Sandia National Laboratories

8th Annual ML/DL Workshop

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Exceptional service in the national interest

DEEP NEURAL OPERATORS AS ACCURATE SURROGATES FOR SHAPE OPTIMIZATION

Applications to Airfoils and Hypersonic Waveriders

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Org. 6741

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PHYSICS-INFORMED MACHINE LEARNING (PIML)

Embed Physics

1. Decide on Problem
   - What are we modeling?
2. Curate Data
   - What data will inform the model?
3. Design an Architecture
   - RNN, CNN, GNN, etc.
4. Craft a Loss Function
   - What models are "Good"
5. Employ Optimization
   - What algorithms to train models?

Main paradigms PIML:

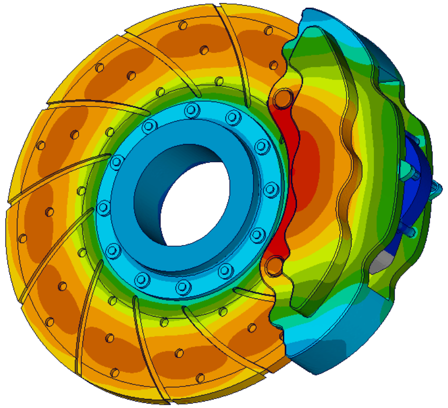
Neural Operators

PINNs

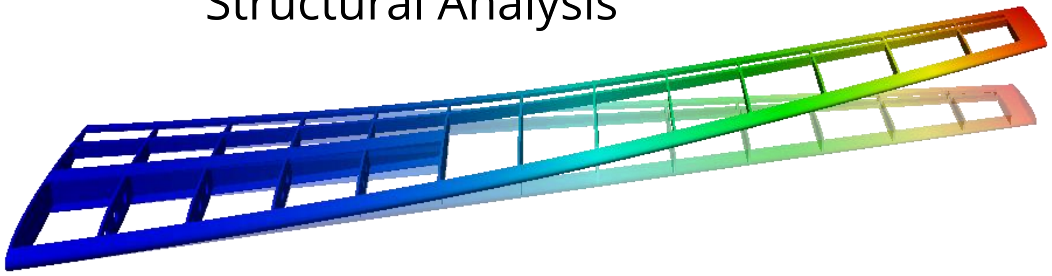
- Equations of motion are simpler in some coordinate frames than others
- We should train on data in formats ML is best able to interpret and learn from based on our physical knowledge
- The simpler the mapping from inputs to outputs, the easier it is to train ML models

SOLVING FORWARD PDE'S (WHY?)

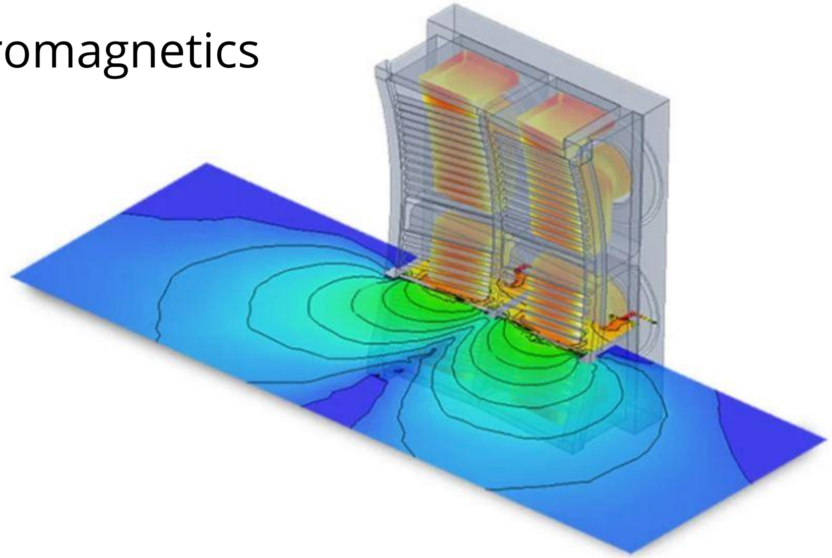
Heat Transfer

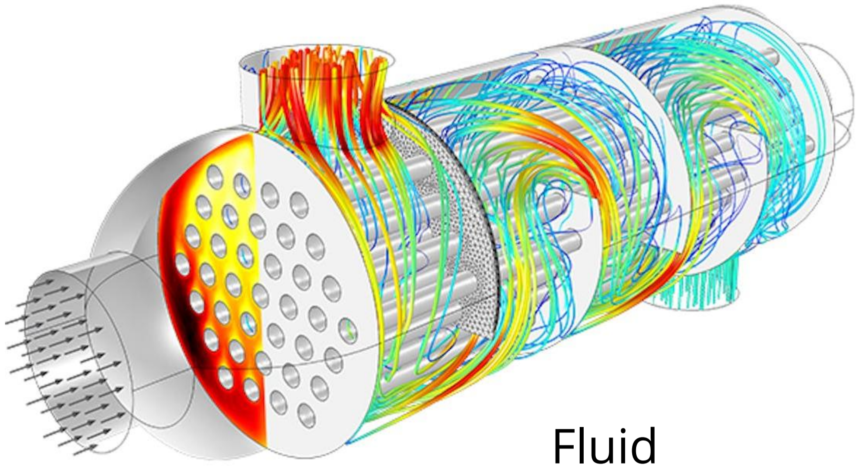


Structural Analysis



Electromagnetics

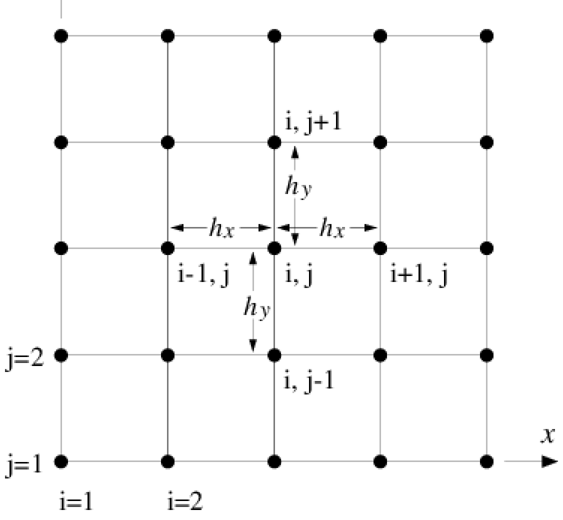




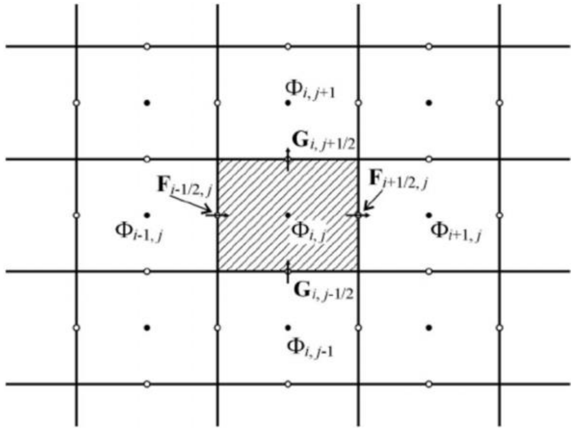
Fluid
Dynamics

TRADITIONAL APPROACHES TO NUMERICAL METHODS FOR PDE'S

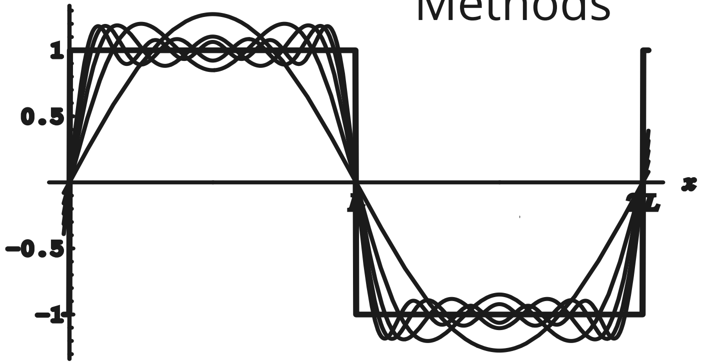
Finite Difference Methods



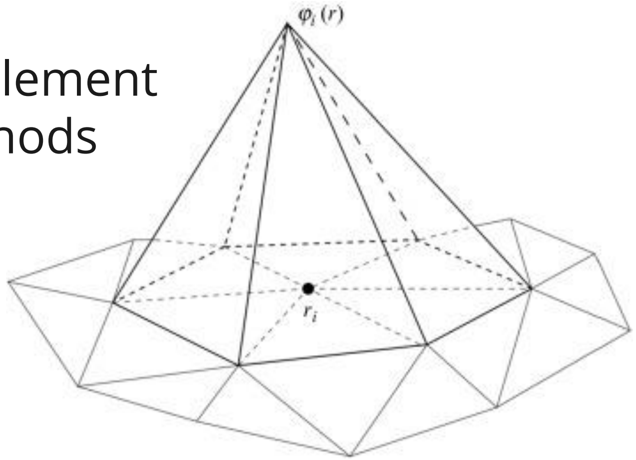
Finite Volume Methods



Spectral Methods



Finite Element Methods



NEURAL OPERATORS

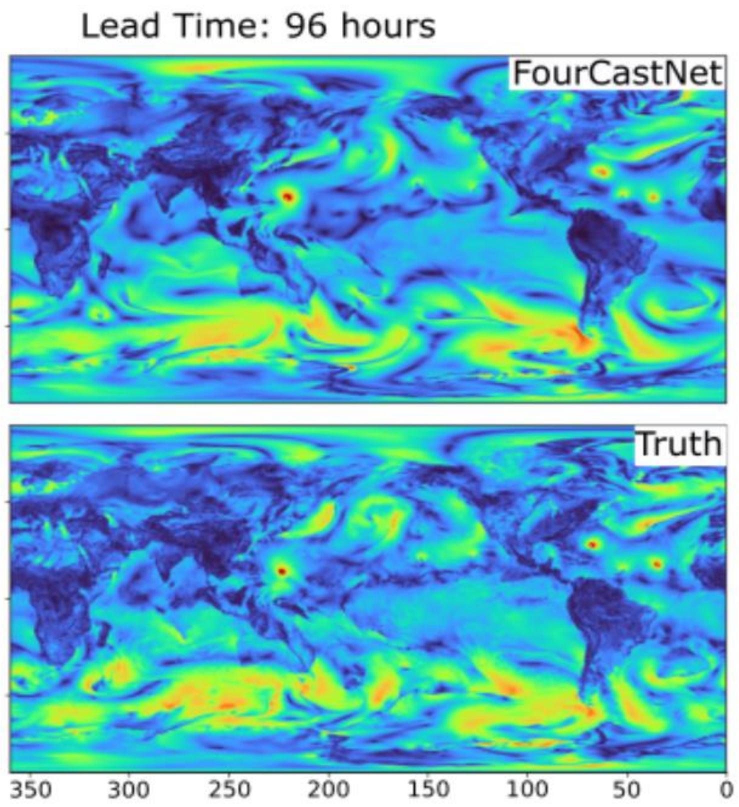
- A neural operator is a general data-driven ML approach which learns infinite dimensional function to function maps

$$G\colon \mathbb{R}^n \to \mathbb{R}^m$$

- Standard PDE solvers can be time consuming and even require super computers
- If you can properly learn the operator between inputs (i.e. PDE initial conditions) and outputs (i.e. PDE solution), then you can predict new solutions with one forward pass of the network (only takes milliseconds) instead of solving each time

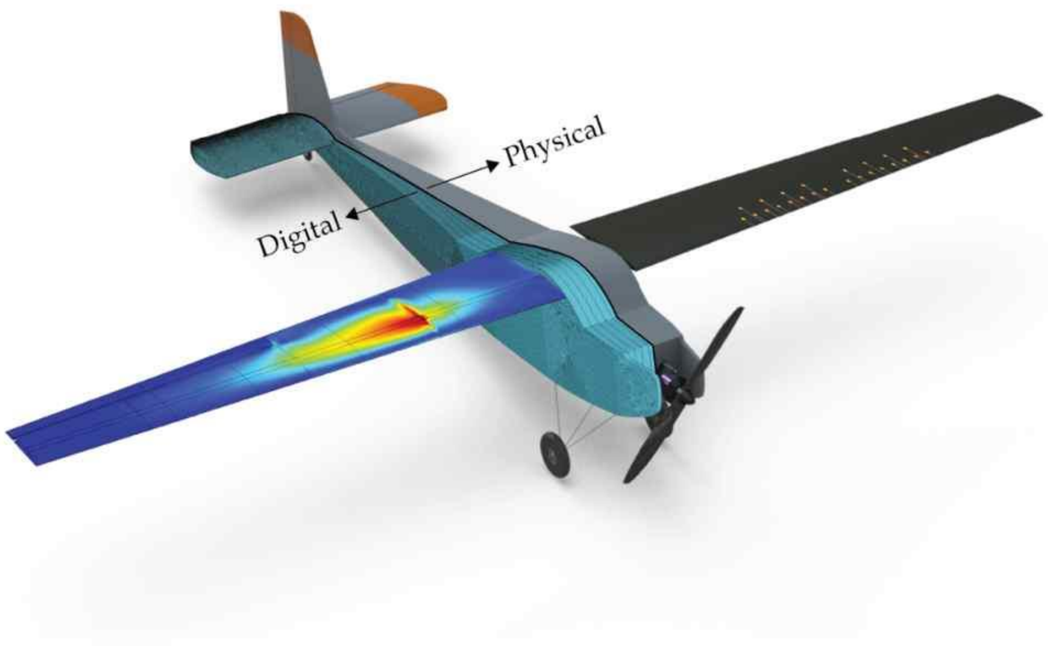
APPLICATIONS OF NEURAL OPERATORS

HPC simulation
(e.g. weather forecasting)



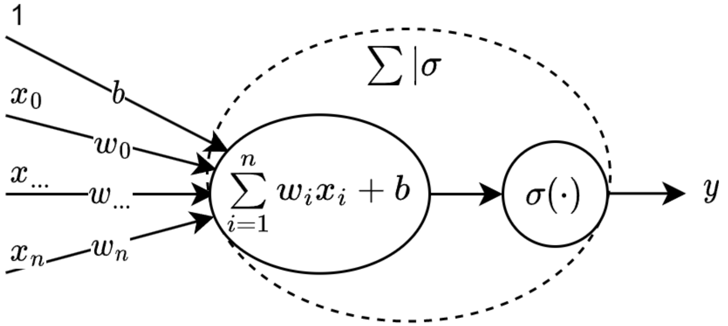
[1]

Digital twins for design, embedded control, etc.

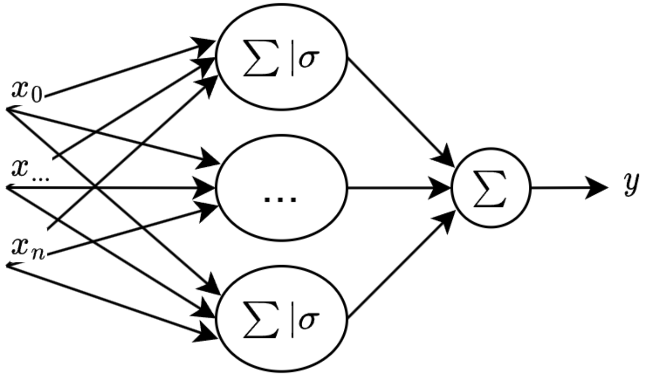


[1] Pathak, Jaideep, et al. "Fourcastnet: A global data-driven high-resolution weather model using adaptive fourier neural operators." *arXiv preprint arXiv:2202.11214* (2022).

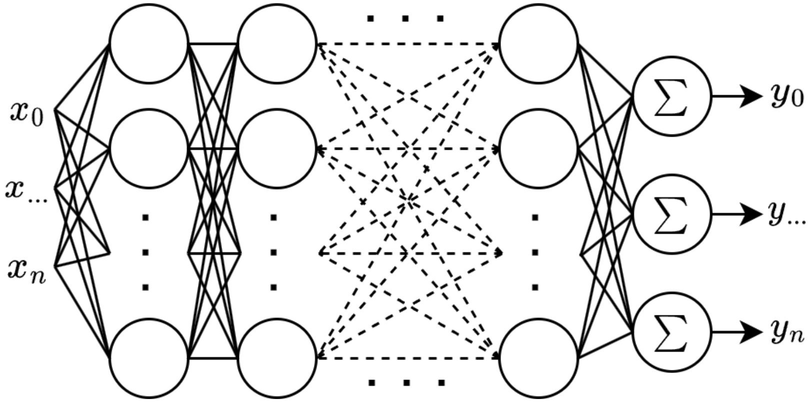
DEEP LEARNING (DL): BRIEF DNN BACKGROUND INFO



- Single artificial neural with (nonlinear) activation function σ



- Arbitrarily large single-layer NN (Universal Approximation Theorem)

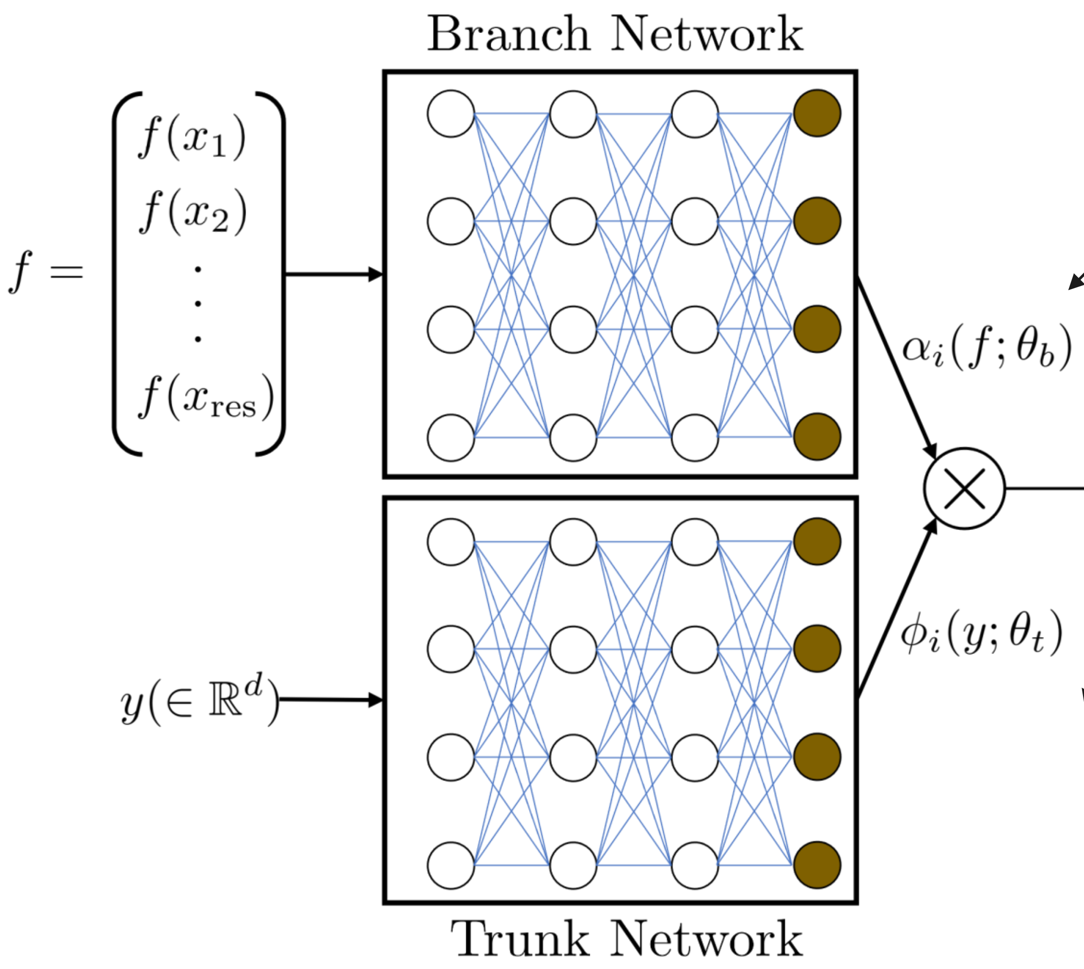


- Fully-connected NN with arbitrary width, depth, and output size

DEEP OPERATOR NETWORK (DEEPONET)

- Based on Universal Approximation Theorem for Operators (Chen & Chen 1995)

$$\left| G(u)(y) - \underbrace{\sum_{k=1}^{p} \sum_{i=1}^{n} c_i^k \sigma \left(\sum_{j=1}^{m} \xi_{ij}^k u(x_j) + \theta_i^k \right)}_{branch} \underbrace{\sigma(w_k \cdot y + \zeta_k)}_{trunk} \right| < \epsilon$$



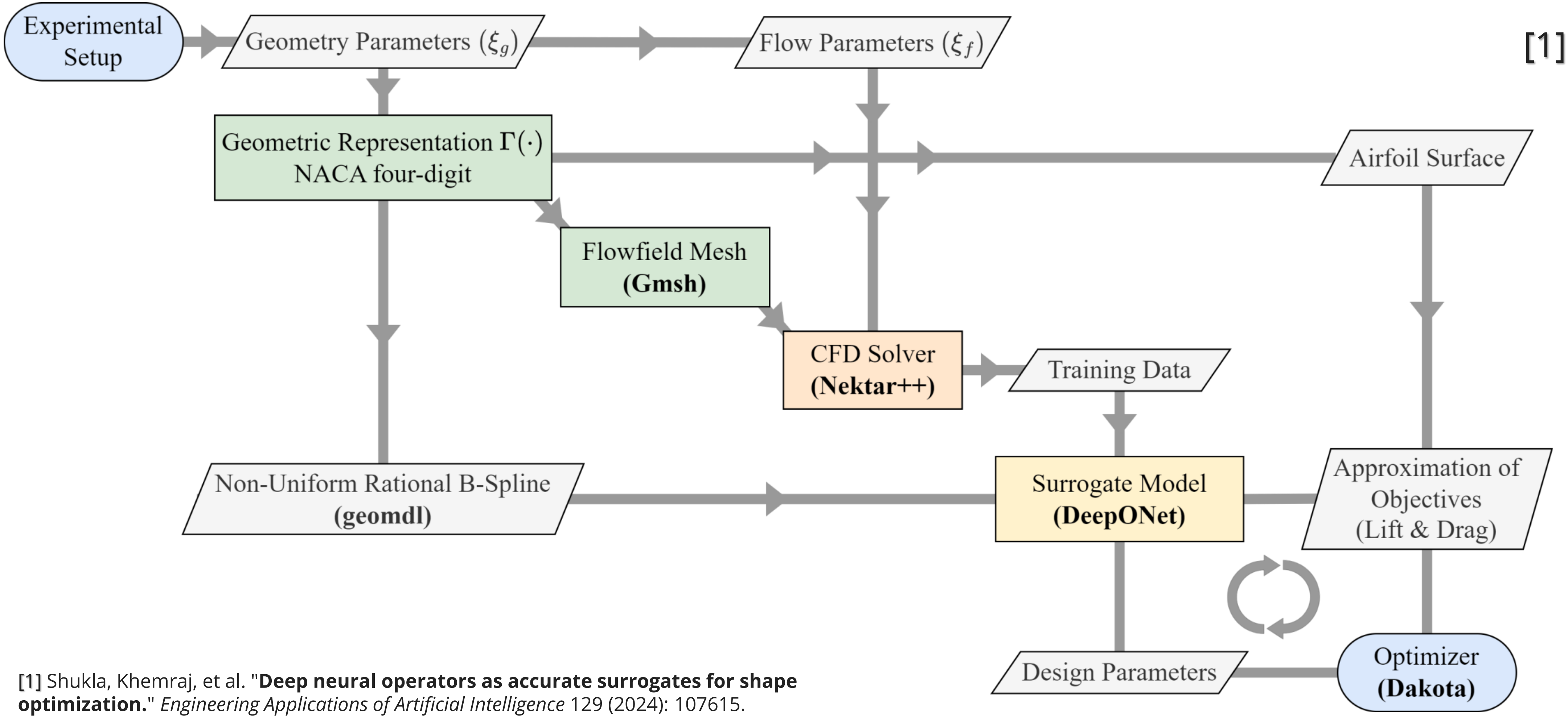
Basis function coefficients

$$\mathcal{G}(f)(y) = \sum_{i=1}^{N_\phi} \alpha_i(f; \theta_b) \phi_i(y; \theta_t)$$

Basis functions

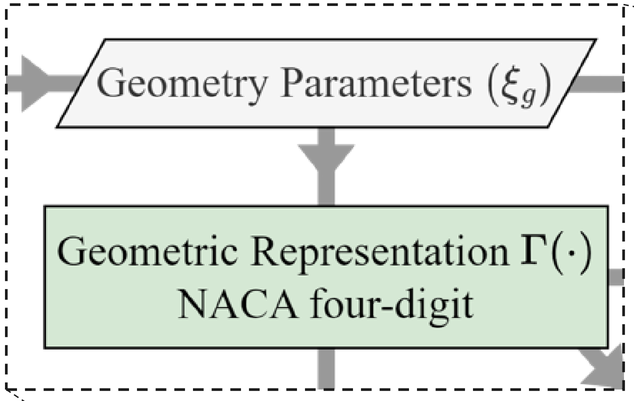
DEEPONET FOR VEHICLE SHAPE OPTIMIZATION

- Using neural operators to discover optimal geometries: a case study on airfoil and hypersonics



[1] Shukla, Khemraj, et al. "**Deep neural operators as accurate surrogates for shape optimization.**" *Engineering Applications of Artificial Intelligence* 129 (2024): 107615.

GENERATE GEOMETRIC DATASET



- Randomly select position of maximum camber (p) and maximum camber (m)

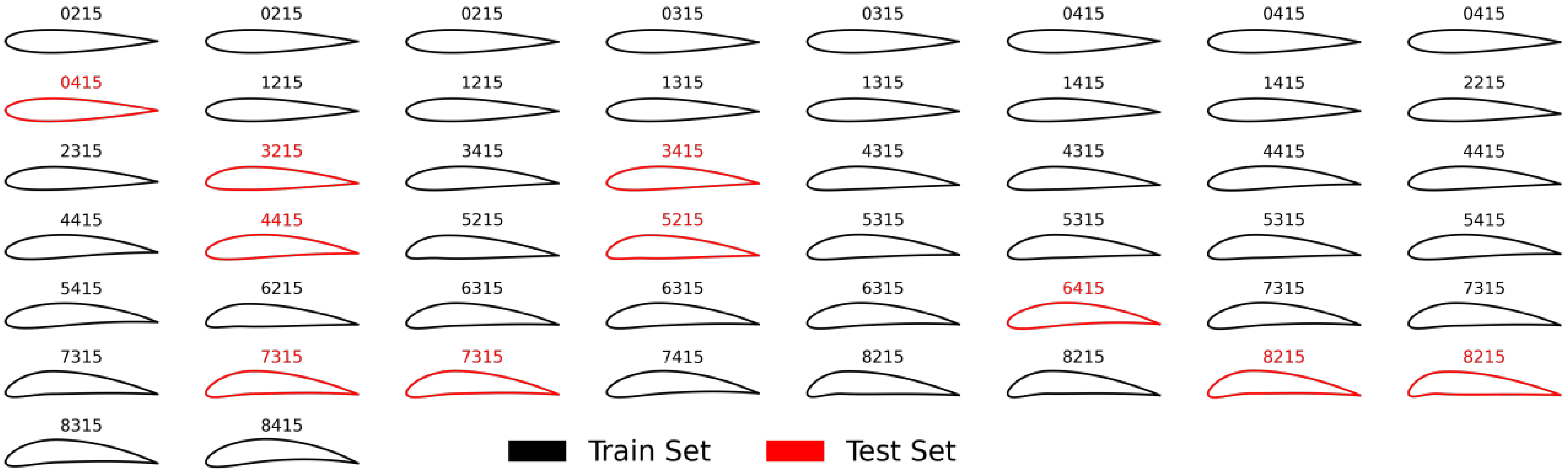
$$y_t = \frac{t}{0.2}\left(a_0\sqrt{x} + a_1 x + a_2 x^2 + a_3 x^3 + a_x x^4\right)$$

$$y_c = \begin{cases} \frac{m}{p^2}\left(2px - x^2\right) & \text{if } x < p \\ \frac{m}{(1-p)^2}\left(1 - 2p + 2px - x^2\right) & \text{if } x > p \end{cases}$$

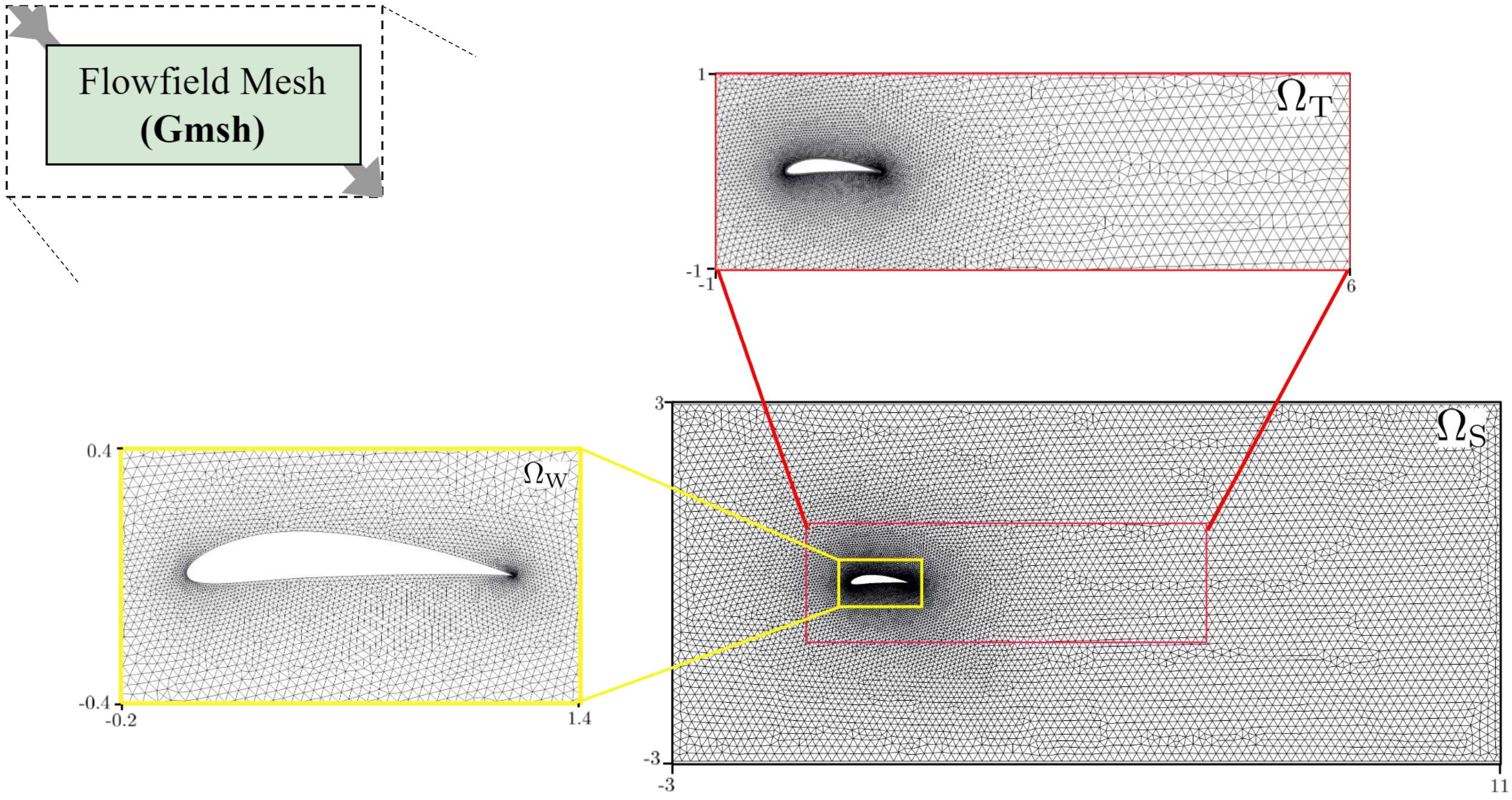
$$x_u = x - y_t \sin(\theta), \quad y_u = y_c + y_t \cos(\theta) \qquad \theta = \tan^{-1}\left(\frac{dy_c}{dx}\right)$$

$$x_l = x + y_t \sin(\theta), \quad y_l = y_c - y_t \cos(\theta)$$

where $a_0 = 0.2969, a_1 = -0.1260, a_2 = -0.3516, a_3 = 0.2843, a_4 = -0.1015.$



MESH TRAINING EXAMPLES (PRE-CFD STEP)



TRAIN SURROGATE MODEL

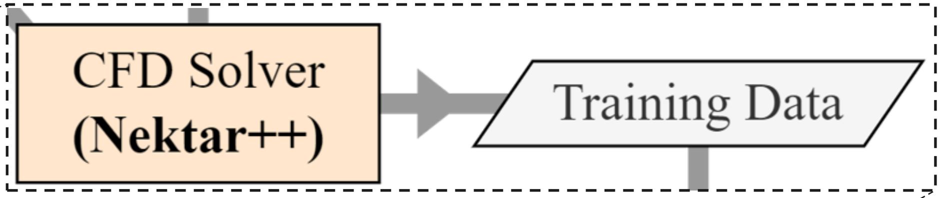
- Solve 2D compressible Navier-Stokes for different airfoils

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0$$

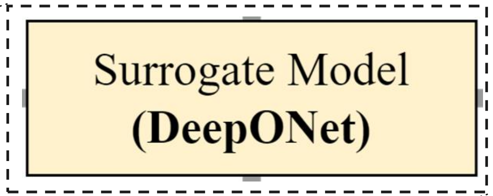
$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + p}{\partial x} + \frac{\partial \rho u v}{\partial y} = \frac{1}{Re}\left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y}\right)$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial \rho u v}{\partial x} + \frac{\partial \rho v^2 + p}{\partial y} = \frac{1}{Re}\left(\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y}\right)$$

$$\frac{\partial E}{\partial t} + \frac{\partial (E+p)u}{\partial x} + \frac{\partial (E+p)v}{\partial y} = \frac{1}{Re}\left[\frac{\partial\left(u\tau_{xx} + v\tau_{xy} + \kappa\frac{\partial T}{\partial x}\right)}{\partial x} + \frac{\partial\left(u\tau_{xy} + v\tau_{yy} + \kappa\frac{\partial T}{\partial y}\right)}{\partial y}\right]$$



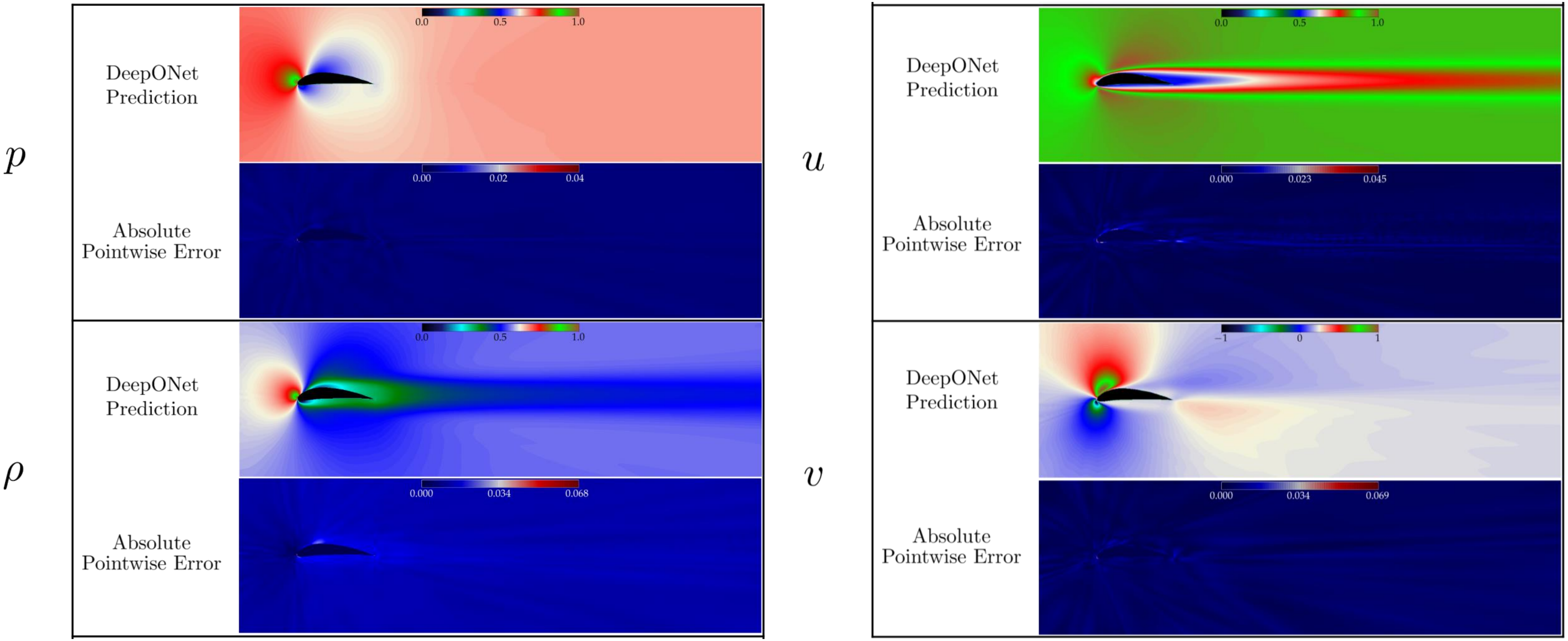
- Train DeepONets to predict pressure, x-y velocity, and density fields



Relative L^2 errors of the state variables trained DeepONet models

	NURBS-DeepONet		Parameter-DeepONet	
	Train rel. L^2 Error	Test rel. L^2 Error	Train rel. L^2 Error	Test rel. L^2 Error
$\mathcal{G}^p$	4.68e-03	6.05e-03	5.23e-03	6.85e-03
$\mathcal{G}^u$	4.97e-03	6.21e-03	4.12e-03	5.38e-03
$\mathcal{G}^v$	3.73e-03	4.60e-03	3.31e-03	4.25e-03
$\mathcal{G}^\rho$	4.57e-03	5.89e-03	4.00e-03	5.18e-03

SURROGATE MODEL MAPS GEOMETRY TO FOUR FIELDS



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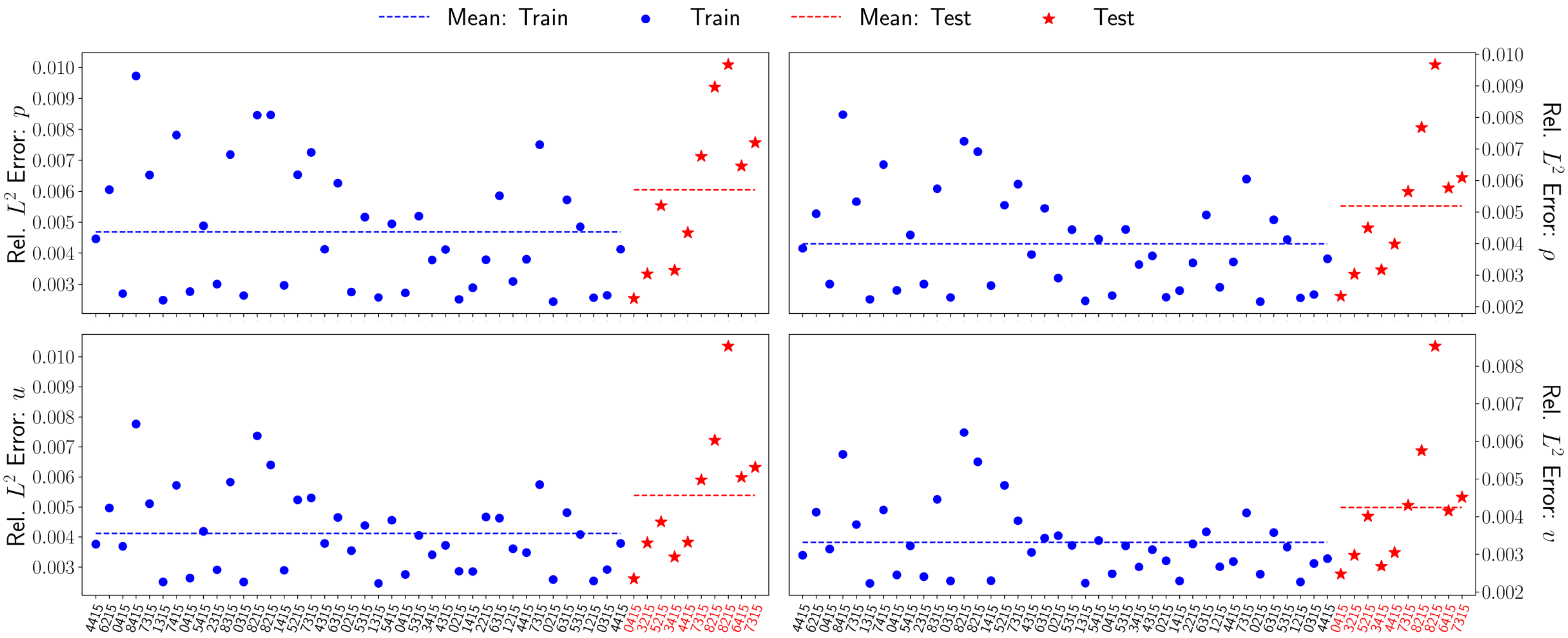
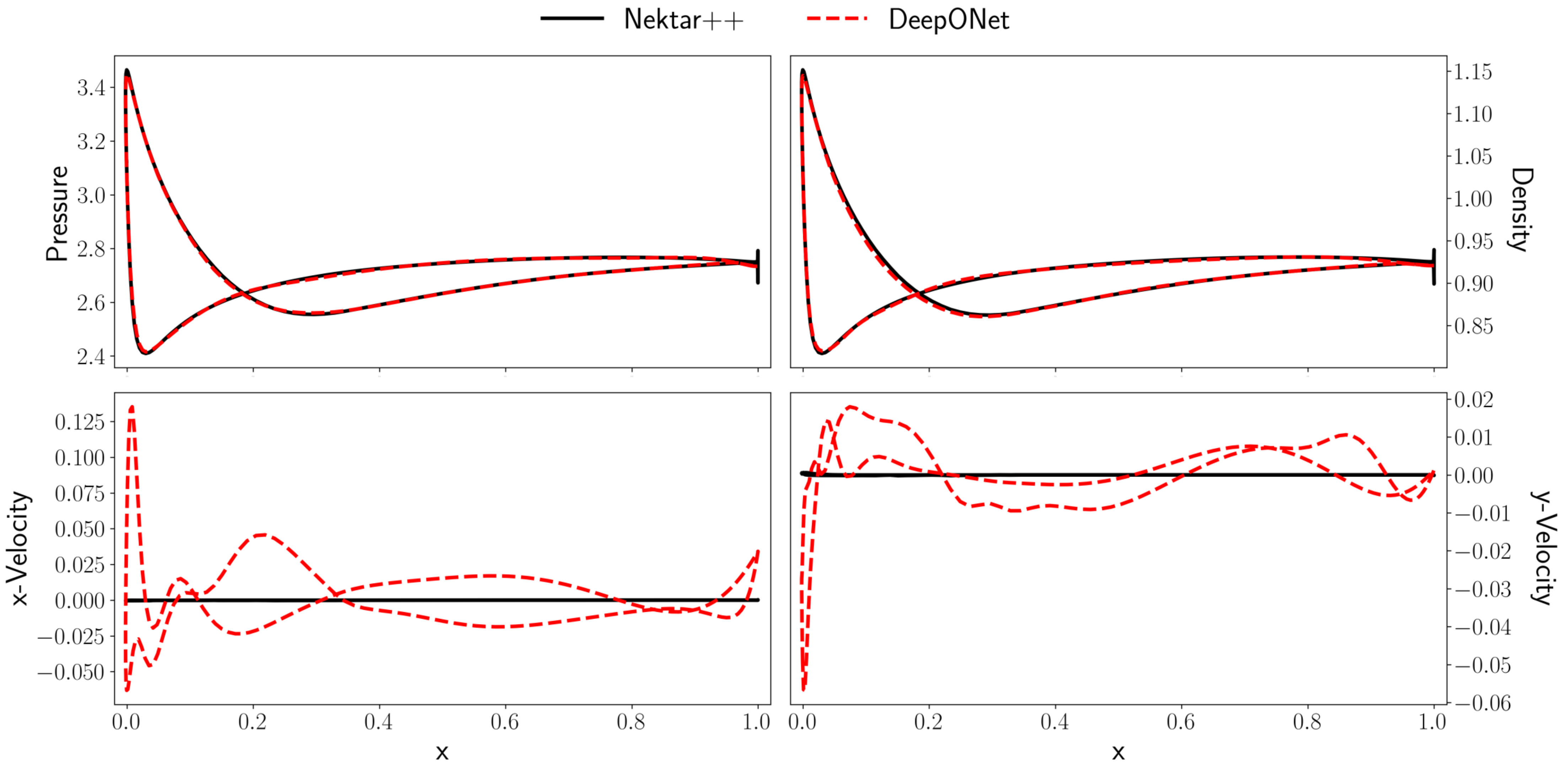
MINIMAL FLOWFIELD GENERALIZATION ERROR



SURFACE OF AIRFOIL PREDICTIONS



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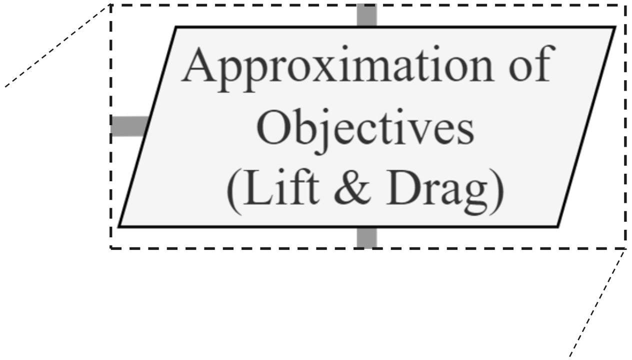
COMPUTE QUANTITIES OF INTEREST

- Compute quantities of interest (QOI) to optimize for (Lift/Drag)



$$\tau_w = \mu \frac{dU}{d\vec{n}}$$

$$L = \int dF_x = \sum p\vec{n_x} dS + \sum \tau_w \vec{t_x} dS$$

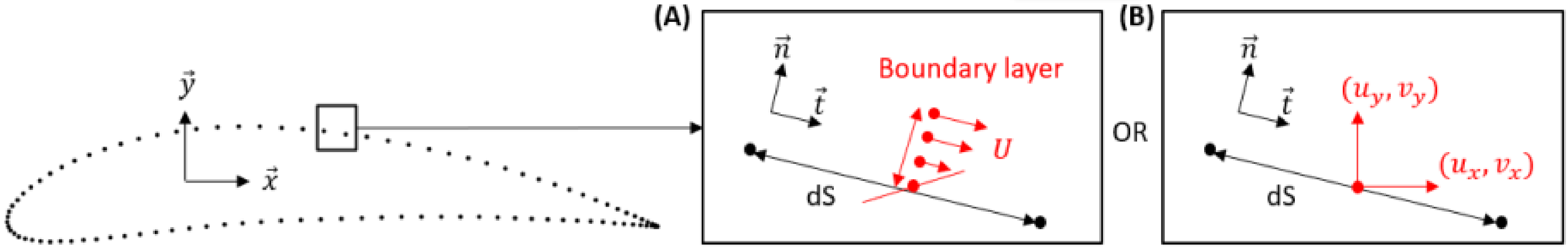
$$D = \int dF_y = \sum p\vec{n_y} dS + \sum \tau_w \vec{t_y} dS$$

1. Finite-difference **(A)**:

$$\frac{dU}{d\vec{n}} = \frac{-U_2 + 4U_1 - 3U_0}{2h}$$

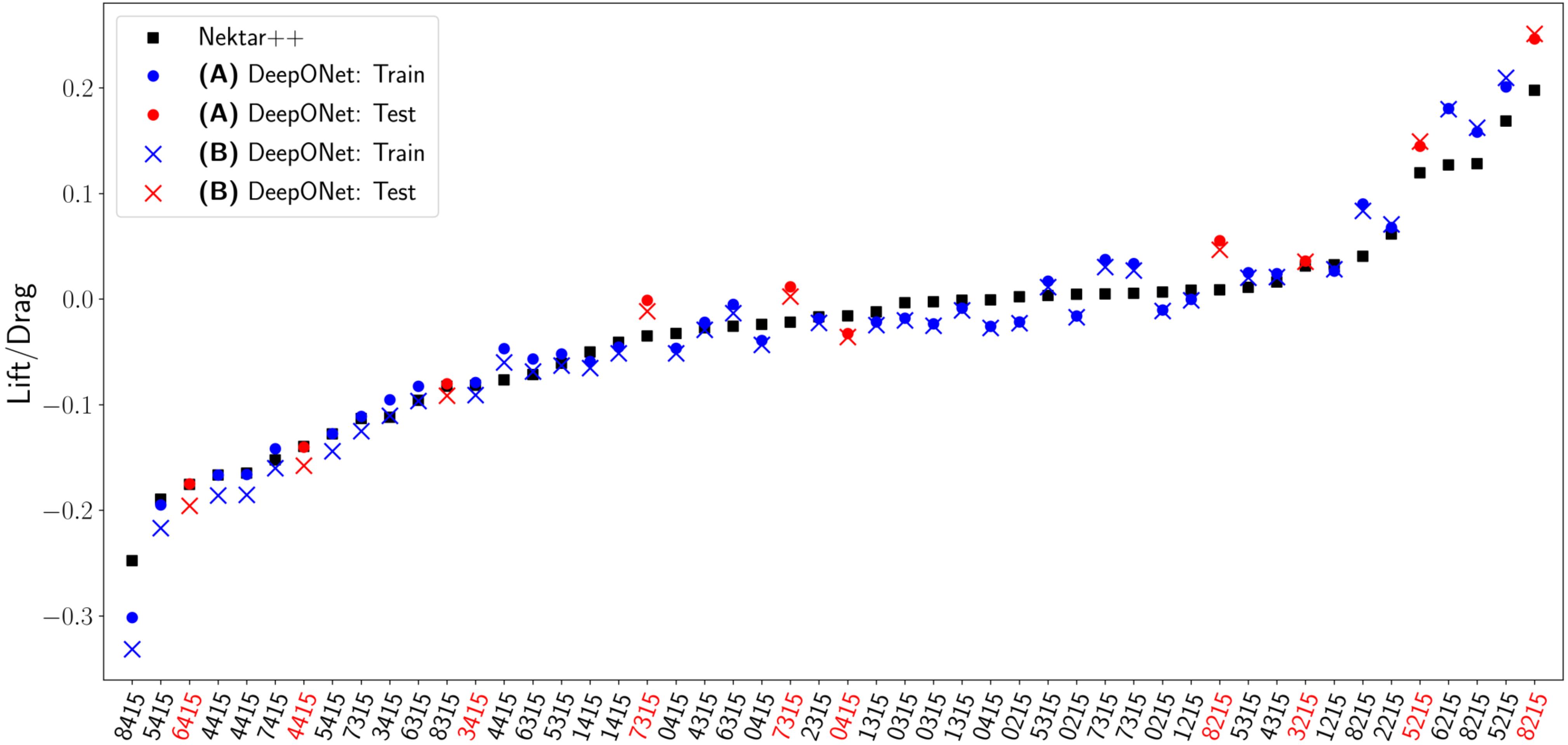
2. Automatic-differentiation **(B)**:

$$\frac{dU}{d\vec{n}} = (v_y - u_x) sin\theta cos\theta - v_x sin^2\theta + u_y cos^2\theta$$

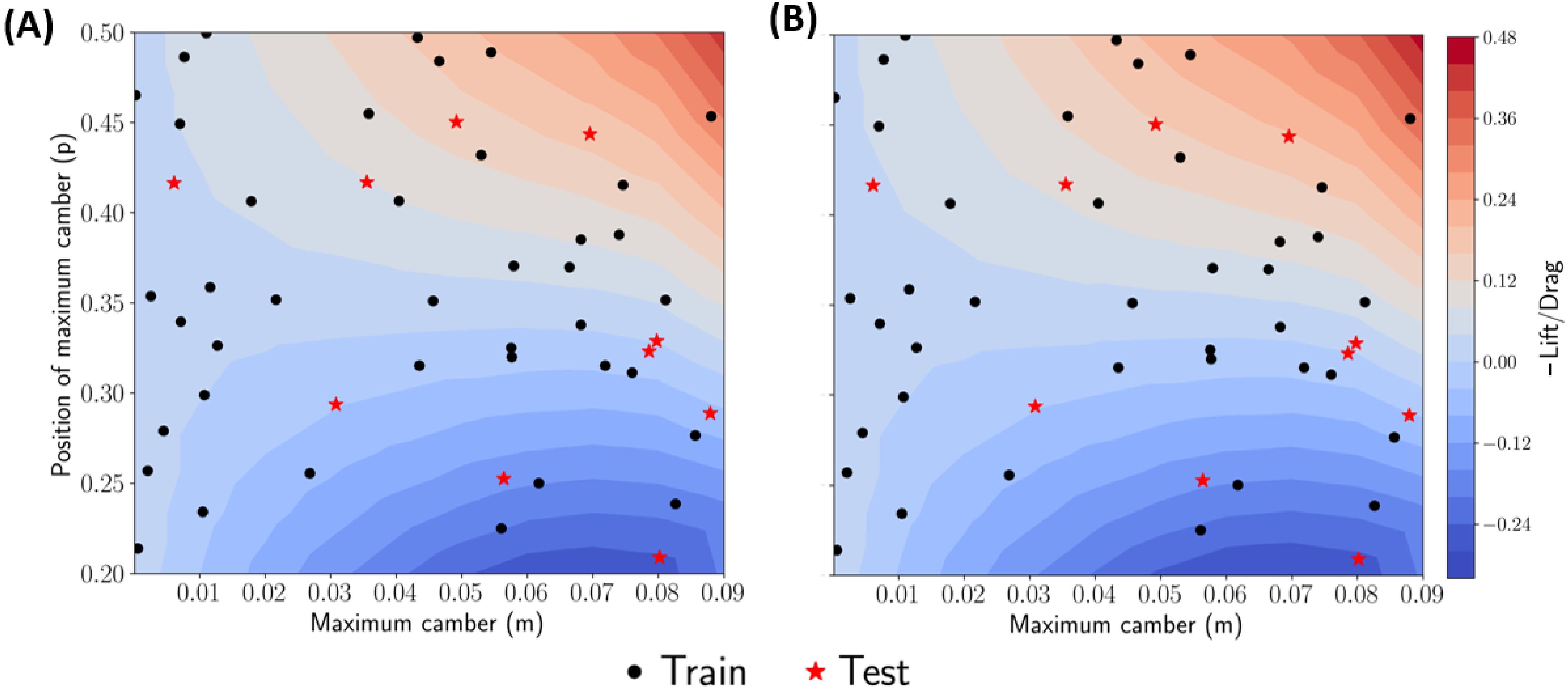


EVALUATING PERFORMANCE

- Lift/Drag QOI is close to Nektar++ (traditional CFD solver) baseline



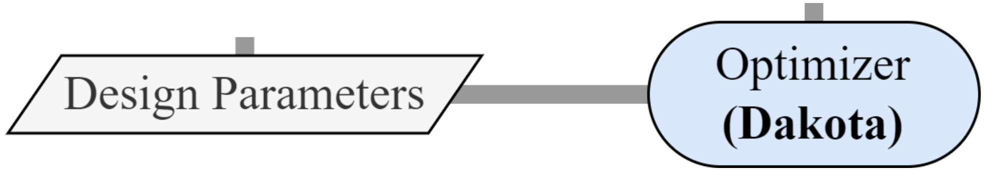
QOI OPTIMIZATION LANDSCAPE

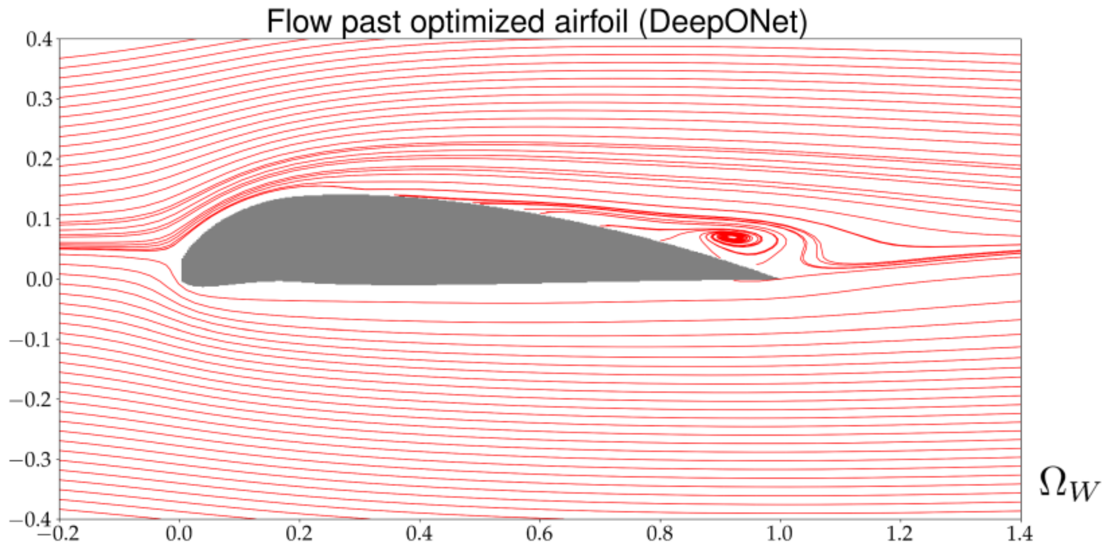


PERFORM GEOMETRY OPTIMIZATION

- Perform optimization

$$
\begin{aligned}
\underset{m,p}{\text{minimize}} \quad & -f(m,p) \\
\text{subject to} \quad & m_{\min} \leq m \leq m_{\max}, \\
& p_{\min} \leq p \leq p_{\max},
\end{aligned}
$$





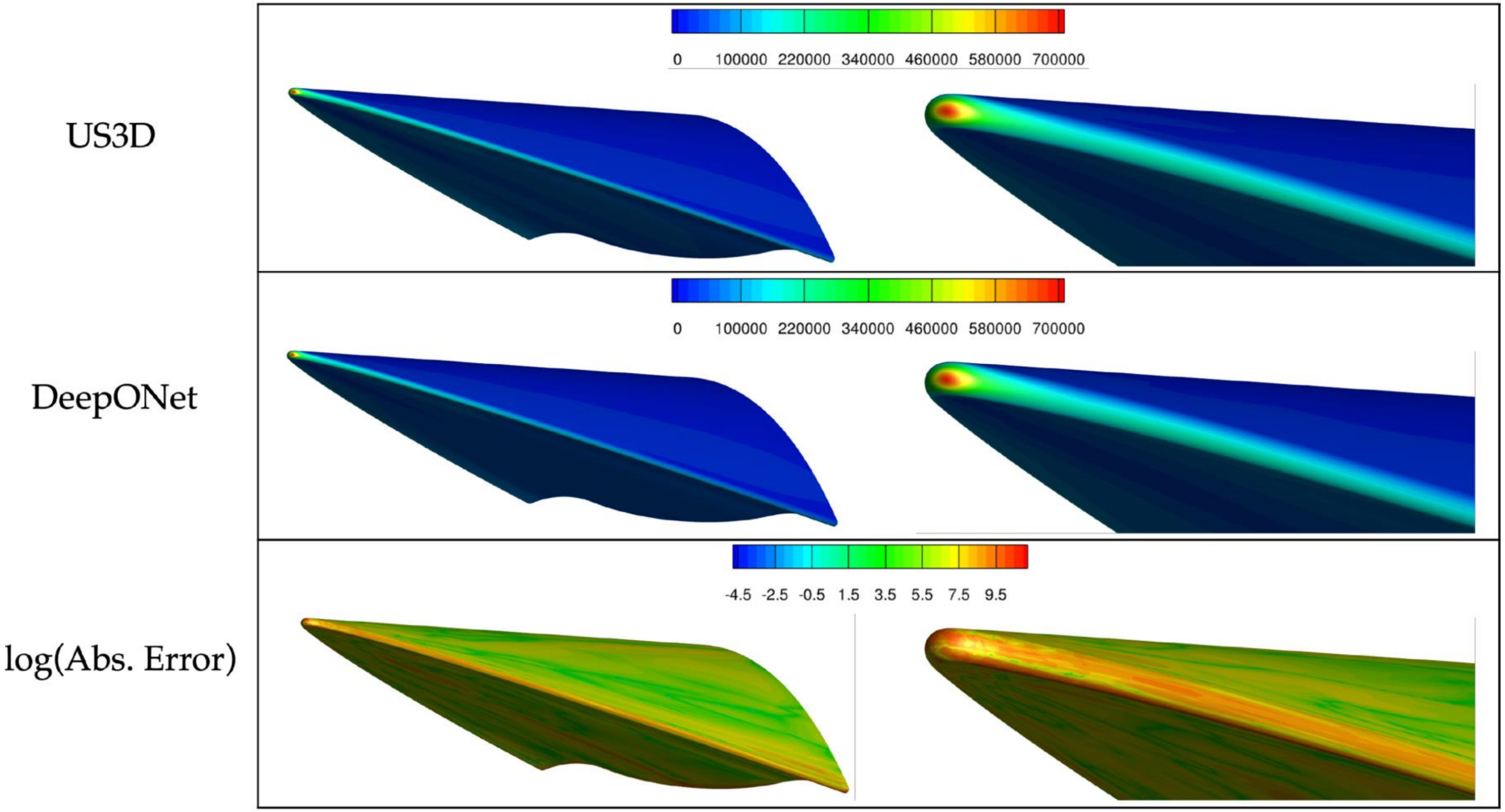
- Four to five orders of magnitude speed-up
- Flexibility to designate new quantities of interest to optimize for without re-training

Model Type	Relative Cost of Single Objective Function Evaluation
Baseline CFD (Nektar++)	32,253
DeepONet (A)	1.34
DeepONet (B)	1

3D AEDC WAVERIDERS AT HYPERSONIC CONDITIONS

- Also done for morphed surfaces for hypersonic waveriders and at different flight conditions
- Neural operators can be used as digital twins for autonomous control due to their real-time physical inferences
- Limited results as most were CUI

Heat flux Q_w at Mach 7.36



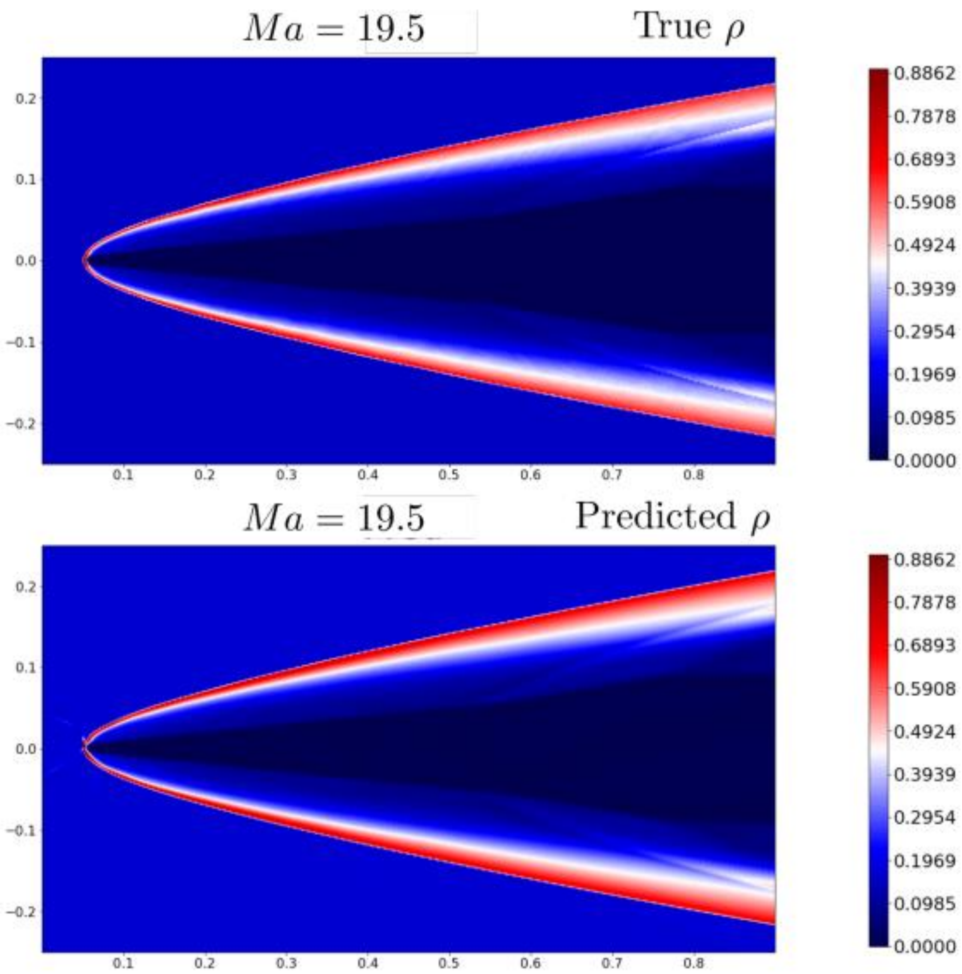
HYPERSONIC AEDC WAVERIDERS

The L^2 norm of relative error between actual and predicted total shear stress τ_y and heat flux Q_w from DeepoNet for the AEDC waverider.

AoA	Sample Type	L^2 error in τ_y	L^2 error in Q_w
-10	Train	0.38%	3.50%
-9	Train	0.34%	3.39 %
-8	Test	0.34%	3.55%
-7	Test	0.38%	4.07%
-6	Train	0.30%	3.35%
-5	Test	0.33%	3.30%
-4	Train	0.29%	3.24 %
-3	Test	0.28%	3.05%
-2	Train	0.28%	2.57 %
-1	Train	0.29%	2.44 %
0	Train	0.28%	2.24%
1	Train	0.32%	2.11%
2	Test	0.36%	2.42%
3	Train	0.37%	2.08%
4	Test	0.40%	2.04%
5	Train	0.45%	2.01%
6	Test	0.50%	1.97%
7	Train	0.51%	1.93%
8	Test	0.54%	1.87%
9	Train	0.57%	1.91%
10	Train	0.61%	2.08%

More UUR results in follow-up preprint:

- Shukla, Khemraj, et al. "Deep operator learning-based surrogate models for aerothermodynamic analysis of AEDC hypersonic waverider." *arXiv preprint arXiv:2405.13234* (2024).



QUESTIONS?

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Research paper

Deep neural operators as accurate surrogates for shape optimization

Khemraj Shukla [a 1], Vivek Oommen [a 1], Ahmad Peyvan [a 1], Michael Penwarden [b 1], Nicholas Plewacki [c], Luis Bravo [c], Anindya Ghoshal [c], Robert M. Kirby [b], George Em Karniadakis [a]