

Editorial **Machine-Learning Methods for Complex Flows**

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1. Introduction

We are delighted to introduce this Special Issue focused on novel machine-learning (ML) methods aimed at predicting, modeling, and controlling a variety of complex fluid flow scenarios. Machine learning, which can be loosely defined as "building models from data", has a progressively wider impact on a wide range of areas in our lives [\[1\]](#page-2-0), and this field is starting to be widely used in the context of fluid mechanics. The research questions posed and analyzed, traditionally, through the pillars of theory, simulations, and experiments are now experiencing a new dimension through the possibilities enabled by ML, thanks to improvements in both the algorithmic aspects and the hardware. The fast development of ML applications, triggered by an exponential increase in performance, resembles what has been experienced over the past decades in terms of high-performance computing (HPC). However, despite the great potential of ML to address a number of open questions in the area of fluid mechanics, it is important to be aware of the limitations of ML techniques, since there are a wide range of established methods which may provide better (and more scientifically sound) answers than some data-driven models [\[2\]](#page-2-1), which, in many cases, lacks the important property of interpretability [\[3](#page-2-2)[,4\]](#page-2-3).

One area where the current trends in ML methods can really benefit fluid mechanics research is when they are used synergistically with high-fidelity simulations, since these can provide a data-rich environment with a sufficiently high number of examples for ML techniques to perform well. Here, we would like to note that data-driven methods should be employed for problems where a governing equation does not exist, and if such an equation can be formulated for the data (or some physical property of the data is known), these should be embedded on any ML model that is used. Note that any property of the data to be studied, e.g., its incompressibility, will have to be learned by the deployed ML model, requiring massive amounts of data (and computer power) for the model to learn a feature that is already known. In addition to the important environmental impact of deploying ML models [\[1](#page-2-0)[,5\]](#page-2-4) (and the responsibility associated with it), the accuracy of the ML model will increase dramatically if the inherent physical properties of the phenomenon that needs to be modeled are embedded in the model itself. This is, for example, the case with physics-informed neural networks (PINNs) [\[6\]](#page-2-5), in which the governing equations of the flow (i.e., the Navier–Stokes equations) are solved via deep neural networks. These ML models are experiencing a very rapid rise in popularity [\[7\]](#page-2-6) due to the possibility of obtaining ML models with interesting generalization properties.

While we anticipate that machine learning will not replace any of the established methods for studying fluid mechanics, it can aid and complement certain areas within existing established methodologies. For instance, when it comes to developing reduced-order models (ROMs), deep learning (which is an area within ML focused on the use of neural networks with more than one hidden layer) has been shown to provide accurate representations of the temporal dynamics of the near-wall region of turbulence [\[8\]](#page-2-7), and has also been introduced as a suitable tool to accelerate numerical simulations in complex flows [\[9,](#page-3-0)[10\]](#page-3-1). In

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this context, other data-driven methods, based on the Koopman operator, also have the potential to provide accurate descriptions of the temporal dynamics in these cases [\[11–](#page-3-2)[16\]](#page-3-3), or even the three-dimensional spatio-temporal reconstruction of spare databases [\[17\]](#page-3-4). Deep learning has also been used to obtain non-linear modal decompositions of fluid flows, using convolutional neural networks [\[18\]](#page-3-5) and autoencoders [\[19\]](#page-3-6), including applications to complex turbulent flows [\[20\]](#page-3-7).

Another area where ML has shown quite high potential is non-intrusive sensing, where the information measured at the wall can be used to obtain details of the flow without disrupting it. This has been achieved via convolutional neural networks (CNNs) [\[21\]](#page-3-8), as well as generative adversarial networks (GANs) [\[22\]](#page-3-9), which have shown great potential for super-resolution tasks in turbulence [\[23\]](#page-3-10). Flow control is another topic where deep learning exhibits potential, in particular, through deep reinforcement learning [\[24](#page-3-11)[,25\]](#page-3-12). Turbulence modelling, e.g., through Reynolds-averaged Navier–Stokes (RANS) methods, has also experienced an important development via ML through interpretable models [\[26](#page-3-13)[–28\]](#page-3-14). Furthermore, flow optimization [\[29\]](#page-3-15) and the development of inflow conditions [\[30\]](#page-3-16) have also been facilitated via recent developments in data-driven methods.

After revising some of the most prominent developments in ML methods applied to fluid mechanics, we summarize the contributions in this Special Issue.

2. Summary of the Contributions

In this Special Issue, we have received contributions from a wide range of researchers and practitioners focused on developing novel ML methods to study complex fluid flows in various configurations. A brief summary of these contributions is provided below:

The first article is entitled "Transition prediction in incompressible boundary layer with finite-amplitude streaks", and it is authored by Martín and Paredes [\[31\]](#page-3-17). In this work, the authors present a parametric stability investigation of the three-dimensional incompressible flat-plate boundary layer with finite-amplitude streaks. The boundaryregion equations (BREs) are used to solve the non-linear evolution of the streaks, and the stability analysis is conducted by the parabolized stability equations (PSEs).

The second paper, "Development and validation of a machine learned turbulence model", written by Bhushan et al. [\[32\]](#page-3-18), focuses on turbulence modelling for steady and unsteady boundary-layer equations. The authors discuss the potential of incorporating physics-based constraints during training, as well as data clustering, to improve the model performance.

The third paper, written by Aguilar-Fuertes et al. [\[33\]](#page-3-19), deals with "Tracking turbulent coherent structures by means of neural networks". In this work, the authors consider a turbulent channel flow, and propose alternatives to track coherent turbulent structures. Their solutions rely on a multi-layer perceptron (MLP) and a long-short-term memory (LSTM) network, both exhibiting very encouraging results.

The fourth article, "Prediction of dead oil viscosity: machine learning vs. classical correlations", was written by Hadavimoghaddam et al. [\[34\]](#page-3-20). In this article they deal with the modelling of the dead-oil viscosity, which is a very important parameter in the context of reservoir-engineering problems. They propose a total of 6 ML models, which can provide very promising results, outperforming some of the established classical methods for the prediction of this parameter.

The fifth article, written by Tokarev et al. [\[35\]](#page-3-21), is entitled "Deep reinforcement learning control of cylinder flow using rotary oscillations at low Reynolds number". The authors focus on reducing the drag in a two-dimensional cylinder, which oscillates around its axis with time-dependent angular velocity. For such an aim, the article applies deep reinforcement learning, developing an active flow control strategy based on the angular velocity.

The sixth article is entitled "Insights into the aeroacoustic noise generation for vertical axis turbines in close proximity" by Viqueira-Moreira and Ferrer [\[36\]](#page-3-22). In this article, the authors predict tonal frequencies, providing theoretical estimates in: an isolated NACA0012 airfoil, an isolated rotating vertical axis wind turbine composed of three rotating airfoils, and a farm of four vertical axis turbines. The results suggest that farms need to be considered and studied as different entities to characterize the aeroacoustic footprint of vertical axis wind turbines located nearby, since a linear combination of sources from isolated turbines is not enough.

The seventh article, by Tiseira Izaguirre et al. [\[37\]](#page-4-0), is entitled "Design and numerical analysis of flow characteristics in a scaled volute and vaned nozzle of radial turbocharger turbines". The article introduces the design of an up-scaled volute-stator model, showing, numerically, that it is representative of the flow patterns, and that enables opticalexperimental-measurement techniques. The limitations of the rotor-stator interactions and the definition of interesting measurement sections for experiments are also presented. The article presents fundamental research that aims to contribute towards improving the aerodynamic development of turbocharger turbines.

The eighth article, "Dynamic mode decomposition analysis of spatially agglomerated flow databases", is written by Li et al. [\[38\]](#page-4-1). This article combines dynamic mode decomposition, a data-driven method suitable to identify flow patterns in fluid dynamics, with several clustering methods, with the aim of reducing the spatial dimensionality of the database. The article compares twelve different clustering algorithms to study the effect of the spatial agglomeration in the results (quantified by measuring the computational performance and the accuracy of the retrieved results). The methodology is applied to three different test cases: a synthetic flow field, the flow around a two-dimensional cylinder, and a turbulent channel flow.

The ninth and last article of this Special Issue is written by Jian et al., and is entitled "A novel algebraic stress model with machine-learning-assisted parameterization", contributing to the further understanding of machine-learning-assisted turbulence modeling. The paper presents a data-driven regression model based on a fully-connected deep neural network, which is tested as suitable for Reynolds-stress closure modeling. This new model, denoted as the tensorial-quadratic eddy-viscosity model (TQEVM), is validated in wall-bounded flows and is tested as suitable for Reynolds-averaged Navier–Stokes (RANS) simulations, showing that the mean-flow quantities of interest agree with the direct numerical simulations (DNSs).

We believe that these articles highlight the exciting research opportunities present in ML applications that can be applied to fluid mechanics, as well as how this dynamic field fosters multi-disciplinary research to achieve novel solutions.

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References

- 1. Vinuesa, R.; Azizpour, H.; Leite, I.; Balaam, M.; Dignum, V.; Domisch, S.; Felländer, A.; Langhans, S.D.; Tegmark, M.; Fuso Nerini, F. The role of artificial intelligence in achieving the Sustainable Development Goals. *Nat. Commun.* **2020**, *11*, 233. [\[PubMed\]](http://www.ncbi.nlm.nih.gov/pubmed/31932590)
- 2. Vinuesa, R.; Brunton, S.L. The potential of machine learning to enhance computational fluid dynamics. *arXiv* **2021**, arXiv:2110.02085.
- 3. Rudin, C. Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead. *Nat. Mach. Intell.* **2019**, *1*, 206–215. [\[CrossRef\]](http://doi.org/10.1038/s42256-019-0048-x)
- 4. Vinuesa, R.; Sirmacek, B. Interpretable deep-learning models to help achieve the Sustainable Development Goals. *Nat. Mach. Intell.* **2021**, *3*, 926. [\[CrossRef\]](http://dx.doi.org/10.1038/s42256-021-00414-y)
- 5. Karnama, A.; Haghighi, E.B.; Vinuesa, R. Organic data centers: a sustainable solution for computing facilities. *Results Eng.* **2019**, *4*, 100063. [\[CrossRef\]](http://dx.doi.org/10.1016/j.rineng.2019.100063)
- 6. Raissi, M.; Yazdani, A.; Karniadakis, G.E. Hidden fluid mechanics: Learning velocity and pressure fields from flow visualizations. *Science* **2020**, *367*, 1026–1030. [\[CrossRef\]](http://dx.doi.org/10.1126/science.aaw4741)
- 7. Eivazi, H.; Tahani, M.; Schlatter, P.; Vinuesa, R. Physics-informed neural networks for solving Reynolds-averaged Navier–Stokes equations. *arXiv* **2021**, arXiv:2107.10711.
- 8. Srinivasan, P.A.; Guastoni, L.; Azizpour, H.; Schlatter, P.; Vinuesa, R. Predictions of turbulent shear flows using deep neural networks. *Phys. Rev. Fluids* **2019**, *4*, 054603. [\[CrossRef\]](http://dx.doi.org/10.1103/PhysRevFluids.4.054603)
- 9. López-Martín, M.; Le Clainche, S.; Carro, B. Model-free short-term fluid dynamics estimator with a deep 3D-convolutional neural network. *Exp. Syst. Appl.* **2021**, *117*, 114924. [\[CrossRef\]](http://dx.doi.org/10.1016/j.eswa.2021.114924)
- 10. Abadía-Heredia, R.; López-Martín, M.; Carro, B.; Arribas, J.I. and. Pérez, J.; Le Clainche, S. A predictive hybrid reduced order model based on proper orthogonal decomposition combined with deep learning architectures. *Exp. Syst. Appl.* **2021**, *187*, 115910. [\[CrossRef\]](http://dx.doi.org/10.1016/j.eswa.2021.115910)
- 11. Eivazi, H.; Guastoni, L.; Schlatter, P.; Azizpour, H.; Vinuesa, R. Recurrent neural networks and Koopman-based frameworks for temporal predictions in a low-order model of turbulence. *Int. J. Heat Fluid Flow* **2021**, *90*, 108816. [\[CrossRef\]](http://dx.doi.org/10.1016/j.ijheatfluidflow.2021.108816)
- 12. Le Clainche, S.; Vega, J. *A Review on Reduced Order Modeling Using DMD-Based Methods*; IUTAM Bookseries; Springer: Cham, Switzerland, 2018; Volume 36.
- 13. Le Clainche, S.; Vega, J. Analyzing nonlinear dynamics via data-driven dynamic mode decomposition-like methods. *Complexity* **2018**, *1*, 6920783. [\[CrossRef\]](http://dx.doi.org/10.1155/2018/6920783)
- 14. Le Clainche, S. Prediction of the Optimal Vortex in Synthetic Jets. *Energies* **2019**, *12*, 1635. [\[CrossRef\]](http://dx.doi.org/10.3390/en12091635)
- 15. Vega, J.M.; Le Clainche, S. *Higher Order Dynamic Mode Decomposition and Its Applications*; Elsevier: Amsterdam, The Netherlands, 2020; p. 320; ISBN 9780128227664.
- 16. Le Clainche, S.; Rosti, M.; Brandt, L. Flow structures and shear-stress predictions in the turbulent channel flow over an anisotropic porous wall. *J. Phys. Conf. Ser.* **2020**, *1522*, 012016. [\[CrossRef\]](http://dx.doi.org/10.1088/1742-6596/1522/1/012016)
- 17. Pérez, J.M.; Le Clainche, S.; Vega, J.M. Reconstruction of three-dimensional flow fields from two-dimensional data. *J. Comput. Phys.* **2020**, *407*, 109239. [\[CrossRef\]](http://dx.doi.org/10.1016/j.jcp.2020.109239)
- 18. Murata, T.; Fukami, K.; Fukagata, K. Nonlinear mode decomposition with convolutional neural networks for fluid dynamics. *J. Fluid Mech.* **2020**, *882*, A13. [\[CrossRef\]](http://dx.doi.org/10.1017/jfm.2019.822)
- 19. Fukami, K.; Nakamura, T.; Fukagata, K. Convolutional neural network based hierarchical autoencoder for nonlinear mode decomposition of fluid field data. *Phys. Fluids* **2020**, *32*, 095110. [\[CrossRef\]](http://dx.doi.org/10.1063/5.0020721)
- 20. Eivazi, H.; Le Clainche, S.; Hoyas, S.; Vinuesa, R. Towards extraction of orthogonal and parsimonious non-linear modes from turbulent flows. *arXiv* **2021**, arXiv:2109.01514.
- 21. Guastoni, L.; Güemes, A.; Ianiro, A.; Discetti, S.; Schlatter, P.; Azizpour, H.; Vinuesa, R. Convolutional-network models to predict wall-bounded turbulence from wall quantities. *J. Fluid Mech.* **2021**, *928*, A27. [\[CrossRef\]](http://dx.doi.org/10.1017/jfm.2021.812)
- 22. Güemes, A.; Discetti, S.; Ianiro, A.; Sirmacek, B.; Azizpour, H.; Vinuesa, R. From coarse wall measurements to turbulent velocity fields through deep learning. *Phys. Fluids* **2021**, *33*, 075121. [\[CrossRef\]](http://dx.doi.org/10.1063/5.0058346)
- 23. Kim, H.; Kim, J.; Won, S. Lee, C. Unsupervised deep learning for super-resolution reconstruction of turbulence. *J. Fluid Mech.* **2021**, *910*, A29. [\[CrossRef\]](http://dx.doi.org/10.1017/jfm.2020.1028)
- 24. Rabault, J.; Kuchta, M.; Jensen, A.; Réglade, U.; Cerardi, N. Artificial neural networks trained through deep reinforcement learning discover control strategies for active flow control. *J. Fluid Mech.* **2019**, *865*, 281–302. [\[CrossRef\]](http://dx.doi.org/10.1017/jfm.2019.62)
- 25. Vinuesa, R.; Lehmkuhl, O.; Lozano-Durán, A.; Rabault, J. Flow control in wings and discovery of novel approaches via deep reinforcement learning. *Fluids* **2022**, *7*, 62. [\[CrossRef\]](http://dx.doi.org/10.3390/fluids7020062)
- 26. Jiang, C.; Vinuesa, R.; Chen, R.; Mi, J.; Laima, S.; Li, H. An interpretable framework of data-driven turbulence modeling using deep neural networks. *Phys. Fluids* **2021**, *33*, 055133. [\[CrossRef\]](http://dx.doi.org/10.1063/5.0048909)
- 27. Weatheritt, J.; Sandberg, R.D. A novel evolutionary algorithm applied to algebraic modifications of the RANS stress-strain relationship. *J. Comput. Phys.* **2016**, *325*, 22–37. [\[CrossRef\]](http://dx.doi.org/10.1016/j.jcp.2016.08.015)
- 28. Weatheritt, J.; Sandberg, R.D. The development of algebraic stress models using a novel evolutionary algorithm. *Int. J. Heat Fluid Flow* **2017**, *68*, 298–318. [\[CrossRef\]](http://dx.doi.org/10.1016/j.ijheatfluidflow.2017.09.017)
- 29. Morita, Y.; Rezaeiravesh, S.; Tabatabaei, N.; Vinuesa, R.; Fukagata, K.; Schlatter, P. Applying Bayesian optimization with Gaussian-process regression to Computational Fluid Dynamics problems. *J. Comput. Phys.* **2022**, *449*, 110788. [\[CrossRef\]](http://dx.doi.org/10.1016/j.jcp.2021.110788)
- 30. Fukami, K.; Nabae, Y.; Kawai, K.; Fukagata, K. Synthetic turbulent inflow generator using machine learning. *Phys. Rev. Fluids* **2019**, *4*, 064603. [\[CrossRef\]](http://dx.doi.org/10.1103/PhysRevFluids.4.064603)
- 31. Martín, J.A.; Paredes, P. Transition prediction in incompressible boundary layer with finite-amplitude streaks. *Energies* **2021**, *14*, 2147. [\[CrossRef\]](http://dx.doi.org/10.3390/en14082147)
- 32. Bhushan, S.; Burgreen, G.W.; Brewer, W.; Dettwiller, D. Development and validation of a machine learned turbulence model. *Energies* **2021**, *14*, 1465. [\[CrossRef\]](http://dx.doi.org/10.3390/en14051465)
- 33. Aguilar-Fuertes, J.J.; Noguero-Rodríguez, F.; Jaen Ruiz, J.C.; García-Raffi, L.M.; Hoyas, S. Tracking turbulent coherent structures by means of neural networks. *Energies* **2021**, *14*, 984. [\[CrossRef\]](http://dx.doi.org/10.3390/en14040984)
- 34. Hadavimoghaddam, F.; Ostadhassan, M.; Heidaryan, E.; Sadri, M.A.; Chapanova, I.; Popov, E.; Cheremisin, A.; Rafieepour, S. Prediction of dead oil viscosity: machine learning vs. classical correlations. *Energies* **2021**, *14*, 930. [\[CrossRef\]](http://dx.doi.org/10.3390/en14040930)
- 35. Tokarev, M.; Palkin, E.; Mullyadzhanov, R. Deep Reinforcement Learning Control of Cylinder Flow Using Rotary Oscillations at Low Reynolds Number. *Energies* **2020**, *13*, 5920. [\[CrossRef\]](http://dx.doi.org/10.3390/en13225920)
- 36. Viqueira-Moreira, M.; Ferrer, E. Insights into the Aeroacoustic Noise Generation for Vertical Axis Turbines in Close Proximity. *Energies* **2020**, *13*, 4148. [\[CrossRef\]](http://dx.doi.org/10.3390/en13164148)
- 37. Tiseira Izaguirr, A.; Navarro García, R.; Benjamin Inhestern, L.; Hervás Gómez, N. Design and Numerical Analysis of Flow Characteristics in a Scaled Volute and Vaned Nozzle of Radial Turbocharger Turbines. *Energies* **2020**, *13*, 2930. [\[CrossRef\]](http://dx.doi.org/10.3390/en13112930)
- 38. Li, B.; Garicano-Mena, J.; Zheng, Y.; Valero, E. Dynamic Mode Decomposition Analysis of Spatially Agglomerated Flow Databases. *Energies* **2020**, *13*, 2134. [\[CrossRef\]](http://dx.doi.org/10.3390/en13092134)