Physical informed learning: stakes in an industrial setting

21st November 2024

William PIAT

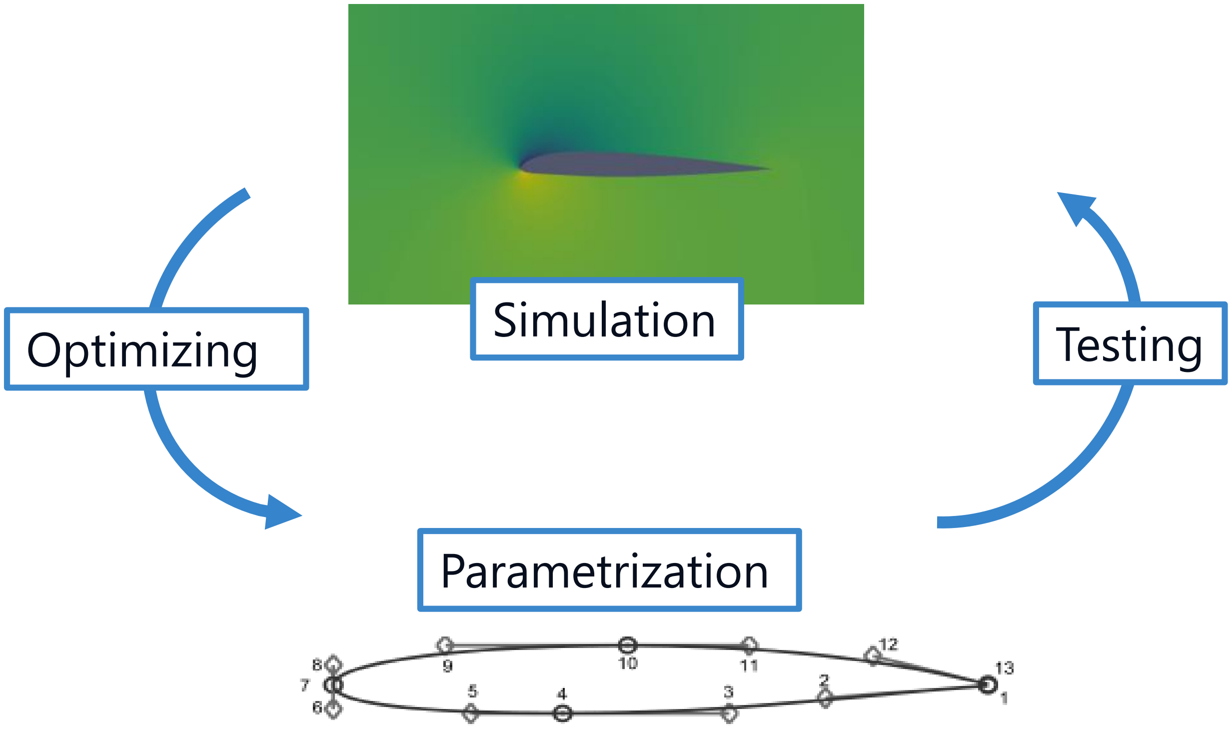
SAFRAN

Chapter 1

Introduction

Introduction

Conception is still lengthy process:



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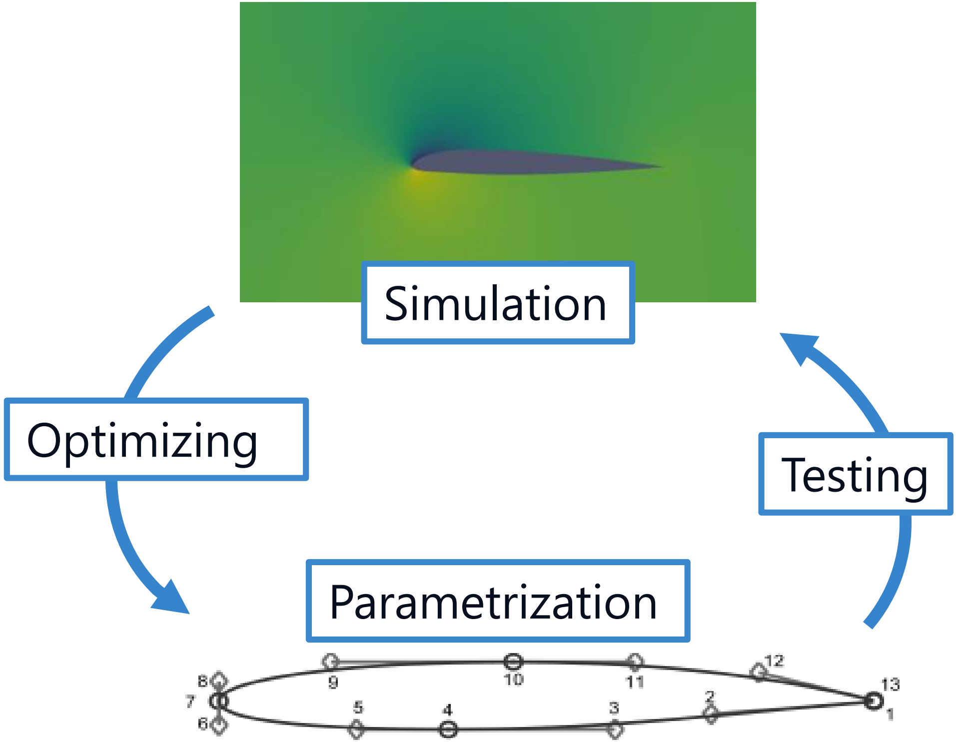
Introduction

Two main ways for speeding up design:



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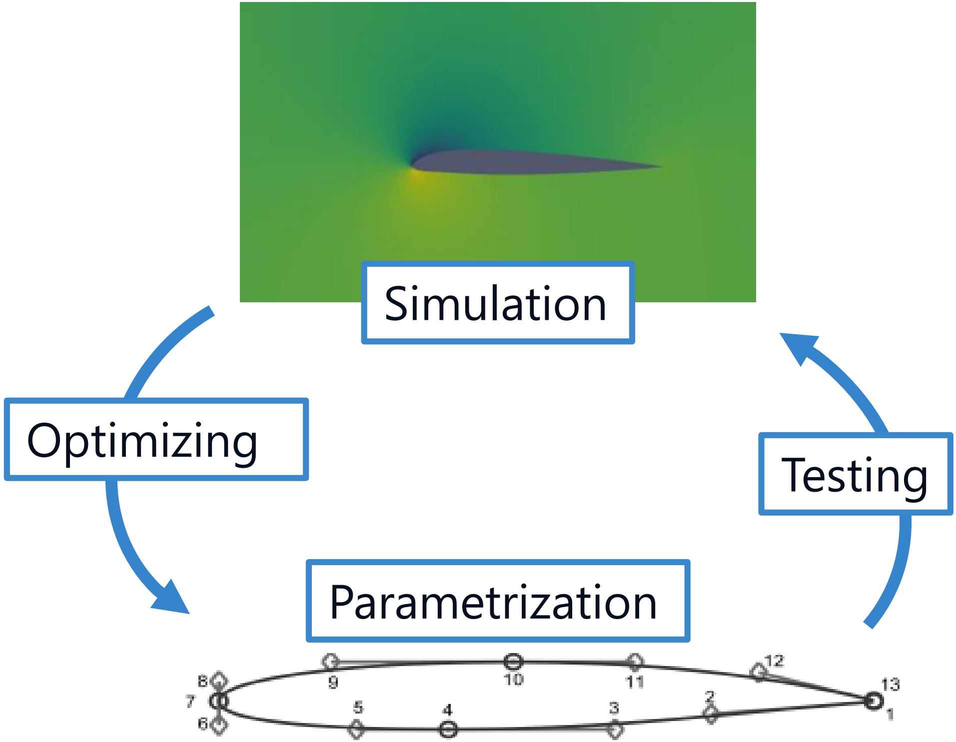
Two main ways for speeding up design:

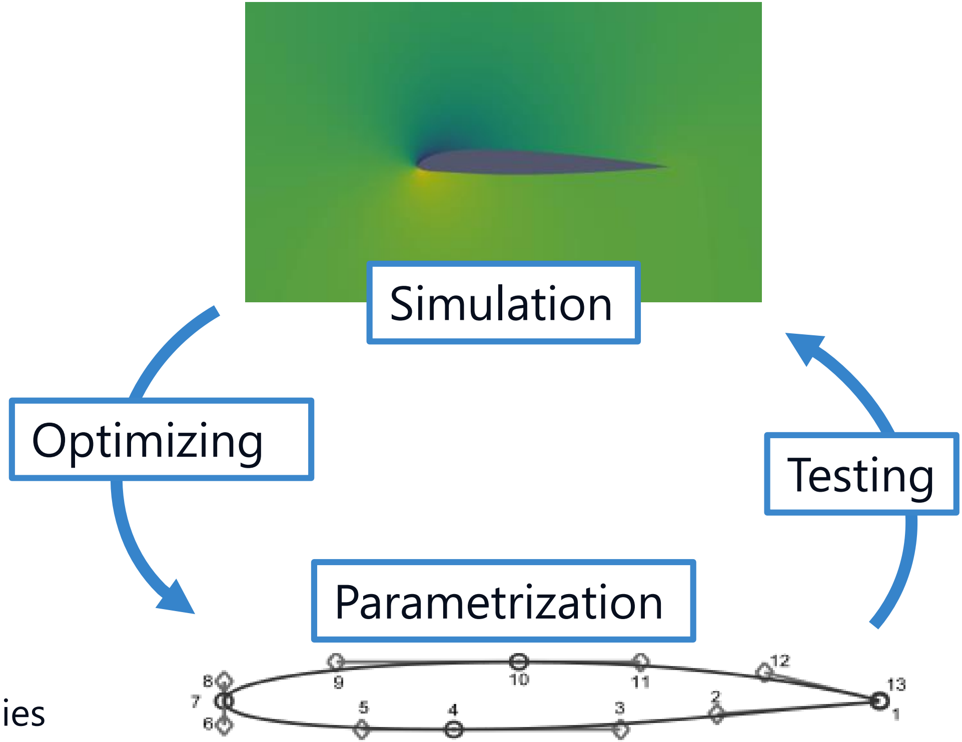
- Accelerate simulation:
    - Use surrogates (Statistical models)



Introduction

Two main ways for speeding up design:

- Accelerate simulation:
  - Use surrogates (Statistical models)
- Set free from parametrization:
  - Make geometry changes non parametric
  - Have a generic datamodel for physical studies

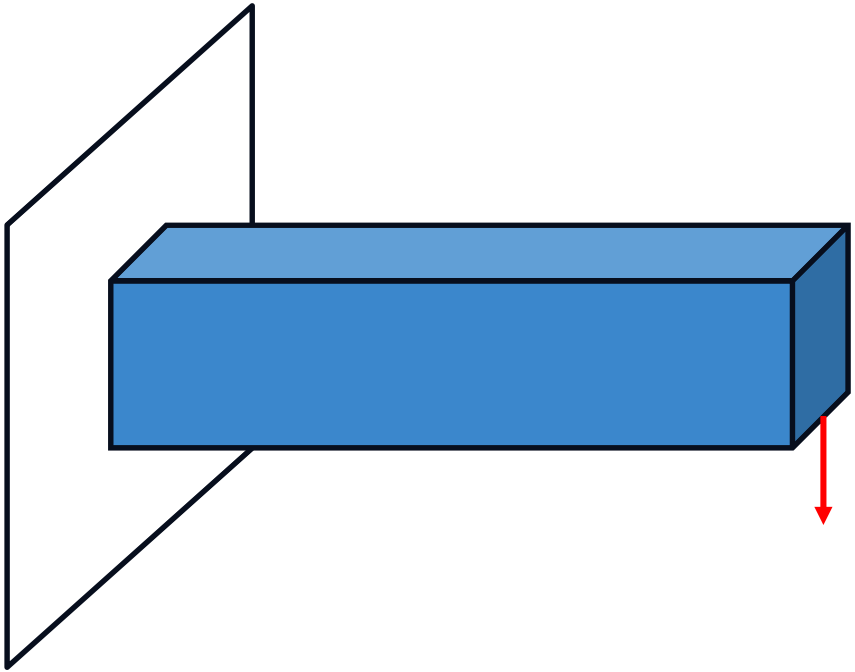


Introduction

Non parametric design taken to the extreme: topology optimisation

1) Nardoni, C., Danan, D., Mang, C., Bordeu, F., Cortial, J. (2022). A R&D Software Platform for Shape and Topology Optimization Using Body-Fitted Meshes. In: Sevilla, R., Perotto, S., Morgan, K. (eds) Mesh Generation and Adaptation. SEMA SIMAI Springer Series, vol 30. Springer, Cham. https://doi.org/10.1007/978-3-030-92540-6_2

Introduction



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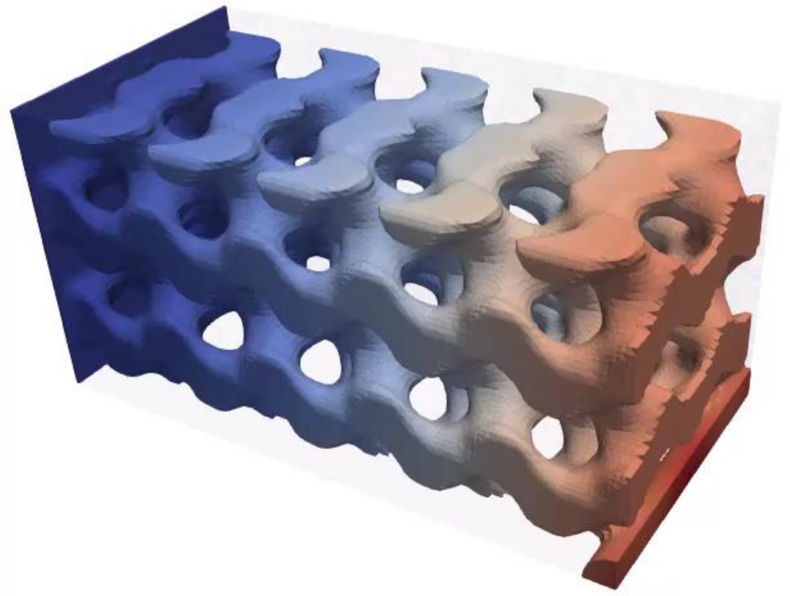

1) https://openpisco.irt-systemx.fr/

Agenda

Chapter 2

Speeding up computations

- Models fit for physical problems
- Physics informed learning: promises and challenges

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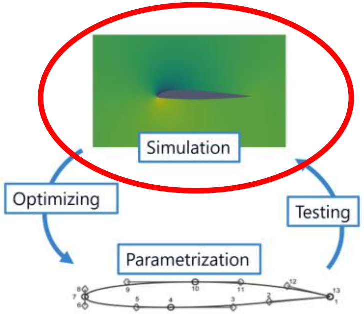
Speeding up computations

- **Models fit for physical problems**
- **Physics informed learning: promises and challenges**



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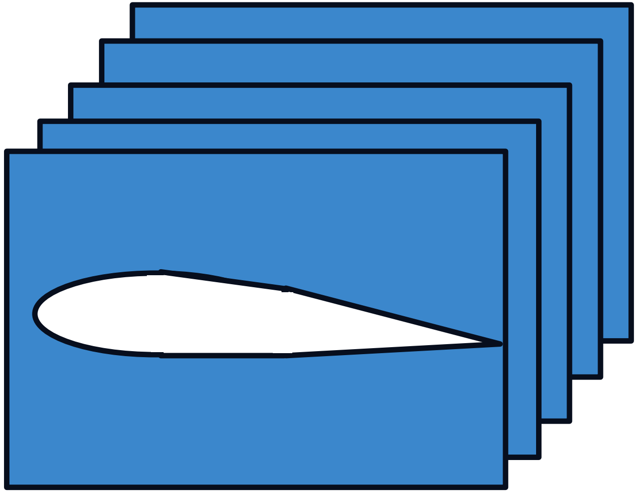
Chapter 2

Speeding up computations

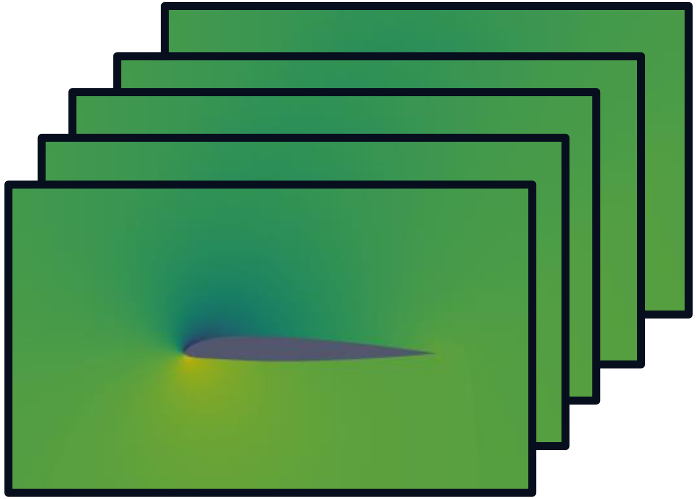
- **Models fit for physical problems**
- **Physics informed learning: promises and challenges**

Speeding up computations:

Models fit for physical problems
Physics informed learning: promises and challenges



Inputs



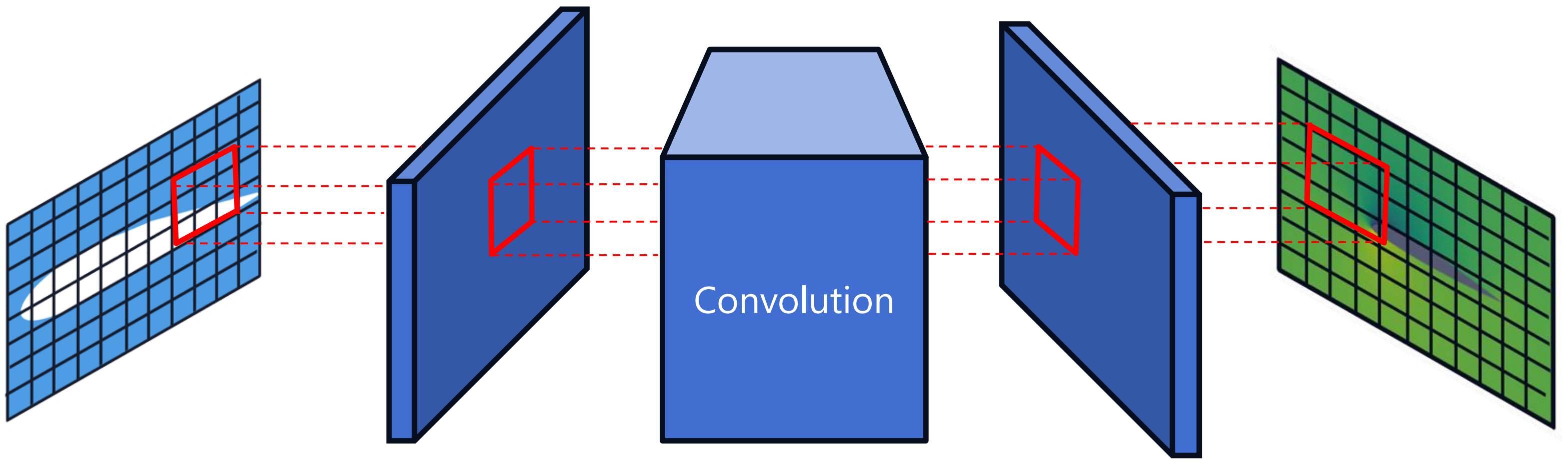
Outputs

High dimensional inputs and outputs

Speeding up computations:

Models fit for physical problems
Physics informed learning: promises and challenges

CNN



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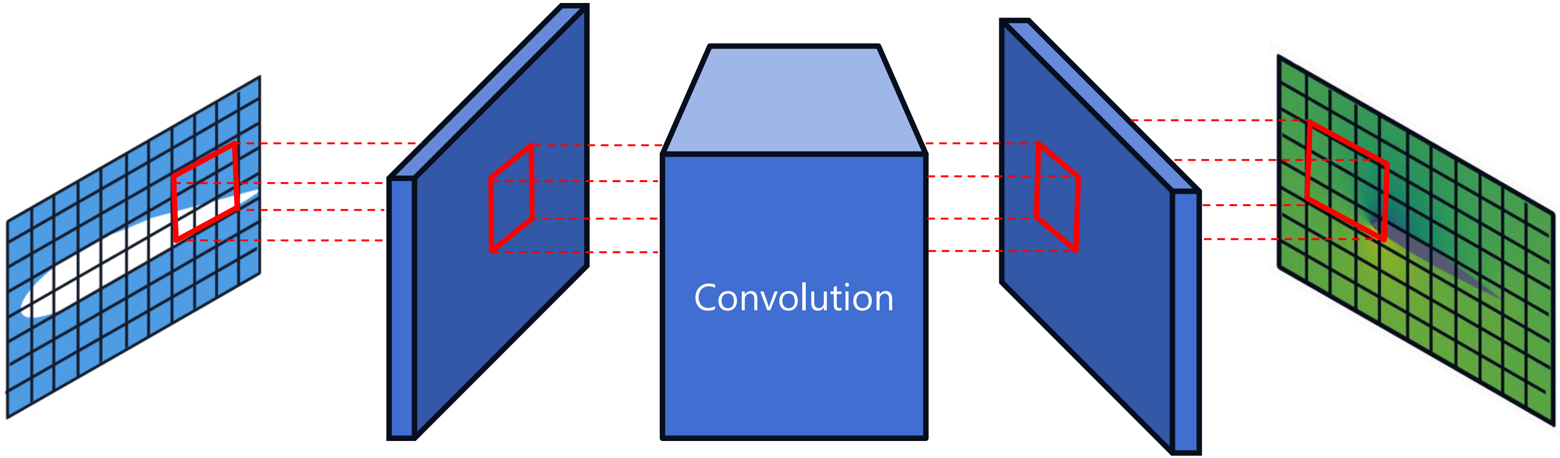

Focuses on local features if number of layers is small

Speeding up computations:

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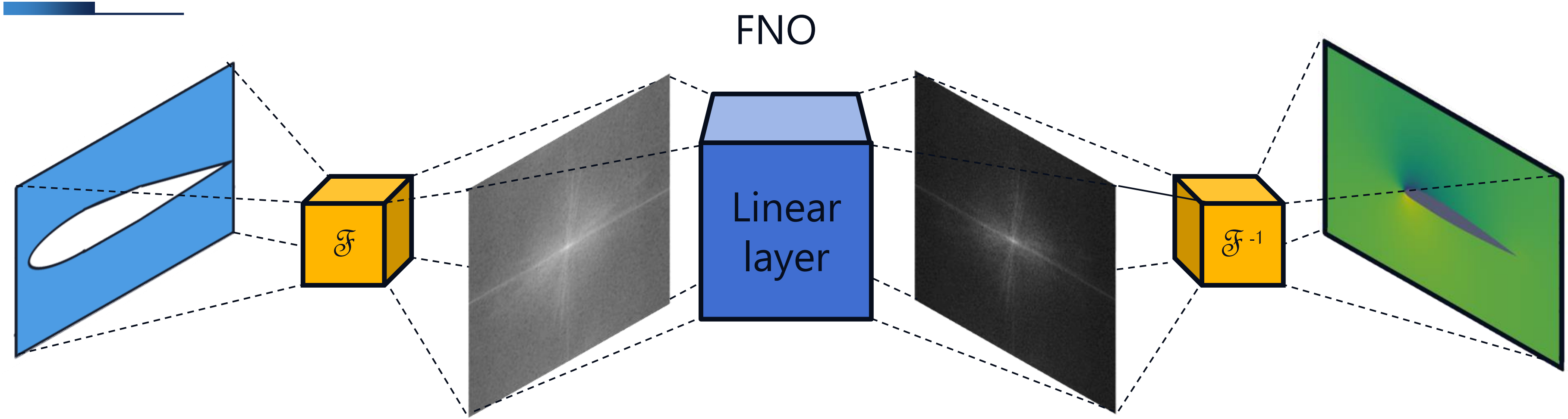

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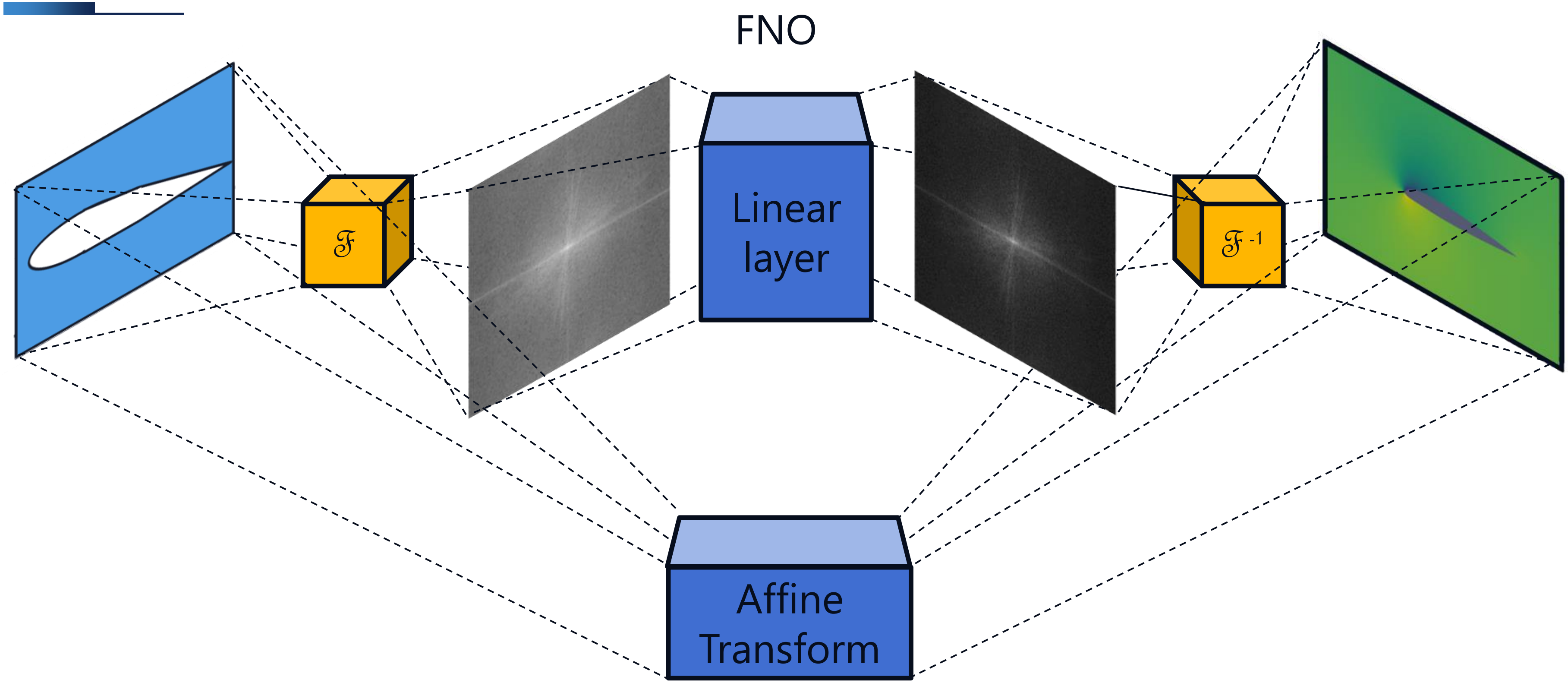

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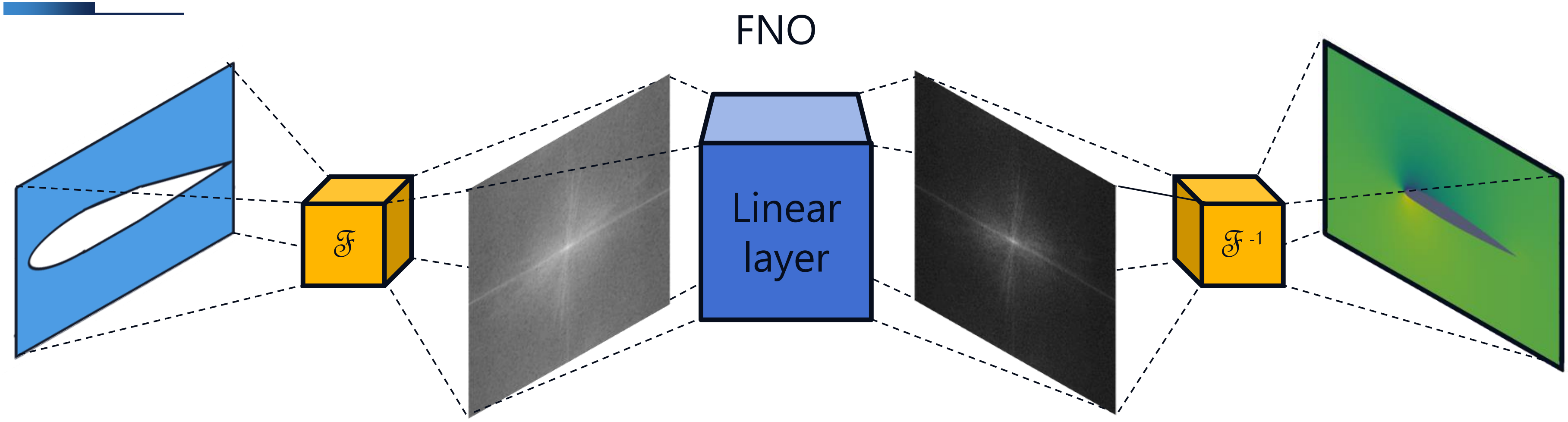

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Models fit for physical problems
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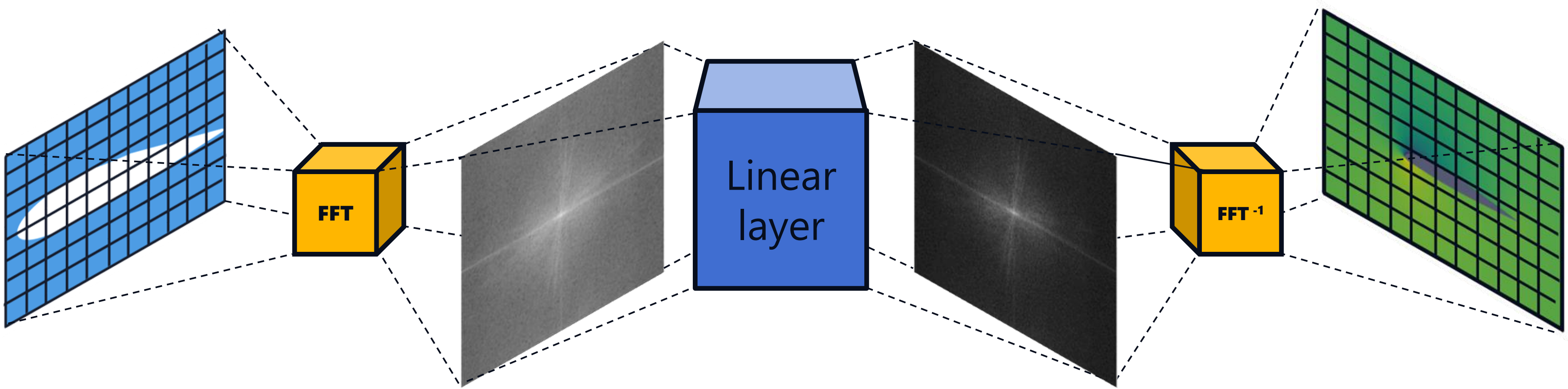
Real FNO



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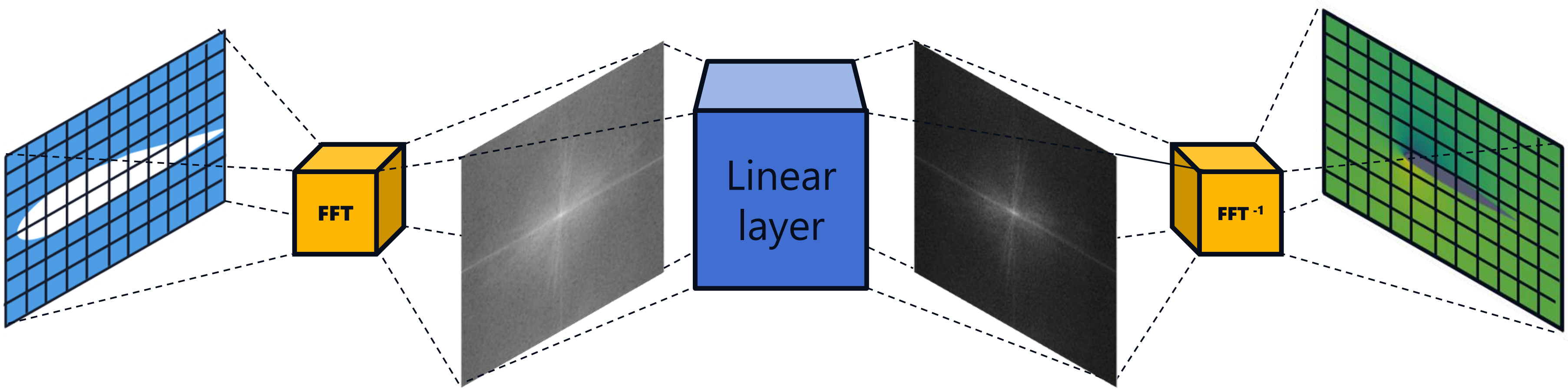

Focuses on global features

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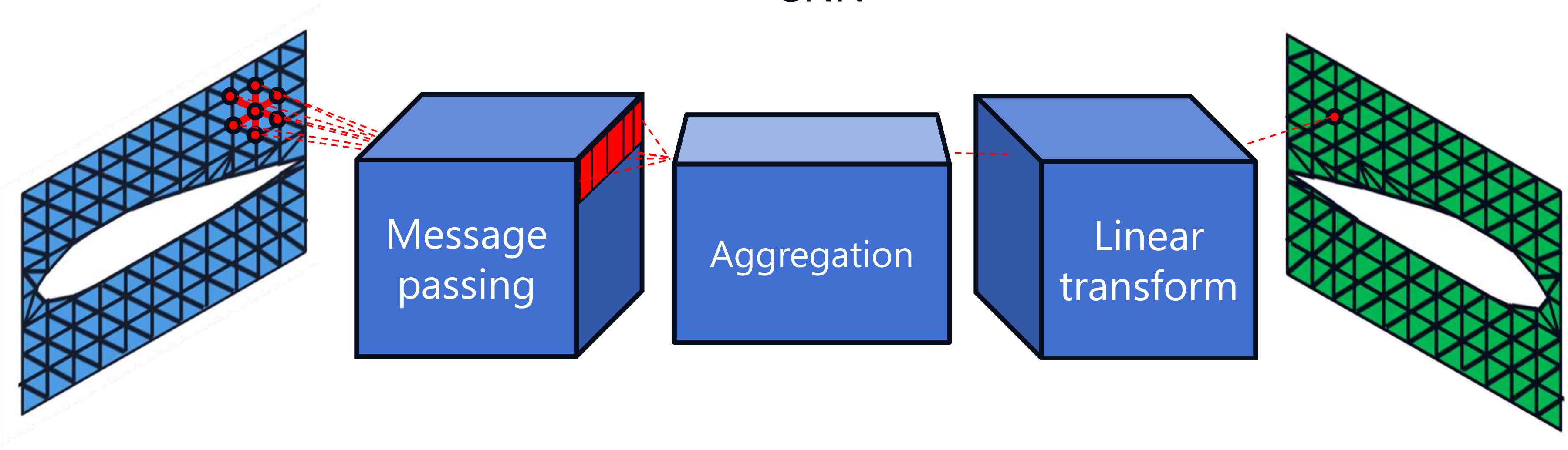
GNN



Tobias Pfaff, Meire Fortunato, Alvaro Sanchez-Gonzalez, Peter W. Battaglia: Learning Mesh-Based Simulation with Graph Networks. ICLR 2021

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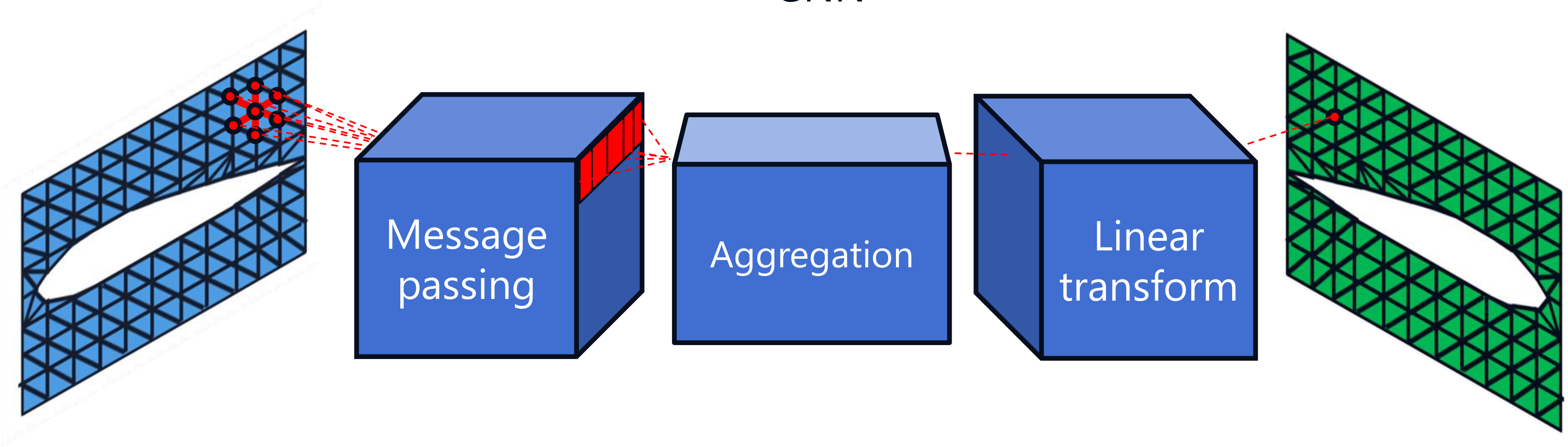

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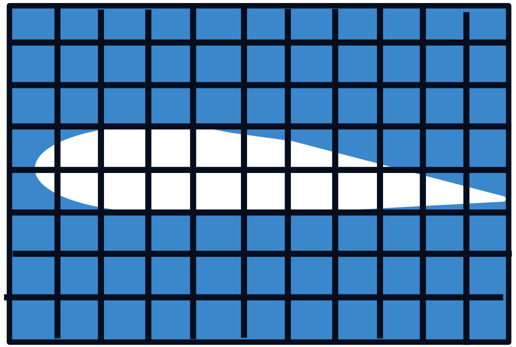
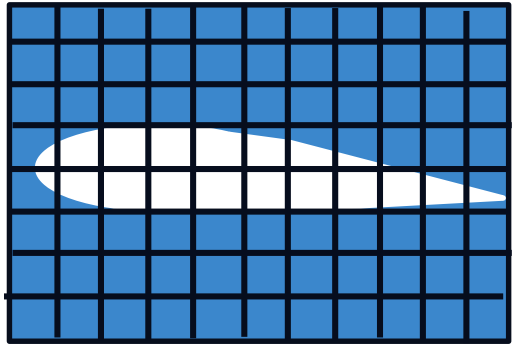


Strenght: local features
Weakness: regular grid

FNO



Strenght: global features
Weakness: regular grid

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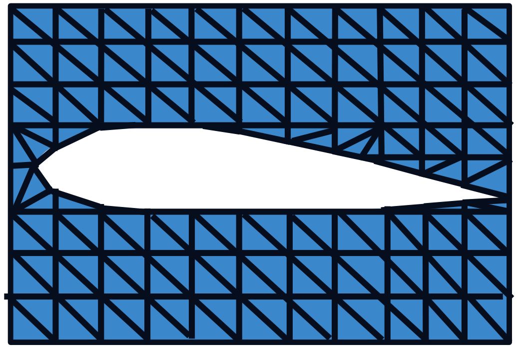

Strenght: generic geometry
Weakness: Mesh sensitive

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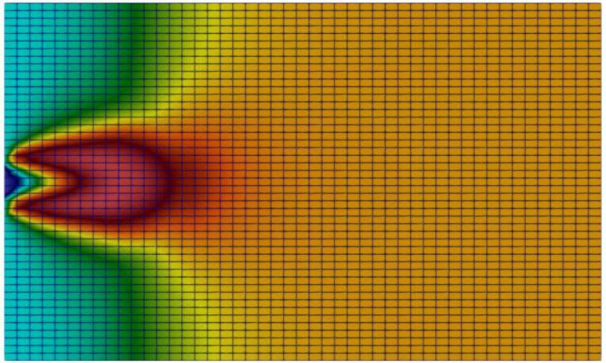
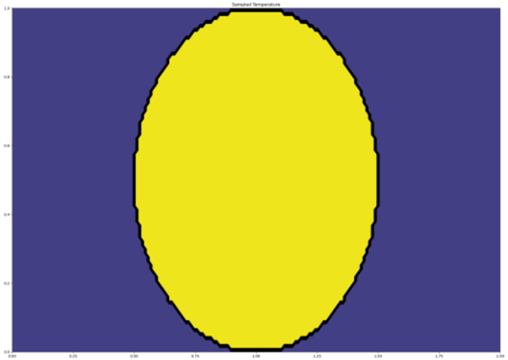


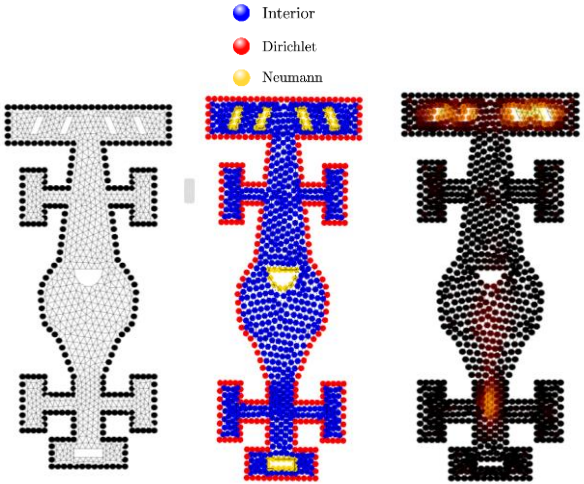
RANS simulation of injector [1]

FNO



Thermal diffusion

GNN



Poisson Equation [2]

1) Akkari N, Casenave F, Daniel T, Ryckelynck D. Data-Targeted Prior Distribution for Variational AutoEncoder. *Fluids*. 2021; 6(10):343. https://doi.org/10.3390/fluids6100343
2) Matthieu Nastorg, Michele Alessandro Bucci, Thibault Faney, Jean-Marc Gratien, Guillaume Charpiat, Marc Schoenauer An Implicit GNN Solver for Poisson-like problems. ArXiv 2023, 10.48550/ARXIV.2302.10891

Speeding up computations:

Models fit for physical problems

Physics informed learning: promises and challenges

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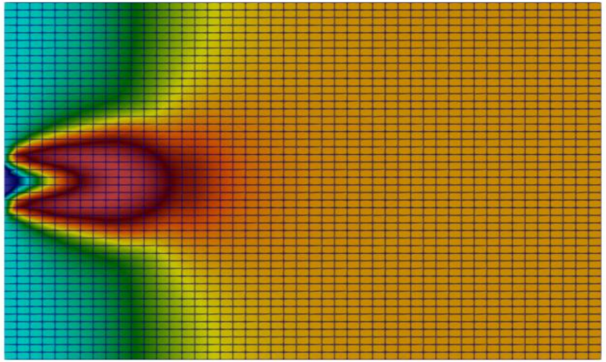

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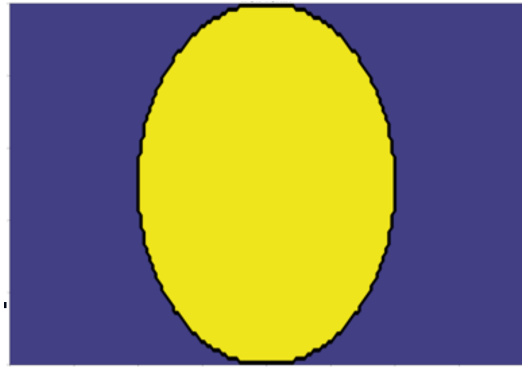

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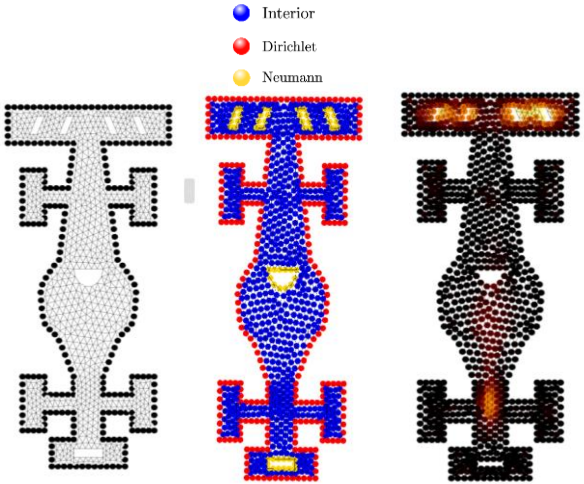

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Speeding up computations:

Models fit for physical problems
Physics informed learning: promises and challenges

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- **Non sparse non linear systems** make the perfect use case due to time and cpu cost…

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- We need to bring forward **inductive bias**: Physical statistical learning

Chapter 2

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Speeding up computations:

Models fit for physical problems
Physics informed learning: promises and challenges

Physics (simulation)	Statistical learning

Speeding up computations:

Models fit for physical problems
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Speeding up computations:

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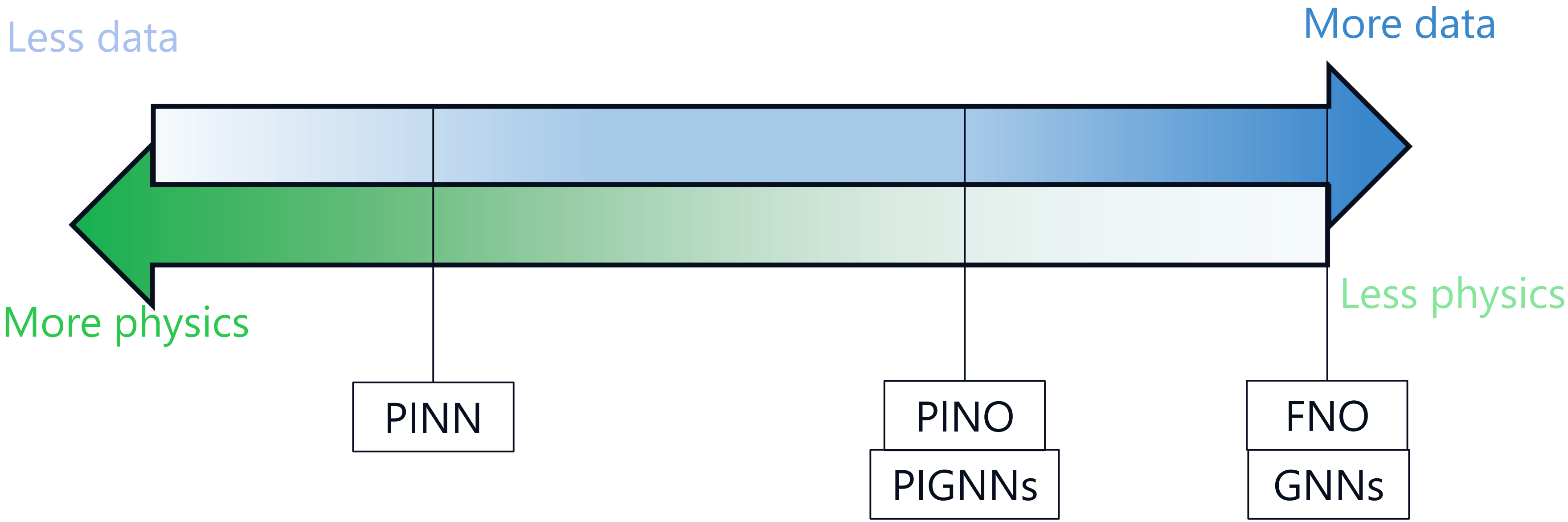

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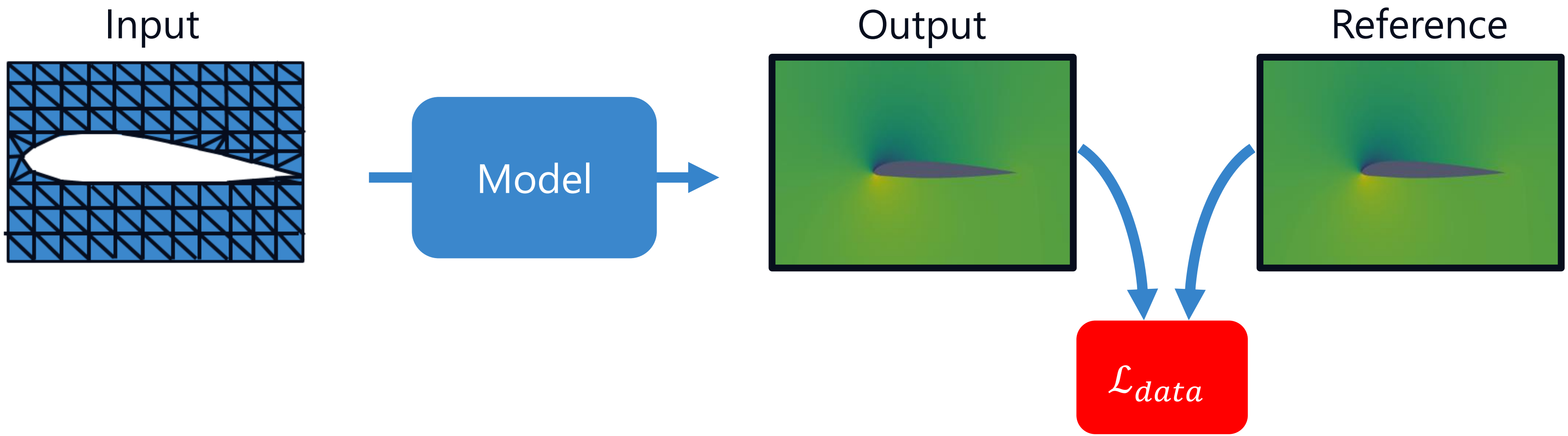

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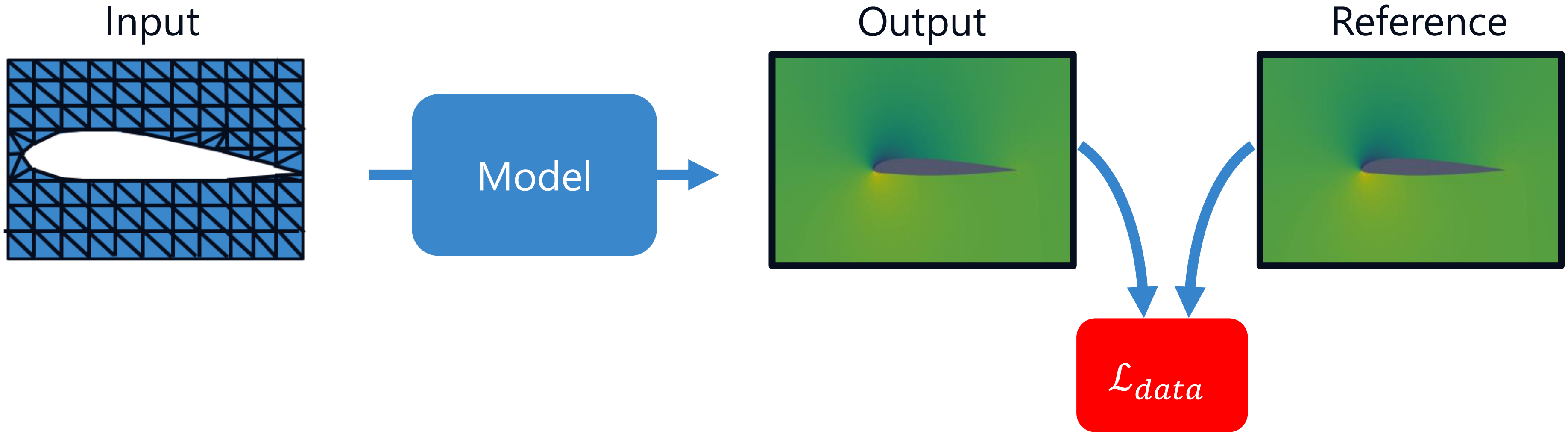

FNO, GNN

Speeding up computations:

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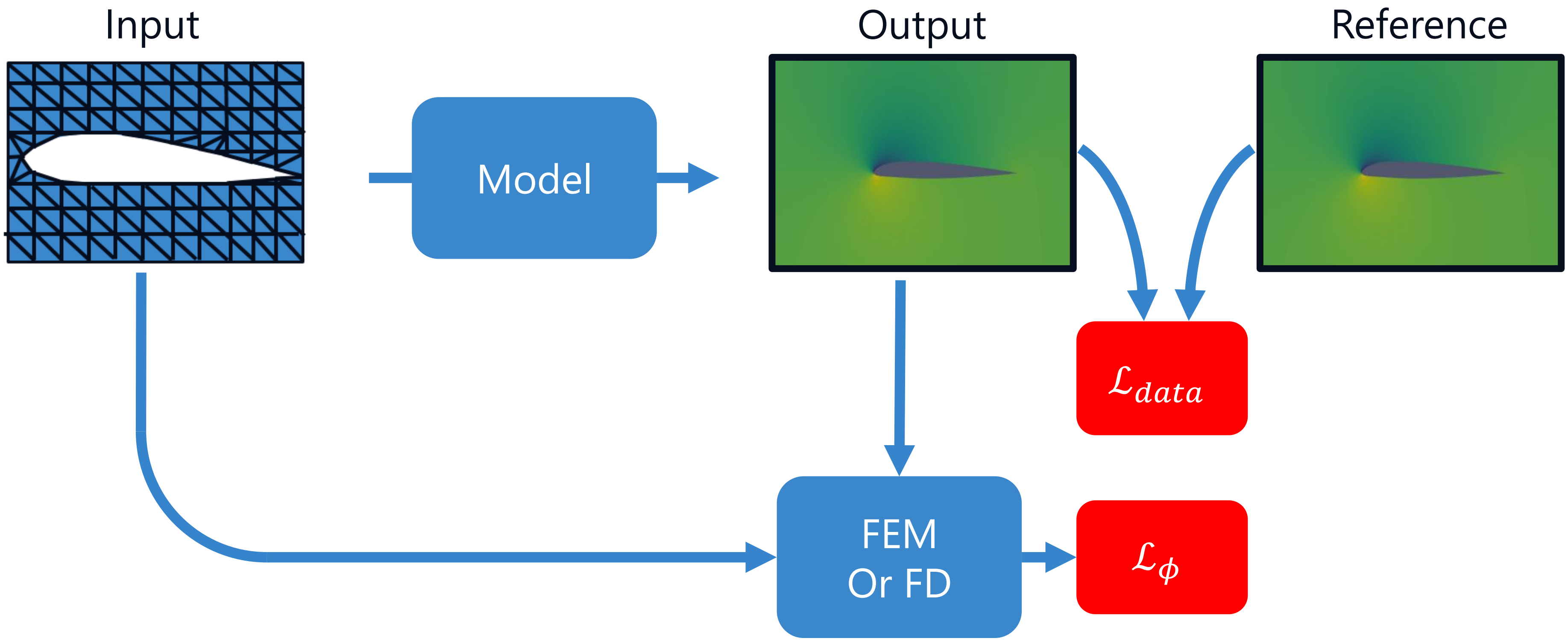

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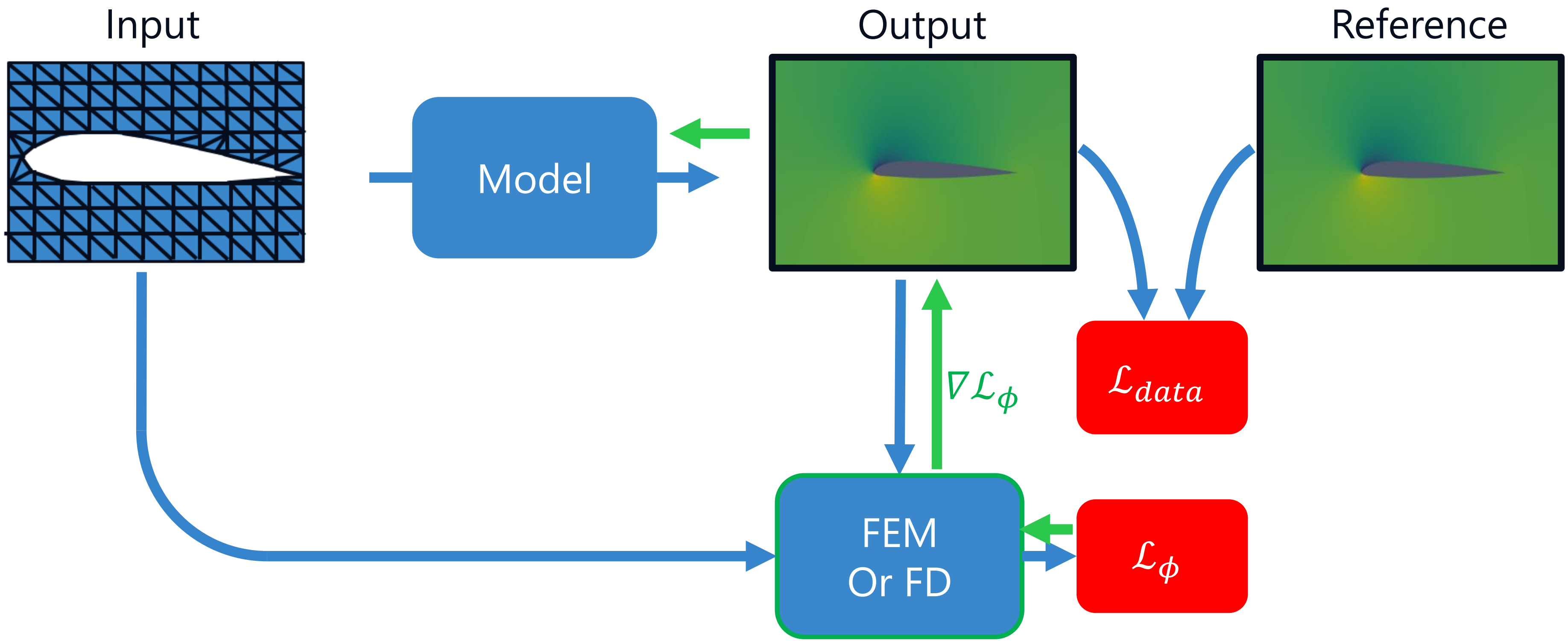

Speeding up computations:

Models fit for physical problems

Physics informed learning: promises and challenges

- FNO and GNNs **are not** relying on physics
- PINOs and Physics informed GNNs **are (usually) trained using numerical method** …

Speeding up computations:

Models fit for physical problems
Physics informed learning: promises and challenges

- FNO and GNNs **are not** relying on physics
- PINOs and Physics informed GNNs **are (usually) trained using numerical method** …
- … that rely on strong hypothesis that might not be verified

Speeding up computations:

Models fit for physical problems

Physics informed learning: promises and challenges

Technology	Extrapolation on unknown cases	Respects physics	Remarks
PINNs	No	Soft constraint using empirical sampling	Can't be applied to multiple problems

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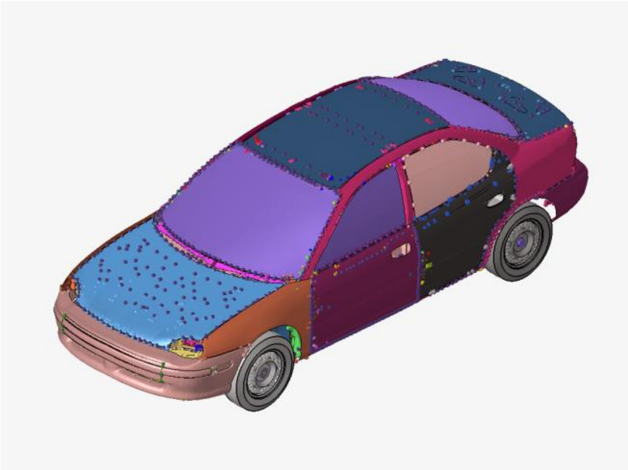
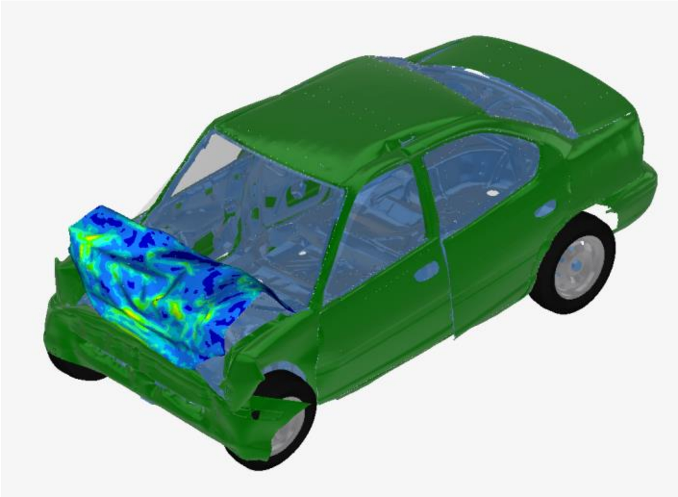
Can only be used for industrial design suggestion but not validation

What is an industrial problem:





HPC Benchmark Models - OpenRadioss - Confluence

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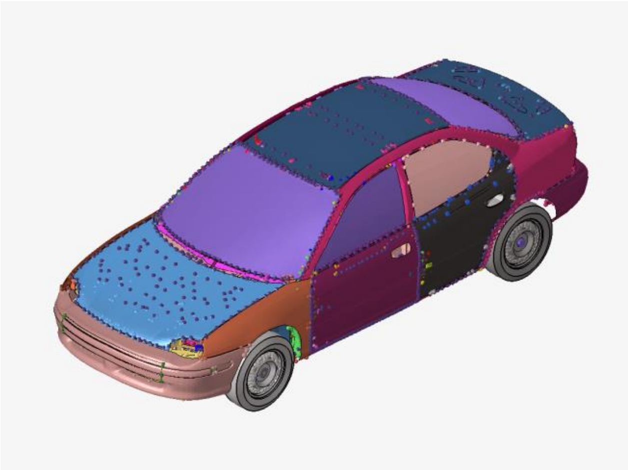
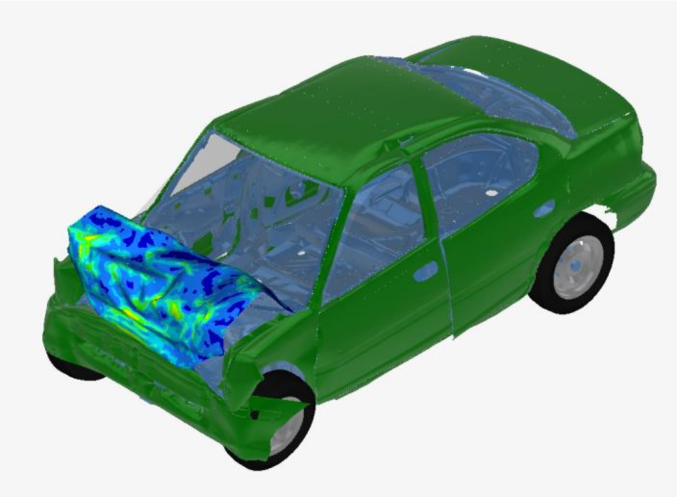




Number of parameters? Where is the regular grid?

[HPC Benchmark Models - OpenRadioss - Confluence]

Conclusions

- Current models are able to take a physical problem as a **whole**
- Some models **are able to take physical non linearities** such as contact into account
- (Non Linear) Statistical learning **could prevent using costly Newton iterations**

Conclusions

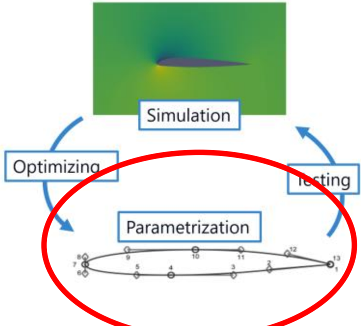
- Current models are able to take a physical problem as a **whole**
- Some models **are able to take physical non linearities** such as contact into account
- (Non Linear) Statistical learning **could prevent using costly Newton iterations**

- Physics informed learning **limits the amount of data needed** by adding **inductive bias**
- We are still **dependant of the numerical method for solving the physics**
- Real use cases are **still out of reach.**

Chapter 3

Speed up design via non parametric design

- **Parametric vs non parametric**
- **PLAID: Physics Learning AI Datamodel**



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Parametric vs non parametric

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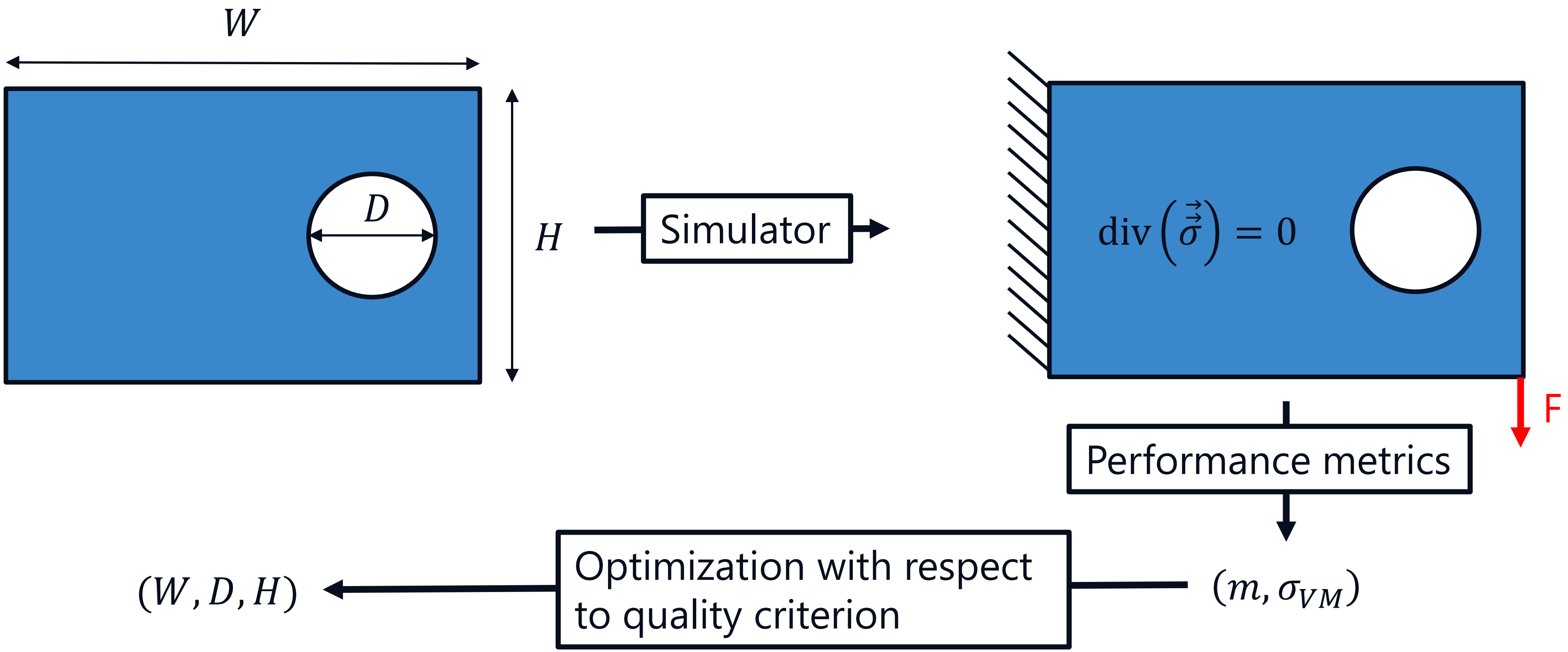

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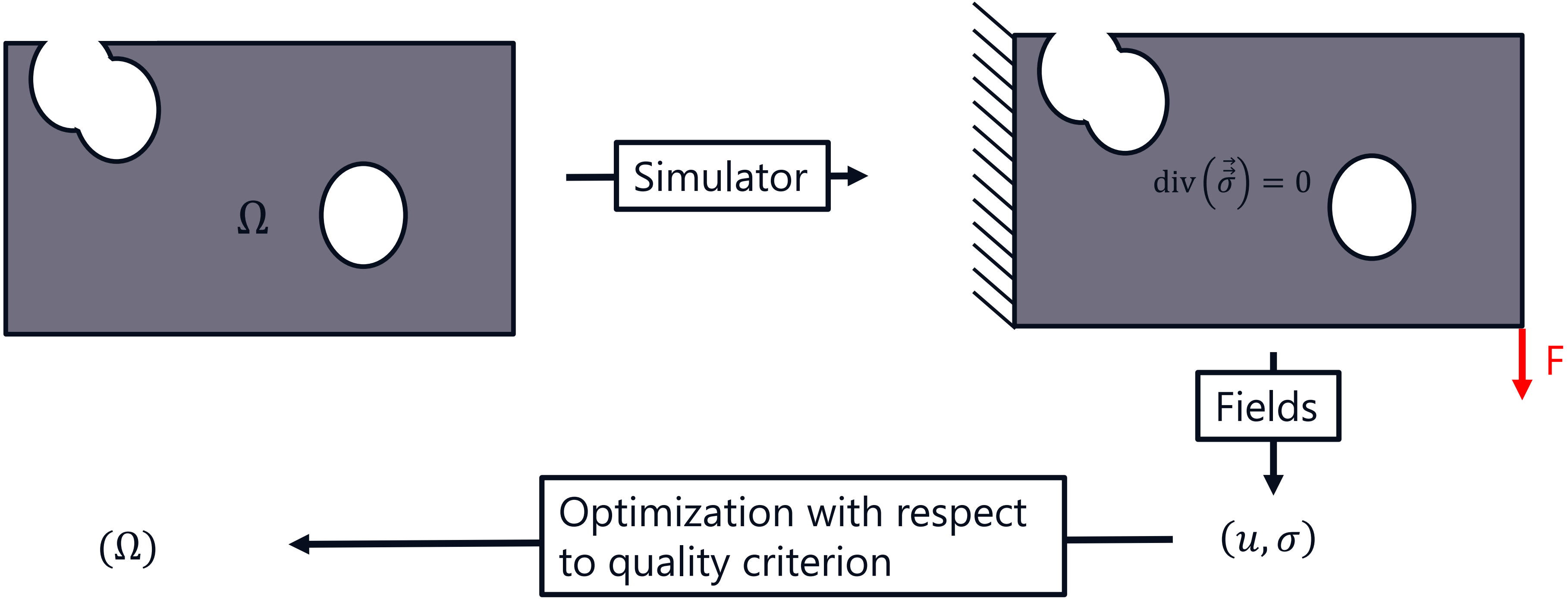
Parametric vs non parametric

PLAID: Physics Learning AI Datamodel



Speed up design via non parametric design

Parametric vs non parametric
PLAID: Physics Learning AI Datamodel

Parametric design	Non Parametric design
Simplifies the problem	More general
Can be tackled with a limited number of simulations	Needs a large number of simulations
Any classical metamodel can be used	Specific metamodels that can take a geometry as an input

What defines a (statistical) physical problem?

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Thankfully, a standard for physical problems already exists:

CFD General Notation System

Speed up design via non parametric design

Parametric vs non parametric
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We made an implementation with commodities for machine learning frameworks

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CFD General Notation System

We made an implementation with commodities for machine learning frameworks

Already compatible with multiple open source readers.

Speed up design via non parametric design

Parametric vs non parametric
PLAID: Physics Learning AI Datamodel

Implementation of a datamodel tailored for AI and ML learning of physics problems

Features

- Based on **CGNS** for physical data (standard, widely used, compact binary files)
- Functions to handle data
- Formalize **ML** problems

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Common DataModel

- Data centric view
- Enables **streamlined workflows** involving different libraries
- Standardization: **share and reuse data produced by others**
- **Human readable** (ascii or paraview compatible files)
- **Heterogeneous** data

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GitLab gitlab.com/drti/plaid

CONDA-FORGE ANACONDA conda-forge/plaid

Read the Docs plaid-lib.readthedocs.io

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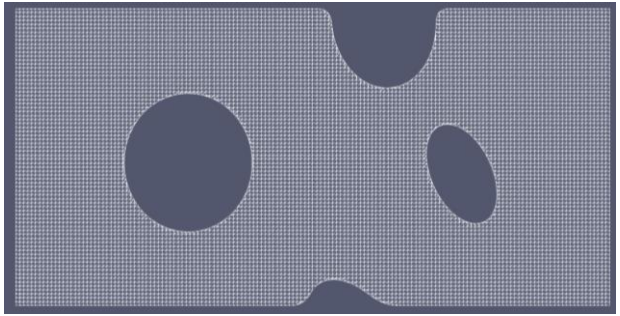
Speed up design via non parametric design

Parametric vs non parametric

PLAID: Physics Learning AI Datamodel

Problème Physique



Données physiques

- Maillage

PLAID model

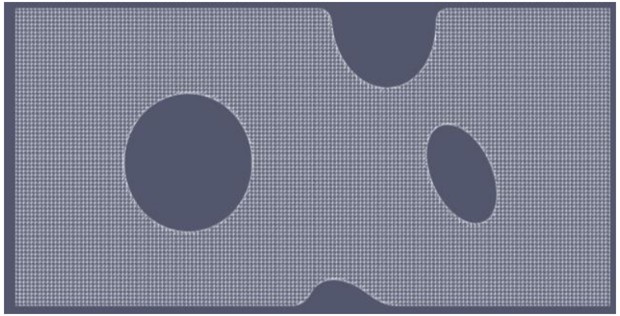
dataset/
|-- samples
    |-- sample_000
        |-- meshes
            |--mesh_000.cgns

Speed up design via non parametric design

Parametric vs non parametric

PLAID: Physics Learning AI Datamodel

Problème Physique



Données physiques

- Maillage

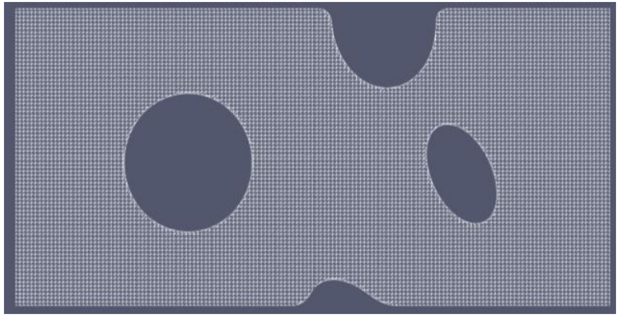
PLAID model

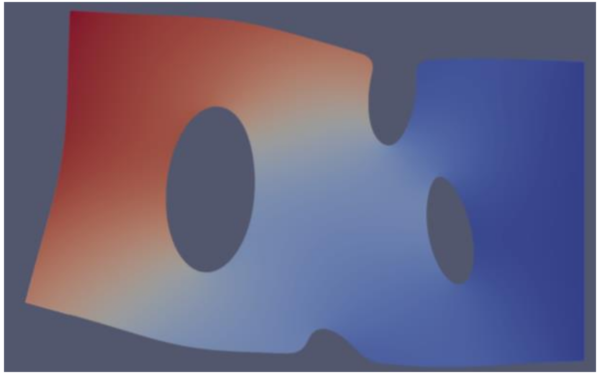
```
dataset/
|-- samples
    |-- sample_000
    |   |-- meshes
    |       |--mesh_000.cgns
    |       |--mesh_001.cgns
    |       |
    |       |--mesh_xxx.cgns
    |
    |
    |-- sample_001
    |
    |-- sample_xxx
```

Speed up design via non parametric design

Parametric vs non parametric
PLAID: Physics Learning AI Datamodel

Problème Physique





Données physiques

- Maillage
- Champs scalaires/vectoriels

PLAID model

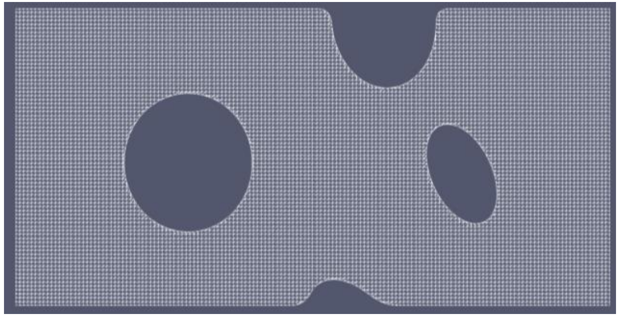
```
dataset/
|-- samples
    |-- sample_000
    |   |-- meshes
    |       |--mesh_000.cgns
    |       |--mesh_001.cgns
    |       |
    |       |--mesh_xxx.cgns
    |
    |
    |-- sample_001
    |
    |-- sample_xxx
```

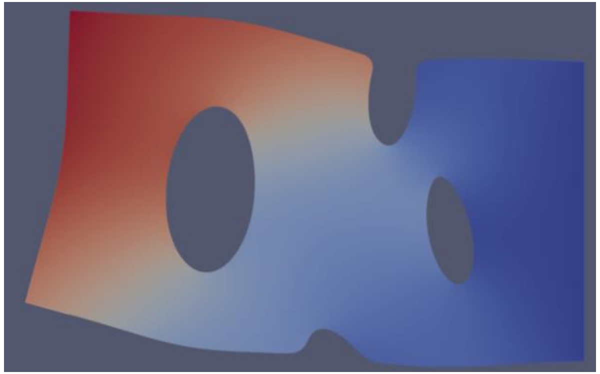
Speed up design via non parametric design

Parametric vs non parametric

PLAID: Physics Learning AI Datamodel

Problème Physique





Données physiques

- Maillage
- Champs scalaires/vectoriels
- Scalaires

PLAID model

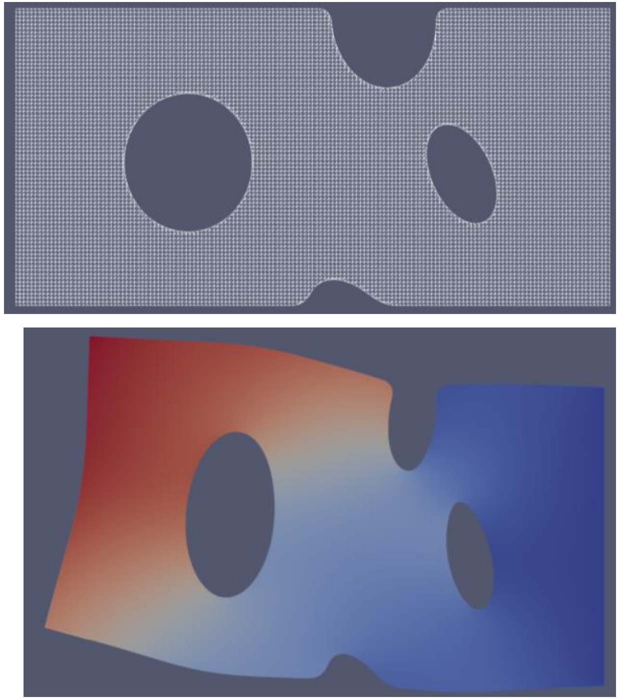
```
dataset/
|-- samples
    |-- sample_000
    |   |-- meshes
    |   |   |--mesh_000.cgns
    |   |   |--mesh_001.cgns
    |   |   |
    |   |   |--mesh_xxx.cgns
    |   |
    |   |-- scalars.csv
    |-- sample_001
    |
    |-- sample_xxx
```

Speed up design via non parametric design

Parametric vs non parametric

PLAID: Physics Learning AI Datamodel

Problème Physique



Données physiques

- Maillage
- Champs scalaires/vectoriels
- Scalaires
- Conditions limites

PLAID model

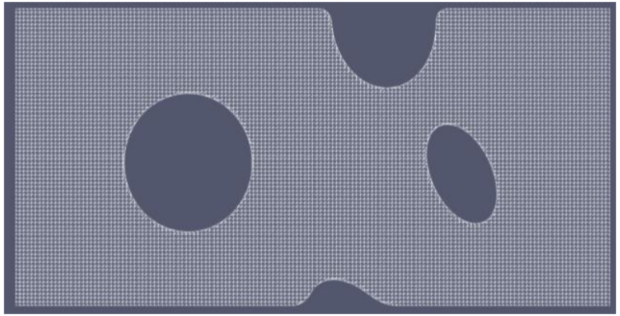
```
dataset/
|-- samples
    |-- sample_000
    |   |-- meshes
    |   |   |--mesh_000.cgns
    |   |   |--mesh_001.cgns
    |   |   |
    |   |   |--mesh_xxx.cgns
    |   |
    |   |-- scalars.csv
    |-- sample_001
    |
    |-- sample_xxx
```

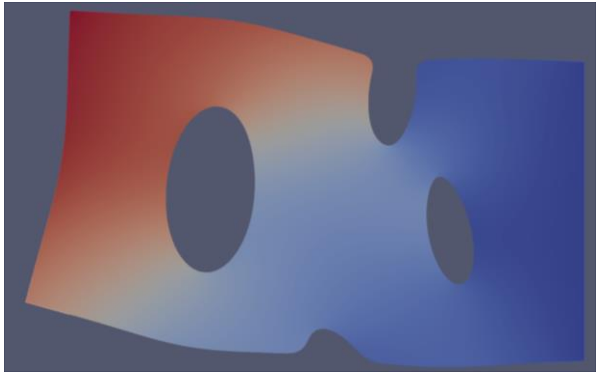
Speed up design via non parametric design

Parametric vs non parametric

PLAID: Physics Learning AI Datamodel

Problème Physique





Données physiques

- Maillage
- Champs scalaires/vectoriels
- Scalaires
- Conditions limites

Données problème

- Identification input/output
- Split train/test

PLAID model

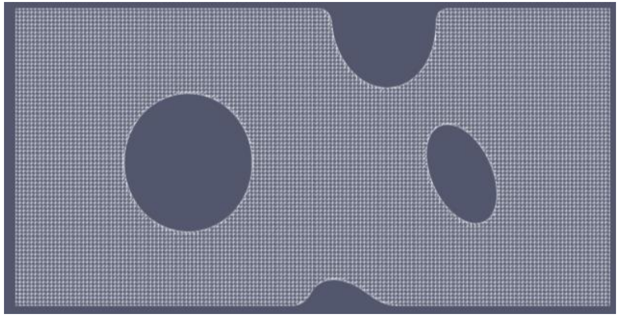
```
dataset/
|-- samples
|   |-- sample_000
|   |   |-- meshes
|   |   |   |--mesh_000.cgns
|   |   |   |--mesh_001.cgns
|   |   |   |
|   |   |   |--mesh_xxx.cgns
|   |   |
|   |   |-- scalars.csv
|   |-- sample_001
|   |
|   |-- sample_xxx
|
|-- problem_definition
    |-- problem_info.yaml
    |-- split.csv
```

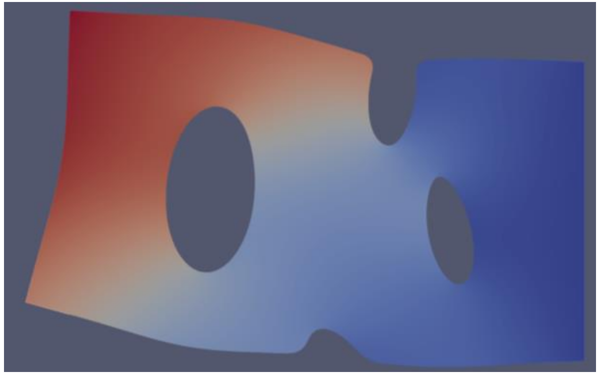
Speed up design via non parametric design

Parametric vs non parametric

PLAID: Physics Learning AI Datamodel

Problème Physique





Données physiques

- Maillage
- Champs scalaires/vectoriels
- Scalaires
- Conditions limites

Données problème

- Identification input/output
- Split train/test

PLAID model

```
dataset/
|-- samples
|   |-- sample_000
|   |   |-- meshes
|   |   |   |--mesh_000.cgns
|   |   |   |--mesh_001.cgns
|   |   |   |
|   |   |   |--mesh_xxx.cgns
|   |   |
|   |   |-- scalars.csv
|   |-- sample_001
|   |
|   |-- sample_xxx
|
|-- problem_definition
    |-- problem_info.yaml
    |-- split.csv
```

Speed up design via non parametric design

Parametric vs non parametric

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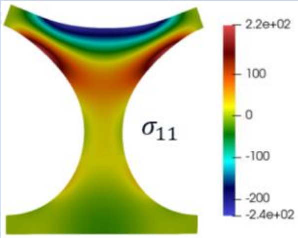
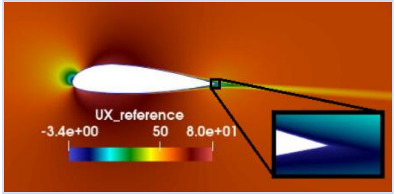
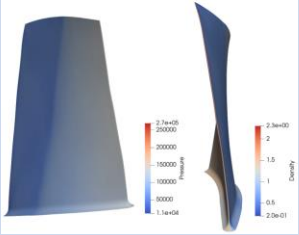
Name	Illustration	Description	Samples and volume	License
Tensile2d		• 2D structural mechanics with EVP constitutive law • Geometry and scalar parameters	• **702 samples** (various splits) • **297 MB**	CC BY SA
		zenodo.org/records/10124594 huggingface.co/datasets/PLAID-datasets/Tensile2d		
AirfRANS		• 2D steady Navier-Stokes • Geometry and scalar parameters	• **1000 samples** (various splits) • **1.5 GB**	**ODbLv1.0**
		zenodo.org/records/12515084 huggingface.co/datasets/PLAID-datasets/AirfRANS_original		**+2 variants**
Rotor37		• 3D steady Navier-Stokes • Geometry and scalar parameters	• **1200 samples** (various splits) • **5 GB**	CC BY SA
		zenodo.org/records/10149830 huggingface.co/datasets/PLAID-datasets/Rotor37		

Conclusions

- Non parametric optimization is made possible when cheap simulation exists (or good surrogates)
- **In non parametric design Design is simpler** but **exploration and testing is more challenging**

- On top of **an existing standard**: we built a library aiming to **streamline physics informed learning problems**

- We provide **open-source** datasets to probe statistical methods methods

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