Università degli Studi di Padova

Machine Learning algorithms for Wall-model LES of high-speed flows for aerospace applications.

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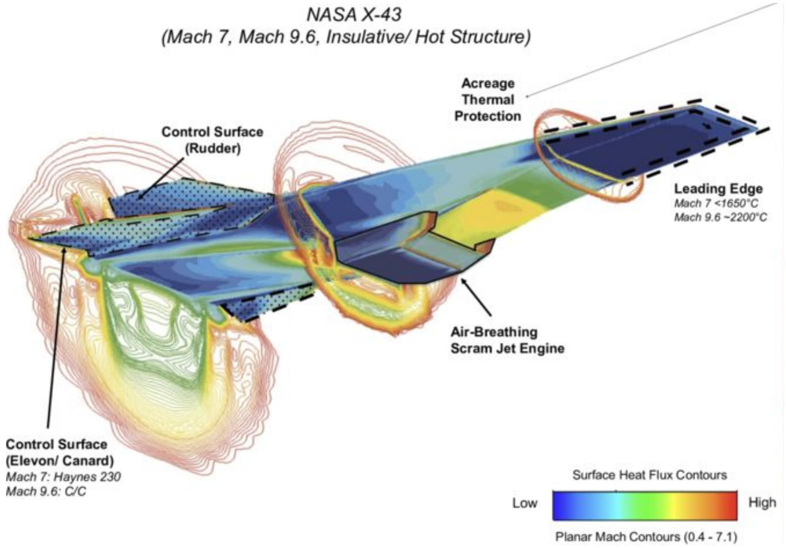
Admission to the second year - 14/10/2025

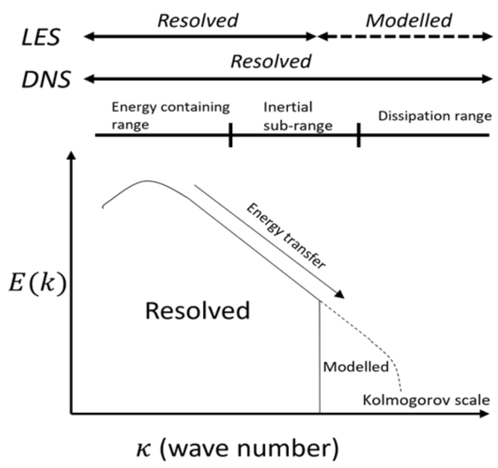
Project Motivation

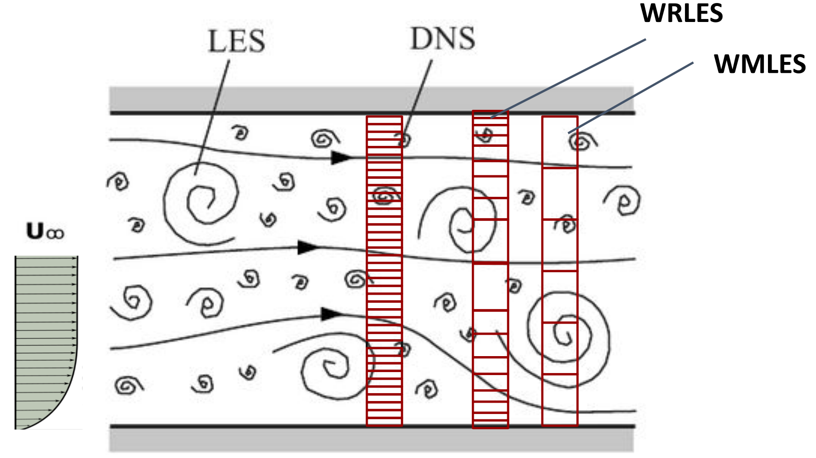
High-speed flow in aerospace applications.

- The presence of turbulent, hot and highly compressible boundary layers increase the mechanical and thermal loads on the vehicle.
- **A detail simulation of the flow dynamics is essential** for the safe design and operation of future missions.
- Solve them directly is computationally intractable, hence **various turbulence closure models have been developed** during the years.



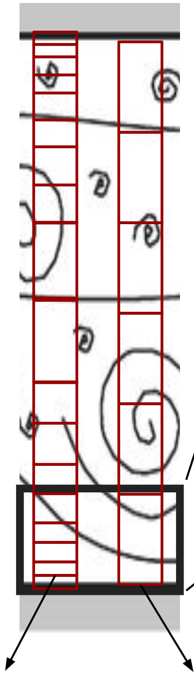
Peters, Adam & Dajie et al. Materials Design for Hypersonics





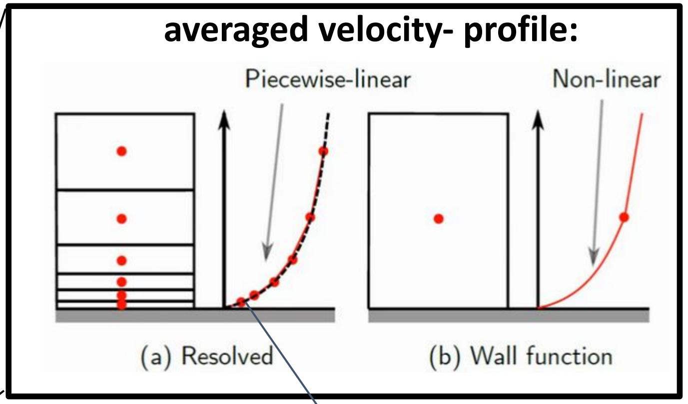
State of the art methodologies

Limitations of current numerical approach employed to simulate unsteady flow.



Resolved

Modeled



$$\tau_w = \mu \left. \frac{\partial u}{\partial y} \right|_{wall}$$

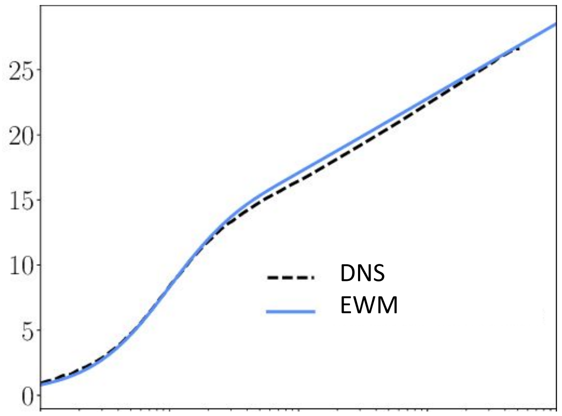
- μ = viscosity
- y = wall-normal direction
- u = streamwise velocity

Equilibrium wall model - EWM

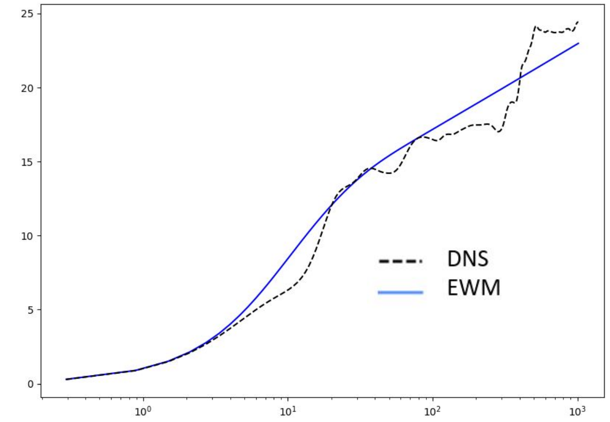
$$u^+ = \frac{1}{\kappa} \ln\left(1 + \kappa y^+\right) + C\left[1 - \exp\left(-\frac{y^+}{A}\right) - \frac{y^+}{A}\exp\left(-0.33\, y^+\right)\right]$$

- averaged profile
- steady, incompressible turbulent flows
- absence of strong pressure gradients
- no flow separation

averaged velocity profile



instantaneous velocity profile

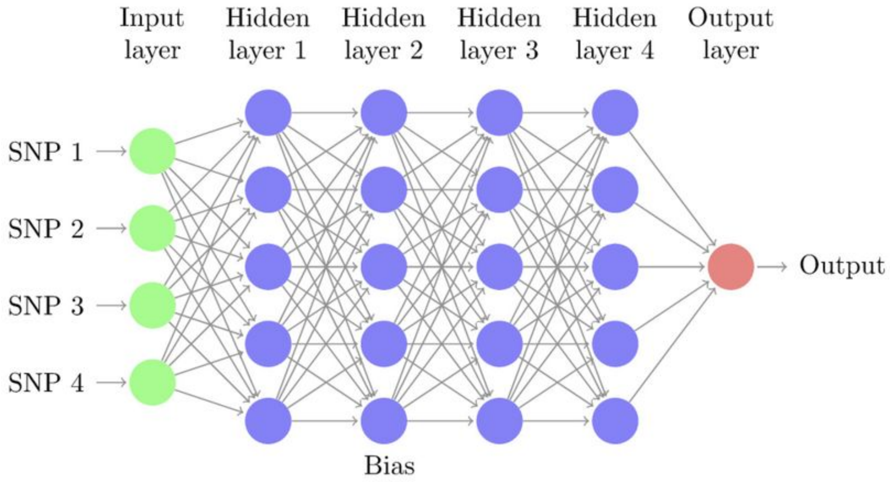


Machine Learning

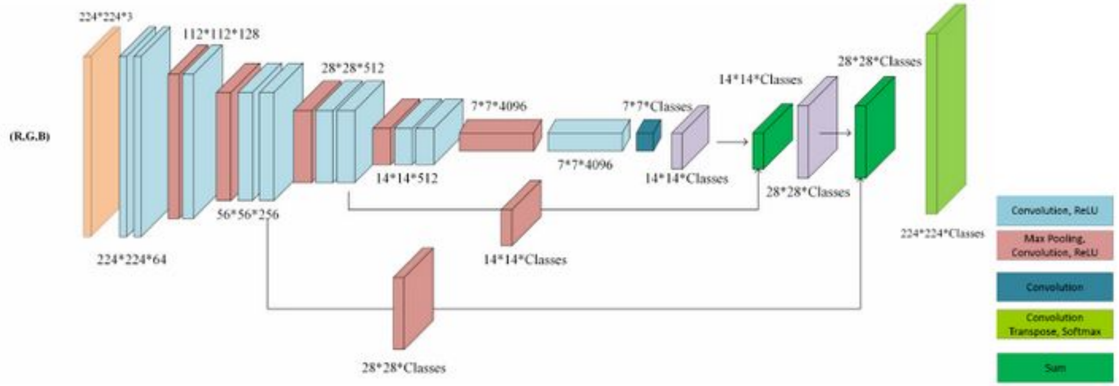
Machine Learning to overcome the limitations of cutting-edge CFD methodologies:

Machine Learning (ML) and Deep Learning (DL) are computational approaches that **enable systems to automatically learn patterns and make predictions from data.**

They are widely used in scientific research to analyze complex datasets, uncover hidden relationships, and accelerate discoveries across fields such as physics, biology, and medicine.



Pérez-Enciso, Miguel & Zingaretti, Laura. (2019). À Guide on Deep Learning for Complex Trait Genomic Prediction.



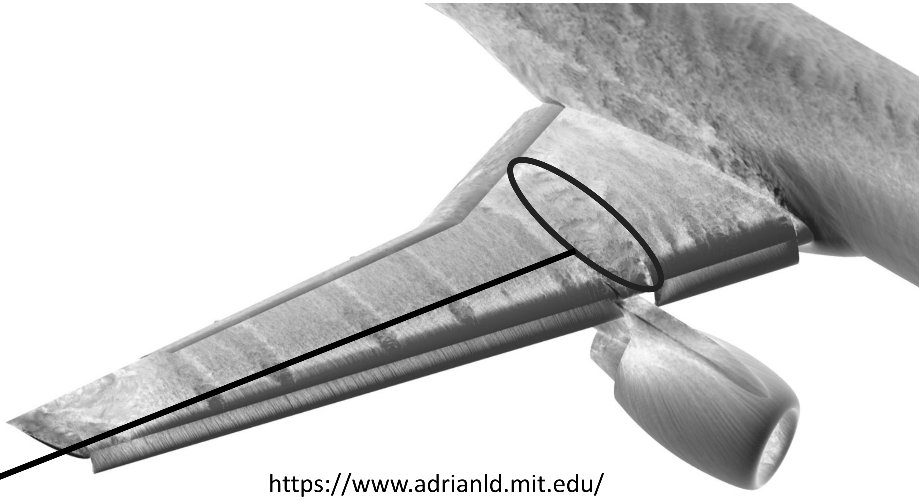
Piramanayagam. Supervised Classification of Multisensor Remotely Sensed Images Using a Deep Learning Framework. Remote Sensing.

Research objectives

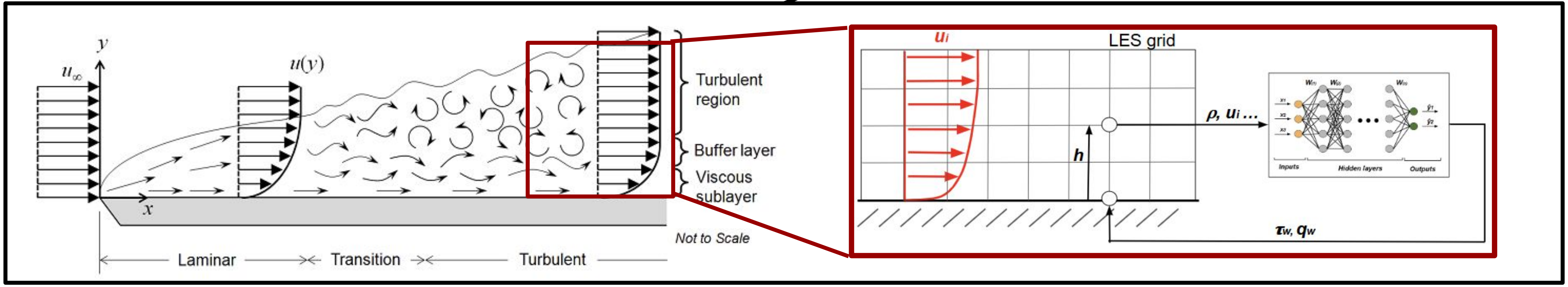
Machine Learning based methods for turbulence modeling.

Key idea: use data-driven **ML algorithms** to develop new turbulence models with:

- ➢ **increase accuracy**
- ➢ **greater generalization**
- ➢ **applicable to complex scenarios** relevant for aerospace applications.

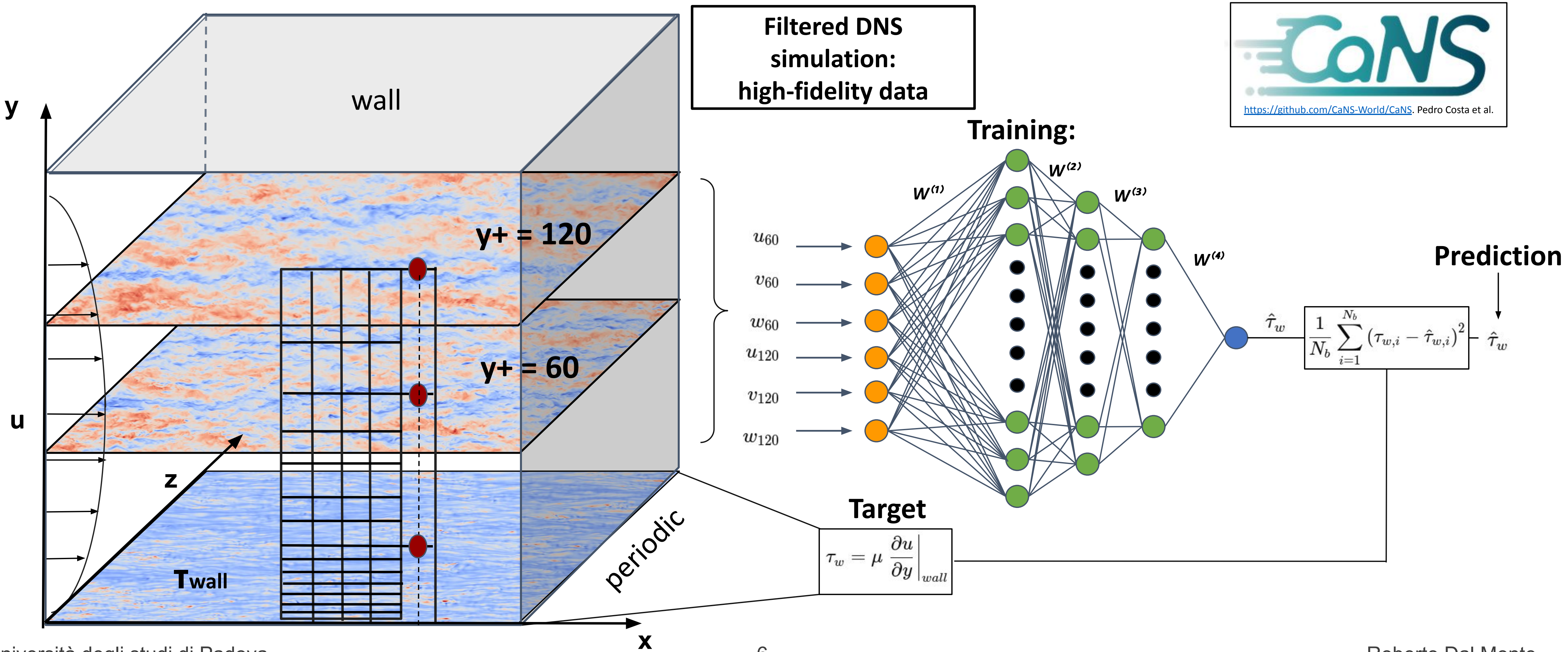


https://www.adrianld.mit.edu/



Activity Breakdown: Task #1

MultiLayer Perceptron (MLP) for predicting friction shear stresses knowing the velocity field far from the wall

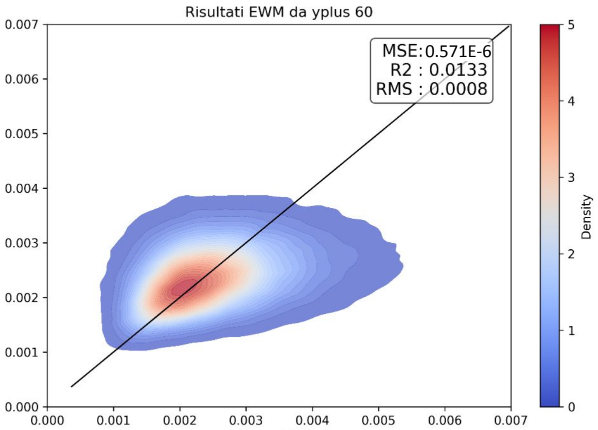


https://github.com/CaNS-World/CaNS. Pedro Costa et al.

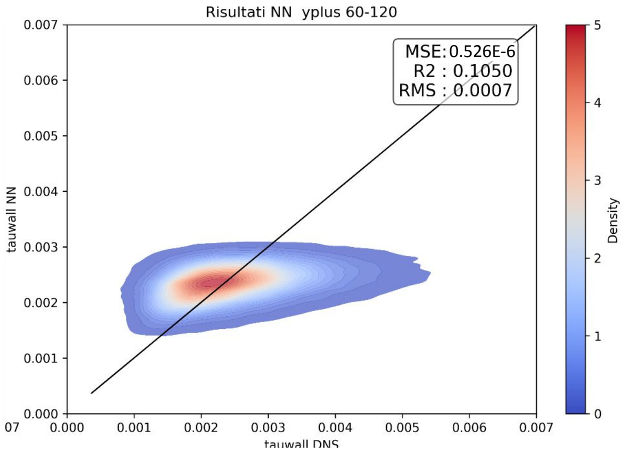
Activity Breakdown: Task #1

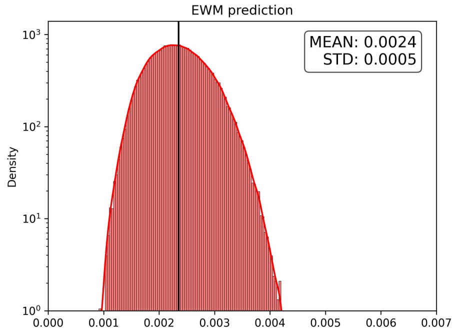
MLP vs EWM: *a priori* analysis

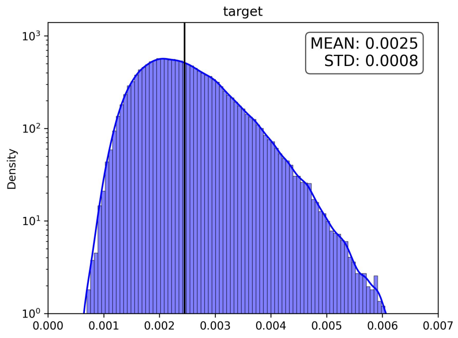
EWM results (reference):

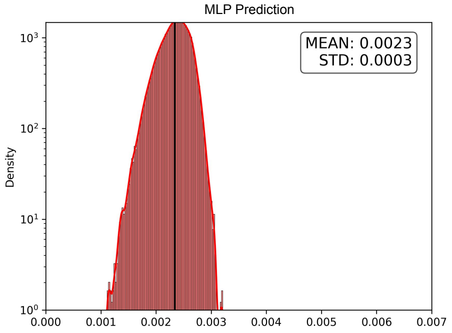


MLP results:



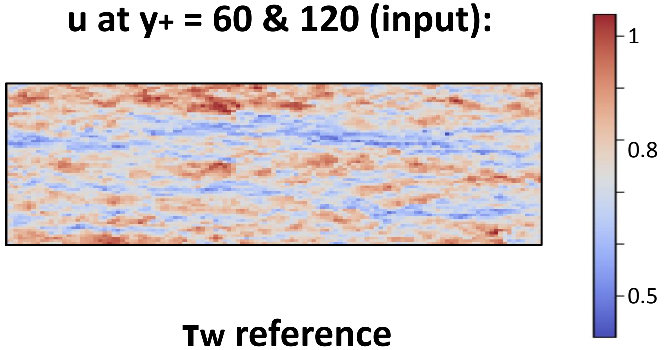




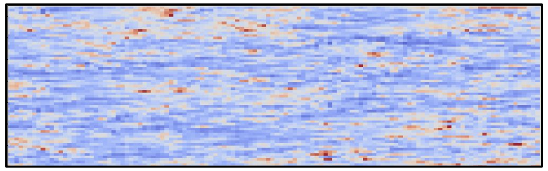


single slice (MLP prediction):

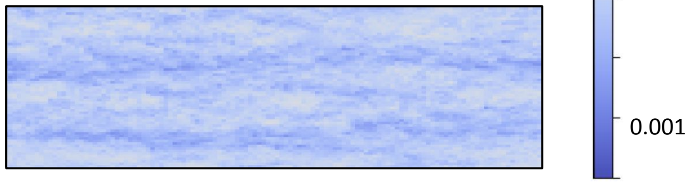
u at y+ = 60 & 120 (input):



τw reference



τw predicted



Activity Breakdown: Task #1

Metrics for evaluating the performance of MLP against EWM: *a priori* analysis

	MLP	EWM
MSE	5.26 E-7	5.71 E-7
R2	0.105	0.0133
RE_u+ (*)	1.48 %	1.92 %
RMS_u+ (*)	2.99%	3.88 %

* RE_u+ :

$$E_{\langle u\rangle^+} = \frac{|\langle u_{\text{NN}} \rangle^+ - \langle u_{\text{DNS}}\rangle^+|}{\langle u_{\text{DNS}}\rangle^+},$$

* RMS_u+ :

$$E_{u^+_{\text{RMS}}} = \frac{\left|u^+_{\text{RMS,NN}} - u^+_{\text{RMS,DNS}}\right|}{u^+_{\text{RMS,DNS}}},$$

$\langle u_{\text{DNS}}\rangle^+$ refers to filtered DNS-data

- **MLP model shows slightly better accuracy compare to EWM**
- **As EWM, MLP struggles to reproduce target variance**
- Fine tuning techniques didn't lead to an improvement of accuracy → **probably the model has reached its maximum performances in term of accuracy and generalizability**

Improvements are expected considering models able to learn spatial correlations in addition to single input-output mapping

Activity Breakdown: Task #2

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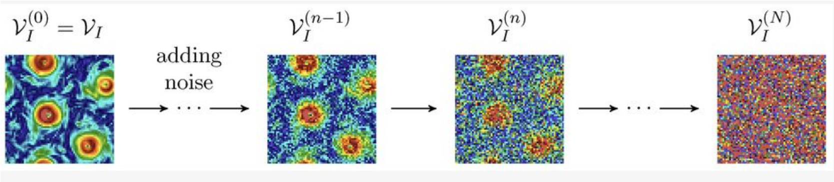
Denoising Diffusion Probabilistic Model (DDPM) to overcome MLP limitations

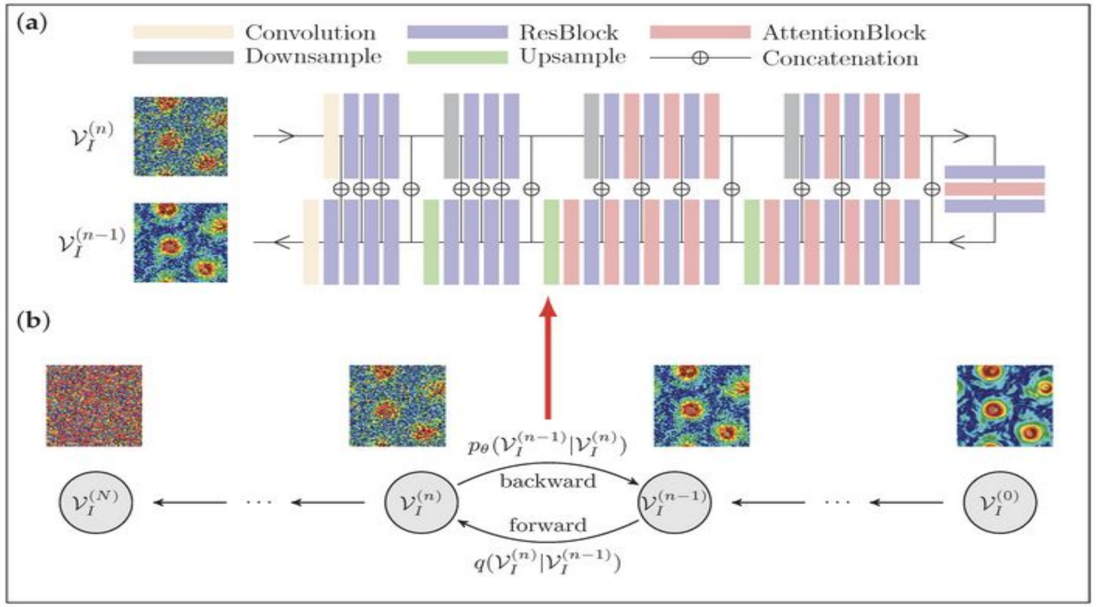
Denoising Diffusion Probabilistic Models (DDPMs) are generative models that **learn data distributions** by gradually corrupting samples with noise (forward process) and then training a neural network to reverse this process (reverse process) .

Through iterative denoising, **they can generate highly realistic samples that capture complex, high-dimensional relationships** present in the training data.

Forward process:



Reverse process:



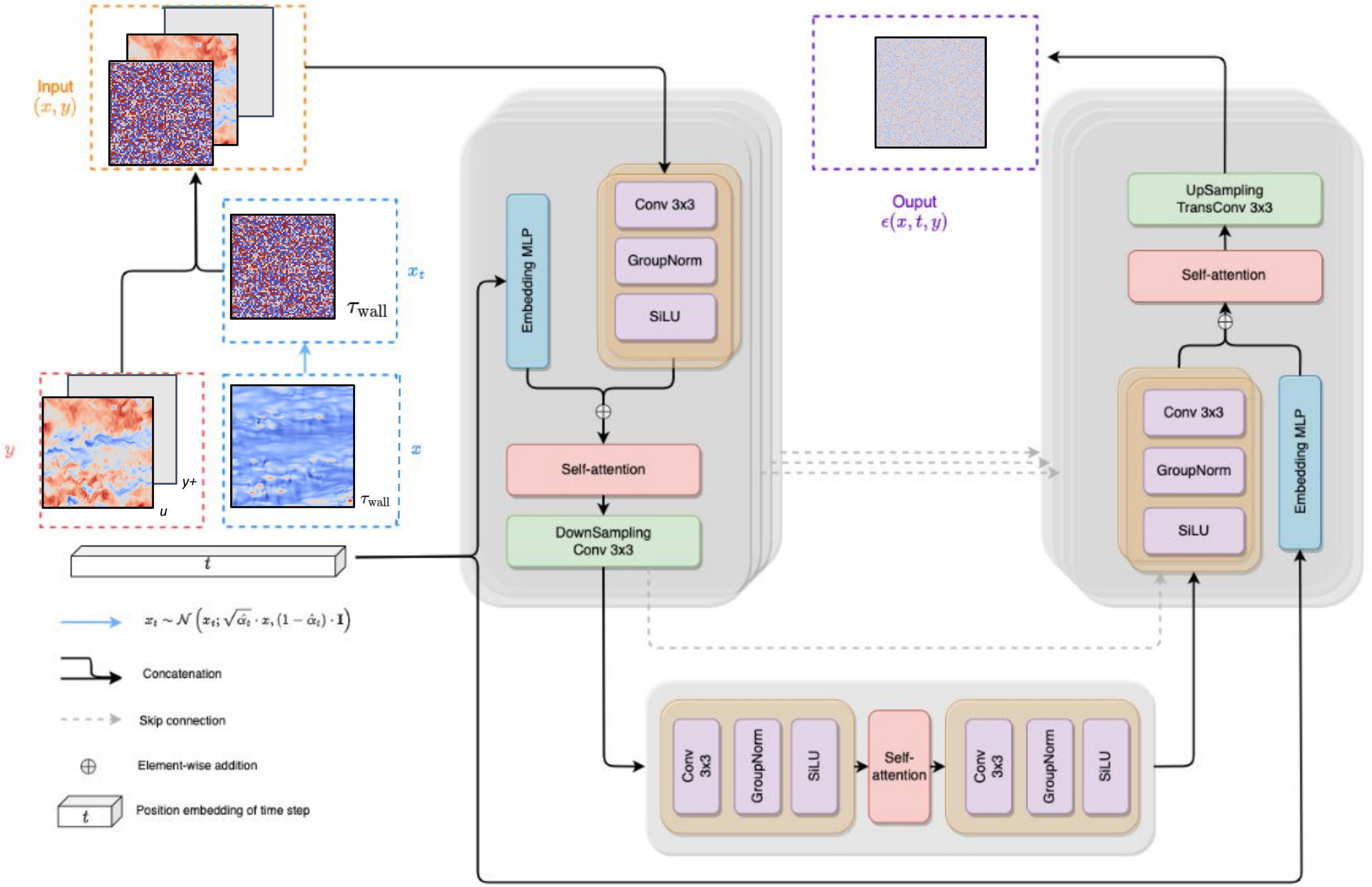
Li, T.; Lanotte, A.S.; Buzzicotti, M.; Bonaccorso, F.; Biferale, L. Multi-Scale Reconstruction of Turbulent Rotating Flows with Generative Diffusion Models.

Activity Breakdown: Task #2

Conditioned DDPM for friction shear stress prediction

- **Input**: small noised portion of τw field
- **Conditions**: corresponding portion of a velocity field and the related matching locations (y+)

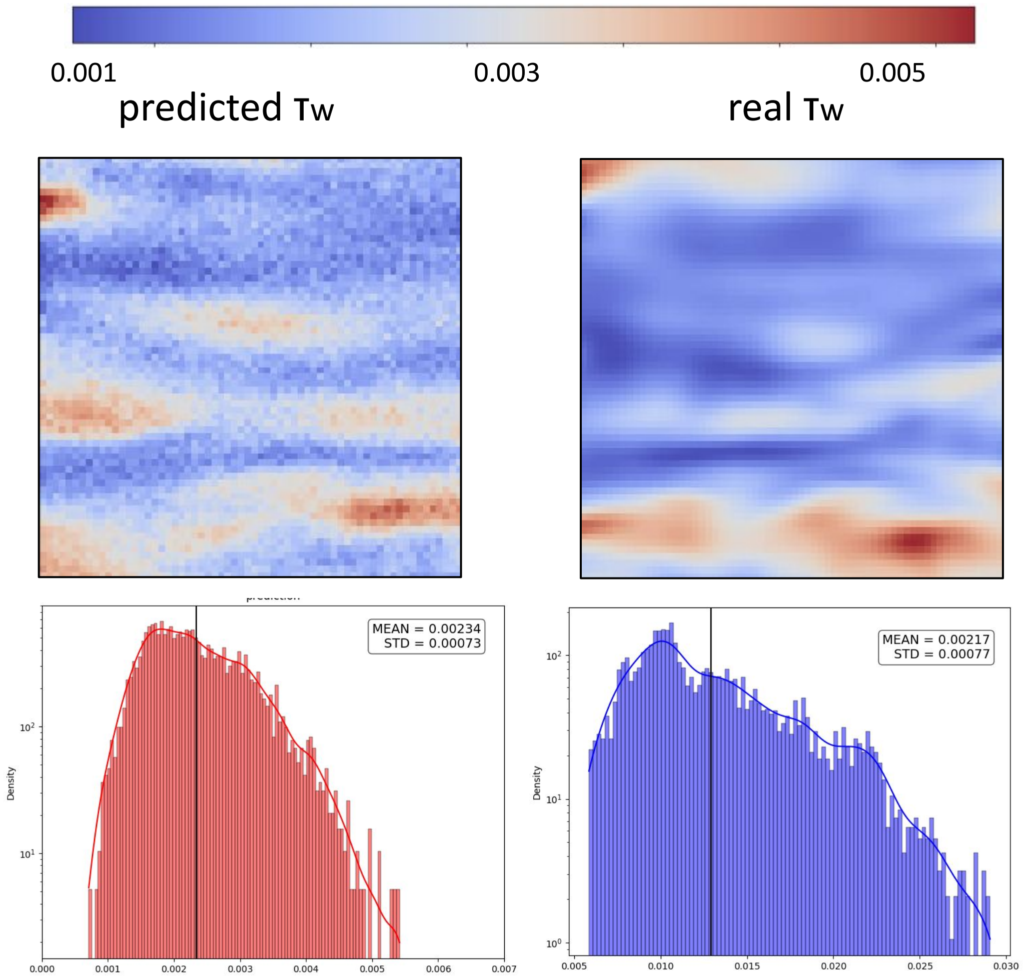
- **Training**:
learn how to re-obtain the real τw reversing the forward process (addition of noise) using the guidance given by the conditions



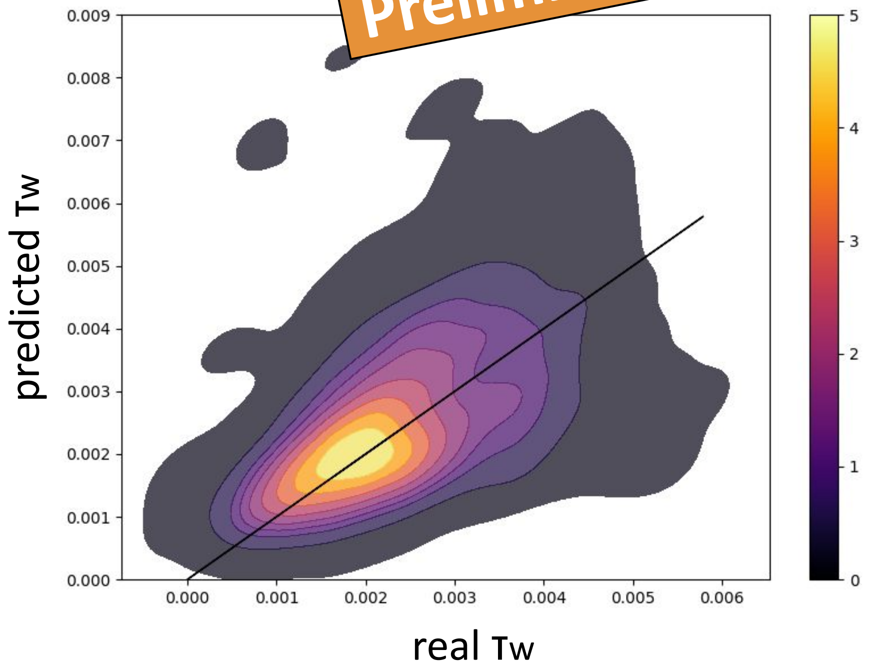
- **Inference**:
generate realistic tauwall that agree with the velocity field given as condition

Activity Breakdown: Task #2

Conditioned DDPM for predicting friction shear stresses: *a priori* analysis



Preliminary Results



y+ = 60

Not really close since they are evaluated on a small portion of the field.

	prediction	target
Mean	0.00234	0.00217
Std	0.0073	0.0077

Conclusion & Next Steps

Conclusion:

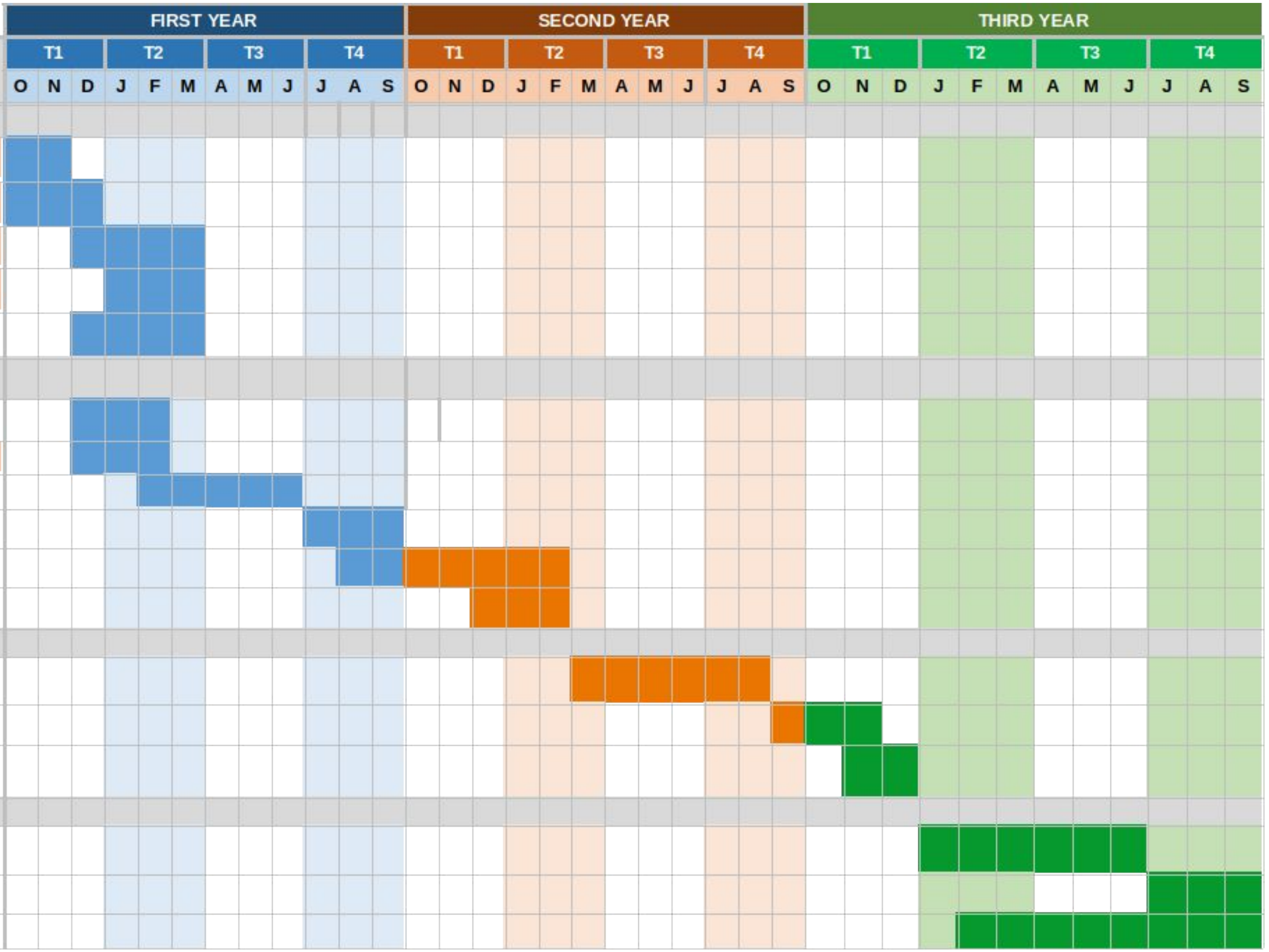
- Simple MLP shows slightly better performances compare to EWM but struggles to represent the rare value of τ_w that are far from the mean
- Diffusion Models are able to learn spatial correlations, hence they describe the τ_w distribution better compare to MLP and EWM

Next Steps:

- Improve current Diffusion Model (fine-tuning the hyperparameters, introduce physical constraints)
- Perform *a priori* analysis on different cases for assessing model generalizability
- Explore different types of Diffusion Models (Score-based, Latent diffusion etc.)
- Explore different strategies to speed-up the inference phase and perform *a posteriori* analysis

GANTT CHART

WBS NUMBER	TASK TITLE	% OF TASK COMPLETE
1	Turbulence Modeling / Numerical approaches (DNS, WMLES)	
1.1	Study of the state of art numerical approaches in CFD (DNS, WMLES)	100%
1.2	Study of the state of art turbulence modeling and statistical characterization of unsteady Dynamic turbulent system	100%
1.3	Setting-up and performing DNS simulations of isotropic turbulent wall-bounded channel flow	100%
1.4	Implementation of EWM on data fields obtaining by DNS simulations and compare them against Ground-truth	100%
1.5	Study the key aspects of Fluid solvers, including programming languages, linux environment And how to use HPC resources	80%
2	Machine Learning / Deep Models – Priori analysis	
2.1	Overview of Machine learning / Deep Learning foundations and models	70%
2.2	Implementation of simple MLP architecture for classification and regression problems	100%
2.3	Developing an optimize deep NN for tauwall prediction and performance analysis	90%
2.4	Studying of generative probabilistic models for high dimensional datasets	60%
2.5	Implementation of Deep Unet architecture for tauwall predictions and performance analysis	60%
2.6	Studying other kind of candidate models and their implementations	15%
3	High speed and compressible flows	
3.1	Repeat the DNS or WMLES for more complex flow, like high speed compressible flow Maybe accounting roughness and/or thermal stresses	0%
3.2	Trainig and testing the chosen Machine Learning model on this framework	0%
3.3	Employ the model for inference testing its accuracy and generalization ability conducting A priori analysis	0%
4	Coupling ML model with CFD solver and Writing the thesis	
4.1	Integrate the ML model chosen into the Fluid solvers and perform simulations under various Conditions	0%
4.2	Assessing the performance reached (a posteriori analysis)	0%
4.3	Collect all the work done and write the final dissertation	0%



Thanks for the attention

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