ERC advanced grant INTECOCIS : Post-doctoral and senior positions in thermoacoustics at IMFT and CERFACS. Theoretical, numerical and experimental work.

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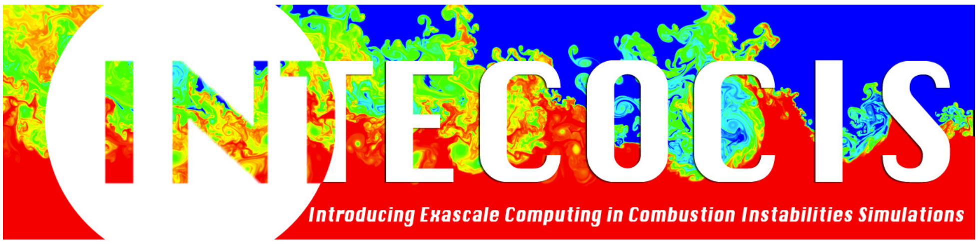


1 OPEN POSITIONS AT IMFT AND CERFACS IN TOULOUSE

The PSC group at IMFT has received an ERC advanced grant in the field of combustion instabilities, called INTECOCIS and starting in February 2013 for five years. In this ambitious project, four PhD, three post-doctoral and two senior positions are open. The topics for the post-doctoral and senior visits can be chosen in the following non exhaustive list :

- Large Eddy Simulation of combustion instabilities in real combustors
- Acoustic tools to predict combustion instabilities
- Experiments in thermoacoustics
- Quantification of Uncertainties (UQ) in the field of thermoacoustics
- High Performance Computing for LES and DNS of reacting flows

Candidates are encouraged to apply by sending mail and complete resumes to Dr Selle or Dr Poinsot. The rest of this document describes the scientific objectives of the project in more details and applicants should read it to see where their expertise can fit.

2 CONTEXT AND OBJECTIVES

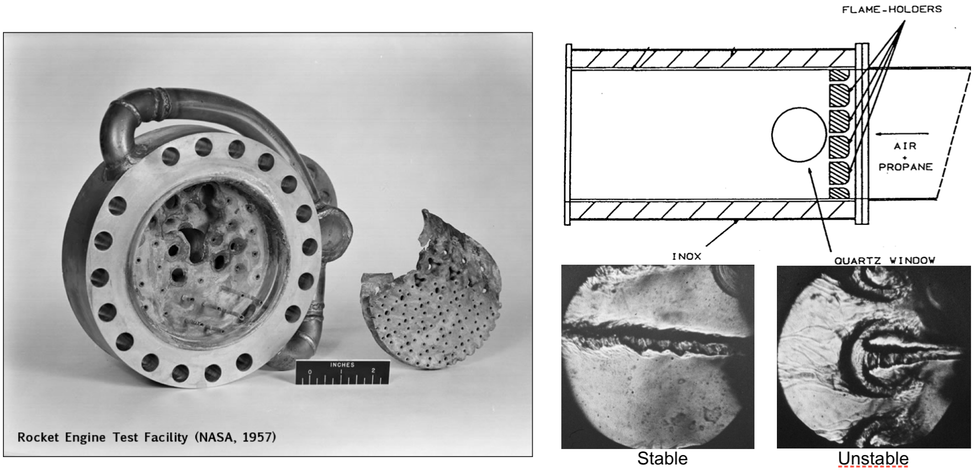
2.1 The ERC project : INTECOCIS

The field of INTECOCIS is combustion instabilities. The project aims at introducing recent progress in the field of High Performance Computing (HPC) for combustion simulation into studies of Combustion Instabilities (CI). The target is to build simulation tools that can predict the occurrence of CI in future combustors before their construction. In order to achieve this goal, the simulation tools used today for CIs must be revolutionized to integrate recent HPC capacities and have the capabilities and brute power required to compute, understand and control CI phenomena. A second objective is to add Uncertainty Quantification (UQ) methods to CI tools. The project will integrate experimental validations and industrial applications. The tools will be made available to European laboratories working in the field of combustion instabilities. INTECOCIS will be based on two teams : the PSC (Particle Sprays and Combustion) team at IMFT (CNRS) that will provide the CI expertise and the CFD team at CERFACS that masters HPC aspects required for combustion simulations.

CIs are a major danger in multiple European programmes where new combustion systems are designed to diminish fossil fuel consumption and pollution as well as to limit climate impact. CIs are due to a resonant coupling of combustion processes with other phenomena, acoustics in most cases. Even though some of the theoretical ground for understanding CIs is available, they cannot be predicted with sufficient precision today and this weakness in our present simulation tools is a major risk : CIs can lead to oscillations of the combustor flow, causing vibration, extinction, loss of control, structural damage, explosions.

The main motivation for computing and understanding CIs is that they represent a major risk for many systems based on combustion while combustion is the key in all future energy production processes. Almost ninety percent of energy on Earth is produced by burning fuel (Law, 2012). One issue that is never subject to controversy is the need to reduce our fuel consumption and to optimize the way we burn fuel. Even with a rapid growth of alternative sustainable energies, combustion will remain the first energy production process for a long time because the global demand for energy keeps increasing and is impossible to satisfy by just novel alternative sources. The fuels burned in combustors can be either non renewable fossil (oil for example) or renewable (hydrogen or biomass) : thus, combustion can be a process to produce renewable energy. Combustion is also required to optimize sun or wind energy production. Indeed, only combustors can replace these systems efficiently on days without sun or wind : hybrid gas turbines are now being developed by Siemens or GE in order to combine solar (or wind) and natural gas at low cost and with limited climate impact.

Combustion is an excellent vector to store or transport energy (by transporting hydrogen for example which can be produced by other means). Finally, certain systems (aircraft, helicopter, rockets) cannot operate at all without combustion. Therefore, the challenge for combustion science is to design systems that can burn fuels without wasting them, increasing pollution or modifying climate. To reach these goals, optimizing combustors and obtaining more power with less fuel, less CO2 emissions and less pollution is the first logical step. This optimization process relies more and more on simulation : instead of building combustors, they are created numerically and used to test optimized designs at low cost. Thanks to HPC, so called ‘virtual combustors’ have appeared in the last five years in some laboratories but at present, none of them can handle CI yet. The fantastic power of modern parallel computers suggests that HPC can now be used to develop these simulation tools and tackle CI problems. This integration of HPC into CI studies represents a significant but risky scientific challenge. However, it is a worthwhile path in terms of fundamental research and industrial applications for Europe.



Stable

Unstable

Figure 1 – Figure 1 : an engine destroyed by combustion instability during the early years of the US rocket program (left) and a laboratory burner exhibiting both stable and unstable behaviours (right, PhD T. Poinsot).

CIs have been known and investigated for a long time. The image on the left of Fig. 1 shows a NASA rocket engine partially destroyed after the engine encountered CI while the right-hand side picture displays high-speed views of the flow in a laboratory burner for both stable and unstable regimes (the burner is built to resist CIs). The instability does change the flow drastically : it creates ‘mushroom’ shaped vortices and an accelerated flame that can destroy the chamber within a few minutes. In a real engine, this can occur within a few seconds. First identified by Lord Rayleigh in 1878 (see a simple video demonstration of combustion instabilities at elearning.cerfacs.fr/combustion/n7masterCourses/acoustic), CIs have been the hidden and feared problem of many combustion programs, starting with solid and liquid fuel rocket engines in the 50s and more recently gas turbines, industrial furnaces or even simple domestic heaters. In the field of NOx mitigation for example, multiple recent European projects (LOCOPOTEC or LOW NOX III) have lead to new combustor designs for gas turbines combustion chambers that were efficient in terms of NOx emissions but exhibited CIs that limited their practical use and required considerable additional developments as shown by the present EC projects where CI has become a central topic (KIAI, LEMCOTEC, TIMECOP).

From the fundamental point of view, CIs constitute one of the most challenging problems in fluid mechanics : they combine chemical kinetics, turbulence, acoustics and two-phase flow in complex geometries (typically real gas turbine engines). An additional difficulty to predict CIs is that the effect of uncertain parameters must be taken into account. Uncertainty Quantification (UQ) is a critical question in this field. Experimentalists have known for years that CIs are very sensitive to many parameters that are not well specified or even identified : small geometry changes (due to manufacturing tolerances but also to wear out effects during operation), air temperature, fuel composition, fuel spray characteristics or wall temperatures affect CIs. A minute geometry change in a gas turbine injection system can be sufficient for a combustor to bifurcate from a stable quiet regime to an unstable one destroying the combustor in a few minutes. This, obviously, is a crucial issue for many combustors. For solid rocket engines, out of ten (supposedly) identical engines, eight can be stable during tests and two unstable : identifying the source of this variation is a critical question. In the context of the introduction of alternative fuels (bio-fuels for example or mixtures of existing fuels with hydrogen as considered in the European initiative H2-IGCC, see www.h2-igcc.eu) in combustors, UQ becomes mandatory : is it possible that by changing slightly the fuel composition or by mixing two fuels, an initially stable combustor might suddenly become unstable ?

The uncertainty problem also extends to the simulation tools themselves and creates new constraints. Predicting the stability map of a combustor (the domain where this combustor can be operated safely) is not sufficient any more : it is also necessary to determine the precision associated to this prediction. Uncertainty sources are linked to physical parameters (geometry, regimes, impedances) but also to modeling difficulties (mesh size, numerical scheme accuracy, sub models). Future simulation codes for CI must include tools to quantify precision associated to both physical and modeling parameters : this cannot be achieved without significant progress in both CI theory and computing technology. In conclusion, today, we do not have design tools allowing to predict CIs before final test phases : thus, CIs remain a major industrial threat and a fundamental scientific challenge that we propose to tackle in this project.

Research on CIs has been quite intense in the last hundred years and Europe has been very active in this field in various groups (Dowling 1997, Sattelmayer 2003, Noiray et al 2008). However, as noted by Culick in his classic 2006 monograph on CIs (and is still true today), High Performance Computing (HPC) applied to Computational Fluid Dynamics (CFD) has not entered the world of CI studies yet. This is somewhat surprising since combustion (with genetics and fundamental physics) simulations have been one of the first HPC applications over the last years : in ASCI projects funded by DOE for example (www.llnl.gov/str/Seager.html), CFD of reacting flows has always been an essential element. Three-dimensional unsteady reacting flows can be computed today with high-accuracy CFD codes using massively parallel computers available in the USA through programs like INCITE or in Europe through PRACE. The PRACE computers available today and the exascale computers that will be available (including in Europe) by year 2020 will revolutionize the field of numerical combustion : massively parallel codes have opened the door to the construction of 'virtual burners' that can entirely be simulated numerically instead of being built and operated experimentally. Interestingly, these HPC CFD codes have had a limited impact for the moment on CIs studies : most CI analysis tools (Crighton et al 1992, Lieuwen and Yang 2005, Poinsot et al 2005) still rely on approaches that do not exploit the power of modern computers. The integration of exascale computing (expected around 2020) in CI methods must begin now because it will bring unprecedented precision in this field and allow CI simulations to become truly predictive methods for practical applications. In particular, future exascale computing will allow using meshes in CI studies with 1000 to 10 000 times more grid points (which means increased precision) than today, thereby taking into account all geometrical details of combustors, which is currently not possible. Similarly, this unprecedented computing power will also allow including more detailed physics. For example one will be able to describe acoustics and two-phase flow (Riber et al 2009), which control the atomization of liquid fuels (kerosene, gasoline or biofuels) in combustors. Two-phase flow is one of the strong topics developed at IMFT (Pr Simonin, Dr Magnaudet).

During the last twenty years, we have developed several HPC CFD codes at CERFACS and CIs studies at IMFT. The moment seems to be opportune to introduce the recent progress in HPC technology into CI studies. The objectives of INTECOCIS are :

- to revolutionize the simulation tools used for CI studies by introducing recent progress achieved for flow simulation on massively parallel computers into this field ;

- to bring UQ methodologies to this field at the same time and
- to validate and apply these methods to a few selected overarching problems in the CI community, including laboratory-scale experiments but also real industrial configurations in collaboration with European industry.

2.2 SIMULATION TOOLS FOR COMBUSTION INSTABILITIES

There are two main numerical methods used today to study CIs which both can be drastically improved by the introduction of high-fidelity large-scale simulation codes running on massively parallel systems :

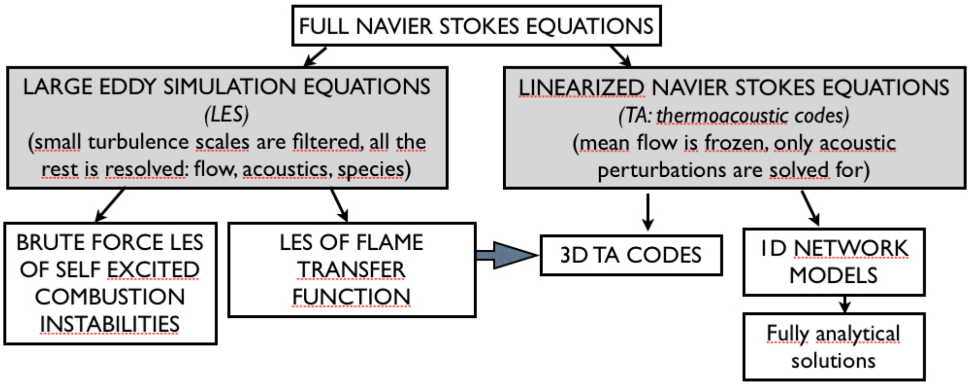


Figure 2 – Numerical methods to study Combustion Instabilities

(1) Brute force Large Eddy Simulation (LES) : recent progress in LES of reacting flows has allowed to simulate full combustion chambers, first for laboratory-scale burners (Branley and Jones 2004, Lartigue et al 2005) and more recently for real industrial configurations (Staffelbach et al 2009, Schmitt et al 2007, Fureby 2010). LES is a method where all flow equations are solved in time on a discretized space (using unstructured grids in most cases). It involves only a limited set of assumptions (mainly a filtering operation of the spatial small scales of the flow), leading to the most precise method today for such geometries but also being the most expensive. The image of a 'virtual burner' can be used here too : a brute force LES of a combustor exhibiting CIs would provide a 'virtual unstable combustor', easier to explore than an experiment. This is an attractive method made possible by recent progress in HPC technologies on machines using 10 000 to 300 000 processors and demonstrated by various research groups in the last years. Many of them use the AVBP code developed in Toulouse in

my group (Sengissen et al 2007, Roux et al 2007, Staffelbach et al 2010). This approach is straightforward, and yet, far from being mature and facing multiple difficulties : a) it does not yet incorporate all details required to mimic CIs in real combustors (acoustic damping, geometrical complexity, detailed kinetics, two-phase flows, wall phenomena, radiation, supercritical flows for future high pressure systems... b) each LES is only a realization of a single operating point (one inlet temperature, one pressure, one fuel, one injection type, one set of acoustic impedances imposed at the inlet(s) and outlet(s) of the combustion chamber...) in a given combustor. The results change as soon as one of these parameters changes. The LES approach in itself does not bring new insight into the reasons why a given chamber is unstable. It does not indicate which change of parameter could lead to a stabilization of the CI. In other words, brute force LES, once sufficiently improved to reproduce real flames, will be able to provide results that are very similar to a perfectly instrumented experiment : it can help us understand CIs provided we have a theory to guide us but it can not replace this theory. Thus a complete method to address and to control CIs must include brute force LES but also smarter theoretical methods as described below. These methods also involve HPC but they have the advantage that they are not restricted to a single operating point. They decompose the physics of CIs in a few building blocks allowing to understand and to control them and not only to observe them. Nevertheless, brute force LES remains a strong asset because it allows testing the accuracy of these ‘smart’ acoustic methods.

(2) Thermoacoustic codes (called here TA codes) coupled to forced response LES : in most CIs, acoustics is the dominant resonant mechanism and multiple studies performed in the last sixty years (most of them inspired by the pioneering work of L. Crocco (1951)) have shown that a proper method to decompose and analyse the physics of CIs was to use ‘acoustic’ codes that can track the propagation of sound waves in the combustor and the growth of eigenmodes. In this approach, the mean flow is frozen and the flames are replaced by active acoustic components (which can be compared to loud speakers that would produce sound waves depending on the acoustic waves they are submitted to). Provided the impact of these active elements can be properly represented, the global stability properties of the combustor can be predicted in the linear as well as in the non-linear regimes. A major interest of this approach is that it allows isolating the elements leading to CIs into different blocks (something a brute force LES cannot do) : a) the acoustics of the combustor, b) the impedances of the outlet(s) and inlet(s) and c) the response of the flame which is quantified by a function called the Flame Transfer Function (FTF) describing the amount of unsteady heat release produced by a flame when it is submitted to an unsteady velocity. TA codes can operate either in the frequency domain or in the time domain but in all cases, they are faster than brute force LES and

their information more useful to mitigate CIs. Their development however, is far from satisfactory today : one main difficulty of TA codes is their dependency on the accuracy of the FTF. FTF can be measured experimentally but they will have to be computed in the future and the proper method to compute FTF is LES again. However, such LES are simpler than brute force LES because FTF can be measured by forcing a part of the combustor using acoustic waves and quantifying the flame response. This response is independent of upstream or downstream boundary conditions and can be viewed as an intrinsic characteristic of the flame. A second difficulty of TA codes is that they must still include the complete combustor geometry and require sophisticated methods to track eigenmodes. The difficulty is no longer to predict the stability of a single case (like in brute force LES) but to predict the effects on stability of multiple parameters on stability. This leads also to a significant challenge in terms of computations, something that until now has not been done with the level of precision required for effective CI control.

2.3 WORK PROGRAM

The objective of this proposal is to develop an integrated framework in which recent progress in HPC (especially in the field of LES but also in TA codes methodology) will be used to improve methods for CI prediction and control. Brute force LES and TA codes are the two basic elements of the project but CI theory (Culick 2006, Poinsot and Veynante 2005, Nicoud and Poinsot 2005) is the third one. Theory remains necessary at all stages of the present proposal. In particular, INTECOCIS will focus on three aspects : Part I : Introducing HPC and LES into combustion instability studies. This will require moving from numerical approaches developed by small teams to an ambitious effort incorporating recent methods for LES and TA codes developed for massively parallel computers. An additional dimension of INTECOCIS is to make these tools available to the scientific community : IMFT and CERFACS are already working with many other actors of the combustion community worldwide and distributing their codes. The LES code AVBP is one example of such an effort where a code developed by CERFACS and IFP-EN has been distributed worldwide and is used today by more than 150 scientists, in laboratories and industry research centers (cerfacs.fr/4-26334-The-AVBP-code.php). Organizing the CI community around existing high-level software tools is a priority : Cambridge (around a low-order code called LOTAN by Pr A. Dowling) or TU Munich (with the tax library (Leandro et al 2010) by Pr Polifke) are good examples of coordinated efforts in the field of CI but without the HPC component : the present proposal will follow a similar path but will focus on LES and TA codes using HPC. Part II : Introducing Uncertainty Quantification (UQ) into LES and TA codes. In most cases, the outcome of CI studies is a discontinuous function : either the combustor is stable or it is not. Making decisions based on this result requires the knowledge of the precision with which it is obtained. Since CIs are known to be very sensitive to multiple physical parameters (flow regime, manufacturing tolerances, fuel changes...) and since the codes (brute force LES as well as TA codes) used to predict CIs are also sensitive to many hidden parameters (number of mesh points, accuracy of numerical methods, boundary conditions...), introducing UQ has become an important issue that is virtually untouched today (see recent IMFT work by Duchaine et al (2010)) and that will be an essential part of the present project. Shape optimization using simulation to mitigate CIs will be a logical addition to the UQ task : being able to predict the effects of geometrical changes or of parameter variations (flow rates, compositions) directly allows searching for the most stable configurations using very similar tools. Part III : Validation in academic burners and application to gas turbine combustion. Such a large-scale numerical effort cannot be successful without experimental validation. These validations are performed at various levels : mean flows (cold and reacting), FTFs, stability maps. IMFT develops its own (small-scale) experiments in the field of CIs and also has a long history of cooperation with most CI groups in the world (Cambridge Univ, Ecole Centrale Paris, TU Munich, Un. Twente, Stanford, Georgia Tech) through many common projects and papers. Upon completion of these academic validation exercises, the last two years of the project will focus on industrial applications with European companies that have been in contact with IMFT and CERFACS for the last ten years and are facing CIs : Turbomeca, Snecma, Alstom, Siemens, Ansaldo are a few examples of European companies with a clear need for an ambitious project to simulate CIs and to control them. These companies will be contacted at the beginning of INTECOCIS and invited to define challenging industry test cases to be used as ultimate proofs of efficiency for INTECOCIS tools. Of course, the validation of INTECOCIS codes will be restricted to “open” configurations (for which results can be published and made available to the community) and not to proprietary cases.

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