Call for candidates: 4 PhD & 4 Post-docs

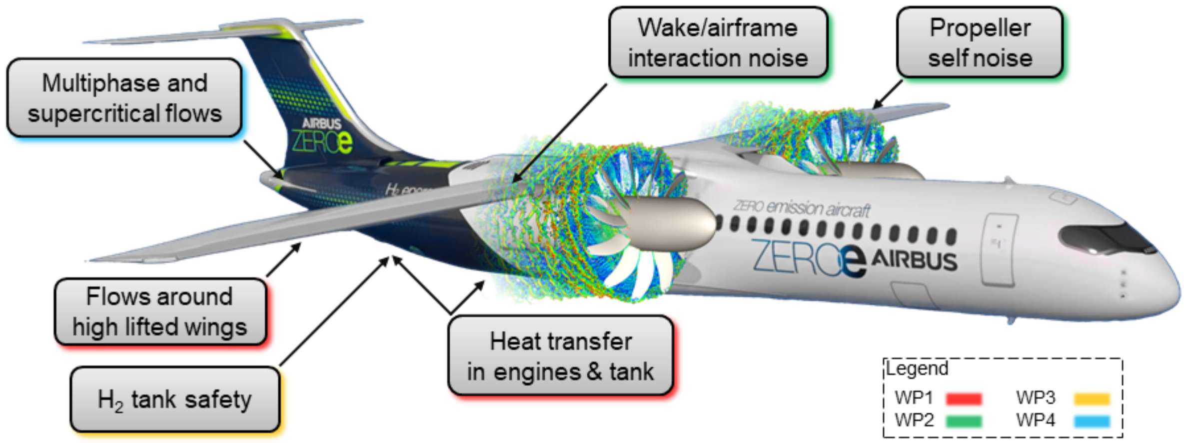
Liberty is an ANR industrial chair and a collaborative effort in the field of computational fluid dynamics applied to the development of new H_2 technologies. It aims at developing efficient Lattice-Boltzmann Methods (**LBM**) for the high-fidelity simulation of multi-species and multi-physics flows in realistic industrial applications such as aerodynamics, aeroacoustics, aerothermal and reacting flows.

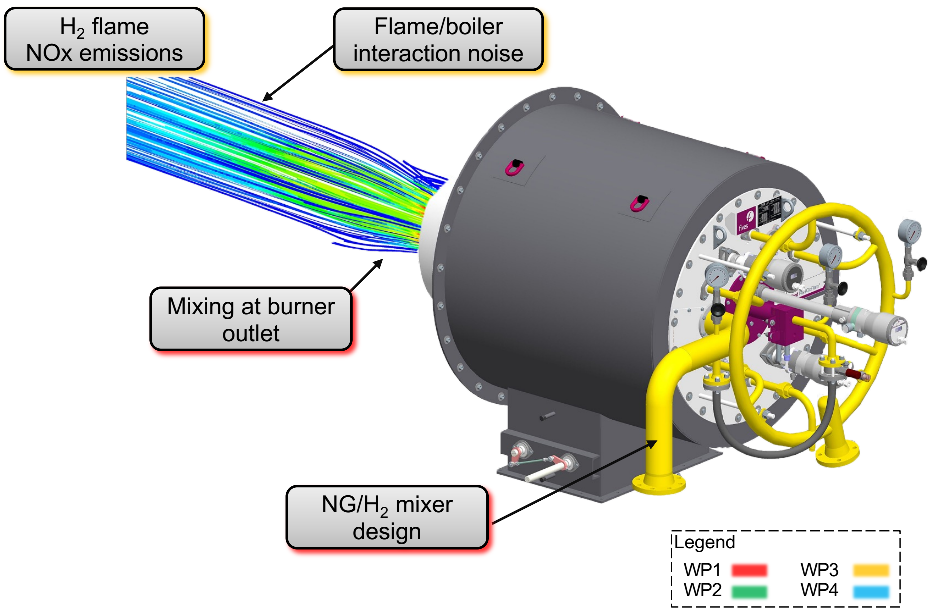
The consortium consists of four partners: the M2P2 lab (AMU/CNRS/Centrale Marseille), two aeronautical manufacturers (**Airbus** and **Safran**), and a burner manufacturer (**Fives-Pillard**). The chair holder is **Dr. Pierre Boivin** (CNRS researcher, CR-HDR), a H_2 combustion and safety specialist from M2P2.

Over the last few years, Lattice-Boltzmann Methods have become very popular for full-scale industrial simulations of isothermal, low Mach, non-reactive flows, as their outstanding computational efficiency and accuracy on complex geometries is no longer in question. Their recent extension to compressible, thermal and multi-species flows opens up a wide new range of applications that needs to be explored and matured. These extensions are crucial in the H_2 transition context for both energy and transport applications, in line with France 2030 objectives.

The research program articulates around four work packages (WP), each focused on a major scientific difficulty in relation with the development of new H_2 technologies:

- **WP1** deals with physical and numerical modeling of solid walls and turbulent boundary layers in aerothermal flows, focusing on the resolution of energy and mass conservativity issues typical of cut-cell approaches.
- **WP2** aims at modelling arbitrary moving and deformable bodies and lay the groundwork for simulating H_2 tank rupture or large propeller deflection.
- **WP3** addresses combustion and safety concerns for future H_2 low NOx combustion chambers, with an emphasis on mixing, flashback and instability studies
- **WP4** explores the possibility of using LBM for high-Reynolds multi-phase flows at high density ratios (both beneath and above critical conditions), such as those encountered in cryogenic and high-pressure H_2 storage.





WP	Flow typology	Applications
1	Aerothermal	Internal flows
2	Moving boundaries	Fans / propellers / turbines
3	Multi-species & reactive	H_2 Combustion and Safety
4	Multiphase	Liquid injection / tanks

Expected outcomes of each work package in terms of field of application

Job offers

- WP1: 1 PhD position, 1 post-doc position
- WP2: 1 PhD position, 1 post-doc position
- WP3: 1 PhD position, 1 post-doc position
- WP4: 1 PhD position or post-doc position, according to profile

PhD positions are fixed term contract for 3 years. Supervision will be assured by the chair holder P. Boivin, Prof. E. Serre (WP1), Prof. J. Favier, (WP2), and the team research engineers J. Jacob & S. Zhao.

Post-doc positions are fixed term contract for 1y, possible extension up to 4 years.

Starting date: negotiable from today.

What to expect from M2P2

- leader for Lattice-Boltzmann methods, with around 30 PhD and post-docs.
- The M2P2 lab co-owns and co-develops the commercial code ProLB.
- A diverse and multi-cultural environment.
- High rate of publication
- High rate of direct recruitment by industrial partners following PhD defense
- Regular interactions with industrial partners
- French classes for foreigners can be offered by the lab.
- In one of the 50 world's greatest places according to Time.

What we expect from you

For PhD position:

- Holder of a MSc or Engineering degree,
- English: working proficiency. French is a plus.
- Rigor and excellence.
- Team work.
- Solid background in fluid mechanics.
- Advanced scientific coding (C++, git,…)

For post-doctoral positions (in addition of the above):

- Holder of a PhD in Fluid mechanics or related field,
- Strong track record,
- Ability to participate in PhD supervision

How to apply

Email to Pierre Boivin and the supervising team (firstname.lastname@univ-amu.fr):

- Detailed CV and cover letter,
- Transcripts (PhD students), PhD defence report (if applicable), a selection of 1-2 relevant research articles.
- References
- Preferred topic.

WP1 : Improved prediction of aerodynamic forces and heat transfer in highly compressible full-scale industrial flows

Keywords : Computational fluid dynamics, Aeronautics, High-speed aerodynamics, Heat transfer, Turbulence modelling, Large eddy simulations

The intrinsic properties of the Lattice Boltzmann method on octree meshes presents a great potential to predict complex flows in realistic conditions. This is already assessed by successful simulations carried out by the M2P2 team for full-scale industrial configurations. However, some key issues have been clearly identified to push forward the reliability and the accuracy of such simulations with LBM: due to the octree (locally cartesian meshes), the grid is not body-fitted meshes, which brings difficulties particularly for flows with compressibility effects that can be induced by both large temperature or pressure variations. The turbulence, the near-wall flows along complex geometries (not aligned on the grid), as well as the presence of steep gradients, flow discontinuities or even shocks raise several numerical and physical modelling issues which will be addressed in this PhD project.

This PhD position focuses on the modelling of solid wall and turbulent boundary layer, which is a key issue to accurately predict aerodynamic forces and heat transfer. The PhD will aim at developing improved boundary conditions at solid walls with an increased physical accuracy and numerical stability. If an efficient mass conservation scheme was recently proposed by the team for isothermal flows (Xu et al. PoF 2022), more work is required for compressible flows, especially when discontinuities are present close to the wall (e.g. attached shock or flame).
A part of the work will be also devoted to heat flux prediction and an accurate estimation of the Nusselt number distribution, dealing both with the modelling of turbulent heat flux and the numerical improvements to damp the spurious wiggles on the fluid quantities along complex geometries non-aligned with the mesh.

Due to the strong unsteadiness expected in the target applications of the project, the turbulence modelling framework will be based on Large Eddy Simulation (WMLES) and the blending RANS/LES strategy based on a simplified constrained Reynolds stress approach with wall functions will be extended to compressible flows with turbulent heat flux constraint.

Supervision will be assured by Eric Serre, Pierre Sagaut and Pierre Boivin.

WP2: Novel algorithms for fluid-structure interaction in realistic industrial conditions in aeronautics using immersed boundary methods

Keywords : Computational fluid dynamics, Aeronautics, fluid structure interactions

Although the motion of immersed solids in rotation is relatively well captured by available numerical codes based on Lattice Boltzmann Method (LBM), the reliable simulation of fully coupled fluid-structure interaction in **realistic conditions** still remain **an open issue for industrial applications in aeronautics**. The objective of the work is to develop novel and efficient algorithms to tackle these configurations involving **complex fluid/solid interfaces**, in the presence of **turbulent** and **compressible** conditions, in the **LBM framework**, including rigid objects in arbitrary motion and deformable objects. The overset and immersed boundary methods, already developed at M2P2 lab, will be compared on testcases of increasing complexity, from **incompressible to high-Mach number regimes**, and novel hybrid methods will be proposed to increase accuracy and robustness of actual methods.

Based on previous works, a crucial aspect of the PhD will be to perform a comprehensive and extensive bibliographical review on the numerical methods to tackle immersed rigid bodies in arbitrary motion (overset mesh, immersed boundary methods, ghost-nodes, etc.) in turbulent and high Mach number conditions, in both Navier Stokes and Lattice Boltzmann frameworks. This task will be performed during the whole PhD in close interaction with the three tasks of the PhD, which correspond to each year:

Rigid bodies with **arbitrary motion** will be considered first with immersed boundary methods, in the presence of **high-Mach** number flows. The presence of **discontinuities** in the pressure fields induced by shocks will be considered, first with **detached shocks** configurations. Based on the bibliographical review, several methods (diffuse, sharps) will be tested and compared in terms of efficiency and accuracy, and a first operational algorithm will be proposed.

Following the same methodology, **attached shocks** will be considered. Several methods available in literature will be tested and a new algorithm will be derived to tackle such problems. The objective will be to preserve the **accuracy** near the walls and obtain a stable algorithm.

Deformable bodies with arbitrary motion will be considered. The focus will be placed on **accuracy** and **local conservation** properties. A new and possibly hybrid algorithm will be proposed in this context.

Supervision will be assured by Julien Favier and Pierre Boivin.

WP3: innovative modelling of novel H_2 industrial burners

Keywords : Computational fluid dynamics, turbulent flows, H_2 combustion and safety

The main open questions for H_2 burners are (i) their thermo-acoustic stability, (ii) proneness to flashback, and (iii) associated NOx emissions. The objective is to develop the required models to carry out the first LBM 3D turbulent simulation of a simplified large-scale burner (1MW), reminiscent from boilers application.

Available and LBM tested models include the thickened flame model and Eddy Dissipation concepts, but more models will be required. In particular, we will focus on the development of ad-hoc LBM turbulent model, based on pdf transport. Revisiting pdf-based transport models is motivated by the fact that LBM is in essence an efficient pdf transport method. Another important issue is the modelling of thermal radiation that dominates heat transfer at the industrial scale. The optimization of radiative property models and radiative transfer equation solver will be an important part of this work-package.

Assuring a smooth H_2 transition requires backward burners compatibility with conventional fuels. This task's objective will be to investigate the effect of H_2 dilution with natural gas on the combustion regime. In particular, the impact of the H_2 content on stability, NOx emissions and radiative losses is not well-understood, in spite of being a priority in the Clean H_2 EU plan. Comparison between aeronautical type burners (e.g. from Safran) and industrial type burners (e.g. from Fives) -- both considered here -- will provide valuable insight and originality to the study. In particular, the PRECCINSTA aeronautical burner test bench, which was recently adapted for H_2 enrichment will be scrutinized.

Adding H_2 lines to existing installations also comes with challenges. The high flammability (and low associated minimum energy) and fugacity of H_2 makes it a capricious gas. This task aims at developing required models to better apprehend safety questions. In particular, we will consider mixture of H_2 with buoyancy effects to observe the formation of flammable pockets. Moreover, we will adapt and improve recent ignition models to help understand the operating conditions to avoid hazardous ignition (maximum leakage rate, ambient temperature, solid part temperatures...). We will also investigate how to successfully arrange flame stoppers in H_2 feed lines, to avoid disastrous flashbacks.

Supervision will be assured by Jean-Louis Consalvi and Pierre Boivin.

WP4: Lattice-Boltzmann modelling of multiphase flows

Keywords : Computational fluid dynamics, multi-phase flows, numerical methods

Supercritical flows are ubiquitous in H_2 applications since H_2 critical pressure is very low (13bar) compared to tank pressures, or even engine pressures. To-date, no LBM method exist to tackle such flows, for which specific equation of states need to be considered. The density ratio encountered across liquid-like / gas-like hydrogen in typical configurations is expected to be close to 20, somewhat larger than across flames, but on the same magnitude order. For such flows, numerical recipes developed for reactive flows are therefore relevant, but require heavy modifications: thermodynamic and transport properties, mesh transitions and boundary conditions all need revisions.

The subcritical regime is also relevant for H_2, in particular in transport applications. Cryogenic conditions are targeted in the main tanks, using autogenous pressurization (e.g. using gaseous H_2). There, encountered density ratios may be much higher, close to 1000, and specific numerical schemes need to be derived. The potential outcomes of this study are important: success open many doors to LBM, from hydro-acoustic to nuclear-cooling applications (among others).

For both regimes, important numerical schemes developments are required to cope with the high density-ratio and high Reynolds flows encountered in the targeted H_2 applications.

Supervision will be assured by Song Zhao, Isabelle Raspo and Pierre Boivin.