Project 10

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Name of the project	Prediction of Aerodynamics Fields around an Airfoil using Machine Learning
Profile of the team leader(s)	Lionel Salesses – Cenaero – Research Engineer in Machine learning applied to physical problems. After completing an engineering degree in 'Applied Mathematics and Computer Science' at Ensimag (Grenoble, France), Lionel Salesses got a PhD thesis in Applied Mathematics at the Jean Kuntzmann laboratory in Grenoble on 'Analysis of some conductivity problems with sign change'. He then worked in a French start-up company on topological optimization of neural networks. In January 2022, he joined Cenaero to work on machine learning applied to physical problems, in particular within the ARIAC project.
Abstract	The aeronautical industry faces enormous challenges in ensuring that it is both environmentally friendly and economically viable. To achieve these goals, significant efforts are undertaken to make the best possible use of the materials and pieces of equipment in the aircraft. For example, by minimizing the weight of the wing and fuselage structures, the kerosene consumption of aircraft engines can be considerably reduced, thereby limiting CO2 emissions. Fortunately, to widely and smartly explore potentially better designs, advanced machine learning and optimization algorithms are constantly being developed and coupled with high-level aerostructural and aerodynamic numerical simulations; such strategies have proved their effectiveness in finding innovative solutions. In this project, the emphasis is put on the aerodynamic design of a well-known 3D wing (based on the ONERA M6 demonstrator). In a first approximation, this design task can be seen as the maximization of the ratio between the lift and drag coefficients, whose values can be post-processed from a Computational

	Fluid Dynamics (CFD) solver. In addition to furnishing scalar values used as objectives and constraints for the shape optimization of the wing, the full CFD analysis also provides a better insight on the physical behavior of the parameterized wing designs (e.g., presence and position of shocks, etc.). Nevertheless, these benefits come at an expensive numerical cost, typically requiring dozens of CPU's on High Performance Computing (HPC) servers running for several hours. For all these reasons, it is of great importance to be able to analyze the physical (e.g., pressure and velocity) fields for any wing geometry without requiring a full CFD analysis on a HPC server. Therefore, Machine Learning (ML) models will be investigated and built to compute the so-called snapshots of the vectorial quantities of interest. Once developed, these ML models can be used to easily generate CFD-like vectorial responses, for example for later use within a sensitivity analysis or an optimization process, or any other many-query tasks.
Project objectives	Based on a dataset of numerical simulations derived from CFD computations on a representative set of 3D wing designs, the objectives of the project consist in developing and testing ML-based models to predict the physical fields of interest for the aerodynamics of the ONERA M6 3D wing (https://dafoam.github.io/mydoc_tutorials_aero_m6.html), i.e., the pressures and velocities. To accomplish this task, different ML architectures can be employed. We can mention the Fourier Neural Operator (FNO) framework, the Graph Neural Network (GNN) or the Convolutional Neural Network (CNN). The main challenge is to be able to predict accurately the physical fields for variable wings geometry. Moreover, a reasonable compromise must be found between accuracy of the prediction and affordability of the ML model in terms of computational cost and resources. It could also be interesting to compare the performance of different ML models on such a task. The proposed models will be trained on an open dataset composed of CFD simulations generated and provided by Cenaero prior to the workshop (additional dataset points might be calculated on demand during the workshop if needed). The purpose is to predict the pressure and velocity fields for any combination of geometrical design variables guiding the parameterization of the wing.

	If successfully built, advanced enrichment strategies could be developed as a bonus, in order to improve the quality of the ML model with new data points carefully selected through a so-called infill criterion. This approach is prevalent in design processes like surrogate-based optimization. Another additional development could consist in estimating the gradients of the vectorial quantities, for further use in a gradient-based optimization.
Background information	CFD models have been developed for decades in aerodynamics (internal and external flows), aeroelasticity, heat transfer, etc. Due to the difficulty of solving the Euler or Navier-Stokes governing equations, advanced discretization methods have been proposed, the prevalent one for a wide range of CFD applications being the finite volume method. An excellent introduction to the topic is available in [1]. Among the open-source codes dedicated to CFD, OpenFOAM has emerged for several years as a versatile and robust solution [2]. Apart from understanding the physics involved in aircraft wings or turbomachinery blades, the CFD simulation can also be efficiently used for helping design the geometry of such components. Shape, and topology optimization algorithms have played a tremendous role in helping designers to reach compromises between performance objectives and operational and manufacturing constraints [3]. When available, these algorithms use the derivatives (also called sensitivities) of the numerical responses with respect to the geometrical (Computer-Aided Design or CAD) parameters. An efficient approach to compute sensitivities is based on an adjoint formulation [4]. In the specific context of multidisciplinary design optimization in aeronautics, DAFoam (Discrete Adjoint with OpenFOAM for High-fidelity Multidisciplinary Design Optimization) is an open-source program implementing an efficient discrete adjoint method to perform high-fidelity multidisciplinary design optimization [5]. While the optimization part of DAFoam will not be used in this project, the full CAD parameterization and fluid simulation process will provide high-fidelity datasets. CFD simulations can provide accurate numerical values that can be used to compare different designs and explore the design space. However, this can be very time consuming in terms of computing power. Machine Learning can be seen as an enabler for accelerating CFD computations, speeding up traditional high-fidelity simulation by several orders of magnitude. In the past few years, the prediction of pressure and velocity around a wing using ML techniques has been investigated using several types of ML models.

	For example, in [7], the authors propose to use Fourier Neural Operators to predict the steady flow around an airfoil under variable boundary conditions. The Fourier Neural Operator (FNO) [8] is a neural network architecture that learns the solution operators of PDEs (the mapping between boundary/initial conditions to the solution). The main benefit of FNO is to be mesh-independent because it learns an operator between function spaces, so its inputs/outputs are a function which can later be discretized on any mesh. In [6], they adapt the Fourier Neural Operator to learn PDEs solutions on arbitrary geometries. Indeed, the classical Fourier Operator Framework relies on Fast Fourier Transform which is limited to rectangular domains with uniform grids. The Graph Neural Network (GNN) has also been used to predict the flow around an airfoil [9]. The main interest of GNN is their ability to work directly on the simulation mesh without requiring any projection on a rectangular grid which is leading to an additional projection error. Some architectures based on Convolutional Neural Networks (CNN) has also been used to predict the flow around a body shape. We can mention the UNet architecture used in [10] which allows to extract and predict features at different scales in images/fields.
Bibliographic references	[1] J. D. Anderson, Jr, “Computational Fluid Dynamics: The Basics with Applications”. McGraw-Hill, 1995. [2] OpenFOAM, 2024, http://www.openfoam.org/. [3] P. Breitkopf and R. Filomeno Coelho, eds., “Multidisciplinary Design Optimization in Computational Mechanics”. Chippenham, UK: ISTE/John Wiley & Sons, April 2010. [4] M. B. Giles and N. A. Pierce, “An Introduction to the Adjoint Approach to Design”, Flow, Turbulence and Combustion 65: 393–415, 2000. [5] P. He, C. A. Mader, J. R. R. A. Martins, and K. J. Maki, “DAFoam: An Open-Source Adjoint Framework for Multidisciplinary Design Optimization with OpenFOAM,” AIAA Journal, vol. 58, no. 4, pp. 1304–1319, 2020. [6] Li, Z., Huang, D. Z., Liu, B., & Anandkumar, A. (2023). “Fourier neural operator with learned deformations for pdes on general geometries”. Journal of Machine Learning Research, 24(388), 1-26. [7] Dai, Y., An, Y., & Li, Z. (2022). “FourNetFlows: An efficient model for steady airfoil flows prediction.” arXiv preprint arXiv:2207.04358. [8] Li, Z., Kovachki, N., Azizzadenesheli, K., Liu, B., Bhattacharya, K., Stuart, A., & Anandkumar, A. (2020). “Fourier neural operator for parametric partial differential equations.” arXiv preprint arXiv:2010.08895.

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Detailed technical description/work plan

1. Technical description

In the context of aerodynamic performance and safety of airfoils (or other complex components of a product), parametric studies based only on wind tunnel experiments are very expensive and time consuming. Therefore, a more efficient and adequate approach is required that allows to reduce the number of physical experiments. Typically, approaches based on numerical simulations such as CFD are used. However, due to the increasing complexity of design problems, the simulation-based methodology is becoming too expensive, and an even cheaper method is making itself increasingly felt.

Machine Learning can change the way computing power is used to solve complex design problems. In particular, ML modelling can be an appropriate solution for fast aerodynamic evaluation of airfoil geometries outside the training database. Compared to more classical surrogate modelling techniques that only approximate scalar, averaged quantities of interest, ML-based approaches allow to exploit the abundant and intrinsic physical information and allow to obtain complete flow field information.

Based on a dataset of numerical simulations derived from CFD computations on a representative set of 3D wing designs, the objectives of the project consist in developing, testing and comparing ML-based models to predict the physical fields of interest for the aerodynamics of the ONERA M6 3D wing. To develop the ML model of the physical fields of interest (pressures and velocities), a dataset of CFD simulations will be provided by Cenaero prior to the workshop. It will be generated through a Design of Experiments or DoE (following a Latin Hypercube Sampling) of representative wing designs. The reference wing is based on the ONERA M6 demonstrator. The parameterization itself contains Free-Form Deformation (FFD) nodal points (defining smooth modifications of the wing geometry from the leading to the trailing edge, and from tip to hub), along with additional global geometrical variables (twist, ...). Around 30 geometrical design parameters will be used to vary the shape of the wing.

For each of these wings, a DAFoam CFD calculation will be run before the workshop, on Lucia's HPC servers (parallel processing on 32 CPU's). As explained earlier, DAFoam relies on an efficient discrete adjoint method to perform high-fidelity multidisciplinary design parameterization and optimization. Using the open-source package OpenFOAM for multiphysics analysis, DAFoam implements a Jacobian-free discrete adjoint approach with competitive speed, scalability, and accuracy.

The corresponding results for all wing designs of the DoE will be available to the participants of the project, through a set of files describing for each sample its geometry and all physical fields of interest. These (compressed) files can be easily parsed, but also visualized, analyzed, and processed with Paraview in order to get a better insight on the physics involved. In addition to the pressure and velocity fields, a scalar response (namely: the ratio CL/CD between the lift and drag coefficients) will also be provided. This quantity is often used as an objective function to maximize in airfoil or wing design optimization.

The different tested ML techniques will be compared on appropriate metrics to identify the ones with the best generalization ability to unseen geometries. One would also test the ability of Fourier Neural Operator to generate accurate fields at different resolutions. A common framework for fair comparison of the proposed ML method should be used, with agreed prediction metrics.

Cenaero develops an optimization software, Minamo, which is daily used to solve engineering optimization problems. The ambition (most probably after the workshop) is to combine the ML-based aerodynamic field prediction with the Cenaero's optimization strategy to optimize the shape of the wing. Investigations on differentiable ML simulators to use gradients to optimize the shape of the wing could also be of interest.

2. Resources needed: facility, equipment, software, staff etc.:

- A laptop equipped with a Python environment (>= 3.9) and a ML framework is needed.
- TRAIL researchers can ask access to Lucia, the Tier-1 supercomputer hosted by Cenaero to train the ML models. However, the full CFD-based simulation chain will not be directly accessible to the participants; if additional data sample points are needed, they can be ordered, and their execution will be taken care of on Lucia by Cenaero.
- The visualization of the physical fields will be done on Paraview, which is freely available (https://www.paraview.org/).
- Good Internet connection.

	A brainstorming session will be organized at the beginning of the workshop to introduce the project in detail, to exchange ideas, and to organize the team (depending on the number of participants, a split off into groups of 2-3 people should be done). Daily scrum meetings with the whole team will be held. A private GitHub repository will be used to collaborate on the code developed during the workshop.
Benefits of the research: expected outcomes of the project	The research targeted within this project will contribute, on its own scale, to improve the quality and/or the cost of the emulation of complex physical systems with AI technologies to take better decisions in engineering processes, in the specific context of aerodynamic wing design. The expected outcome of the project is to develop machine learning methodology to predict a physical field with high accuracy, but an affordable computational cost. Although the use case targeted in this project concerns aerodynamic external flows, it should be possible to extend the developed methodology to other design processes involving expensive numerical simulations. The tangible outputs / deliverables of the project at this workshop should include: - Python codes on GitHub to perform prediction of the pressure and velocity fields using ML models. When mature enough, the codes will be released on the TRAIL Factory. The dataset could be stored with the code on the TRAIL Factory. - Final slides and reports presenting the methodology and the results (with appropriate visualization plots). - Depending on the results, the writing of a scientific paper could be considered after the end of the workshop. This project is linked to the Grand Challenge 1 “Hybrid Modelling Methods towards an Augmented Engineering” led by Cenaero. As for the use case of AI-enabled additive manufacturing, the main purpose is to investigate how machine learning can accelerate numerical simulations (CFD, FEM, ...), making them faster and more accessible to take better decisions to optimize products and processes. Indeed, the demand for real-time CFD simulations has increased significantly in recent years.
Other remarks	Potential team members (to be confirmed on May 16, 2024): - Lionel Salesses – Cenaero - Rajan F. Coelho – Cenaero - Caroline Sainvitu – Cenaero - Florent De Geeter – ULiège - Yann Claes – ULiège

	- Omer Rochman – ULiège - ...