Workshop in Data-driven methods, machine learning and optimization in fluid mechanics.

Speaker Abstracts

Name:	Luca Magri
Email:	l.magri@imperial.ac.uk
Institution:	Imperial College London
Abstract	

Physics-aware data-driven methods for unsteady fluids: Real-time and machine learning approaches

To predict the evolution of physical systems, we need a model that tells us "what happens next" given "what we know so far".
This can be enabled by physical principles and data-driven approaches.
On the one hand, physical principles, for example conservation laws, are extrapolative because they can provide predictions on phenomena that have not been observed, but they are "rigid".
On the other hand, data-driven modelling provides correlation functions within data, but they are "adaptive".

In this talk, the complementary capabilities of both approaches will be exploited to achieve adaptive modelling and optimization of nonlinear, unsteady, and uncertain flows.
This is the subject of physics-aware data-driven methods.

The focus of the talk is on computational methodologies for modelling and optimization of complex flows: (i) real-time data assimilation with a Bayesian approach to infer model errors (bias) with applications to thermoacoustic oscillations; and (ii) and auto-encoders and reservoir computers for reduced-order modelling of turbulent flows, which generalise POD/DMD methods to nonlinear dynamics, for the prediction of extreme events.

Name:	Saleh Rezaeiravesh
Email:	Saleh.rezaeiravesh@manchester.ac.uk
Institution:	The University of Manchester
Co-authors and their institutions	Timofey Mukha, tmu@mech.kth.se, KTH Royal Institute of Technology, Sweden Philipp Schlatter, pschlatt@mech.kth.se, KTH Royal Institute of Technology, Sweden

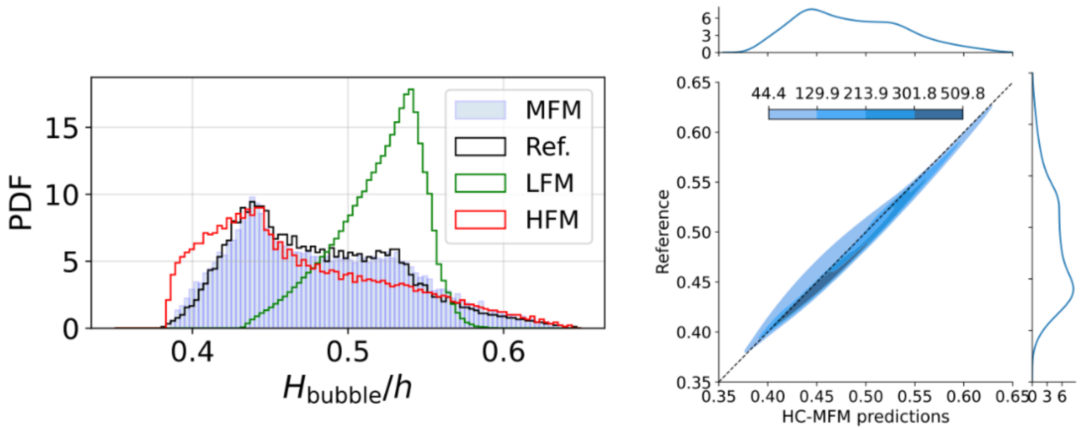
Abstract

A Bayesian hierarchical multifidelity model for turbulent flow problems

Conducting high-fidelity experiments and scale-resolving numerical simulations of turbulent flows can be prohibitively expensive particularly at high Reynolds numbers which are relevant to engineering applications. On the other hand, it is necessary to develop accurate yet cost-effective models for data-driven outer-loop problems involving turbulent flows which include uncertainty quantification (UQ), data fusion, prediction, and robust optimization. In these problems, exploration of the space of inputs and design parameters demands a relatively large number of flow realizations. A solution can be using multifidelity models (MFMs) which aim at accurately predicting quantities of interest (QoIs) and their stochastic moments by combining the data obtained from different fidelities. When constructing MFMs, a given finite computational budget is optimally used through running only a few expensive (but accurate) simulations and many more inexpensive (but potentially less accurate) simulations.

The present study reports our recent progress on further development and application of a class of Bayesian hierarchical multifidelity models with automatic calibration (HC-MFM) which rely on the Gaussian processes. At each fidelity level, which can be associated to any of the turbulence simulation approaches, both model inadequacy and aleatoric uncertainties in the process of data fusion are considered. As a main advantage of the present multifidelity modelling approach, the fidelity-specific and cross-fidelity calibration parameters as well as the hyperparameters appearing in the Gaussian processes are simultaneously estimated within a Bayesian framework using a limited number of flow realizations. The Bayesian inference of the posterior distribution of various parameters is done using a Markov Chain Monte Carlo (MCMC) approach. As a major strong point of the HC-MFM, the predictions will be accompanied by the estimation of the associated confidence intervals. Given the generality of the HC-MFM, they can be applied to various problems related to fluid mechanics and turbulent flows. For the latter, when combining the data of RANS (Reynolds-averaged Navier-Stokes) simulations with those of scale-resolving approaches such as direct numerical simulation (DNS) and large-eddy simulation (LES), where a small correlation between the data exists, the HC-MFM leads to accurate predictions. This is important, noting that the correlation-based MFMs which are widely used in the community are incapable of providing such level of accuracy. In the talk, we will discuss various aspects of the HC-MFM for several problems related to wall-bounded turbulent flows.

Figure



(Left) Histogram of the height of the separation bubble in a turbulent flow over periodic hills due to the geometrical uncertainties, estimated by low-fidelity (LFM, 125 RANS simulations), high-fidelity (HFM, 5 DNS), and multifidelity (MFM, LF+HF data) models and compared to the ground truth (Ref., 9 DNS). (Right) Scatter plot of the MFM predictions against the reference data for samples of the uncertain parameters. The DNS data are taken from Xiao et al., 2020 (https://doi.org/10.1016/j.compfluid.2020.104431). For details, see Rezaeiravesh et al. 2022 (https://doi.org/10.48550/arXiv.2210.14790).

Name:	Andrew Mole
Email:	andrew.mole@manchester.ac.uk
Institution:	University of Waterloo, Canada
Co-authors and their institutions	Ryley McConkey *, Alex Skillen*, Alistair Revell*, Eugene Yee^, Fue-Sang Lien^ *: University of Manchester, UK ^: University of Waterloo, Canada

Abstract

XGBoost-augmented RANS closure modelling of complex 3D flows

Though growing computational capabilities enable wider use of Large Eddy Simulation (LES), Reynolds-averaged Navier-Stokes (RANS) simulations remain the dominant method for simulating turbulent flows of engineering importance. This dominance is expected to continue for the next few decades due to the significant computational resources required to perform LES of industrially relevant flows. Therefore, for the next decades, industries such as wind energy, hydroelectric energy, aerospace engineering, automotive engineering, nuclear engineering, and chemical engineering will continue to rely on RANS simulations for engineering design. However, there are numerous well-known deficiencies with RANS which are detrimental to the accuracy of these simulations. In particular, the “linear eddy viscosity hypothesis”, which is used in nearly all RANS simulations, fails to accurately predict turbulence in flows with stagnation, curvature, non-equilibrium shear, and other phenomena of engineering relevance. Previously proposed “non-linear eddy viscosity” models somewhat address these shortcomings, but are not widely used due to stability issues, lack of generalization to new flows, and the reliance on hand-tuning numerous coefficients.

Machine learning offers a way to leverage high-fidelity turbulent flow datasets (e.g, direct numerical simulation and LES), and avoid heuristically tuning closure coefficients. While various techniques for improving the accuracy of RANS simulations have been investigated, the most promising techniques target a main deficiency in RANS: the closure relationship. However, nearly all techniques have only been tested on simple flows such as channel flows, periodic hills flows, and square duct flows. Due to their data-driven nature, the applicability of these techniques for complex 3D flows of industrial relevance remains an open question.

In this work, we adapt a previously presented augmented closure framework to a complex 3D flow to demonstrate that these techniques are suitable for industrially relevant flows. We leverage a large dataset of over 20 million datapoints to augment the k-omega shear stress transport (SST) turbulence model via a series of XGBoost models. This training dataset is the largest used to-date in augmented RANS closure modelling. The augmented RANS model can generalize to new variations of flow over wall-mounted cubes, producing results that closely match the LES mean fields. These results spur further interest in applying nascent machine learning techniques to other industrial cases. Our findings enable industrial users to leverage in-house and public datasets for fast and accurate simulations of turbulent flows.

Name:	Omid Bidar
Email:	obidar1@sheffield.ac.uk
Institution:	The University of Sheffield
Co-authors and their institutions	Dr Sean Anderson, and Prof Ning Qin The University of Sheffield

Abstract

Sensor Placement for RANS-based Data Assimilation Using Eigenspace Perturbation

Sensor Placement for RANS-based Data Assimilation Using Eigenspace Perturbations

In recent years a plethora of data assimilation techniques have been introduced for improved Reynolds-averaged Navier-Stokes (RANS) turbulence modelling [1]. A number of frameworks have been shown to achieve considerable improvements using limited, experimentally measurable, data. However, most applications thus far have been primarily dictated by the availability of existing data, usually generated for benchmarking and validation. In the present study, we introduce a strategy that addresses the important task of sensor placement for generating the experimental data in the first place, specifically tailored for RANS-based data assimilation. We employ the eigenspace perturbation approach which involves systematically perturbing the eigenvalues and eigenvectors predicted by a given RANS turbulence model (e.g. k-omega SST). Specifically, six CFD simulations are run in total: one simulation with the baseline model, two simulations perturbing the eigenvectors, and three simulations perturbing the eigenvalues [2]. All six simulations result in as many flow predictions, allowing us to generate sensitivity maps–based on the variances–for various quantities of interest (QoI). Then, for a prescribed number of sensors and for a given QoI, a gradient-free optimisation problem is solved where the sum of variance over all possible sensor locations is maximised to ensure sensors are placed in regions of flow field with highest uncertainty. A regularisation term, based on maximising the distance between the sensors, is introduced to avoid excessive clustering of sensors. Potential advantages of the approach include: not requiring experimental data; in principle, informing experiment design by directly accounting for structural errors in RANS modelling which is the basis for the eigenspace perturbation method; and relatively low computational costs compared to the methods based on deep neural networks [3], or other variational approaches [4].

To investigate the effectiveness of the method, we perform data assimilation using the adjoint-based field inversion approach, with the separated flow over the 2D NASA hump as a test case. Once, the data for a given QoI has been prepared (presently using an LES dataset to emulate experimental scenarios), the field inversion process involves perturbation of the transport equation(s) for the RANS model, k-omega SST in the current study, and an optimisation solution where the goal is to minimise the error between the RANS output and the higher-fidelity data [5]. Early results based on the current method, compared to uniform and random sensor placement strategies, demonstrate significant improvements in flow reconstruction.

Name:	Taraneh Sayadi
Email:	taraneh.sayadi@sorbonne-universite.fr
Institution:	Sorbonne University, Paris France

Abstract

XGBoost-augmented RANS closure modelling of complex 3D flows

Though growing computational capabilities enable wider use of Large Eddy Simulation (LES), Reynolds-averaged Navier-Stokes (RANS) simulations remain the dominant method for simulating turbulent flows of engineering importance. This dominance is expected to continue for the next few decades due to the significant computational resources required to perform LES of industrially relevant flows. Therefore, for the next decades, industries such as wind energy, hydroelectric energy, aerospace engineering, automotive engineering, nuclear engineering, and chemical engineering will continue to rely on RANS simulations for engineering design. However, there are numerous well-known deficiencies with RANS which are detrimental to the accuracy of these simulations. In particular, the “linear eddy viscosity hypothesis”, which is used in nearly all RANS simulations, fails to accurately predict turbulence in flows with stagnation, curvature, non-equilibrium shear, and other phenomena of engineering relevance. Previously proposed “non-linear eddy viscosity” models somewhat address these shortcomings, but are not widely used due to stability issues, lack of generalization to new flows, and the reliance on hand-tuning numerous coefficients.

Machine learning offers a way to leverage high-fidelity turbulent flow datasets (e.g, direct numerical simulation and LES), and avoid heuristically tuning closure coefficients. While various techniques for improving the accuracy of RANS simulations have been investigated, the most promising techniques target a main deficiency in RANS: the closure relationship. However, nearly all techniques have only been tested on simple flows such as channel flows, periodic hills flows, and square duct flows. Due to their data-driven nature, the applicability of these techniques for complex 3D flows of industrial relevance remains an open question.

In this work, we adapt a previously presented augmented closure framework to a complex 3D flow to demonstrate that these techniques are suitable for industrially relevant flows. We leverage a large dataset of over 20 million datapoints to augment the k-omega shear stress transport (SST) turbulence model via a series of XGBoost models. This training dataset is the largest used to-date in augmented RANS closure modelling. The augmented RANS model can generalize to new variations of flow over wall-mounted cubes, producing results that closely match the LES mean fields. These results spur further interest in applying nascent machine learning techniques to other industrial cases. Our findings enable industrial users to leverage in-house and public datasets for fast and accurate simulations of turbulent flows.

Name:	Alexandros Kontogiannis
Email:	ak2239@cam.ac.uk
Institution:	University of Cambridge
Co-authors and their institutions	Matthew Juniper, University of Cambridge

Abstract

Physics-informed compressed sensing for PC-MRI: an inverse Navier--Stokes problem

We formulate a physics-informed compressed sensing (PICS) method for the reconstruction of velocity fields from noisy and sparse phase-contrast magnetic resonance signals. The method solves an inverse Navier--Stokes boundary value problem, which permits us to jointly reconstruct and segment the velocity field, and at the same time infer hidden quantities such as the hydrodynamic pressure and the wall shear stress. Using a Bayesian framework, we regularize the problem by introducing a priori information about the unknown parameters in the form of Gaussian random fields. This prior information is updated using the Navier--Stokes problem, an energy-based segmentation functional, and by requiring that the reconstruction is consistent with the k-space signals. We create an algorithm that solves this inverse problem, and test it for noisy and sparse k-space signals of the flow through a converging nozzle. We find that the method is capable of reconstructing and segmenting the velocity fields from sparsely-sampled (15% k-space coverage), low (~10) signal-to-noise ratio (SNR) signals, and that the reconstructed velocity field compares well with that derived from fully-sampled (100% k-space coverage) high (>40) SNR signals of the same flow.

Figure

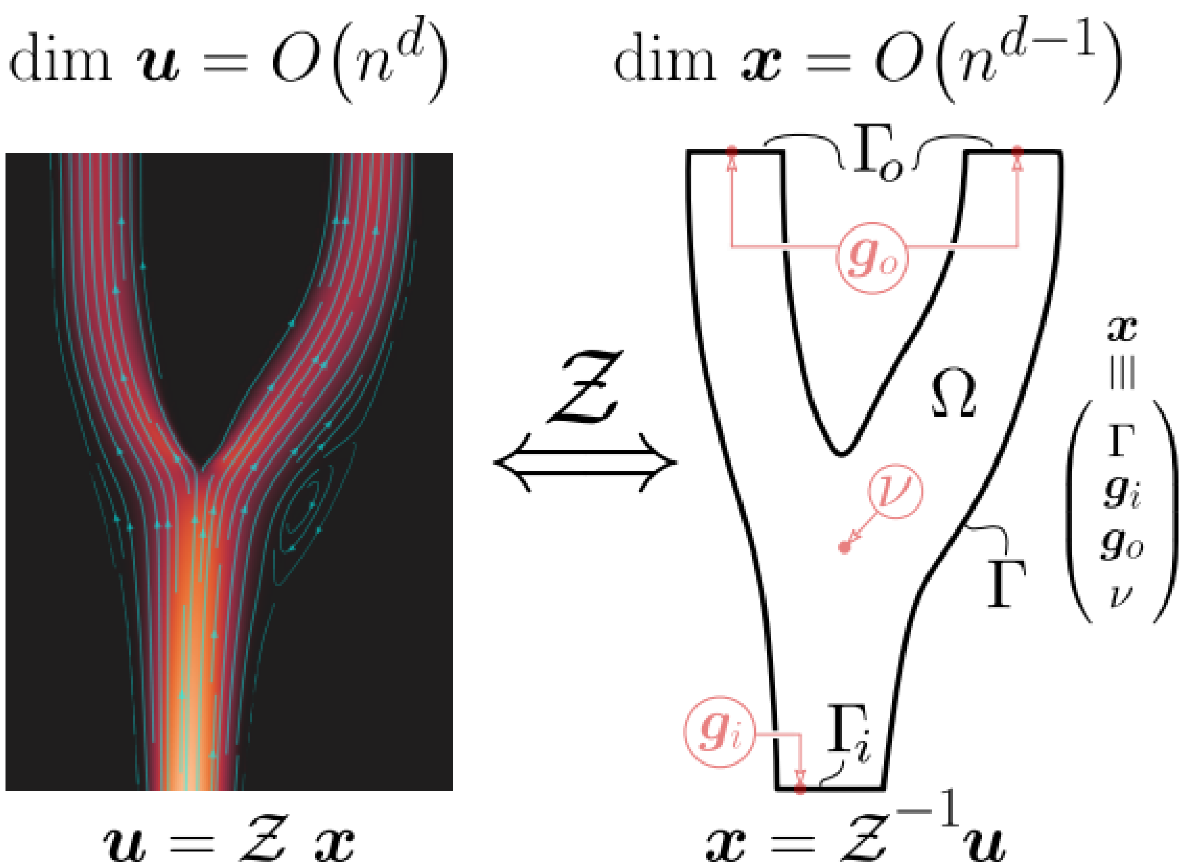


Figure: A d-dimensional velocity field (u) that can be described by a Navier--Stokes problem (Z) has an underlying (d-1)-dimensional structure ($x=Z^{-1}u$), which is the parameter vector containing the shape of the object (Γ), the boundary conditions (g_i, g_o), and the kinematic viscosity (v). Images of n^d voxels depicting the d velocity components can be compressed/decompressed by solving an inverse/forward N--S problem.

Name:	Daniel Kelshaw
Email:	djk21@ic.ac.uk
Institution:	Imperial College London
Co-authors and their institutions	Georgios Rigas, Imperial College London Luca Magri, Imperial College London & Alan Turing Institute

Abstract

Super-resolution of sparse spatial-observations of Navier-Stokes: a physics-informed convolutional neural network approach

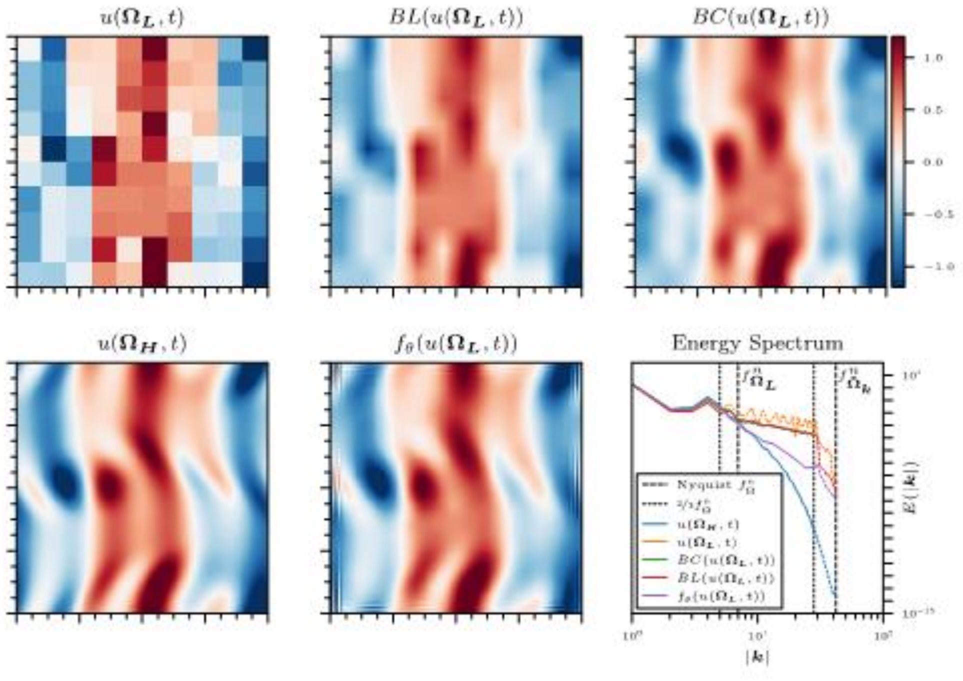
In the absence of high-resolution samples, super-resolution of sparse observations on dynamical systems is a challenging problem with wide-reaching applications in experimental settings. Access to only sparse, or partial, observations obscures the underlying dynamics and limits the scientific analysis which can be conducted. Super-resolution methods offer the means for high-fidelity state reconstruction from limited observations, a problem of fundamental importance in fluid dynamics.

Classical approaches rely on existing high-resolution samples, an assumption which does not always hold. In the absence of these ground-truth labels, a common approach is to impose prior knowledge of the physics; regularising predictions with respect to known governing equations. In this work, we introduce a physics-informed convolutional network for super-resolution of sparse observations on grids, learning to super-resolve observations by employing knowledge about the underlying dynamical system.

Results are demonstrated for the chaotic-turbulent Kolmogorov flow, increasing the resolution by fifteen times. We provide a comparison with naive interpolation methods, highlighting the ability of the method to retrieve the true high-resolution field. Analysis of the turbulent energy spectrum shows the ability to resolve finer scales of turbulence, alleviating the spectral folding which occurs as a result of sampling at low spatial frequency. By recovering finer scales of turbulence, we show that by imposing knowledge about the dynamical system a priori, it is possible to reconstruct missing physics.

This work opens opportunities for physics-informed super-resolution in experimental settings where it is infeasible to collect dense spatial measurements.

Figure



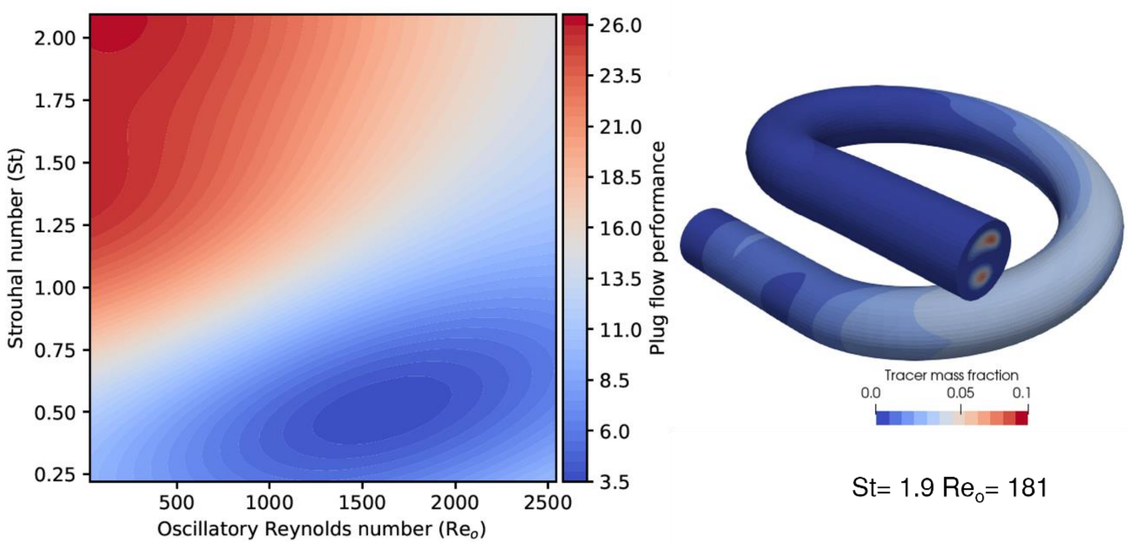
Name:	Nausheen Basha
Email:	nausheen.basha@imperial.ac.uk
Institution:	Imperial College London
Co-authors and their institutions	Thomas Savage(1), Jonathan McDonough(2),Ehecatl Antonio del Rio Chanona(1), Omar K. Matar(1) (1) Imperial College London (2) Newcastle University

Abstract

Data-driven optimisation of coiled reactors

Optimisation based on surrogate models is becoming popular for engineering problems due to its reduced computational efforts. In this research, we aim to maximise the plug flow performance of coiled reactors operating under oscillating conditions for a fixed geometry. This is done through Bayesian optimisation that uses Gaussian processes as a surrogate

model and is coupled with computational fluid dynamics (CFD) simulations in OpenFOAM through the PyFoam library. We run a transient analysis with ScalarTransportFoam solver where the tracer is injected into the water as a working fluid to obtain residence time distribution which is then fitted with the tank-in-series model to get the plug flow performance. We explore the parameter space for amplitude (1-8 mm) and frequency (2-8 Hz) for a fixed Reynolds number of 50. The optimal conditions for plug-flow performance correspond to the Strouhal number St > 1 and oscillatory Reynolds number Re_0<500. At these conditions, a pair of rotating vortices are observed that promote radial mixing and reduce axial mixing. We expect this low-cost, open-source, automated, closed-loop integrated modelling approach could be easily applied to a wide range of industrial mixing reactors to identify opportunities for performance improvement.
Figure



St= 1.9 Re_o= 181

Name:	Léo Cotteleer
Email:	leo.cotteleer@ulb.be
Institution:	Université Libre de Bruxelles, École Polytechnique de Bruxelles, Aero-Thermo-Mechanics Laboratory, Brussels, Belgium Université Libre de Bruxelles and Vrije Universiteit Brussel, Brussels Institute for Thermal-Fluid Systems and Clean Energy (BRITE), Brussels, Belgium

Co-authors and their institutions	Alessandro Parente Université Libre de Bruxelles, École Polytechnique de Bruxelles, Aero-Thermo-Mechanics Laboratory, Brussels, Belgium Université Libre de Bruxelles and Vrije Universiteit Brussel, Brussels Institute for Thermal-Fluid Systems and Clean Energy (BRITE), Brussels, Belgium

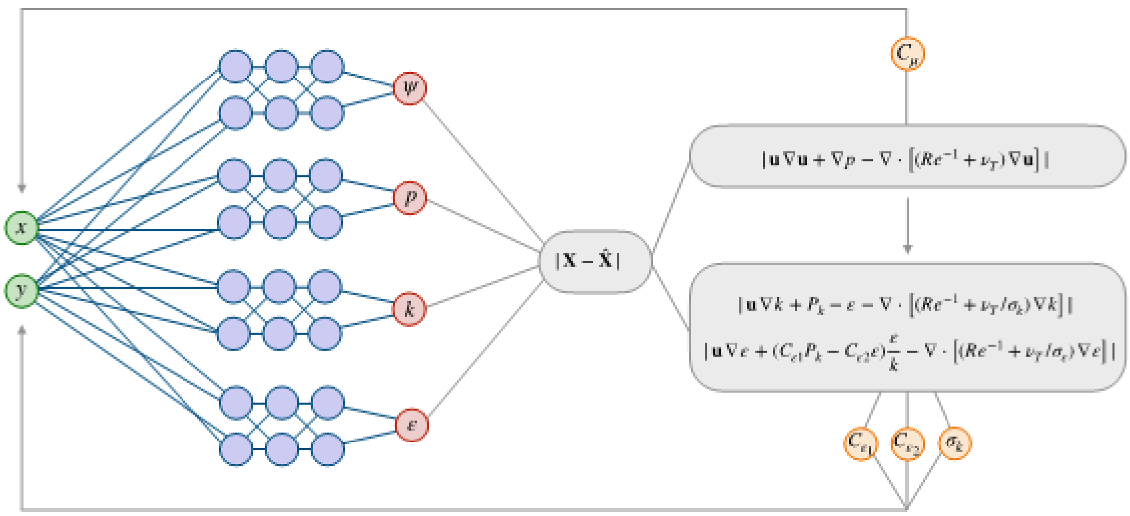
Abstract

Inversion of Turbulence Model Constants with Physics-Constrained Deep Learning:

Numerical analyses of fluid flows usually rely on the Reynolds-Averaged Navier-Stokes (RANS) equations that are solved into a discretized domain. However, due to the nonlinearity of the convective term, the averaging process yields to an unclosed set of equations. The most used turbulence model to close the RANS equations is the k-[Equation] where two additional transport equations are solved for the turbulent kinetic energy and the turbulent dissipation rate. As the model does not strictly rely on first principles, several empirical constants are introduced to calibrate the solution with respect to canonical flows. The calibration of those constants is usually case-dependent and requires numerous numerical simulations e.g. to build a surrogate model or to perform Bayesian optimization. However, the computational cost of such processes can be prohibitive for many engineering applications. Deep Learning with embedded physics has shown to be a promising tool for inverse problem in fluid dynamics. In this research, we introduce a general framework for the estimation of the k-[Equation] turbulence model constants via a physics-constrained deep learning architecture to leverage the computational cost of solving multiple times the governing equations into a discretized domain.

Firstly, and as a proof of concept, the ability of the present methodology is demonstrated through the estimation of the nominal constants of the k-[Equation] model. For that purpose, a RANS solution is used as training data and the RANS equations are embedded into the loss function of the deep neural network to guide the training process. The results show that the architecture is able to predict accurately the nominal coefficients within 4% of relative error for different test cases (e.g. Periodic Hill, Backward facing step, etc). Subsequently, high-fidelity (well-resolved LES or DNS) data are provided as training data and the results show that an optimized calibration of the constants helps to improve the predictive capabilities of low-fidelity simulations.

Figure



Name:	Jacob Page
Email:	jacob.page@ed.ac.uk
Institution:	University of Edinburgh
Abstract	

Automatic differentiation for the dynamical systems view of turbulence

In the last few decades the application of ideas from dynamical systems theory has significantly improved our understanding of transitional and weakly turbulent shear flows. The discovery of unstable periodic orbits (UPOs) embedded in turbulent attractors provides a unique insight into the underlying self-sustaining mechanisms, while there is hope that periodic orbit theory may yield a quantitative understanding of the role of various physical processes in the flow statistics. However, progress towards the latter goal has been incrementally slow due to both an inability to identify guesses for candidate UPOs and the poor performance of the Newton-Raphson methods used for convergence.

In this talk I will discuss a new approach to the UPO search based on automatic differentiation (AD) that appears to dramatically overcome the past limitations, using two-dimensional Kolmogorov flow as an example. By using a fully-differentiable flow solver and an appropriate loss function, robust guesses for UPOs with specific properties can be generated via a gradient descent algorithm, before being converged with a few iterations of standard Newton solver. I will use this approach to find hundreds of solutions at high Reynolds numbers where past methods have been ineffective. The solutions span the full range of observed turbulent dissipation rates, and a simple data-driven method can be applied to reconstruct a wide range of statistical properties from a fit to a single statistic. I

will also demonstrate how AD can be used to systematically search for more complex simple invariant solutions (homoclinic and heteroclinic orbits).

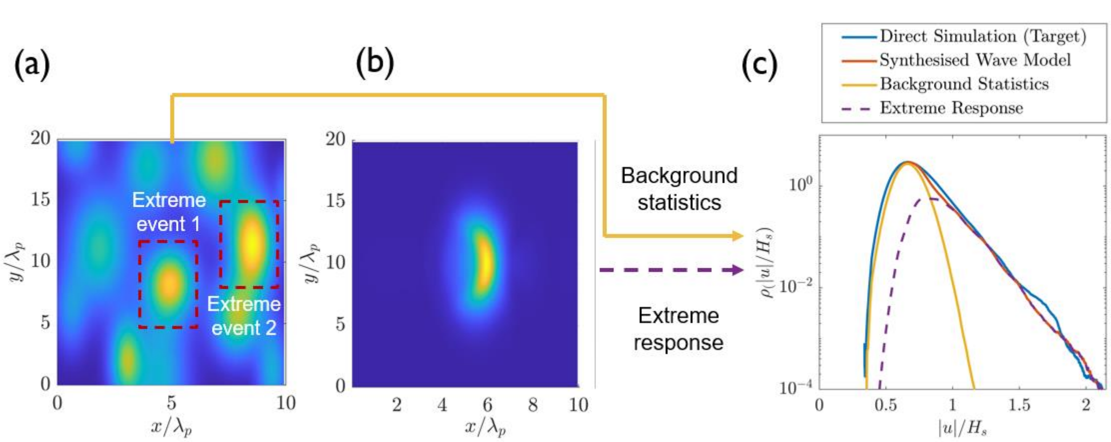
Name:	Tianning (Tim) Tang
Email:	tianning.tang@eng.ox.ac.uk
Institution:	University of Oxford
Co-authors and their institutions	Thomas Adcock University of Oxford

Abstract

A reduced order model for space-time wave statistics using probabilistic decomposition-synthesis method

We present a reduced order model for predicting space-time extreme wave statistics for directionally spread water waves. This reduced order model relies on the probabilistic decomposition-synthesis framework. In this framework, the probabilistic distribution is decomposed into a `background' region, where there are negligible nonlinear effects and a `instability' region where the nonlinear physics leads to heavy-tailed statistical behaviour. In our reduced order model, we approximate the statistics in the background region with linear simulations to reduce the computational cost. The statistics in the instability region are estimated with nonlinear simulations of focused wave groups with carefully chosen initial conditions to capture the nonlinear effects during the formation of the extreme waves. The probabilistic statistics from these two components are synthesised with analytical expressions to model the overall behaviour of weakly nonlinear waves. This reduced order wave statistical model can provide accurate predictions of nonlinear space-time wave statistics at a fraction of computational cost of direct nonlinear Monte-Carlo simulations.

Figure



Schematic diagram for the wave-current prediction model. (a): Linear undisturbed envelope field with extreme wave detected. (b): Simulation of extreme wave group with nonlinear Schrodinger equation. (c): Comparison of synthesised wave envelope distribution for undisturbed space-time wave statistics against direct numerical simulation.

Name:	Peter Nagy
Email:	peter.nagy@strath.ac.uk
Institution:	University of Strathclyde
Co-authors and their institutions	Scott Bennie, University of Strathclyde Marco Fossati, University of Strathclyde

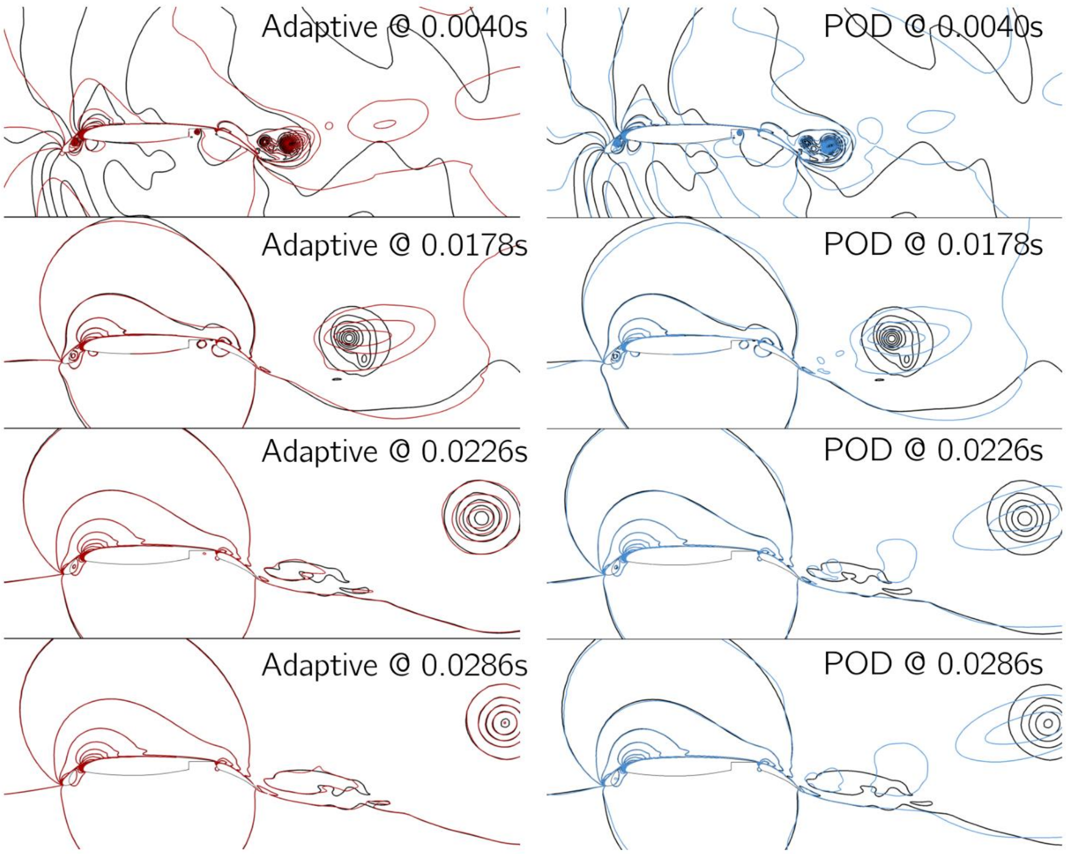
Abstract

Data-driven Adaptive Model Order Reduction Framework for Aerodynamics

Model Order Reduction (MOR) approaches have garnered continued interest in the community for their applicability to various aerodynamics problems. Through MOR, complex flow phenomena of high dimensionality can be represented in a substantially lower-dimensional space while preserving flow physics. As such MOR is well suited for reducing the computational complexity associated with the high-fidelity CFD simulation of such flows. Reduced Order Models (ROMs) can be used in the context of parameter space exploration or design and optimisation (multi-query) problems. An example is the enrichment of time dynamics for unsteady flows ROMs or the exploration of operating conditions or various geometries for steady flows. However, a limitation of various reduced order methods lies with their ability to capture and recover highly nonlinear phenomena common to the aerodynamic problems of interest; nonlinearities can be observed for example in the time evolution of unsteady flows or the presence of transonic shocks as a result of varying flight conditions. Other MOR formulations can be chosen to better cope with this circumstance, though ultimately for a given problem usually no best-in-class or globally best performing formulation can be found.

Hence, the motivation behind this work is to introduce a so-called Adaptive MOR Framework that synergistically combines a number of reduced order methods with the aim of maximising accuracy of solution reconstruction (within a pre-defined parameter space). This is achieved by adaptive selection of the locally best performing method. The selection process is driven by a user-defined error metric according to which the reconstruction (approximation) error is evaluated throughout the parameter space for all available ROMs. The framework itself is data-driven and non-intrusive: the low-dimensional models are constructed from an ensemble of correlated flow solutions and new solutions are reconstructed by coupling the ROMs to an interpolation technique. The computationally intensive aspects of the framework (namely a-priori CFD, low-dimensional model generation, and error estimation) are executed offline, thus new solutions can be

obtained fast, in the online stage. In this presentation we will focus on an overview of the adaptive framework and its applications for various unsteady and steady test cases.
Figure
Comparison of Density field reconstruction near 30P30N multi-element airfoil using Adaptive (left) vs. Single-ROM/POD (right) approach. Black contour lines are reference CFD solutions, coloured contour lines are reconstructions.



Name:	Anna Guseva
Email:	A.Guseva@leeds.ac.uk
Institution:	Department of Applied Mathematics, University of Leeds
Co-authors and their institutions	Steven Tobias, Department of Applied Mathematics, School of Mathematics, University of Leeds

Abstract

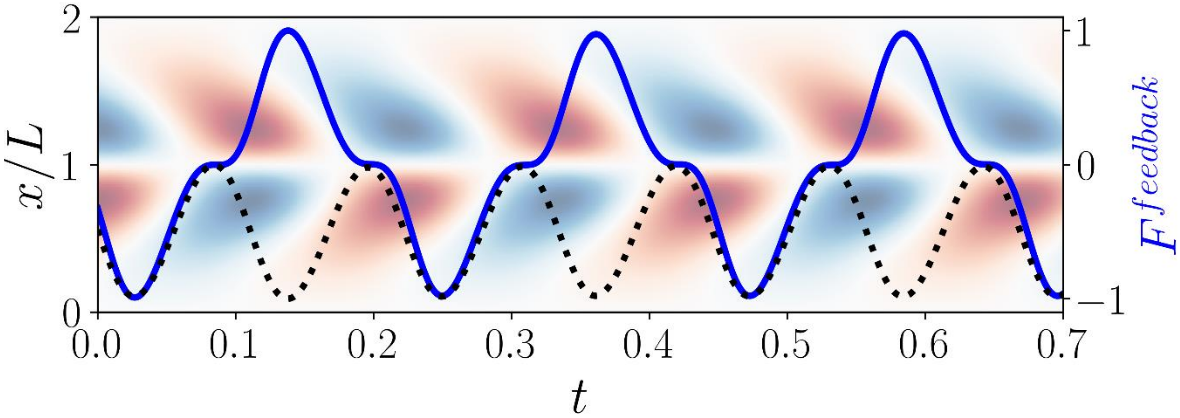
Data-driven reduced-order modelling of dynamo waves

Coherent in time and space magnetic fields of planets and stars are prominent footprints of their inner dynamical activity. They appear in a dynamo process which is supported by turbulent motions of conducting fluid inside these astrophysical objects and opposed by the Ohmic dissipation. Stellar magnetic activity frequently manifests itself through oscillating dipolar or quadrupolar magnetic fields, generated through stretching of the field by small-scale helical flows (so-called alpha-effect). These dynamos can be considered as nonlinear chaotic dynamical systems, whose saturated states depend on the nonlinear interaction between the flow and the magnetic field. A rigorous description of these saturation mechanisms is important for better understanding of long-term behaviour and variations in large-scale stellar and planetary flows.

In this work, we employ a data-driven approach to describe these nonlinearities. As a benchmark system, we use the one-dimensional dynamo model of Bushby (2003). The partial differential equations (PDE) of this system resemble dynamically more realistic three-dimensional dynamo flows: the magnetic field evolution is influenced by the flow velocity through an “induction” term, and the velocity is affected by the magnetic field through the quadratic feedback term – Lorentz force. We explore a range of dynamo numbers D, which is a parameter representing the strength of the alpha-effect in this system. We found that dipolar dynamo waves appear at $D=D_{cr}$ through a supercritical Hopf bifurcation. As the dynamo number increases, the quadrupolar mode also becomes unstable, and eventually, the magnetic field become modulated or chaotic.

Here, we use Principal Orthogonal Decomposition (POD) to extract the main dynamical components corresponding to the large-scale patterns of magnetic and velocity field. We related their temporal coefficients in a nonlinear reduced-order system of ordinary differential equations using the method of Sparse Identification of Nonlinear Dynamics (SINDy). The resulting nonlinear model is consistent with the original PDE equations of the system; in particular, its solutions saturate through velocity field without artificial damping terms. This model reproduces the Hopf bifurcation to dynamo and helps to understand which nonlinear interactions are dynamically important in this system. Finally, we construct a reduced-order model describing the interaction between the dipolar filed, the quadrupolar field and the flow velocity.

Figure



The evolution of dynamo waves, together with the temporal coefficient of the main velocity field mode (dotted line) and the feedback of velocity on the waves from the reduced-order SINDy model (solid line).

Name:	Dania Ahmed
Email:	d.ahmed18@imeprial.ac.uk
Institution:	Imperial College London
Co-authors and their institutions	Catriona Stokes, Stavroula Balabani, Vanessa Diaz and George Papadakis

Abstract

Flow reconstruction in thoracic aorta from 4D-MRI data

Patient-specific geometry of the thoracic aorta is used to investigate the potential of reconstructing the unsteady, three-dimensional blood flow from 4D-MRI plane (4-Dimensional Flow Magnetic Resonance Imaging) using a linear dynamic estimator. Rigid-wall geometry with patient-specific boundary conditions are considered for the simulation. Three-dimensional Proper Orthogonal Decomposition (POD) is used to reduce the model order based on the kinetic energy of the fluctuated flow. The flow field is approximated using the first four most energetic POD modes, which carry 98% of the total kinetic energy. The dynamic estimator is identified using a subspace system identification algorithm, N4SID, with the fluctuated streamwise velocity on the aorta arch as input (shown in figure 1) and the time coefficients of the POD modes as output. The estimator performance is validated using sensor signals from actual 4D-MRI data on the aorta arch. The reconstructed flow field is then compared to the CFD (Computational Fluid Dynamics) and 4D-MRI data at other planes. With reference to the training data from CFD, the average estimation accuracy is around 85%. It reduced to 50% when compared to the 4D-MRI flow field. These values are calculated based on the velocity field at the different planes along the thoracic aorta, part of

which are shown in figure 1. The estimation accuracy was found to strongly depend on the match between the CFD and the 4D-MRI, where higher accuracy is expected for a lower difference between the two data sets. This mismatch could be attributed to the uncertainty of the 4D-MRI, which has a limited spatiotemporal resolution compared to the CFD. With the current approximations, the estimation accuracy looks very promising. Further investigations into improving it are currently being considered. To the authors' knowledge, this represents the first study to reconstruct the blood flow using a linear dynamic estimator from planar 4D-MRI data.

References:

[1] Stokes, C., Bonfanti, M., Li, Z., Xiong, J., Chen, D., Balabani, S., & Díaz-Zuccarini, V. (2021). A novel MRI-based data fusion methodology for efficient, personalised, compliant simulations of aortic haemodynamics. Journal of Biomechanics, 129, 110793.

Figure

4D-MRI CFD Reconstructed flow

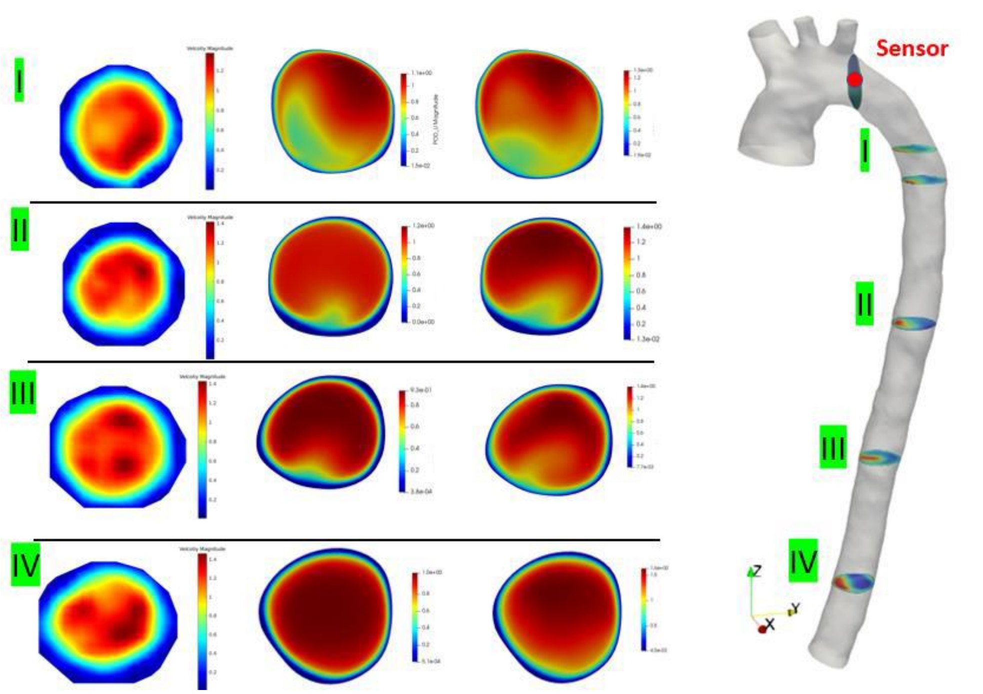


Figure 1 Schematic of the thoracic aorta and a comparison of the velocity magnitude between the 4D-MRI, CFD and the reconstructed flow on different sections (I-IV) along the descending aorta.

Name:	Georgios Rigas
Email:	g.rigas@imperial.ac.uk
Institution:	Imperial College London
Abstract	

Data-enabled flow control

Model-free Reinforcement Learning (RL) algorithms have been employed recently to discover flow control strategies using data obtained from direct intraction with the flow system (i.e. simulation environment). In case of bluff bodies, for example, efficient drag reduction has been successfully demonstrated by suppressing vortex shedding at laminar regimes using probes located in the flow downstream of the body to achieve full-state observability and control. In the present study, we consider partial measuremnts, due to sensor limitations in practical applications, i.e. by restricting sensing to pressure probes mounted on the base of a bluff body. The performance of the RL under partial observability is significatly degraded, limiting drag reduction by 65% compared to probes optimally located downstream of the body. A method integrating memory into the control architecture is proposed to improve performance in partially observable systems. By augmenting the input to the controller (neural network) with a time series of lagged observations, the dynamic controllers discovered using RL completely stabilise the vortex shedding using only surface mounted sensors. Finally, the hardware implementation of RL algorithms in turbulent flows will be discussed for reducing the drag of fully turbulent wakes by real-time interaction with the wind tunnel setup, at regimes that are intractable using simulations. These results are a first step towards realistic implementation of reinforcement learning of partially observable and intractable flows.

Name:	Mohammad Jadidi
Email:	Mohammad.jadidi@manchester.ac.uk
Institution:	The University of Manchester
Co-authors and their institutions	Marta Camps Santasmasas, Ximeng Kang, Xutong Zhang, Saleh Rezaeiravesh, Alistair Revell. Department of Mechanical, Aerospace and Civil Engineering, The University of Manchester, UK.
Abstract	

Towards a framework for prediction, UQ and data analysis of urban wind flows

Computational Fluid Dynamics (CFD) is widely used as a tool to model urban wind flow for a variety of applications including pedestrian comfort, pollutant dispersion and wind energy. However, despite employing various modelling approximations, predicting wind patterns in

urban environments in real-time remains challenging due to the limited computational resources and the potential uncertainties due to both physical and numerical parameters. The present study reports our recent progress on developing a data analytic framework based on wind flow simulations in a part of the city of Manchester, UK. CFD simulations are performed for selected values of the uncertain parameters; their results are used as input to generate a surrogate model which is significantly less computationally expensive than CFD and can predict the flow field over the space of the uncertain parameters as well as the physical space. The uncertain parameters include the wind velocity magnitude and direction over the boundaries of the simulation domain. The surrogates are constructed by Gaussian Process Regression (GPR) which naturally predicts the uncertainty in the data and estimates confidence intervals for the predictions. The UQ (Uncertainty Quantification) forward problem and global sensitivity analysis are performed using non-intrusive generalized polynomial chaos expansion (gPCE) and analysis of variances (ANOVA), respectively. Blending these techniques with the GPR, the effects of combined uncertainties from the data and parameters/inputs can be studied. The integrated data analytics framework based on the combination of the CFD simulations, surrogate modelling and UQ analyses is being optimized to make accurate real-time predictions and analyses possible. The turbulent flow simulations are performed using RANS (Reynolds-averaged Navier-Stokes) approach in OpenFOAM. A workflow is designed to create a computational mesh for the imported topology of urban areas, set initial and boundary data, perform simulations on high-performance computing resources, extract the resulting flow fields, create the surrogate, and perform UQ analyses for wind direction and reference velocity magnitude. The inflow boundary conditions represent a fully developed neutral surface layer, which is specified using a logarithmic profile for velocity, a constant turbulence kinetic energy, and a profile for the turbulent dissipation rate. As the next development stage, large eddy simulations (LES) and hybrid RANS-LES will be performed which together with the RANS data can be used for constructing efficient multi-fidelity predictive models for urban flows.
Figure

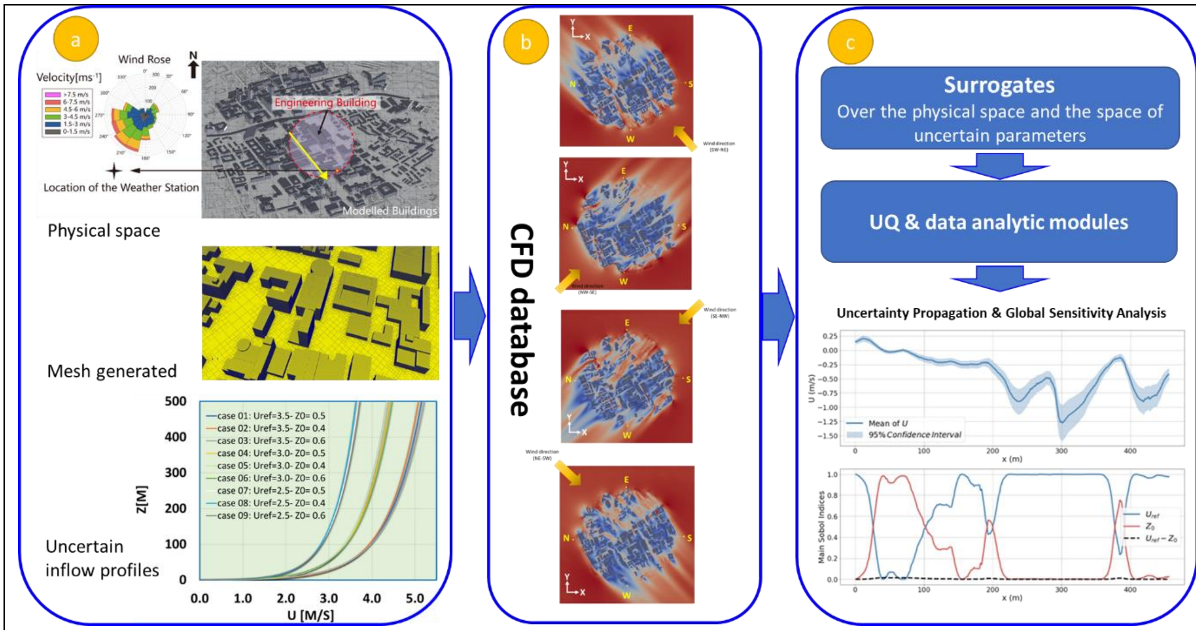


Figure 1. Summary of the workflow; from left to right: (**a**) The CAD geometry of the urban region, (**b**) CFD simulations to create training data for constructing surrogate models for prediction, and (**c**) UQ, and other data analytic approaches.

Name:	Ira Shokar
Email:	ira.shokar@maths.cam.ac.uk
Institution:	DAMTP, University of Cambridge
Co-authors and their institutions	Peter Haynes, Rich Kerswell, both DAMTP, University of Cambridge
Abstract	

Presentation Title: Learning Stochastic Dynamics with Neural Networks to study Zonal Jets

Machine Learning has emerged as a powerful tool for identifying patterns in datasets and increasingly has been applied to the field of fluid dynamics to either provide insight into or to attempt to model fluid flows. We look to provide both by using deep neural networks to provide a reduced-order model of the Beta-Plane approximation - a barotropic,

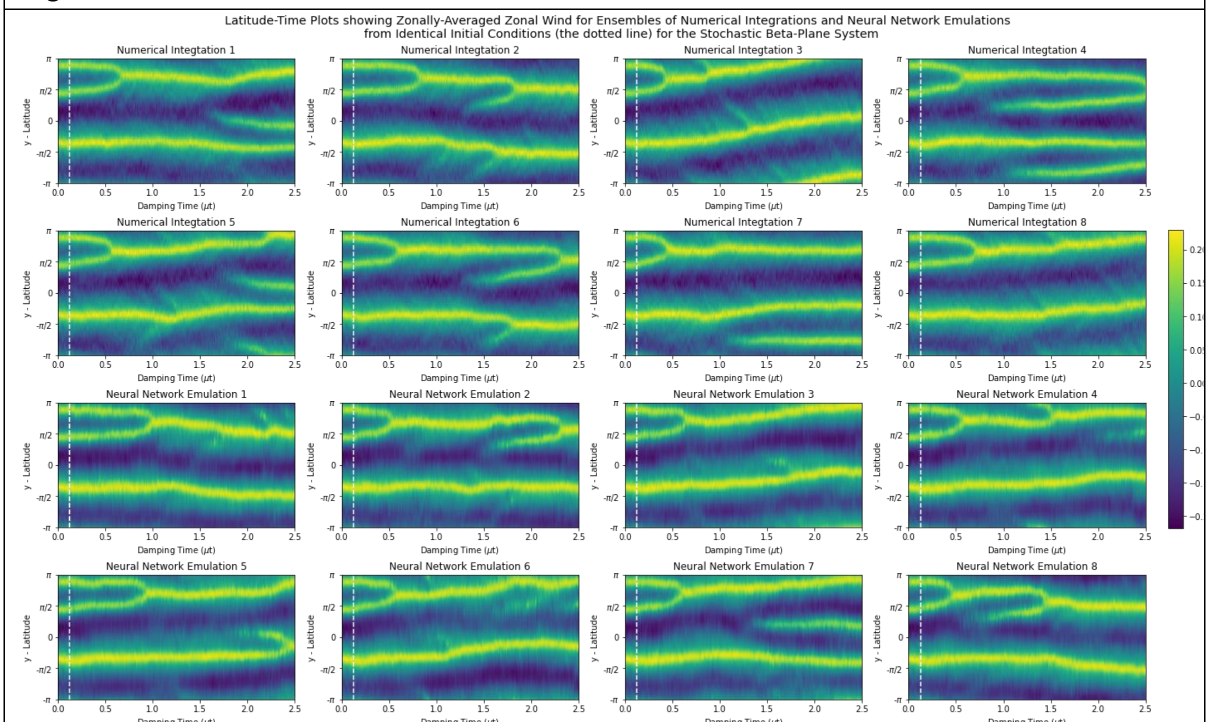
stochastically forced turbulent flow on a beta-plane - that provides an analogue for tropospheric mid-latitudinal dynamics, describing European weather.

The system lies on a 2D plane, with the lack of baroclinicity due to the absence of stratification resulting in the requirement for small-scale eddies, that generate turbulence, to be parameterised by a stochastic forcing. The idealised model allows us to study the formation of zonal jets and their variability, with the formulation of a reduced-order model providing insight into the underlying dynamical mechanisms.

We utilise methods in manifold learning and adversarial training to learn the system dynamics using a stochastic neural network - accounting for the nature of the underlying system. The model is able to produce an emulation of the system, 4 orders of magnitude faster than numerical integration from a physics-based model.

As the underlying system is non-deterministic, model verification is evaluated between an ensemble of predictions from the deep learning model, obtained by sampling in the latent space of the model, and an ensemble of numerical integrations with different realisations of noise - with information gained from both the size of the neural network's latent space as well as the information within it, enabling for the exploration of this newly defined state-space, yielding insight into the dynamics of the system.

Figure



Name:	Fergus Shone
Email:	Mm16f2s@leeds.ac.uk
Institution:	University of Leeds
Co-authors and their institutions	Erica Dall'Armellina2, Alejandro Frangi3,4, Zeike Taylor3,4, Peter Jimack1,4 1CDT Fluid Dynamics, University of Leeds, 2LICAMM, University of Leeds, 3CISTIB, University of Leeds, 4School of Computing, University of Leeds

Abstract

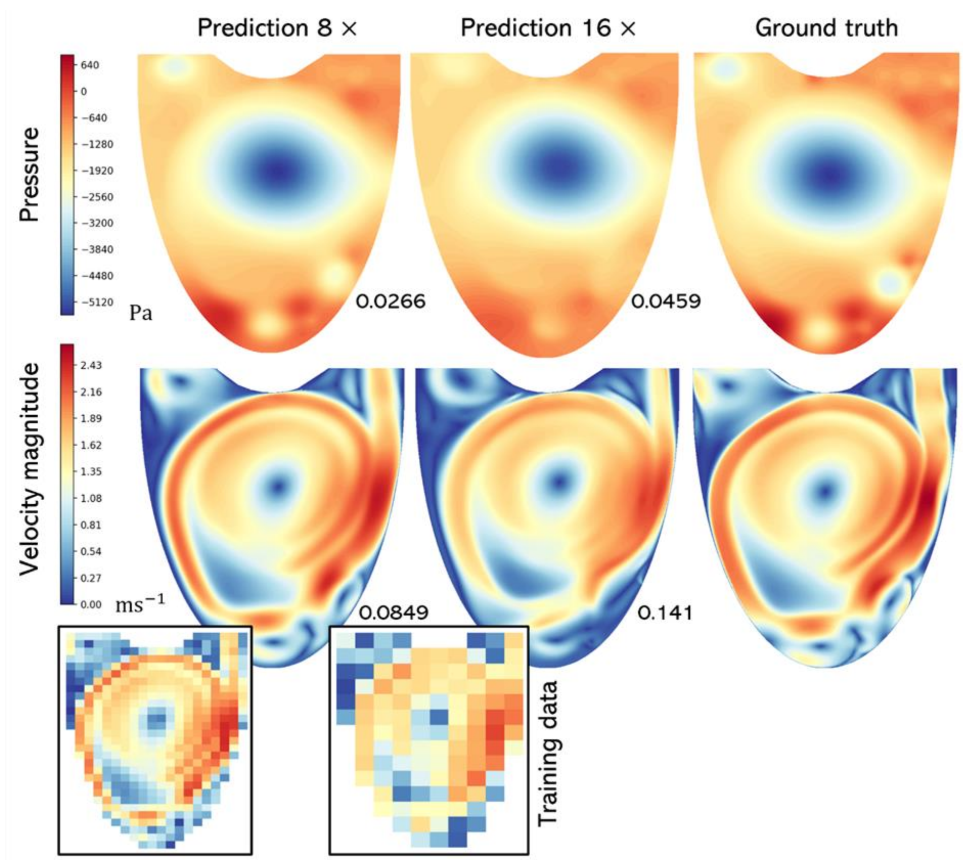
A physics-informed machine learning approach to super-resolution of 4D-flow MRI in the left ventricle

As is well-established in the vasculature, it is hypothesised that haemodynamic flow abnormalities within the heart chambers can provide insights into how and why particular pathologies evolve. 4D-flow magnetic resonance imaging (MRI), which provides non-invasive blood flow reconstructions in the cardiovascular system, has the potential to be a key tool such research. However, to realise it's potential, there are certain issues associated with the modality that must be addressed. Low spatio-temporal resolution and significant noise artifacts are present, reducing the quality of the acquired velocity field. Moreover, clinically relevant derived quantities like pressure, vorticity and wall shear stresses are not directly measured, and thus highly susceptible to effects of corruption in the data. Therefore, the effectiveness of the modality to establish links between flow abnormalities and pathologies is limited, and recent efforts have been made to super-resolve and denoise 4D-flow MRI data to improve the accuracy of predictive haemodynamic quantities.

We propose a physics-informed super-resolution approach to address the aforementioned shortcomings associated with 4D-flow MRI data, presenting the first application of this approach to super-resolve flow data in both the left ventricle and moving domains in general. Weak regularisation of the model is performed using the Navier-Stokes equations and the no-slip condition on the endocardium, which not only constrains model predictions to accurately super-resolve the velocity field, but also uncovers the underlying pressure field without the use of pressure data or boundary conditions.

We demonstrate the feasibility of our model through two computational fluid dynamics (CFD)-generated cases, namely a 2D idealised ventricle and a computed tomography-acquired, patient-specific left ventricle. For each case, we generate multiple synthetic 4D-flow data sets from our CFD results at various downsampling rates and noise levels, establishing the effective range of the model with regard to data degradation. We show robustness to both effects, achieving normalised velocity RMSE values of under 16% at extreme spatial and temporal upsampling rates of 16x and 10x respectively, using a signal-to-noise ratio of 7.

Figure



Name:	Paola Cinnella
Email:	paola.cinnella@sorbonne-universite.fr
Institution:	Sorbonne University, Paris France
Abstract	
Turbulence modeling: artificial vs human intelligence Reynolds-averaged Navier-Stokes (RANS) models of turbulent flow remain the cornerstone of flow analysis and design in fluids engineering, despite several inherent limitations that prevent them from capturing the correct physics of flows even in simple configurations. Instead, these models are developed and tuned to match certain quantities	

of interest to the engineer while providing reasonable performance over a wide range of flow situations.
On the other hand, the increased availability of high-fidelity data from both advanced numerical simulations and flow experiments has fostered the development of a multitude of “data-driven” turbulence model based on data-assimilation, Bayesian calibration, as well as machine learning techniques. Although these models can provide significantly better results over classical models for the narrow class of flows for which they are trained, their generalization capabilities remain far inferior to those of classical models, while the computational cost of model training and validation is significant.
In this talk I will first review the qualities and drawbacks of RANS model derived from human or artificial intelligence. Then I will present a methodology for developing data-driven models with improved generalization capabilities while delivering estimates of the predictive uncertainty. I will conclude with an outlook on future research avenues for the development of industry-ready data-driven models.

Name:	Defne Ege Ozan
Email:	d.ozan@imperial.ac.uk
Institution:	Imperial College London
Co-authors and their institutions	Luca Magri Imperial College London, The Alan Turing Institute, Technion

Abstract

Hard-constrained thermoacoustic neural networks

In thermoacoustic systems, if the heat release is sufficiently in phase with the pressure, self-excited oscillations with finite amplitudes can occur. Thermoacoustic oscillations can have detrimental consequences for gas turbines and rocket engines. Typical nonlinear regimes are limit cycles, quasiperiodic and chaotic oscillations. We develop physics-aware feedforward neural networks that learn thermoacoustic oscillations from data with a focus on limit cycles, which are characterised by periodic orbits in the phase space. In addition to a data-driven loss, a physical residual penalises solutions that violate the conservation of momentum and energy as a soft constraint. Further, we explore hard constraints in time and space domains. We impose periodicity by periodic activation functions and a trainable angular frequency. We employ acoustic eigenfunctions as spatial modes, while a jump discontinuity in velocity at the flame is captured by discontinuous modes. We test the algorithm on synthetic data generated from a time-delayed model of a Rijke tube and a higher-fidelity model with a kinematic flame. We find that (i) physics constraints significantly improve the predictions from noisy or sparse data, (ii) periodic activations outperform conventional activations in terms of extrapolation capability, and (iii) boundary conditions and discontinuities can be hard-coded with a-priori selected spatial modes. This work opens up possibilities for the prediction of nonlinear thermoacoustics by combining physical knowledge and data.

Name:	Matthew Yoko
Email:	mjy29@cam.ac.uk
Institution:	Cambridge University
Co-authors and their institutions	Matthew Juniper, Cambridge University

Abstract

Data assimilation in thermoacoustics: generating a quantitatively-accurate model of an electrically-heated Rijke tube.

We perform 7000 experiments at 175 stable operating points on an electrically-heated Rijke tube. We pulse the flow and measure the acoustic response with eight probe microphones distributed along its length. We assimilate the experimental data with Bayesian inference by specifying candidate models and calculating their optimal parameters given prior assumptions and the data. We model the long timescale behaviour with a 1D pipe flow model driven by natural convection into which we assimilate data with an Ensemble Kalman filter. We model the short timescale behaviour with several 1D thermoacoustic network models and assimilate data by minimizing the negative log posterior likelihood of the parameters of each model, given the data. For each candidate model we calculate the uncertainties in its parameters and calculate its marginal likelihood (i.e. the evidence for that model given the data) using Laplace's method combined with first and second order adjoint methods. We rank each model by its marginal likelihood and select the best model for each component of the system. We show that this process generates a model that is physically-interpretable, as small as possible, and quantitatively accurate across the entire operating regime. We show that, once the model has been selected, it can be trained on little data and can extrapolate successfully beyond the training set.

Name:	Mario Lino
Email:	mal1218@ic.ac.uk
Institution:	Department of Aeronautics, Imperial College London

<table>
<tr><td>Co-authors and their institutions</td><td>Stathi Fotiadis2, Anil A. Bharath2 and Chris Cantwell1
1. Department of Aeronautics, Imperial College London
2. Department of Bioengineering, Imperial College London</td></tr>
<tr><td colspan="2">Abstract</td></tr>
<tr><td colspan="2">Multi-scale rotation-equivariant graph neural networks for unsteady Eulerian fluid dynamics

Multi-scale rotation-equivariant graph neural networks for unsteady Eulerian fluid dynamics
The simulation of fluid dynamics, typically by numerically solving partial differential equations, is an essential tool in many areas of science and engineering. However, the high computational cost can limit application in practice and may prohibit exploring large parameter spaces. Recent deep-learning approaches have demonstrated the potential to yield surrogate models for the simulation of fluid dynamics. While such models exhibit lower accuracy in comparison, their low runtime makes them appealing for design-space exploration. We introduce two novel graph neural network (GNN) models, multi-scale (MuS)-GNN and rotation-equivariant (RE)MuS-GNN, for inferring the time evolution of the fluid flow on a fluid domain discretised into an unstructured set of nodes. In both models, the previous state is processed through multiple coarsenings of the graph, which enables faster information propagation through the network and improves the capture and forecast of the system state, particularly in problems encompassing phenomena spanning a range of length scales. Additionally, REMuS-GNN is architecturally equivariant to rotations, which allows the network to learn the underlying physics more efficiently, leading to improved accuracy and generalisation. We analyse these models using two canonical fluid models: advection and incompressible flow around an elliptical cylinder. Our results show that the proposed GNN models can generalise from uniform advection fields to high-gradient fields on complex domains. The multi-scale graph architecture allows for inference of incompressible Navier-Stokes solutions, within a range of Reynolds numbers and design parameters, more effectively than a baseline single-scale GNN. Simulations obtained with MuS-GNN and REMuS-GNN are between two and four orders of magnitude faster than the numerical solutions on which they were trained.</td></tr>
<tr><td colspan="2">Figure</td></tr>
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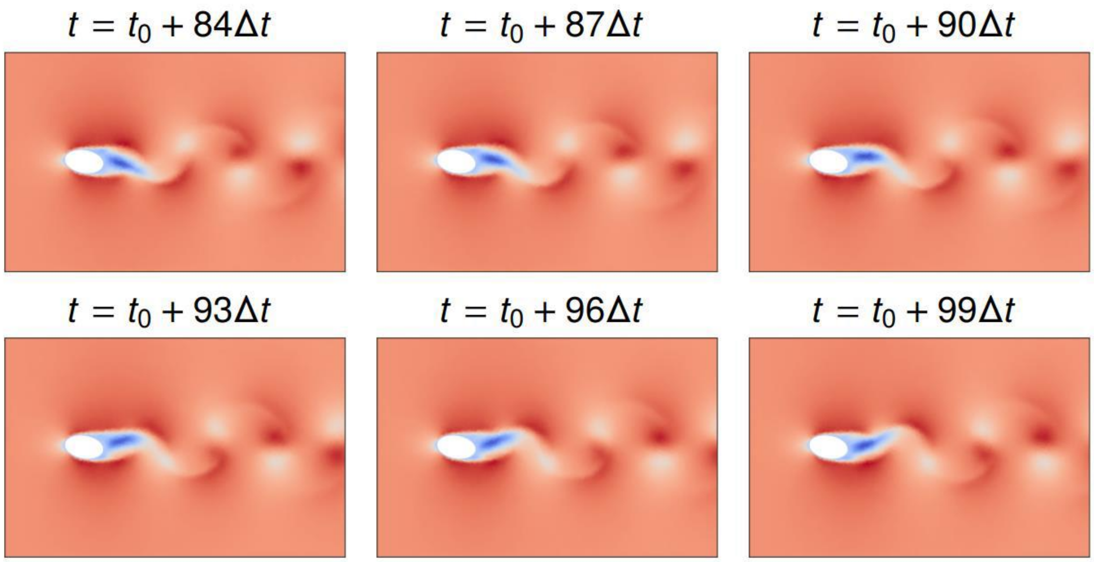

Poster Abstracts

Name:	Alasdair Roy
Email:	Scatr@leeds.ac.uk
Institution:	University of Leeds, CDT for Fluid Dynamics
Co-authors and their institutions	Prof. Steven Tobias: University of Leeds, School of Maths Prof. Christopher Jones: University of Leeds, School of Maths Prof. Phil Livermore: University of Leeds, School of Earth and Environment Dr. Wayne Arter: Culham Centre for Fusion Energy Dr. Stanislas Pamela: Culham Centre for Fusion Energy

Abstract

Reduced-Order Models for Magnetoconvection in 2D

Direct numerical simulation of full state equations can be computationally intensive and result in high dimensional datasets. While the numerical data is high-dimensional, the flows themselves can exhibit much lower dimensional behaviour. This has led to an interest in finding reduced order models for such systems.

Derivation of a reduced-order model typically relies on knowledge of the underlying equations, in which the analytic modes are projected back on the governing equations. While this encodes the appropriate physics of the system, the governing equations are not always known making this method intrusive. Recently, data-driven model discovery techniques have been shown to be able to find reduced-order models purely from measurements of the system, automating this process. Data driven methods have the advantages that an optimal set of modes can be used to describe the data through proper orthogonal decomposition. The time series of these modes projected on the measurements can then be used to generate a reduced order model via the sparse identification of nonlinear dynamics [1].

We apply this method to 2D magnetoconvection, where traditional convection can be inhibited by the presence of a magnetic field. These convective processes are important, for instance, at the surface of stars. It was shown that the governing equations for magnetoconvection admit weakly nonlinear solutions given by a system of 5 ODEs [2]. These are instructive as they can predict features such as whether convection first sets in as a direct instability or overstability. Stability criteria can then be determined with much greater ease than by simulation of the full PDE system. However, these equations are only valid near the onset of instability, when the velocities are small.

Data-driven methods provide a new avenue to find reduced order models in magnetoconvection, further from the onset of instability. We first apply these methods to understand if recovery of the analytic solutions near fixed points is possible, before looking for reduced order models further from onset in regimes with aperiodic motion. By comparison with the solutions of the full PDEs, we assess the utility of the reduced models both for prediction and for reproducing the statistics of the full system; we further test how well a model derived for a certain set of parameters reproduces the dynamics for parameter sets for which no direct data is available.

[1] E. Knobloch, N. O. Weiss, and L. N. Da Costa. Oscillatory and steady convection in a magnetic field. Journal of Fluid Mechanics, 113:153–186, 1981.

[2] Steven L. Brunton, Joshua L. Proctor, and J. Nathan Kutz. Discovering governing equations from data by sparse identification of nonlinear dynamical systems. Proceedings of the National Academy of Sciences, 113(15):3932–3937, 2016.

Figure

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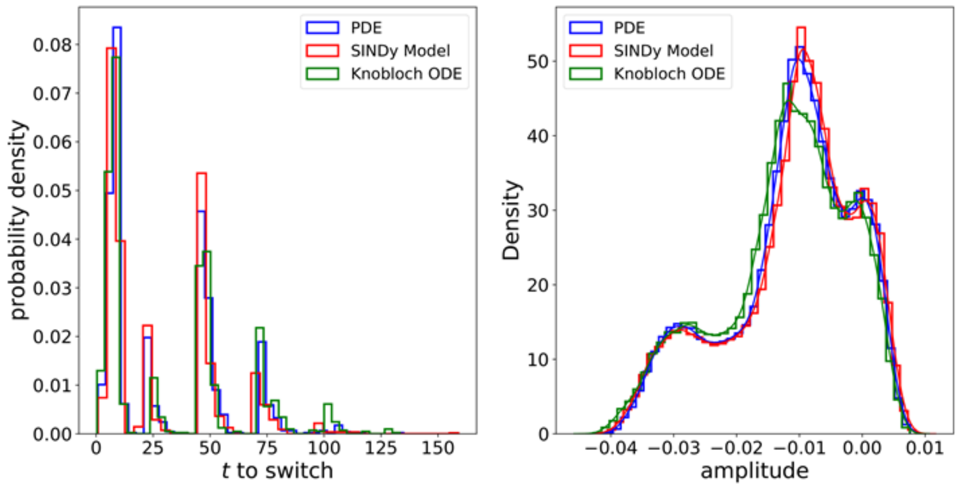


Name:	Alessandro Giannotta
Email:	ag2274@cam.ac.uk
Institution:	Polytechnic of Bari, University of Cambridge
Co-authors and their institutions	Matthew Yoko, University of Cambridge Matthew Juniper, University of Cambridge Stefania Cherubini, Polytechnic of Bari Pietro De Palma, Polytechnic of Bari

Abstract

Assimilating physics-based flame models from flame images

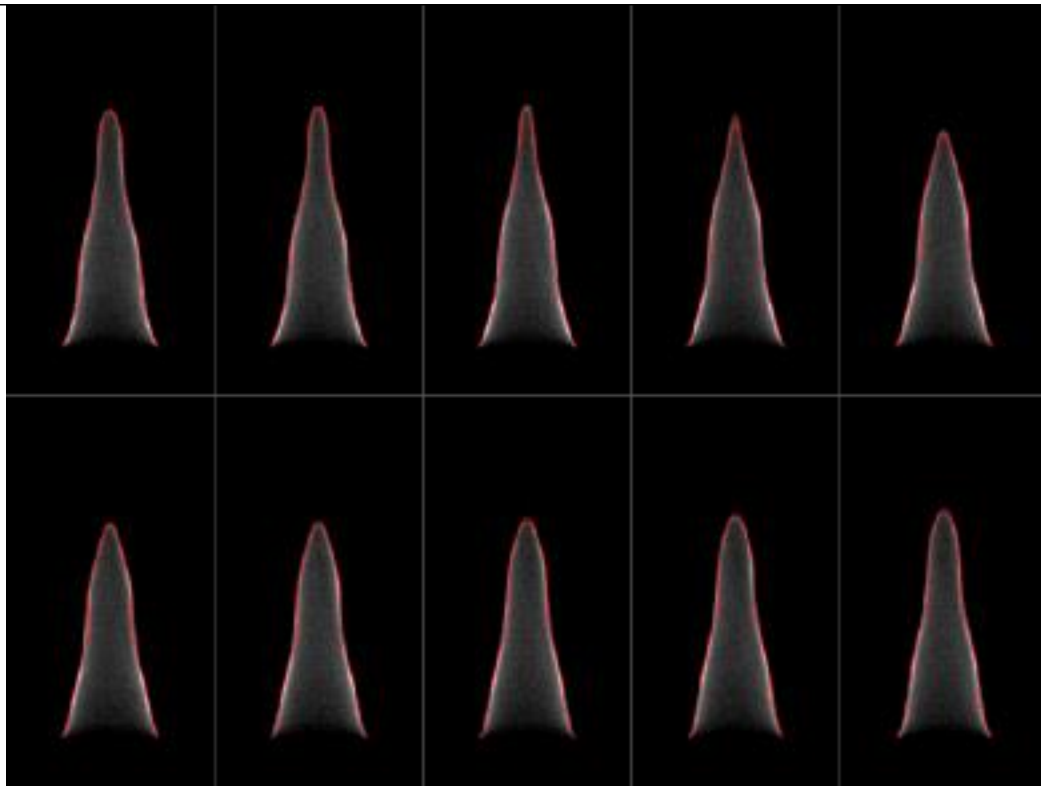
We perform experiments with an acoustically forced laminar premixed bunsen flame and assimilate experimental data into a physics-based premixed flame model.
The experimental rig is a ducted Bunsen flame supplied by a mixture of methane and ethylene. Flames produced by a wide range of equivalence ratios and mass flow rates are studied. These cover both stable and unstable operating conditions. In the stable regime, the flame is harmonically forced by a loudspeaker and the forced response is recorded. In the unstable regime, the flame is initially stabilised using active control. When the active control is switched off, the self-excited oscillations are recorded. A high-speed camera is used to capture the dynamics of the perturbed flames, as well as snapshots of the stable flame shape.

For the model, we assume that the flame thickness is much shorter than the hydrodynamic length. The flame is then approximated by an axisymmetric surface dividing the reactants by the products. Each point of the surface is in kinematic equilibrium between the local flame speed and the reactants velocity field. The flame speed is dependent on the flame stretch with the Markstein length. We assume that the velocity field can be expressed by the sum of a steady flow and an unsteady perturbation. A shape parameter linearly determines the velocity profile of the steady flow such that when it is set to zero the flow corresponds to a uniform flow, and when it is set to one the flow corresponds to a Poiseuille flow. The perturbation is assumed to be generated by the harmonic acoustic forcing and takes the form of a wave originating at the burner rim and traveling in the longitudinal direction with constant phase speed.

We tune the model parameters by minimising the Euclidean distance between the flame-front positions predicted by the model and the ones captured by the experimental snapshots, during a limit cycle. This process is accelerated by adjoint methods which give the sensitivity of the flame-front position predicted by the model with respect to the model parameters. Adjoint methods are also used to find a periodic solution of the model equations for each set of parameters.

This study is preliminary to the generation of a physics-based quantitatively accurate model of a flame-driven Rijke tube with Bayesian inference, in which the model parameters are assimilated with their uncertainties using Laplace's method combined with first and second-order adjoint methods.

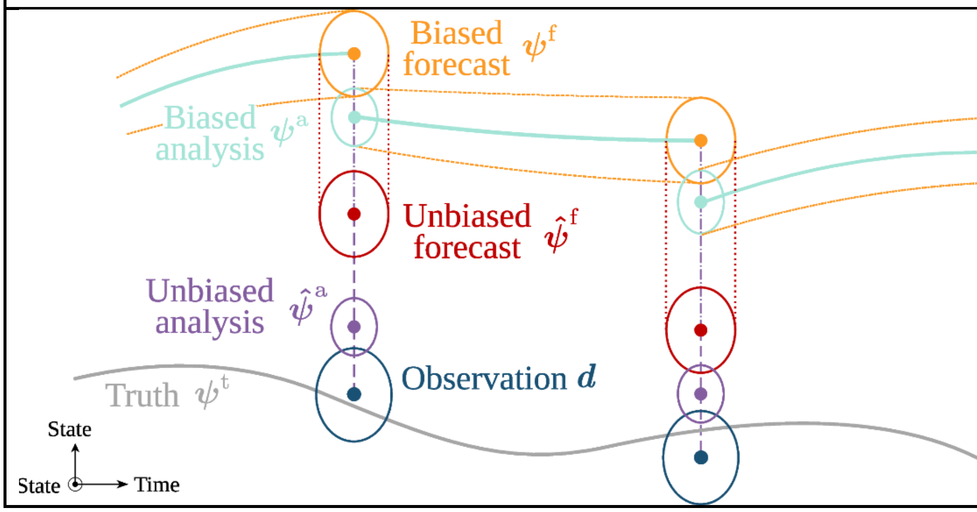
Figure



Name:	Andrea Nóvoa
Email:	an553@cam.ac.uk
Institution:	University of Cambridge
Co-authors and their institutions	Alberto Racca (University of Cambridge) Luca Magri (University of Cambridge, Imperial College, Alan Turing Institute)
Abstract	
Real-time bias-aware data assimilation with echo state networks Low-order models provide qualitative-accurate estimates at low computational cost. However, they only capture the dominant physical mechanisms of the quantity of interest, in statistical terminology: low-order models are biased. Real-time data assimilation are Bayesian inference methods that optimally combine reference data (from experiments or high-order models) with knowledge given by a numerical model. This real-time update improves the quantitative accuracy of the model estimate, bypassing the need for data storage and postprocessing. Nevertheless, these methods assume that there is no systematic error in the model. We propose a bias-aware data assimilation framework where	

we prescribe the model bias with an echo state network, which is a form of reservoir computing. This enables the application of real-time data assimilation to low-order models which simultaneously infers the physical state, as well as the key parameters, and the bias of a low-order model. The echo state network is trained a priori and then runs in parallel to an ensemble data assimilation algorithm. Every time that reference data becomes available, we (1) perform a Bayesian update on the model state and parameters, and (2) re-initialise the echo state network with a new estimate of the model bias. We test this method on a low-order thermoacoustic model, using synthetic reference data from a higher-order model. Results show that, with a short training time, the echo state network is able to self-adapt and learn the hidden dynamics of unseeing bias data of the low-order model. This work opens new possibilities for uncertainty quantification in real-time applications.

Figure

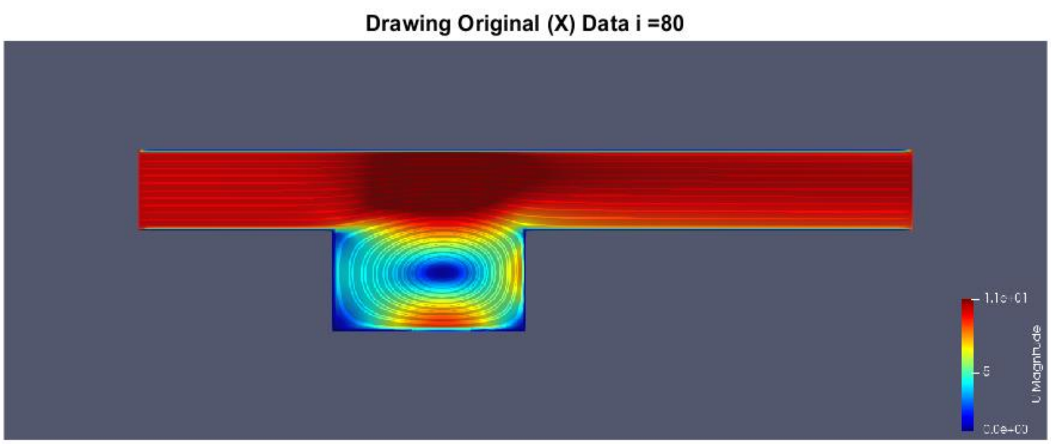


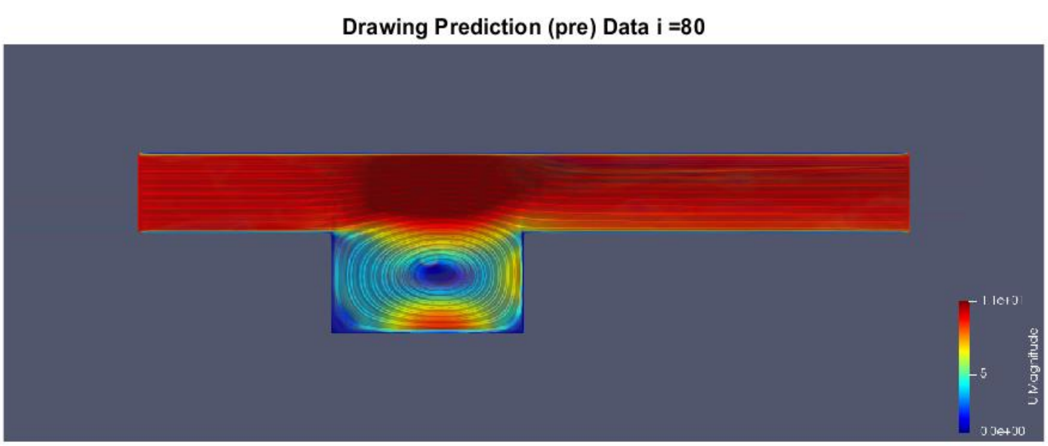
Name:	Dr. Gamze YUKSEL
Email:	G.Yuksel@leeds.ac.uk
Institution:	Mugla Sitki Kocman Univ. Faculty of Science Department of Mathematics Visiting Researcher at Univ of Leeds School of Mathematics
Co-authors and their institutions	M. Hicret YAMAN Mugla Sitki Kocman Univ. Graduate School of Naturel and Applied Sciences Department of Mathematics

Abstract

Dynamic Mode Decomposition for Channel Flow with Cavity Fluid Flows

Dynamic Mode Decomposition (DMD) is a powerful technique in Fluid Mechanics that can extract fundamental information from snapshots of the fluid flows. Dynamic Mode Decomposition algorithm reveals the Spatio-temporal coherent structures of the model by using only the data, without the governing equations so DMD is a fully data-driven technique. The aim of this study is to diagnose the flow characteristic of the model and reconstruct the flow by revealing the pattern found in the flow by using DMD. DMD is applied to a fluid flow model called “Channel Flow with Cavity Flow’’ obtained by the flow Channel flow over a square cavity, and the turbulent flow field is investigated. The data obtained by OpenFoam solutions of this flow and reconstructed by DMD are in the Figure. In this Figure, the above illustration is obtained by OpenFoam and the below is obtained by DMD for iteration number i=80.
Figure





Name:	Dr Calum S. Skene
Email:	c.s.skene@leeds.ac.uk
Institution:	University of Leeds
Co-authors and their institutions	Prof Steve M. Tobias – University of Leeds

Abstract

Simulating zonal flows using Markov neural operators

Many astrophysical and geophysical systems of interest take place in a parameter regime that is beyond the scope of direct numerical simulation (DNS). Furthermore, even when DNS is accessible the fact that these systems often contain multiple temporal and spatial scales renders them stiff, meaning they require substantial computational resources. However, despite needing a fine resolution in order to obtain an accurate solution many flow features of interest, such as large scale zonal flows, occur on a much larger scale than the fluctuations that produce them. Hence, there is a possibility that reduced order models which aim to capture these large scale features could help in efficiently modelling these flows, and ultimately in extrapolating them to regimes that are currently inaccessible.

In this poster we explore one such possibility for modelling these flows based on a machine learning framework. Namely the Markov neural operator (MNO) proposed by Z. Li et al. (Learning Dissipative Dynamics in Chaotic Systems, NeurIPS 2022), which has been shown to accurately capture the statistics of chaotic flows including Kolmogorov flow. We consider learning a MNO for the Busse annulus, a model for rotating convection that is capable of giving rise to large scale zonal jets. Despite its simplicity, the Busse annulus exhibits complex phenomena such as the formation of multiple jets and bursting, making it an ideal system in which to assess the suitability of using an MNO for predicting zonal flows. Special attention is given to two main questions. Firstly, can the MNO approach predict the large scale statistics of zonal flows when the step size is larger than that of the underlying DNS? Secondly, does the MNO accurately predict the dynamics of different phenomena such as bursting?

Figure

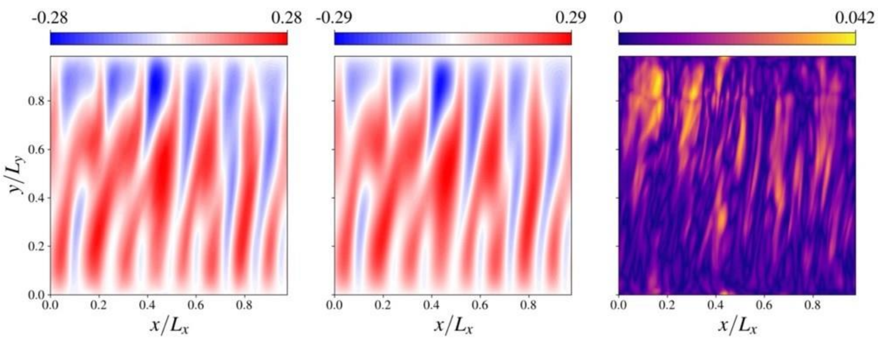


Figure 4: (left) Snapshot of θ produced by the Markov neural operator (centre) True value of θ from DNS (right) The absolute error.

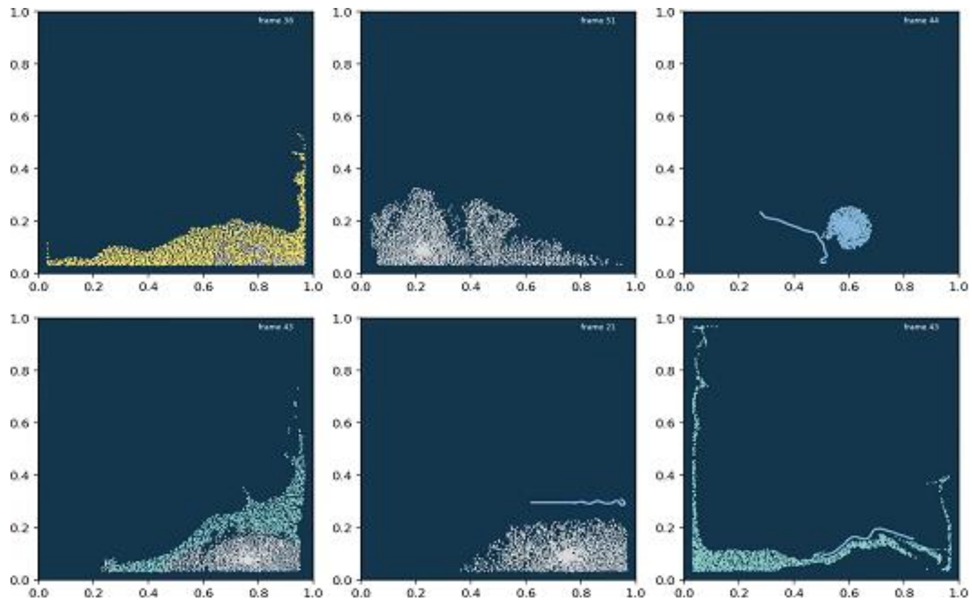
Name:	Dody Dharma
Email:	scddh@leeds.ac.uk
Institution:	University of Leeds

Abstract

Experiment of 2D Multi-material fluid-deformable solid simulation on LSTM Network

The goal of this experiment is to conduct a qualitative and quantitative study of the fluid and solid simulation to minimize the error of the simulation in the long prediction using Recurrent neural network. In this experiment, we try to combine LSTM (*Long short-term memory*) with MLP (Multilayer Perceptron) to combine temporal and spatial modelling. We use a window of 2 frames as the input and add dropout after the 1st and 2nd LSTM layer for regularization in improving the performance of the network. In the third layer of LSTM, we remove the loop to transform the dimension of the output shape from 2x1250 to 1x 250 to match the dimension of the next MLP network. In the end, the network upscaled to to match the output. The prediction results shows that compared with LSTM, the MLP model is better at predicting the shape of the liquid but suffers badly in temporal modelling (e.g. prediction *drifting* - jumping to certain state of simulation and showing a different flow). The LSTM, on the other hand, is able to maintain the trajectory of the fluid state but struggles to maintain the expected shape of liquid. The Combination of LSTM with MLP gives the best results. To analyze the error of the forward step method quantitatively, we compute the average MSE of particle positions and velocities at each frame with respect to the ground truth.

Figure



Name:	Chotirawee Chatpattanasiri
Email:	chotirawee.chatpattanasiri.21@ucl.ac.uk
Institution:	University College London
Co-authors and their institutions	Gaia Franzetti[b], Vanessa Diaz-Zuccarini[a,b], Stavroula Balabani[a,b] [a]Department of Mechanical Engineering, University College London, London, UK [b]Wellcome/EPSRC Centre for Interventional and Surgical Sciences (WEISS), Department of Medical Physics and Biomedical Engineering, University College London, London, UK

Abstract

Reduced Order Models of Aortic Flow via Robust Proper Orthogonal Decomposition

Computational Fluid Dynamics (CFD) is a widely-used tool in cardiovascular biomechanics since it can provide insights into the haemodynamics of cardiovascular conditions. However, CFD is extremely expensive in terms of computational resources, hindering their use in cardiovascular clinics. This challenge can potentially be overcome with the help of data-driven methods, especially with Reduced Order Models (ROMs). In the present work, we present the implementation of Robust Proper Orthogonal Decomposition (RPOD) compared to the traditional Proper Orthogonal Decomposition (POD) applied to the flow inside a human aorta. The flow data is obtained from an in vitro PIV experiment using a patient-specific phantom and patient-specific boundary conditions. The kinetic energy contents in POD/RPOD modes are calculated, and multiple ROMs are created to reconstruct the flow fields for each case. When using the same number of modes, RPOD outperforms POD in terms of reconstruction performance and efficiency. The ROM, consisting on the first two RPOD modes, is able to capture more than 98% of the total kinetic energy, while the first two POD modes amount to only about 86%. The RPOD reconstructed flow field also appears to be spatially and temporally smoother than the original flow field, making the algorithm suitable for noise reduction purposes. This might be beneficial in enhancing in vivo velocity data obtained via medical imaging modalities such as 4D MR making them more suitable for data driven modelling.

Figure

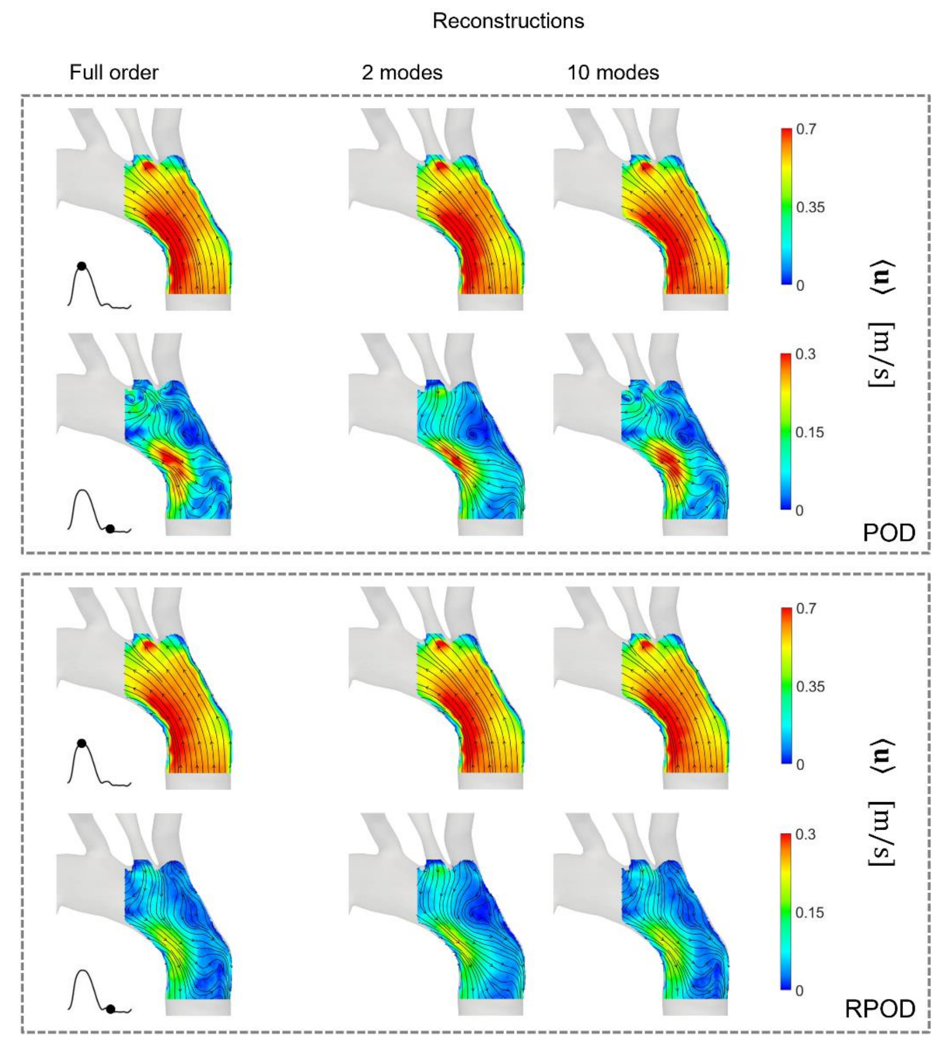


Figure 1 The reconstructions of aortic flow (top) by 2 and 10 POD modes, and (bottom) by 2 and 10 RPOD modes

Name:	Traverso Tullio
Email:	ttraverso@turing.ac.uk
Institution:	The Alan Turing Institute, London (UK)
Co-authors and their institutions	T. Y. Abadie (*Department of Chemical Engineering, Imperial College London*) O. K. Matar (*Department of Chemical Engineering, Imperial College London*) L. Magri (*Department of Aeronautics, Imperial College London*)

Abstract

Data-driven optimization of multiphase flows

The prediction of the drop size distribution (DSD) in liquid atomization and sprays is key to the optimization of multi-phase flows, from gas-turbine combustion, through agriculture to healthcare. On the one hand, it is interesting to predict certain global features of the DSD with known accuracy. Examples are the mean of the distribution (or higher order moments), as well as the cumulative probability at a finite number of points, i.e., the probability of having drops smaller than certain sizes of interest. On the other hand, the detailed continuous DSD is necessary when using generative approaches, e.g., to produce synthetic population of drops.

We use multi-task Gaussian process regression (GPR) to infer from data the mean and an arbitrary number of cumulative probabilities of the DSD as a function of the input parameters. The input parameters are the spray angle, the Reynolds, and Weber number of the jet, and the data (i.e., empirical populations of drops) are obtained from high-fidelity simulations. In a second step, we perform another GPR to infer the continuous DSD at any arbitrary point in input space. This provides an estimator of the DSD that is unbiased independently of the binning scheme, as the GPR framework lets us impose the mean of the predicted DSD, while consistently consider its uncertainty. Moreover, the predicted DSD is associated with confidence intervals which account for the fact that the data from simulations have different level of fidelity for different drop sizes. The work opens up opportunities for data-driven surrogate modelling and optimization of atomizers.