

# A Point-Cloud Deep Learning Framework for Prediction of Fluid Flow Fields on Irregular Geometries

Ali Kashefi Davis Rempe Prof. Leonidas Guibas

#### Manuscript

A Point-Cloud Deep Learning Framework for Prediction of Fluid Flow Fields on Irregular Geometries

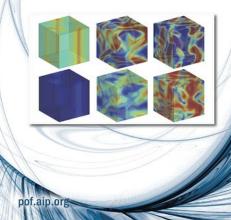
#### A Point-Cloud Deep Learning Framework for Prediction of Fluid Flow Fields on Irregular Geometries

Ali Kashefi,<sup>1, a)</sup> Davis Rempe,<sup>1, b)</sup> and Leonidas J. Guibas<sup>1, c)</sup> Stanford University, Stanford, CA 94305, USA

We present a novel deep learning framework for flow field predictions in irregular domains when the solution is a function of the geometry of either the domain or objects inside the domain. Grid vertices in a computational fluid dynamics (CFD) domain are viewed as point clouds and used as inputs to a neural network based on the PointNet architecture, which learns an end-to-end mapping between spatial positions and CFD quantities. Using our approach, (i) the network inherits desirable features of unstructured meshes (e.g., fine and coarse point spacing near the object surface and in the far field, respectively), which minimizes network training cost; (ii) object geometry is accurately represented through vertices located on object boundaries, which maintains boundary smoothness and allows the network to detect small changes between geometries; and (iii) no data interpolation is utilized for creating training data; thus accuracy of the CFD data is preserved. None of these features are achievable by extant methods based on projecting scattered CFD data into Cartesian grids and then using regular convolutional neural networks. Incompressible laminar steady flow past a critical method. various shapes for its cross section is considered. The mass and momentum of predicted fields ar July 2013 For the first time, our network generalizes the predictions to multiple objects as well as an airfoil, only single objects and no airfoils are observed during training. The network predicts the flow field AIP Physics of of times faster than our conventional CFD solver, while maintaining excellent to reasonable accu

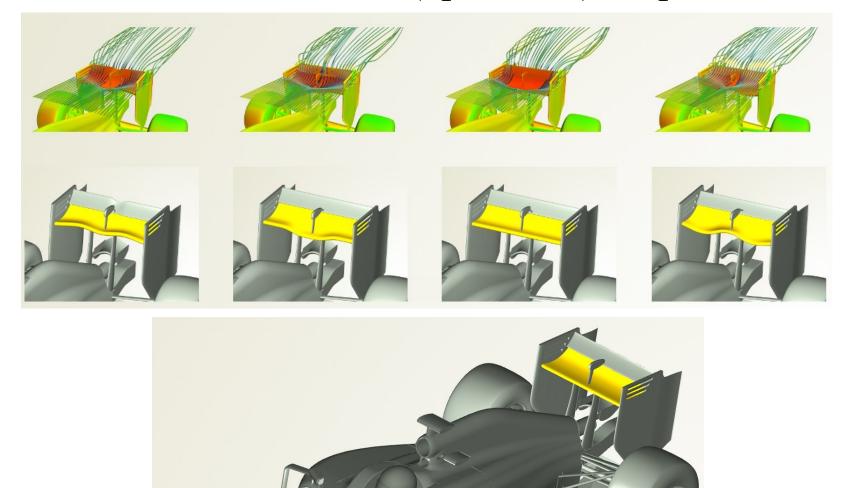
#### I. INTRODUCTION AND MOTIVATION

One of the main contributions of machine learning techniques to Computational Fluid Dynamics (CFD) simulations is reducing the computational costs. Even with the presence of high performance computing tools (see e.g., Refs. 11-5) and efficient numerical schemes (see e.g., Refs. 6-11) to accelerate CFD simulations, investigation of design parameters for device optimization remains computationally expensive mainly because a huge a network, and thus, an effective data reprecrucial. The connection of neural networks sian grids is straightforward. For this scenari and three-dimensional CNNs is a popular r among the CFD community (see e.g., Refs. this method, each vertex of a Cartesian grid to a pixel of an image processed by a CNN. real-world applications with complex geometri ing unstructured grids is unavoidable. In co Cartesian grids, the connection of unstruction

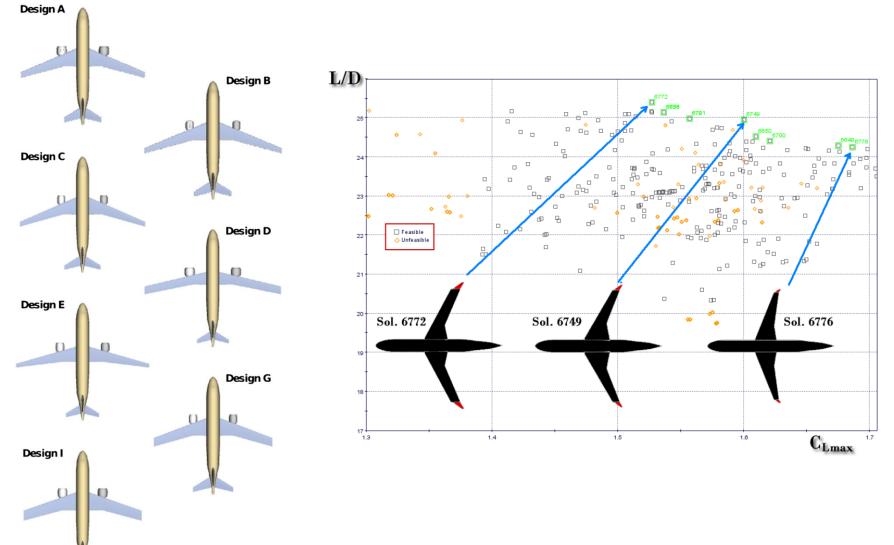


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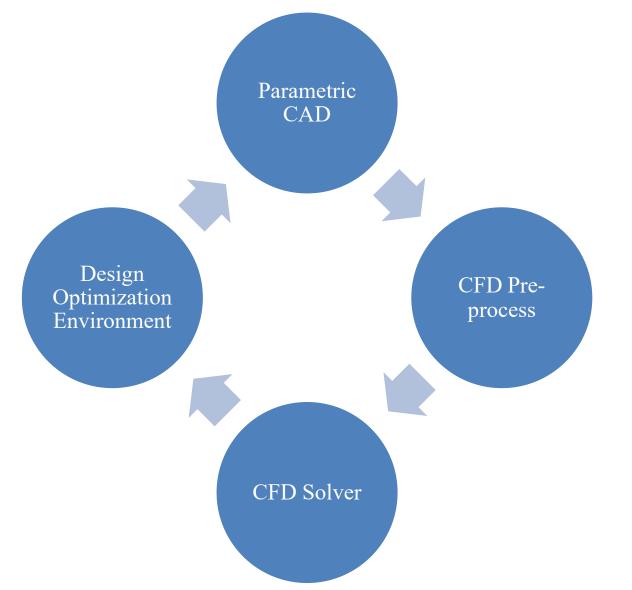
### What is the best (optimized) shape?



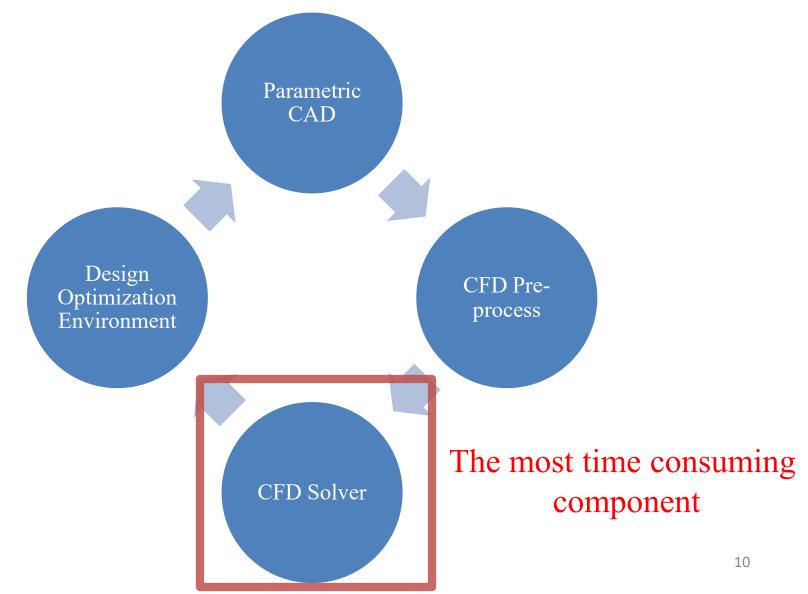
### What is the best (optimized) shape?



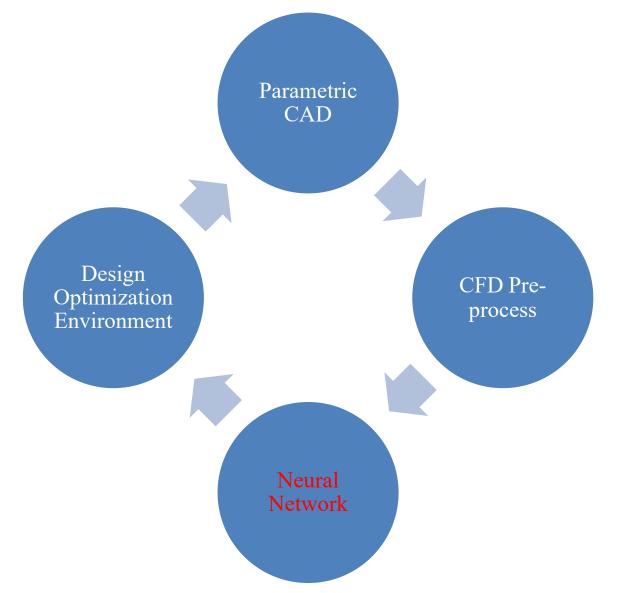
### Shape optimization based on geometric parameters



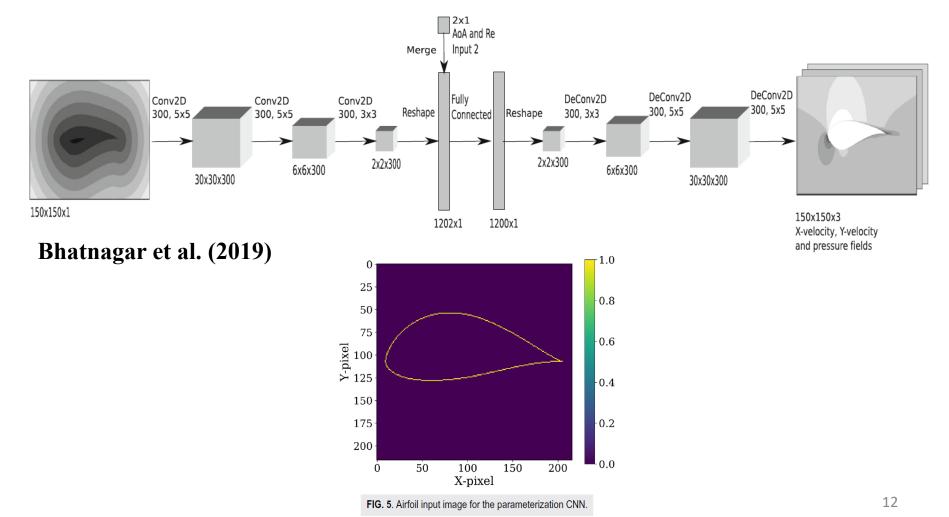
### Shape optimization based on geometric parameters



### Shape optimization based on geometric parameters

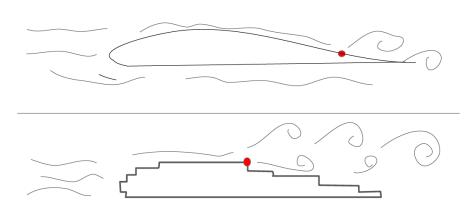


### How to represent the geometry? **"Pixelation"**, a so-far-used strategy for this purpose!



### **5** main shortcoming

**1**# Pixelation leads to coarsening previously-smooth boundaries of a shape and introduces artificial roughness to its surface. This error can dramatically change the flow features such as the location of the detachment point on the surface of an airfoil.



Detachment points for an airfoil and its voxelisation.

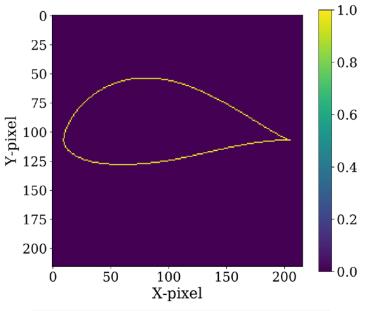
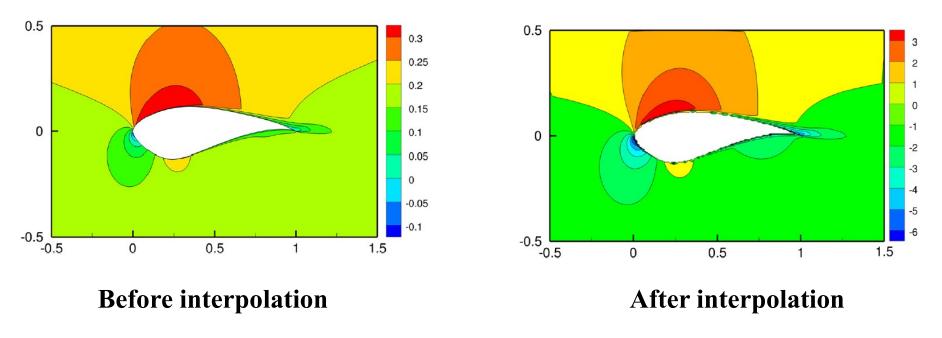


FIG. 5. Airfoil input image for the parameterization CNN.

Sekar et al. (2019)

### **5** main shortcoming

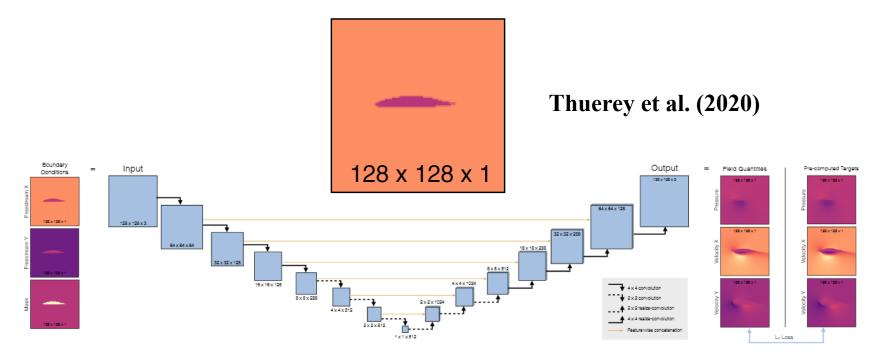
**2**# Decreasing the order of accuracy of CFD data due to the data interpolation/extrapolation.



Bhatnagar et al. (2019)

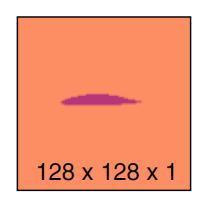
### **5** main shortcoming

**3**# While the flow field around an object is highly sensitive to small changes (e.g., rotation or length increment of the object), the pixelation method cannot capture these changes unless a CNN with super resolution input is used, which by itself imposes high computational cost to the system.

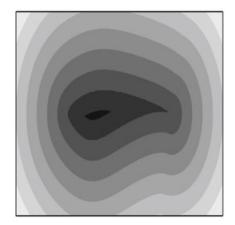


## **5** main shortcoming

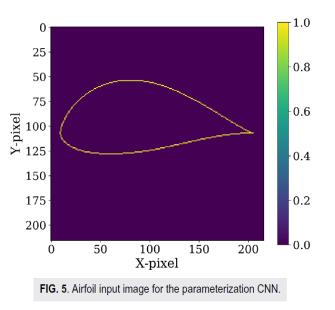
4# It is common to mask the interior points of objects However, this procedure leads to ignoring the corresponding pixels of a CNN and, in fact, some portions of its computational potential.



Thuerey et al. (2020)



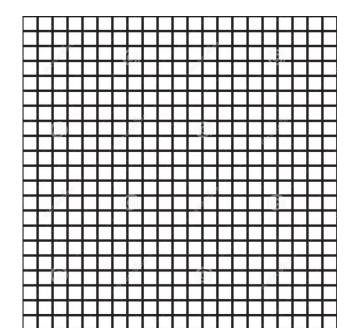
150x150x1 Bhatnagar et al. (2019)

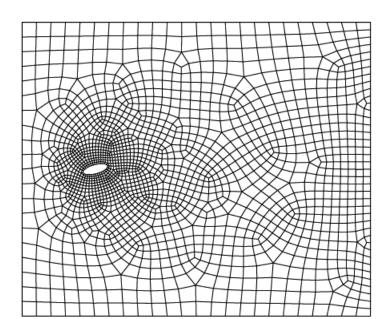


Sekar et al. (2019)

### **5** main shortcoming

**5#** The importance of information in a CFD domain is not equal. For instance, the velocity and pressure fields near the surface of an airfoil and in its wake region are more important than other areas. Nonetheless, using pixelation and consequently Cartesian grids, the distribution of CNN pixels is uniform everywhere in the domain!





# **2** Problem formulation

### **2. 1 Governing equations of fluid dynamics**

### Navier-Stokes & continuity for incompressible flows

$$\rho \left[ \frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla) \boldsymbol{u} \right] - \mu \Delta \boldsymbol{u} + \nabla p = \boldsymbol{f} \text{ in } V, \qquad (1)$$

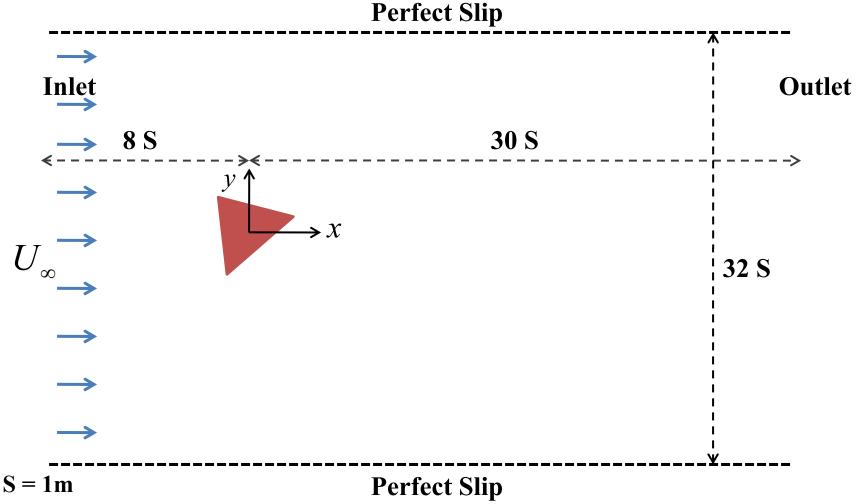
$$\nabla \cdot \boldsymbol{u} = 0 \text{ in } V, \tag{2}$$

$$\boldsymbol{u} = \boldsymbol{u}_{\Gamma_D} \text{ on } \Gamma_D, \tag{3}$$

$$-p\boldsymbol{n} + \mu \nabla \boldsymbol{u} \cdot \boldsymbol{n} = \boldsymbol{t}_{\Gamma_N} \text{ on } \Gamma_N, \qquad (4)$$

Velocity vector: 
$$\boldsymbol{u} = (u, v, w)$$
  
Pressure:  $p$   
Fluid density:  $\rho$   
Fluid viscosity:  $\mu$ 

### **2. 1 Governing equations of fluid dynamics** Geometry and boundary conditions



**2.1 Governing equations of fluid dynamics** 

Mesh Generator: **Gmsh** (open source)



http://gmsh.info/

CFD Solver: **OpenFoam** (open source)

Open∇FOAM

https://openfoam.org/

### **2. 1 Governing equations of fluid dynamics**

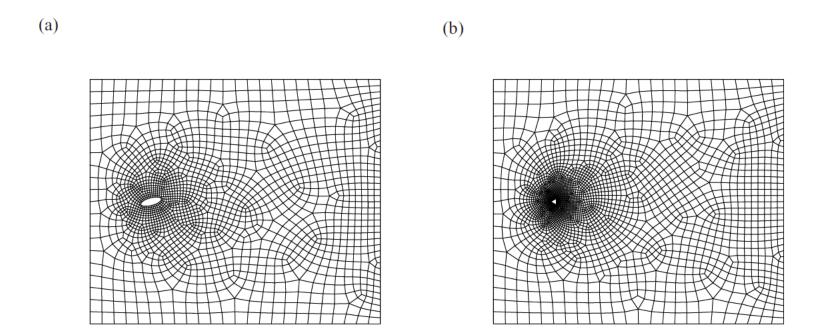


Figure 1: Representation of the finite volume meshes used for solving the continuity and Navier-Stokes equations in the simulation of flow over a cylinder; **a** An elliptical cross section, 2672 vertices; **b** A triangular cross section, 2775 vertices

### **2.1 Governing equations of fluid dynamics**

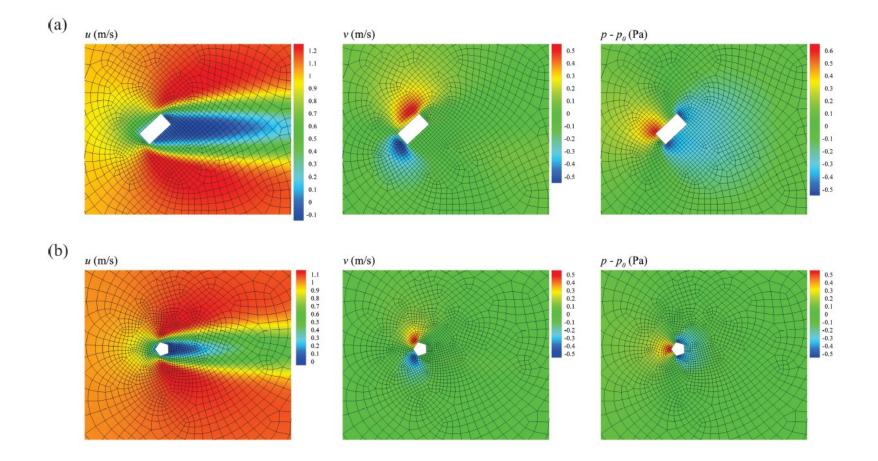


Figure 2: Velocity and pressure fields for the steady-state flow over a cylinder with **a** rectangular cross section and **b** pentagonal cross section;  $p_0$  is the atmospheric pressure

### 2. 2 Data generation

Shape	Schematic figure	Variation in orientation	Variation in length scale	Number of data
Circle		-	a = 1  m	1
Equilateral hexagon		$3^{\circ}, 6^{\circ}, \ldots, 60^{\circ}$	a = 1 m	20
Equilateral pentagon		$3^{\circ}, 6^{\circ}, \ldots, 72^{\circ}$	a = 1 m	24
Square	↓ª ∧ ↑	$3^{\circ},  6^{\circ},  \dots,  90^{\circ}$	a = 1  m	30
Equilateral triangle		$3^{\circ},  6^{\circ},  \dots,  180^{\circ}$	$a = 1 \mathrm{m}$	60
Rectangle	$b \rightarrow t$	$3^{\circ},  6^{\circ},  \dots,  180^{\circ}$	$a = 1$ m; $b/a = 1.2, 1.4, \dots, 3.6$	780
Ellipse		$3^{\circ},  6^{\circ},  \dots,  180^{\circ}$	$a = 1$ m; $b/a = 1.2, 1.4, \dots, 4.2$	960
Triangle		$3^{\circ},  6^{\circ},  \dots,  360^{\circ}$	a = 1  m; b/a = 1.5, 1.75 $\gamma = 40^{\circ}, 60^{\circ}, 80^{\circ}$	720

TABLE I. Description of the generated data

### **2. 2 Data generation**

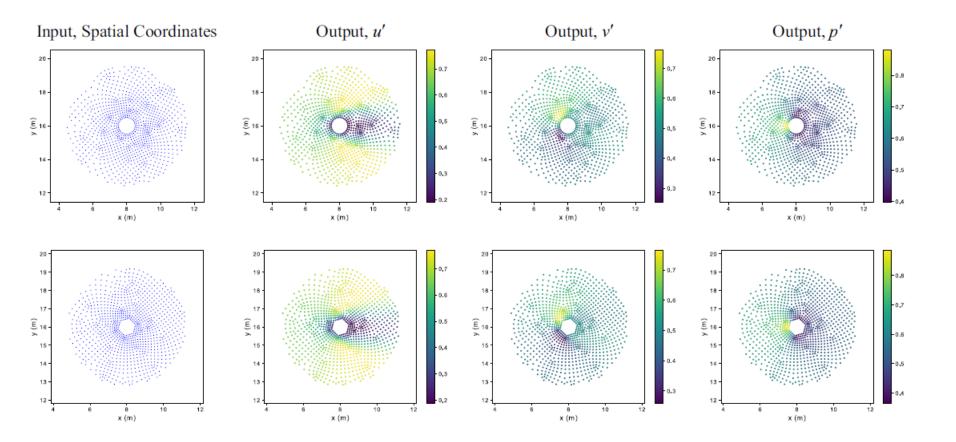


Figure 4: Examples of input and output data

#### **2.3 Data generation**

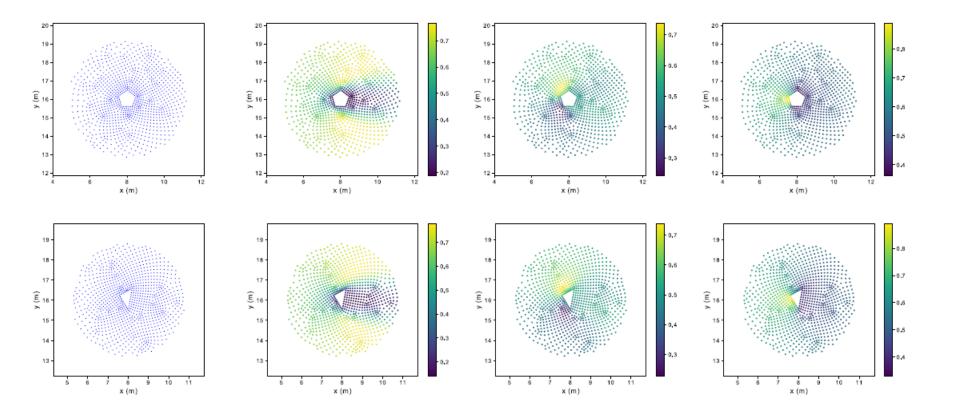


Figure 4: Examples of input and output data

#### **2.3 Data generation**

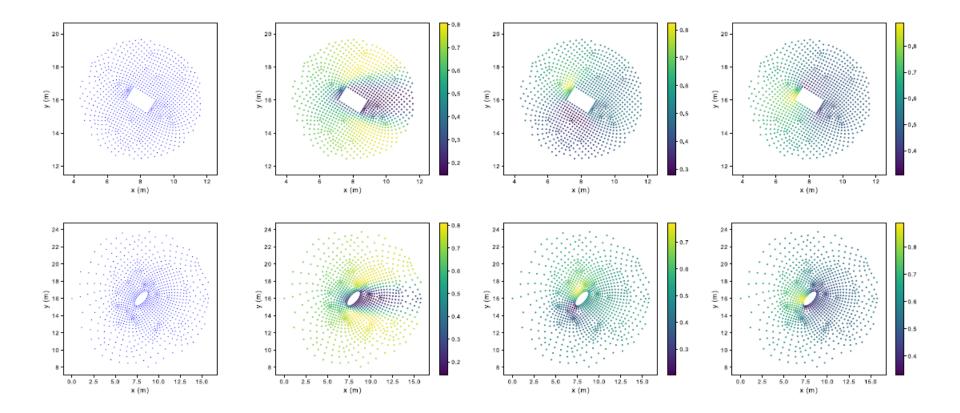


Figure 4: Examples of input and output data

#### 2. 3 Neural network architecture

### Segmentation component of PointNet

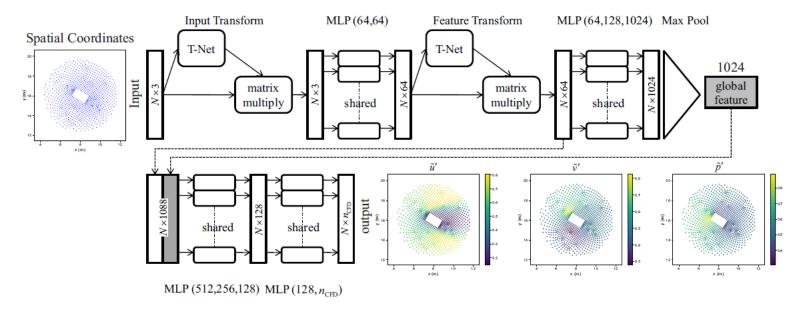


FIG. 5. Structure of our neural network; Labels in the format of (A, B) demonstrate the size of the first layer, A, and the second layer, B, of the MLP. Labels in the form of (A, B, C) are similarly classified for three layers.  $n_{\text{CFD}}$  indicates the number of CFD variables; in this study,  $n_{\text{CFD}} = 3$ . The figure shows the structure for handling three-dimensional problems; though we consider two-dimensional problems in this study. Some parts of this figure are reproduced from Ref. [37].

### 2.4 Training

$$\mathcal{L} = \frac{1}{3 \times N} \left( \sum_{i=1}^{N} \left[ (u'_i - \tilde{u}'_i)^2 + (v'_i - \tilde{v}'_i)^2 + (p'_i - \tilde{p}'_i)^2 \right] \right)$$

- Adam optimizer
- Batch size of 256
- 3552588 parameters
- Three sets of training (80%), validation (10%), and test (10%) through a random process
- Train the neural network over 2076 data; 260 data for the validation and the remaining 259 for evaluation
- NVIDIA TITAN Xp graphics card with the memory clock rate of 1.582 GHz and 12 Gigabytes of RAM
- Stop after 4000 epochs
- Approximately takes 10 hours

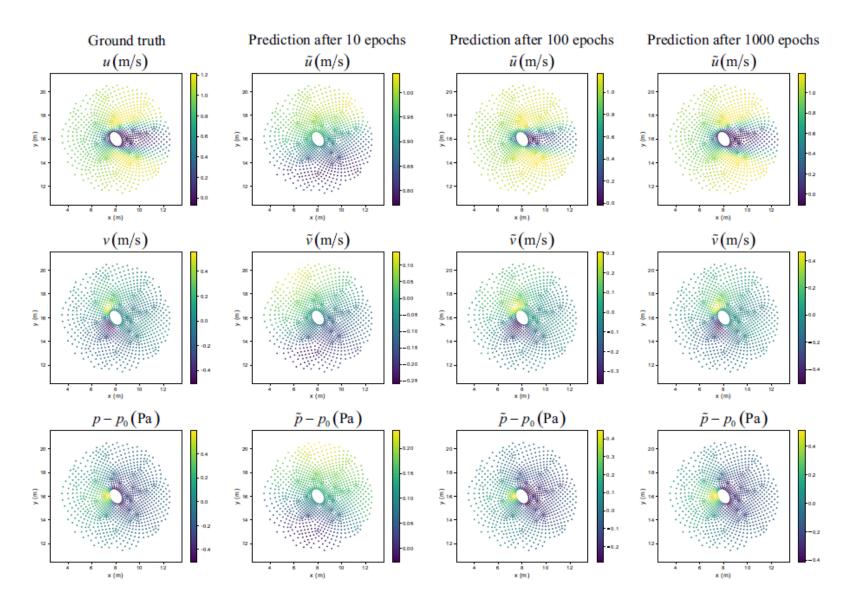


FIG. 6. A comparison between the ground truth and prediction of the network for the velocity and pressure fields after 10, 100, and 1000 epochs

# **3 Results and discussion**

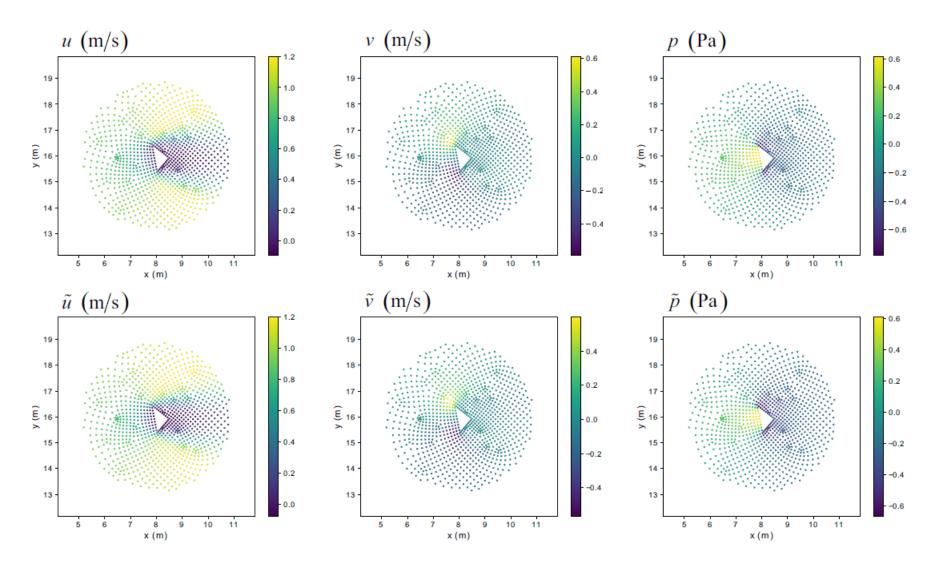


Figure 6: A comparison between the ground truth and our network prediction for the velocity and pressure fields for two different cross sections; the first set of examples

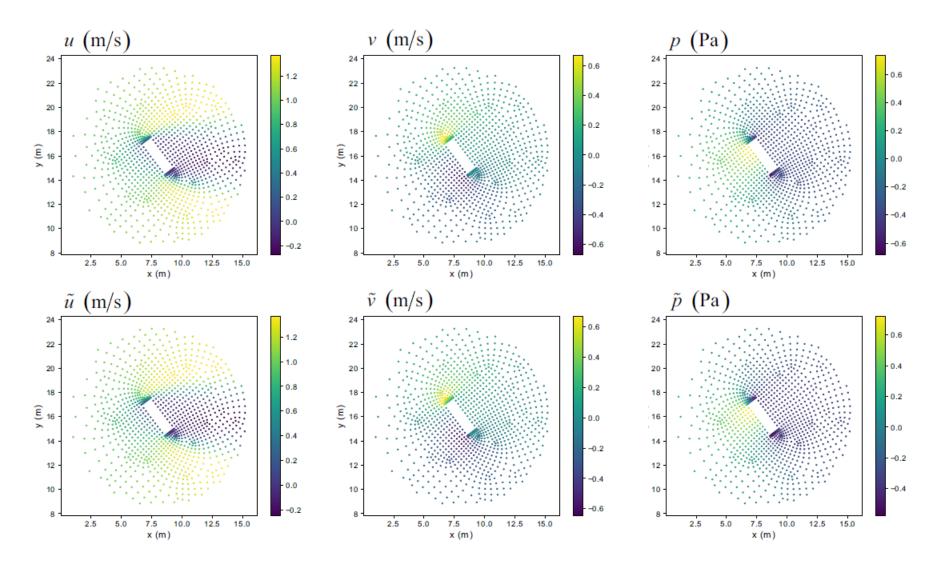


Figure 6: A comparison between the ground truth and our network prediction for the velocity and pressure fields for two different cross sections; the first set of examples

**3.1 General analysis** 

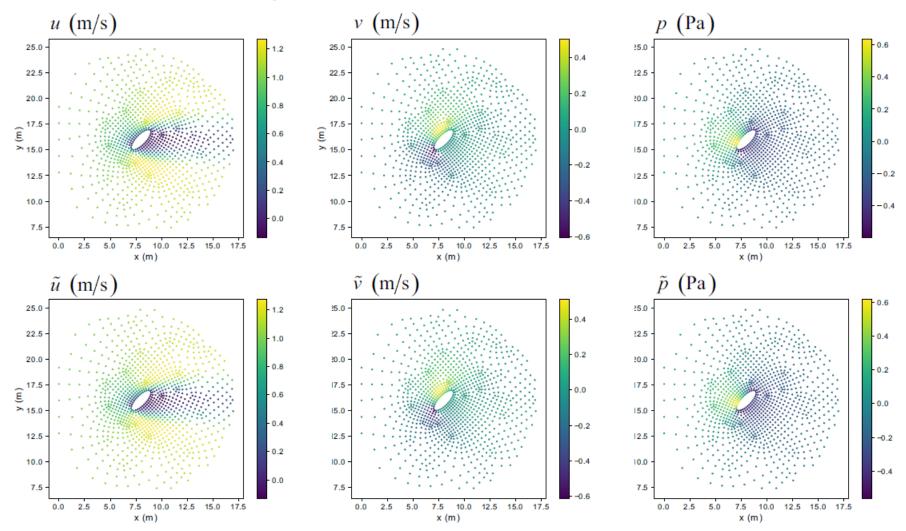


Figure 7: A comparison between the ground truth and our network prediction for the velocity and pressure fields for two different cross sections, the second set of examples

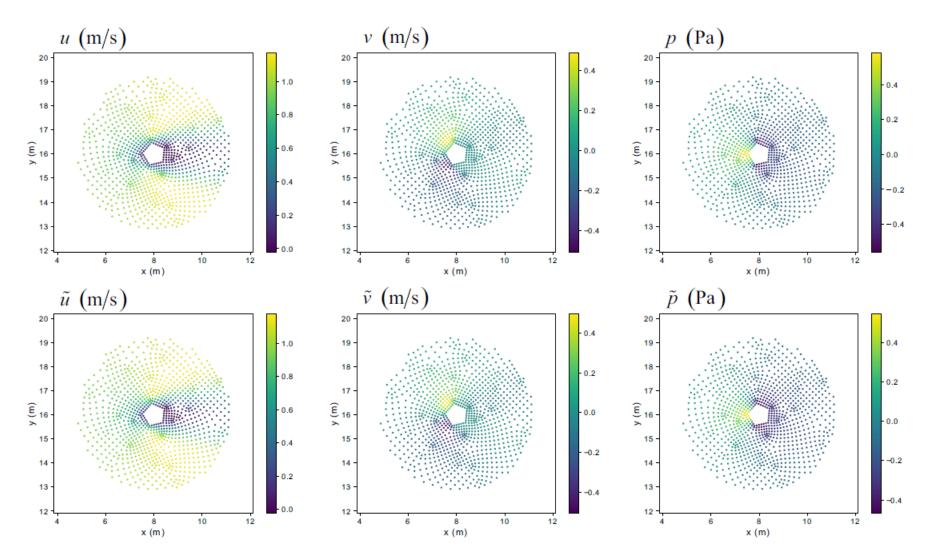


Figure 7: A comparison between the ground truth and our network prediction for the velocity and pressure fields for two different cross sections, the second set of examples

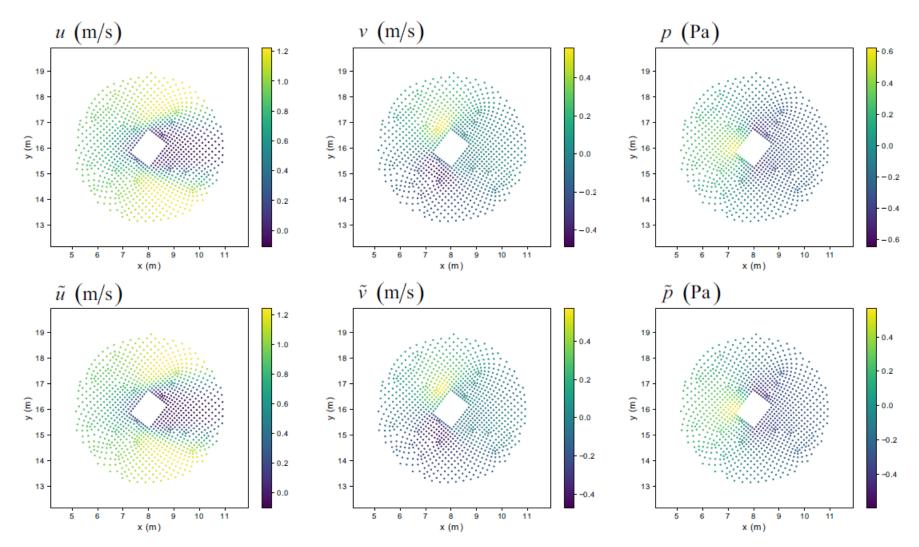


Figure 8: A comparison between the ground truth and our network prediction for the velocity and pressure fields for two different cross sections, the third set of examples

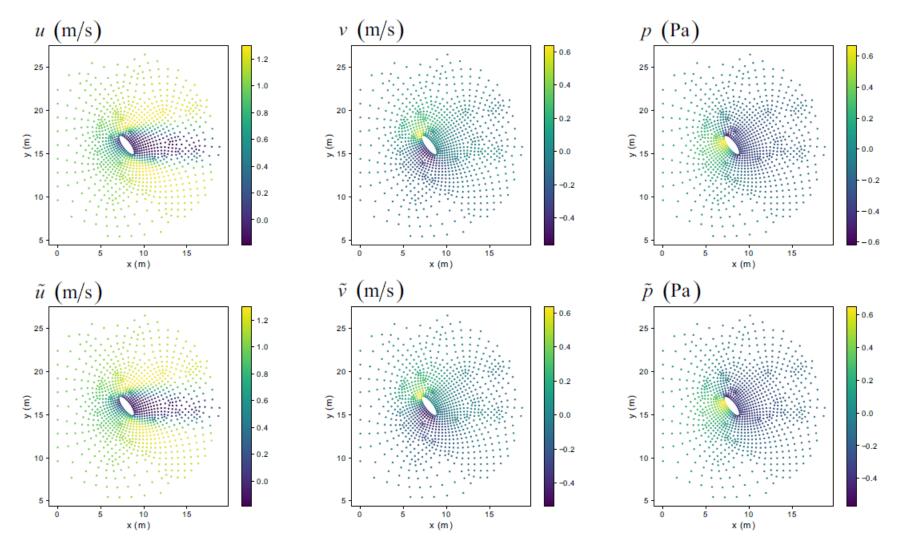


Figure 8: A comparison between the ground truth and our network prediction for the velocity and pressure fields for two different cross sections, the third set of examples

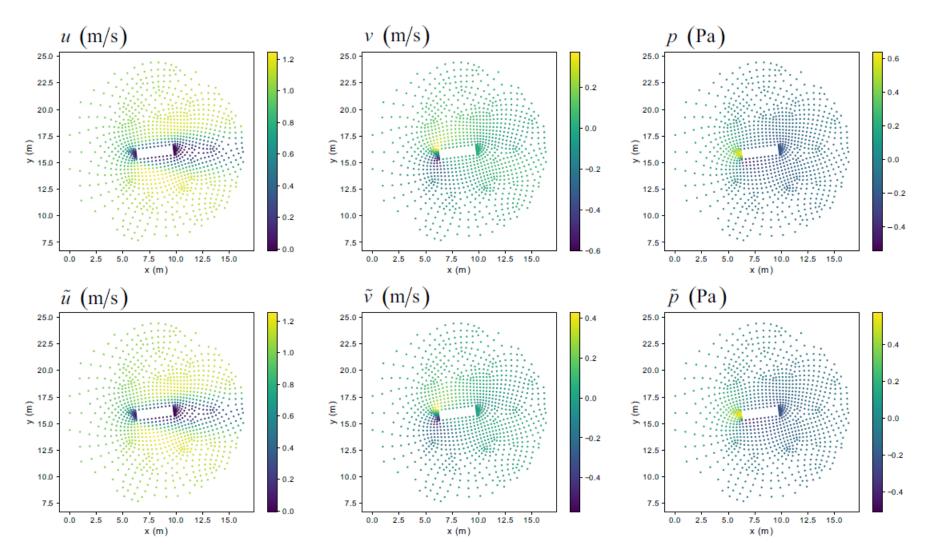


Figure 9: A comparison between the ground truth and our network prediction for the velocity and pressure fields for two different cross sections, the fourth set of examples

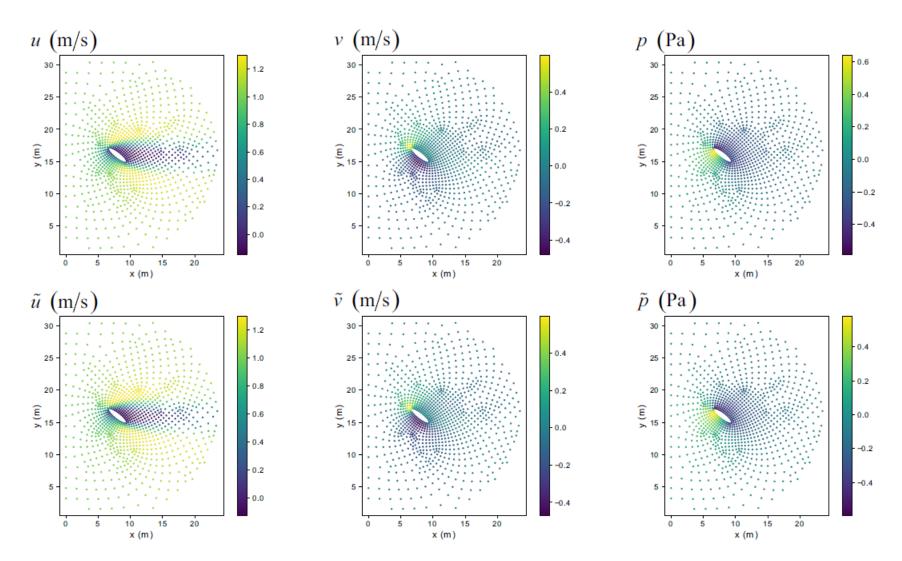


Figure 9: A comparison between the ground truth and our network prediction for the velocity and pressure fields for two different cross sections, the fourth set of examples

#### **3.1 General analysis**

TABLE II. Error analysis of the velocity and pressure fields predicted by our neural network for 259 unseen data;  $|| \dots ||$  indicates the  $L^2$  norm.

	$  u - \tilde{u}  $	$  v - \tilde{v}  $	$  p - \tilde{p}  $
Average	4.49666E - 2	$3.70540\mathrm{E}{-2}$	2.71661E - 2
Maximum	$2.49088 \mathrm{E}{-1}$	$2.34281\mathrm{E}{-1}$	$1.16901 \mathrm{E}{-1}$
Minimum	1.10453E - 2	9.20977E - 3	$7.58447 \mathrm{E}{-3}$

#### **3.1 General analysis**

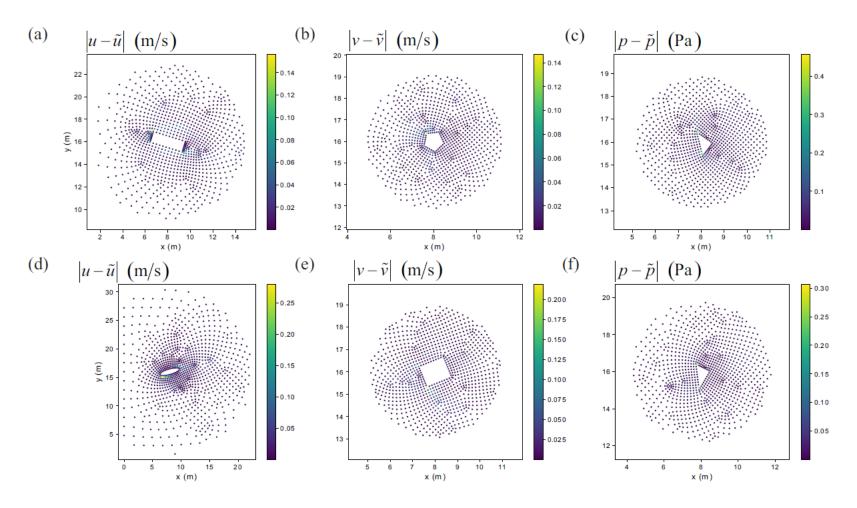


FIG. 11. Distribution of absolute pointwise error when the mean square error becomes **a** maximum for  $\tilde{u}$ , **b** maximum for  $\tilde{v}$ , **c** maximum for  $\tilde{p}$ , **d** minimum for  $\tilde{u}$ , **e** minimum for  $\tilde{v}$ , and **f** minimum for  $\tilde{p}$ .

#### **3.1 General analysis**

• Speed-up:

Wall time for prediction of the 259 unseen data: 6 seconds

Simulation of the flow fields for these 259 geometries using the CFD software: **11071 seconds** (about 3 hours)

Average achieved speedup: **1846** 

This is not an absolute number and depends on the framework of our available computational facilities!

#### **3.2 Investigation of conservation of mass and momentum**

$$\rho \left[ \frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla) \boldsymbol{u} \right] - \mu \Delta \boldsymbol{u} + \nabla p = \boldsymbol{f} \text{ in } V, \qquad (1)$$

$$\nabla \cdot \boldsymbol{u} = 0 \text{ in } V, \tag{2}$$

$$\boldsymbol{u} = \boldsymbol{u}_{\Gamma_D} \text{ on } \Gamma_D, \tag{3}$$

$$-p\boldsymbol{n} + \mu \nabla \boldsymbol{u} \cdot \boldsymbol{n} = \boldsymbol{t}_{\Gamma_N} \text{ on } \Gamma_N, \qquad (4)$$

## **Residuals:**

$$r_{momentum_{x}} = (16)$$

$$\left| \int_{V_{NN}} \left( \rho \left( \tilde{u} \frac{\partial \tilde{u}}{\partial x} + \tilde{v} \frac{\partial \tilde{u}}{\partial y} \right) + \frac{\partial \tilde{p}}{\partial x} - \mu \left( \frac{\partial^{2} \tilde{u}}{\partial x^{2}} + \frac{\partial^{2} \tilde{u}}{\partial y^{2}} \right) \right) dV \right|,$$

$$r_{momentum_y} = (17) \\ \left| \int_{V_{NN}} \left( \rho \left( \tilde{u} \frac{\partial \tilde{v}}{\partial x} + \tilde{v} \frac{\partial \tilde{v}}{\partial y} \right) + \frac{\partial \tilde{p}}{\partial y} - \mu \left( \frac{\partial^2 \tilde{v}}{\partial x^2} + \frac{\partial^2 \tilde{v}}{\partial y^2} \right) \right) dV \right|,$$

$$r_{continuity} = \left| \int_{V_{NN}} \left( \frac{\partial \tilde{u}}{\partial x} + \frac{\partial \tilde{v}}{\partial y} \right) dV \right|, \qquad (18)$$

#### **3.2 Investigation of conservation of mass and momentum**

TABLE III. Investigation of conservation of mass and momentum of the flow fields predicted by our neural network for 259 unseen data. All values are reported in the International Unit System.

	$r_{momentum_{x}}$	$r_{momentum_y}$	$r_{continuity}$
Average	$4.14958E{-3}$	$2.46155E{-3}$	2.99411E - 3
Maximum	3.38842E - 1	$3.59399E{-2}$	8.74008E - 2
Minimum	$5.69245 \text{E}{-6}$	$9.03372E{-7}$	3.58928E - 6

#### **3.3 Neural network generalizability**

# What does it mean?!

#### In computer graphics:

For instance, Qi et al. tested PointNet for the semantic segmentation of unseen categories such as "face", "house", "rabbit", and "teapot", while these objects did not exist in their data set.

In computational mechanics:

???

#### **3.3 Neural network generalizability**

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#### In computer graphics:

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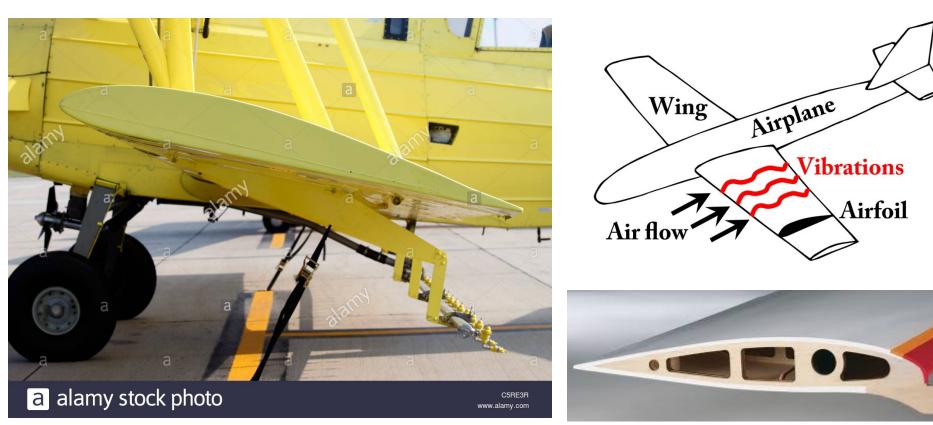
#### **3.3 Neural network generalizability**

For the first time:

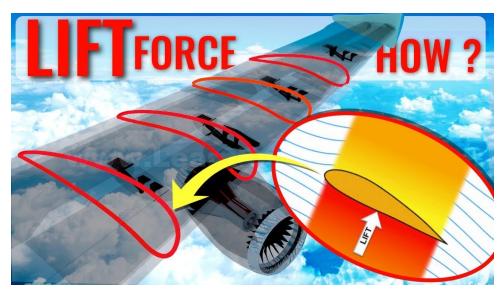
our network generalizes the predictions to **multiple objects** as well as an **airfoil**, even though **only single objects** and **no airfoils** are observed during training.

# NACA 0028

## Applications of airfoils in airplane wings

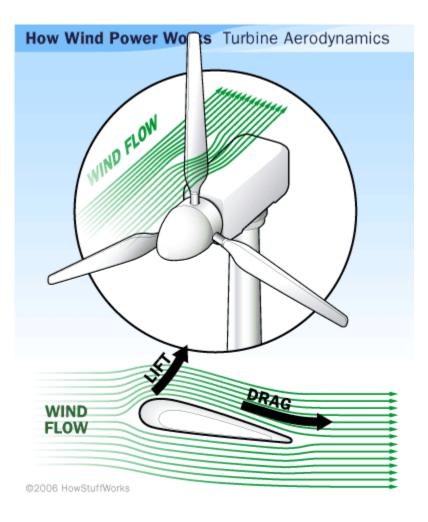


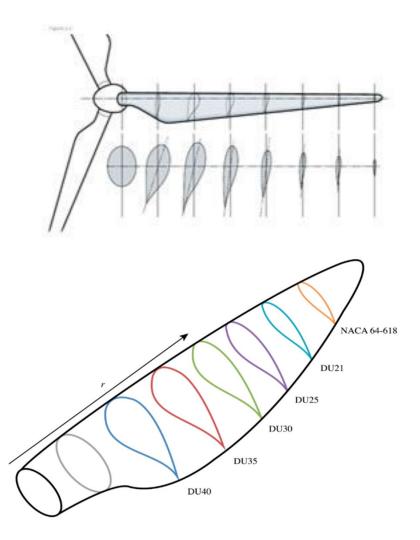
## Applications of airfoils in airplane wings



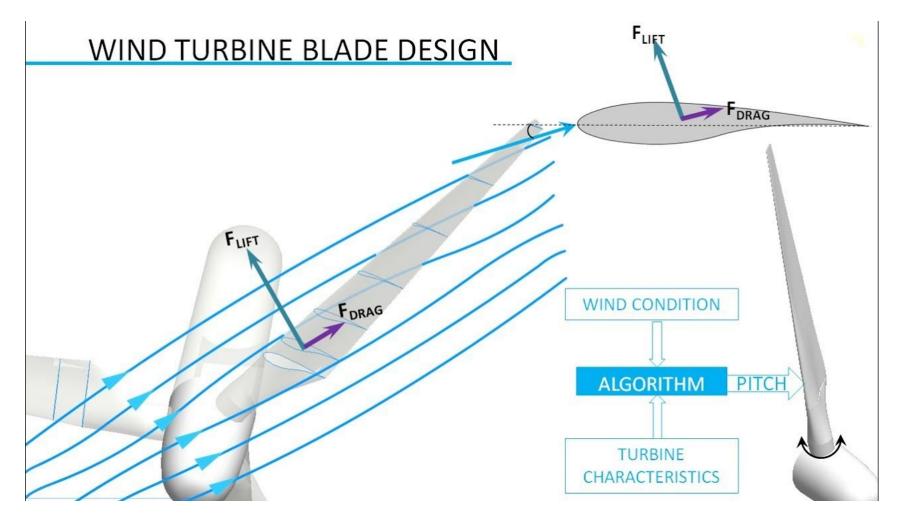


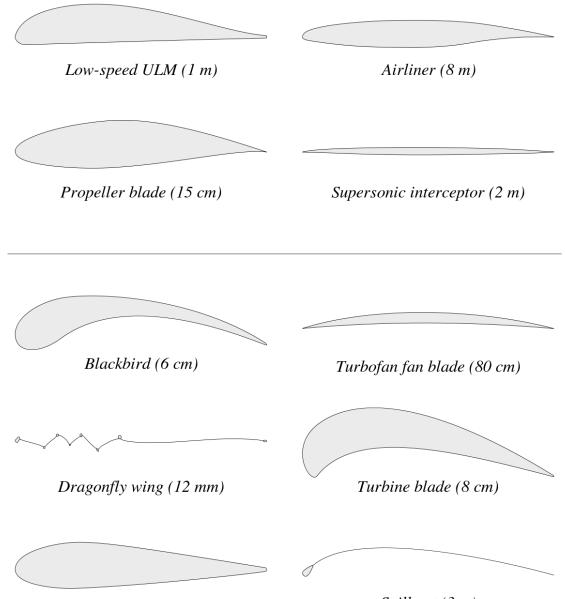
## Applications of airfoils in wind turbines





## Applications of airfoils in wind turbines

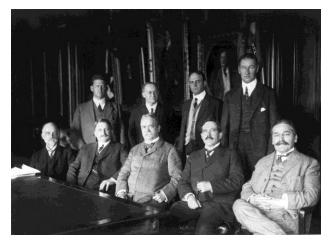




Dolphin flipper fin (10 cm)

Sailboat (3 m)

## National Advisory Committee for Aeronautics (NACA)



The first meeting of the NACA in 1915



The NACA Test Force at the High Speed Flight Station in Edwards, California.



Formed: March 3, 1915

Dissolved: October 1, 1958

**Superseding agency:** NASA

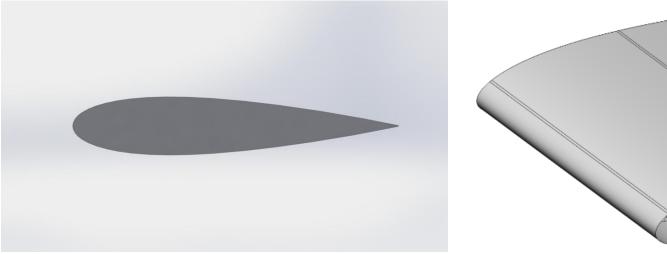


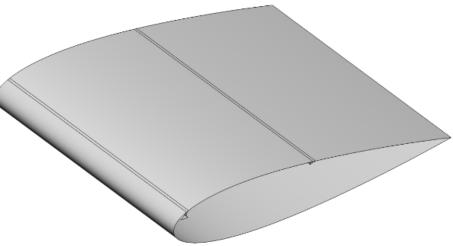
National Advisory Committee for Aeronautics (NACA)

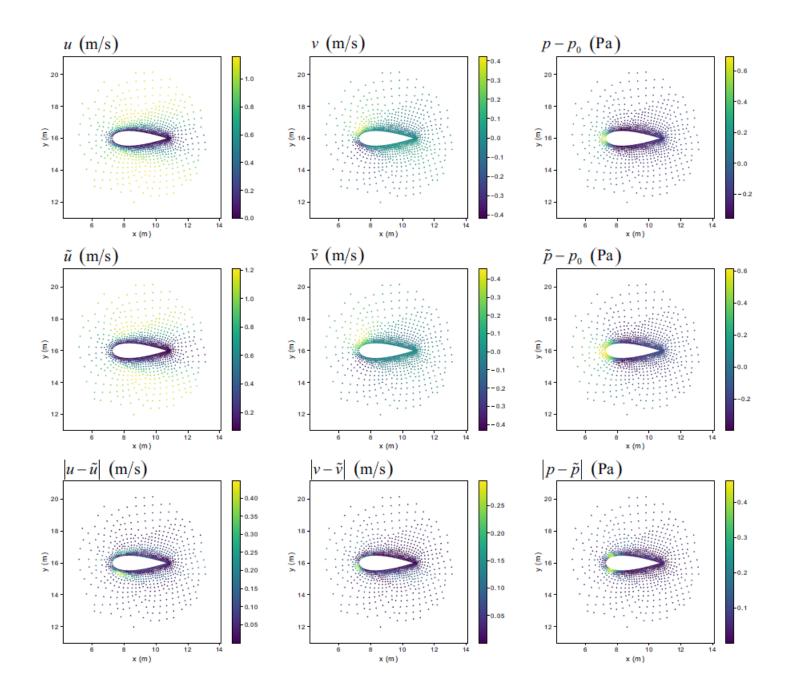
4 Digits NACA airfoils: https://en.wikipedia.org/wiki/NACA\_airfoil

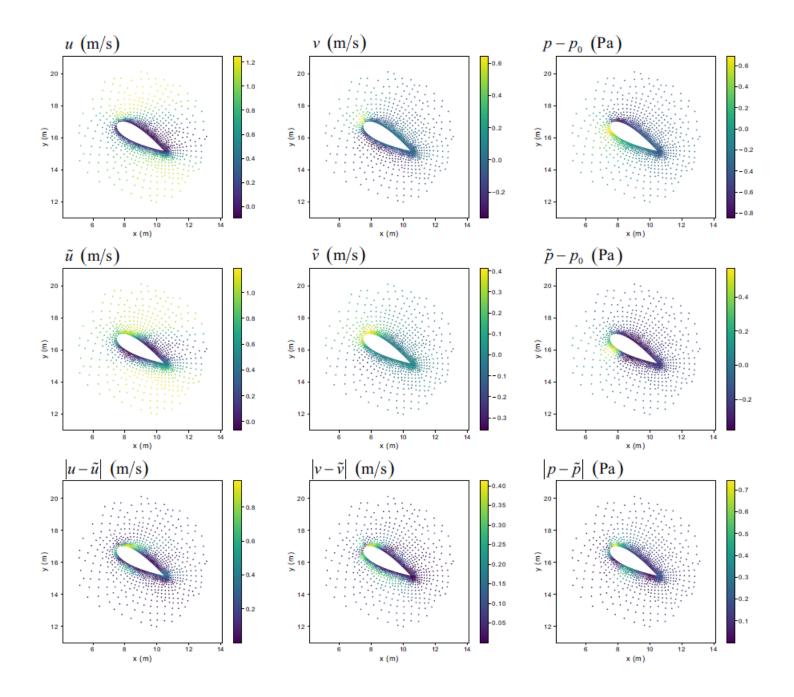
## NACA 0028

NACA 0028









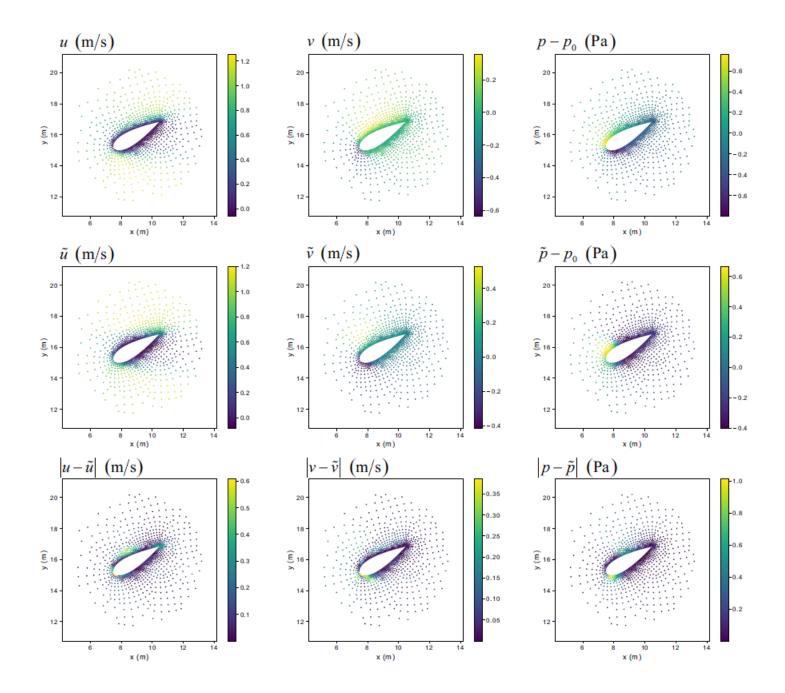
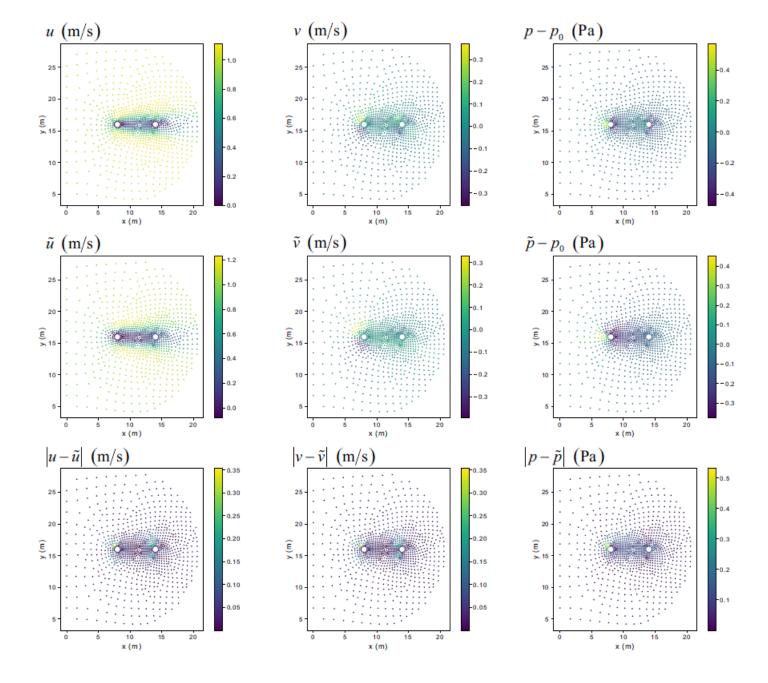
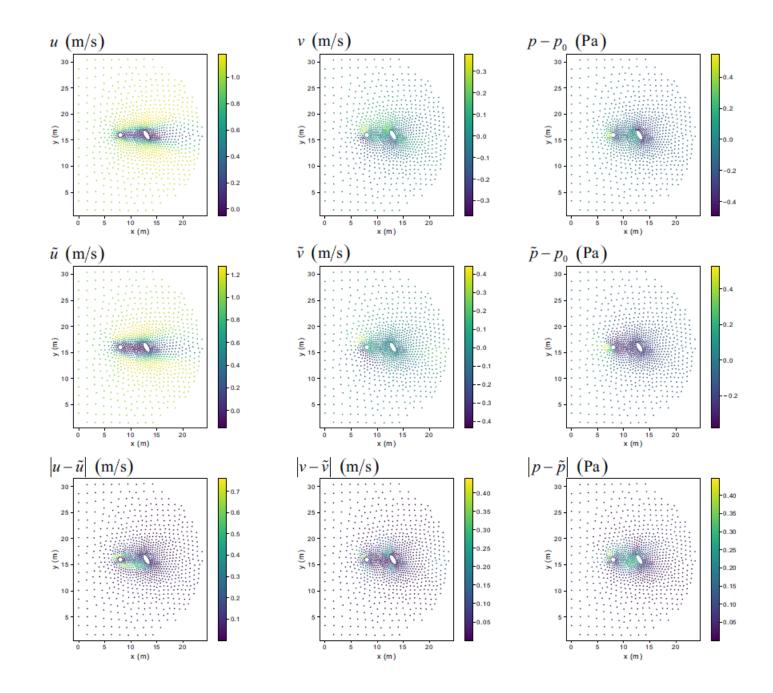


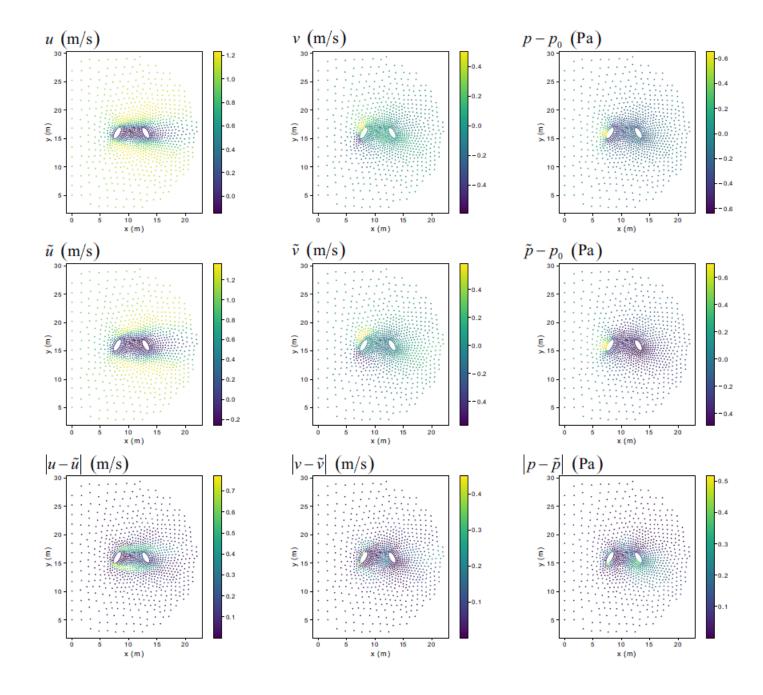
TABLE V. Error analysis of the velocity and pressure fields predicted by our neural network for NACA 0028;  $|| \dots ||$  indicates the  $L^2$  norm.

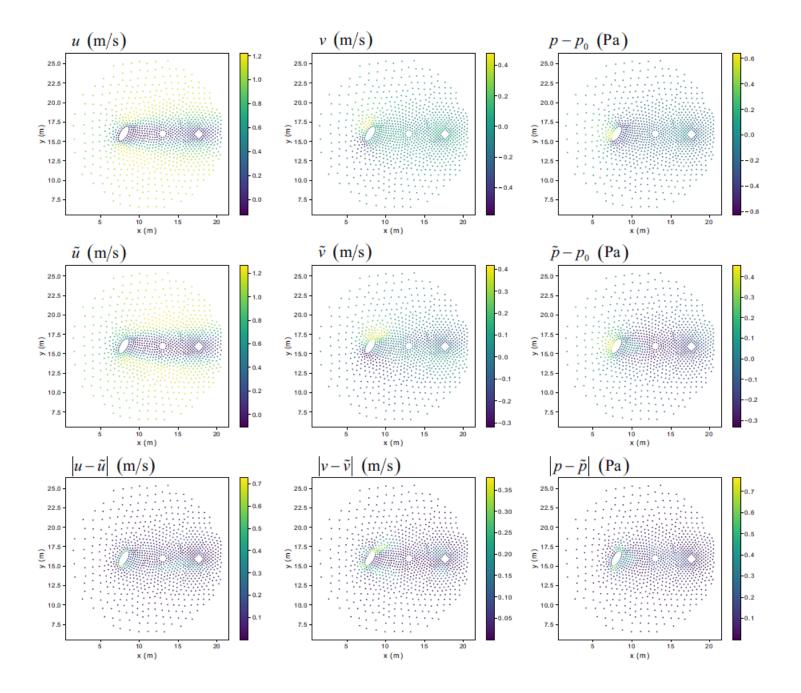
Angle of attack	$  u - \tilde{u}  $	$  v - \tilde{v}  $	$  p - \tilde{p}  $
$0^{\circ}$	1.05631E - 1	5.47357E - 2	1.04842E - 1
$30^{\circ}$	2.83492E - 1	$1.30977 \mathrm{E}{-1}$	2.07335E - 1
$-30^{\circ}$	$1.62185 \mathrm{E}{-1}$	$1.00821 \text{E}{-1}$	$2.42353E{-1}$

#### **3.3.2 Prediction of flow around multiple objects**









#### **3.4 Prediction of flow around multiple objects**

TABLE IV. Error analysis of the velocity and pressure fields predicted by our neural network for multiple bodies;  $|| \dots ||$ indicates the  $L^2$  norm.

	$  u- ilde{u}  $	$  v - \tilde{v}  $	$  p - \tilde{p}  $
Two circular cylinders (Fig. 12)	$1.51130E{-1}$	5.80172E-2	9.22659E - 2
Circular and elliptical cylinders (Fig. 13)	$1.63664E{-1}$	7.50613E - 2	1.09544E - 1
Two elliptical cylinders (Fig. 14)	2.19626E - 1	8.93397E-2	1.35396E - 1
Elliptical, circular, and rectangular cylinders (Fig. $15$ )	1.30335E - 1	8.59303E - 2	1.33239E - 1

$  u - \tilde{u}  $	$  v - \tilde{v}  $	$  p - \tilde{p}  $
$1.51130E{-1}$	$5.80172 \text{E}{-2}$	$9.22659E{-2}$
$1.63664 \mathrm{E}{-1}$	$7.50613 \mathrm{E}{-2}$	$1.09544 \mathrm{E}{-1}$
2.19626E - 1	8.93397 E - 2	$1.35396E{-1}$
$1.30335 \mathrm{E}{-1}$	8.59303E - 2	1.33239E - 1

# **4 Conclusions and future directions**

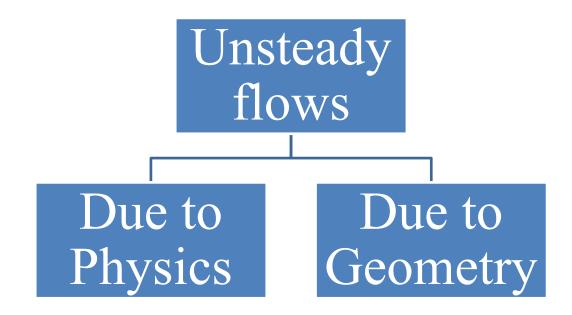
# **Future directions:**

- 1) Unsteady CFD problems due to moving objects and mesh deformation
- 2) Unsupervised learning of CFD problems in variable geometries
- 3) Multidisciplinary design optimization

# Unsteady Flows with Moving Objects and Boundaries

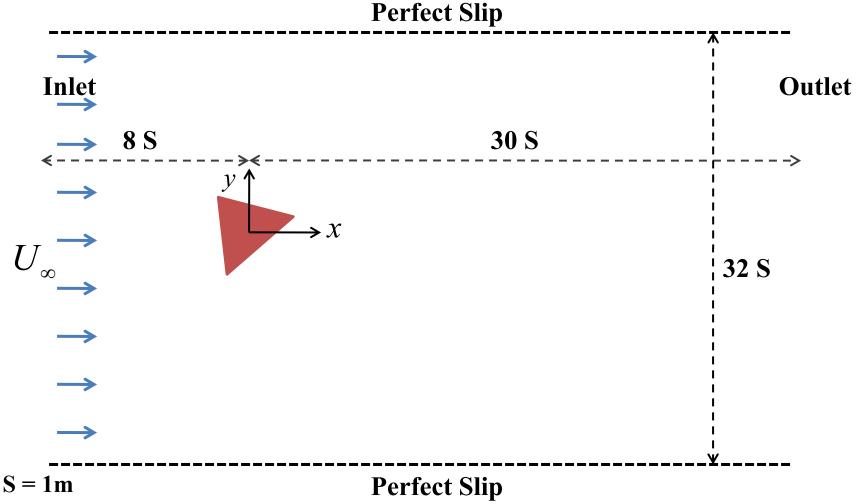
# **Future directions:**

1) Unsteady CFD problems

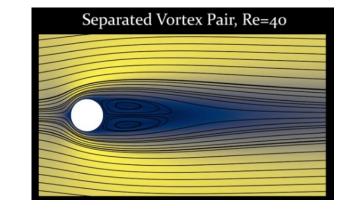


#### **2.1 Governing equations of fluid dynamics**

Unsteady flows due to the physics but with a fixed geometry

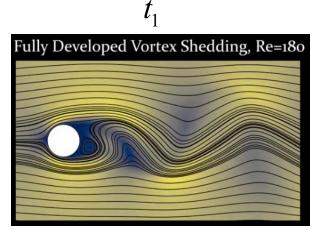


Unsteady flows due to the physics but with a fixed geometry

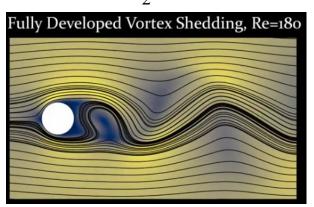


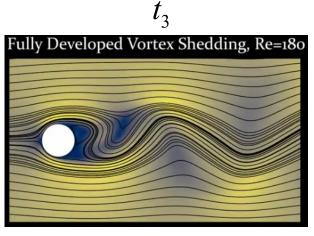
Steady-State

 $t_{\gamma}$ 



 $Re = \frac{\rho L u_{\infty}}{\mu}.$ 

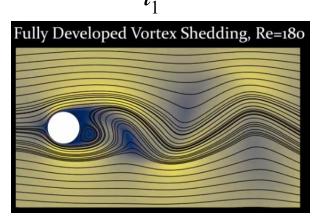


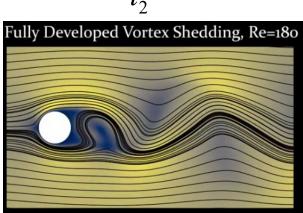


## Unsteady

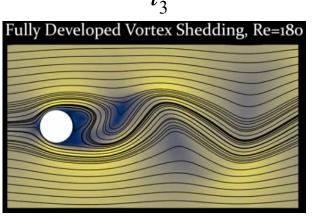
Unsteady flows due to the physics but with a fixed geometry

$$Re = \frac{\rho L u_{\infty}}{\mu}.$$
But we are not  
interested in these types  
of problems,  
because the geometry  
is fixed in time!



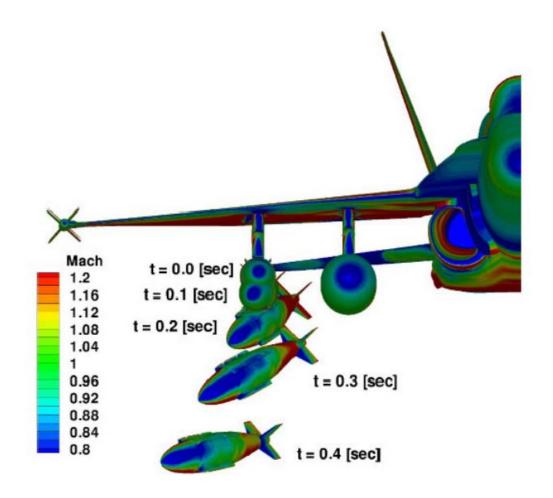


Unsteady

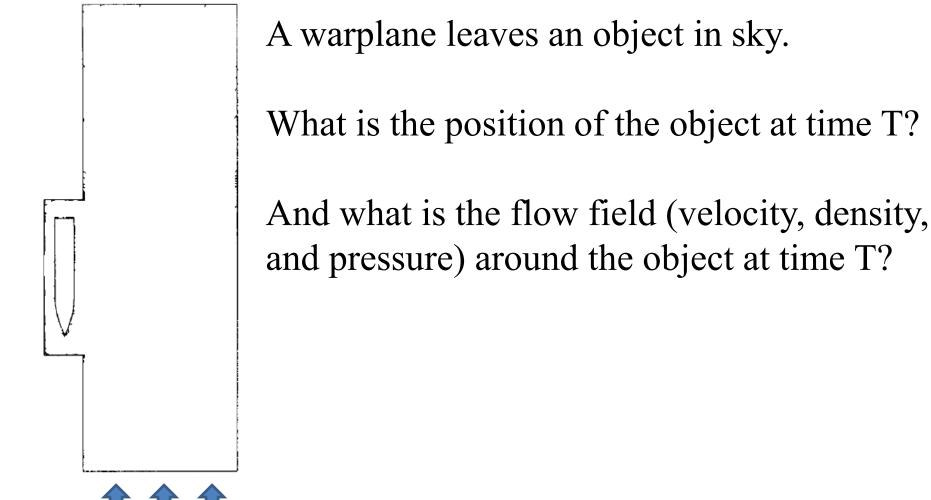


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Unsteady flows due to the inconsistent geometry

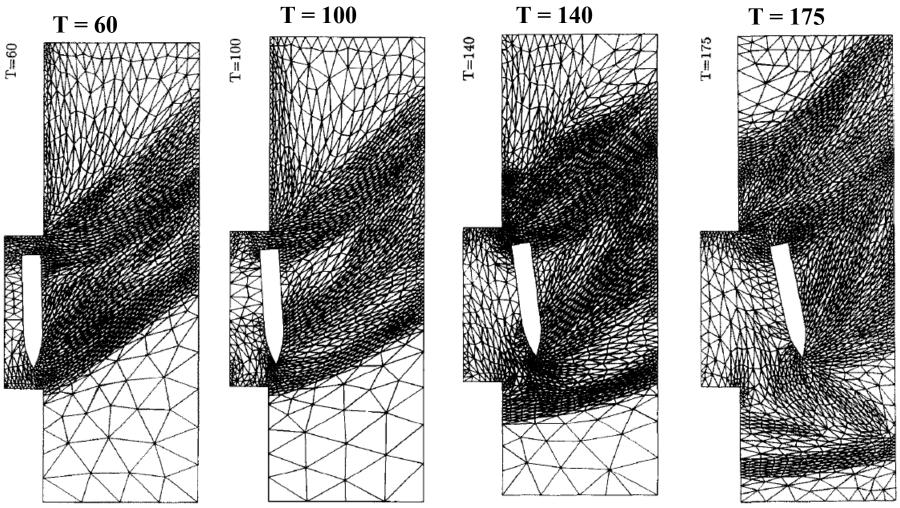


Unsteady flows due to the inconsistent geometry

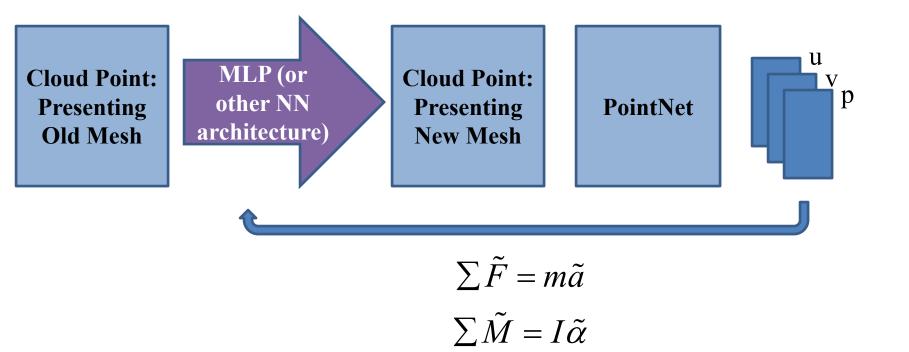


**Supersonic Flow (compressible)** 

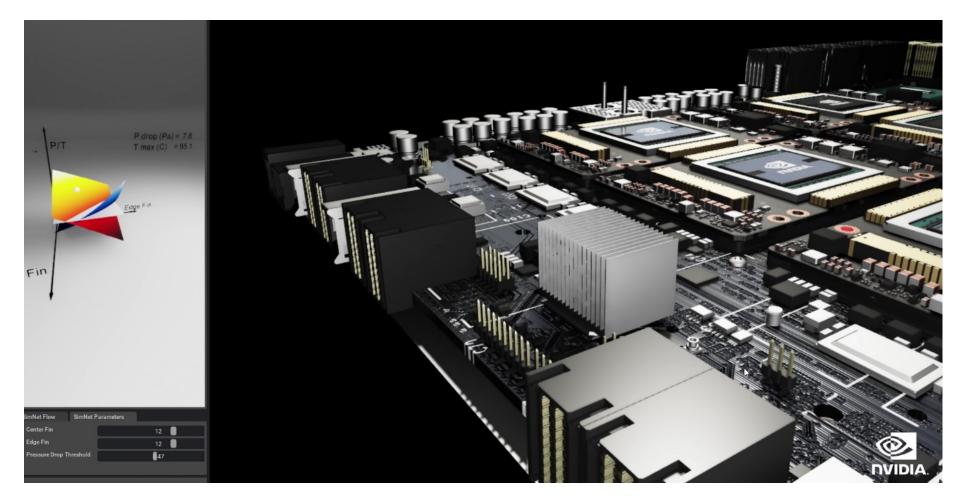
Unsteady flows due to the inconsistent geometry

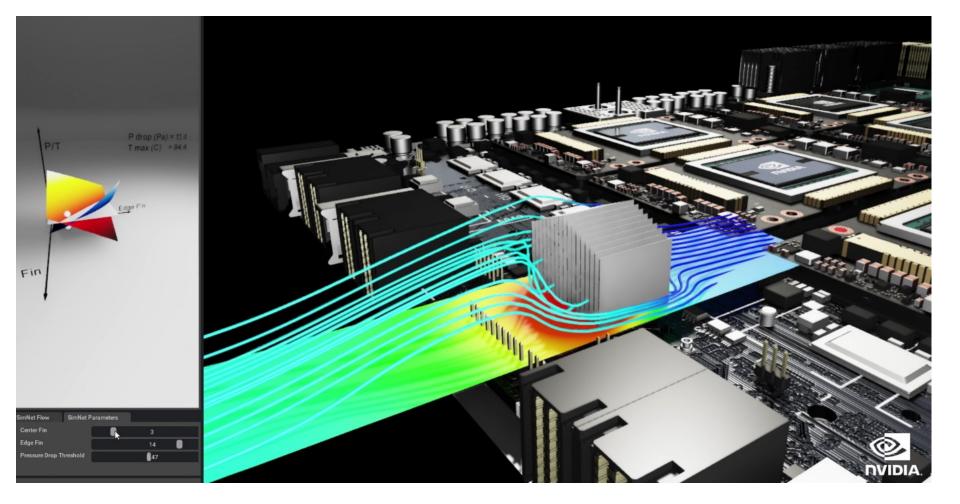


# Unsteady flows due to the inconsistent geometry Using LSTM (at each time step)



# Physics Informed Neural Network: An-unsupervised DL approach





- The idea of Physics Informed Neural Network (PINN) first introduced at Brown University and has become popular recently. Here are a few papers discussing this approach:
- Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations <u>https://www.sciencedirect.com/science/article/pii/S0021999118307125</u>
- NSFnets (Navier-Stokes Flow nets): Physics-informed neural networks for the incompressible Navier-Stokes equations https://arxiv.org/abs/2003.06496
- Physics-informed neural networks for high-speed flows <u>https://www.sciencedirect.com/science/article/pii/S0045782519306814</u>

To say the idea of PINN at a high level, we enforce the loss function to minimize the residual of governing equations. Specifically, let's see how it works for continuity and Navier-Stokes equations.

## **Continuity & Navier-Stokes Equations:**

$$u_{t} + uu_{x} + vu_{y} = -p_{x} + Re^{-1}(u_{xx} + u_{yy}), v_{t} + uv_{x} + vv_{y} = -p_{y} + Re^{-1}(v_{xx} + v_{yy}) - \eta_{tt}, u_{x} + v_{y} = 0.$$

## **Residuals:**

$$e_{1} := u_{t} + uu_{x} + vu_{y} + p_{x} - Re^{-1}(u_{xx} + u_{yy}),$$
  

$$e_{2} := v_{t} + uv_{x} + vv_{y} + p_{y} - Re^{-1}(v_{xx} + v_{yy}) + \eta_{tt},$$
  

$$e_{3} := u_{x} + v_{y}.$$

**Loss function:** 
$$\sum_{i=1}^{3} \sum_{n=1}^{N} (|e_i(t^n, x^n, y^n)|^2)$$

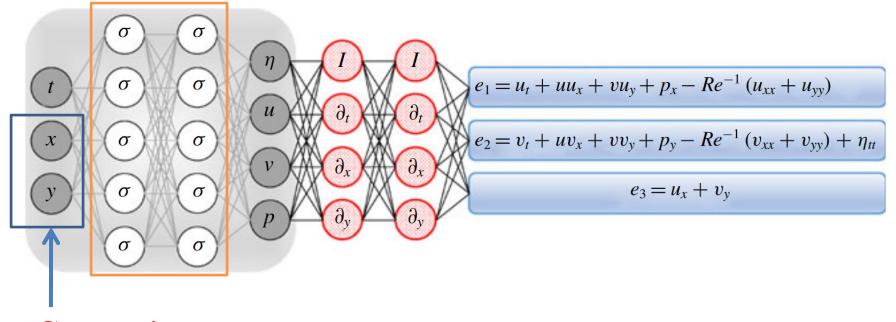
## **Neural Network for PINN**

All figures in this section are taken from Raissi et. al. (2018) and Mao et. al. (2020)

None of the current PINN can capture variable geometries! They have designed for the fixed geometries!

Connection to Point Cloud and PointNet

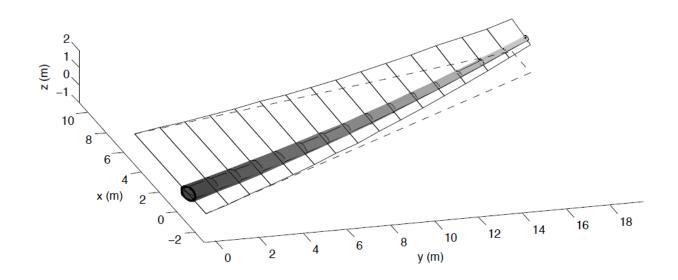
#### **Replace the MLP by our CFD PointNet**



Connection to Point Cloud and PointNet

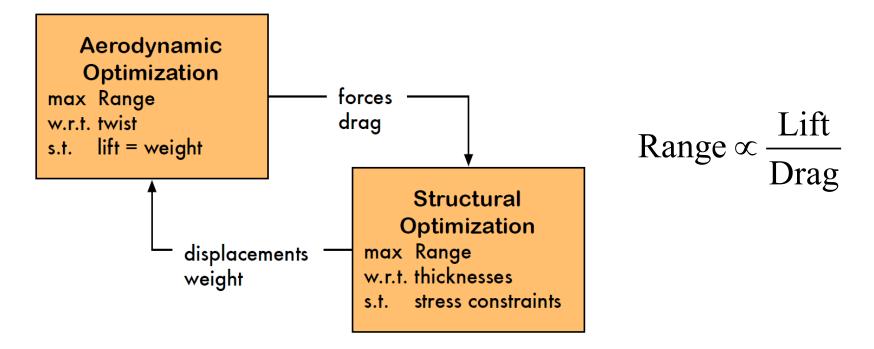
## **Future directions:**

## 3) Multidisciplinary Design Optimization





## 1) Multidisciplinary Design Optimization



So many directions exist to incorporate neural networks!

Needs literature review to take a "evolutionary" direction!

## Thank you!