Implicit Neural Representations for surrogate modeling of transonic aerodynamics.

1st Workshop on Machine Learning for Fluid Dynamics.

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Introduction and Objectives

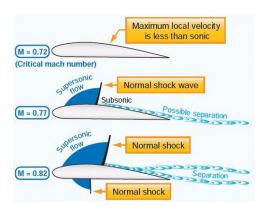
Surrogate Modeling of Transonic Flows

Introduction - Transonic Flows

Transonic Flows are of paramount importance in commercial and military aviation.

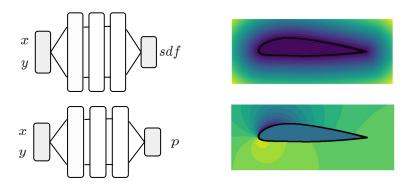
Accurate wing design for transonic conditions can lead to significant **drag reduction** and fuel savings.

Challenges in developing surrogate models for transonic flows are represented by the presence of **shock waves**.



Introduction - Implicit Neural Representations.

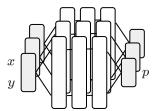
Neural Networks can continuously approximate signals on general domains: Implicit Neural Representation (INRs).



A **shape** can be parametrized by a NN that outputs the **Signed Distance Function** value at each point [2].

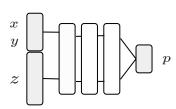
Similarly, for a **physical field** on a mesh (es. a pressure field) [3].

Distinct NN for each sample





Latent code conditioning



Introduction - Objectives

Demonstrate the potential of an INR based approach in predicting transonic aerodynamics, namely the shock region.

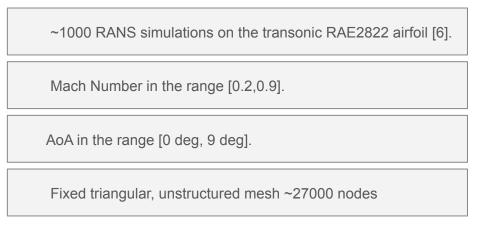
Compare the approach with traditional and state of the art surrogate models.

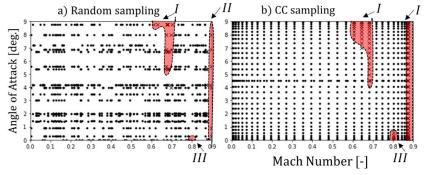
Analyze the effect of the INR architecture, namely in terms of input encoding.

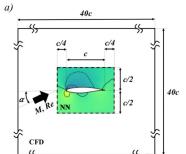
Show the advantages of using a multiscale Implicit Neural Representation architecture.

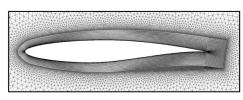
Methodology

Methodology - RAE 2822 Dataset.









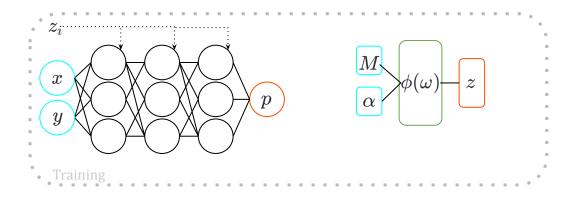
Methodology - INR Model Overview

Dataset consists of multiple pressure field samples $\{X_i\}_{i=1,\dots,M}$ where each sample consists of coordinate and pressure values tuples: $X_i = \{(\mathbf{x_j}, p_j)\}_{j=1,\dots,N}$

Latent codes $\{z_i\}_{i=1,...,M}$ and network weights are jointly learnt: $\underset{\theta,\{z_i\}_{i=1}^M}{\operatorname{argmin}} \sum_{i=1}^M (\sum_{j=1}^N \mathcal{L}(f_{\theta}(z_i,\mathbf{x_j}),p_j))$

At training time, a subset of nodes is **dynamically subsampled** to speed up training.

The latent space dynamics is learnt with a regressor (MLP) $\phi(\omega)$



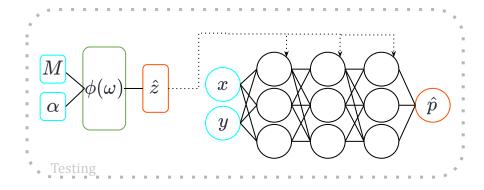
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Methodology - Multiscale Architecture

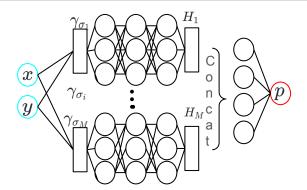
Fourier Feature Networks [5] perform positional encoding via the Fourier Basis functions. The standard deviation controls the **kernel bandwidth** and the overfitting behaviour of the model.

To enhance convergence to the high frequency components and to limit at the same time overfitting, inspired by [6] we propose a multiscale FF-NN architecture:

Multiple Gaussian encodings are operated on the input coordinates:

$$egin{aligned} \gamma_{\sigma_i}(v) = [sin(2\pi \mathbf{B}_{\sigma_i} v), cos(2\pi \mathbf{B}_{\sigma_i} v)] & b_{\sigma_i} \sim \mathcal{N}(0, \sigma_i^2) & i = 1, ..., M \end{aligned}$$

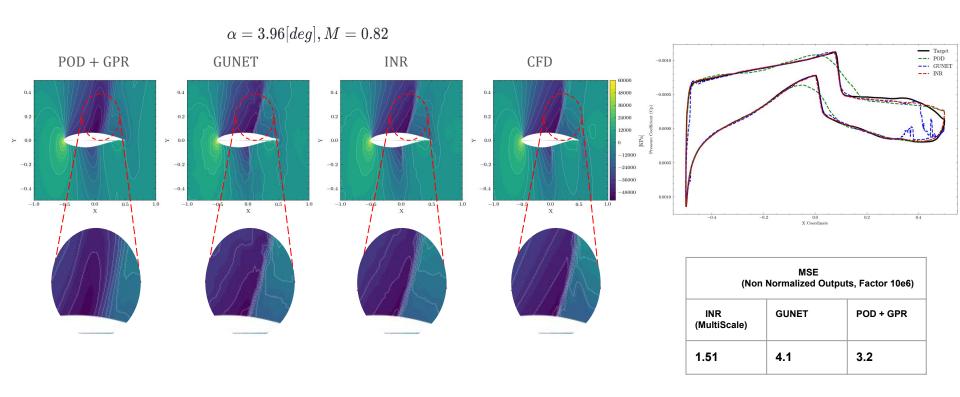
— The intermediate outputs H_i i = 1, ..., M are concatenated and passed through a final linear layer.

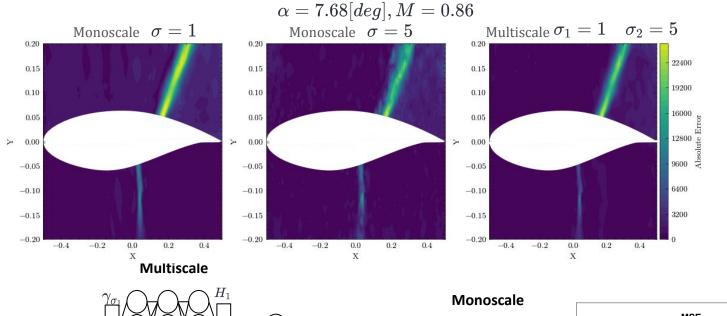


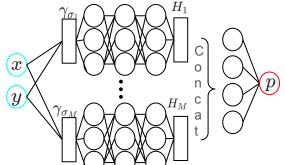
^[5] Tancik, Matthew, et al. "Fourier features let networks learn high frequency functions in low dimensional domains." Advances in Neural Information Processing Systems 33 (2020)

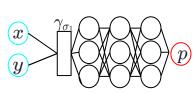
^[6] Wang, Sifan, Hanwen Wang, and Paris Perdikaris. "On the eigenvector bias of Fourier feature networks: From regression to solving multi-scale PDEs with physics-informed neural networks." Computer Methods in Applied Mechanics and Engineering 384 (2021): 113938.

RAE2822 Airfoil Dataset





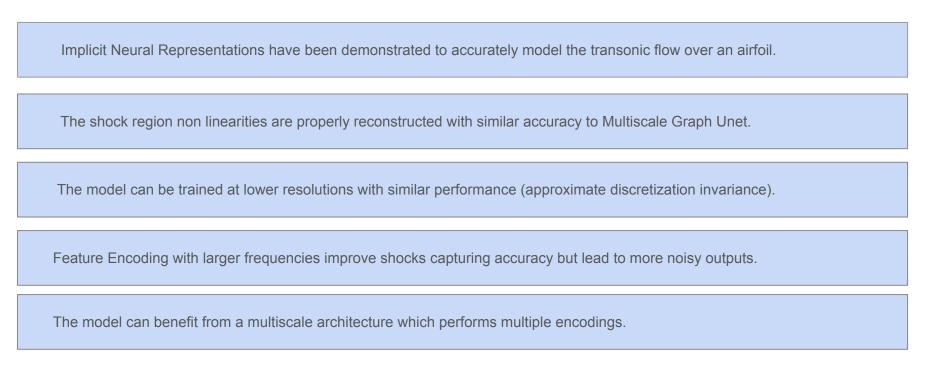




	MSE (Non Normalized Outputs, Factor 10e6)		
)	$\sigma = 1$	$\sigma = 5$	$\sigma_1=1$ $\sigma_2=5$
	1.61	1.67	1.51

Conclusions and Recommendations

Conclusions



Recommendations

The approach should be demonstrated for learning complex aerodynamics on manifolds in 3D.

The frequency encoding should be adapted to the frequency spectrum of the training dataset.

Discretization invariance is an important aspect that should be investigated for extension to large mesh simulations where full graph training is not feasible.

Thanks for listening!

Reach out at: giovanni.catalani@airbus.com

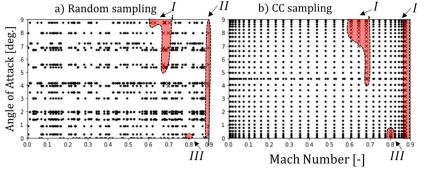
Appendix - RAE 2822 Dataset.

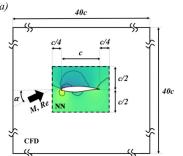
~1000 RANS simulations on the transonic RAE2822 airfoil [6].

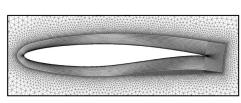
Mach Number in the range [0.2,0.9].

AoA in the range [0 deg, 9 deg].

Fixed triangular, unstructured mesh ~27000 nodes







Appendix - Fourier Feature Networks

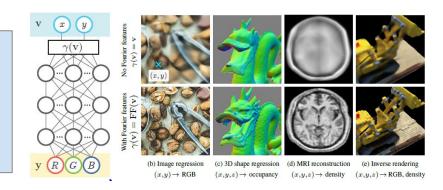
Simple MLPs are characterized by **spectral bias**: slow convergence to high frequency feature Positional encoding: Fourier
Feature Networks [5] perform
positional encoding via the
Fourier Basis functions.

Fourier Feature mapping make the regression kernel function **stationary**. Convergence to higher frequency content of the data is enhanced.

Gaussian Encoding

 $\gamma(v) = \left[a_1 \cos(2\pi b_1^T v), a_1 \sin(2\pi b_1^T v), \dots, a_m \cos(2\pi b_m^T v), a_m \sin(2\pi b_m^T v) \right]^T$ $b \sim \mathcal{N}(0, \sigma^2)$

The standard deviation controls the **kernel bandwidth** and the overfitting behaviour of the model.



Appendix - Baseline Methods

Proper Orthogonal Decomposition + Gaussian Process Regression

POD Formulation

$$\begin{split} & \max_{\boldsymbol{\phi}_1,...,\boldsymbol{\phi}_M} \sum_{j=1}^M \sum_{i=1}^M |\langle \boldsymbol{p}^{(j)}, \boldsymbol{\phi}_i \rangle|^2 \\ & \mathbf{p}^{(j)} = \sum_{l=1}^N \widehat{\boldsymbol{a}_l} \widehat{\boldsymbol{\phi}_l} \widehat{\boldsymbol{\phi}_l} \quad for \quad j=1,..,M \\ & a_{lj} = \langle \boldsymbol{\phi}_l, \mathbf{p}^{(j)} \rangle. \end{split}$$

Gaussian Process Regression

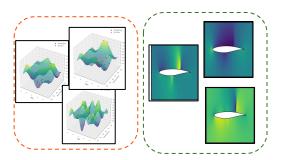
$$\{\hat{a}_{lj}\}_{l=1,...r} = f^{GPR}(\mu_{\mathbf{j}})$$

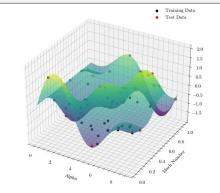
Radial Basis Function Kernel with optimized hyperparameters [7].

Final Prediction

$$\mathbf{\hat{p}}^{(j)} = \sum_{l=1}^r \hat{a}_{lj} oldsymbol{\phi}_l$$

r=128 component are retained (latent dimension)

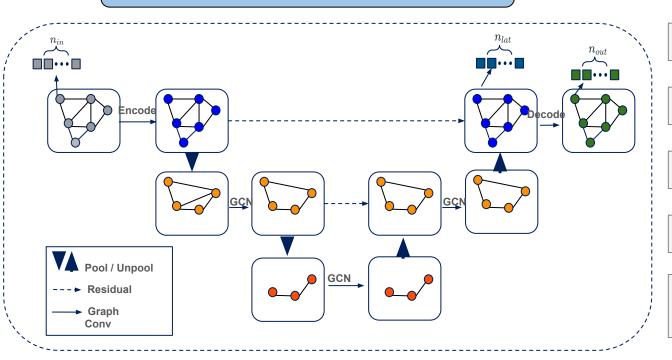






Appendix - Baseline Methods

Graph UNET [8]



Encoder - Process - Decode

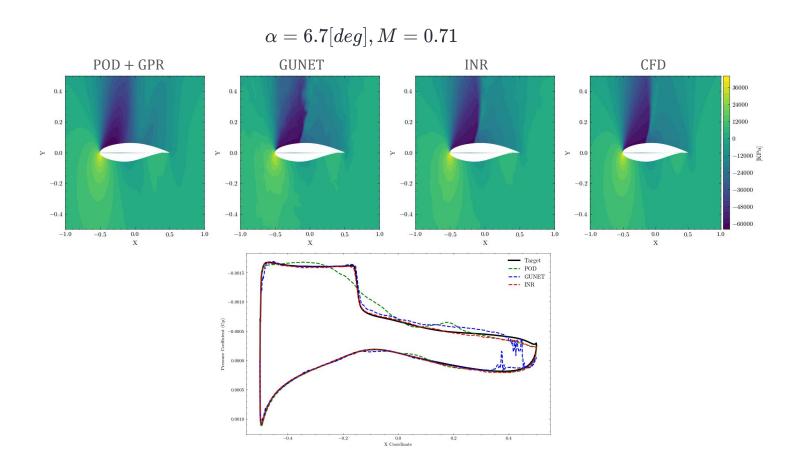
SageConvolution Layers

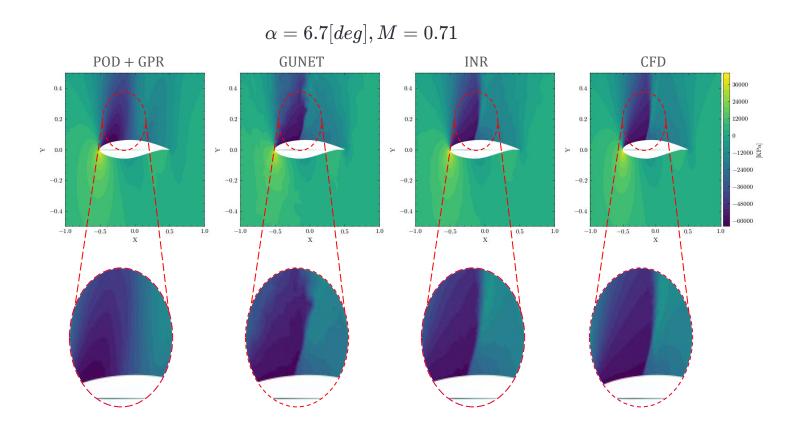
TopKPooling (3 Levels)

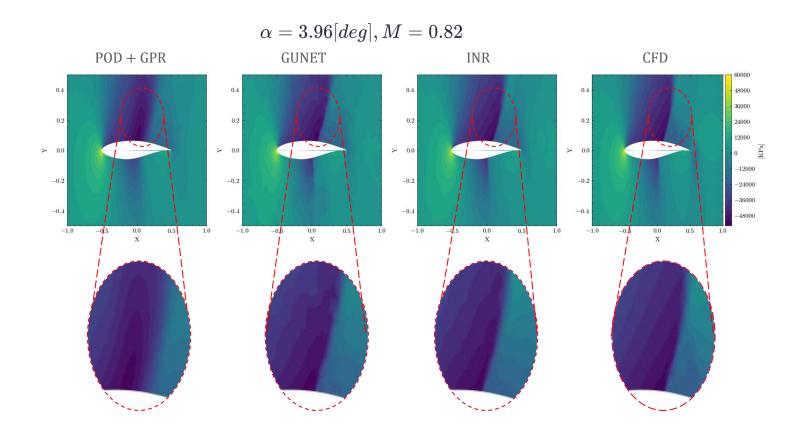
Latent dimension of 128

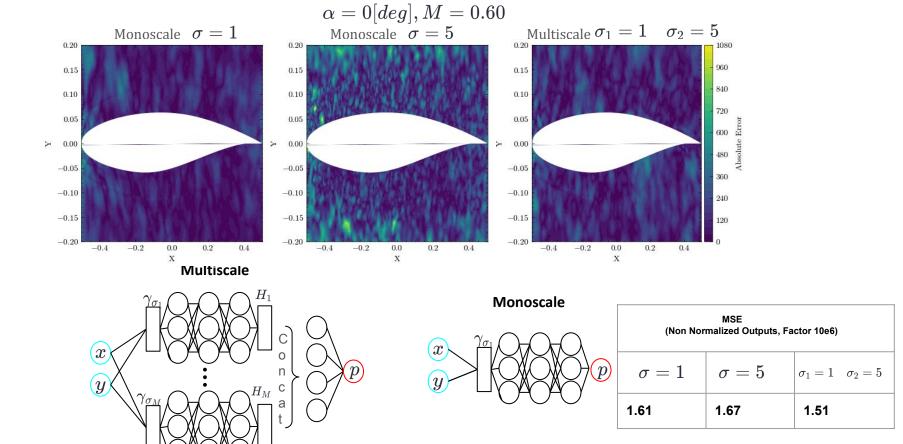
Inputs: x,y,Mach,alpha
Outputs: Pressure

[7] Gao, Hongyang, and Shuiwang Ji. "Graph u-nets." international conference on machine learning. PMLR, 2019..



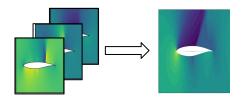






Appendix - Landscape of Surrogate Models

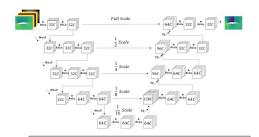
Modal Based Methods (POD)



Limitations

- Fixed Discretization.
- Non-linearities.
- Discontinuities.

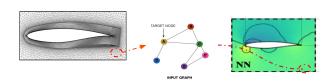
Convolutional Neural Nets



Limitations

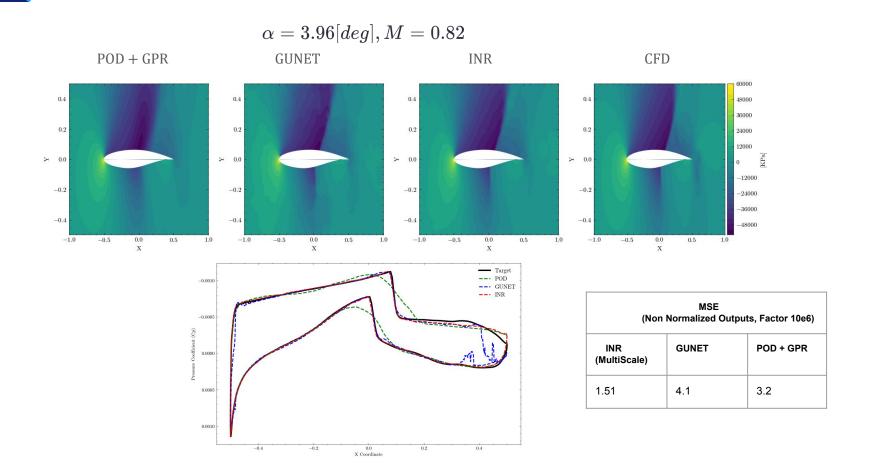
- Uniform Grids.
- Large resolutions required

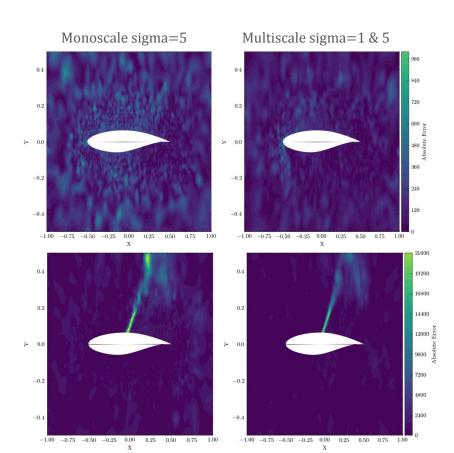
Graph Neural Nets



Limitations

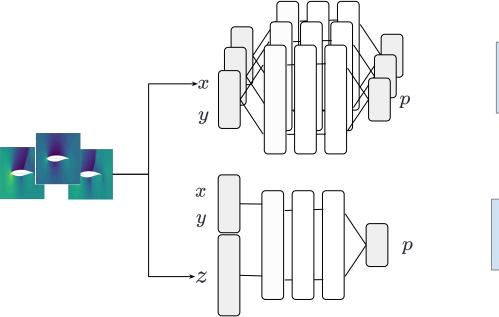
- Overmoothing.
- Large mesh applications.
- Multiscale operators.





INR: continuous representation of data.

Learning classes of objects for parametric systems on general domains.



Learn a distinct NN for each sample

Condition a global NN with a latent code z, modulating the network outputs [4].

