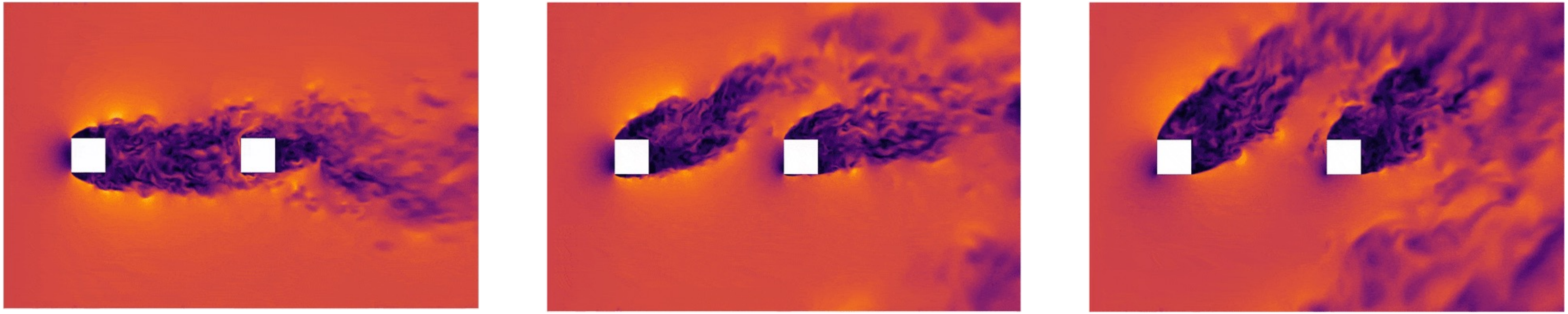

XGBoost-augmented RANS closure modelling of complex 3D flows

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Introduction

- NASA CFD 2030 plan demonstrates need for accurate models for ***industrial*** flows (Slotnick et al. 2014).
- ***RANS*** still not as accurate as required for industry.
- Accurate methods (***LES***) exist but will be ***expensive*** for decades (Widtherden 2016).
- **How can we improve RANS in the meantime?**

Slotnick et al. 2014, Vincent et al. 2016

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Introduction

Corrective, Data-driven RANS closure models

Main idea: Run a RANS simulation, correct the Reynolds stress tensor, then re-run simulation

Machine learning: Trains a model to predict a "better" Reynolds stress tensor (e.g., from DNS or LES) from a RANS simulation

Key issues:

- Training dataset
- Machine learning model architecture & input features
- Conditioning & injection

Introduction

Novelties:

- Explore applicability of machine learning techniques for an industrially relevant, ***complex, 3D flow***.
  - Previous studies have focused on ***canonical 2D*** flows (Ling et al. 2016, Kaandorp & Dwight 2020, McConkey et al. 2022)

- Explore stability and robustness of injected ***XGBoost*** predictions
  - Previous studies have used random forests (Kaandorp & Dwight 2020), and neural networks (Ling et al. 2016, McConkey et al. 2022)

Methodology

What should we ***predict*** with the model?

Model predicts: $\nu_t^\dagger$, $a^\perp$

$$\nabla \cdot (\vec{U}\vec{U}) = -\nabla p + \nu \nabla^2 \vec{U} - \nabla \cdot \tau$$

$$a \equiv \tau - \frac{1}{3}\mathrm{tr}(\tau) I$$

$$a = -2\nu_t^\dagger S + a^\perp$$

"Optimal eddy viscosity"

$$\nu_t^\dagger = \arg\min_{\nu_t \geq 0} ||a - (-2\nu_t S)||$$

"Remainder"

$$a^\perp = a - (-2\nu_t^\dagger S)$$

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Methodology

What ***input features*** should we use?

Key fields:
U, p, k

Tensors:
S, R, Ap, Ak

$$\begin{bmatrix} 0 & -\partial_z k & \partial_y k \\ \partial_z k & 0 & -\partial_x k \\ -\partial_y k & \partial_x k & 0 \end{bmatrix}$$

Form a **minimal integrity basis** for these 4 tensors

Extract the maximum ***invariant information*** from these fields.

47 basis tensors

Take **tensor invariants**

$$I_1(A) = \mathrm{tr}(A)$$
$$I_2(A) = \frac{1}{2}[(\mathrm{tr}(A))^2 - \mathrm{tr}(A^2)]$$

94 invariant scalars

Input features

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Methodology

Input Features

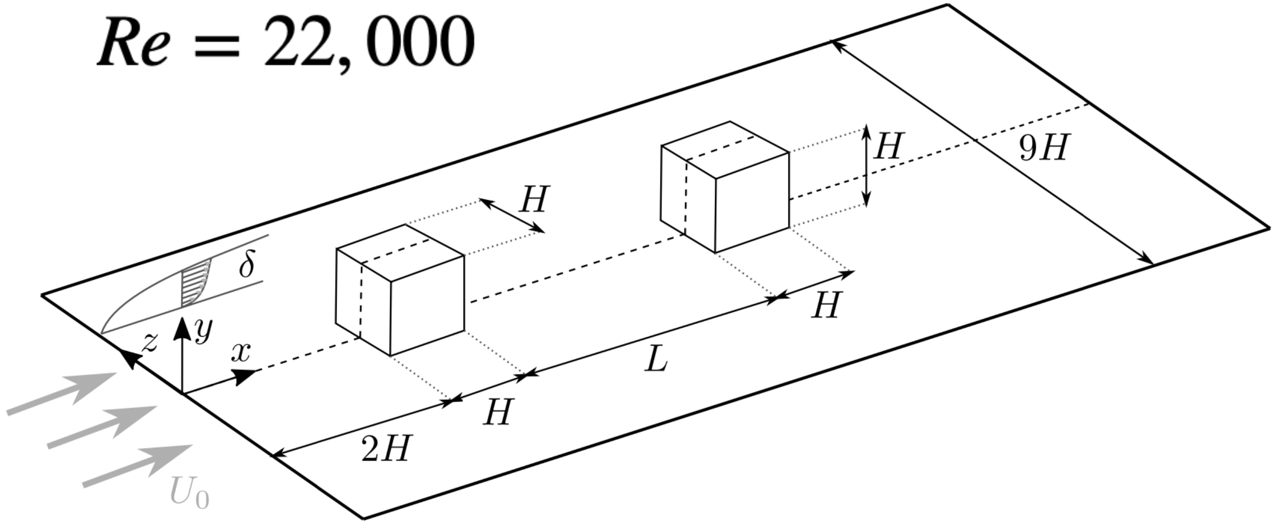
94 invariant scalars derived from U, p, k

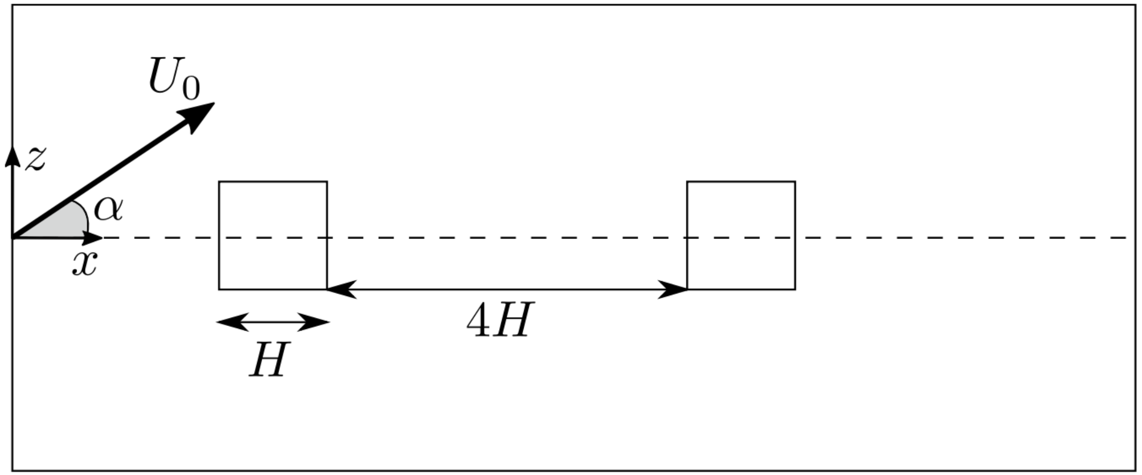
Model Target

Model predicts: $\nu_t^{\dagger}$, $a^{\perp}$

- ***XGBoost*** - gradient boosted decision trees (Chen 2016)
  - Outperforms neural networks for ***tabular data regression*** problems (Shwartz-Ziv 2022)
  - Training performed using ***multi-GPU*** HPC nodes (4xA100), due to large dataset size

3D flow description





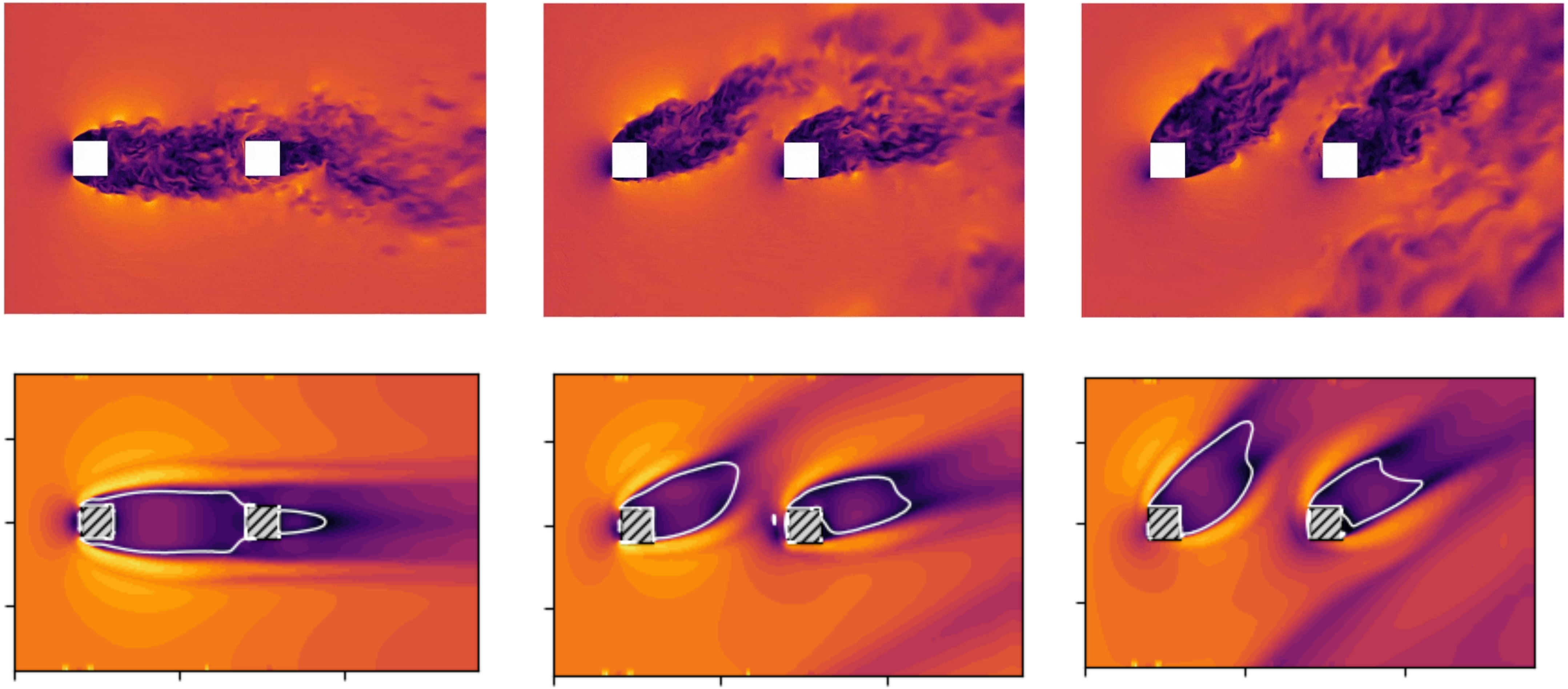
- An array of ***tandem*** wall mounted ***cubes***.
- A range of ***inlet flow angles*** are explored between α=0º and α=45º

Coupling between cubes changes with variations in the parameter space.

Training

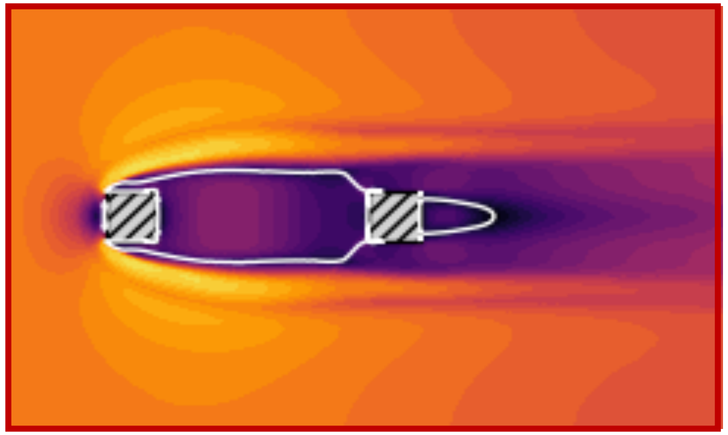
LES dataset

RANS Dataset

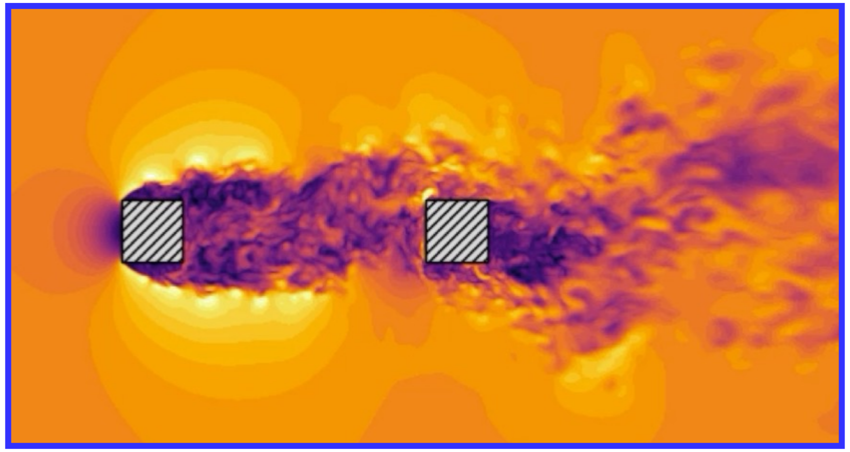


Training

RANS Dataset



LES dataset

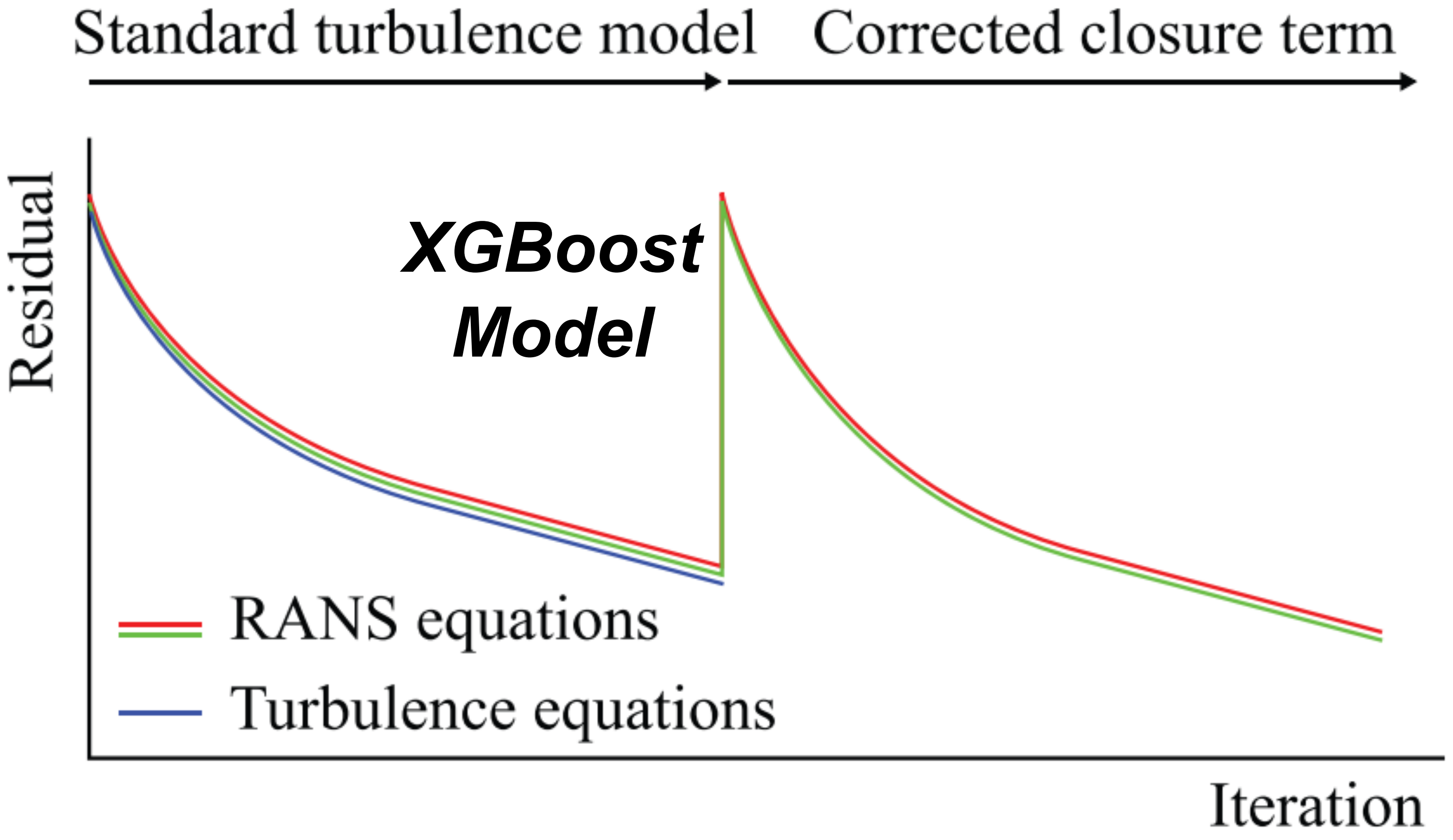


94 invariant scalars derived from U, p, k

XGBoost

Model trained to predict: $\nu_t^{\dagger}$, $a^{\perp}$

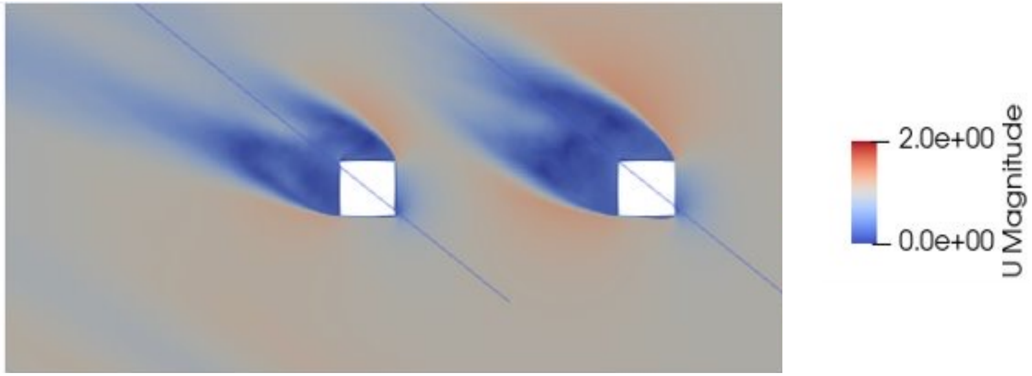
Injection



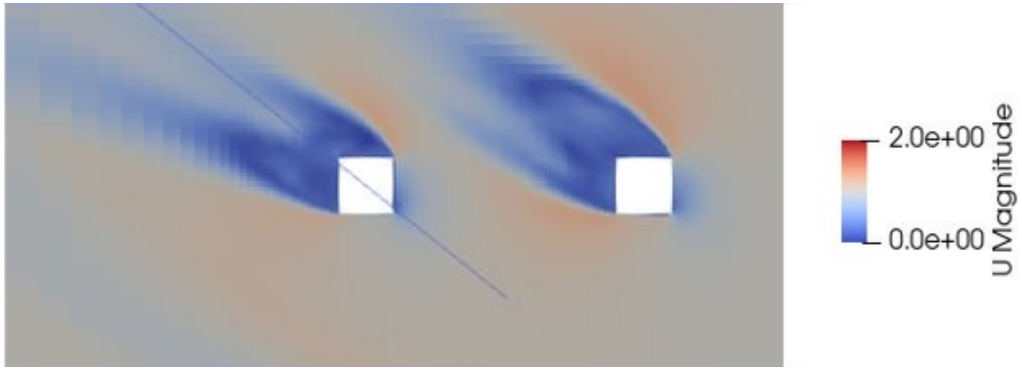
(McConkey et al. 2022) "Qualitative" residual plot showing injection procedure

Results

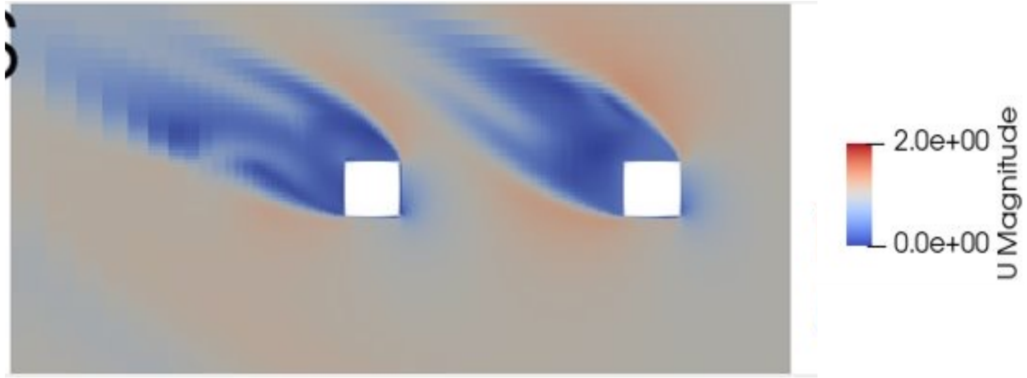
LES



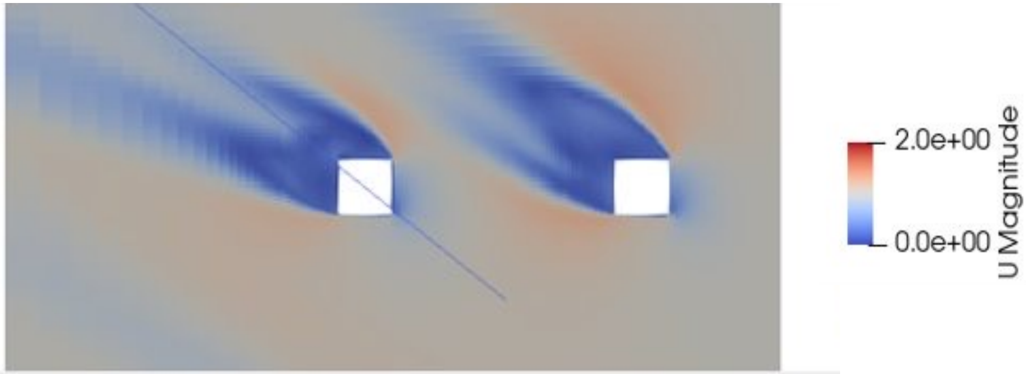
Label Injection



RANS



ML-RANS



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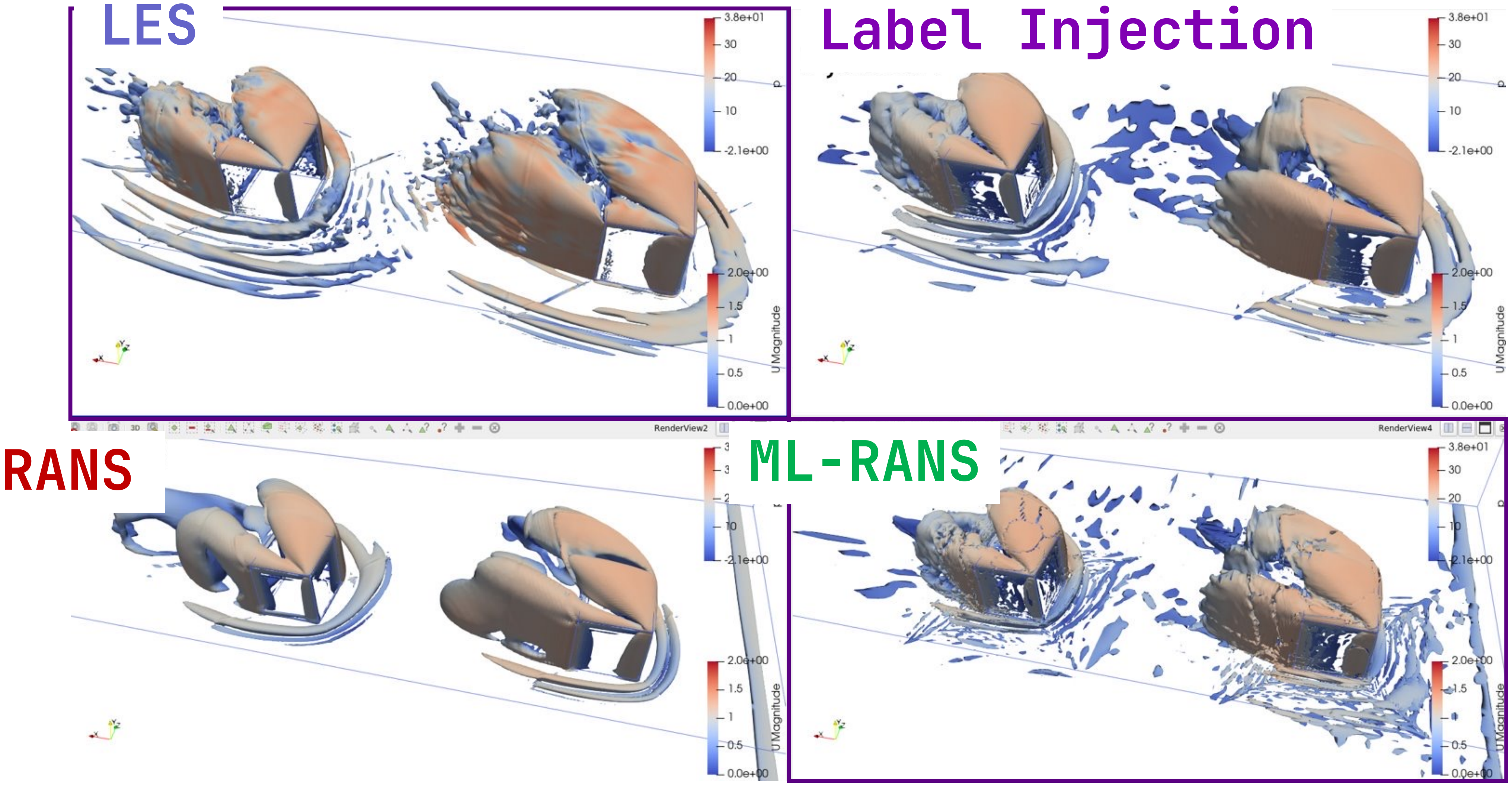
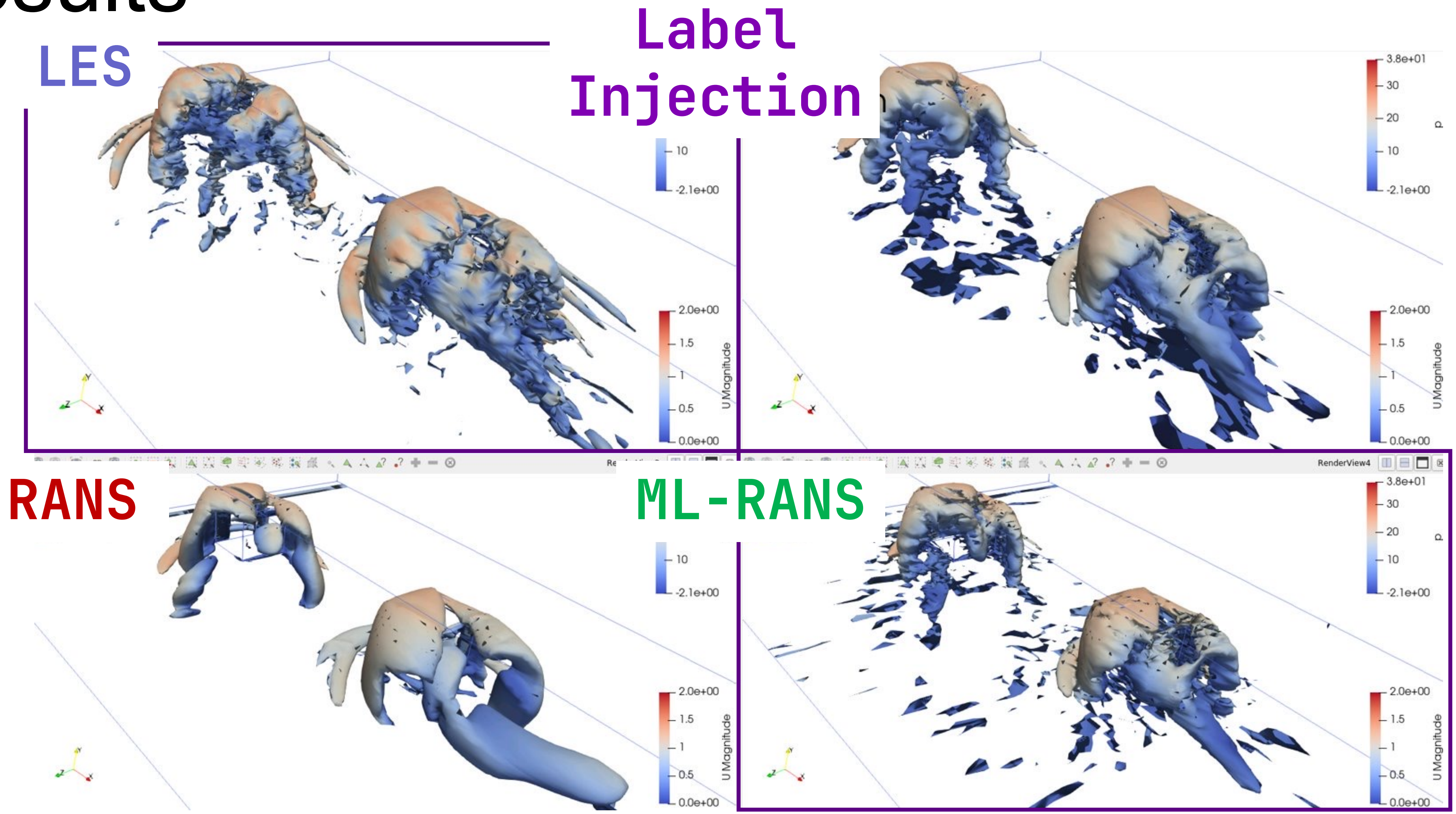
Results

Pressure contours, coloured by velocity magnitude



Results

Pressure contours, coloured by velocity magnitude



Conclusions

- Confirmed applicability and practicality of machine learning techniques for ***industrially relevant***, massively separated ***3D flows***.
- Confirmed ***stability*** of injected XGBoost predictions into RANS equations.
- Developed distributed, ***multi-GPU*** XGBoost training code for training ***large data-driven turbulence models*** using large LES datasets on HPC.

Future work

- Extending framework to ***unsteady*** flows.
- Incorporating XGBoost directly into ***turbulence model***.

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