PROPOSITION DE SUJET DE THESE

Intitulé : **Synthetic reacting flow generation from a non-dimensional elementary data-driven model**

Référence : **MFE-DMPE-2024-23**

Début de la thèse : Octobre 2024	**Date limite de candidature :** juillet 2024

Mots clés : Combustion, Artificial Intelligence, Machine Learning, CFD, Physics Informed Neural-Network

Profil et compétences recherchées : Master of Science or Master of Engineering in fluid mechanics. Courses and experiences in AI are highly considered. Combustion knowledge is also appreciated. Fluent English is required.

Présentation du projet doctoral, contexte et objectif

Numerical simulations while applicable in predicting reactive flows occurring in combustion chambers of aerospace engines are extremely costly due to high-resolution grids, numerous species, and detailed models necessary to capture the existing chemical reactions and their interaction with the underlying flow. Solutions to reduce the cost of these models while maintaining their accuracy and predictability would hence constitute a great contribution to the combustion and chemical propulsion communities.

Techniques based on machine learning, and in particular, deep Learning, can offer an alternative to classical physics-based approaches. In particular, machine learning has proven to be very efficient in predicting combustion-based quantities of interest (temperature, chemical product concentrations, pressure, reaction rate, etc.) with much lower cost. According to Lapeyre *et al.* [1], the convolutional neural network is able to predict the transient behavior of detailed simulations better than algebraic (physics-based) models. AI tools also have the ability to clarify links and establish correlation between quantities involved in complex physical phenomena, such as, for instance, the MILD combustion for which the PDF shape is found substantially different from that of a conventional flame [2]. The AI approach can also bypass very difficult mathematical optimization problems for choosing the most adapted numerical model for a particular region of the flow field while reducing the computation cost [3]. Furthermore, using unsupervised learning strategies (such as clustering algorithms), it is possible to identify different regions of the flow (dynamically or reactively) for which separate and dedicated modeling approached can be employed [4].

However, most of studies, involving AI algorithms in combustion modeling, use a single geometry and/or operational condition to build the necessary training data [5]. Consequently, they lack of generalizability and interpretability [6]. This is not just a problem faced in combustion modelling but pertains to most AI-driven approaches applied in scientific domains dealing with non-linear or unsteady systems. The infusion of physical insight into the training has shown to improve generalizability in some scientific application [6, 7]. Nevertheless, the ability to transpose the obtained results to another flow configuration is yet to be demonstrated, and remains an open question. Such a statement prevents the regular use of AI-based CFD simulations since the confidence in the trained model is a critical aspect [6].

The underlying unsteady flow, the mixing efficiency, the chemical power distribution and resulting instabilities are intimately related to the geometry of the chamber. However, the current methodologies do not warrant the extrapolation of the models from one geometry to the other. One way of integrating the geometry in the model is to use data obtained in multiple geometrical configurations [8]. However, this approach is too expensive to be feasible in practice, since it requires the generations of a large amount of data, and compromises the advantage of using AI. In order to avoid generating expensive and time-consuming data, some studies use Transfer Learning approaches [9] so as to integrate the change in the geometry with limited data. This technique consists in transferring the knowledge obtained by a training realized in one domain to another one using minimal data from the new configuration. This transfer is however only possible when the two domains are sufficiently similar and can thereby significantly reduce the amount of data required for training the model on the target domain. However, in the case of industrial combustion chambers, whereby geometries are very different from one to the other, the results are not warranted which justifies further investigation.

Hitherto, training cases are very close to the application case. Hereafter, the effects of less obvious database on results must be measured to assess the generalization capability of the data-driven approaches for reacting flow CFD simulations. The non-linear interaction between elements of the database could lead to a completely unexpected new flow configuration, potentially unphysical. Research works on the measurement of the result alterations, the database structure and the training processes are therefore required to propose a framework to enlarge the generalization capability of the data-driven approaches for CFD flow field generation.

Objectives:

The main objective of the thesis is to develop a framework to design an efficient database and organize the training able to promote the geometrical generalization capability of a data-driven model for CFD reacting flow field generation. An underlying objective is to measure the alterations of the ML algorithm results when considering different geometry configurations.

Thesis approach:

The present work is focused on a 2D configuration of a duct CH_4/Air reacting flow with a shaped wall (Fig. 1) as reference case. CEDRE, the CFD's software of ONERA, will be used for the computations. The top wall is altered according to the geometry configuration to study whereas the bottom wall remains unchanged. The study will start with subsonic steady compressible 2D laminar reacting and frozen flows. As the thesis progresses, turbulence and unsteadiness will be added. The walls are no-slip and adiabatic. The equivalence ratio of reference is 0.82, corresponding to the case of the step flow treated in MICAEDI facility [14].

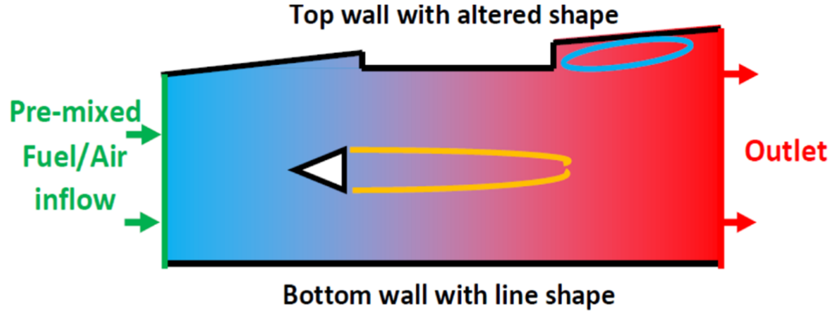

Figure 1: Reference work case.

The ML-based algorithm will use, as input, the geometry and the boundary conditions of the combustion chamber (Fig.2). Non-dimensional approach will be used to maximize the applicability range. The output will be the pressure, the temperature, the species mass fractions and the velocity flow fields. ML-framework is designed to generate flow fields from a complex combustion chamber geometry and specific boundary conditions. In the present thesis, all walls are assumed no-slip and adiabatic. ML algorithm is trained from a database built from selected basic elements provided by numerical simulations of variations of the elementary reference case with changing the shape of the top wall. The selection, treatment, division and training organization processes are part of the objects of the thesis: several methods will be studied and assessed to provide some understanding elements to control the non-linear trends of the synthesis process and limit the occurrence of non-physical solutions due to the strongly non-linearity of reacting flow Navier-Stokes equations and ML approaches.

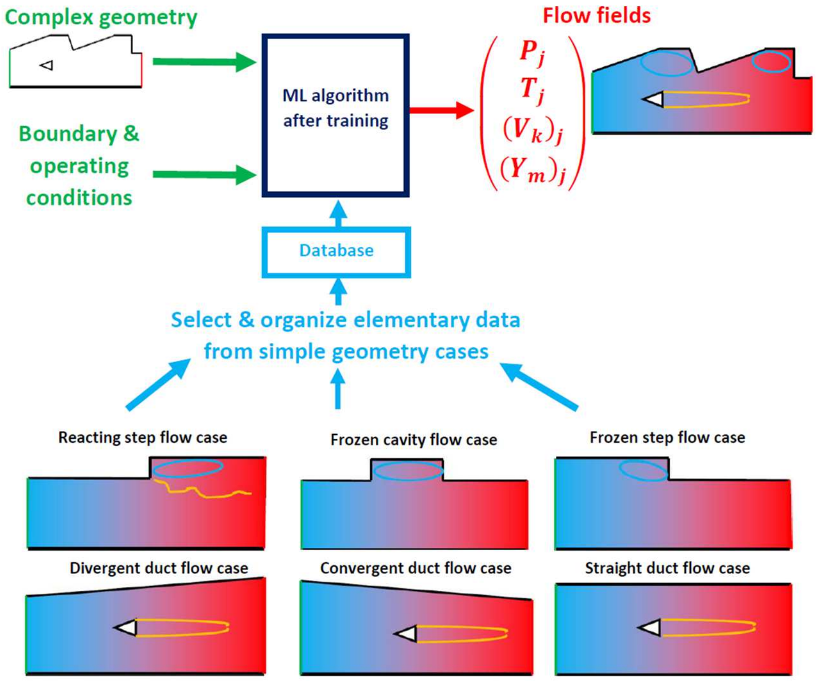

Figure 2: Principle scheme of the elementary data-driven method and approach for producing synthetically flow fields.

For all the databases, the considered maximum ranges are from 0.1 to 0.6 for the Mach number and from 100 to 10000 for Reynolds number. The Damköhler number range is from 0.01 to 100. The meshes refinement will be intentionally reduced to simulate with a reasonable cost the overall considered cases, as the objective will be assessed qualitatively.

The database generation processes will target to provide a minimal number of elementary cases for maximal applicability in the context of combustion chamber. For that, several kinds of database must be built. Four levels of database is considered:

- Homogeneous frozen flow: the treated cases display the most numerous configurations comparing with others. Only one represented species is used, as only aerodynamics is regarded;
- Heterogeneous frozen flow: the treated cases consider a heterogeneous distributions. Arbitrary source terms or inflows with different species distributions are considered to get a database of the heterogeneous effects of the species transportation in the flow;
- Premixed flame flow: the treated cases consider a reacting flow with a pre-mixed inflow. In those cases, the geometry or a body will be used to hold the flame;

- Non-premixed flame flow: the oxidizer and the fuel are injected separately in positions defined by the configurations.

Several geometrical configurations of the top wall used for the database allow to form a set of canonical problems (convergent, divergent duct flows, step-flow, flame-holder in a duct, etc.). For each configurations, geometry variations will be considered (step wall, injector positions, length to height ratio, slope angle of the top wall, etc.). The maximum calculations will be around one thousand. However, each flow field will be divided on hundreds of elements to feed the ML algorithm.

The main target is to measure the ability of the database methodology and the ML design to reproduce the dominant flow patterns as well as reasonable estimation of quantities of interest. The criteria to assess the quality of the results are the ability to reproduce the main phenomena involved in the flow field (recirculation zones, flame shape and position, unsteadiness, etc.), the magnitude of the characteristic non-dimensional numbers (Re, Da, Ma, etc.), and the conformity with the fundamental physical conservation laws.

Our ML approach consists of a two-sided idea, which is capable of dealing with unknown underlying function spaces, uncertainty in data and possible explanations w.r.t data generating scenarios. First part covers two types of PINNs (classical Physics-informed neural networks), which is a type of deep learning that can take into consideration the knowledge of the physical phenomenon in question. The knowledge can be governing partial differential equations (PDEs), for example. This approach allows to be more faithful to the physic with a lower amount of dataset, compared to a data-driven deep learning. Based on the discussion opened in [6] and the possible problems w.r.t classical PINNs, we are also looking for epistemic and aleatoric uncertainty, which is covered by the Bayesian view in terms of data and model prediction. The methodical equivalent in this approach is the Baysian-PINN [10, 11]. Last but not least, we would like to examine the conditions of the data-generating distribution through the possibilities of the Generative Adversarial Networks (GAN). Those GANs (might be considered as an alternative approach when PINNs turns out to be difficult to integrate.) are a promising tool for recovering data generating processes, which we would like to map back to the different settings with methods coming from Latent Space Arithmetic's [12]

To validate and assess the performances of the several developed ML approaches, an experimental database, provided by ONERA, will be used to validate the approach for comforting its practical use in industrial case. Those data are provided by a set of test cases obtained previously at ONERA in configurations close to propulsive systems. They consist of combustion imaging data obtained at high acquisition rates, e.g., [13, 14]. The studied cases can be treated in 2D gaseous phase only, fitting with the scope the present thesis. The exact geometries and operating conditions will be used in the ML input and the results are treated and compared with experimental visualization results. Here, the purpose is mainly qualitative, which is in line with the main objective of the thesis. Stable flows are considered. However, unstable cases could be foreseen to assess the capability of the ML approaches to catch the critical cases of industrial configurations.

Methodologically, a classical approach is firstly adopted, consisting on considering one configuration for the database and training the ML algorithm with it to synthetize flow fields from an input geometry of the same configuration. A first performance assessment is carried out. Then, the database is altered with other configurations. The performances of the ML algorithm is assessed again, giving a first measurement of the effects of geometry configuration on the flow field generations of the ML algorithm. According to the obtained results, more complex approaches will be considered.

The first part of thesis will be dedicated to building the training data using CEDRE's simulations and generalization framework at ONERA Palaiseau's center. The frozen database is firstly built to assess the effects of geometry on aerodynamics in frozen flows generated by a first design of the ML algorithms. Then the premixed database is used to start the study of the reacting flows. The MICAEDI results will be considered in the validation process of the database and ML design. The last database to build is the diffusion flame database. Several meetings with DLR's team are planned to build the first steps of ML algorithms. The second part of the thesis will be dedicated to the ML development and assessment of the database strategies and the chosen methodology, at DLR Cologne's center.

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Collaborations envisagées : DLR/ONERA

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