Understanding and Predicting Hydrogen Combustion

Detailed program

Current EU decarbonization strategies are promoting the use of green hydrogen across different sectors from energy and power generation to transportation i.e., automotive, marine, or aerospace. In these applications, the hydrogen is converted directly into electricity by using fuel cells or heat by combustion. In the Center of Excellence in Combustion (CoEC), new methodologies for the simulation of these technologies in future Exascale systems are developed and applied to some fundamental challenges in these sectors.

Within this frame, this training course brings together a set of experts to discuss the challenges and opportunities for the utilization of hydrogen and provide the attendees with some fundamental understanding of the physics and methodologies that can be used to simulate hydrogen flames in practical applications.

The course is divided into three main parts:

1. Description of the context from production, and storage to utilization.
2. Theory and fundamentals of H2 combustion.
3. Numerical methods and tools for post-processing and analysis.

This training is split into 3 days from Monday, 18th of December, to Wednesday, 20th of December, and is hosted at the Barcelona Supercomputing Center (BSC), which is a national research facility managing the supercomputer MareNostrum 4. During these days, discussions on the use of hydrogen to assist in the decarbonization strategies of the EU for different sectors will be discussed across the three days along with lectures describing the modelling and simulation requirements of different application. The contents of the program are given below:

18/12/2023 – Day 1: Role of Hydrogen in the Energy and Transportation Green Transition

This session introduces the context and market opportunities of hydrogen across different sectors from production to utilization. External speakers from industry and academia will give lectures on the application of hydrogen for power generation and transportation.

Part I: The Hydrogen Economy: A Background

9:00 - 9:15 *Welcome and introduction*

9:15-10:15 **The Role of Hydrogen in a Sustainable Energy System**
Albert Tarancon (IREC)

10:15 - 11:15 **Fuel Cells and Their Applications**
Maria Serra (CSIC-UPC)

11:15 - 11:45 *Coffee break*

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Part II: Utilization of Hydrogen by Industrial Sector

11:45 - 12:30 **Challenges and Current Developments for Hydrogen Ground Mobility**
Olivier Laget (IFPEN)

12:30 - 13:15 **Hydrogen-powered Aircraft - Introduction to the Main Challenges**
Anais Marie Gay (Airbus)

13:15 - 14:45 *Lunch*

14:45 - 15:30 **Challenges for Ammonia Engines**
Christine Rouselle (University of Orléans)

15:30 - 16:15 **Clean Hydrogen Power Generation in Gas Turbines**
Lukasz Panek (Siemens AG)

16:15 - 17:00 **Potentials and Challenges of Hydrogen to Decarbonize the Steel Sector**
Sébastien Caillat (Fives Stein)

17:00 - 17:15 **Conclusions and Outlook**

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19/12/2023 – Day 2: From Theory to Simulation of Hydrogen Flames

This session introduces the fundamentals of hydrogen combustion from theory to simulations using high-fidelity methods. It includes lectures and hands on activities where the students can utilize the physical models and numerical methods described in the lectures.

9:30 - 11:00 **Theory and Fundamentals of H2 Combustion I**
Prof. Heinz Pitsch (RWTH Aachen University)

This lecture aims to highlight the effects of hydrogen thermo-physical properties on the combustion process. First, the hydrogen combustion chemistry will be discussed in the context of the high burning velocities. Then, the focus will be on hydrodynamic and thermo-diffusive instabilities including the physical mechanisms behind them, the impact on laminar premixed flames and on lean turbulent flames, and the possibility of modelling such non-linear phenomena.

11:00 - 11:30 Coffee break

11:30 - 13:00 **Theory and Fundamentals of H2 Combustion II**
Prof. Thierry Poinsot (IMFT)

In this lecture, all the necessary numerical and modelling aspects for the simulation of hydrogen flames will be reviewed. This will include chemical models, transport models, as well as turbulence and flame / turbulence interaction models in the context of Large Eddy Simulation (LES). The various flame combustion regimes will be described, and some particular flame behaviours will be highlighted, like flame-wall interaction, and flame stabilization. The lecture will end with the numerical study of some technical challenges raised using hydrogen as a fuel in practical systems.

13:00 - 14:30 Lunch break

14:30 - 16:00 **Numerical Methods for Turbulent Reactive Flows** - Prof. Ananias Tomboulides (Aristotle University of Thessaloniki) and Dr. Daniel Mira (Barcelona Supercomputing Center)

This part provides an overview and perspective on the computational requirements to simulate turbulent flames in the context of DNS and LES. It will introduce different levels of modelling like RANS, LES, and DNS, solution approaches low Mach or fully compressible, discretization strategies, and high-order methods, with an overview of different algorithms and strategies that can be used to accelerate the computations. The last part of the lecture will introduce some practical applications of LES for hydrogen combustion with a focus on the numerical and modelling aspects described in previous lectures.

16:00 - 17:30 **Hands-on Exercises I**

This hands-on session is focused on the computation and characterization of hydrogen flames using the Cantera software. The effects of chemistry and transport will be discussed in the context of 1D flames with emphasis on the chemistry description and the flame structure.

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20/12/2023 – Day 3: Understanding and Predicting Hydrogen Flames

9:30 - 11:00 **Hands-on Exercises II**

This hands-on session is focused on the study of numerical methods applied to the solution of reactive flow simulations. The students will have the opportunity to select different numerical methods and explore their influence on the accuracy and cost of the simulations in the context of hydrogen flames. Laminar flames and weakly turbulent flames will be used as examples.

11:00 - 11:30 Coffee break

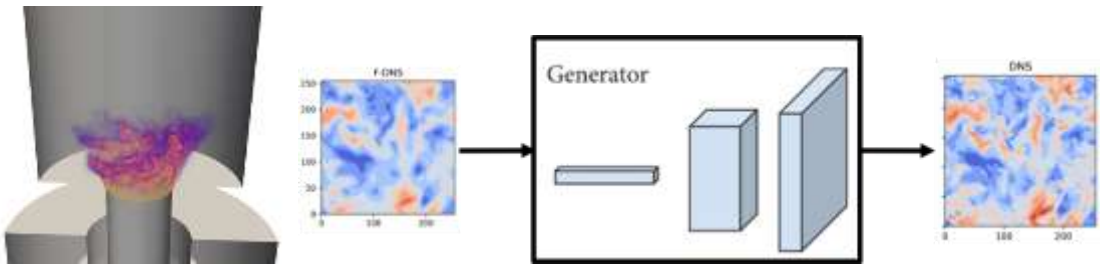
11:30 - 13:00 **Data-driven Analysis of Turbulent Reactive Flows** – Prof. Alessandro Parente (Université libre de Bruxelles) and Alberto Procacci (Université libre de Bruxelles)

The use of machine learning algorithms to predict the behaviors of complex systems is booming. The present talk reviews some open opportunities for applying data-driven, reduced-order modelling to tackle some of the challenges associated with combustion modelling: the large dimensionality of detailed chemical mechanisms and the complex turbulence-chemistry interactions. Examples of feature extraction in turbulent combustion data, empirical low dimensional manifold identification, classification, regression, and reduced-order modelling are provided.

13:00 - 14:30 Lunch break

14:30 - 17:30 **Hands on Exercises III**

The last hands-on session is focused on the study of the methodologies used for the analysis of massive databases. These methodologies are a common feature to be able to automatically extract non-linear dependency among the quantities of interest. The students will have the possibility to learn more about the structure of data-driven algorithms, explore the effects of tuning parameters on the models extracted and their accuracy. Laminar flames and weakly turbulent flames will be used as examples.



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