Accélérateur
de la transformation
numérique

On some approaches of deep learning for physical simulation in Industry

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Workshop « Leveraging AI-based Physical Simulation for Industry »
Versailles, November 9, 2023

AI, Data, Robotics Forum
#ADRF23

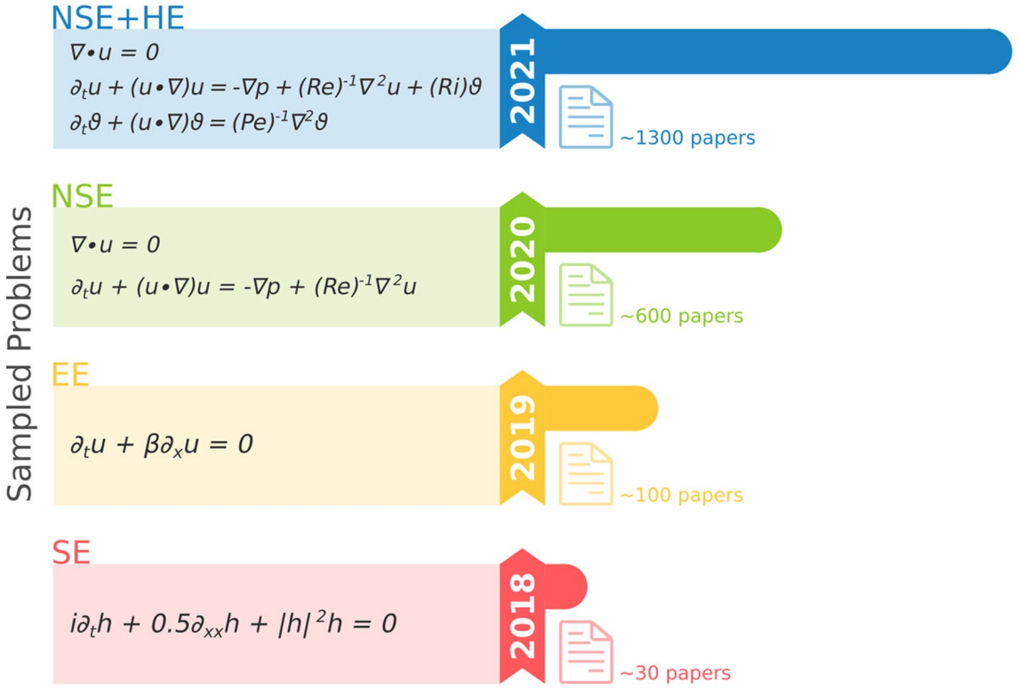
Outline

- Scientific challenges and Approaches
- Industrial context
- SystemX's Contributions
- Perspectives

Scientific Context: Physics-Informed Machine Learning

➔ Enable 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 modeling: combining ML and Physical Simulation

In engineering, it allows

➔ the integration of analytical knowledge derived from physical laws governing the studied systems,

- to augment th statistical knowledge learned from observed/measured data
- for reducing the high cost of physical simulation, in particular in the industrial sector

➔ *Promising* : 1st recommendation from the French Academy of Technologies in its 2020 report:

It will be ncessary to build hybrid approaches, combining basic physics and learning:
i.e. Knowledge and physico-mathematical modeling <u>With</u> Information extracted by deeplearning from data.

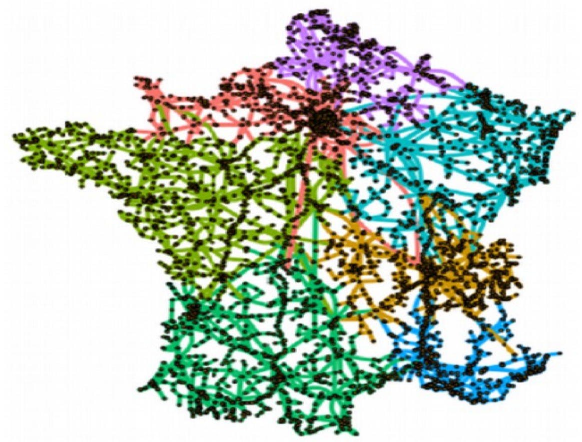
➔ Despite its scientific challenges, this hybridization is suitable for numerical simulation in the industrial sector

«Calcul et données : nouvelles perspectives pour la simulation numérique à haute performance,» Rapport de l'Académie des Technologies, Décembre 2020. ISBN : 979-10-97579-23-4. Lire en ligne

ML for Physical Simulation in Industry

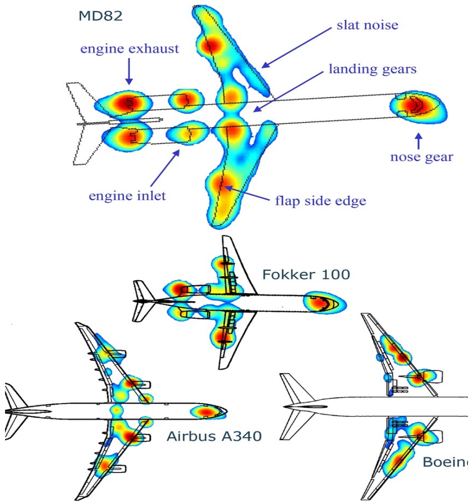
- Covering various fields in physics (mechanics, fluid dynamics, aerodynamics, electromagnetism …)
- In a wide variety of Applications in industry, in particular in numerical simulation

Electricity (power grids)



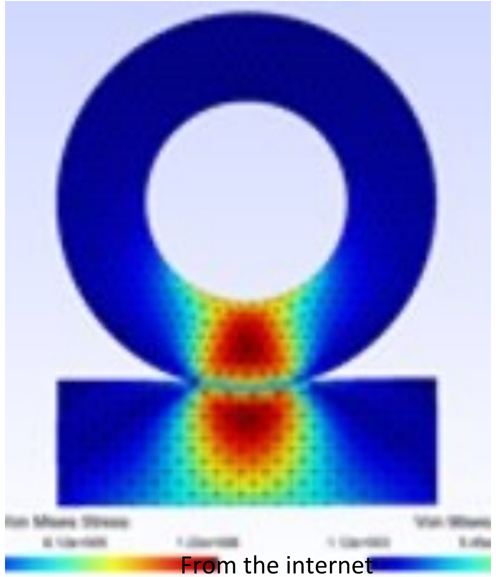
Picture from Marot, A., et al. (2018, October). Guided machine learning for power grid segmentation. In *2018 IEEE PES Innovative Smart Grid Technologies Conference Europe (ISGT-Europe)* (pp. 1-6).

Aerodynamics



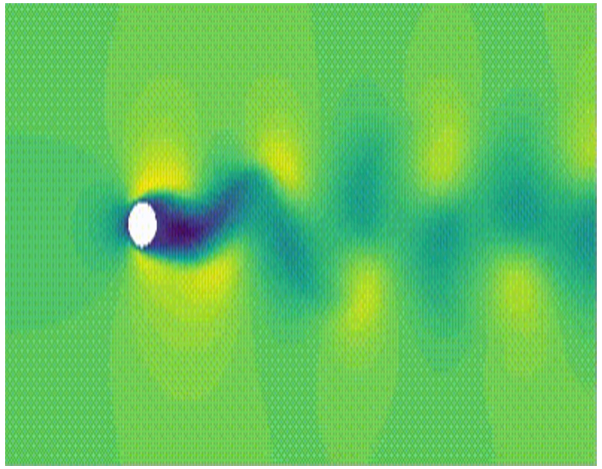
Merino-Martínez *et al. CEAS Aeronautical* Journal (2019).

Solid Mechanics pneumatics



From the internet

Fluid Flows/Dynamics



Picture from Emmanuel Menier

Challenges : Physical systems that are
- Complex to model/solve analytically

- Compuationally expensive to solve numerically

eg. , Computational Fluid Dynamics – CFD, Turbulance, Flows

Scientific Challenges
- Problems highly-nonlinear, high-dimensional, with complex structures (eg. organized in graphs…
- Need for adapted NN architectures: Graph NNets, Deep AE ..

Deep NNets for Unsupervised representation Learning

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

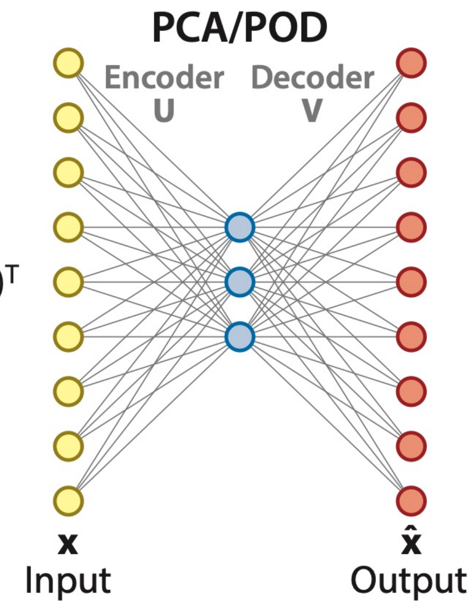
Shallow / Linear

$$\bar{\mathbf{x}} = \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n$$

$$\mathbf{S} = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n - \bar{\mathbf{x}})(\mathbf{x}_n - \bar{\mathbf{x}})^T$$

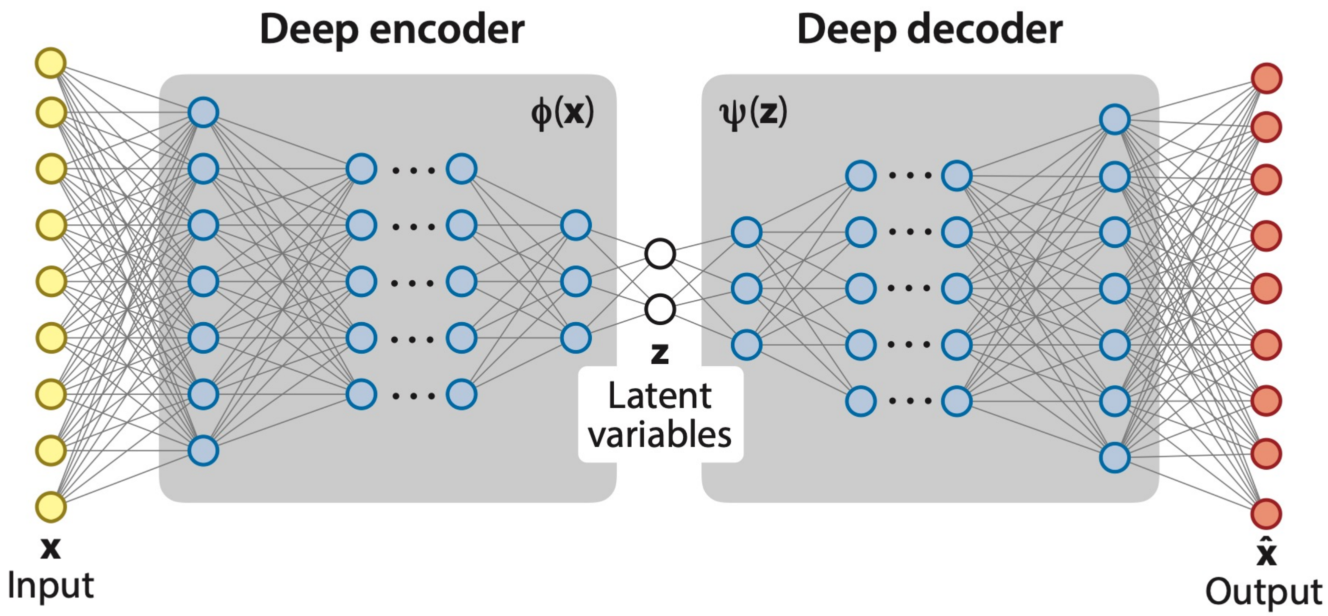
$$\mathbf{S}\mathbf{u}_i = \lambda_i \mathbf{u}_i$$

Retain $M < D$ eigenvectors



POD: proper orthogonal decomposition
PCA: principal component analysis

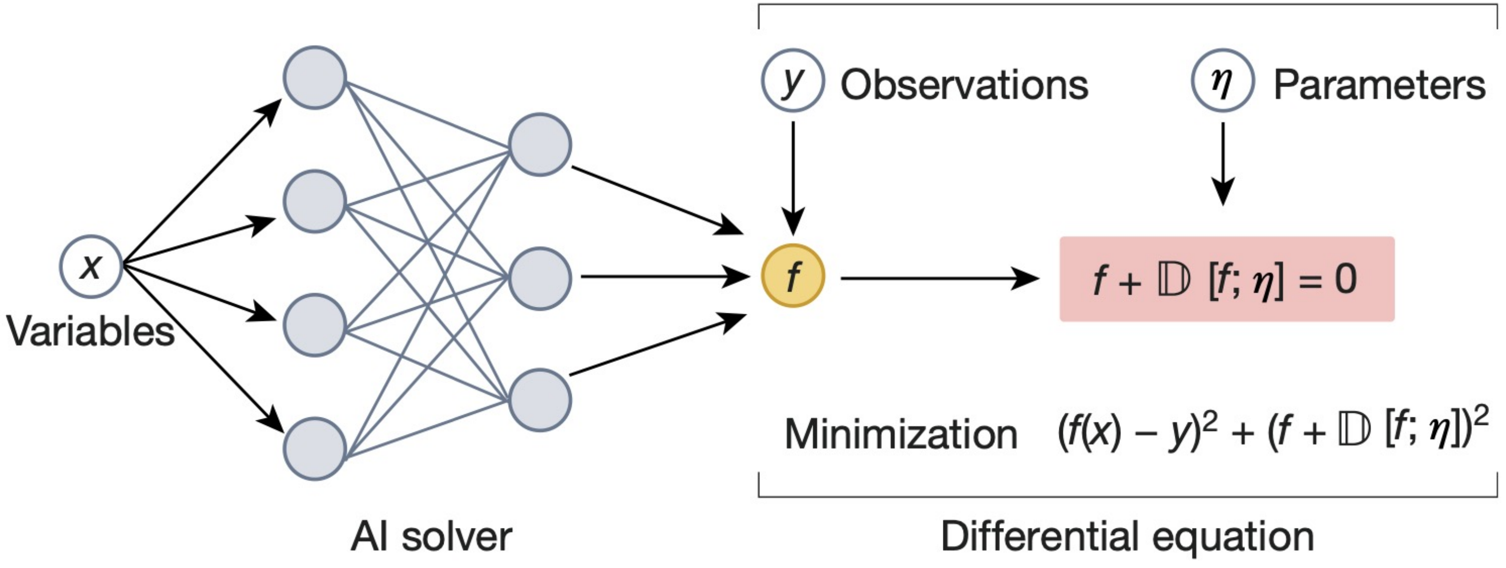
Deep / Non-Linear



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

Hybrid ML modeling for solving Partial Differential Equations



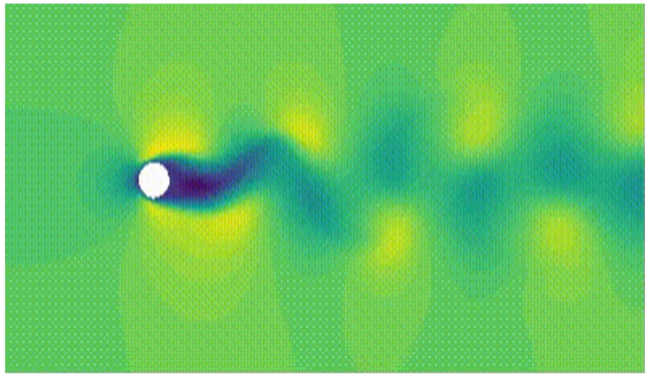
- Eg. Learning Computational Fluid Dynamics

- 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



Simulation from Emmanuel Menier

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 **D(*f;η*)** is unknown (parameterized by ***η***), it can be estimated by solving a multi-objective loss that optimizes both the functional form of the equation and its fit to observations ***y***.

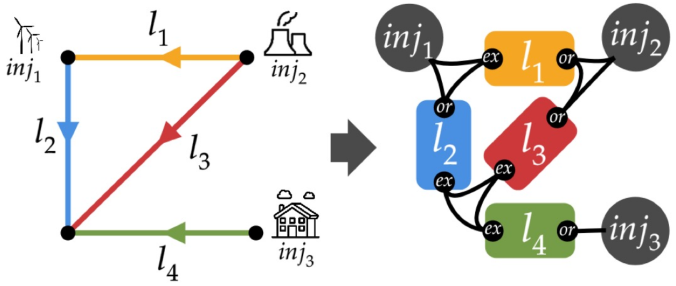
Wang & al. (2023). Scientific discovery in the age of artificial intelligence. Nature, 620. Read Online

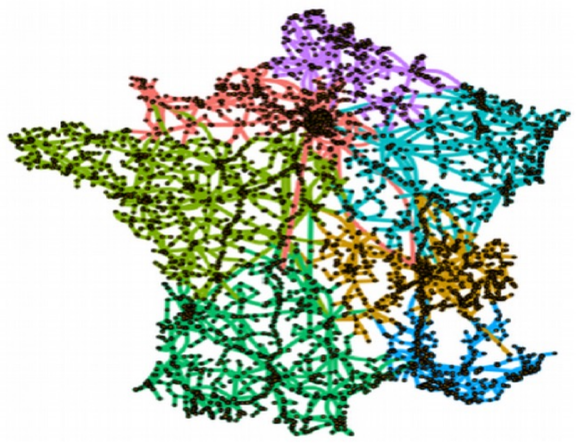
Hybrid ML and Physical Simulation in Industry

Eg. Deep Statistical Solvers (DSS)

Context: Simulation of a Power Grid flow

Problem:
Given injections (productions and consumptions) inj_1, inj_2, inj_3, compute the flows of electricity in all lines l_1, l_2, l_3, l_4.





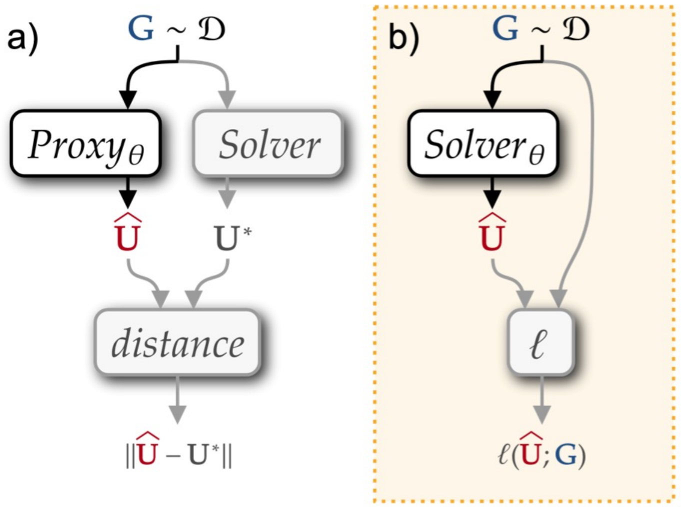
Picture from Marot, A., et al. (2018, October). Guided machine learning for power grid segmentation. In *2018 IEEE PES Innovative Smart Grid Technologies Conference Europe (ISGT-Europe)* (pp. 1-6).

The "proxy" approach (SoTA): learning from known solutions of the problem, provided by a classical solver.
➔ Cons: needs a huge number of training examples (*i.e., **U^(G)**):* too costly to obtain and no exact solutions

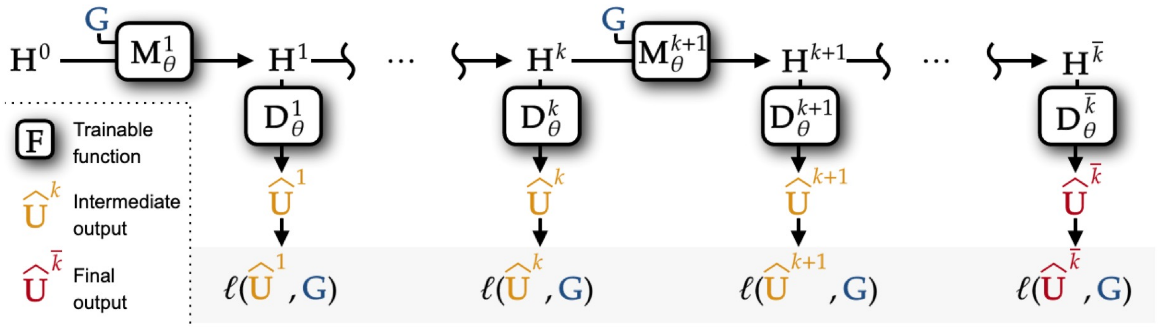
➔ The **DSS** directly trains $Solver_\theta$ by minimizing the loss ℓ with no need for such examples.

Learn the *states* **U**$=(U_i)$
of the Interaction Graph **G** :

$$\mathbf{U}^\star(\mathbf{G}) = \underset{\mathbf{U}\in\mathcal{U}}{\operatorname{argmin}}\ \ell(\mathbf{U},\mathbf{G})$$



Proxy approach (a) *vs. Deep Statistical Solver* - DSS (b)



Graph Neural Network architecture of a DSS

- 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

Contributions @ SystemX: The Research Program IA2

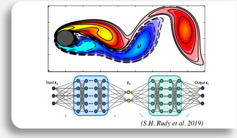
Intelligence artificielle et ingénierie augmentée

Artificial Intelligence
an Augmented Engineering

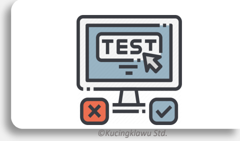
- a program with **6 R&D collaborative projects** based on concrete **industrial** use cases
- Area: Hybrid AI

Advance project
Thesis / Postdocs / Shared work

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

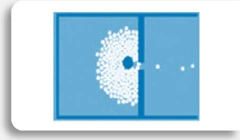


AFS: Agility and fidelity of simulations
How to imporve agility and fidelity of simulation in complex systems design? 02



S2I: Industrial infrastructure supervision
How to improve decision-making on distubuted industrial systems via machine learning technices ? 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 the expert 06

Credit to IA2 Program

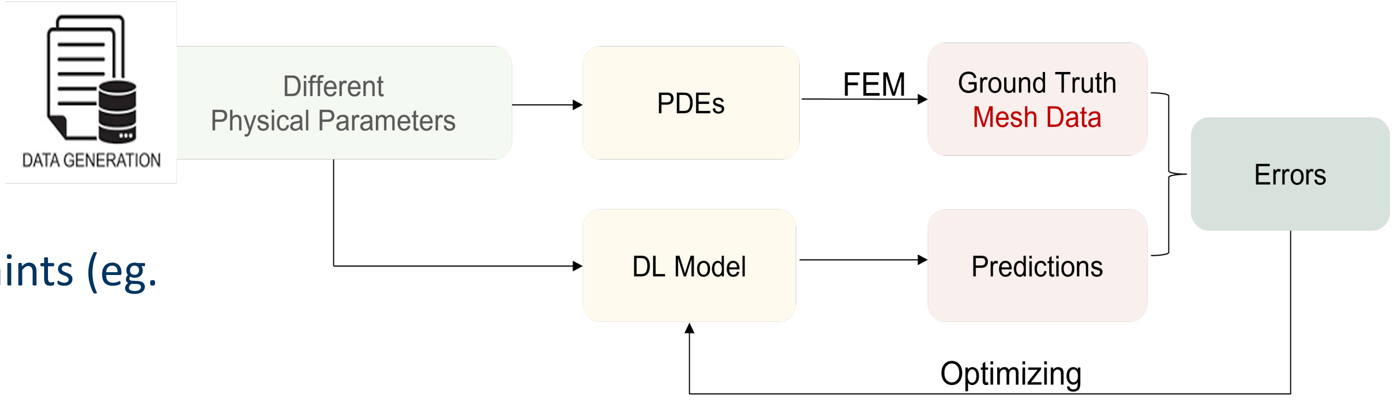
Hybrid Machine Learning for Physical Simulation in Industry

Challenges

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

Possible solutions (studied as part of the **HSA project**):

- Hybrid Machine Learninrg as surrogate models for physical simulation, aiming to Replace physical solvers with



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

Data-driven methods to solve PDEs. PhD thesis of W. Liu 2023 (LISN, INRIA/SystemX).). [Read Online]

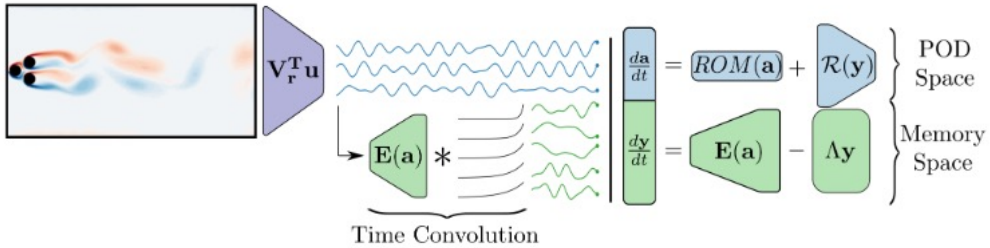
HSA Project : Simulation/machine learning hybrid modeling

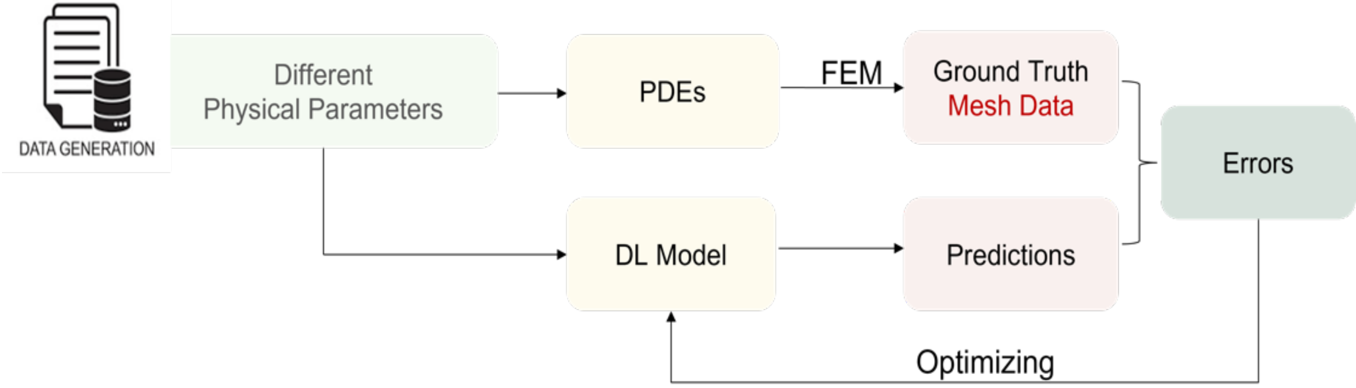
Intelligence artificielle et ingénierie augmentée

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

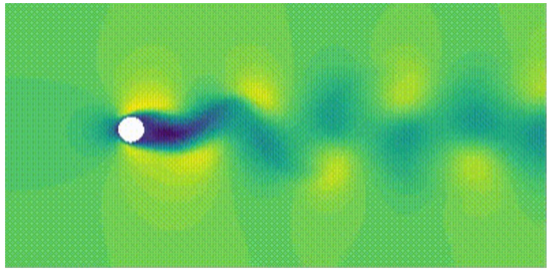
- Augementing/Replacing physical solvers with data-driven models that integrate physical constraints
- Hybrid Machine Learninrg as surrogate models for physical simulation

=> Deal with high-dimensional, non-linear, and complex structured systems (e.g reduced modeling, ..)





High-Dimensional non-linear Physical Equations



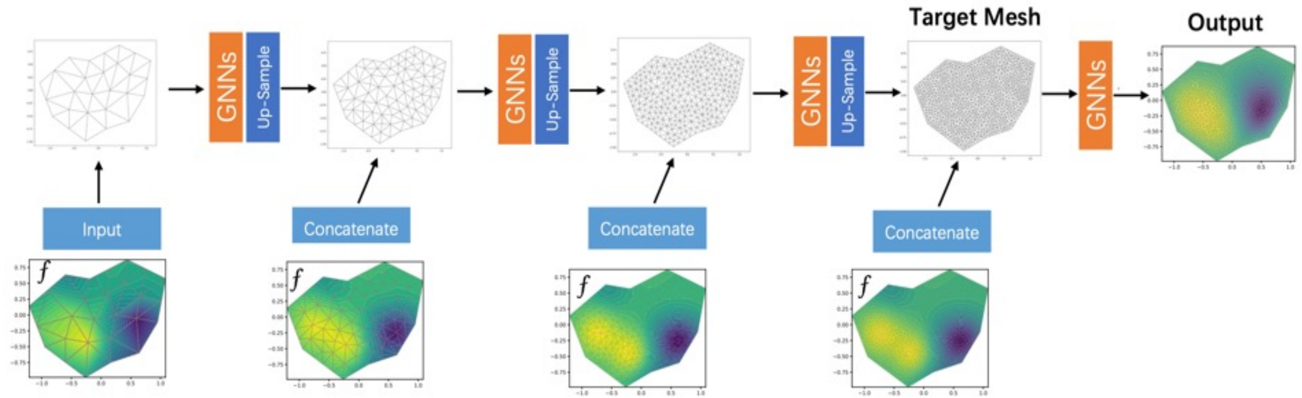
Deep Graph Neural Networks for Numerical Simulation of PDEs
PhD thesis de W. Liu. 2023 (LISN, Inria/SystemX). Read Online

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

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

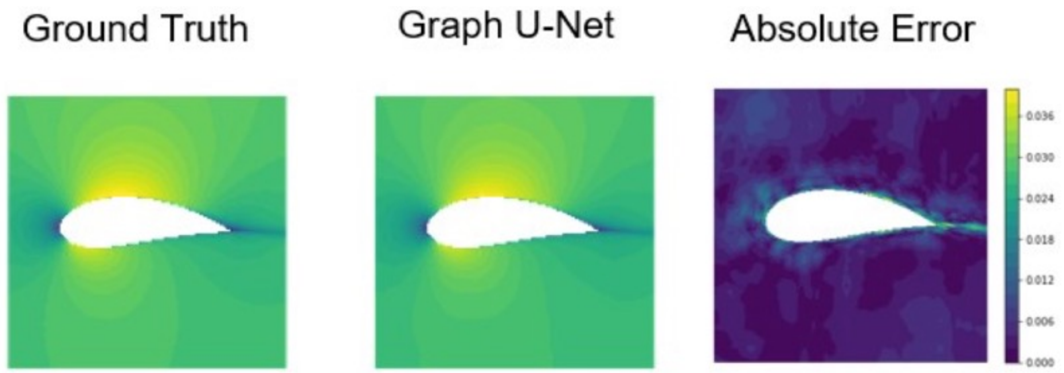
Project HSA : simulation and deep learning of graphs

Graph Neural Nets for 3D **meshes**
More suitable, as they operate by construction on graphs



Prediction of the air**flow** profile around an aircraft wing (Air Foil)

Physics: Navier-Stokes equations



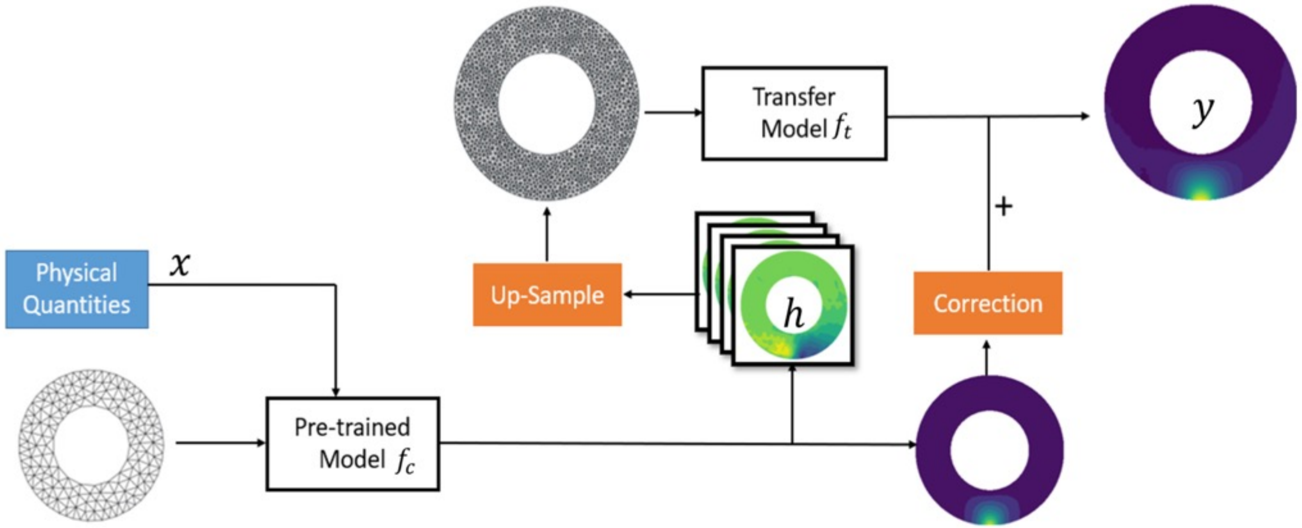
PhD theis of W. Liu, 2023 (LISN, Inria/SystemX)

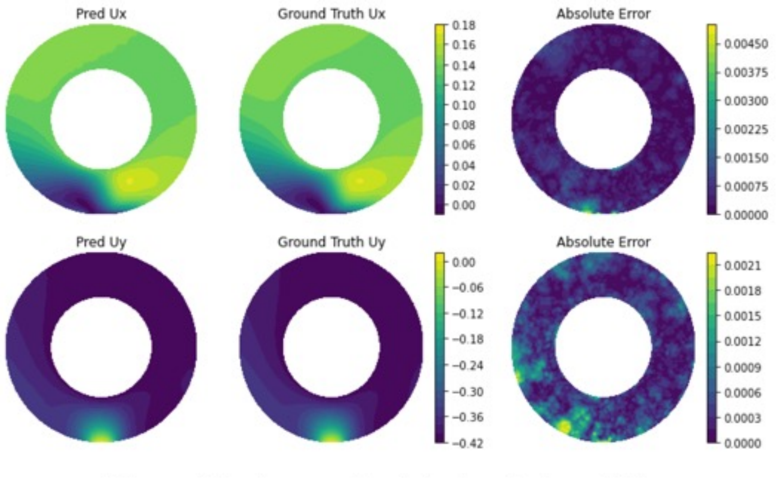
HSA Project: Hybridization and transfer learning

- 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

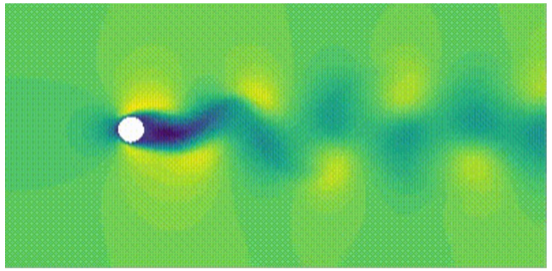
Physics: contact equations





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

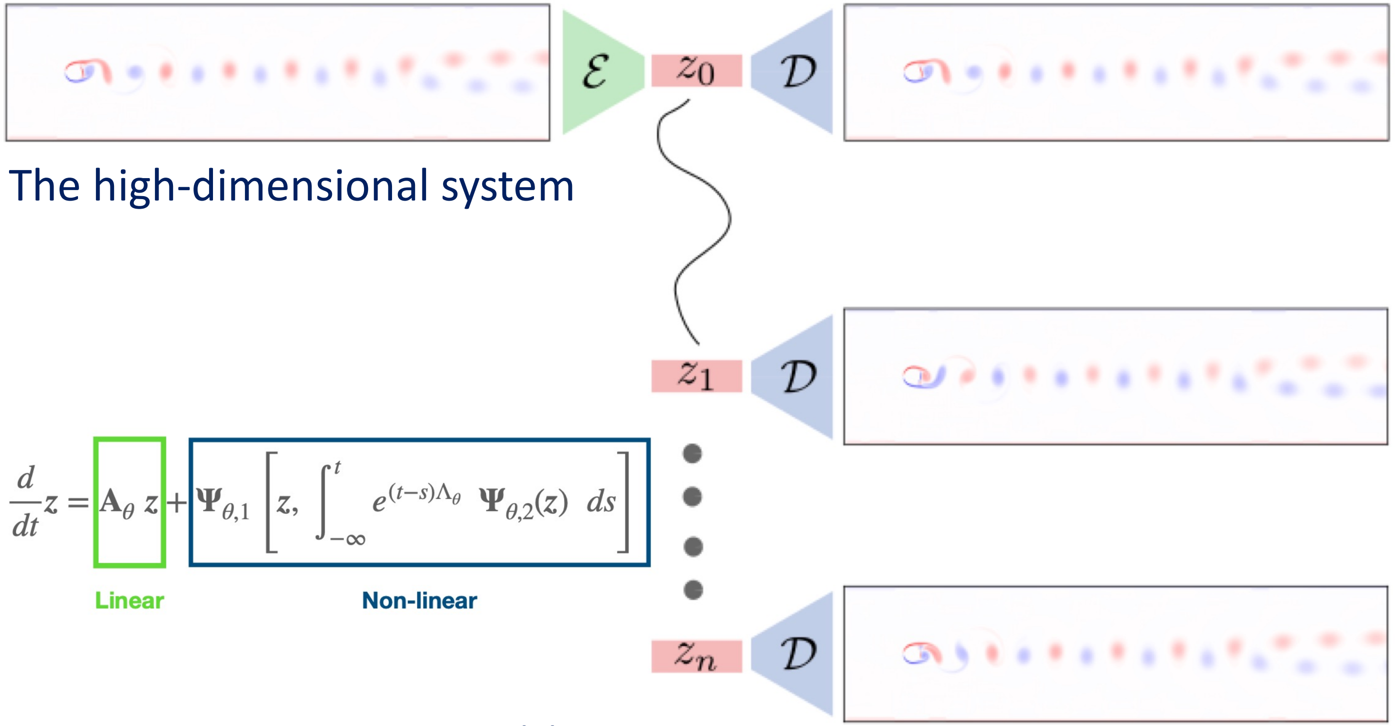
Dynamics: Hybrid ML for HD dynamical physical systems



High-Dimensional non-linear Dymical Systems:

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

Interpretable learning of effective dynamics (ILED) architecture:



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

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]

Perspectives worth exploring

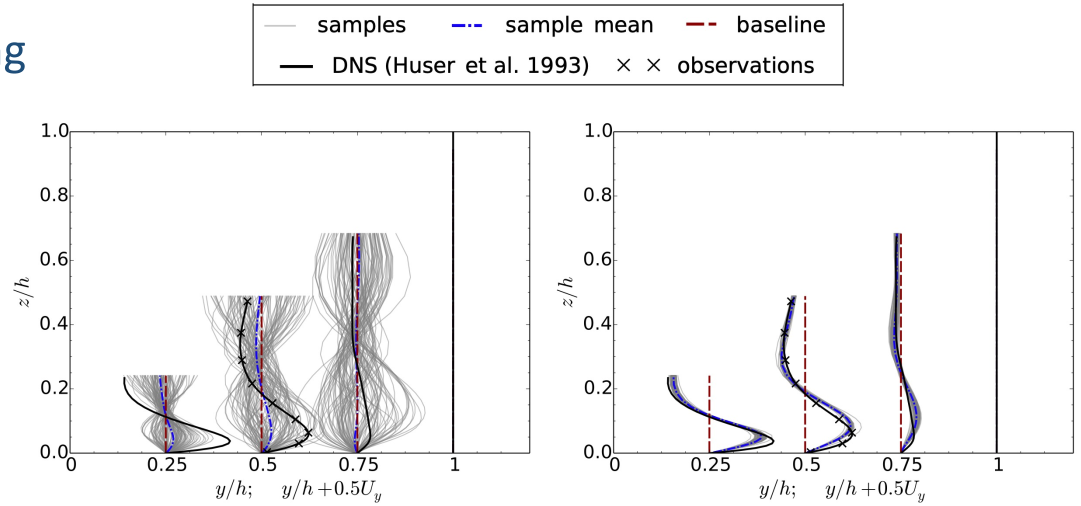
Topics for progress: Uncertainty Quantification (UQ)

➔ UQ should be inherent to hybrid models and systems engineering

- quantify and guarantee desirable learning and prediction performance, by characterizing/controlling data and model bias

➔ **Bayesian learning** is a principled framerwork to account for uncertainty

Eg. posterior ensemble mean prediction improves upon prior ensemble mean and the baseline
RANS - Reynolds-Averaged Navier–Stokes prediction



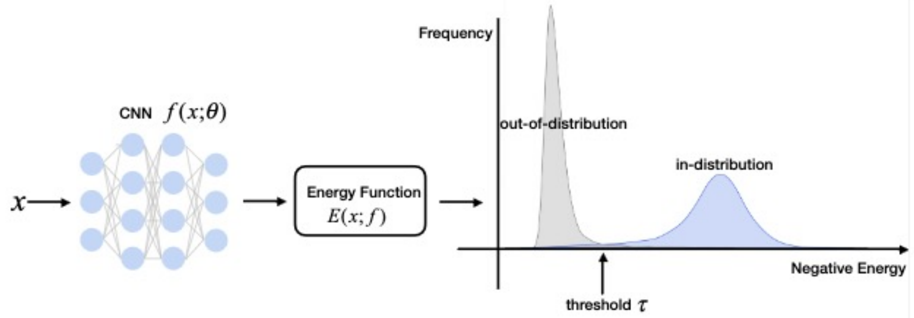
(Left) Prior velocity ensemble and (Right) posterior velocity ensemble with comparison to baseline (RANS) and benchmark results

Xiao, H. et al., .(2016). Quantifying and reducing model-form uncertainties in Reynolds-averaged Navier–Stokes simulations: A data-driven, physics-informed Bayesian approach. *Journal of Computational Physics*, *324*, 115-136. [Read Online]

➔ Beyond the Bayesian approach of learning

- e.g., UQ **anomaly detection**, **monitoring**, through deep architectures with probabilistic constructions to detect distribution deviations

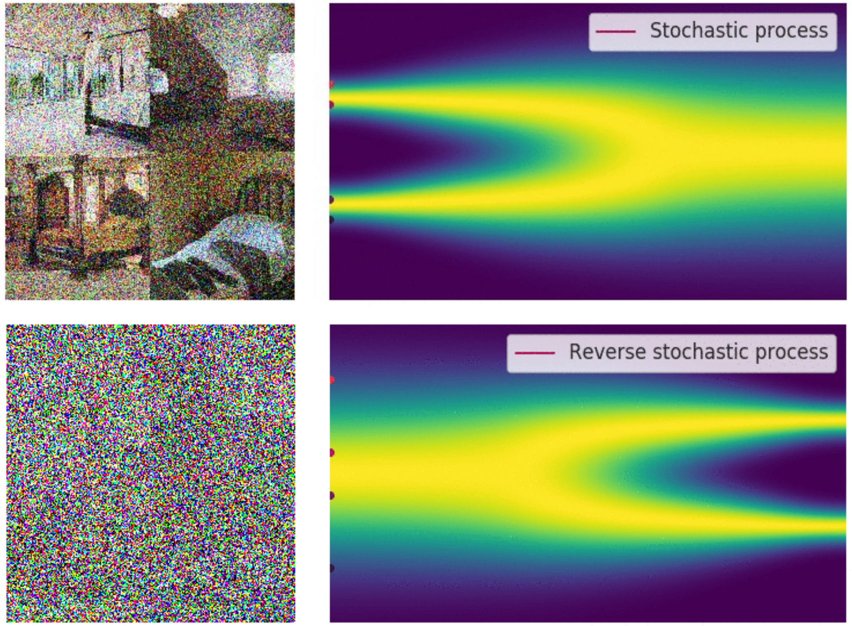
(Out OF Distribution - **OOD**)



Liu et al. (2020), Energy-based Out-of-distribution Detection, NeurIPS. [Read Online]

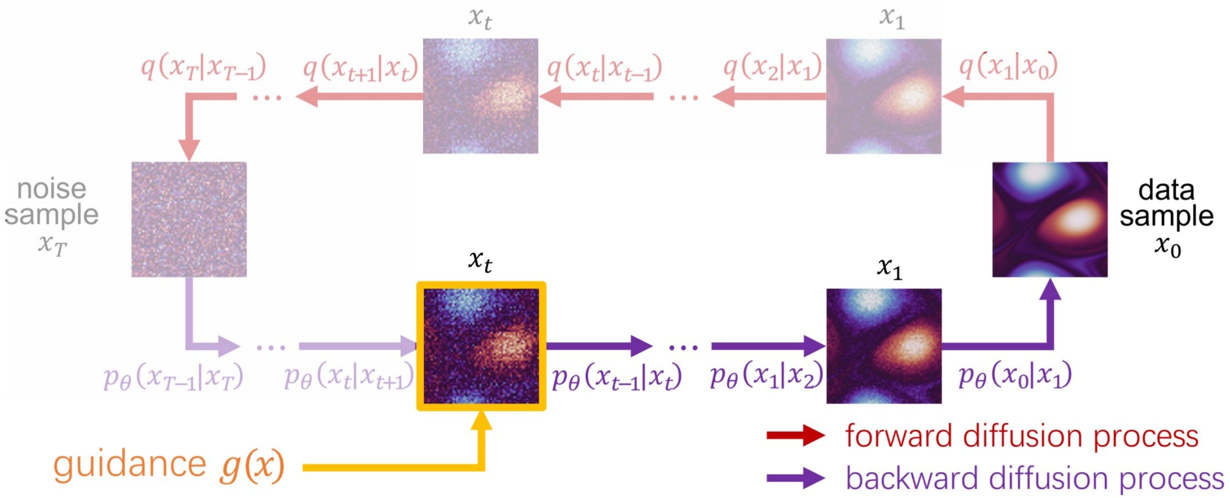
Hybrid Generative AI: a topic worth exploring

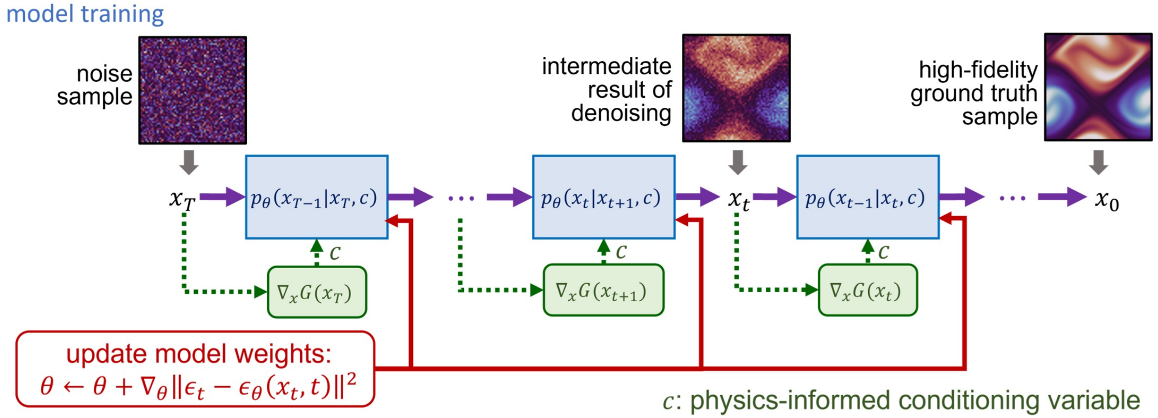
1. Generative approach to Improve the quality of physical simulation samples



Yang Song Blog

high-fidelity CFD data reconstruction from low-fidelity data using **DDPM-** Denoising Diffusion Probabilistic Model model





* **Denoising Diffusion Probabilistic Model** : a principle that is not very intuitive at first: progressively destructure the input until it is completely degraded, then reconstruct it by reversing the process.

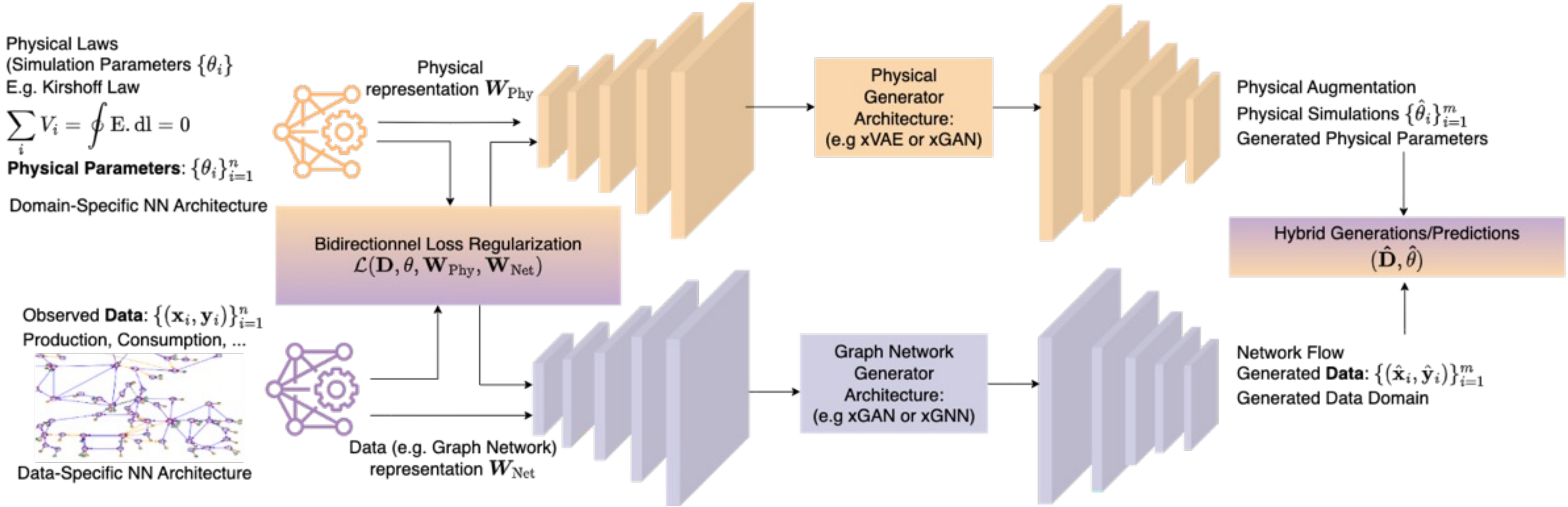
➔ Excellent in image synthesis, despite a costly training (MCMC to learn the iverse transition distribution $q(.|.)$)

Ho et al. 2022. Denoising diffusion probabilistic models. Adv. NeurIPS., 33 (2020), pp. 6840-6851. 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

Hybrid Generative AI: a topic worth exploring

- 2. Generative Models for the augmentation of physical simulation
- 3. Data augmentation to improve learning quality and reduce the cost of physical simulation



A potential architecture for a generative hybdrid ML/physical model to augmented simulation

An upcoming workshop on the topic

Call for participation and abstract contributions:

3rd International Workshop on
Artificial Intelligence Advanced Engineering (AIAE'2023)

7/12/2023 at Institut Pascale Saclay. Free registration

Possible abstract contribution and presentation
Deadline for abstracts 16/11,

Website: https://aiae23.sciencesconf.org/

Intelligence artificielle et ingénierie augmentée

Thank you for your attention!