Dati, Calcoli & Intelligenza Artificiale per i Gemelli Digitali

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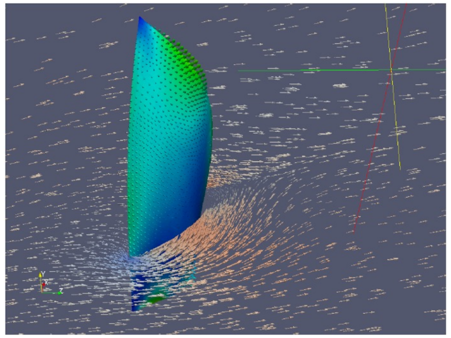
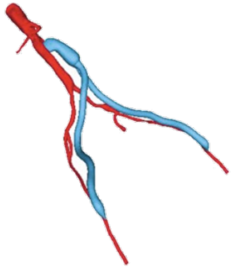
Introduction and Leading Motivations

Leading Motivation: Computational Sciences challenges

- **Reduced Order Modelling** is a quickly emerging field in applied mathematics and computational science and engineering for speeding up **Numerical Simulations**

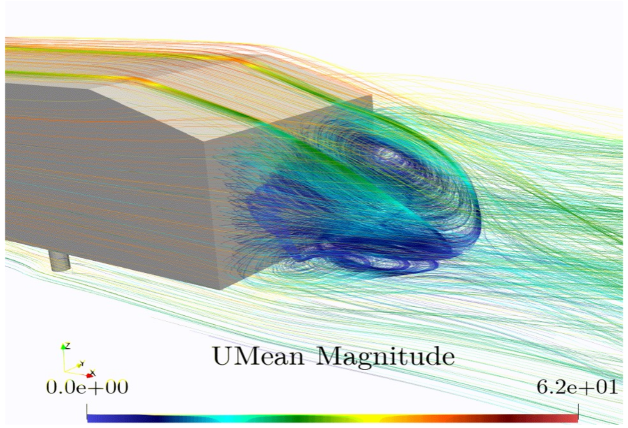
- Growing demand of
  - **efficient computational tools**
  - **many query** and **real time** computations
  - **parametric formulations**
  - **uncertainty quantification**
- The need of a computational collaboration rather than a competition between **High Performance Computing** (HPC) and **Reduced Order Methods** (ROM), as well as Full/High Order and Reduced Order Methods.



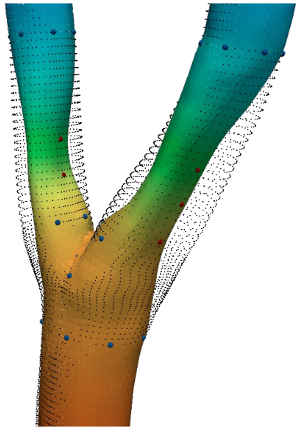


Physical Parametric Differential Problems Overview

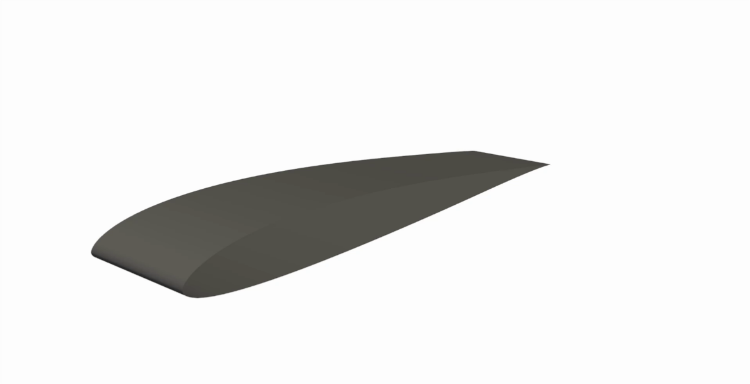
Parametric Differential Problem are ubiquitous in many field of Natural Science from **naval** and **nautical** engineering, to **aeronautical** engineering and **industrial** engineering.



automotive



biomedics



aeronautics

References:

1. *Rozza, Gianluigi, Giovanni Stabile, and Francesco Ballarin (2022) eds. Advanced Reduced Order Methods and Applications in Computational Fluid Dynamics. Society for Industrial and Applied Mathematics.*

SISSA mathLab: our current efforts and perspectives

Goals of our research group:

- ➔ Face and overcome **several limitations** of the state of the art for parametric ROM by means of **Deep Learning**
- ➔ Improve capabilities of reduced order methodologies for **more demanding applications** in industrial, medical and applied sciences settings
- ➔ Carry out important **methodological developments** in Numerical Analysis, with special emphasis on **mathematical modelling** and a more extensive exploitation of Computational Science and Engineering

- ➔ Focus on Computational Fluid Dynamics as a central topic to enhance broader applications in multiphysics and coupled settings (e.g. aeronautical, mechanical, naval, cardiovascular surgery, …)

Towards real-time computation (hardware)

OFFLINE (full order)
High Performance Computing

- **Very expensive** and time demanding;
- basis calculation done once after suitable parameters sampling (ex: **Proper Orthogonal Decomposition, RB, PGD**, ...);
- *HPC facilities.*

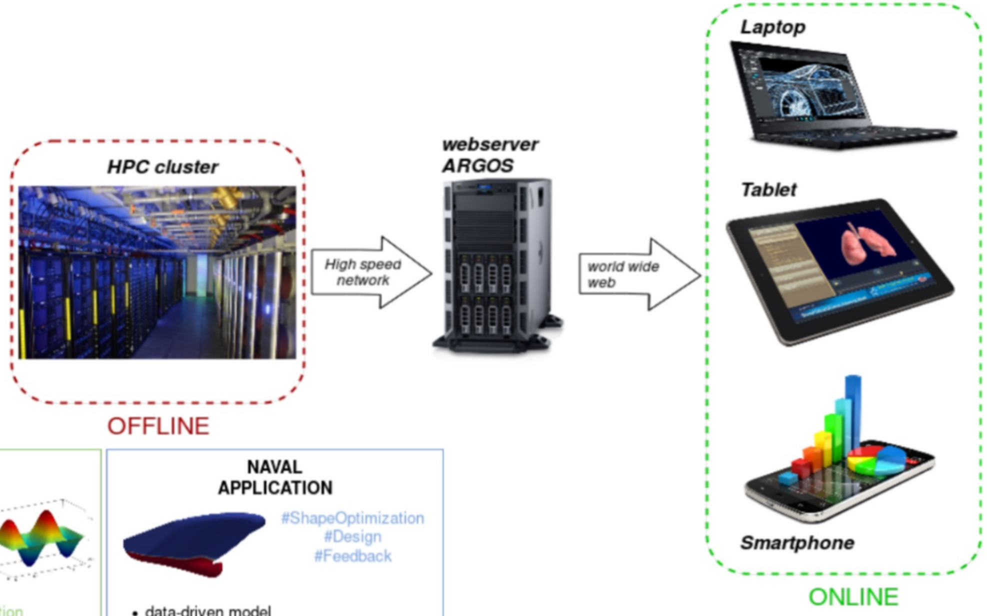
ONLINE (reduced order)
Advanced ROM techniques

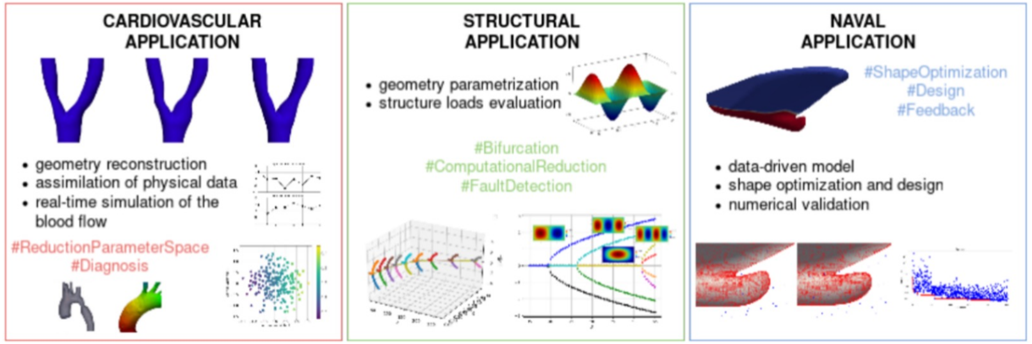
- **Extremely fast**;
- **real-time** input-output evaluation;
- computational **webserver** via browser;
- *in situ, tablets or smartphones.*

Computational Webserver/Computational Apps

Model order reduction for computational web server: to real world applications
argos.sissa.it

- HPC
- data science
- Digital twin
- SMACT Industry 4.0
- 3D Printing





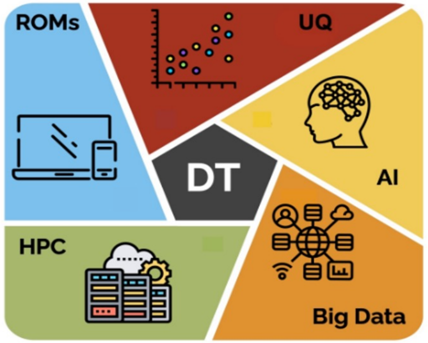
Digital Twin (DT): integration of emerging fields

A large amount of data (**Big Data**) can be collected, **Artificial Intelligence** (AI) can help to store and **organize** them (data-driven approaches).

By using **black box models**, AI techniques are able to find **fitting functions**. They do not require knowledge about the physics of the problem, even if we do prefer integrated "**Big Models**" Physics informed approaches.

The development of **High Performance Computing** (HPC) and its integration with reduced order models allowed to reach better performances.

* **Uncertainty quantification** (UQ),
* **Data analytics**,
* **Artificial intelligence** (AI),
* **Digital Twins** of products and processes.

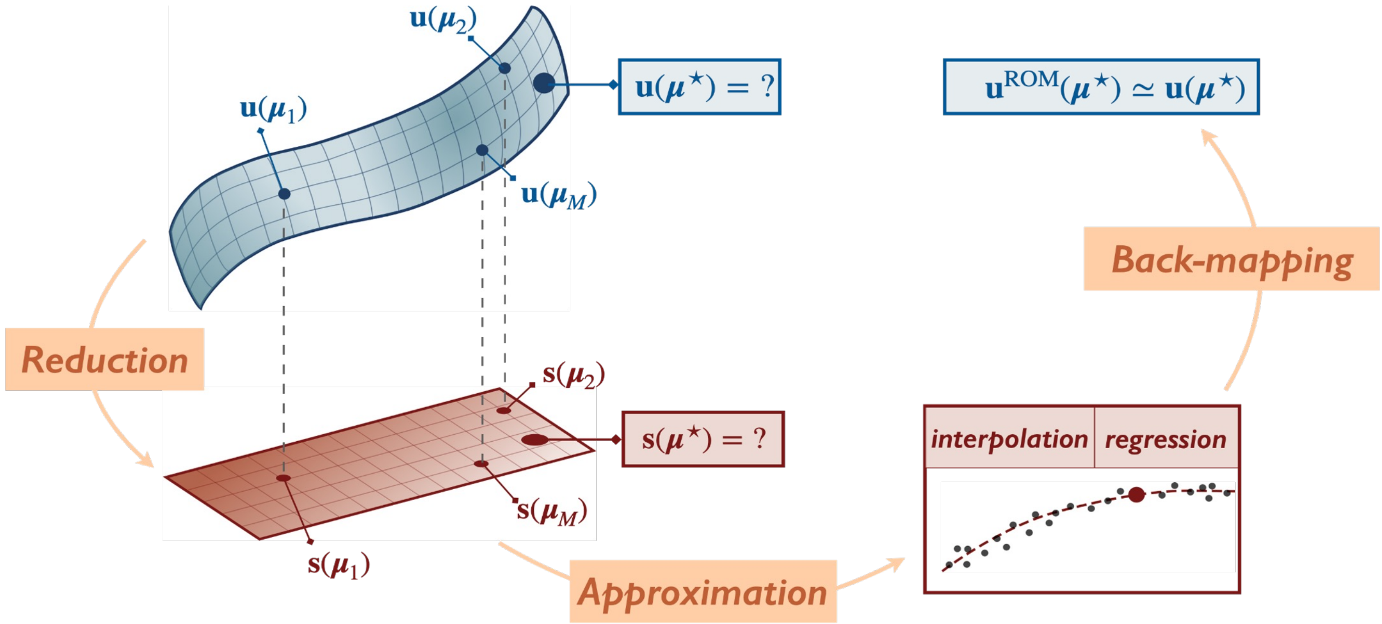


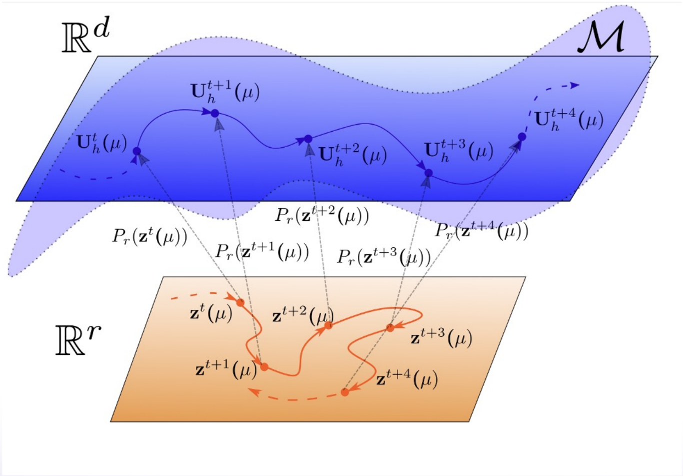
Thanks to ROMs we have a more sustainable framework, energy savings, reduced computational times and resources.

The Data-Driven Approach to Reduced Models

ROM approximate the high dimensional solution manifold by dimensionality reduction and perform interpolation to predict for unseen parameters

- ➔ Reducing Parameter Space
- ➔ Applicable for Sensor and Incomplete Data
- ➔ Fast Online Phase





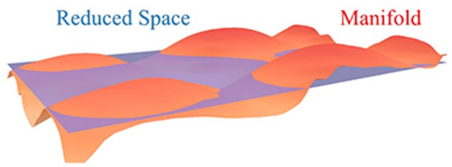
SISSA mathLab: our current efforts and perspectives

➔ Development of new open-source tools based on reduced order methods:
  - **ITHACA**, In real Time Highly Advanced Computational Applications, as an add-on to integrate already well established CSE/CFD open-source software
  - **RBniCS** as educational initiative (FEM) for newcomer ROM users (training).
  - **Argos A**dvanced **R**educed order modellin**G O**nline computational web server for parametric **S**ystems
  - **PINA** a deep learning library to solve differential equations
  - **EzyRB** data-driven model order reduction for parametrized problems
  - **PyDMD** a Python package designed for Dynamic Mode Decomposition (in collaboration with University of Texas, CERN, and University of Washington)

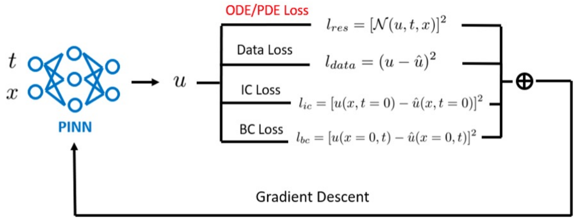
PINA ITHACA ITHACA - FV PyDMD ITHACA-DG RBniCS multiphenics ARGOS ATLAS EZyRB

Reduced Order Models enhanced by Deep Learning and Scientific Machine Learning

Scientific Machine Learning for PDEs



Linear Algebra based Reduced Order Models



Physics Informed Machine Learning

Symmetries, High Dimensional Systems, Stochastic Equations, …

2017

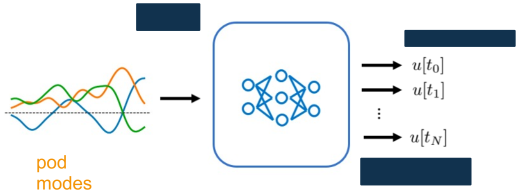
2021

< 2017

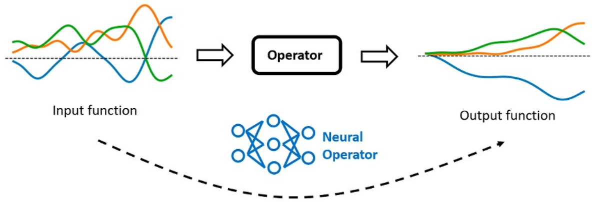
2019

….

Artificial Neural Networks as Reduced Order Models



Neural Operator Learning

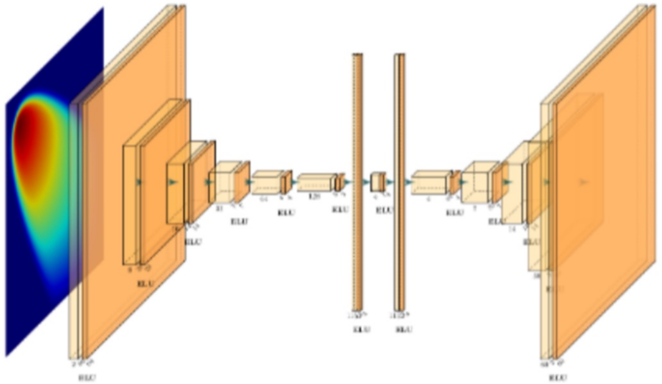


Enhancing ROM techniques by Deep Learning

Artificial Intelligence can **enhance** classical ROM techniques for **Computational Fluid Dynamics**

Enhancing data-driven reduction methods

- Approximation in Reduced Order Model (POD-NN, AE-NN)
- Automatic preprocess data for **dominant advection models**
- Auto-encoders for **dimensionality reduction** and **manifold learning**
- Reduction in **wide parameter space** by means of deep learning **parameter domain decomposition**



References:

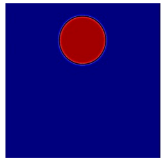
1. *F. Romor, G. Stabile, and G. Rozza, (2023). "Non-linear manifold ROM with Convolutional Autoencoders and Reduced Over-Collocation method." Journal Scientific Computing.*
2. *D. Papapicco, N. Demo, M. Girfoglio, G. Stabile, and G. Rozza, (2022). "The Neural Network shifted-proper orthogonal decomposition: A machine learning approach for non-linear reduction of hyperbolic equations.", accepted for Computer Methods in Applied Mechanics and Engineering.*

How to solve PDEs by Scientific Machine Learning

The **ML pipeline can be divided into four stages**

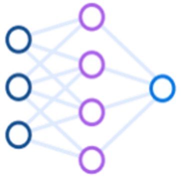
1. Select a **problem to solve** e.g. fluid dynamics, stochastic pdes, …
2. Generate the **data**, e.g. high fidelity simulations, scattered data from the domain, …
3. Build a **ML model**, e.g. NNs, POD + Interpolation, Neural Operators, …
4. **Optimize** the model, e.g. by Supervised, Physics-Informed losses and gradient descent

$$\partial_t \phi + \mathbf{u} \cdot \nabla \phi = 0$$

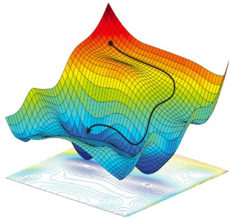


problem to solve

data generation



build ML model



optimization

How to solve PDEs by Scientific Machine Learning

Deep Learning can be a powerful tool for solving **Differential Equation** with l**ittle data.**

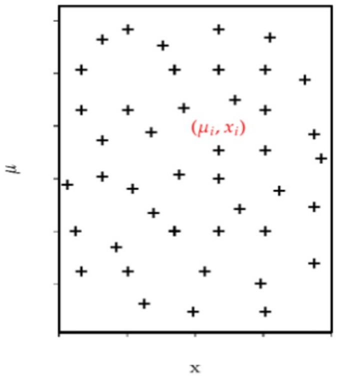
Physics-Informed Neural Networks

- Solving PDEs by including physical laws and symmetries in Neural Networks

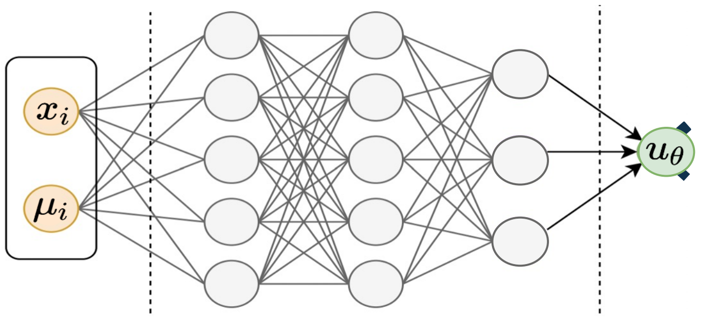
Deep Operator Learning

- Approximate PDEs operators leveraging neural networks
- Data-driven with possibility to make it physics-informed

PiNA



$$\{(x_i, \mu_i)\}_{i=1}^{N}$$



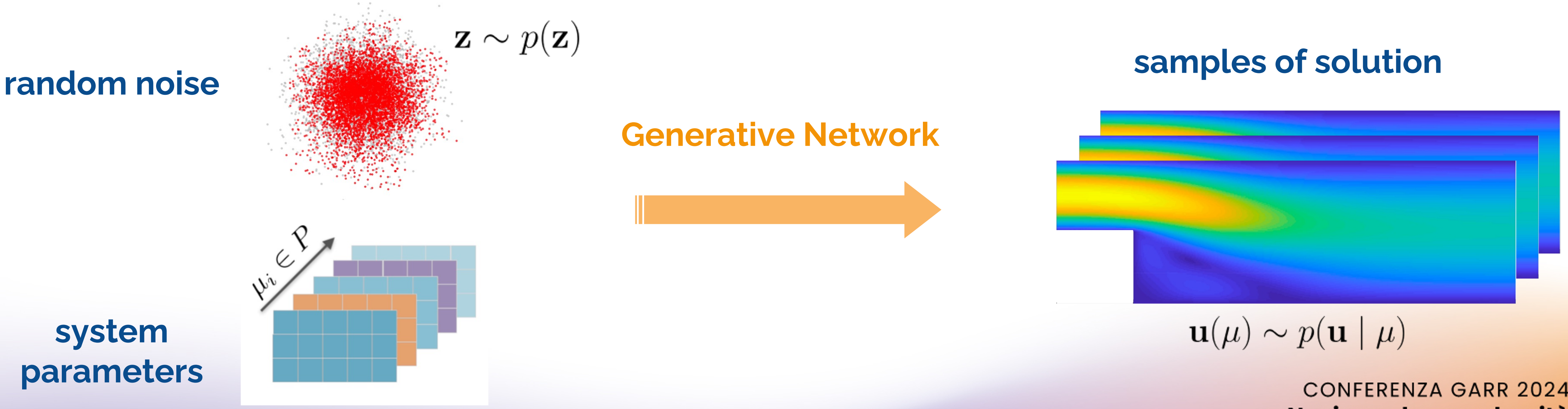
approximate solution

extract coordinates from the domain

pass it through a DL model

Generative Models – Quantify Model Uncertainty

- → Generative modelling learns **probability distributions** on the data, capturing the intrinsic characteristics of the original ones
- → **Generation of differential equation solutions** for parametric/time-dependent problems
- → **Optimize meshes** by preserving the structural properties and generating new ones
- → **Uncertainty Quantification** already integrated given the probabilistic approach
- → **Upsampling** high fidelity solution databases only data-driven



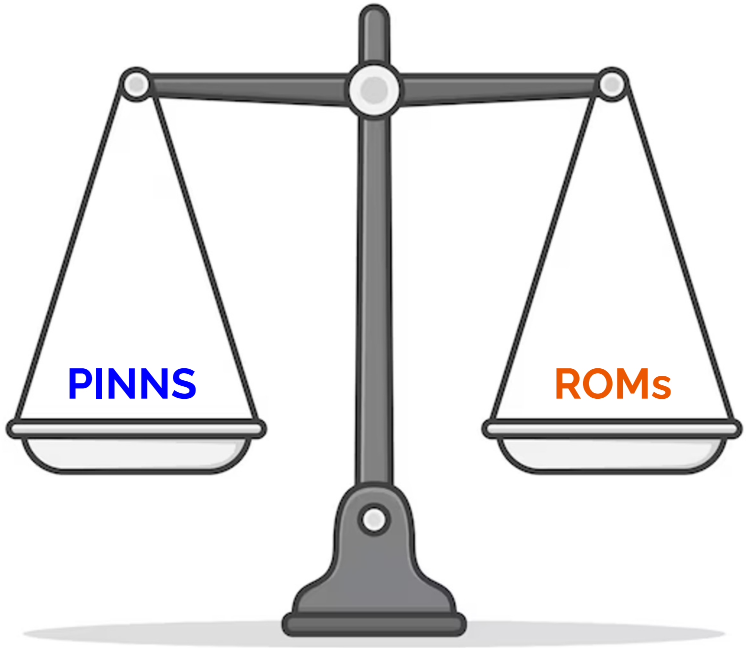
Inductive Bias vs Real Data

➔ Data and Physical knowledge must be **balanced** to build a **truthful** and **reliable** ML model

Inductive Bias

Physical Equations

Constraints and Symmetries



Data

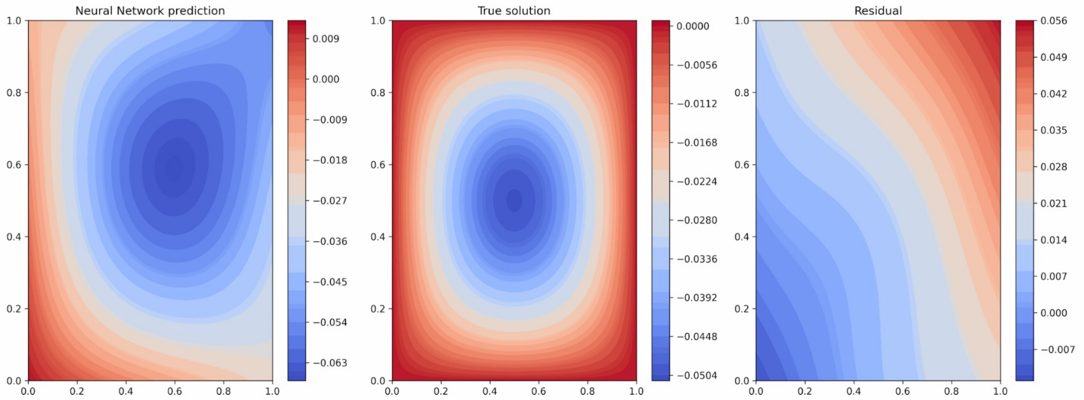
Full Order Models simulations

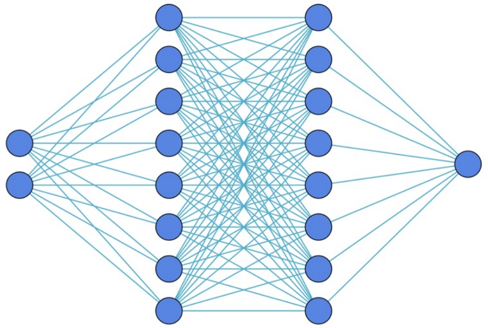
Sensor Data

PINA: Physics Informed Neural Network and ROMs Software

PINA is much more than a simple software for PINNs

- SOTA Neural Operators and customizable trainings
- TensorBoard API for model training visualization
- Data-Driven Reduced Order Modelling
- Deformation Models by Physics Informed Networks
- User friendly
- Multiple HPC Devices (GPU, TPU, …)
- ROMs, PINNs, NOs, and all the state-of-the-art methods implemented





PiNA

PyTorch

PyTorch Lightning
Created by Lightning AI

SMACT – ODYSSEA

Empowering Industry 4.0 with Integrated Digital Innovation

SM ACT competence center

SMACT ODYSSEA

WARTSILA

Smart Hybrid Energy System (SHEMS-VIEW)

WARTSILA

Wartsila Live Demo

DANIELI AUT.

Danieli Live Demo

FINCANTIERI

FINCANTIERI SHOPROMs

ELECTROLUX

Fridge CFD Multiphase & ROM

ELECTROLUX

Drying Cycle Optimization

ELECTROLUX

Electrolux Live Demo

Wartsila Live Demo

Motivation:
Early identification of deviations from the diesel/gas engine ideal behaviour, already at test time.

Goals:

- **Data acquisition/cleaning:** Collection of data from sensors and then perform data cleaning to remove noise and outliers
- **Modelling:** use non-linear models as ANNs
- **Model integration** with GUI

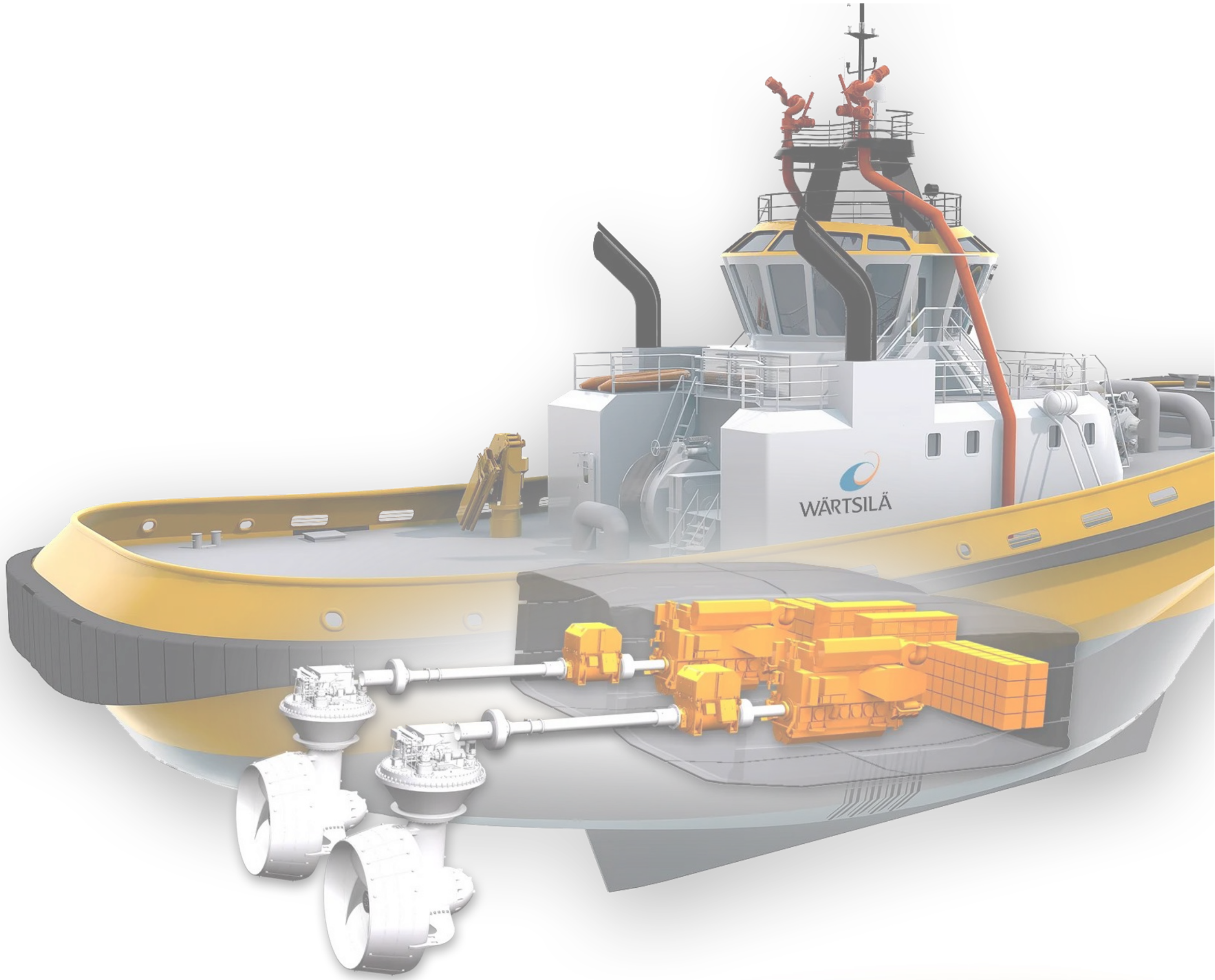
WÄRTSILÄ

SM ACT competence center

Wartsila Live Demo

Motivation:
Optimization of the efficiency of Wärtsilä's Energy Management System for hybrid engines.

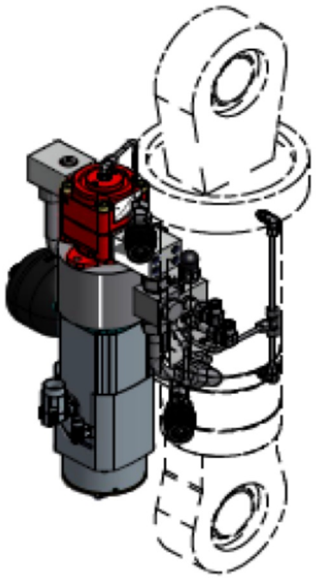
Goals:
- → **Data collection from sensors**
- → **ANN algorithm** for demand prediction
- → Find **Best operational parameters**
- → **Specialization** of the procedure depending on external conditions

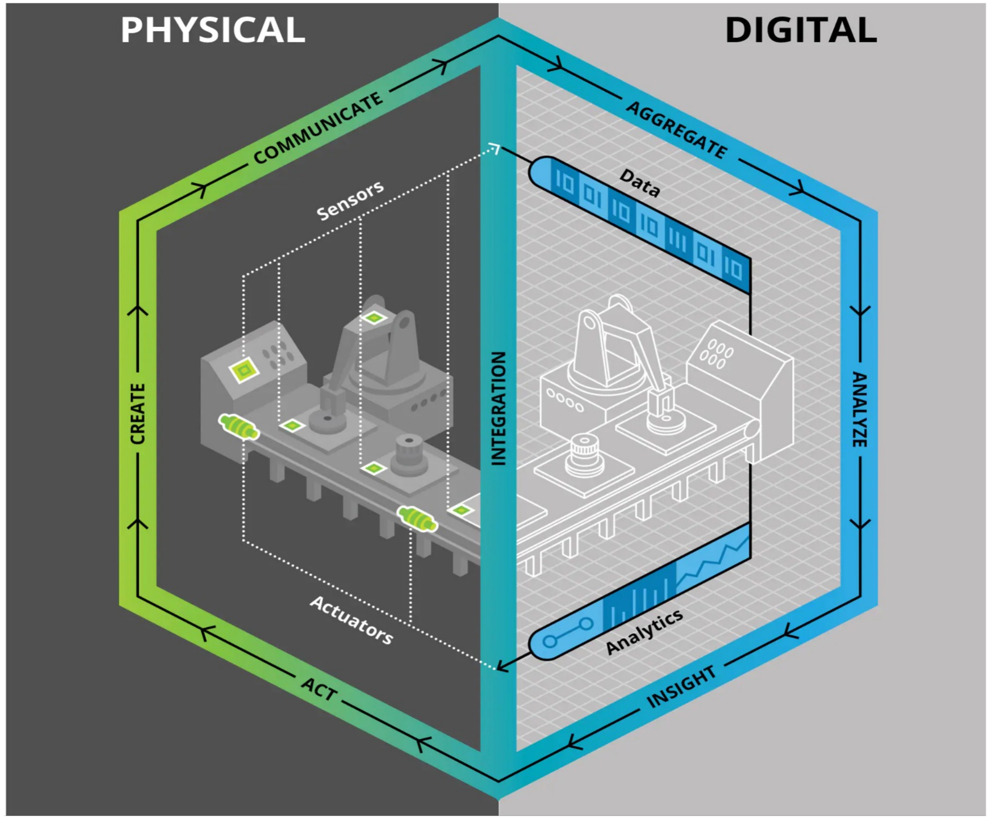


Danieli Live Demo

Motivation:
Implementation of the **Digital Twins** concept to the **electro-hydraulic actuator (Hy-Power)** produced by Danieli and used in the process of steel casting to obtain a virtual replica of the machine that can **communicate** with its real counterpart, **monitor** machine health, **predict** future failure and **optimize** performance.

Goals:
→ **Fault detection**
→ **Condition classification**
→ **Predictive maintenance**





Italiadomani
PIANO NAZIONALE
DI RIPRESA E RESILIENZA

iNEST

Interconnected Nord-Est Innovation Ecosystem

iNEST - Spoke 9

11 founding members

13 affiliates

9 Spokes

SISSA

Spoke 9

Spoke 9: Models, Methods, Computing Technologies for Digital Twins

Leader:

SISSA (Mathematics Area), SISSA mathLab

Partners:

- **UNIPD** (Mathematics Dept.),
- **OGS** (Oceanographic Dep.),
- **UNITS** (math and geosciences dept.)

Themes:

- Mathematical, numerical and data-driven modeling
- Model Order Reduction
- Automatic Learning for Digital Twins
- Applications of DT in industry, medicine, Environmental Sciences, Daily life

Conclusions

- ➔ It is time to better integrate **Data, Modelling, Analysis, Numerics, Control, Optimization and Uncertainty Quantification** in a new parametrized, reduced and coupled paradigm;
- ➔ We need to draw the attention to the fact that "**Science and Engineering could advance with Mathematics (CSE)**"
- ➔ **Applied Mathematics as propeller for methodological innovation and technology transfer** by a new generation of talented computational scientists