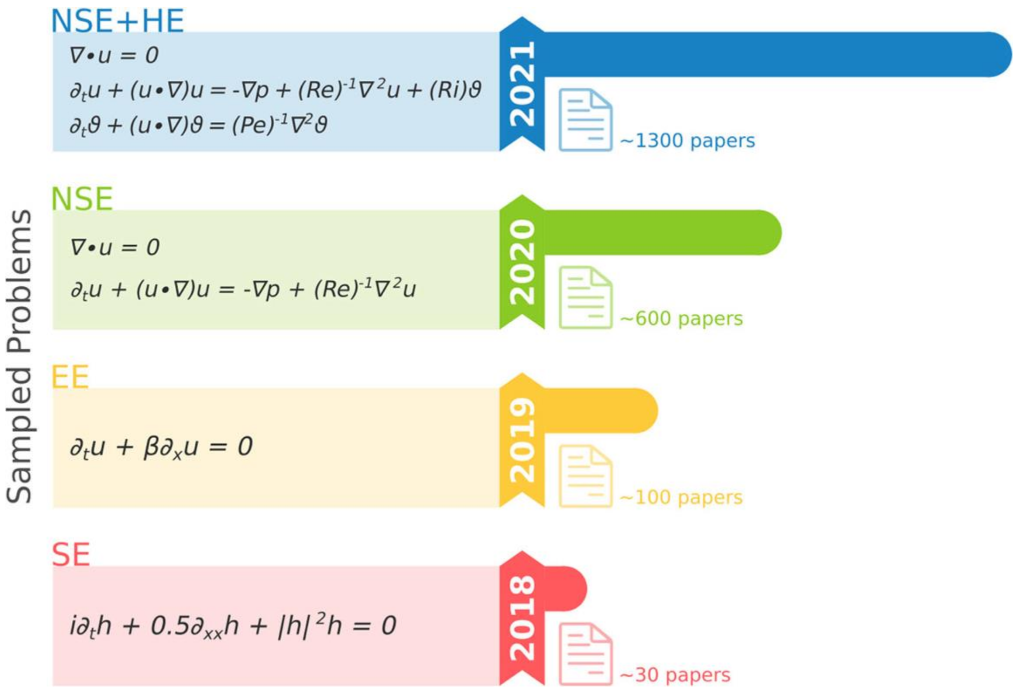
Scientific Challenges

- 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 :

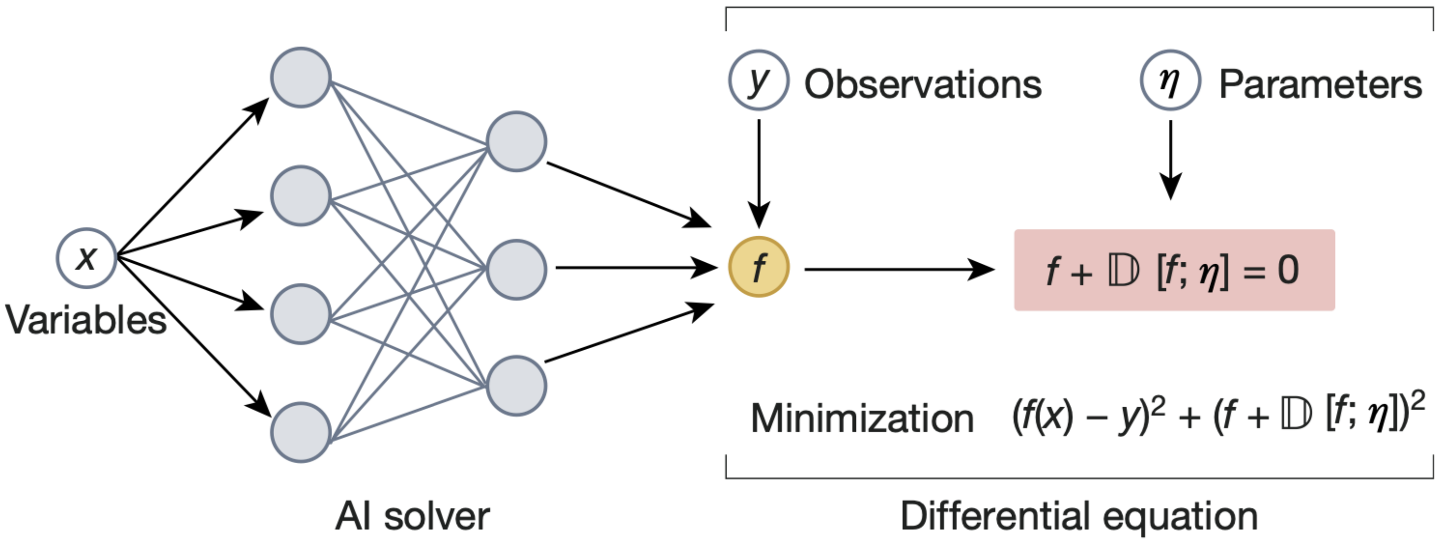


- Solving Navier–Stokes equations coupled with the corresponding temperature equation for analyzing heat flow convection (NSE+HE). Cai et al, 2021
- Solving incompressible Navier–Stokes equations (NSE). Jin et al., 2020.
- Solving Euler equations (EE) that model high-speed aerodynamic flows. Mao et al,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

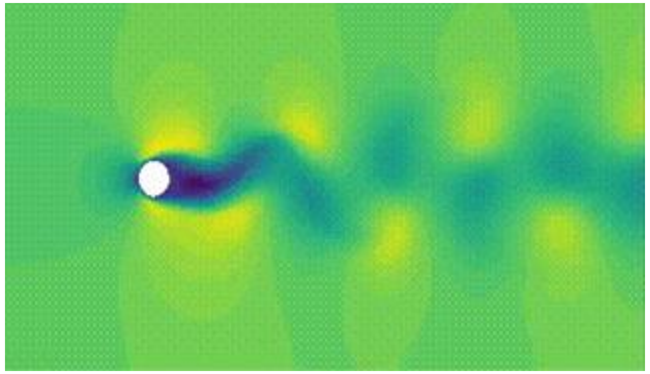
Wang & al. (2023). Scientific discovery in the age of artificial intelligence. Nature, 620. Read Online

- 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



Credit: Emmanuel Menier, PhD LISN/SystemX

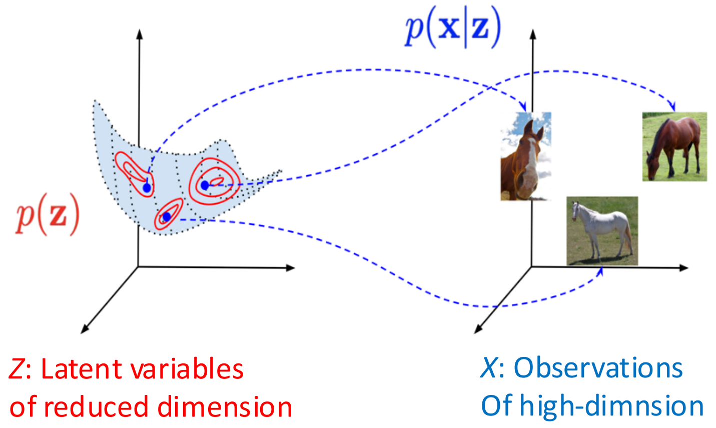
Deep NNets for unsupervised representation Learning

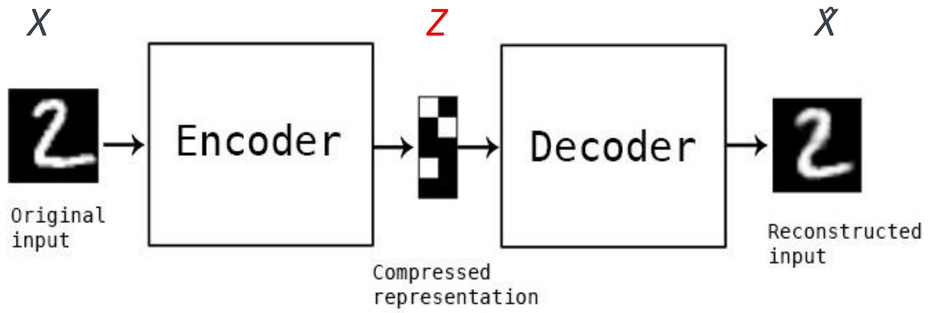
Latent Variable Models: A family of probabilistic models capable of inferring the intrinsic latent structure (of reduced dimension) of the data

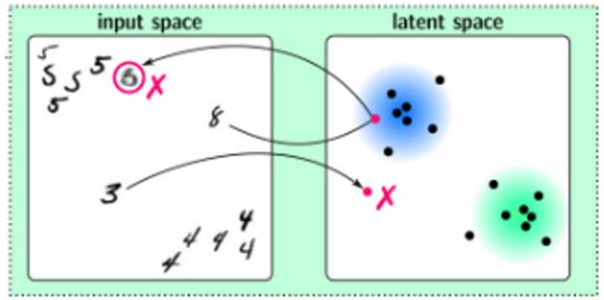
- **Auto-Encoders - AE** (LeCun 1987): The **encoder** projects the input ***X*** (of high-dimension dimension) in a compressed latent representation ***Z*** (the **code**) to reconstruct it using the **decoder** with outpu $\hat{X}$
- ➔ Learning by minimizing the reconstruction error between $\hat{X}$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



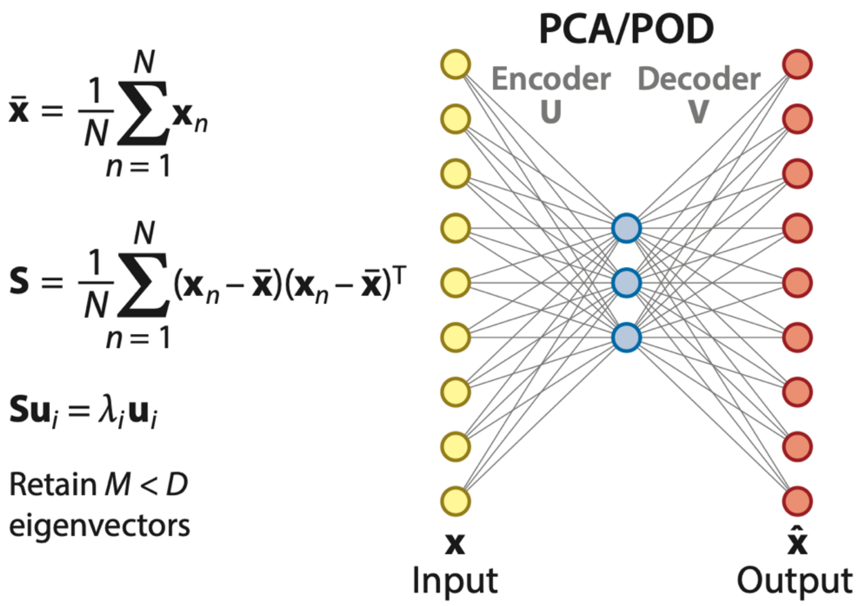




Deep NNets for unsupervised representation Learning

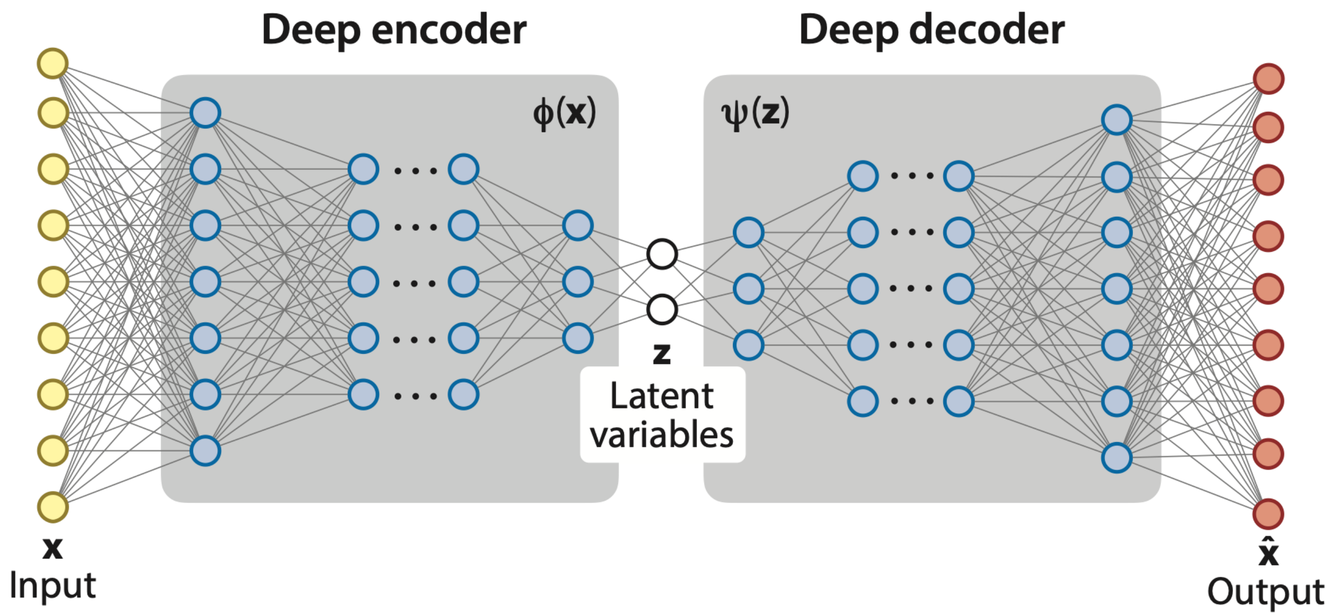
- Nnets are capable to recover highly non-linear relationships in the data
- Adapted architectures that work in a low-dimensional (latent) space

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

The Research Program IA2: AI and Augmented Engineering

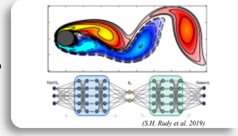
Intelligence artificielle et ingénierie augmentée

Artificial Intelligence and Augmented Engineering

- a program with **6 R&D collaborative projects** on concrete **industrial use cases**
- Area: Hybrid AI
- 20+ industrial and academic partners
- ~12M€

Advance project
Thesis / Postdocs / Shared work

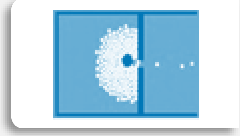
HSA: Simulation/machine learning hybrid modeling
How industrial solvers and learning models can enrich each other ?
01



AFS: Agility and fidelity of simulations
How to imporve agility and fidelity of simulation in complex systems design?
02

S2I: Industrial infrastructure supervision
How to improve decision-making on distubuted industrial systems via machine learning techniques ?
03

SAA: Augmented multi-agent simulation
How can multi-agent models benefit from real data and bring out atypical situations?
04



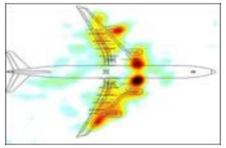
SMD: Business Semantics for Multi-source Data Mining
How to link heterogeneous data with established practical knowledge?
05

CAB: Cockpit and Bidirectional Assistant
How to develop a virtual assistant that learns from expert and learns to the expert
06

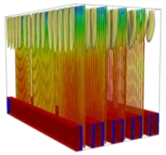
Diagram/pictures credit to [IA2 Program]

HAS Project: Industrial use cases

AIRBUS: Aircraft aero-acoustic performance



Air Liquide: Steam methane reforming

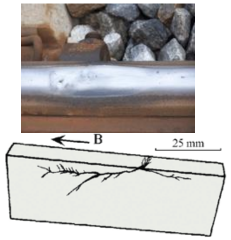


EDF: Energy modeling of buildings

Michelin: 3D rolling tire

RTE : Augmented simulator for electrical grid management

SNCF: Forecasting crack propagation in rails



HSA Project : Simulation/machine learning hybrid modeling

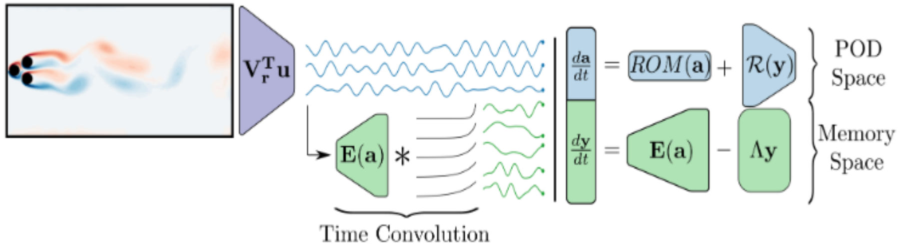
Challenges and possible solutions (studied as part of the HSA project):

- Augmenting physical solvers with data-driven models that integrate physics constraints
- Building model architecture adapted to the complex physical structures/systems
- Reducing the simulation cost

➔ Surrogate models for physical simulation, aiming to Replace physical solvers with

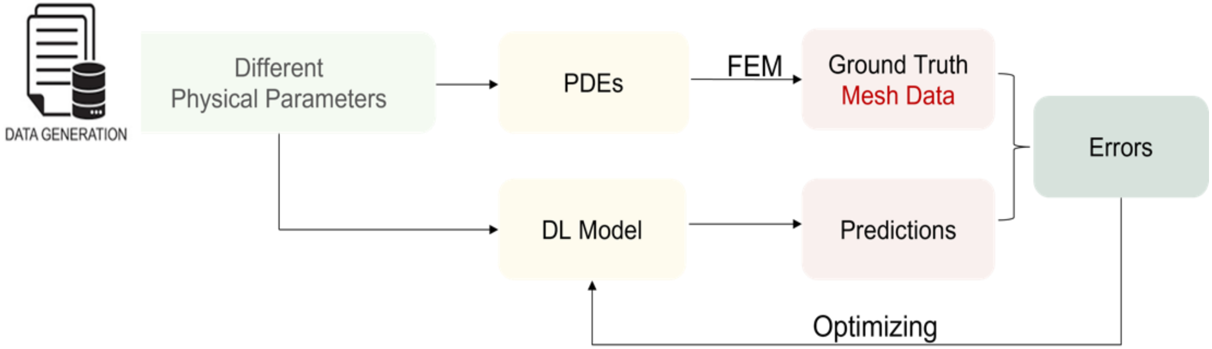
➔ Deep learning intergrating physical constraints (eg. Deep Graph Nets for PDEs)

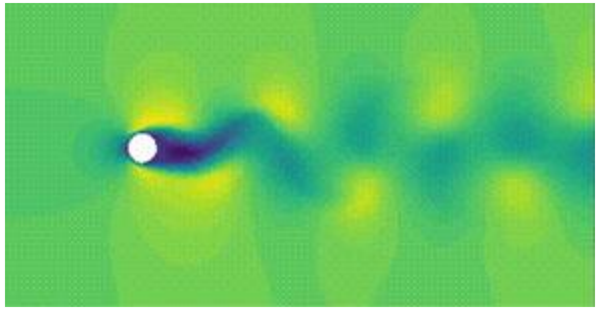
➔ Deal with high-dimensional, non-linear, and complex structurs (e.g reduced modeling, ..)



High-Dimensional non-linear Physical Equations

HSA





Reduced models and deep learning for PDEs
PhD Thesis of E. Menier, 2024 (LISN, Inria/SystemX)

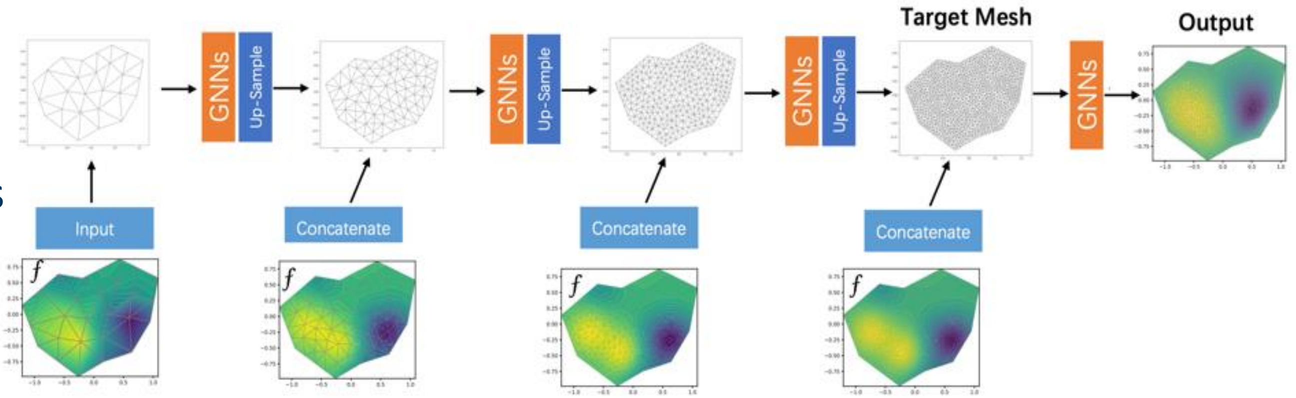
Deep Graph Neural Networks for Numerical Simulation of PDEs. PhD of W. Liu. 2023 (LISN, Inria/SystemX). Read Online

E. Menier et al., 2023. CD-ROM: Complementary Deep-Reduced Order Model. *Computer Methods in Applied Mechanics and Engineering* 410. Read Online

https://www.irt-systemx.fr/projets/HSA/

Project HSA : simulation and deep learning of graphs

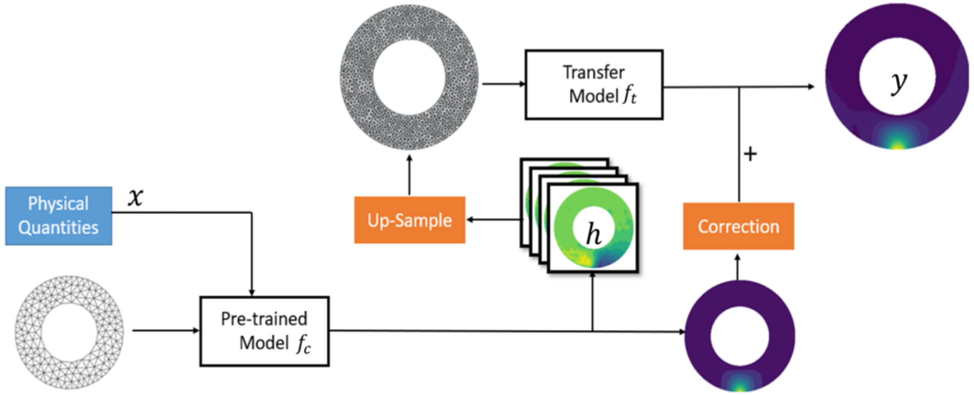
Graph Neural Nets for 3D **meshes**



More suitable, as they operate by construction on graphs

- Generic nature of the learned models
- Transfer learning for improved results
- Prediction can be improved via transfer learning:

from low fidelity (coarse mesh) to high fidelity (finer mesh) models



Wheel contact profile

Physics: contact equations

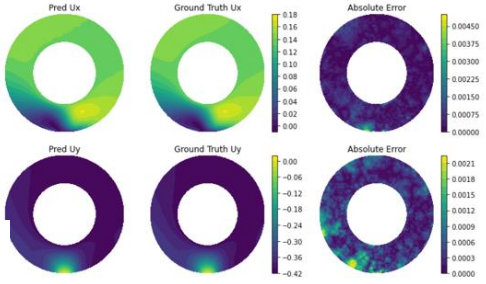
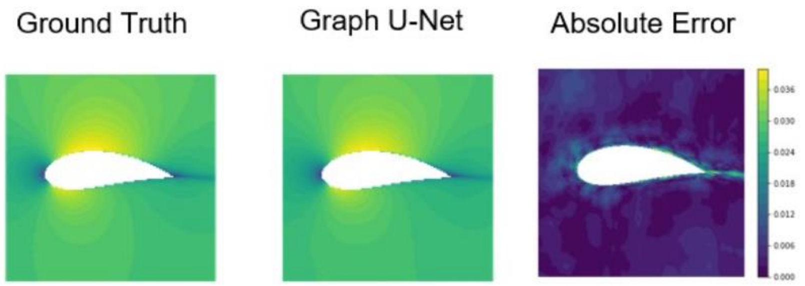


Figure 6.3: An example of wheel contact prediction

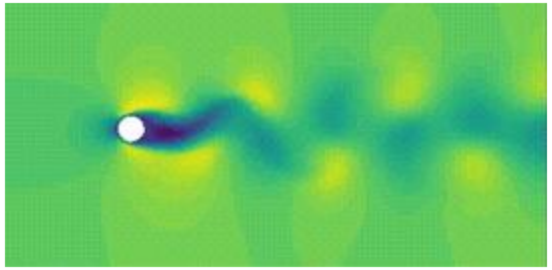
Modeling of the **airflow** profile around an aircraft wing (Air Foil)

Physics: Navier-Stokes equations



PhD theis of W. Liu, 2023 (LISN, Inria/SystemX)

Dynamics: Hybrid ML for HD dynamical physical systems

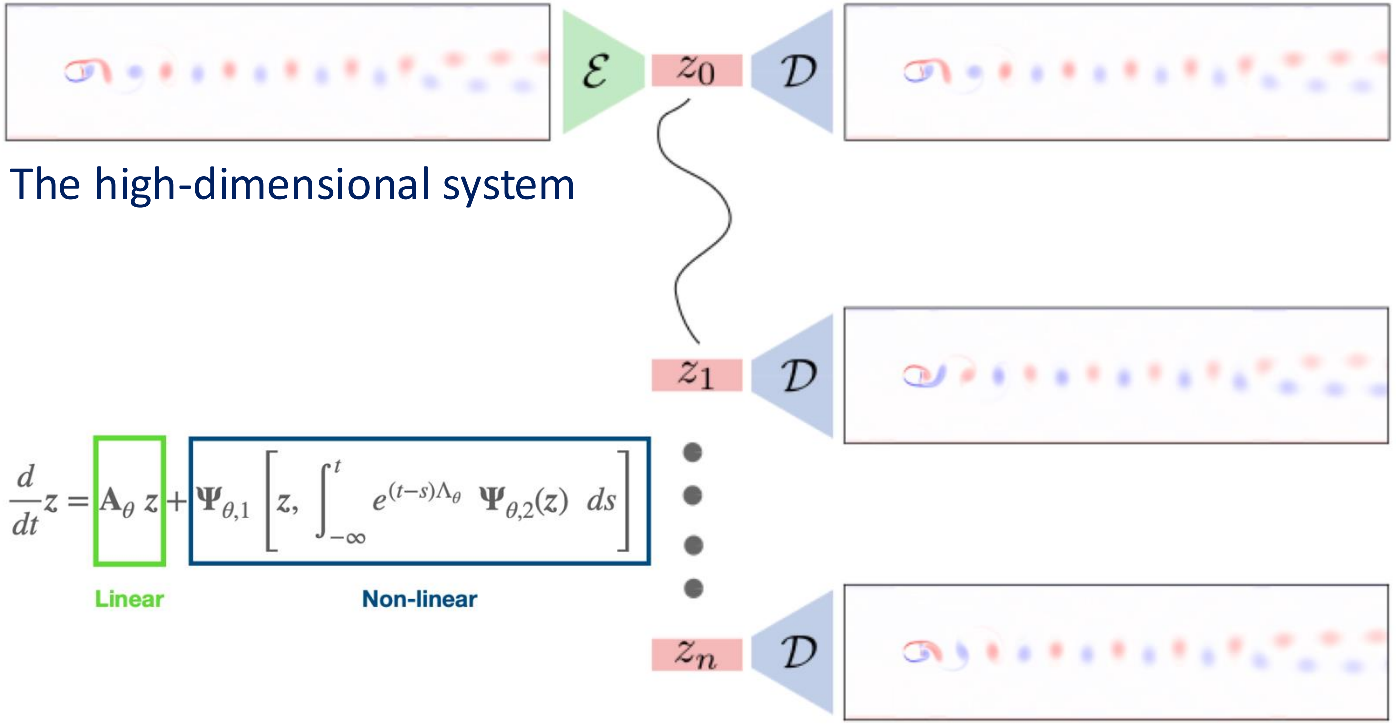


High-Dimensional non-linear Dymical Systems:

Goals:
Recover the dynamics, non-linearity in a high-dimensitonal setting

An Auto-Endore based architecture

Interpretable learning of effective dynamics (ILED) architecture:



$$\frac{d}{dt}z = \underbrace{\boxed{\mathbf{A}_\theta\, z}}_{\text{Linear}} + \underbrace{\boxed{\mathbf{\Psi}_{\theta,1}\left[z, \int_{-\infty}^{t} e^{(t-s)\Lambda_\theta}\ \mathbf{\Psi}_{\theta,2}(z)\ ds\right]}}_{\text{Non-linear}}$$

The high-dimensional system

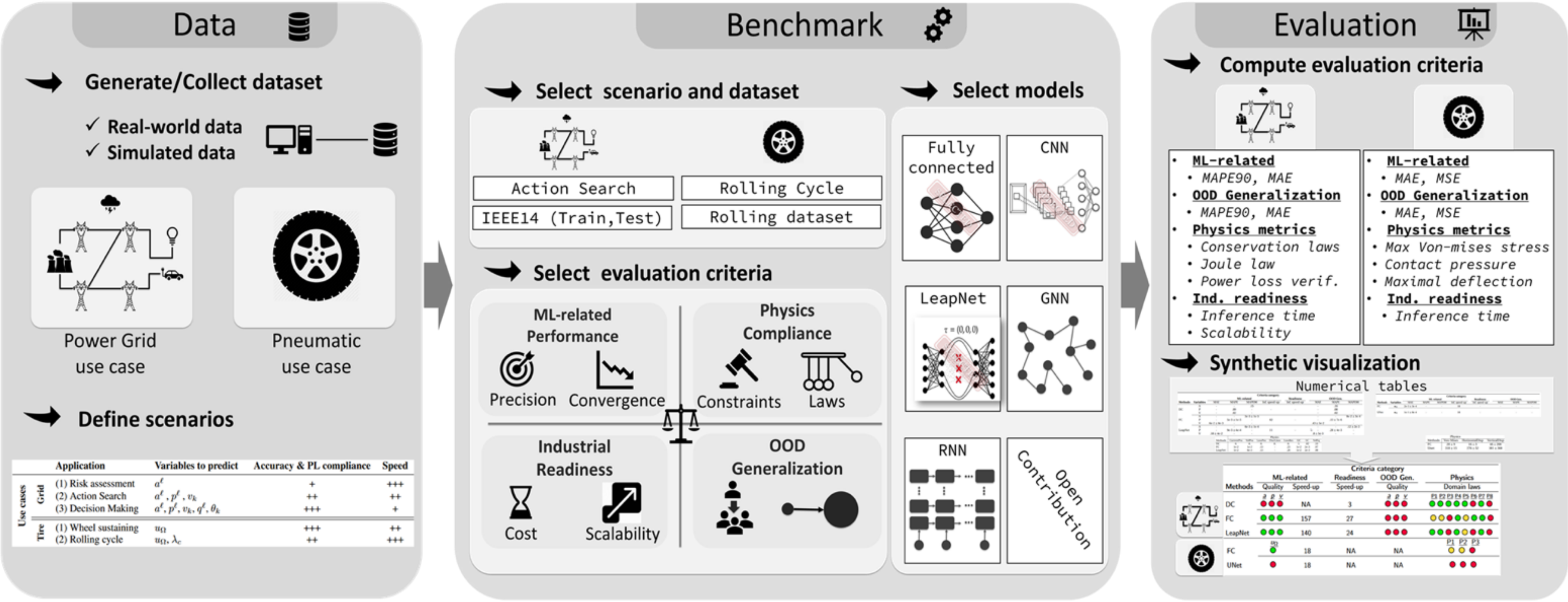
The lower-dimensional representation (**z**) is propagated in time using a linear and a non-linear part based on the Mori-Zwanzig formalism

The decoder D reconstructs the high-dimensional systems.

Menier, E., et al. (2023). Interpretable learning of effective dynamics for multiscale systems. *arXiv preprint arXiv:2309.05812*. Read Online
PhD Thesis of E. Menier, 2024 (LISN, Inria/SystemX), 2024

Validation of hybrid physical-ML systems: LIPS Platform

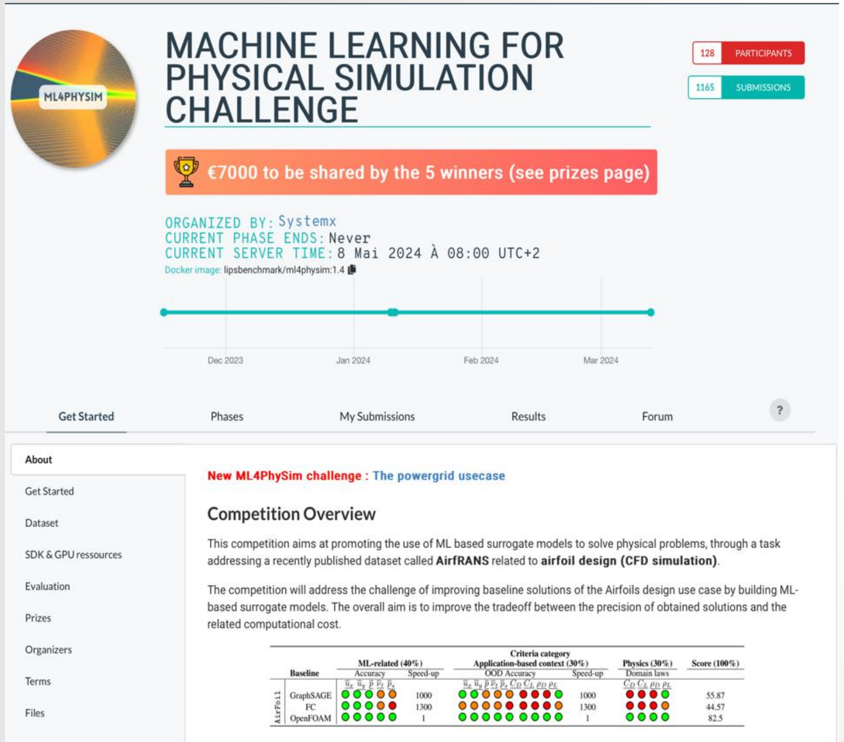
- **How to validate hybrid (with physics) ML approaches** ?
  - Several evaluation criteria are required (statistical performance, physical compliance, generalization, etc)
  - Comparison of # ML methods on several specific physical problems => need for a common evaluation framework
- Proposed solution for industry : LIPS "Learning Industrial Physical Simulation" benchmark suite (*Result of the project HSA-IA2)*
  - 1st framework for the evaluation of physical simulators augmented by machine learning
  - 7 use cases integrated
  - Open-source Framework https://github.com/IRT-SystemX/LIPS [Published at NeurIPS2022](#)



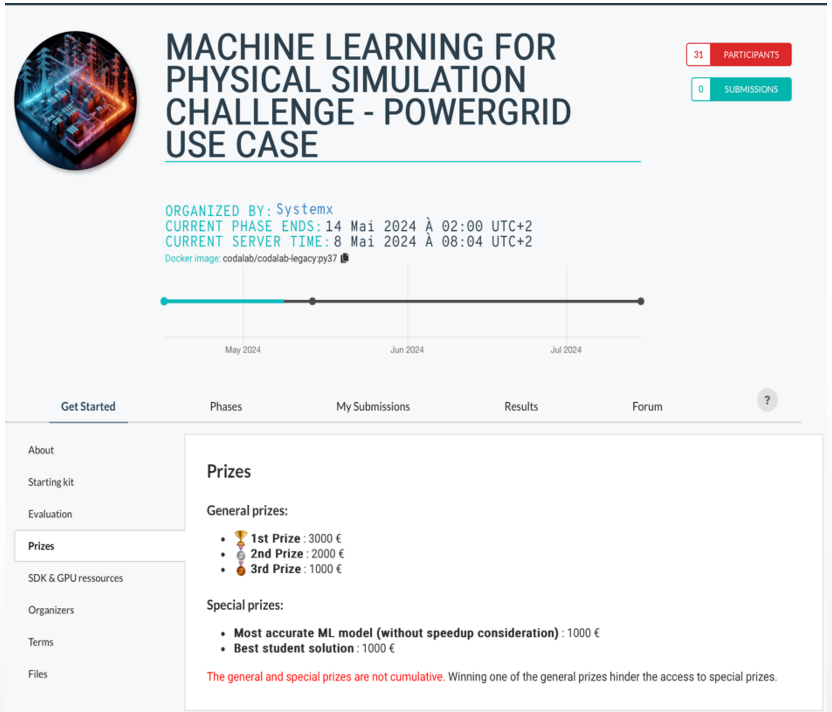
Competitions on Codabench/codalab, NeurIPS’24

LIPS hosts/ed the three following competitions:

https://www.codabench.org/competitions/1534/



https://www.codabench.org/competitions/2378/



https://www.codabench.org/competitions/3282/

Running !

Challenges and industrial applications in

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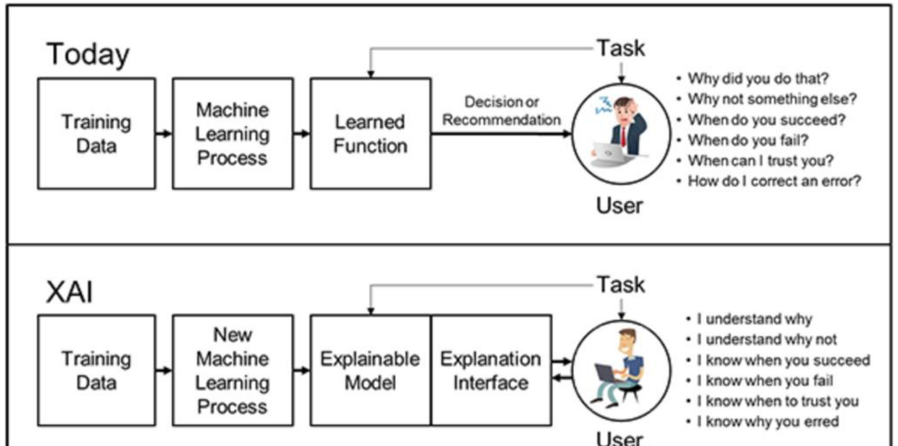
Symbolic approaches and Machine Learning (ML and ***Semantics***)

➔ The challenge: **Producing explanations**

There are several ways of producing explanations:

1. training the NNet to produce arguments at the same time as prediction
2. => or using a **hybrid approach** combining symbolic and neural methods

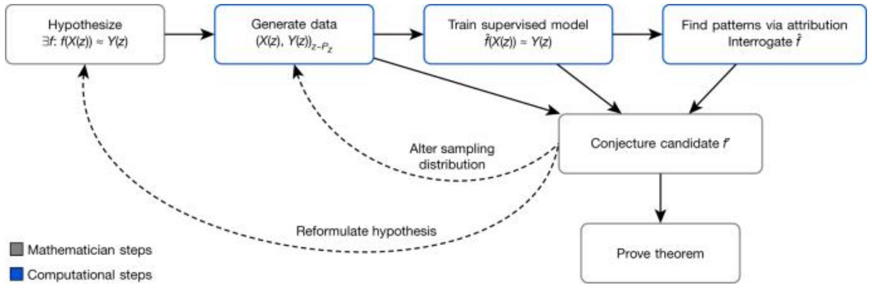
- Combining learning and knowledge graphs enables **business expertise to be integrated** and results to be **explained**.

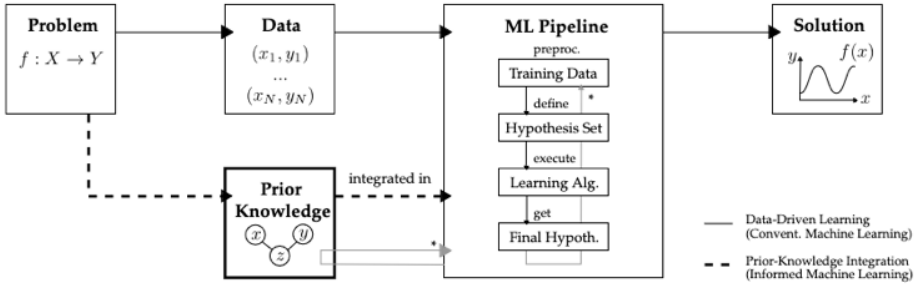


Source: DARPA.mil

➔ Neuro-symbolic methods aim at bridging techniques from symbolic AI and deep learning:

- integrating a symbolic paradigm into a neural network
- E.g The ML model uses explicit symbolic knowledge, in the form of logic rules/ontologies, to specify desired properties for the NNet.





- Formal rules for explainability (Audemard, 2023)
- Improving Neural-Based Classification with Logical Background Knowledge (Ott 2023) (Battagla 2018)

Integrating Expert/Business *semantics* in ML (Project SMD)

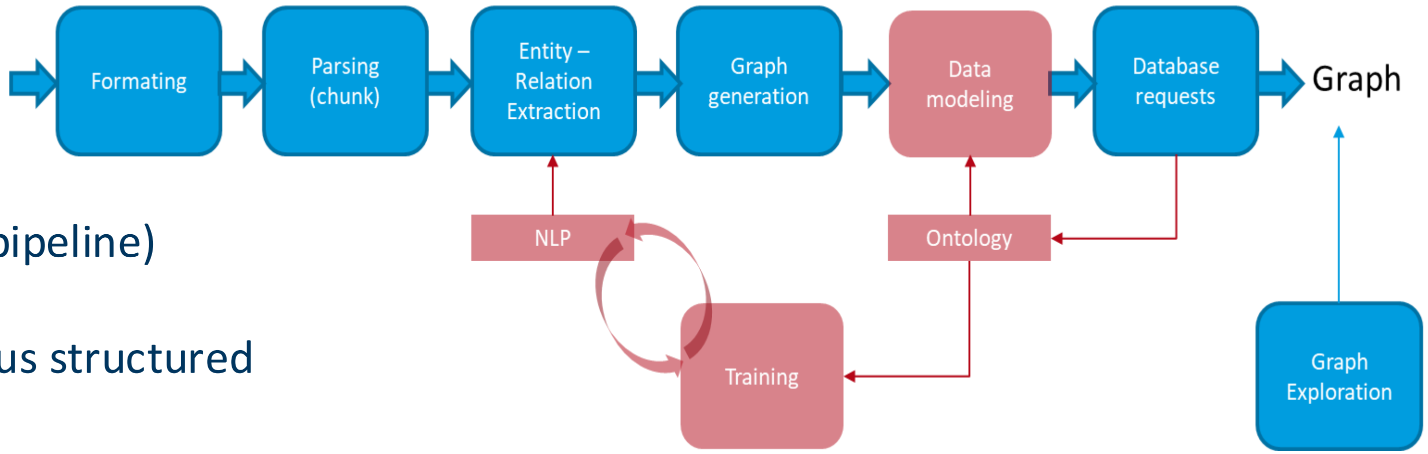
https://www.irt-systemx.fr/projets/SMD/

Framework:
Building ML-based on knowledge graphs from expert/business language data

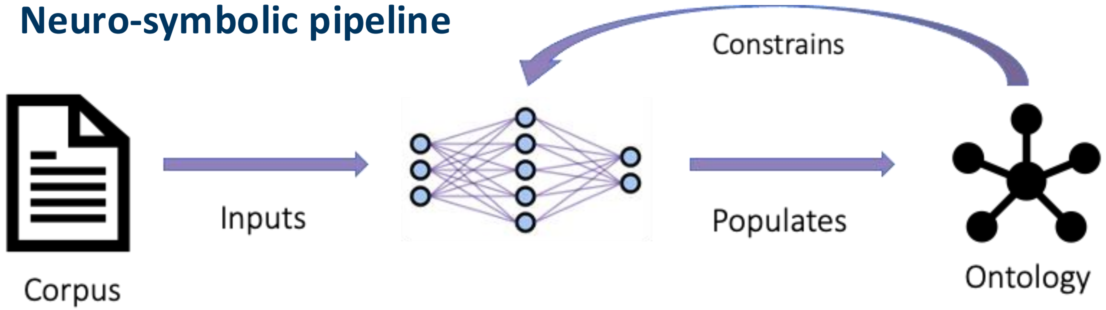
Approach (The Neuro-symbolic engineering pipeline)

- Information extraction from heterogeneous structured and semi-structured text corpora...:
- NLP approach; Semantic annotation
- Taking into account domain rules/constraints in the numerical-AI based decision

The Neuro-symbolic engineering pipeline:



Neuro-symbolic pipeline

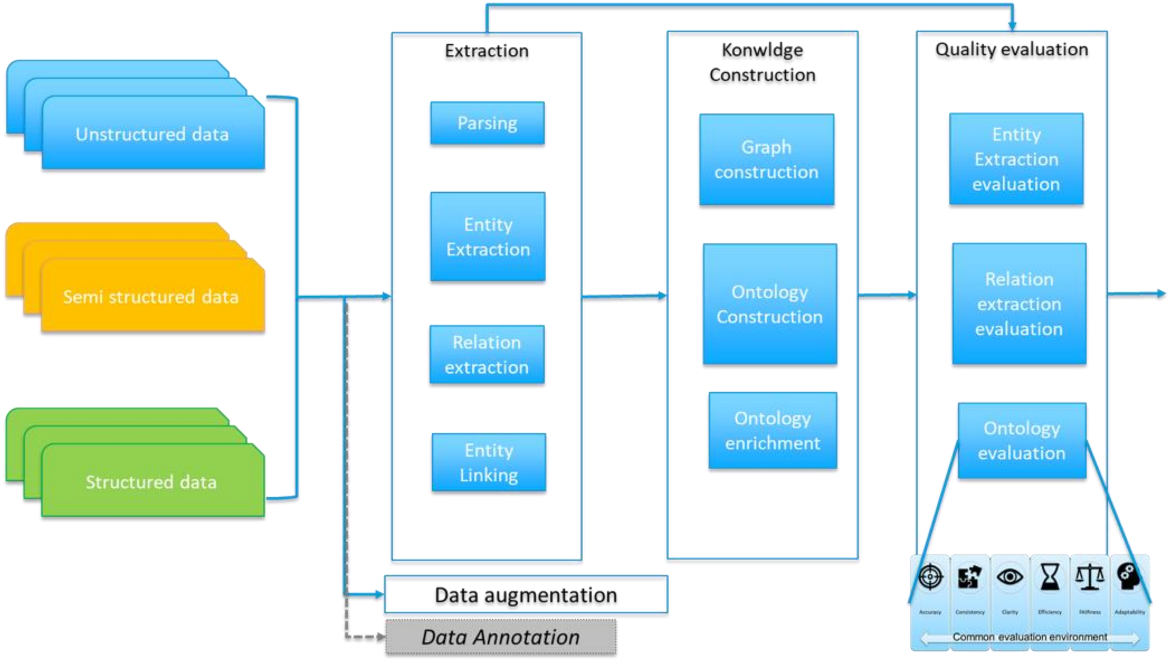


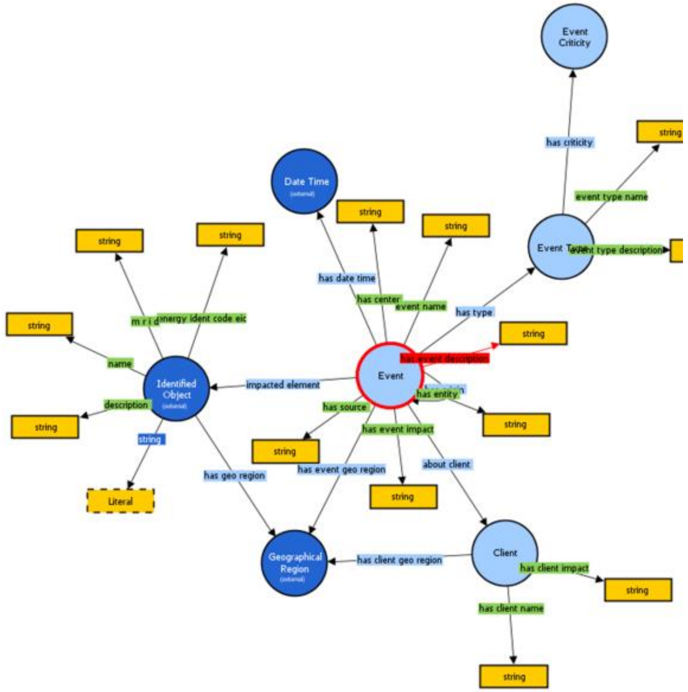
Intelligence artificielle et ingénierie augmentée

SMD Project

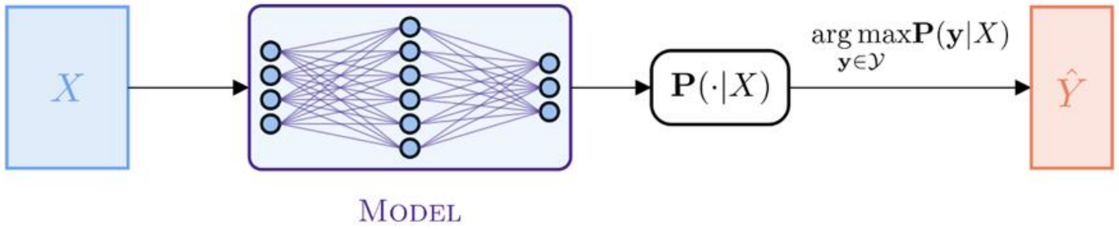
Integrating Expert/Business semantics in ML (Project SMD)

Ontology-based explanations :





Logic rules, to specify desired properties for the Nnet:



=> Insertion of logical rules at the inference step :

- Recalculate P(y|X, α) in lieu of the learnt P(y|X)
- α is a rule encoding the validity of the prediction $\hat{y}$

Ontologies and (machine/transfer) learning for multimedia document analysis. PhD thesis of A. Ledaguenel (in progress, MICS/SystemX)

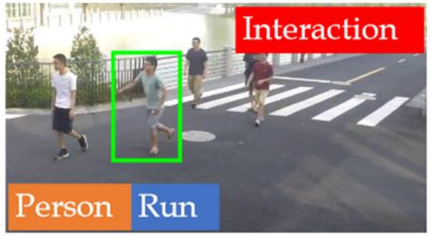
Some use cases

**these shown examples are obtained on Public (not industrial) data*

Use case : Detection and characterization of atypical scenes in surveillance videos for crisis management

AIRBUS DEFENCE & SPACE

- identifying anomalies in video streams
- scene analysis and construction of contextualized graphs



ShanghaiTech data (437 videos on 13 different locations, containing 130 abnormal events)

Fighting

Explosion

Road accident

UCF-crime data (128 hours videos contain realistic anomalies including Abuse, Arrest, Arson, Assault, etc.)

Credit: SystemX's SMD Project

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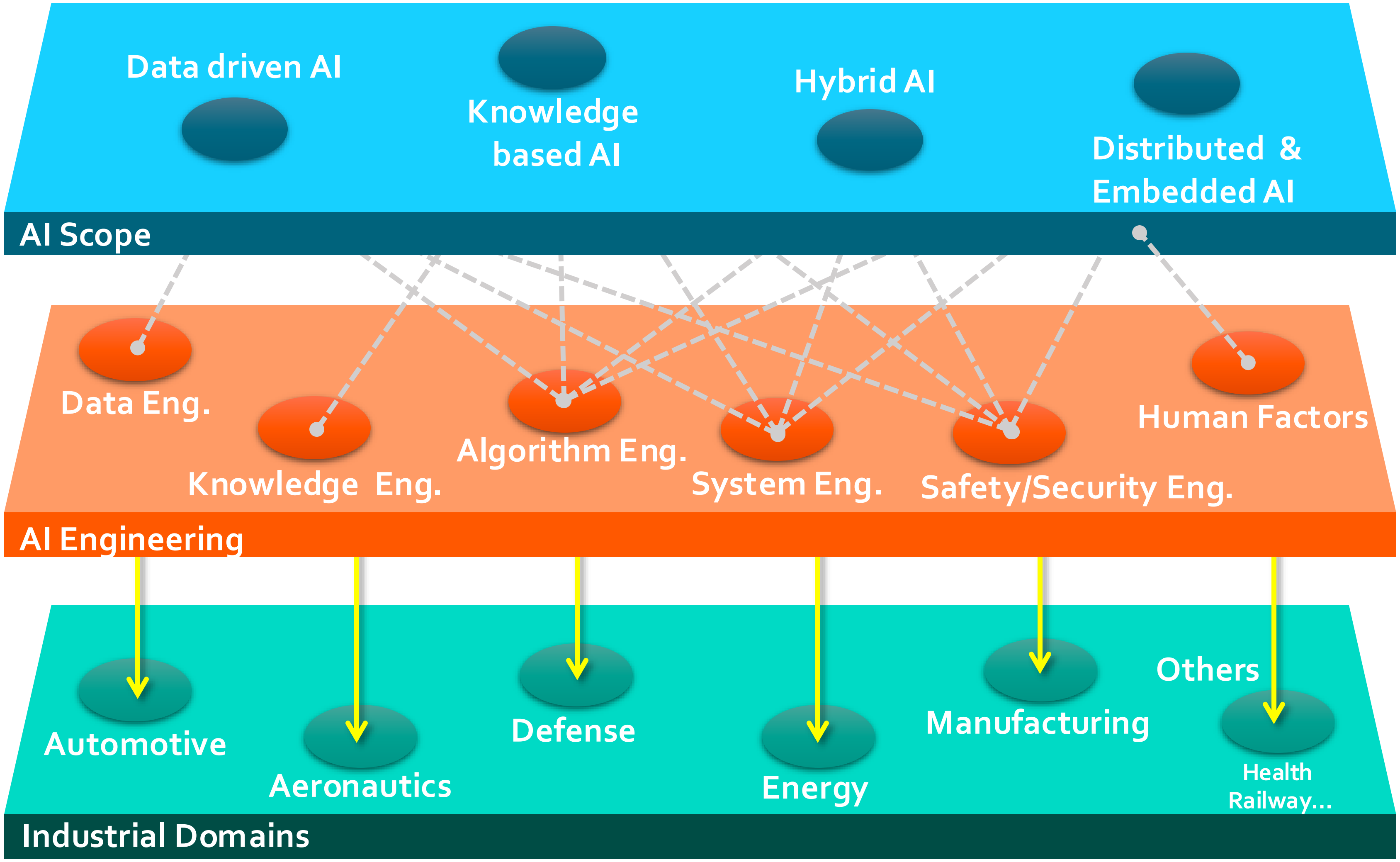
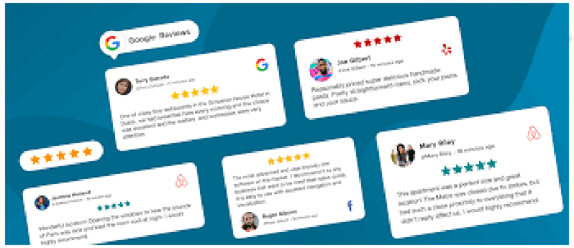
- Generative AI for industry: How to evaluate and advance specialized generative AI models for industrial applications

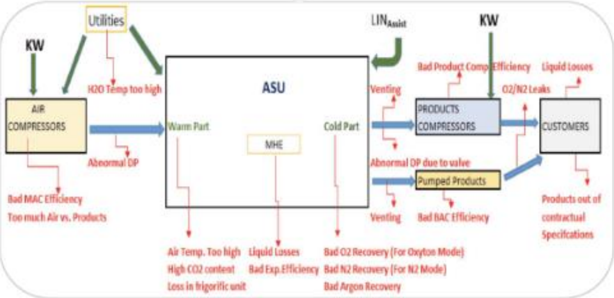
Confiance.AI programme: A French unique community to design and industrialise trustworthy AI-based critical systems



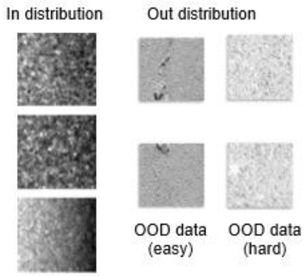
Credit : Confiance.ai

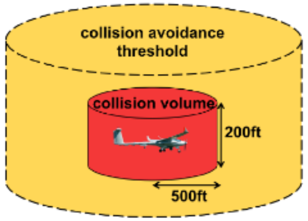
Some Use Cases





Theme	Primary	Secondary
2D Vision	**Scene understanding** (Valeo) In autonomous driving	Aerial pictures (Thales LAS)
Visual inspection	**Welding inspection** (Renault)	Industrial control (Safran)
Time series prediction	**Demand forecasting** (Air Liquide) Eg. oxygen	
Time series anomaly detection	Plant efficiency monitoring (Air Liquide)	Virtual sensor (Airbus Helicopter)
Tabular data	ACAS XU (Airbus)	
NLP	Opinion mining (Renault)	
Hybrid ML Symbolic	**Time dependent planning** (Safran)	
Visual similarity	Re-identification (ATOS)	





Credit : Confiance.ai

Scientific challenges of confiance.ai

- **confiance.ai:** methods and tools for trusted AI.
- High expectations for industry
- **3 groups** of **scientific challenges** to cover all aspects of trust

    1) **Trust and learning data**
    2) **Trust and human interaction**
    3) **Trust and AI-based system engineering**

- Organization in **7 projects:**
    - EC1: Integration & **use cases**
    - EC2: Process, **methodology** and guidelines
    - EC3: Characterization & **qualification** of trustworthy AI
    - EC4: **Design** for Trustworthy AI
    - EC5: Data, information and knowledge **engineering** for trusted AI
    - EC6: **IVV&Q** strategy toward homologation / **certification**
    - EC7: Target **Embed**ded AI

Scientific challenges as part of the ongoing PhD theses within confiance.ai

- **confiance.ai:** methods and tools for trusted AI ➔ High expectations for industry
- many scientific challenges (as part of the confiance.ai doctoral programme)
  - **Data** coverage and operational **domain design** ODD in Computer Vision (PhD Theis of Adrien Le Coz)
  - **Robustness** to ‘patch’ adversarial attacks in Computer Vision (PhD Thesis of Paul La Barbarie)
  - Robust **Reinforcement** learning (PhD Thesis of Lucas Schott)
  - Statistical control of **Fairness**/Bias in Machine Learning (Stat) (PhD Thesis of Gayane Taturyan)
  - Towards hardware **deployment** using BO & Neural Architecture Search) (PhD Theis of H Ouertatani)
  - **Monitoring** of (deployed) AI algorithms using conformal prediction (PhD Thesis of Abdelmouaiz Tebjou)

Confiance.ai : Key figures

4 YEARS

Duration

9

Large industrial groups

4

Research centers

7

Thematic projects

+300

FTP involved over 4 years

2

Sites: Paris-Saclay and Toulouse

45 M€

Budget

12

Associate partners (laboratories, SMIs, startups)

Outline

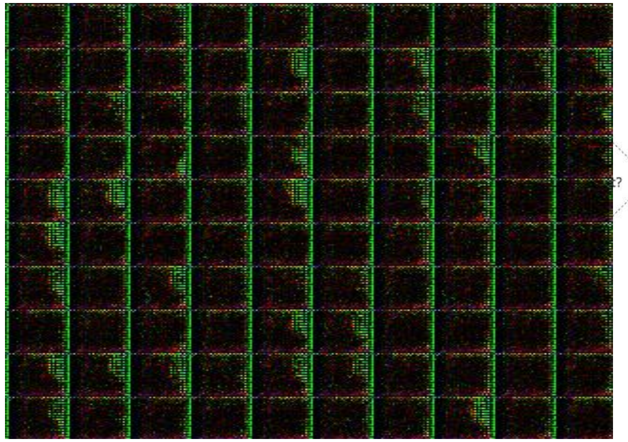
Challenges and industrial applications in

- Hybrid AI: How to exploit industry knowledge of physical (scientific) and symbolic (semantic) nature in data-driven learning models.
- Trustworthy AI: Towards integrating AI into critical system engineering
- Generative AI for industry: How to evaluate and advance specialized generative AI models for industrial applications

GenAI : AE, GANs, Diffusion Models, Transformers

*__GANs__ (Goodfellow 2014): A **generator G** and a **discriminator D** subjected to two contradictory training (ie. *adversarial* aspect)

- ➔ impressive results in images,…
- ➔ **IRT** work advancing the state of the art on the subject: in particular, work on EPI, RTI Confiance.AI/EC3,4,5 projects.

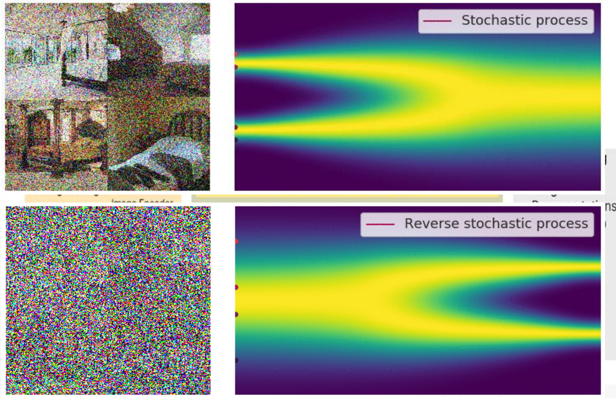


OpenAI

*__Diffusion models__ (Ho 2020; Yang 2023; Rombach 2022): an unintuitive principle at the basis : progressively **destructure** the input

until it is completely degraded,
then **reconstruct** it by reversing the process.

- ➔ Excellent performance in image synthesis, despite costly training
- ➔ Research work at**IRT** (Confiance.AI, EC4/Explo; e.g. NeurIPS'23)

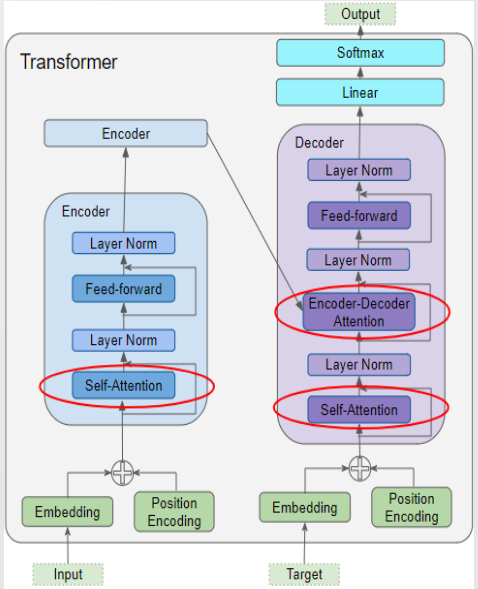


Yang Song Blog

*__Transformers__ (Vaswani 2017): have revolutionized generative AI, particularly in NLP.

- ➔ highly parallelizable (unlike sequential architectures like RNNs)
- ➔ Use an AE and relies on **an attention mechanism** to integrate global I/O and context dependencies into a variable-length sequence.
- ➔ High NLP capabilities {eg. ChatGPT-3.5: responses of up to ~ 3000 words}.
- ➔ NLP models and transformers are studied in R&D at IRT

(eg. Confiance.AI, SMD)



Generative AI for Industry : Main challenges

- **Main scientific challenge in GenAI in industry** (Hybridization, Frugality, Multimodalities, Evaluation/Benchmarking, ..)
    - the **frugality** of foundation models (related to data, model, and learning),
    - operating on different **multi-modalities** (beyond text : time-series, diagrams, images..),
    - their **hybridization** to integrate knowledge (expert and or scientific **knowledge**),
    - their **specialization** (eg. fine-tuning, RAG) to different **use cases**,
    - and their **evaluation** to guarantee industrial use,
- Preparation to the implementation of the AI act
- Hybrid AI (GenAI, Physics-Simulation, Data augmentation, Uncertainty Quantification, ..)

Discussion

- **Hybrid AI**, with its inclusive approach to human knowledge, overcomes the limitations of “classic” AI (based exclusively on data) : The
  - **accuracy** of physical simulations can be improved by hybrid modeling that takes advantage of data.
  - joint use of data and scientific laws **reduces the complexity and cost** of physical simulations.
  - joint use of data & knowledge graphs enables **business expertise to be integrated** and results to be **explained**.
- Approaches that hybridize data and knowledge models (physical/semantic) have emerged fairly recently, and **have not yet reached maturity ==>** R&D efforts are needed to bring the subject to maturity in engineering/industry.
- An avenue in AI to the preparation of the implementation of the AI act for the entreprise, is Trusted AI. Need for the Human in the loop
- **Generative AI** is beginning to make slight progress in industry...

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