



INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Team CONCHA

*Complex flow simulation Codes based on
High-order and Adaptive methods*

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1. Team

CONCHA is a joint project of INRIA Futurs and LMA (Laboratoire de Mathématiques Appliquées– CNRS UMR 5142), UPPA (Université de Pau et des Pays de l'Adour).

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2. Overall Objectives

2.1. Introduction

The main objective of this project is the development of innovative algorithms and efficient software tools for the simulation of complex flow problems. On the one hand, our contributions concern modern discretization methods (high-order and adaptivity) and goal-oriented simulation tools (prediction of physical quantities, numerical sensitivities, and inverse problems) on the other hand. Concrete applications originate from flows related to propulsion devices featuring important and challenging problems for numerical simulations in this field; see Section 4.1.

Reactive flow problems lead to very complex coupled systems of equations which are often very difficult to handle in routine way with industrial software. The difficulties are due to the physical complexity of the system of equations to be solved and the mathematical problems they imply: the extremely stiff reaction terms in combustion, the different flow regimes ranging from low Mach numbers to hypersonic flow, the presence of turbulence, and two-phase flows.

Our medium-term goal is to develop flow solvers based on modern numerical methods such as high-order discretization in space and time and self-adaptive algorithms. Adaptivity based on a posteriori error estimators has become a new paradigm in scientific computing, first because of the objective to give rigorous error bounds, and second because of the possible speed-up of simulation tools. A systematic approach to these questions requires an appropriate variational framework and the development of corresponding software tools.

It is our goal to study at hand of concrete applications the possible benefits and difficulties related to these numerical approaches in the context of complex fluid mechanics. Therefore, prototypical applications are chosen in order to represent important challenges in our field of application.

The main ingredients of our numerical approach are adaptive finite element discretizations combined with multilevel solvers and hierarchical modeling. In view of our applications described below in Section 4.1, it is natural to consider discontinuous and stabilized finite element methods, for example the so-called discontinuous Galerkin approach (DGFEM), since it generalizes classical finite volume methods and offers a unified framework for the development of adaptive higher order methods. The enhancements of these methods and their application to challenging physical problems induce numerous mathematical investigations.

Our long-term goals are described as follows. Having appropriate software tools at our disposal, we may attack questions going beyond sole numerical simulations: parameter identification, optimization, and validation of different numerical techniques (including validation of software relying on the particular technique). The disposal of such tools is also a prerequisite for testing of physical models concerning for example turbulence, chemical kinetics, and their interaction.

Nowadays it seems clear that many engineering problems in the field of complex flow problems can neither be solved by experiments nor by simulations alone. In order to improve the experiment, the software has to be able to provide information beyond the results of simple simulation. Here, information on sensitivities with respect to selected measurements and parameters is required. The parameters could in practice be as different in nature as a diffusion coefficient and a velocity boundary condition. CONCHA has as long-term objective the development of the necessary computational framework and to contribute to the rational interaction between simulation and experiment.

Goals of the project are to evaluate the potential of recent numerical methods and to develop new approaches in the context of industrial CFD problems.

We intend to validate our software with respect to other commercial and research tools in the domain, such as *Aéro3d* (INRIA-Smash), *AVBP* (CERFACS), *Cedre* (ONERA), *Fluent* (ANSYS), *FluidBox* (INRIA-Scallaplix), *OpenFoam* (OpenCfd).

The development of CFD software benefits in an important measure from in-house experiments. With this respect, we emphasize that there exists a test facility of confined inert flows developed in another research program at UPPA. Its flow geometry and the metrology are adequate for the purpose of comparison with our simulations. It is planned to create an open data basis which serves for comparison with other simulation software and experiments. As outlined above, the project is based and generates different research topics. Especially, the interaction between fluid mechanics and numerical analysis as well as the interaction between software development and experiments is crucial for this project. The composition of the project team consists of mathematicians and physicists, and the support from in-house experiments is available.

In the first phase we intend to develop high-order adaptive flow solvers. The availability of such tools is crucial for DNS-based turbulence and combustion model development. The software to be developed in the first phase of the project is a necessary condition for the realization of the more advanced algorithms related to model prediction, inverse problems, and numerical sensitivity analysis. Testing of new numerical methods from the mathematical community at hand of concrete problems is a necessary research task. What is the practical gain of discontinuous Galerkin schemes for a realistic flow simulation ? What can be expected from adaptive discretization algorithms ? Is it possible to guide hierarchical modeling and model reduction based on a posteriori error analysis ? What might be the gain in computing numerical sensitivities ?

Interaction with industry should profit from the different research networks listed above. The purposes of this project being to develop, analyze, and test new algorithms, collaboration with industry through the presented

test problems will be natural. We intend to evolve these test problems by feed-back with our industrial partners. Technology transfer in form of integration of new methods into existing industrial codes is intended and could be the goal of phd-theses.

2.2. Highlights

CONCHA has been created as an 'equipe INRIA' in april 2007.

3. Scientific Foundations

3.1. Introduction

Keywords: *Euler equations, Navier-Stokes equations, discontinuous Galerkin, finite element method, reactive flow, stabilization, turbulent flow.*

We first give a short overview on typical systems of equations arising in the considered domain of applications. Then we describe some typical difficulties in this field which require the improvement of established and the development of new methods. Next we describe the research directions underlying our project for the development of new software tools. They are summarized under the two headlines 'high-order methods' and 'adaptivity'. Our approach for the discretization of the Euler and related equations is based on the discontinuous Galerkin finite element method (DGFEM), which offers a flexible variational framework in order to develop high-order methods. Finally some perspectives are outlined.

3.2. Goals: accuracy and efficiency

Accurate predictions of physical quantities are of great interest in fluid mechanics, for example in order to analyze instabilities, especially in reacting and/or turbulent flows. Due to the complex and highly nonlinear equations to be solved, it is difficult to predict how fine the spatial or temporal discretization should be and how detailed a given physical model has to be represented. We propose to develop a systematic approach to these questions based on high-order and auto-adaptive methods.

We note that most of the physical problems under consideration have a three-dimensional character and involve the coupling of models. This makes the development of fast numerical methods a question of feasibility.

3.3. Difficulties related to numerical simulations of reacting flows

For the modeling of reactive flows see [35], [124]. Numerical simulations of reactive flows have rapidly gained interest [37], [38], [111]. For an overview on state-of-the-art modeling of combustion and turbulent reactive flows see [112], [122].

3.3.1. Physical coupling

The coupling between the variables describing the flow field and those describing the chemistry is in general stiff. Our efforts will therefore be concentrated on coupled implicit solvers based on Newton-type algorithms. A good speed-up of the algorithms requires a clever combination of iteration and splitting techniques based on the structure of the concrete problem under consideration.

3.3.2. Reaction mechanisms

The modeling of chemistry in reactive flow is still a challenging question. On the one hand, even if complex models are used, estimated physical constants are frequently involved, which requires an algorithm for their calibration. On the other hand, models with detailed chemistry are often prohibitive, and there exists a zoo of simplified equations, starting with flame-sheet-type models. The question of model reduction is of great interest for reacting flows, and different approaches have been developed [100], [115].

Although first attempts exist for generalization of a posteriori error estimators to model adaptation [39], [56], [57] and [110], it remains a challenging question to develop numerical approaches using a hierarchy of models in a automatic way, especially combined with mesh adaptation.

3.3.3. *All-Mach regimes*

The development of solvers able to deal with different Mach regimes simultaneously is a challenging subject. For a long time, the CFD community has been divided into two communities: one oriented towards the Euler equations and the other towards incompressible flow equations. The main reason for this is that both fields have to deal with major difficulties which have few in common: The first is the approximation of - and in addition physically correct - shock positions, and the second difficulty is the stable approximation of the pressure and the bad conditioning of the systems. The methods that have been developed are consequently of quite different nature: finite volumes with sophisticated numerical fluxes based on approximate Riemann solvers combined with fast explicit time stepping schemes on the one hand, and special finite elements with implicit time discretization and multigrid solvers on the other. For the first family we refer to the text books [81], [99], [101], [119] whereas for the second one we cite exemplarily [74], [79], [82]. The recent interest in questions related to low-Mach number flows is for example documented in the proceedings [34], [52], [76].

3.3.4. *Turbulence*

The flows under consideration are in general turbulent. This is a major difficulty from the computational point of view, since the resolution of the finest scales still requires a prohibitive number of unknowns in the flow field alone. We note that special difficulties are due to coupling of the flow with chemistry. Recently, it has been observed that certain turbulence models have similarities to finite element stabilization techniques for the Navier-Stokes equations, and the corresponding idea that rational turbulence models might be based on adaptive techniques has gained much attention, see [78], [88] and related work.

3.4. Numerical tools: High-order discretization methods

3.4.1. *Motivation for discontinuous finite elements*

The discontinuous Galerkin finite element method (DGFEM) offers interesting perspectives, since it offers a framework for the combination of techniques developed in the incompressible finite-element (well-founded treatment of incompressibility constraints, pressure approximation, and stabilization for high-Reynolds-number flows) and the compressible finite-volume community (entropy solutions, Riemann solvers and flux limiters).

In addition, the order limit of finite volume discretizations is broken by the variational formulation underlying DGFEM, which makes it possible to develop discretization schemes with local mesh refinement and local variation of the polynomial degree (*hp*-methods). At the same time, the well-established finite-element knowledge for saddle-point problems can be set on work.

Noting that different approaches based on discontinuous Galerkin methods have been used in recent years for the solution of challenging flow problems, DGFEM seems to be a natural framework for the present project. Since the project team members have experience with (these and other) stabilized finite element methods, a combination of the different techniques is expected to be beneficial in order to gain efficiency.

3.4.2. *Overview on discontinuous Galerkin and other stabilized finite elements*

Overview articles concerning DGFEM and stabilized finite element methods are available, see for example [66], [36]. The literature on these methods has an important growth rate since the last decade of the last century. Here, we only give a very short introduction concerning the most important aspects in light of the present project.

3.4.2.1. Hyperbolic equations.

The first discontinuous Galerkin method for hyperbolic equations is generally attributed to Reed and Hill [113], where the authors propose a scheme for the neutron transport equation. The first analysis of the method has been presented by Lesaint and Raviart [103]. Their result has been further improved and the analysis substantially broadened by Johnson, Pitkäranta and Nävert [95], [96]. We illustrate DGFEM for the linear first-order scalar equations $\beta \cdot \nabla u = f$ in Ω with boundary conditions $u = g$ on the inflow part of the boundary $\partial\Omega^-$ (defined by the condition $\beta \cdot n \leq 0$ with n the unit outer normal field at $\partial\Omega$). We seek an approximation u_h which is allowed to be discontinuous across all interior edges of a given mesh h . On a given cell K of the mesh, the restriction u_K of u_h to K is a polynomial. It is determined by the equation to be satisfied by all local test functions v_K :

$$-\int_K u_K \beta \cdot \nabla v_K dx + \int_{\partial K} F(u_h, n_K) v_K ds = \int_K f v_K dx, \quad (1)$$

where $F(u_h, n)$ is a numerical flux function which is used to distinguish between in- and outflow values. Since we are only allowed to prescribe boundary data on the inflow (think of $K = \Omega$), $F(u_h, n)$ equals for example $(\beta \cdot n)g$ on $\partial K \cap \partial\Omega^-$ and $(\beta \cdot n)u_K$ on ∂K^+ .

DGFEM became popular only ten years later when it was applied to nonlinear hyperbolic equations within the work of Cockburn and Shu [67], [69] who combine a spatial DGFEM discretization with an explicit Runge-Kutta method in time. The breakthrough of DGFEM for the Euler equations was achieved by Bassi and Rebay [46]. Since then, there is a growing research activity concerning the application of DGFEM to complex flow problems. It even found its way into lecture notes, see for example [73].

3.4.2.2. Elliptic equations.

Also around 1970, DGFEM for elliptic and parabolic equations were proposed. The different variants were generally called interior penalty (IP) methods and their development remained independent of the development of the DGFEM methods for hyperbolic equations. The starting point of these methods is the celebrated paper of Nitsche [109] where a variational scheme for the so-called weak implementation of Dirichlet boundary conditions was developed and analyzed. In order to solve the Dirichlet problem $-\Delta u = 0$ in a bounded polygonal domain Ω with boundary condition $u = g$ on $\partial\Omega$, Nitsche's method determines a finite element approximation u_h to u in a finite element space V_h as the solution of the variational equation to be satisfied for all test functions $v_h \in V_h$:

$$\int_{\Omega} \nabla u_h \cdot \nabla v_h dx - \int_{\partial\Omega} F_{\gamma}(u_h) v_h ds - \int_{\partial\Omega} u_h F_{\gamma}(v_h) ds = - \int_{\partial\Omega} g \tilde{F}_{\gamma}(v_h) ds, \quad (2)$$

where $F_{\gamma}(w_h) = \frac{\partial w_h}{\partial n} - \gamma w_h$ and \tilde{F}_{γ} is defined by consistency. The beauty of this formulation lies in its symmetry and obvious consistency properties.

The next step made by Arnold in his 1979 thesis (summarized in [40]) was based on the fundamental idea to enforce continuity of finite element approximations on the interior edges of a given mesh in a similar way as the Nitsche method does for the boundary conditions; see also Wheeler [123] for a collocation finite element method and the methods of Douglas and Dupont [70] and Baker [43] where similar ideas have been used in order to enforce the continuity of the derivatives of finite element functions across interior edges. It seems that these early methods could not gain much attention at that time and have therefore been fallen into sleep for twenty years.

The renewed interest in discontinuous finite element methods for elliptic equation seems to be related to the success of the DGFEM methods for hyperbolic equations. Being known to lead to accurate and robust discretization of the transport equation, the next step is to consider the convection-diffusion, see for example [48]. In order to deal with the Navier-Stokes equations, new ideas for the discretization of the diffusive terms have been developed in Bassi and Rebay [45] and Cockburn and Shu [68]. A unified framework of DGFEM methods for elliptic equations has been developed in [42].

The DGFEM framework offers many interesting possibilities. We mention here a robust scheme for the elasticity system [85], the discretization of Maxwell's equation [75], [89], its use for the discretization on non-matching meshes without Mortar spaces [50], and hp -methods [90], [117].

It is generally accepted that an important advantage of DGFEM beside its flexibility is the fact that it is locally conservative. At the same time, its drawback is its relative high numerical cost. For example, compared to continuous P^1 finite elements on a triangular mesh, the number of unknowns are increased by a factor of 6 (and a factor of 2 with respect to the Crouzeix-Raviart space); considering the system matrix even leads to a more disadvantageous count. Concerning higher-order spaces, standard DGFEM has a negligible overhead for polynomial orders starting from $p = 5$, which is probably not the most employed in practice. The question of how to increase efficiency of DGFEM is an important topic of recent research. Our approach in this field is based on comparison with stabilized FE methods.

3.4.2.3. New generation of stabilized FE methods.

Standard finite element schemes do not lead to satisfactory schemes for convection dominated problems. Modifications of standard Galerkin methods by introducing additional so-called stabilization terms in order to increase robustness have been introduced by Hughes and co-workers for the Stokes equations and convection-dominated problems [59], [91], [92]. In case of the linear transport equation $\beta \cdot \nabla u = f$ in Ω with boundary conditions $u = 0$ on the inflow part of the boundary $\partial\Omega^-$ a typical variational formulation reads: Find $u_h \in V_h$ such that for all test functions $v_h \in V_h$ there holds

$$\int_{\Omega} \beta \cdot \nabla u_h v_h dx + \int_{\partial\Omega^-} |\beta \cdot n| u_h v_h ds + \int_{\Omega} \delta(\beta \cdot \nabla u_h - f)(\beta \cdot \nabla v_h) dx = \int_{\Omega} f v_h dx. \quad (3)$$

The third term on the left of (3) is the stabilization term which allows to control the streamline derivative of the discrete solution. The resulting so-called streamline diffusion method SDFEM (or sometimes Galerkin least squares or SUPG) has been analyzed in detail by Johnson and co-workers [98], [97]. The method has been extended in many variants to the incompressible Navier-Stokes equations, see for example [77], [118].

One difficulty in the application of these methods to complex flow equations is the coupling of various terms and unknowns which can be anticipated from (3) if $f = f(u)$ depends on u . These difficulties are avoided by a new family of methods which replace the stabilization term in (3) by terms of the form $\int_{\Omega} \delta(\beta \cdot \nabla u_h - \widetilde{\beta \cdot \nabla u_h})(\beta \cdot \nabla v_h - \widetilde{\beta \cdot \nabla v_h}) dx$ where $\widetilde{\beta \cdot \nabla u_h}$ is a different approximation of $\beta \cdot \nabla u$, constructed for example with the help of an additional coarser mesh, see Guermond's two-level scheme for the transport equation [83] and the local projection stabilization [1], [55]. Another approach in this family is the stabilization based on the jumps of the derivatives of finite element functions which goes back to [70] and has recently been developed in a systematic way for convection-diffusion and incompressible flow problems by Burman and Hansbo [61], [64].

3.4.2.4. Relation between DGFEM and other stabilized FE methods.

There are many similarities between DGFEM and SDFEM (streamline-diffusion FEM) based on piecewise linear elements for the transport equation from a theoretical point of view, see for example the classical text book [94]. Recently, attempts have been made to shed brighter light on the relations between these methods [58] [60], [65]. There is also a renewed interest in stabilizing non-conforming finite elements for the Navier-Stokes equations [104], [62], [63].

A better understanding of the relations between these methods will contribute to the development of more efficient schemes with desired properties. As outlined before, the goal is to cut down the computational overhead of standard DGFEM, while retaining its robustness and conservation properties.

3.4.3. Challenges related to DGFEM

Formulation of discretization schemes based on discontinuous finite element spaces is nowadays standard. However, some important questions remain to be solved:

- How to combine possibly higher-order spaces with special numerical integration in order to obtain fast computation of residuals and matrices ? How to stabilize such higher-order DGFEM ?
- Treatment of quadrilateral and hexahedral meshes:
Hexahedral meshes are economical for simple geometries. However, arbitrary hexahedra (the image of the unit cube under a trilinear transformation) lead to challenging questions of discretization. For example, some standard methods such as mixed finite elements surprisingly lead to bad convergence behavior [41]. Standard conforming Q^p finite elements are costly to compute and have disadvantages on anisotropic meshes.
- Time-discretization:
The choice of DG time-discretization is natural in view of its good stability and conservation properties. However, the higher-order members of this family lead to coupled systems which have to be solved in each time-step.
In order to be fully conservative, the time discretization has to be implicit: for example for the transport equation it seems reasonable not to distinguish between time and space variables and it is therefore natural to discretize both time and space with discontinuous finite elements. Fortunately, taking into account the tensor-product structure of the space-time mesh, it is still possible to organize a code in a time-marching procedure. The DG time-discretization leads to implicit Runge-Kutta schemes [72], which are quite costly, since one has to solve for several levels of unknowns simultaneously. Therefore, a competitive realization has to take advantage of the special structure of these systems.
- Solution of the discrete systems:
The computing time largely depends on the way the discrete nonlinear and linear systems are solved. Concerning the solution of the nonlinear systems, we note that the strong stiffness induced by combustion requires special solvers, based on homotopy methods, time-stepping and specially tuned Newton algorithms.
Although direct solvers are often competitive in two-dimensional computations, the complexity of three-dimensional problems makes iterative solvers unavoidable; here, multilevel solvers are able to ensure optimal complexity for stationary problems. It should however be denoted, that time-dependent problems lead to different situations, and the most efficient solution largely depends on the concrete application. The question of parallelization is intrinsically related and is of particular importance for the solution of the systems resulting from higher-order space- or even time- discretization.

3.4.4. Approximation of solutions with shocks

The shock capturing term for DGFEM plays a similar role as flux limiters in classical finite volume schemes. The choice of an effective shock capturing term is important for the success of the discretization. Authors seem to agree about this point, but the precise form differs significantly. It can be noticed that there is a lack of theory. This also concerns the treatment of the resulting additional nonlinearity. Within the framework of discontinuous Galerkin methods, it is possible to formulate methods which allow to locally adapt the approximation without necessarily adapting the mesh. Such a procedure has been proposed in [84] and applied to fracture problems in solid mechanics in [87]. We propose to develop a similar approach for the tracking of shock waves and combustion fronts.

3.4.5. All-Mach approach

There are many attempts to improve codes for compressible flows in order to deal with small Mach numbers, see for example [114], as well as attempts to generalize codes for incompressible flows to deal with high Reynolds numbers and varying densities. It is important to notice that there is a *physical* difficulty in finding an appropriate model and a *numerical* difficulty in finding a stable discretization. Concerning the *numerical* difficulty, we know from the theory of numerics for incompressible flows that the pressure gradient has to be discretized in a stable manner. However, this causes important difficulties in a solver for the compressible

flow equations since here, the pressure is not a direct variable but is instead determined by the state equation. There is a modern tendency to use a stable discretization for the incompressible flow equations also in the compressible case. This can either be done by respecting certain relations between pressure and velocity approximation [79] or by introduction of stabilization terms [91] (or for more recent techniques [1],[13], [55], [64]).

As a general technique which allows to obtain a discretization which is stable for all Mach number regimes we consider the discontinuous Galerkin method (DGFEM). On the one hand, it is relatively easy to generalize standard finite element schemes to the discontinuous case. On the other hand, discontinuous finite elements have a long tradition [95], [103] and have recently regained attention [66], [44], [45]. We remark here, that the discretization of second-order terms as the diffusion terms has a sound theoretical background [49], [50], [40], [80].

Despite its potential for robust and accurate discretization, further research has to be carried out in order to make the DGFEM approach competitive. Among the different questions arising in this context we cite:

- Which variables to use ?
Whereas conservation properties are expressed in *conservative* variables and accurate shock approximation necessitates their use, diffusion and boundary conditions are expressed in *primitive* variables.
- How to solve the coupled system ?
Decoupling algorithms as the pressure correction schemes for transient incompressible flows are well understood. However, the generalization to higher Mach numbers, in particular for combustion, does not seem to be straightforward due to the different role of the pressure.

Concerning the *physical* difficulties, one has to be aware that the full system of flow equations comprises different physical phenomena with different time-scales. One standard technique consists in developing the pressure with respect to the Mach number [108], [105]. One is then able to construct numerical schemes for the resulting equations in the small Mach number limit [125], [120]. However, in that case fast scales as acoustic waves need to be captured, and consequently, it is important to develop separate equations since an efficient numerical treatment has to take these different aspects into account.

3.5. Numerical tools: Adaptivity

3.5.1. Mesh and order adaptation

The possible benefits of local mesh refinement for fluid dynamical problems is nowadays uncontested; the obvious arguments are the presence of singularities, shocks, and combustion fronts. The use of variable polynomial approximation is more controversial in CFD, since the literature does not deliver a clear answer concerning its efficiency. At least at view of some model problems, the potential gain obtained by the flexibility to locally adapt the order of approximation is evident. It remains to investigate if this estimation stays true for the applications to be considered in the project.

The design and analysis of auto-adaptive methods as described above is a recent research topic, and only very limited theoretical results are known. Concerning the convergence of adaptive methods for mesh refinement, only recently there has been made significant progress in the context of the Poisson problem [53], [107][2], based on two-sided a posteriori error estimators [121]. The situation is completely open for p -adaptivity, model-adaptivity or the DWR method¹. In addition, not much seems to be known for nonlinear equations. It can be hoped that theoretical insight will contribute to the development of better adaptive algorithms.

3.5.2. Automatic model selection

An important parameter of adaptation is the level of modeling. Here, the ideal situation is to dispose of a hierarchy of models which can be locally adapted in order to yield a desired accuracy at lowest possible cost.

¹Dual-weighted-residual method [3], see below.

A general approach towards the systematic a posteriori error estimation of modeling errors has been developed in [39], [56], [57] and [110]. The crucial point for practical purposes seems to be the parameterization of different models. In the context of reacting flows, model reduction techniques in order to reduce the great number of unknowns are used. It is of interest to understand, how the errors produced by the model reduction can be controlled in a systematic way.

3.5.3. DWR-method (*dual-weighted residual*)

The four outlined fields of adaptation have in common the following questions:

- What is the criterion ?
- Does, and if so, how fast does the algorithm converge ?
- How to practically adapt the parameters ?
- How to realize an efficient adaptive algorithm ?

Concerning the first point, we note that most of the mathematical literature deals with a posteriori error estimators in the energy norm related to linear symmetric problems.

A more praxis-oriented approach to error estimation is the DWR method, developed in [4]; see also the overview paper [3], application to laminar reacting flows in [47], and application to the Euler equations in [86]. The idea of the DWR method is to consider a given, user-defined physical quantity as a functional acting on the solution space. This allows the derivation of a posteriori error estimates which directly control the error in the approximation of the functional value. This approach has been applied to local mesh-refinement for a wide range of model problems [3]. Recently, it has been extended to the control of modeling errors [56]. The estimator of the DWR method requires the computation of an auxiliary linear partial differential equation. So far, relatively few research has been done in order to use possibly incomplete information from, e.g., coarse discretization of this equation.

3.5.4. *Parameter identification and numerical sensitivities*

Numerical simulations generally involve parameters of different nature. Some parameters reflect physical properties of the materials under consideration, or describe the way they interact. In addition to these parameters the values of which are often determined by experiments and sometimes only known with accuracy under certain conditions, the development of a computational model involves additional quantities, which could for example be related to boundary and initial conditions.

The generalization of the DWR method to parameter identification problems has been developed in [51], and [16] for time-dependent equations. The case of finite-dimensional parameters, which is theoretically less challenging than the infinite-dimensional case and has therefore been less treated in the literature, is of particular interest in view of the presented applications (for example the estimation of a set of diffusion velocities).

The goal of numerical simulations are in general the computation of given output values I which are obtained from the approximated physical fields by additional computations, often termed *post-processing*. The DWR method places these output values in the center of interest and aims at providing reliable and efficient computations of these quantities.

In the context of calibration of parameter values with experiments, it seems to be natural to go one step beyond the sole computation of I . Indeed, the computation of numerical sensitivities or condition numbers $\partial I / \partial q_i$ where q_i denotes a single parameter can be expected to be of practical and theoretical interest, either in order to improve the design of experiments, or in order to help to analyze the outcome of an experiment.

It turns out, that similar techniques as those employed for parameter identification can be used in order to obtain information on parameter sensitivities and corresponding a posteriori error analysis [5].

3.6. Further topics

Here, we list some possible research topics of interest for the long-term perspective of the project.

- thermal, acoustic couplings
- hierarchical turbulence modeling
- other complex flows such as polymers
- direct computation of turbulent flows
- stability prediction

4. Application Domains

4.1. Introduction

Keywords: *Process engineering, environment.*

The targeted applications belong to the field of fluid mechanics with special emphasis on numerical simulation of complex flows. Of special interest are generic flow configurations related to the development of combustion chambers for jet or helicopter engines.

In the following, we shortly review the physics of combustion chambers. Then we present concrete example problems illustrating the challenging numerical difficulties described above. These examples serve as prototypical test problems.

4.2. Targeted issues related to combustion chamber development and engine certification

4.2.1. Working principle of combustion chambers

As an introduction, we briefly remind hereafter the very basic aspects of airplane propulsion. The engine provides a certain amount of energy thanks to the heat released in the combustion chamber by the oxidation of kerosene. The usable part of this energy is used to increase the kinetic energy of the mass flow rate of air channeled by the air inlets. The combustion chamber is the place where the initial amount of energy is being brought to the system before being transformed into mechanical energy and losses. The pressure drops through the different turbine stages are used to entrain the compressor stages and the remainder serves to produce thrust through the diverging exhaust (turbojet) or to entrain a propeller (turboshaft engine) or a rotor (helicopter). A schematic view of a diluted jet engine is given in Figure 1. The air mass flow streamed by the air intakes is then divided into two streams, the first one passing through the combustion chamber and the second one whose energy increases when passing through the fan. The dilution is the ratio between these two air fluxes. The higher this ratio, the better the propulsive efficiency since the ejection velocity decreases. Figure 1 presents an overview of a recent jet engine (by Rolls-Royce) where it appears clearly that the combustion chamber, which can be considered as the primary source of energy for the system, has a rather modest volume compared to that of the complete engine!

Thermodynamically speaking, the efficiency of the relevant cycle is directly controlled by the temperature level reached at the exit of the combustion chamber. So, the tendency through decades of engines development is to increase as much as possible the temperature and pressure levels in the chamber. However, there is a limit due to the resistance of the various parts of the chamber and turbine (spatial homogeneity of the temperature profile in front of the turbine) and due to the respect of objectives in term of pollutants emission.

4.2.2. Development of new combustion chambers

In the following, we describe four major issues in the development of new combustion chambers: the environmental norms for pollution, the safety constraints, improved wall cooling efficiency, and combustion in micro-devices.

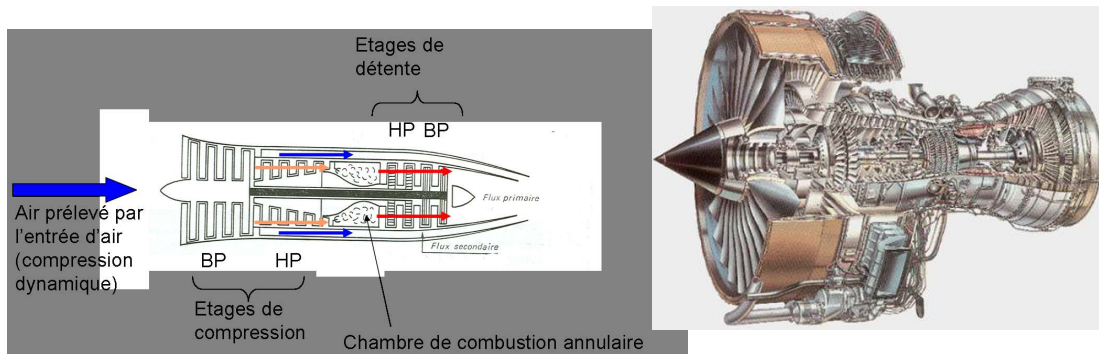


Figure 1. Functioning diagram of a diluted jet engine (left) and recent commercial plane engine (right, Rolls-Royce Trent 500).

4.2.2.1. Pollution

The combustion chamber being at the source of most of the engine pollutants emissions, it is naturally the subject of continuous efforts aimed at reducing as much as possible the level of its pollutants emissions in order to satisfy to the constantly more stringent international certification procedures.

ENGINE IDENTIFICATION:		CFM56-5B1/2P					
MODE	POWER SETTING (%F ₀₀)	TIME minutes	FUEL FLOW kg/s	EMISSIONS INDICES (g/kg)			SMOKE NUMBER
				HC	CO	NOx	
TAKE-OFF	100	0.7	1.32	0.1	0.8	23.3	0.5
CLIMB OUT	85	2.2	1.07	0.1	1.9	16.4	0.3
APPROACH	30	4.0	0.37	3.7	23.1	7.3	0.5
IDLE	7	26.0	0.12	2.9	36.5	4.1	2.1
LTO TOTAL FUEL (kg) or EMISSIONS (g)			473	891	9197	5024	-
NUMBER OF ENGINES				2	2	2	2
NUMBER OF TESTS				4	4	4	4
AVERAGE D _p /F ₀₀ (g/kN) or AVERAGE SN (MAX)				6.8	70.5	37.9	2.1
SIGMA (D _p /F ₀₀ in g/kN, or SN)				-	-	-	-
RANGE (D _p /F ₀₀ in g/kN, or SN)				6.2-7.4	66.2-74.7	37.5-38.3	2.0-2.3
REMARKS			BYPASS RATIO:		5.7		
DAC-II Combustor P/N 1968M99G04			PRESSURE RATIO (π ₀₀):		30.5		
			RATED OUTPUT (F ₀₀) (kN):		133.5		

Figure 2. Example of sheet established during the certification process (CFM-International family).

Among the different undesirable chemical species, one can cite the various carbon oxides (which leads to ozone formation, greenhouse effect), the nitrogen oxides (provoking ozone formation locally and in the high atmosphere) and sulfur (which causes atmosphere acidity), unburned hydrocarbons (provoking ozone formation locally, greenhouse effect) and soot (dangerous for human health). The International Civil Aviation Organization (ICAO) is in charge of setting up the various procedures required to measure the pollutant

emission levels that any new engine must undergo before being marketable. A standard sequence of take-off/flight/landing is thus defined in Annex 16 - Volume II [93]. In this framework, the monitored species are unburned hydrocarbons, soot, carbon monoxide, nitrogen oxides. Figure 2 presents a typical result produced during such tests of a new engine (source www.qinetiq.com). Bearing in mind the various mechanisms that produce such oxides, new combustion systems are actively developed and tested especially in the framework of European research programs such as LOPOCOTEP and MOLECULES which group academic and industrial partners around this common objective. Many of the present device improvements rely on the recourse to Lean Premixed Prevaporized (LPP) combustion based systems characterized by a tight control of the stoichiometry field properties within the combustion chamber. Such innovative concepts prove to be very promising but they still suffer from intrinsic instabilities over the range of operational conditions and therefore additional studies are still required to minimize, if not suppress, the negative impact of these phenomena. With this respect, the development of reliable and efficient CFD tools incorporating up-to-date and extensively validated physical modeling is of paramount importance in order to supplement experiments.

4.2.2.2. Safety issue: accidental boring of a combustion chamber

The development of new combustion chambers is not only concerned by pollution or efficiency matters but also by safety problems. Indeed, if the engine manufacturer has to demonstrate the various capabilities of its engine regarding reliability, easy servicing or low operating costs, the airplane manufacturer (Airbus or Boeing for instance) who powered its plane with such engines has also to face some certification rules regarding safety issues. For instance, it is of its responsibility to demonstrate that the plane and its passengers will not be endangered in the case of an accidental boring of one of the engines combustion chambers (this happens from time to time, often near the kerosene injection ports). In that respect, the FAR 25903 (d)(1) stipulates the type of testing that can ensure that such conditions are satisfied. During such a test, the pylon truss must stand a three-minute impact of an highly underexpanded supersonic jet whose stagnation conditions are strictly imposed (see Figure 3).

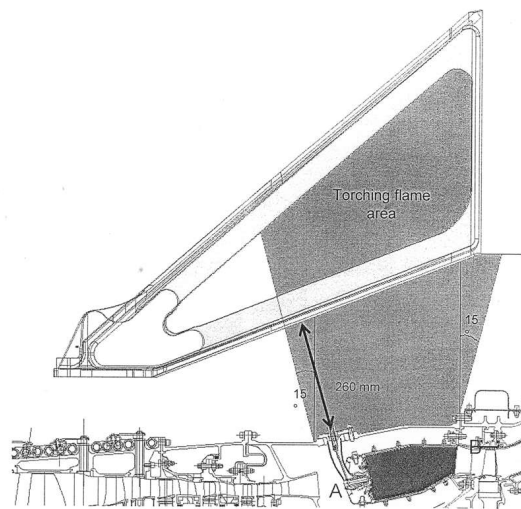


Figure 3. Domain of possible interaction between the jet created by the boring of a combustion chamber and the engine pylon (from Airbus).

This three-minute period of time is thought of as being sufficient for the pilot to take any necessary action to detect and stop the faulty engine. For instance, Airbus France recently developed a partnership with the

Moscow Aviation Institute to carry out this type of test. Considering the wide family of airplanes that a single manufacturer can offer, with different engines, pylon positioning and so forth as well as the cost and the difficulty of conducting the experiments required by the certification authorities, it is clear again that accurate numerical simulations conducted *a priori* or jointly with the experiments are of great help in the course of the certification procedure. Now, what is the type of flow, simulations would have to deal with in such a case? If one considers a reservoir discharging into a quiescent atmosphere, it is the nozzle pressure ratio (NPR) between the static pressure at the nozzle exit and that of the ambient atmosphere that can be used to discriminate between the various possible flow patterns.

For weak or moderate NPR's (typically for $1 < \text{NPR} < 2$), these jets are characterized by three main zones: i) the near field, whose "diamond-like" shock structure is a repetition of incident and reflected oblique shock waves; ii) the transition region, wherein these structures are swallowed by the development of the shear layer; and finally, iii) the far field, with a more classical self-similar jet. In these cases, the jet core remains mainly supersonic so that the global features of the flow structure are reasonably predicted just by taking into account the compressible effects on turbulence. This is not the case for situations involving much higher NPR's. In that case, the expansion fan gives rise to a highly curved incident "barrel" shock which irregularly reflects through a strong, curved "Mach Disk" which strongly interacts with the jet shear layer, while a large subsonic zone develops within the jet core. This flow configuration represents a great challenge as far as the modeling of the prominent phenomena is concerned, e.g. compressible turbulence, interaction between turbulence and shock, strong compression or expansion zones, curvature and non-equilibrium effects on the shear layer growth. A comprehensive survey of the sensitivity of the flow structure to various parameters is given in [102]. When such a flow is impacting a solid surface, the resulting flow structure is even more complex and extremely sensitive to the impact angle, the distance between the nozzle and the surface and the NPR. In the case of a normal impact, a double shock structure (Mach disk and the so-called plate shock) may appear and the interaction with the boundary layer developing on the impacted surface can lead to the appearance of recirculation bubbles prone to low frequency unsteadiness. In the case of a non-normal impact, the near surface flow morphology changes again (additional reflected shocks and triple points) and can yield a pressure field that can reach peak values on the impacted surface three times as much as those observed when the impact is normal. Considering the complexity of such a type of flow, it appears that the preliminary necessary step paving the way towards accurate simulations of such type of fluid-surface interaction, is the development of numerical tools able to simulate accurately the structure of free highly underexpanded supersonic jets involved in such an interaction. In addition, such jets are well suited for testing newly developed numerical tools since they can be simulated by considering increasingly complex physical modeling, starting with the Euler equations (2D, 2D-axisymmetric, and 3D), then considering the Navier-Stokes equations before going to turbulence modeling.

4.2.2.3. *Engine efficiency: improved cooling of a combustion chamber wall*

The film cooling technique is now widely used in combustion chambers. The continuous injection of air through numerous holes drilled through the combustion chamber wall permits the formation of a film which protects the wall from the high temperature resulting from the kerosene+air combustion process. If this type of wall flows has been extensively studied in order to determine the layout of the holes that maximizes the cooling efficiency, the knowledge of the influence of the hole shape on the near wall flow structure is not extensively documented. This issue has to be addressed, since it is well known that the drilling techniques usually employed in industry (laser or electron beams) produce holes of different shapes.

A partnership between LMA and Turbomeca in order to address this topic exists. This collaboration has led to the installation of a test facility at UPPA, see Figure 4. Its goal is to study experimentally confined wall flows representative of those present in a real combustion chamber. This experimental rig is intended to be used in order to compare with computational results.

4.2.2.4. *Generating compact propulsive systems: mixing processes and combustion in micro-devices*

If jet or helicopter engine combustion chambers are the primary systems in sight, it is worth noticing that recently, micro combustion chambers have received a renewed interest either as a propulsive tool for drones or to produce electricity for various portable devices. In France, ONERA, who is the leader in this domain, has recently developed a test facility in Palaiseau to study experimentally the various aspects and problems related



Figure 4. Experimental bank at UPPA.

to these devices. A doctoral thesis on a related question with a UPPA-ONERA co-supervision is planned. Since the codes developed in the present project should have the capability of dealing with laminar and turbulent reacting flows, the numerical simulation of the flow in this type of micro-combustion chamber is an interesting step to assess the capability of the developed tools to deal with reacting flows.

4.3. Test problems related to the targeted issues

4.3.1. Highly underexpanded supersonic jets

This kind of flow corresponds to the jets experimentally studied by Yüceil and Ötügen [126] and Ötügen et al. [127]. Figure 5 presents a schematic view of the flow configuration along with the main flow parameters to be considered. The main objective of this test configuration is to correctly predict the Mach disk location as well as its radial extension. The complex shock pattern including the Mach disk is presented in Figure 6 (taken from [102]). The underlying model are the standard Euler equations.

Highly underexpanded supersonic jets have been the subject of the doctoral thesis of G. Lenasch (supervisor: P. Bruel). The computational and experimental results obtained in this thesis showed the necessity to increase the accuracy of computations for this type of problems. They form an ideal basis for comparison with the software to be developed.

The objective of this test problem is to evaluate the potential gain in efficiency of high-order and adaptive methods based on the discontinuous Galerkin finite element methods applied to the Euler equations. A natural extension of this test problem is to include viscous terms.

4.3.2. Subsonic jet in cross flow

This kind of flow corresponds to the experimental configuration investigated by Miron et al. [106]. Figure 7 presents a schematic view of the flow configuration.

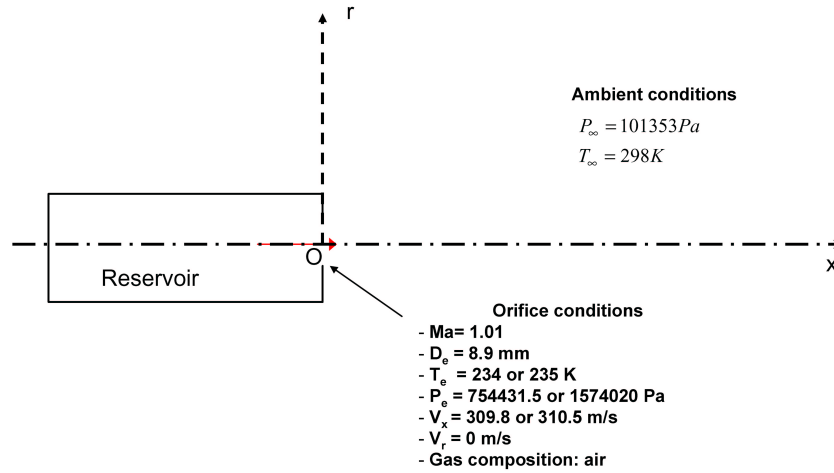


Figure 5. Underexpanded jet: main parameters of the flow.

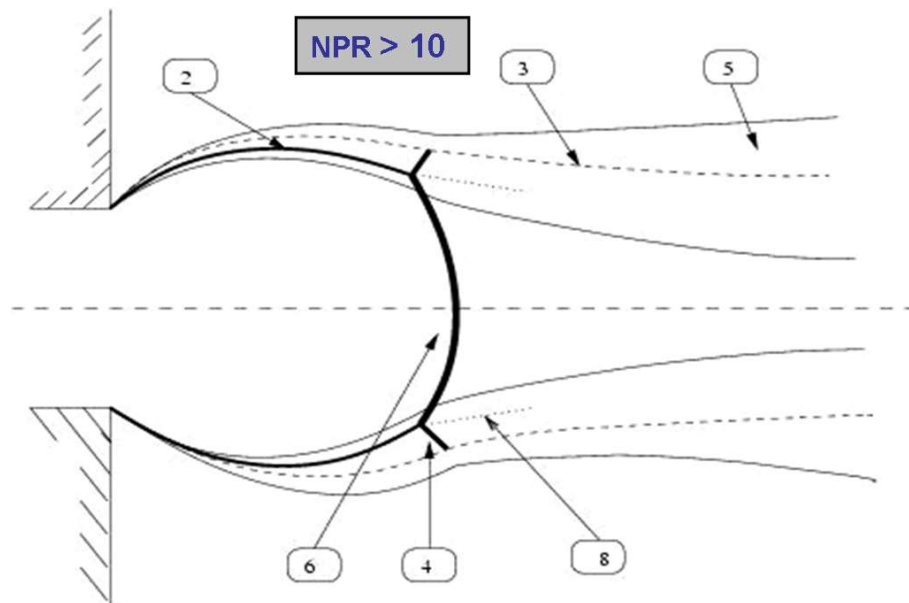


Figure 6. Schematic plot of the structure of an highly underexpanded supersonic jet : 2. incident shock, 3. isobaric line of the shear layer, 4. Reflected shock, 5. Jet shear layer, 6. Mach disk, 8. Mach disk shear layer.

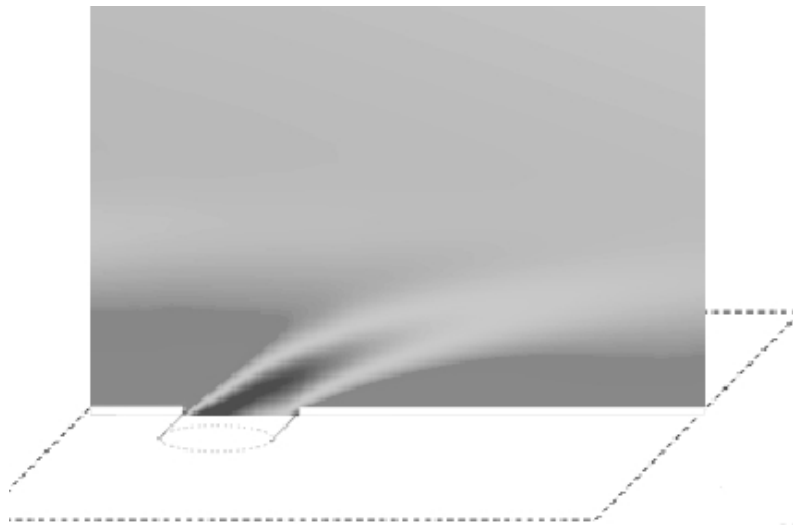


Figure 7. Subsonic jet in a cross-flow.

The first objective is to simulate accurately the flow within the hole and the near field of the jet to cross-flow interaction zone, in order to be able to assess the discharge coefficient sensitivity to the detailed shape of the hole which is in general non-circular. The flows are turbulent, thus this geometry will be specifically used for testing the capability of the numerical tools developed in the project, especially combined with turbulence modeling.

The discharge coefficient is the mean of the normal velocity component over a whole, and can therefore be considered as a functional of the velocity. Our particular interest is in deriving self-adaptive methods for the efficient computation of this functional. We therefore intend to employ the DWR-method [3] in order to perform automatic mesh selection. As a mid-term goal we wish to develop a similar approach for self-adaptive turbulence modeling. A first effort in this direction is the post-doctoral work of Phuc Nguyen Danh (supervised by P. Bruel and R. Becker), which is financed by the CDAPP².

4.3.3. DNS of mixing in micro-channels

This kind of flow has been experimentally studied in the doctoral thesis of Dumand [71] at ONERA (supervised by V. Sabel'nikov). The flow geometry is sketched in Figure 8.

It represents a view of the mixing channel, e.g., the channel used to mix the oxidizer stream of air and the fuel stream which is simulated by an injection of nitrogen and acetone. The objective of this device is to mix the two streams as quickly as possible in order to feed the combustion chamber with a mixture as homogeneous as possible. Due to the very small dimensions of the channel, the Reynolds number of the flow is below 500, and the Mach number is very small.

In order to compute the flow of this test problem, we intend to develop an incompressible flow solver. In addition to the pressure and velocity field, the concentration of each considered species has to be determined. We intend to extend the solver to the case of compressible low-Mach number flows.

5. Software

²Communauté d'agglomération de Pau Pyrénées

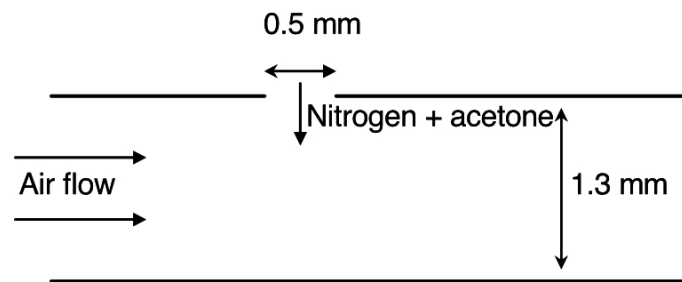


Figure 8. Micro combustion chamber: overview of the mixing channel geometry.

5.1. Toolkit Concha

Keywords: *DG, FEM, SDFEM, nonconforming elements.*

Participants: David Trujillo [correspondant], Roland Becker.

Since the goals of the project are to evaluate the potential of recent numerical methods and to develop new approaches in the context of industrial CFD problems, it is important to possess flexible and extendable software which is able to integrate the methods under consideration such as local adaptive mesh refinement, anisotropic meshes, hierarchical meshes, *hp*-methods, and DGFEM. At the same time the codes have to be able to deal with the physics of complex reactive flow problems.

We have started the development of a toolkit Concha which serves as a basis for specialized solvers. The software architecture is designed in such a way that a group of core developers can contribute in an efficient manner, and that independent development of different physical applications is possible. Further, in order to accelerate the integration of new members and in order to provide a basis for our educational purposes (see Section 9.1), the software proposes different entrance levels. The development is made under the INRIA Gforge.

5.2. ConchaEuler

Keywords: *DG, Euler equations, FEM.*

Participants: Eric Schall [correspondant], Roland Becker, Robert Luce.

Based on the toolkit Concha, we have developed a code for the two-dimensional Euler equations based on the lowest-order discontinuous finite element method. The objective is to compare the efficiency of different well-known Riemann solvers, and to understand the computational bottlenecks in order to guide the further development concerning adaptive higher order methods.

5.3. ConchaNavierStokes

Keywords: *FEM, Navier-Stokes equations, incompressibility, stabilization.*

Participants: Daniela Capatina [correspondant], Roland Becker, David Trujillo.

Based on the toolkit Concha, we have developed a code for the two-dimensional Navier-Stokes equations based on different stable and stabilized pairs of elements (P1-P1, P2-P2, P2-P1, CR1-P0). The objective is to compare the properties and efficiency of different stabilization methods for higher Reynolds numbers in order to guide the further development concerning adaptive higher order methods, especially in three dimensions.

6. New Results

6.1. Experimental results

Keywords: *FEM, convergence, error estimation, stabilization.*

Participants: Pascal Bruel, Phuc Danh Nguyen, Aurelien Most.

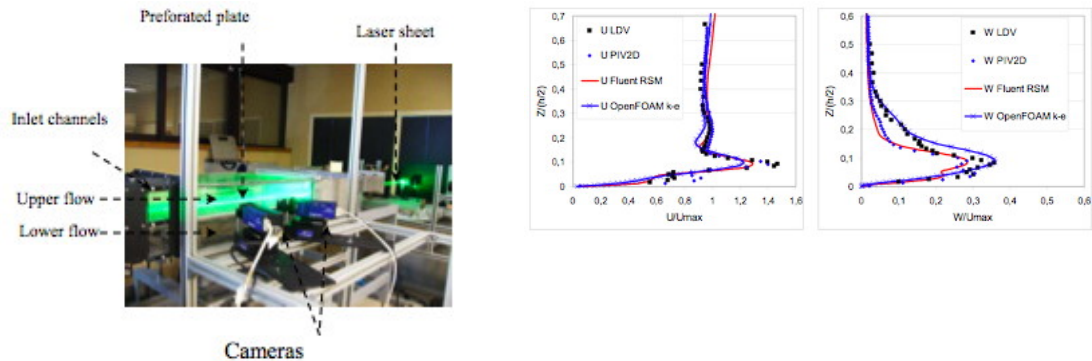


Figure 9. The experimental bank MAVERIC (left), comparison of numerical simulations (right).

The test facility MAVERIC (MAquette pour la Validation et l'Expérimentation sur le Refroidissement par Injection Contrôlée) has been installed and the particle image velocimetry (PIV) system has been fitted. The first velocity data were produced in June 2007. In Figure 9, a detailed view of the test section of MAVERIC is presented. The right image of Figure 9 gives an example of profiles that have been extracted from the PIV data and compared to i) LDV measurements available in the literature and ii) RANS simulations carried out in parallel [26], [25]. A first analysis of the sensitivity of the wall flow to the shape of the perforation hole has also been carried out [11].

6.2. Stabilized finite elements for Navier-Stokes

Keywords: *FEM, convergence, error estimation, stabilization.*

Participants: Roland Becker, Peter Hansbo, Daniela Capatina, David Trujillo.

Stabilized FEM for the Stokes problem are very popular in applications, since they allow for equal-order interpolation (same 'simple' FE space for both pressure and velocities) [91]. In recent years, the trend is to move from residual-based schemes such as GLS [91] to consistent penalty methods like LPS [1] [54], [64]. Especially the method of [54] is advocated, since it avoids the explicit introduction of stabilization parameters. We have recently found an even simpler approach [14] which only used the difference of the mass matrix and its lumped variant. The optimal convergence rate has been established, as well as a generalization to higher order elements.

The stabilization of higher Reynolds-number flow is the subject of [13]. The approach is based on introduction of the vorticity as an additional unknown. The method has been analyzed, and computational comparisons have been made.

6.3. Convergence of adaptive finite element algorithms

Keywords: *AFEM, complexity, convergence, mixed FEM, nonconforming FEM.*

Participants: Roland Becker, Shipeng Mao.

Adaptive finite element methods are becoming a standard tool in numerical simulations, and their application in CFD is one of the main topics of CONCHA. However, their theoretical analysis is very recent, and the known results have a lot of limitations with respect to the underlying PDE, which is supposed to be elliptic, but also with respect to important practical issues. In general, the mesh refinement is supposed to be done by the 'newest vertex algorithm', which generates interior nodes in the newly refined triangles. In addition the standard treatment of an unavoidable data-oscillation term either prohibits the control of the complexity (MNS-algorithm [107]), or leads to additional iteration [116]. In order to overcome these difficulties, we have developed a new adaptive marking strategy, which allows us to prove geometric convergence and optimal complexity [15]. We have extended this result to the case of the Courant FE with standard red-green refinement [32], mixed FE [31], as well as nonconforming FE [33].

7. Contracts and Grants with Industry

7.1. Turbomeca

Turbomeca (SAFRAN Group)³ is a leading constructor of turbines for helicopters and turbojet engines for aircraft and missiles. It is located in Bordes, close to Pau. The interest of collaboration between UPPA and Turbomeca on different levels has been manifested and lead to the establishment of a 'contrat cadre'⁴.

CFD plays a crucial role in the development and certification of turbomachines and is used at Turbomeca in different contexts : heat transfer, cooling, compressors, and combustion. Reactive flow problems and combustion are an important field of collaboration between UPPA and the manufacturer of turbines Turbomeca. Although numerical approaches have been part of it, the collaboration is at the moment mostly centered on experiments. Due to its experimental banks, the TURBOMECA site of Pau-Bordes is a reference center in the field of turbo machinery on the European level.

It is to be noted that the need to concentrate applied research in combustion from an industrial point of view had lead to the foundation of INCA (Advanced Combustion Initiative)⁵.

8. Other Grants and Activities

8.1. Other Grants and Activities

Numerical methods for complex fluid mechanical applications is a very huge subject. Here we focus on the most significant aspects related to reactive flow simulations.

- Research network: Pôle de compétitivité AESE⁶
The themes of this project enter the 'pôle de compétitivité' AESE (aéronautique, espace et système embarqués) which brings together research activities in this domain and is located in the south-west of France.
- Research network: INCA
Concerning the field of combustion, ONERA, CNRS, and the group SAFRAN (containing TURBOMECA), have created in 2002 the common project INCA which aims to extract added value from French combustion research, and to position Snecma among the world leaders in this technology. As a consequence, INCA provides a natural framework for technology transfer in the field of combustion.

³<http://www.turbomeca.com/>

⁴contract coordinating common research

⁵<http://www.cerfacs.fr/inca>

⁶<http://www.aerospace-valley.com>

We intend to collaborate in the framework of these research networks. The participation is important since they provide a forum for discussion of industry relevant research topics. We intend to participate by means of doctoral thesis.

9. Dissemination

9.1. Education

The LMA has proposed a new Master program starting in 2007, which is called MMS (Mathématiques, Modélisation et Simulation) and has a focus on analysis, modeling, and numerical computations in PDEs. The core of this education is formed by lectures in four fields : PDE-theory, mechanics, numerical analysis, and simulation tools. Our software has a special part devoted to educational purposes (library 'ConchaBase'⁷). It is intended to have a simple transparent structure in order to allow teaching of the low-level details of modern finite element programming. The purpose is to provide a basis for teaching and to gradually introduce the student to the use and development of more elaborated tools.

The second year of this master program includes lectures on physical applications, one of the three proposed fields is CFD; lectures are provided by the members of the project. The second semester of the second year is devoted to internships in industry, which defines a practical means of collaboration with our industrial partners such as CERFACS, ONERA, TOTAL, and Turbomeca.

9.2. Scientific community

The participants have activities as referees in international journals such as *Int. J. for Numer. Methods in Fluids, Combustion Science and Technology, Int. Symposium on Combustion, J. Thermophysics, J. Comp. Phys., Numer. Math., SIAM J. on Opt. and Control, SIAM J. Numer. Anal., SIAM J. Sci. Comp., J. of Comp. Mech., Computing.*

The participants of the project participate in international scientific conferences such as *Mafelap06, Finite Element Fair 2006, Oberwolfach 2007, ECM 2007, ICDERS 2007, CFM 2007, 43rd Joint Propulsion Conference and Exhibit 2007, FLOCOME07, ICIAM07, ICFD07, MAMERN07, Euro-Mediterranean Conference on Biomathematics, Le Caire, 26-29 juin 2007.*

Finally we mention the one-month visits of Shipeng Mao (Chinese academy of Sciences) and Francesco-Javier Sayas (University of Zaragoza).

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