Global Conference on Mechanical and Mechatronics Engineering 2021

Invited presentation - Computational Design in Mechanical Engineering Applications via CFD: Uncertainty Quantification and Optimisation

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InovScitech

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OVERVIEW

- Introduction
- Case 1: UQ impinging swirling jet for heat transfer
- Case 2: UQ NASA ARN nozzle
- Case 3: ML/Optimisation in a Micro Heat Exchanger
- Conclusions

- INTRODUCTION

INTRODUCTION

- Engineering practice is nowadays inconceivable without the presence of computational tools. Within this context, Computational Fluid Dynamics (CFD) are an essential tool for fluid-based machine design, such as heat exchangers, turbines, cooling processes or aerodynamic performance of vehicles.

- Among the simulation capabilities of modern softwares, Reynolds-Averaged Navier Stokes (RANS) simulations are the most popular industrial approach, due to the decent computation elapsed times and accuracy for a vast range of applications. RANS < LES < DNS

- However, some engineering applications that simulate complex flows may exhibit certain discrepancies as a consequence of neglected sources of uncertainty. -> Uncertainty Quantification (UQ)

UNCERTAINTY QUANTIFICATION

- The aim of Uncertainty Quantification (UQ) is to quantify how the output of a model is varied due to the variability of its inputs.
- UQ can provide measures of confidence, which are important for realistic validation.
- In some scenarios, UQ can even provide risk measures. E.g. *Black-Swans.*
- UQ can be combined with sensitivity analysis studies to develop relevant industrial decision making procedures.

UNCERTAINTY QUANTIFICATION

- Aleatoric uncertainties take place due to physical variability, which leads to certain variance in the results

- Aleatoric uncertainties can be modelled as probabilistic distributions as their behavior can be interpreted probabilistically.

- Aleatoric uncertainties can be reduced by more controlled experiment/performance conditions, accurate machining processes, etc.

  - Examples: variability in aircraft velocity, small variations in the angular velocity of a pump, variations in ambient pressure or velocity, etc.

UNCERTAINTY QUANTIFICATION

- Epistemic uncertainties arise due to a lack of knowledge. These are result of incompleteness in the modelling of real physics.

- Whilst aleatoric uncertainty is represented by probabilistic measures, epistemic uncertainties are represented by means of intervals of belief.

- The recommended approach to reduce epistemic uncertainty is to increase the knowledge. This can be overcome by using more accurate model.

  - Example: turbulence modelling in RANS simulations

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MACHINE LEARNING IN CFD

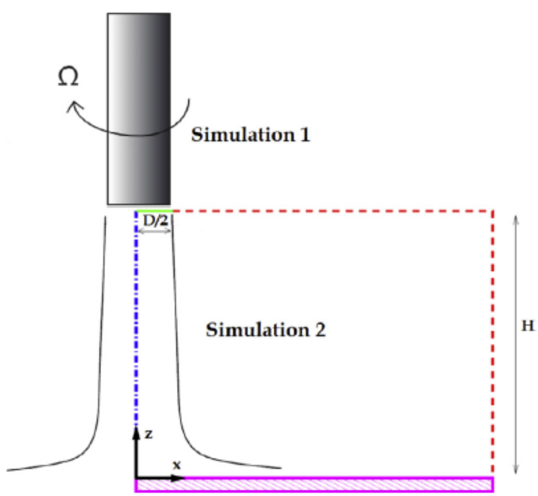
- In a nutshell, Machine Learning (ML) is about building machines that learn and/or think in an automatic manner.
- CFD/Fluid dynamics is a field where ML is being applied “recently”. There is much potential, specially in turbulence modelling.
- Examples:
  - Data-driven turbulence modelling: *Zhang, Z. J., & Duraisamy, K. (2015). Machine learning methods for data-driven turbulence modeling. In 22nd AIAA Computational Fluid Dynamics Conference (p. 2460).*
  - Physics-informed Learning Machines: infer the flow characteristics from scattered snapshot data. The authors further demonstrated that from smoke or dying visualisations one can use these AI techniques and extract flow quantities of interest, namely ``Hidden Fluid Dynamics", whose work has been published this year in Science: *Raissi, M., Yazdani, A., & Karniadakis, G. E. (2020). Hidden fluid mechanics: Learning velocity and pressure fields from flow visualizations. Science, 367(6481), 1026-1030.*
  - Prediction of erosion in pipe elbows due to solid particles: *Zahedi, P., Parvandeh, S., Asgharpour, A., McLaury, B. S., Shirazi, S. A., & McKinney, B. A. (2018). Random forest regression prediction of solid particle Erosion in elbows. Powder Technology, 338, 983-992.*
  - Risk of aneurysm using classification methods supported by CFD: *Aranda, A., & Valencia, A. (2018). Study on cerebral aneurysms: Rupture risk prediction using geometrical parameters and wall shear stress with CFD and machine learning tools. Machine Learning and Applications: An International Journal (MLAIJ) Vol, 5.*

- CASE 1: IMPINGING SWIRLING JET

CASE 1: IMPINGING JET

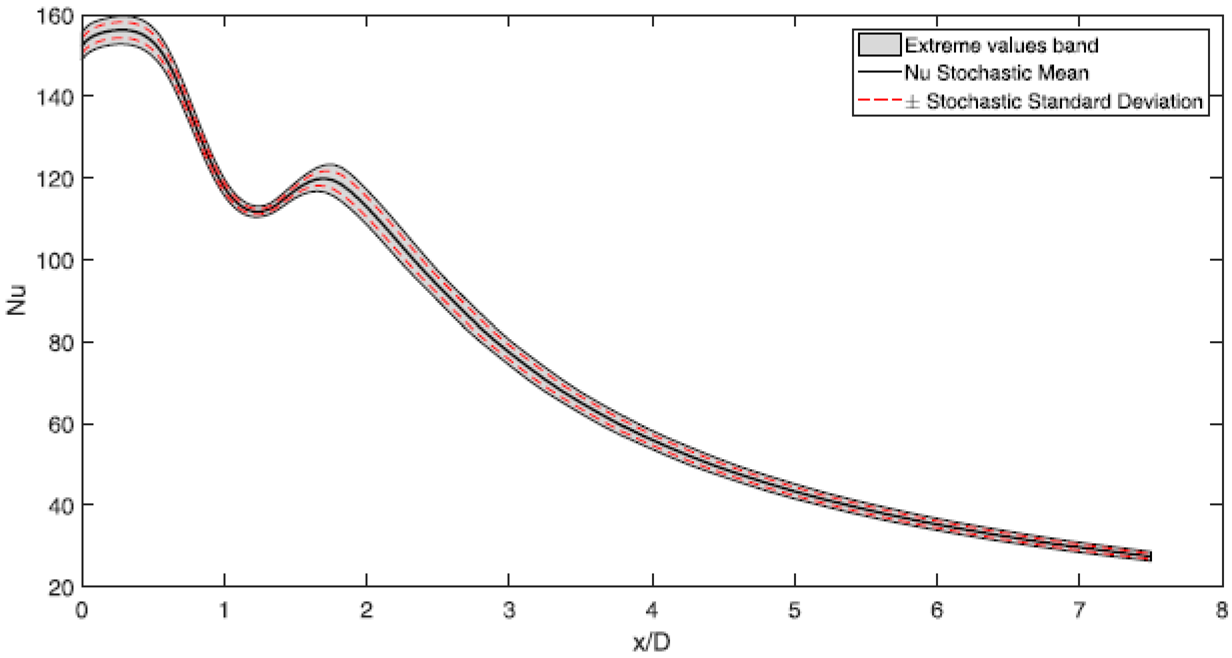
Granados-Ortiz, F. J., Ortega-Casanova, J., & Lai, C. H. (2020). Propagation of uncertainty in a rotating pipe mechanism to generate an impinging swirling jet flow for heat transfer from a flat plate. Engineering with Computers, 1-30.

- Reynolds number: $Re = \frac{U\rho D}{\mu} = 23000$. Swirl intensity: $S = \frac{\Omega R}{U} = \frac{\pi D^3 \Omega}{8Q} = 0.5$, due to rotation of a pipe with angular velocity Ω.
- Uncertainty of a 5% in Q and 0.5% in Ω (observed in experiments) modelled as:
  - $Q \sim Unif(0.95\bar{Q}, 1.05\bar{Q})$, where $\bar{Q}$ corresponds to $Re = 23000$
  - $\Omega \sim Unif(0.995\bar{\Omega}, 1.005\bar{\Omega})$, where $\bar{\Omega}$ is the deterministic value for S=0.5



CASE 1: IMPINGING JET

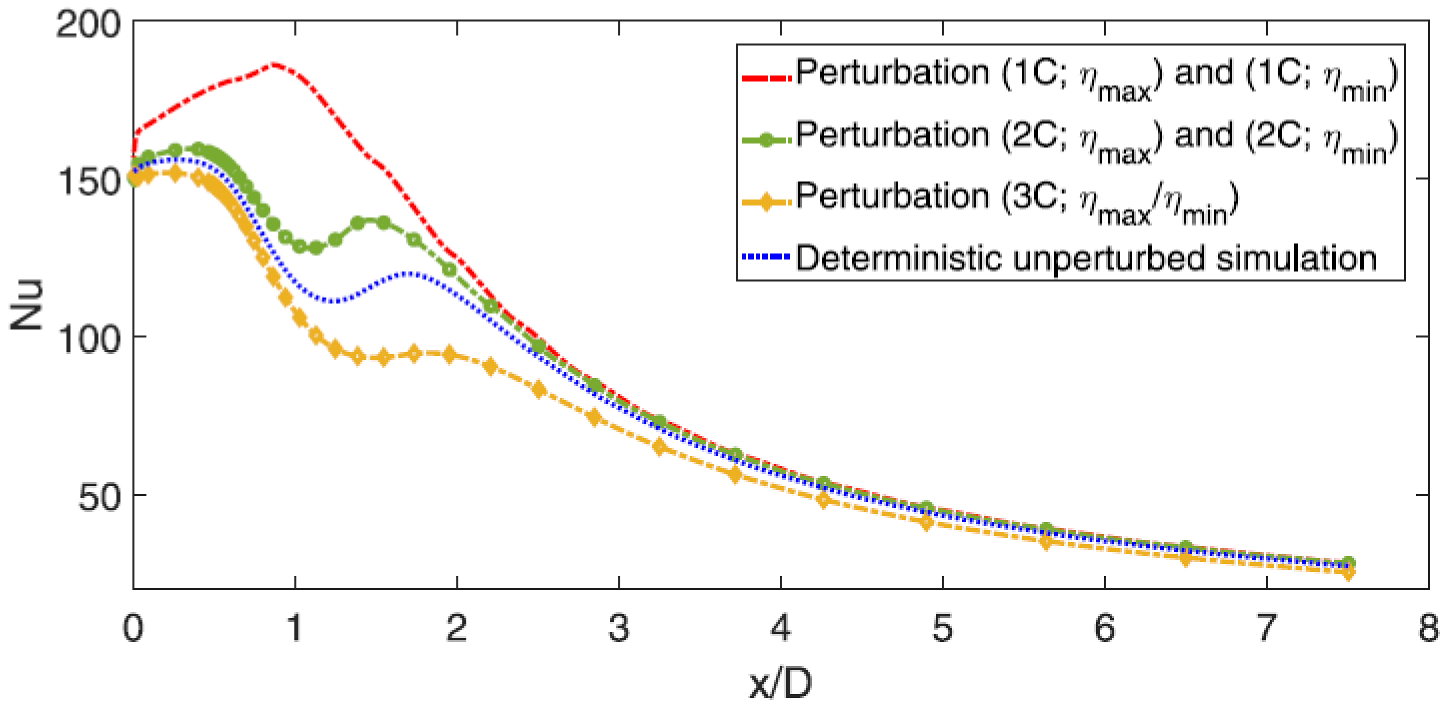
Aleatoric UQ



$$Nu = \frac{hD}{k}$$

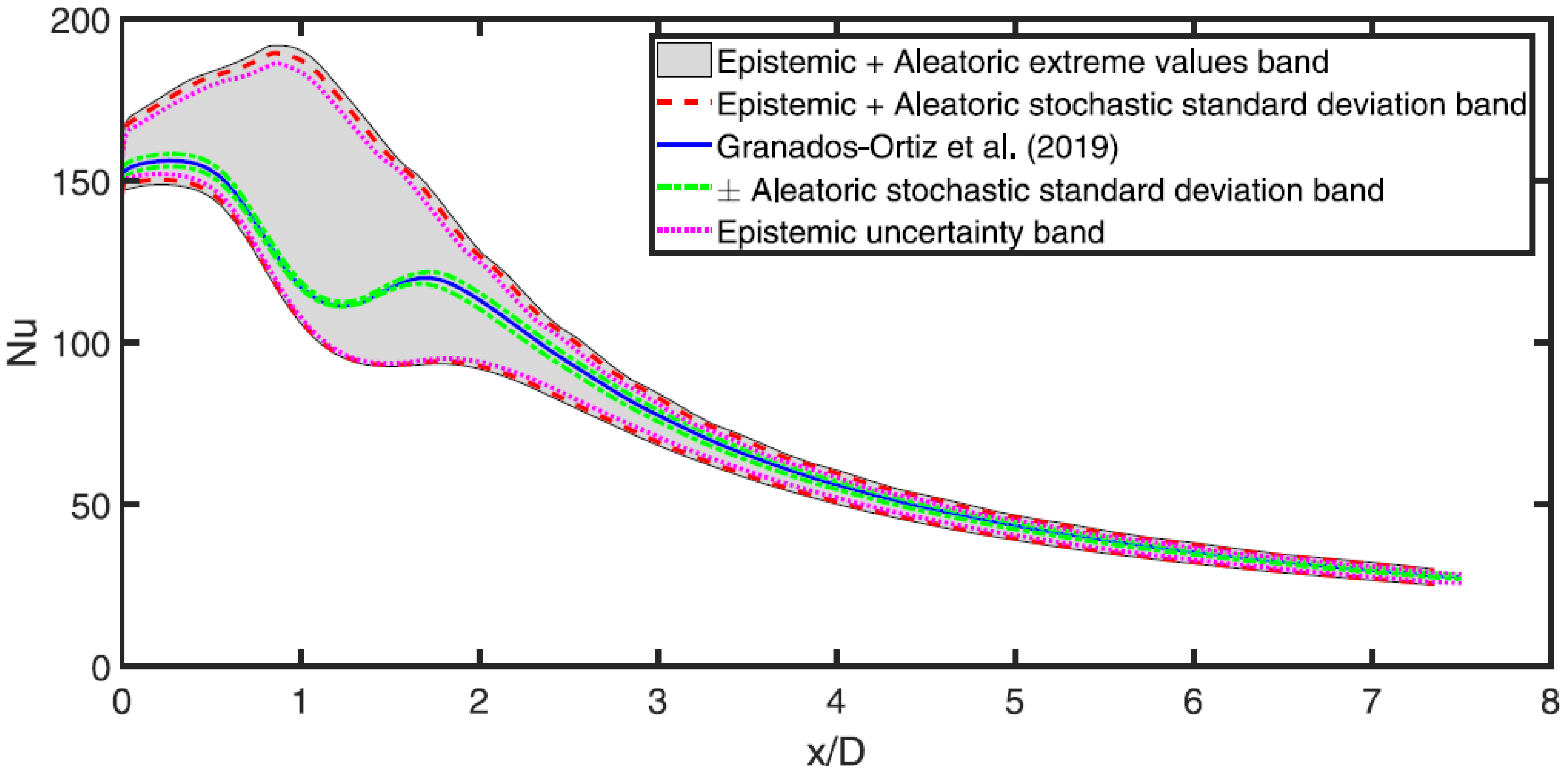
CASE 1: IMPINGING JET

Epistemic UQ



CASE 1: IMPINGING JET

Mixed UQ



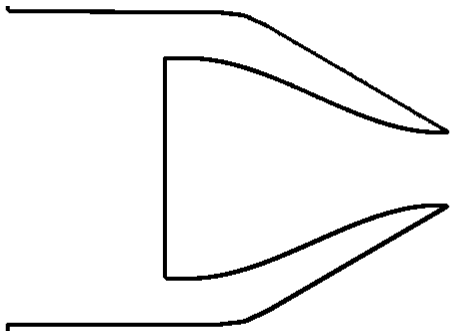
- CASE 2: NASA ARN NOZZLE

CASE 2: NASA ARN NOZZLE

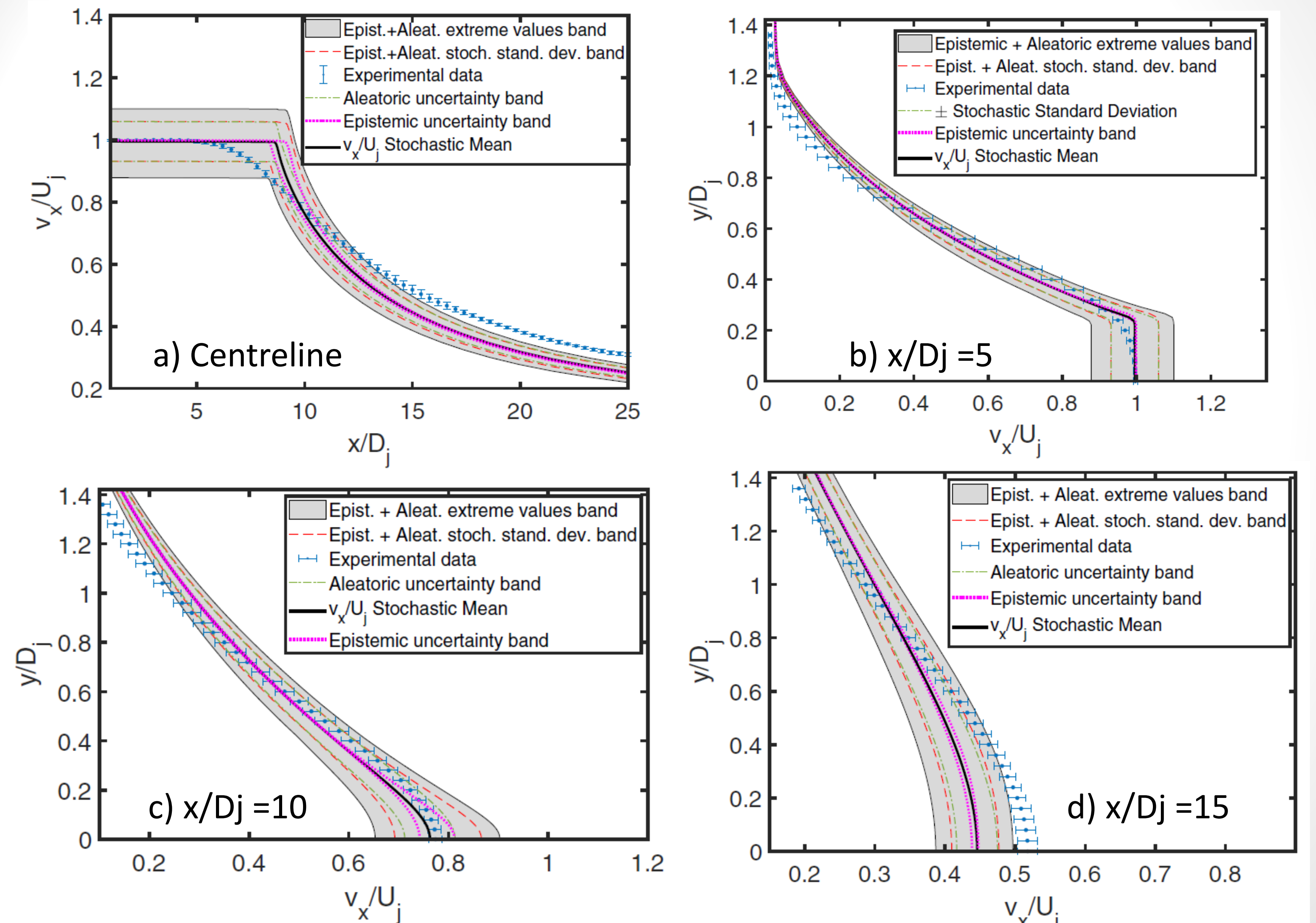
Granados-Ortiz, F. J., & Ortega-Casanova, J. (2020). Quantifying & analysing mixed aleatoric and structural uncertainty in complex turbulent flow simulations. International Journal of Mechanical Sciences, 188, 105953.

https://turbmodels.larc.nasa.gov/jetsubsonic_val.html

- Acoustic Mach jet : $Ma = 0.513.$
- Static to ambient temperature: $T_j/T_0 = 0.950$
- 4% of uncertainty on the turbulent intensity and pressure inlet, as observed in the work of Bridges & Wernet (2010, 2011), where the variability of the parameters is approximately ranging between a 3% and 5%.
  - $I(\%) \sim Unif(0.96\bar{I}, 1.04\bar{I})$, where $\bar{I} = 0.104\%$
  - $p_j \sim Unif(0.96\overline{p_j}, 1.04\overline{p_j})$, where $\overline{p_j}$ = 120995.8 Pa



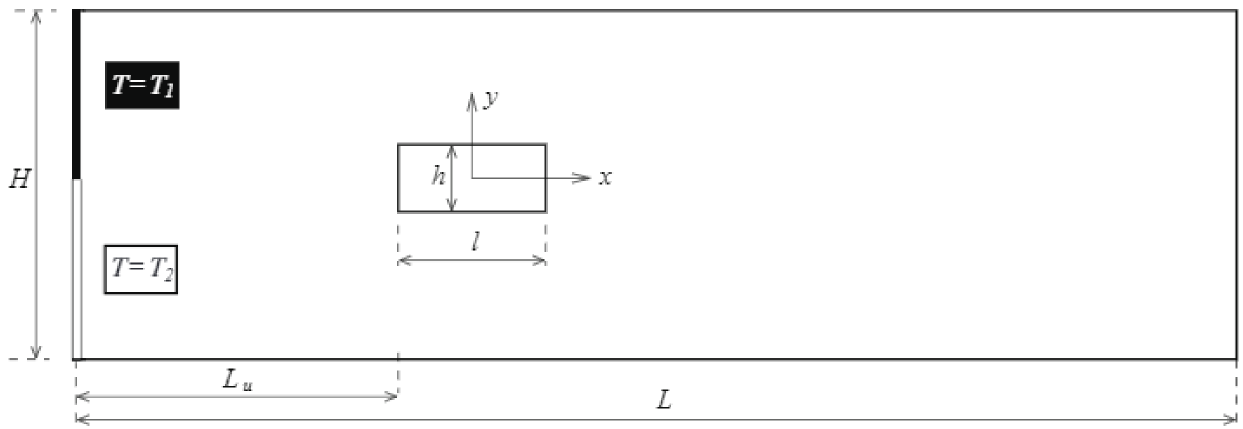
CASE 2: NASA ARN NOZZLE



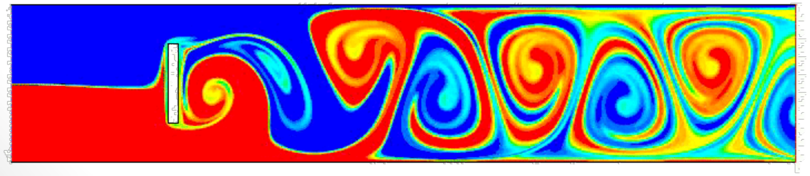
- CASE 3: Optimisation Micromixer

OPTIMISATION MICROMIXER

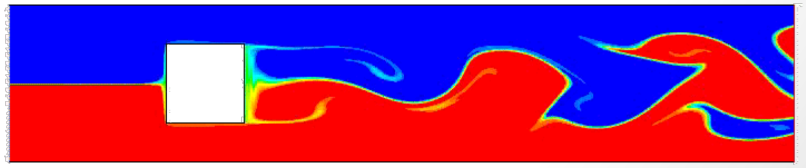
- 2D Micromixer considered in this work:



$Re = 200, BR = 0.2 , AR = 1$



$Re = 200, BR = 0.5, AR = 0.125$



$Re = 200, BR = 0.5, AR = 1$

OPTIMISATION MICROMIXER

- Random Forest (RF) predictor
  - Classification problem: prediction of configurations with vortex shedding (VS=1) and without vortex shedding (VS=0).
  - Dataset balanced enough (VS= 0 in 33.75% cases). 80 simulations from the combinations amongst:

$$Re = \{120, 140, 160, 180, 200\}$$
$$BR = \{0.2, 0.3, 0.4, 0.5\}$$
$$AR = \{0.125, 0.25, 0.5, 1\}$$

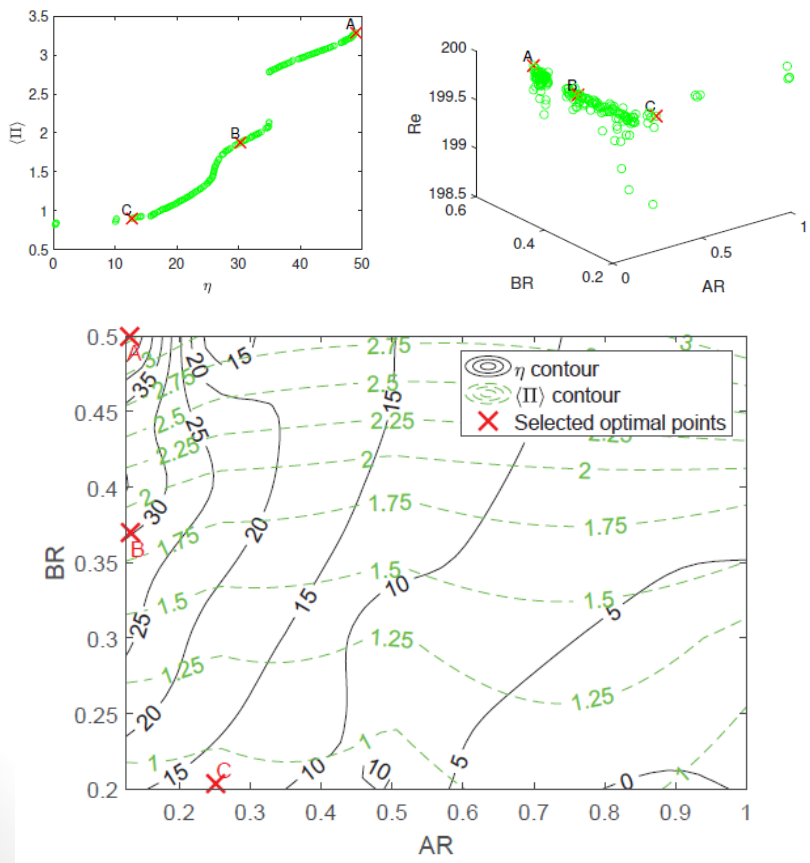
  - RF: Bootstrap randomised sampling on the training dataset in order to train several decision trees that will be ensembled:

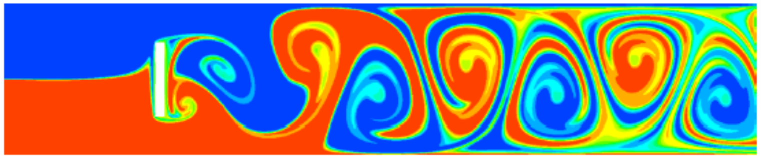
$$C^{RF}_{D_t,\Theta_1,\Theta_2,\ldots,\Theta_M} = arg\ max \sum_{m=1}^{M} (h(\mathbf{X}, \Theta_m) = c)$$

  - This bootstrap method with replacement (samples can be re-utilised to train the trees).

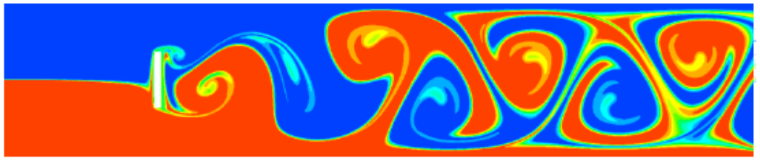
OPTIMISATION MICROMIXER

- Genetic Algorithms are applied onto the surrogates to find the optimal solutions:

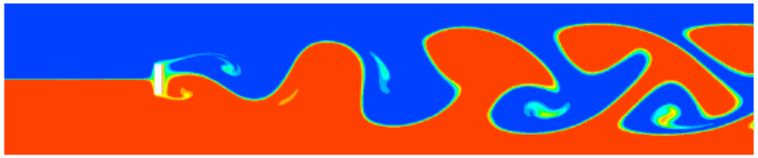




Config. A



Config. B



Config. C

CONCLUSIONS

- Aleatoric and epistemic uncertainty are important in the simulation of complex flow.
- Classically, UQ of both types of uncertainty have been considered in an isolated approach. Mixed uncertainty in CFD shows underlying interactions between aleatoric and epistemic uncertainty.
- Efficient surrogates can be incorporated to a framework to improve CFD optimization studies, since this model predicts quantities of interest.
- All the abovementioned conclusions supports the idea that CFD is an invaluable tool both in industry and academia, with increasing importance and in continuous development.

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Thank you!