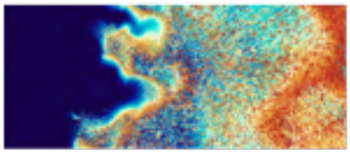
CERFACS

EUROPEAN CENTRE FOR RESEARCH AND ADVANCED TRAINING IN SCIENTIFIC COMPUTING

Ph.D. Students' Day (JDD 2022)

Thursday 30 June 2022

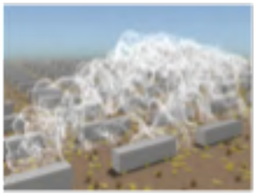
Algo-Coop

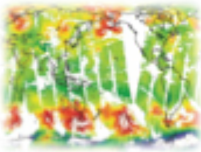


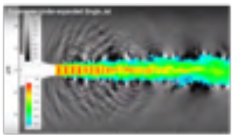
Climate Modeling

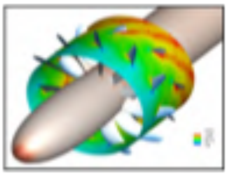
&

Global Change

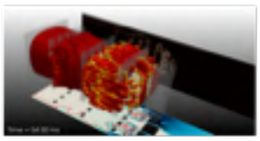


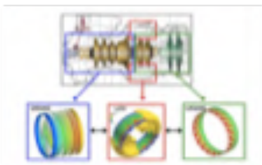


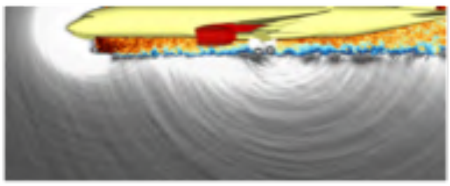




Computational Fluid Dynamics







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09:00	**Welcome Speech: Catherine Lambert**			
Ma thèse en 3 minutes		Chair : Matthieu Pouget		
09:15	DURANTON Thibault	*Advanced LES Modeling of Multiperforated Plates for New Generation Aircraft Engines*	p. 5	CFD
09:20	CANCES Mathieu	*Low-Order Modeling for the Prediction of Thermoacoustic Instabilities*	p. 5	CFD
09:25	GIOUD Thibault	*Injection Modelling in LOx/GCH4 Rocket Engines with a Diffuse Interface Method*	p. 6	CFD
09:30	DEFONTAINE Théo	*Extension of Discharge Forecasting Lead-Time with Machine Learning*	p. 6	GLOBC
09:35	DABAS Jérôme	*Development of LES-based Engineering Models for the Design and Control of Floating Off-Shore Wind Turbine Farms*	p. 7	CFD
09:40	BRIANT Jérémy	*Multi-Fidelity Ensembles for High Performance Ensemble-Variational Data Assimilation for Earth Systems*	p. 7	ALGO
09:45	VIGOT Gabriel	*Development of Numerical Tools for Hall Effect Thruster Design*	p. 8	CFD
09:50	PEDEN Benoît	*Large Eddy Simulation of Atomization in Evaporating and Reactive Conditions*	p. 8	CFD
09:55	LESAFFRE Thomas	*Alternative Fuels Combustion Modelling and Simulation*	p. 9	CFD
10:00	BAUR Susanne	*Analysis of Spatially Resolved Solar Radiation Modification Impacts using an Impulse-Response Emulator*	p. 9	GLOBC
10:05	**Voting for the best “Ma thèse en 3 minutes” presentation**			

Session 1		Chair: Olivier Thual		
10:20	FOUDAD Mohamed	*Impact of Climate Change on Clear-Air Turbulence for Aviation*	p. 11	GLOBC
10:25	HOK Jean-Jacques	*Modelling of Chemistry-Turbulence Interactions for the Large-Eddy Simulation of Explosion*	p. 11	CFD
10:30	MEZIAT RAMIREZ Francis	*Large Eddy Simulations of Hydrogen/Air Gas Explosions in Big-Scale, Complex Geometries*	p. 12	CFD
10:35	GENTIL Yann	*Modelling of Combustion Noise in Turbines*	p. 12	CFD
10:40	STREMPFL Patrick	*LES of Flow and Combustion in A Rotating Detonation Engine Coupled to a Turbine*	p. 13	CFD
10:45	VANBERSEL Benjamin	*Adaptive Mesh Refinement Methods for Large-Scale Simulations of Gas Explosions.*	p. 13	CFD
10:50	GIANOLI Thomas	*Turbomachinery S-Duct Simulation using the Lattice-Boltzmann Method*	p. 14	CFD
10:55	PEYRON Mathis	*Latent Data Assimilation by using Deep Learning*	p. 14	ALGO
11:00	**40 min coffee break and poster session n°1: Foudad, Hok, Duranton, Gentil, Defontaine, Gioud, Gianoli**			

Session 2		Chair: Olivier Thual		
11:40	COULON Victor	*AI-Assisted Turbulent Combustion Models for Sustainable Hydrogen Combustion in Helicopter Engines*	p. 16	COOP
11:45	GAUCHERAND Jessica	*Numerical Investigation of a Carbon Free Fuel for Internal Combustion Engines*	p. 16	CFD
11:50	GARNIER Felicia	*LES of Hydrogen Jet Flames with and without Cross Flow*	p. 17	CFD
11:55	NAESS Thomas	*Prediction of Pollutants Production in Aeronautical Engines*	p. 17	CFD
12:00	LUMET Eliott	*Data Assimilation from Mobile Sensors for the Study of Pollutant Dispersion At Micro-Scale*	p. 18	GLOBC
12:05	COSTES Raphaël	*Wall Modeling for the Prediction of Heat Transfers in an Aeronautical Combustion Chamber*	p. 18	CFD
12:10	VILLARD Jean	*Simulation of the Combustion of Metal Particles*	p. 19	CFD
12:15	ZAPATA USANDIVARAS Jose Felix	*Surrogate Models Based on LES for the Multi-Disciplinary Design of Liquid Rocket Engines*	p. 19	CFD
12:20	MOCQUARD Clément	*Large Eddy Simulation of Afterburners in Fighter Aircraft Engine*	p. 20	CFD
12:25	WERNER Paul	*Aerothermal Modelling of Bore-Cooling Cavities using the Lattice-Boltzmann Method*	p. 20	CFD
12:30	**Lunch**			

13:15	**45 min poster session n°2: Naess, Lumet, Zapata, Villard, Werner, Mocquard**			
Session 3		Chair: Laurent Gicquel		
14:00	RUIZ GIRONA Julia	*Projection of Regional Ocean Circulation Climate Change in the Pacific Est: Implications for Marine Associated Ecosystem Services*	p. 22	GLOBC
14:05	VARGAS RUIZ Héctor	*High Performance Simulations of Industrial Gas Turbines Decarbonization through H2/NH3/CH4 Mixtures*	p. 22	CFD
14:10	ANTOLIN William	*Improvement of the Representation of the Fuel for Fire/Atmosphere Coupled Modeling for the Simulation of Wildfires*	p. 23	GLOBC
14:15	ALAS Rémi	*Data-Driven Atmospheric Wall Models for Unmeshed Topologies*	p. 23	CFD
14:20	CIZERON Mehdi	*Wall Modeling for Large-Eddy Simulations of Turbomachinery Flows*	p. 24	CFD
14:25	EL MONTASSIR Rachid	*Hybrid Physics-AI Approach for Cloud Cover Nowcasting*	p. 24	ALGO
14:30	HAMMACHI Riwan	*Numerical Investigation of Laminar Flow Control of Boundary Layers with Wall Porous Coatings*	p. 25	CFD
14:35	**25 min coffee break**			

Session 4		Chair: Catherine Lambert		
15:00	SANKURANTRIPATI Shriram	*High Fidelity Simulations to Study the Propagation of Airborne Viruses in Closed Environment*	p. 27	CFD
15:05	ROULAND Nathanaël	*Modelisation and Simulation of Enriched Hydrogen Turbulent Flames*	p. 27	CFD
15:10	HOLZER Markus	*Code Generation in A Lattice Boltzmann Framework for Exascale Computation*	p. 28	COOP
15:15	DETOMASO Nicola	*LES Simulation of Constant Volume Combustion*	p. 28	CFD
15:20	GOUX Olivier	*Accounting for Correlated Observation Error in Variational Ocean Data Assimilation: Application to Wide-Swath Altimeter Data*	p. 29	ALGO
15:25	COUDRAY Alexandre	*Modeling and Simulation of SAF (Sustainable Aviation Fuel) Combustion Including Soot Production in Aeronautical Engine Conditions*	p. 29	CFD
15:30	SALLES Suzanne	*Impact of Climate Change on Aviation: Uncertainty Cascade linked to Climate and Engine Modelization on the Take-Off Phase of a Commercial Aircraft.*	p. 30	GLOBC
15:35	CONCHA Emilio	*Meridional Modes of the Southern Hemisphere: Triggering Mechanisms and Sensitivity to Mean State Changes*	p. 30	GLOBC
15:40	**Voting for best poster and results of the votes**			
16:00	**Closing Speech: Catherine Lambert**			

Ma thèse en 3 minutes

Some students have chosen to do their presentation under the "Ma thèse en 3 minutes" format, which is a theatrical science communication exercise. They entered a specific training course given by Dr. Matthieu Pouget, who holds a PhD in Performing Arts from the Université de Toulouse and is a professor at the Conservatoire d'art dramatique de Toulouse. He guided them throughout the process of writing the script, creating their performance, and learning how to communicate their research subject to a wide audience in the format of the national competition "Ma thèse en 180 secondes".

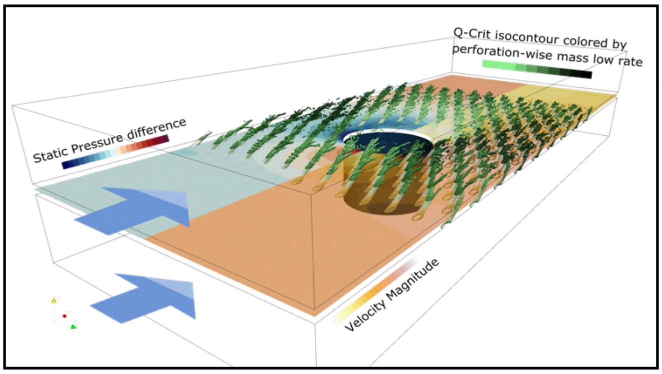
The presentations will be in French. The participants who have prepared a poster will move on to a regular poster session in English.

Thibault Duranton

09:15 - Poster 11:00

Advanced LES Modeling of Multiperforated Plates for New Generation Aircraft Engines

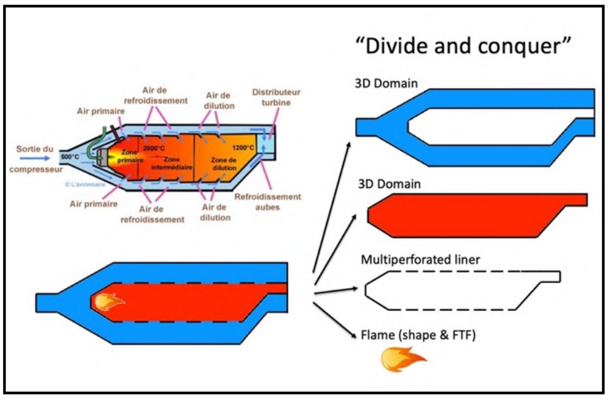
To respect current and incoming environmental regulations, aeronautical engine manufacturers are in constant need of improving gas turbines efficiency. By increasing the pressure ratio of the compressor, the overall efficiency is improved but the temperature of the burnt gases in the combustion chamber increases, undermining the integrity of the walls. To deal with it, walls are perforated by thousands of submilimetric holes generating an effusion film cooling. To reduce computational and engineer costs, multiperforations must be modeled. To enhance the current low cost multiperforation model and prevent local damage from the flame, the non-uniform pressure drop field across the plate holes is now to be taken into account to properly reproduce the mass flow repartition along the plate.



Mathieu Cances

09:20

Low-Order Modeling for the Prediction of Thermoacoustic Instabilities



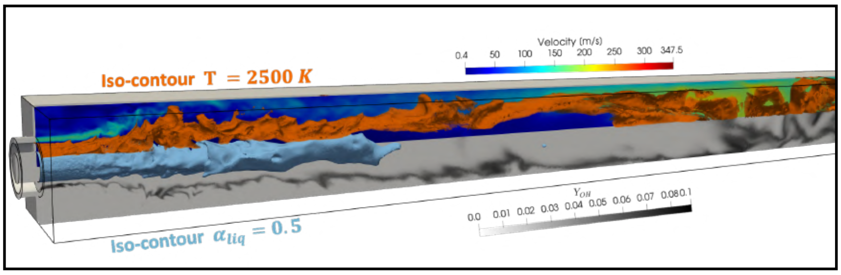
Thermoacoustic instabilities are a major concern for industrial as SAFRAN, they could have destructive effects on gas turbines and combustion chamber. Understanding these instabilities required a solid comprehension of the coupling between the acoustic waves and flames dynamic. A new method started to be developed 3 years ago, with the work of C.Laurent (CERFACS), and provide positive and consistent results. Following this method, a global system such as combustion chamber, can be decomposed in elementary sub-domains, such as a 3D geometry, a flame, a multiperforated liner, etc. Subdomains are characterized by different system of equations (acoustic equations) and then connected each other in order to reconstruct the global system. Thermoacoustic modes are finally computed from the matrix of the assembled system.

Thibault Gioud

09:25 - Poster 11:00

Injection Modelling in LOX/GCH4 Rocket Engines with a Diffuse Interface Method

Liquid propellants rocket engines feature a liquid injection which atomizes to feed the turbulent flame. This atomization has a strong impact on the subsequent flame structure and should be accurately described in numerical models. To represent liquid injection and atomization in a computationally-efficient way in 3D calculations, a diffuse interface method relying on a 3-equations multi-fluid model and accounting for surface tension forces has been implemented in the LES AVBP solver. The PhD thesis intends to assess this methodology on both non-reactive and reactive test-cases representative of LOx/GCH4 engines. Comparisons against experimental measurements performed at Technical University of Munich (TUM) are conducted for the pressure losses and wall heat fluxes. Future work will focus on the implementation of an Eulerian-Lagrangian transition model for primary atomization.



Théo Defontaine

09:30

Extension of Discharge Forecasting Lead-time with Machine Learning

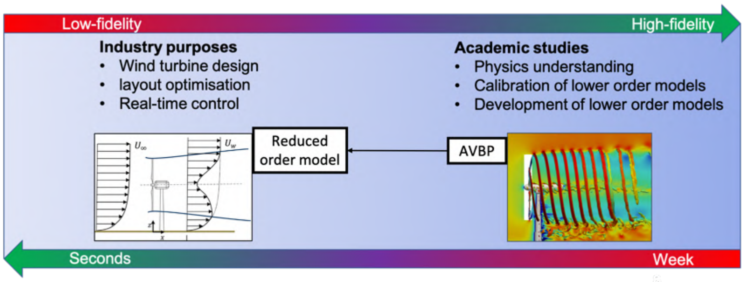
Flood prediction is still nowadays a thorny problem to assess. Hydraulic simulation techniques have proven their usefulness when the topology of the field is well defined. But, when the topology is not well known, other simpler empirical lag and route models are used. The Toulouse's Garonne basin is in such a case. Those models have limitations when new unseen floods happen. The aim of this PhD Thesis is to extend the discharge forecasting lead time of the lag and route models used in Toulouse by means of Machine Learning. The case is a challenge to learning techniques due to the low number of floods events in the Toulouse basin.

3

Jérôme Dabas

09:35

Development Of LES-Based Engineering Models for the Design and Control of Floating Offshore Wind Turbine Farms



Wind farm flows are highly turbulent and feature interacting structures on a wide range of scales that impact their power production and efficiency. In particular, the wake produced by a wind turbine is a region of low mean velocity and increased turbulence intensity that reduces the power production and the lifetime of the wind turbines located inside. In the context of floating offshore wind farms, additional complexity is added to the wake structure due to the coupling between the waves and the wind turbine platform. The wall-modelled LES approach can be used to capture the main features of wind turbine wakes, yet the computational cost of this approach is not compatible with the simulation of a complete wind farm. Nonetheless, these high-fidelity simulations are required to develop and calibrate accurate lower order models compatible with industrial use. The purpose of this thesis is to develop such reduced order models with wall-modelled LES of wind turbines subjected to wave motions.

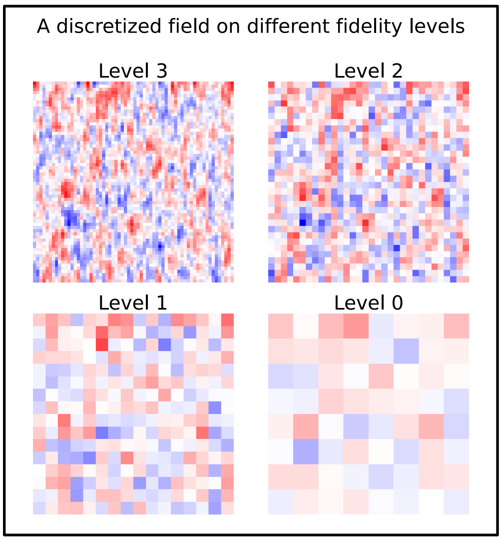
3

Jérémy Briant

09:40

Multi-Fidelity Ensembles for High Performance Ensemble-Variational Data Assimilation for Earth Systems

In data assimilation algorithms used for geosciences, the background error covariance matrix B is estimated using an ensemble of realisations. But the computation of a single realisation is costly and thus the ensemble size is very limited, which cause the estimation to have a large sampling error. Multi-level Monte Carlo methods aims to reduce this sampling error by combining high fidelity realisations which are cosly but accurate with lower fidelity realisations which are cheaper but also less accurate. We are working to adapt those multifidelity methods to the estimation of B and also on improving them by studying possible links with multigrid methods.

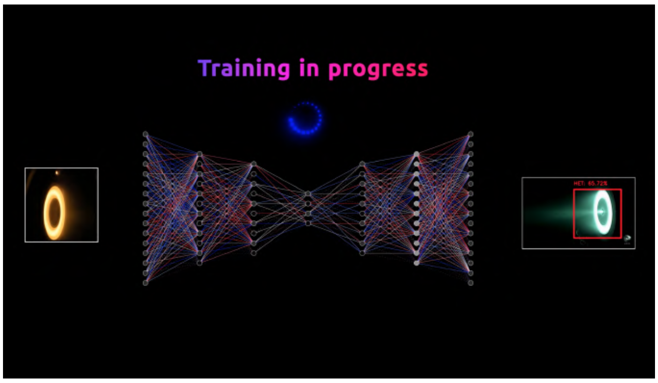


Gabriel Vigot

09:45

Development of Numerical Tools for Hall Effect Thruster Design

Machine Learning has recently expanded its applications in many areas further than initially conceived, like climate and atmospheric sciences, neurosciences, fluid mechanics, cognitive sciences, biology, chemistry, and physics. In this presentation, we will discuss the impact of machine learning in the world of physical numerical simulations and the prospects of solving the Poisson equation using machine learning for physical purposes. This presentation will also illustrate the importance of using machine learning, for instance, to reduce drastically the computation cost of solving elliptic problems and enhancing computational solving. Solve the Poisson equation will enable us to decode physical equations that depend upon it, like plasma physics, fluid mechanics, and for my thesis: Hall-effect thrusters.

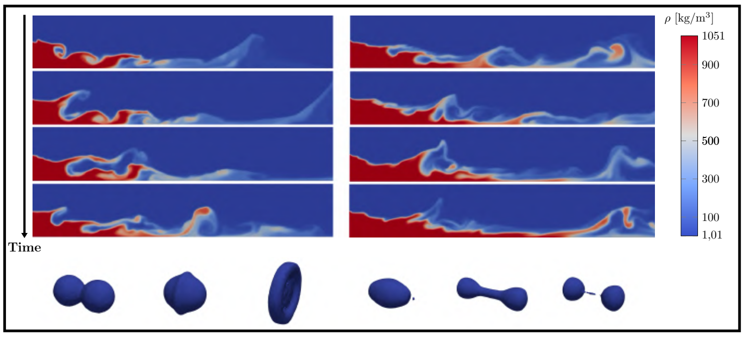


Benoît Péden

09:50

Large Eddy Simulation of Atomization in Evaporating and Reactive Conditions

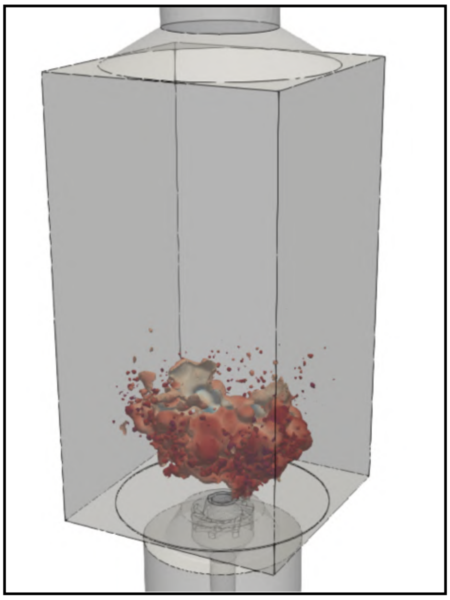
Combustion in aeronautical engines is based on fuel atomization from liquid core into spray. This phenomenon allows fuel evaporation and mixing with surrounding air. The numerical prediction of these atomization processes remains a challenge today because the mesh resolution to capture the liquid-gas interface has to be very fine what will induce high CPU cost. The primary atomization is for now ignored in most of Large Eddy Simulations and models are used for the liquid part. The purpose of this PhD is to predict primary atomization using a diffuse interface method, as well as a recently developped Euler-Lagrange transition model. The considered thermo-dynamics is extended to allow proper NSCBC boundary conditions, as well as evaporating and reactive conditions.



Thomas Lesaffre

09:55

Alternative Fuel Combustion Modelling and Simulation



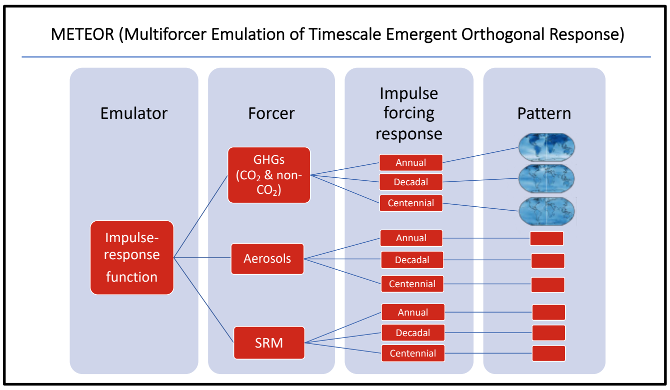
The international community aims at reducing greenhouse gas emissions from aviation to reach climate targets. The use of new energy sources seems inevitable as air traffic growth is expected to have a greater impact than the projected technology improvements. A short-term solution is the use of alternative drop-in fuels, also called Sustainable Aviation Fuels (SAFs) or simply bio-fuels. The objective of this PhD is to improve existing models to be able to simulate the combustion of such fuels within a LES framework. Two main characteristics of SAFs must be taken into account: they are liquid when they are injected in a combustion chamber, and they are composed of many different species. Therefore, chemistry and two-phase flow effects are particularly studied during this PhD.

Susanne Baur

10:00

Analysis of Spatially Resolved Solar Radiation Modification Impacts using an Impulse-response Emulator

Solar Radiation Modification (SRM) is a form of geoengineering that intends to artificially lower global climate change impacts by modifying the radiative energy budget of the Earth system. Proposed techniques include stratospheric aerosol injection (sulfur-SRM) or the placement of reflective objects in space (solar-SRM). The aim of this work is to look at global and regional impacts of solar- and sulfur-SRM by running targeted SRM-simulations with the CNRM-ESM2-0 Earth-system model and using the output to train a surrogate model, the emulator METEOR-SRM (Multiforcer Emulation of Timescale Emergent Orthogonal Response). The novelty of METEOR is the ability to emulate gridded surface climate response to greenhouse-gas overshoot-pathways and therefore enables the analysis of SRM implementation in various greenhouse-gas scenarios.



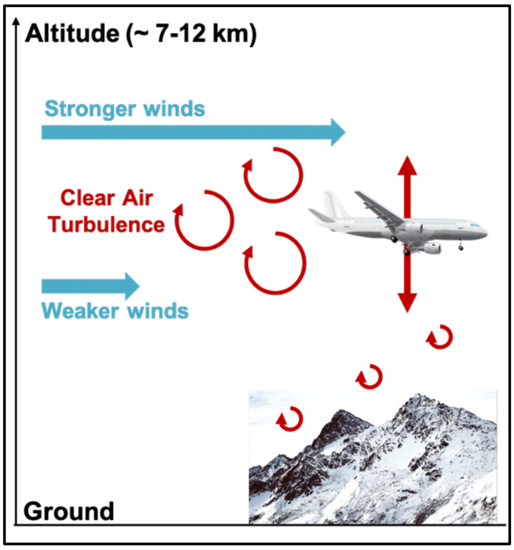
SESSION 1

Mohamed Foudad

10:20 - Poster 11:00

Impact of Climate Change on Clean-Air Turbulence for Aviation

Airplanes spend about 1% of cruise time in Moderate-Or-Greater (MOG) Clear-Air Turbulence (CAT), which is defined as any turbulence occurring in the atmosphere away from a visible convective activity and which is particularly difficult to detect. MOG CAT events can injure passengers, cause structural damage to planes, and induce considerable economic loss. This PhD thesis aims at assessing CAT sensitivity to global warming. The first stage consists in analyzing CAT trends in the present climate in atmospheric reanalysis and investigate future CAT changes by using climate models. The second stage will focus on designing a dynamical downscaling procedure through a coupling of different atmospheric models to characterize changes in severe CAT episodes at finer scales.

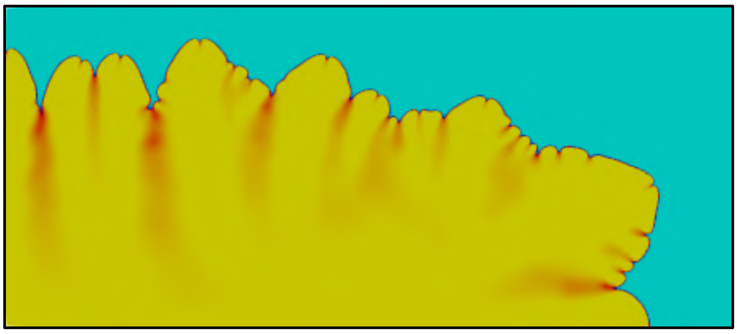


Jean-Jacques Hok

10:25 - Poster 11:00

Modelling of Chemistry-turbulence Interactions for the Large-Eddy Simulation of Explosions

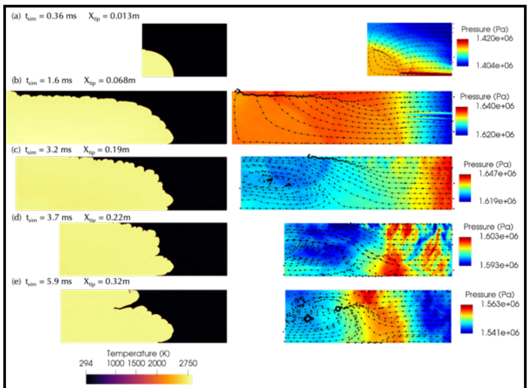
The use of hydrogen for energy generation in combustion engines has become attractive to many industrials as it is decarbonated. However, this combustible exhibits wider flammability limits than usual fuels and the relatively small size of H2 molecules make leakages and explosions likelier. Part of the LEFEX (Large-Eddy Simulation for EXplosions) project, my PhD thesis aims at providing a better understanding of the impact of H2 chemical properties on its combustion. In particular, attention is paid on the response of H2-air flames to stretch due to their non-unity Lewis number. Besides, my work will also analyze the formation mechanisms of flame front instabilities for lean hydrogen flames. Influence of both phenomena on flame acceleration will be assessed.



Francis Meziat Ramírez

10:30

Large Eddy Simulations of Hydrogen/Air Gas Explosions in Big-scale, Complex Geometries



Finger flame propagation in a tube explosion

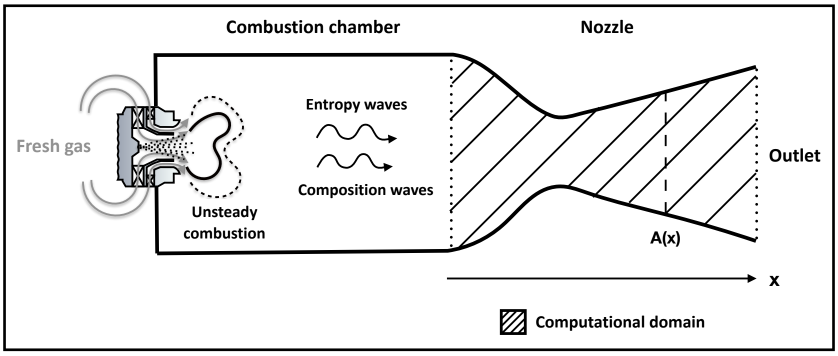
Large Eddy Simulations (LES) coupled with High Performance Computing have shown great potential to reproduce the flow characteristics of hydrogen explosions: a priority for many industrial sectors due to the characteristics and the raising importance of this fuel. However, the simulation of big-scale, non-academic configurations is still a challenge in the field. The objective of this thesis will be to develop the last algorithmic and modeling elements required for the simulations of hydrogen/air explosions in big-scale, complex geometries with AVBP. New metrics for Adaptive Mesh Refinement on fast hydrogen flames and LES models for flame-turbulence interaction of hydrogen/air flames will be studied. Finally, the developments will be validated on big-scale, complex configurations.

Yann Gentil

10:35

Modelling of Combustion Noise in Turbines

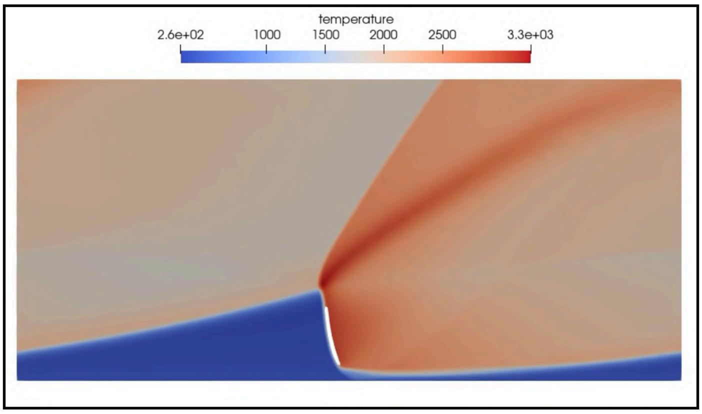
Indirect noise is created when entropy waves cross turbine stages and is a significant contribution of gas turbine engines. Composition noise is part of indirect combustion noise mechanism, due to waves of chemical composition entering the turbine stage. Its importance and definition are revisited here: a new decomposition of entropy is proposed, which provides an independent set of variables to describe an ideal, non-reacting gas mixture. Composition noise is actually shown to be caused by the acceleration/deceleration of fluctuations of the specific gas constant. This new theory is verified by comparing the model predictions with direct numerical simulations of nozzle flows in which temperature and composition fluctuations are pulsed separately.



Patrick Strempfl

10:40

LES of Flow and Combustion in a Rotating Detonation Engine coupled to a Turbine



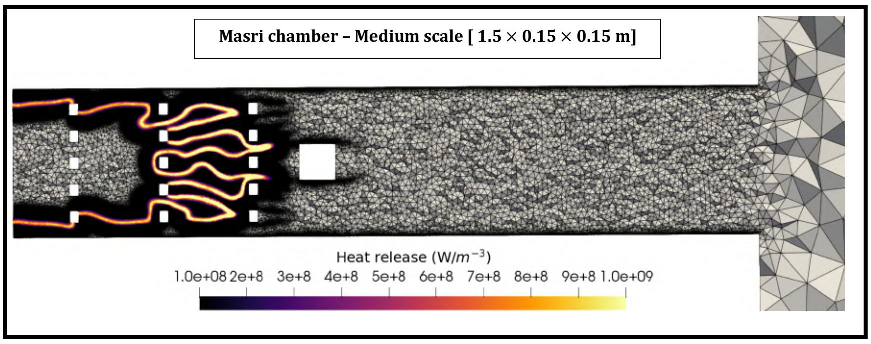
Rotating detonation engines (RDE) are a novel pressure gain combustion (PGS) system for thrust generating devices such as rocket engines or generation of thermal energy for gas turbines. In theory RDEs are capable to deliver higher thermal efficiency than conventional combustion systems. In the last years, the interest in these combustors has increased significantly, which led to the emergence of a number of experimental setups worldwide dedicated to understanding the performance of RDEs. The utilization of Large Eddy Simulations (LES) can play an important role to gain insight into the flow phenomena in RDEs, such as mixing, reaction or losses.

Benjamin Vanbersel

10:45

Adaptive Mesh Refinement Methods for Large-Scale Simulations of Gas Explosions.

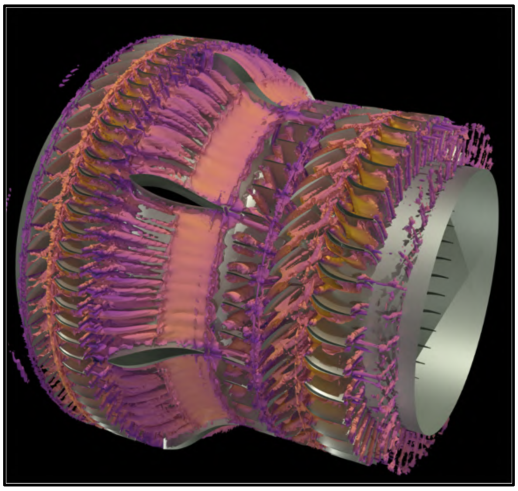
The most limiting parameter in numerical simulation is computational time. To capture all the physics of a turbulent flame, the mesh needs to be refined enough to solve flame and turbulence. This mesh can reach several billion cells in industrial configurations. These simulations are unaffordable in the context of LES. That is why mesh adaptation is used. It aims to refine the mesh in regions where the important quantities are detected and to coarse it otherwise. In the case of explosions, the mesh adaptation needs to be dynamic because the flame and turbulence evolve in the whole domain. The strategy is to follow these quantities and develop criteria to trigger mesh adaptation to keep an acceptable computational cost.



Thomas Gianoli

10:50 - Poster 11:00

Turbomachinery S-duct Simulation Using the Lattice-Boltzmann Method

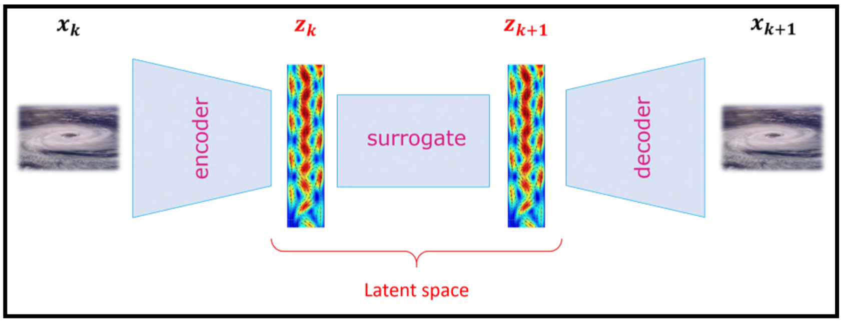


In the last years, the bypass-ratio of modern aero-engines has continuously increased to improve engine efficiency, forcing the radial offset between the Low-Pressure Compressor and the High-Pressure Compressor. However, these two parts are connected via an annular S-shaped duct which is an aerodynamic passage used to redirect the fluid from one radial position to another without significantly altering the flow direction. The designer's goal is to have an S-duct as short as possible for weight savings aspect while maintaining a low level of losses and distortion. However, classical RANS computations have shown to underestimate the losses, hence the desire to switch to a fast high-fidelity method, the Lattice Boltzmann Method (LBM).

Mathis Peyron

10:55

Latent Data Assimilation by using Deep Learning



Performing Data Assimilation at a low cost is of prime concern in Earth system modeling. Capitalizing on the ability of Neural Networks techniques for approximating the solution of PDE's, we incorporate Deep Learning methods into a DA framework. More precisely, we exploit the latent structure provided by autoencoders to design an Ensemble Transform Kalman Filter with model error in the latent space. Model dynamics are also propagated within the latent space via a surrogate neural network. This novel ETKF-Q-Latent (ETKF-Q-L) algorithm is tested on a tailored version of Lorenz 96 equations along with the quasi-geostrophic model. Numerical experiments evidence that the ETKF-Q-L approach both reduces the computational cost and provides better accuracy than state of the art algorithms.

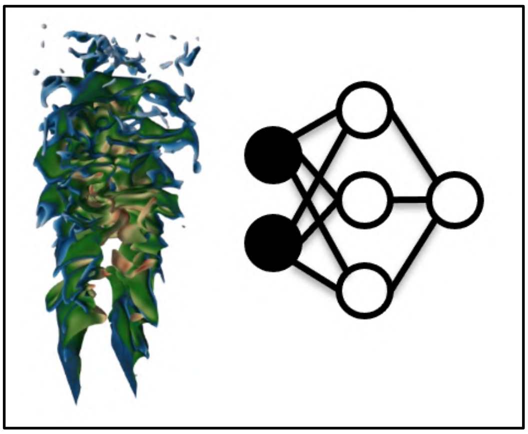
SESSION 2

Victor Coulon

11:40

AI-Assisted Turbulent Combustion Models for Sustainable Hydrogen Combustion in Helicopter Engines

Combustion wears the double hat of being a source of harmful polluting emissions and a promising technology for the 2050 horizon. Hydrogen is coming to the forefront thanks to its interesting physical properties, making it possible to use it in the aeronautical sector in particular. However, the dynamics of these flames are totally different because of the very low Lewis number. It is therefore more than necessary to develop a robust subgrid model for the LES formalism still widely used. To this end, the objective is to explore the path of Artificial Intelligence in a context of supervised learning in order to use neural networks to infer the highly non-linear link between both chemical kinetics and turbulence phenomena.

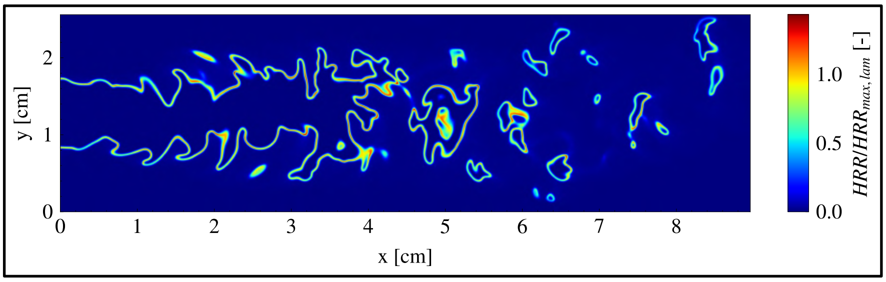


Jessica Gaucherand

11:45

Numerical Investigation of a Carbon Free Fuel for Internal Combustion Engines

Ammonia (NH_3) is a fuel of interest in the hydrogen economy framework as it is an efficient hydrogen carrier. However, it has a low laminar burning velocity. But to counteract this, it is possible to make fuel blends with fuels such as hydrogen, and the mixture can be tuned to match the properties of well-known flames such as the laminar flame speed of a methane-air flame. Investigations are carried out to study an ammonia/hydrogen-air flame, first looking into a one-dimensional flame, then a two-dimensional laminar flame in a Bunsen burner like configuration, and finally a 3D turbulent Bunsen burner configuration. This investigation is carried out using Cantera and direct numerical simulation and uses analytically reduced chemistry.



Felicia Garnier

11:50

LES of Hydrogen Jet Flames with and without Cross Flow

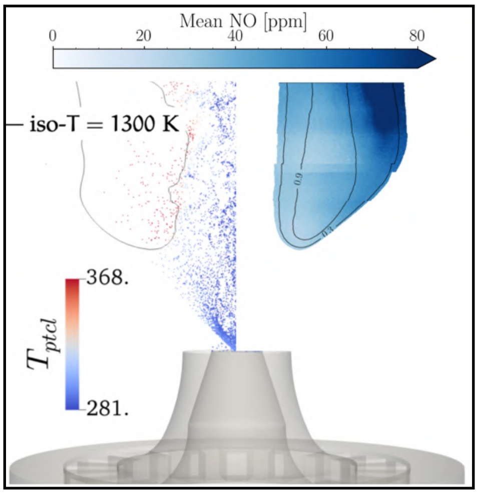
The introduction of hydrogen in aircraft raises significant issues in terms of safety. The present PhD aims to address a specific safety scenario: leaking fuel leading to a large hydrogen plume around an aircraft, on the ground and in flight. The resulting turbulent plume may ignite, possibly causing major damage to its surroundings. Using the compressible LES (Large Eddy Simulation) solver AVBP, various reacting and non-reacting leak configurations will be studied, and simulation tools will be developed so as to meet the numerous challenges raised by the unusual properties of hydrogen. Focuses of work include atmospheric and under-expanded releases of hydrogen, in quiescent air as well as in a crossflow.

Thomas Naess

11:55 - Poster 13:15

Prediction of Pollutants Production in Aeronautical Engines

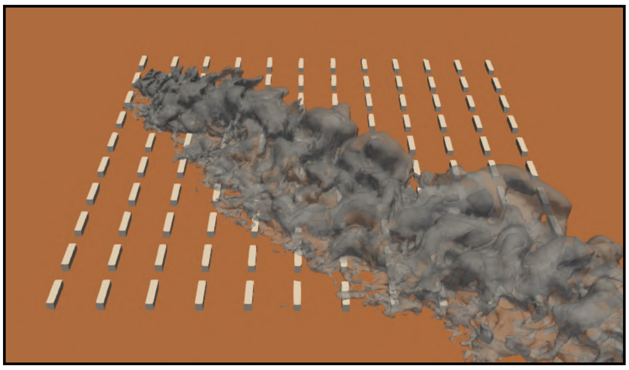
New aeronautical technologies must comply with international regulations and answer the public environmental concern about global warming and human health. In particular, focus is made on the emission of soot and NOx. Combustion in real engines implies chemistry, turbulence, and spray interaction in addition to pollutant emissions description. Reactive Large Eddy Simulation has been shown a powerful tool to understand these interactions, combining accurate chemistry (for fuel oxidation, NOx, and soot precursors) and a Lagrangian framework to describe both the fuel spray and the soot particles. This Ph.D. aims to predict NOx and soot emissions with a reasonable degree of confidence in real-like combustors. For that purpose, the confrontation of simulations with experimental measurements will assess the pollutants prediction accuracy.



Elliot Lumet

12:00 - Poster 13:15

Data Assimilation from Mobile Sensor for The Study of Pollutant Dispersion at Micro-Scale



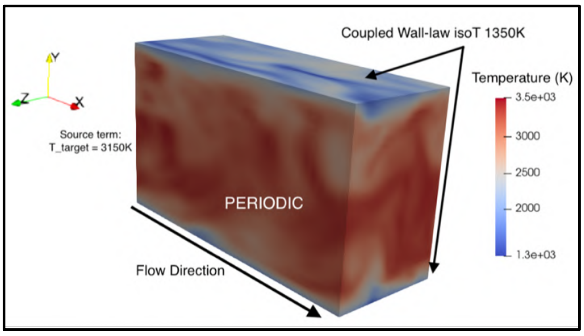
The ability to predict pollutant dispersion in the bottom part of the atmospheric boundary layer is key to monitor urban air quality, accidental exposure to pollutant or even wildfire smoke. To improve our understanding of the complex multi-physics processes at stake, we use high-fidelity, scale-resolving models. Still, important differences remain between model estimations and experimental data. The objective of this PhD is to design a data assimilation strategy to optimally combine Large-Eddy Simulation predictions and sensors measurements to reconstruct the best possible plume representation. In order to reduce even more the model uncertainties, optimal sensor placement methods are designed to take advantage of the sensor mobility to acquire the most informative data.

Raphaël Costes

12:05

Wall Modeling for The Prediction of Heat Transfers in an Aeronautical Combustion Chamber

Accurate prediction of wall heat transfer is required in Large Eddy Simulation (LES) of aeronautical combustion chambers in order to compute the wall heat flux and wall shear stress. In the industrial context, wall-modeled approaches are considered to allow an affordable computational cost by assuming several assumptions of a Reynolds Averaged Navier-Stokes (RANS) context. Wall models however involve significant couplings between numerical methods at the boundary and physical modeling. For this reason, this PhD intends to propose an accurate numerical framework to implement wall-laws in the cell-vertex, finite element context of AVBP, as well as to propose a physical model for heat transfer prediction in aeronautical combustion chambers where strong temperature gradients take place.

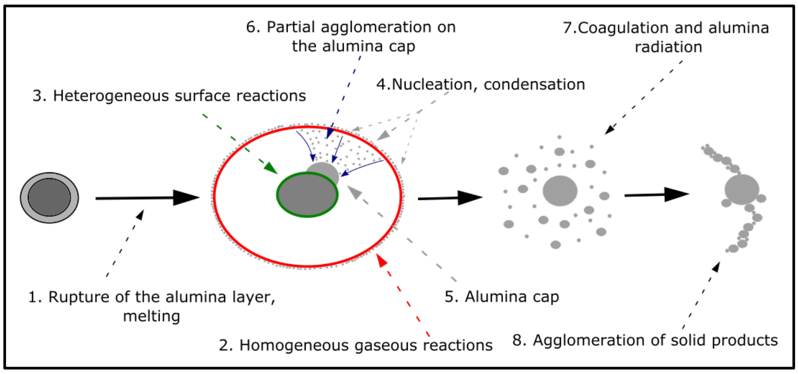


Jean Villard

12:10 - Poster 13:15

Simulation of the Combustion of Metal Particles

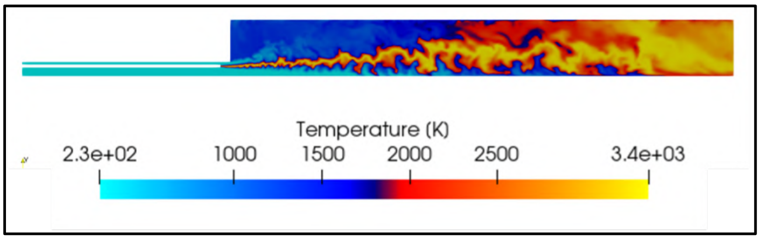
Metal as a fuel has been used in the space and arms industry for many years for its high energy density and release. This type of flame is very complex to stabilize, experimentally and numerically. Therefore, few numerical simulations exist in the literature. Recently, metal fuels have been considered as promising alternatives to fossil fuels due to their carbon free combustion process. Moreover, metal combustion products can be transformed back to fuel, effectively creating a clean and renewable energy carrier over long distances. During the first half of this PhD thesis, several physical phenomena such as surface reaction and nucleation have been added to AVBP. Thus, allowing a better numerical simulation of these capricious, yet very promising flames.



José Félix Zapata Usandivaras

12:15 - Poster 13:15

Surrogate Models Based on LES for the for the Multi-Disciplinary Design of Liquid Rocket Engines

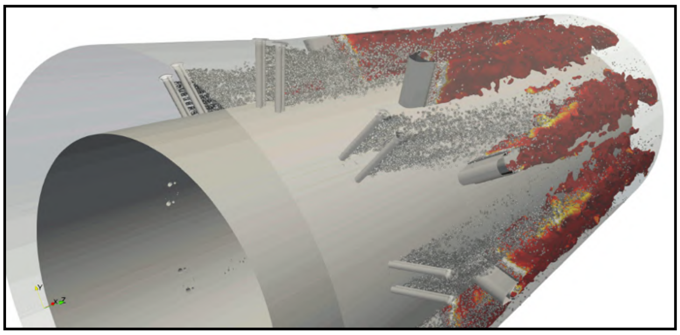


Rocket propulsion systems design is under growing pressure of reducing development costs. CFD codes for the simulation of combustion chambers can provide a low-cost alternative to experiment-driven design. Nonetheless, a holistic approach for design optimization is not yet practical, as the exploration of the entire engine design space through full-scale CFD evaluations is too expensive. Surrogate models may avoid this conundrum through fast inference times, without significant accuracy loss. The main goal of this thesis is the development of surrogate models of a rocket combustion chamber injectors plate, comprised of gaseous oxygen-methane shear-coaxial injectors. These are to be derived through the leveraging of machine-learning techniques, particularly deep learning, in combination with LES data of the target system.

Clément Mocquard

12:20 - Poster 13:15

Large Eddy Simulation of Afterburners in Fighter Aircraft Engine



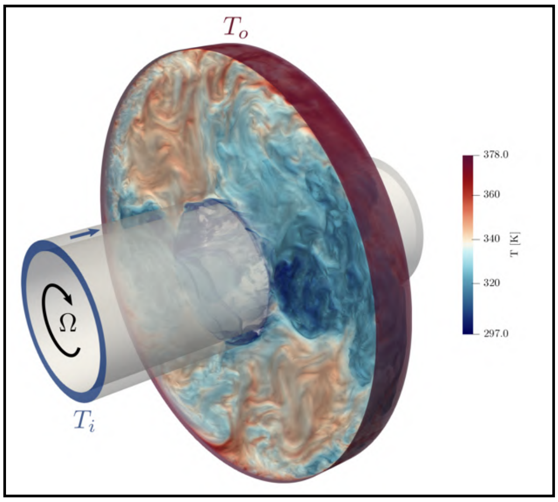
The simulation of post-combustors is a useful tool during the design phase of an after-burner. Post-combustors imply several phenomena such as liquid jets atomization and evaporation in turbulent wakes of burnt gases at elevated pressure (~ 5 bars), two-phase combustion, and high frequency transverse thermo-acoustic instability known as "screech". Large Eddy Simulations is a method which has been proven able to capture complex flame/flow/acoustic interactions as well as gaseous/liquid phase interactions. However, the coupling between these different phenomena is still an active field of research and some improvements are needed. In particular chemical schemes and combustion models must reproduce accurately auto-ignition delays which are very important in this
context.

Paul Werner

12:25 - Poster 13:15

Aerothermal Modelling of Bore-Cooling Cavities Using the Lattice-Boltzmann Method

Reduction in compressor blade clearance has improved engine efficiency for decades. However, it pertains directly to a meticulous control of the thermal dilatation of rotor disks, which is ensured by the bore-cooling system. It is composed of a cold, swirled axial throughflow and of consecutive rotating cavities where natural convection induced by centrifugal forces and large temperature gradients occurs. The LBM is perfectly suited to such unsteady flow and complex geometry but lacks maturity in modeling rotating perfect gases. The objectives are to extend the LBM in a rotating frame and validate the model on academic and experimental configurations. A major challenge is to correctly predict heat exchange through rotor disks, which may lead to optimized cooling techniques.



SESSION 3

Julia Ruiz Girona

14:00

Projection of Regional Ocean Circulation Climate Change in the Pacific Est: Implications for Marine Associated Ecosystem Services

The global ocean is a major sink of anthropogenic carbon dioxide (CO2). Current estimates of CO2 uptake contain considerable uncertainty, particularly EBUS in the Southern Hemisphere, historically least observed and sampled. Here we investigate the interannual CO2 variability in the Humboldt System, which is one of the most productive EBUS and experiences large climate fluctuations associated with El Niño-Southern Oscillation (ENSO). Due to the scarcity of historical data, particularly during extreme El Niño events, we use the Community Earth System Model (CESM) model output. Results show two main centers of peak CO2 flux variability located off Central Peru and Chile, being the magnitude of the response to El Niño extreme events higher off Peru than off Chile.

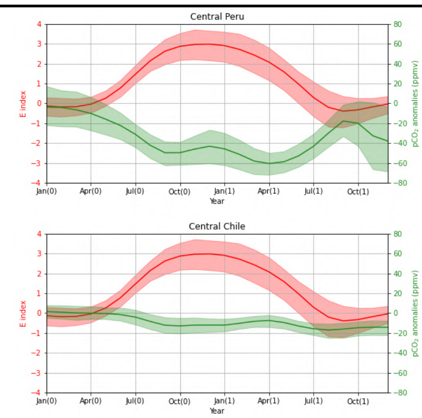
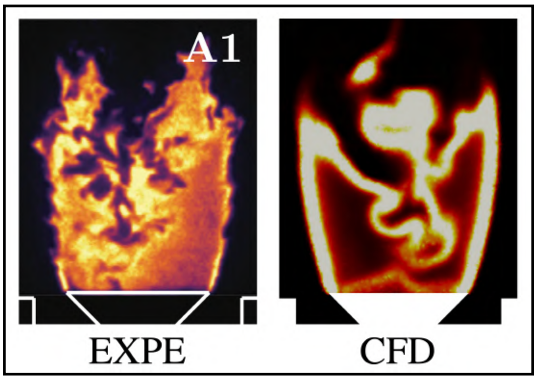


Figure 1: *Eastern Pacific (E) index (red) and pCO2 anomalies during extreme El Niño events corresponding to 35 realisations in the CESM-LENS model. The extreme events where defined as those in which the E index was over 1.5 for at least 6 months. 222 extreme El Niño events were identified. The thick line shows the mean values among all events in all realisations, while the shading indicates the range of values between the 25th and 75th percentiles of the distribution.*

Héctor José Vargas Ruiz

14:05

High Performance Simulations of Industrial Gas Turbines Decarbonization through Hydrogen - Ammonia - Methane Mixtures



Decarbonization on off-grid off-shore oil platforms can be foreseen through the adoption of new fuel blends relying on H2/NH3/CH4 mixtures. Such a choice is indeed of interest because it could potentially limit the initial capital investment induced by the retrofitting of the existing gas turbine fleet. Moreover, ammonia can be inexpensively transported and stored as opposed to hydrogen, which is bulky and unpractical.

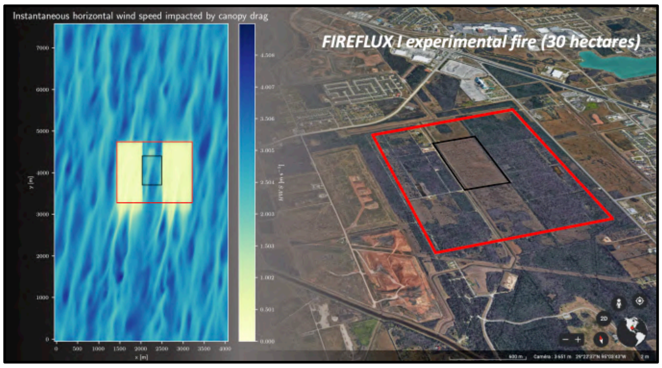
However, ammonia combustion presents us with both opportunities and challenges. Firstly, the use of ammonia increases the risk of producing fuel-related nitrogen oxides. Secondly, the less reactive nature of ammonia may entail flame stability issues. For that reason, it is interesting to enhance ammonia's combustion properties by incorporating more reactive fuels such as hydrogen or methane. The objective of this work is thus to understand and adequately model the effect of such fuel changes on the gas turbine burner using LES of ammonia-hydrogen flames.

William Antolin

14:10

Improvement of the Representation of the Fuel for Fire/Atmosphere Coupled Modeling for the Simulation of Wildfires

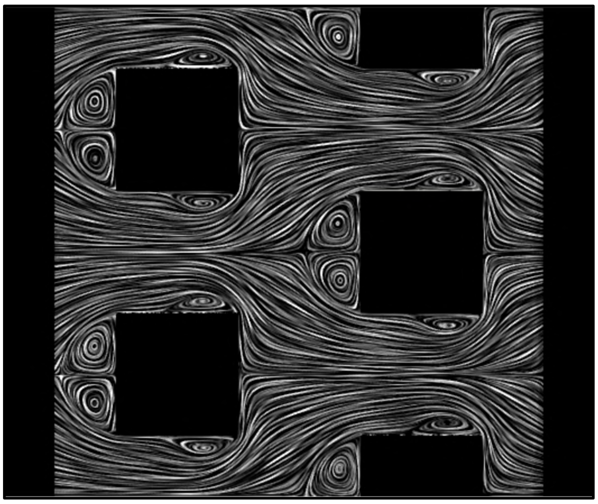
Extreme wildfires are no longer isolated events in the context of a changing climate. Being able to simulate and understand these events is key to discriminate between situations at risk, in order to help decision makers and land managers when facing new wildfires. Coupled fire/atmosphere modeling is particularly promising to simulate wildfire behavior by representing the fire-induced flow and its retroactive feedback on the fire propagation as well as the smoke plume dynamics. In this PhD project (Cerfacs/CNRM), we aim at including a more realistic representation of the vegetation in the Meso-NH/Blaze coupled model. This is essential to account for the dynamical effects of the living fuel due to canopy drag and to better characterize living/dead fuel properties.



Rémi Alas

14:15

Data-Driven Atmospheric Wall Models for Unmeshed Topologies

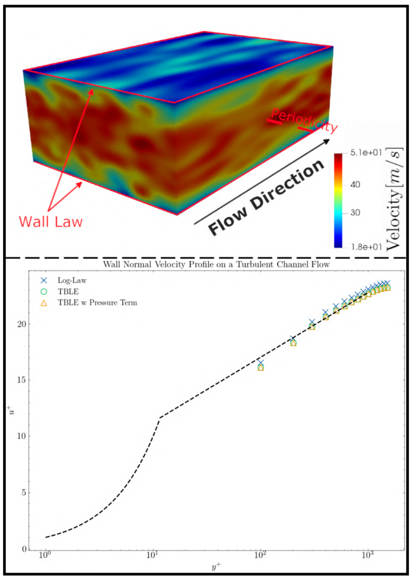


Capturing the relevant scales of motion is crucial to perform accurate simulation. The task gets tricky when the flow is subjected to strong scale disparity resulting in a very high computational cost. The aim of the present study is to accelerate LES of flow with strong scale disparity while guaranteeing an appropriate accuracy. The Urban Boundary Layer (UBL) problem, where the flow encounters elements size varying form few meters (threes, housing...) to hundreds of meters (buildings) over a boundary layer of depth $\delta = 1$km, is the perfect example to illustrate the scale disparity problem. A data-driven approach to model the impact of the smallest elements in the UBL is being implemented to drastically reduce the computational cost.

Mehdi Cizeron

14:20

Wall Modeling for Large-Eddy Simulations of Turbomachinery Flows



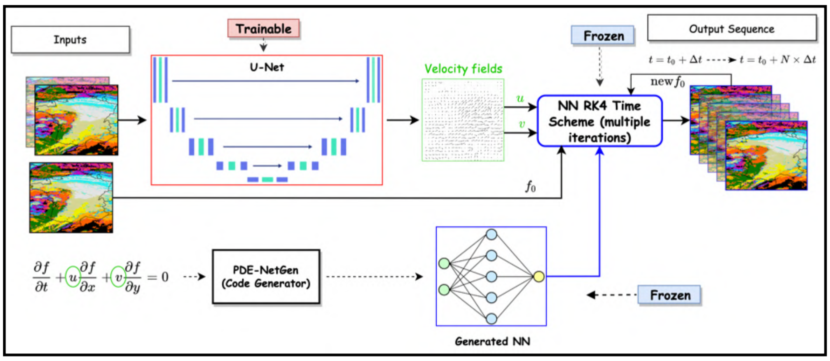
In the industrial context, the numerical resolution of the boundary layers developing along the walls is too expensive for high Reynolds numbers. These boundary layers are modeled by analytical laws, developed in the RANS context. Many assumptions are underlying this modeling (stationary, fully developed turbulent flow on a flat plate, with no pressure gradient). Despite the unsteady and complex context of Large Eddy Simulations (LES), these wall laws are still used, thus presenting weaknesses. Models of increasing complexity will be considered, the first one being the 1D thin boundary layer model, to capture the pressure gradient effect. LES dedicated to turbomachinery will be treated in order to establish the importance of the various contributions on the predictions.

Rachid El Montassir

14:25

Hybrid Physics-AI Approach for Cloud Cover Nowcasting

Recent works using AI have explored cloud cover nowcasting, showing that a future sequence of satellite images can be predicted from a sequence of past observations. But, using numerical resources (data, computation) to learn physical processes that are already known, e.g. the advection, to the detriment of more complex processes, appears to be a waste of resources. To tackle these issues, we propose a novel hybridization between physics and AI, where part of the known physical equations is mixed with state-of-the-art Deep Learning techniques. In this work we designed a hybrid Physics-AI model that enforces a physical behaviour, transport dynamics, as a hard constraint for a trained U-Net architecture.

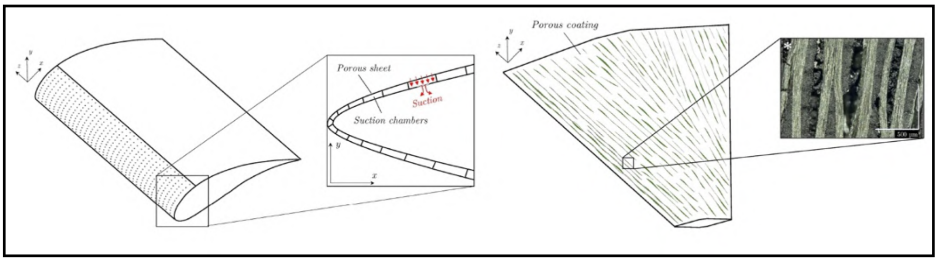


Riwan Hammachi

14:30

Data Assimilation from Mobile Sensor for The Study of Pollutant Dispersion at Micro-Scale

Scenarios for natural transition to turbulence are studied in subsonic/transonic and hypersonic boundary layers. Linear stability theory (LST) is used to identify the features of primary instabilities that lead to turbulence in order to determine the optimal conditions that generate the most unstable disturbances inside the boundary layer. The study is aimed at describing in great detail the influence of nonlinear interactions of disturbances of different wavelengths. For this reason, and in order to overcome the restrictive assumptions of LST, direct numerical simulations are employed. Furthermore, the stabilizing effect of porous walls is investigated via time-domain impedance boundary conditions modelling the effect of porous walls coupled with flow suction in the subsonic cases.

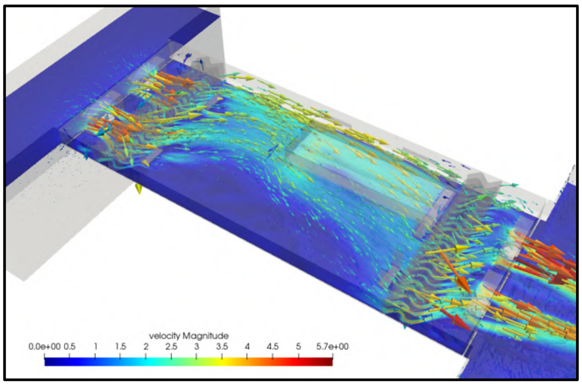


SESSION 4

Shriram Sankurantripati

15:00

High Fidelity Simulations to Study the Propagation of Airborne Viruses in Closed Environments



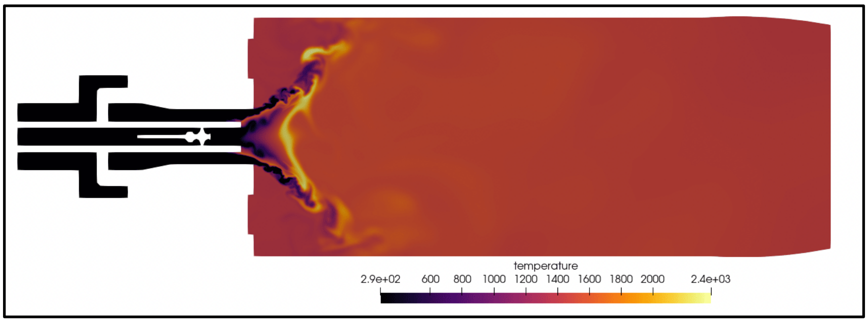
Airborne viruses such as COVID-19 can infect an individual through direct or indirect transmissions. Research suggests that the survivability of these virus-laden droplets is heavily dependent on numerous factors such as humidity, room temperature, turbulence dispersions, wind speed and orientation. To provide a mitigation solution, one has to accurately simulate and understand the flow physics of these droplets inside a closed environment (eg: Bus). In collaboration with VALEO, UV purifier design is proposed to install inside a bus to bring down the infection spread. Large Eddy Simulations coupled with a Lagrangian tracking of droplets and a radiation solver will be used to simulate this purifier setup. Then, simulations will be carried inside a bus with an installed purifier.

Nathanaël Rouland

15:05

Modelling and Simulation of Enriched Hydrogen Turbulent Flames

The use of hydrogen in combustion, either pure or mixed with other fuels, is promising to achieve an efficient energetic transition. However, modelling and simulating those flames remains a challenging scientific and technological issue. The first objective of this thesis is to handle the particular issue of modelling transport phenomena in multicomponent gas phases, which requires new strategies balancing complexity and accuracy. Then, it has been shown in multiple burners that the diffusion flame regime is dominant in H2 combustion. Consequently, the second main objective is to propose an efficient model to deal with those cases. The slot burner case and a reactive mixing layer with a blend of H2 and methane in air are mainly studied.



Markus Holzer

15:10

Code Generation in a Lattice Boltzmann Framework for Exascale Computation

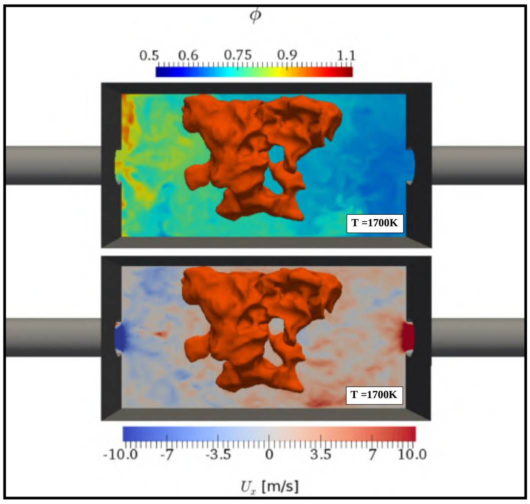
Adapting codes to new heterogenous systems is challenging and time-consuming. Therefore, higher-level methods such as code generation must be researched to reduce the burden on developers and legacy codes. Code generation entails taking a step back from the code, tackling the problem from the equation level, and automatically generating compute kernels adapted to the physics of the problem and the target architecture to be used for the computation. The PhD project will study and develop this new approach to scientific software in the context of lattice Boltzmann simulations for fluid flow and apply it on accelerator hardware and complex flow configurations.

Nicola Detomaso

15:15

LES Simulation of Constant Volume Combustion

Classical gas turbine thermodynamic cycle has undergone no change over the last decades. Pressure Gain Combustion represents an interesting solution to break out current technological limits. Cycle models show that a pressure raise across the combustion process would reduce the fuel consumption, increasing the efficiency. Constant Volume Combustion represents a viable solution that still needs to be studied. In the current project, the CV2 (Constant-Volume Combustion Vessel) installed at the Pprime laboratory is numerically investigated using the high-fidelity compressible solver AVBP. The successive phases of the cycle, i.e., air intake, fuel injection, spark-ignited combustion and exhaust, are considered in the LES. Spark ignition, flame-turbulence interaction and cycle-to-cycle variation will be deeply analyzed in terms of physics and modeling.

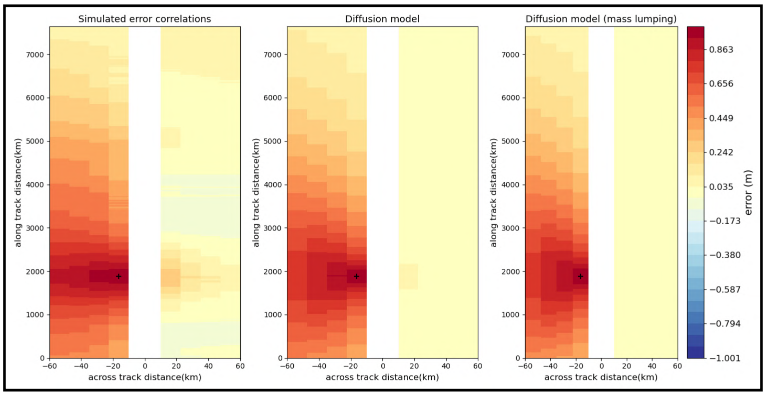


Olivier Goux

15:20

Accounting for Correlated Observation Error in Variational Ocean Data Assimilation: Application to Wide-Swath Altimeter Data

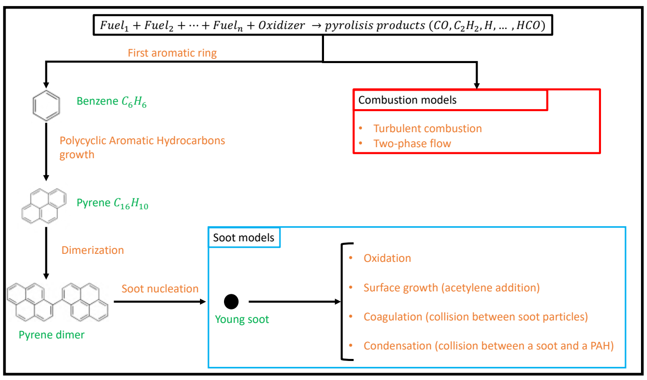
Variational data assimilation is a standard procedure for determining the best possible estimate of the state of an Earth system component (atmosphere, ocean, land, sea-ice) by iteratively minimizing a cost function that measures the weighted least squares fit of the model state to a background state and to observations. The weights contain information about the accuracy of the background state and observations and are defined in terms of an estimate of their respective error covariance matrices. The goal of this PhD is to develop methods to estimate correlated observation errors, account for them in variational data assimilation, and assess their impact on the quality of the solution.



Alexandre Coudray

15:25

Modeling and Simulation of SAF (Sustainable Aviation Fuel) Combustion Including Soot Production in Aeronautical Engine Conditions



With the objective of moving towards a fossil fuel free kerosene, this thesis focuses on the use of 100% SAFs (Sustainable Aviation Fuels) through the modelling of soot in the case of turbulent combustion.

The chemical description of fuel pyrolysis, oxidation of pyrolysis products, soot precursors and gaseous pollutants is delicate because it requires a large number of species.

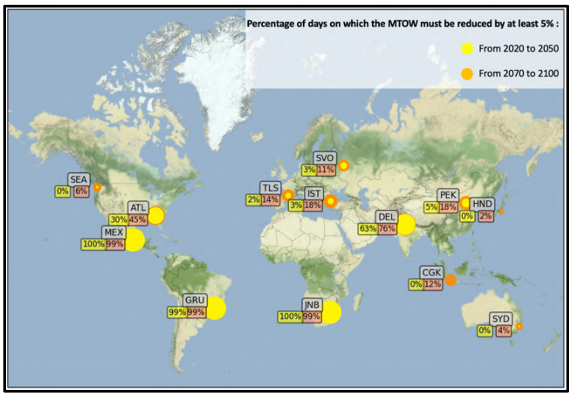
To reduce the computational cost, several strategies need to be developed aiming two main axes. The first axis is the gaseous phase description where soot precursors need to be correctly described while keeping the number of species low then soot models will be used. The second axis focuses on the interaction of premixed turbulent combustion models and multicomponent fuels.

Suzanne Salles

15:30

Impact of Climate Change on Aviation: Uncertainty Cascade Linked to Climate and Engine Modelling on the Take-Off Phase of a Commercial Aircraft.

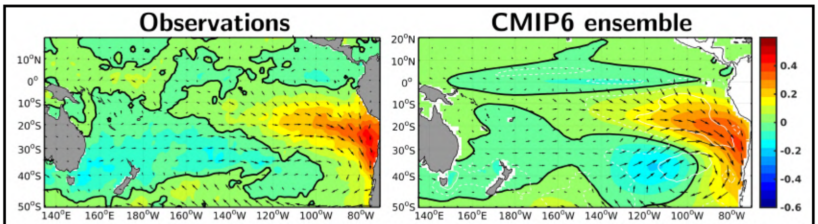
The aircraft performance, both in terms of lift and thrust, is impacted by the modification of atmospheric conditions due to climate change. The project focuses on the role of temperature and humidity on the take-off phase, relying on 1) the forecast of temperature and humidity conditions simulated with CNRM-CM6 climate model and 2) the modeling of the engine thrust and aircraft aerodynamic response to these uncertain parameters. A global sensitivity analysis is carried out to quantify the influence of atmospheric uncertainties on restrictions on the weight of the aircraft. This shows that the number of days with restrictions on the weight as well as the dependency of the weight restriction on atmospheric variables vary depending on local climate.



Emilio Concha

15:35

Meridional Modes of the Southern Hemisphere: Triggering Mechanisms and Sensitivity to Mean State Changes



Spatial pattern of Chile El Niño for: Observations from HadISST + NCEP(left) (1948-2020) and CMIP6 mean ensemble (right) (1850-2014, 41 models) of historical runs. Colors show SST anomalies in °C, black contour corresponds to the isotherm of 0°C, arrows show surface wind anomalies and white contours show standard deviation of the ensemble (segmented line for 0.05°C and continuous for 0.07°C)

A new interannual climate mode of variability in the south-eastern Pacific has been recently described, called the Chile El Niño (CENI) because its center of action is located off Central Chile. This mode results from air-sea interaction near the coast and can be triggered by either perturbations of equatorial origin (e.g oceanic coastal Kelvin wave) or of extra-tropical origin (e.g storms). Here we evaluate how this regional mode of variability is simulated in the historical runs of the models participating to the CMIP phases 5 and 6. We further document the changes of its characteristics (amplitude, frequency of occurrence, seasonality) in the simulations with climate change scenarios RCP8.5/SSP5-8.5.