IN PARTNERSHIP WITH:
CNRS

Université de Pau et des Pays de l'Adour

Activity Report 2017

Project-Team CAGIRE

Computational AGility for internal flows sImulations and compaRisons with Experiments

IN COLLABORATION WITH: Laboratoire de mathématiques et de leurs applications (LMAP)

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Numerical schemes and simulations

Table of contents

Project-Team CAGIRE

Creation of the Team: 2011 June 01, updated into Project-Team: 2016 May 01

Keywords:

Computer Science and Digital Science:

A6.1.1. - Continuous Modeling (PDE, ODE)
A6.2.1. - Numerical analysis of PDE and ODE
A6.2.7. - High performance computing

Other Research Topics and Application Domains:

B4.2. - Nuclear Energy Production
B5.2.1. - Road vehicles
B5.2.3. - Aviation
B5.2.4. - Aerospace

1. Personnel

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2. Overall Objectives

2.1. Turbulent flows with complex interactions

This interdisciplinary project brings together researchers coming from different horizons and backgrounds (applied mathematics and fluid mechanics) who progressively elaborated a common vision of what should be the simulation tool of fluid dynamics of tomorrow. Our application will be focused on wall bounded turbulent flows and featuring complex phenomena such as aeroacoustics, hydrodynamic instabilities, phase change processes, complex walls, buoyancy or localized relaminarization. Because such flows are exhibiting a multiplicity of time and scale fluctuations resulting from complex interactions, their simulation is extremely challenging. Even if various methods of simulation (DNS [1]) and turbulence modeling (RANS [2], LES [3], hybrid RANS-LES) are available and have been significantly improved over time, none of them does satisfy all the needs encountered in industrial and environmental configurations. We consider that all these methods will be useful in the future in different situations or regions of the flow if combined in the same simulation in order to benefit from their respective advantages wherever relevant, while mutually compensating their known limitations. It will thus lead to a description of turbulence at widely varying scales in the computational

[1] Direct numerical simulation
[2] Reynolds averaged Navier-Stokes
[3] Large-eddy simulation

domain, hence the name *multi-scale simulations*. For example, the RANS mode may extend throughout regions where turbulence is sufficiently close to equilibrium leaving to LES or DNS the handling of regions where large scale coherent structures are present. However, a considerable body of work is required to:

- Establish the behavior of the different types of turbulence modeling approaches when combined with high order discretization methods.
- Elaborate relevant and robust switching criteria between models, similar to error assessments used in automatic mesh refinement, but based on the physics of the flow in order to adapt on the fly the scale of resolution from one extreme of the spectrum to another (say from the Kolmogorov scale to the geometrical large scale, i.e., from DNS to RANS).
- Ensure a high level of accuracy and robustness of the resulting simulation tool to address a large range of flow configurations, i.e., from a generic lab scale geometry for validation to practical systems of interest of our industrial partners.

But the best agile modeling and high order discretization methods are useless without the recourse to high performance computing (HPC) to bring the simulation time down to values compatible with the requirement of the end users. So, a significant part of our activity will be devoted to the proper handling of the constantly evolving supercomputer architectures. But even the best ever simulation library is useless if it is not disseminated and increasingly used by the CFD community as well as our industrial partners. In that respect, the significant success of the low order finite volume simulation suite OpenFOAM [4] or the more recently proposed SU2 [5] from Stanford are considered as examples of quite successful dissemination stories that could be if not followed but at least considered as a source of inspiration. Our natural inclination though will be to promote the use of the library in direction of our present and future industrial and academic partners with a special interest on the SMEs active in the highly competitive and strategic economical sectors of energy production and aerospace propulsion. Indeed, these sectors are experiencing a revolution of the entire design process especially for complex parts with an intimate mix between simulations and additive manufacturing (3D printing) processes in the early stages of the design process. For big companies such as General Electric or Safran (co-developing the CFM Leap-1 engines with 3D printed fuel nozzles) as well as medium-size companies such as Aerojet Rocketdyne, this is a unique opportunity to reduce the duration and hence the cost of development of their systems while preserving if not strengthening their capability of designing innovative components that cannot be produced by classical manufacturing processes. On the other side, for the small companies of this sector, this may have a rather detrimental effect on their competitiveness since their capability of mastering both these new manufacturing processes and advanced simulation approaches is far more limited. Thus, through our sustained direct (EDF, Turbomeca, PSA, AD Industrie) or indirect (European programs, WALLTURB, KIAI, IMPACT-AE, SOPRANO) partnership with different companies, we are able to identify relevant generic configurations from our point of view of scientists to serve as support for the development of our approach. This methodological choice was motivated by the desire to lead an as efficient as possible transfer activity while maintaining a clear distinction between what falls within our field of competence of researchers from what is related to the development of their products by our industrial partners. The long-term objective of this project is to develop, validate, promote and transfer an original and effective approach for modeling and simulating generic flows representative of flow configurations encountered in the field of energy production and aeronautical propulsion. Our approach will be combining mesh (h) + turbulence model (m) + discretization order (p) agility. This will be achieved by:

- Contributing to the development of new turbulence models.
- Improving high order numerical methods, and increasing their efficiency in the constantly evolving High Performance Computing context.
- Developing experimental tools.

[4] http://www.openfoam.com
[5] http://su2.stanford.edu/

Concerning applications, our objective are :

- To reinforce the long term existing partnership with EDF and Safran group, and the other European partners involved in the same European projects as we are.
- To consolidate and develop partnership with SMEs operating in the aeronautical sector.

3. Research Program

3.1. The scientific context

3.1.1. Computational fluid mechanics: modeling or not before discretizing ?

A typical continuous solution of the Navier Stokes equations at sufficiently high values of the Reynolds number is governed by a spectrum of time and space scales fluctuations closely connected with the turbulent nature of the flow. The term deterministic chaos employed by Frisch in his enlightening book [32] is certainly conveying most adequately the difficulty in analyzing and simulating this kind of flows. The broadness of the turbulence spectrum is directly controlled by the Reynolds number defined as the ratio between the inertial forces and the viscous forces. This number is not only useful to determine the transition from a laminar to a turbulent flow regime, it also indicates the range of scales of fluctuations that are present in the flow under consideration. Typically, for the velocity field and far from solid walls, the ratio between the largest scale (the integral length scale) to the smallest one (Kolmogorov scale) scales as $Re^{3/4}$ per dimension. In addition, for internal flows, the viscous effects near the solid walls yield a scaling proportional to Re per dimension. The smallest scales play a crucial role in the dynamics of the largest ones which implies that an accurate framework for the computation of turbulent flows must take into account all these scales. Thus, the usual practice to deal with turbulent flows is to choose between an a priori modeling (in most situations) or not (low Re number and rather simple configurations) before proceeding to the discretization step followed by the simulation runs themselves. If a modeling phase is on the agenda, then one has to choose again among the above mentioned variety of approaches. As it is illustrated in Fig. 1, this can be achieved either by directly solving the Navier-Stokes equations (DNS) or by first applying a statistical averaging (RANS) or a spatial filtering operator to the Navier-Stokes equations (LES). The new terms brought about by the filtering operator have to be modeled. From a computational point of view, the RANS approach is the least demanding, which explains why historically it has been the workhorse in both the academic and the industrial sectors. It has permitted quite a substantial progress in the understanding of various phenomena such as turbulent combustion or heat transfer. Its inherent inability to provide a time-dependent information has led to promote in the last decade the recourse to either LES or DNS to supplement if not replace RANS. By simulating the large scale structures while modeling the smallest ones supposed to be more isotropic, LES proved to be quite a step through that permits to fully take advantage of the increasing power of computers to study complex flow configurations. At the same time, DNS was progressively applied to geometries of increasing complexity (channel flows with values of Re_τ multiplied by 10 during the last 15 years, jets, turbulent premixed flames, among many others), and proved to be a formidable tool that permits **(i)** to improve our knowledge on turbulent flows and **(ii)** to test (i.e., validate or invalidate) and improve the modeling hypotheses inherently associated to the RANS and LES approaches. From a numerical point of view, if the steady nature of the RANS equations allows to perform iterative convergence on finer and finer meshes, the high computational cost of LES or DNS makes necessary the use of highly accurate numerical schemes in order to optimize the use of computational resources. To the noticeable exception of the hybrid RANS-LES modeling, which is not yet accepted as a reliable tool for industrial design, as mentioned in the preamble of the Go4hybrid European program [6], once chosen, a single turbulence model will (try to) do the job for modeling the whole flow. Thus, depending on its intrinsic strengths and weaknesses, the accuracy will be a rather volatile quantity strongly dependent on the flow configuration. The turbulence modeling and industrial design communities waver between the desire to continue to rely on the RANS approach, which is unrivaled in terms of computational cost, but is still not able to accurately

[6] https://cordis.europa.eu/result/rcn/177053_en.html

represent all the complex phenomena; and the temptation to switch to LES, which outperforms RANS in many situations but is prohibitively expensive in high-Reynolds number wall-bounded flows. In order to account for the deficiencies of both approaches and to combine them for significantly improving the overall quality of the modeling, the hybrid RANS-LES approach has emerged during the last decade as a viable, intermediate way, and we are definitely inscribing our project in this innovative field of research, with an original approach though, connected with a time filtered hybrid RANS-LES and a systematic and progressive validation process against experimental data produced by the team.

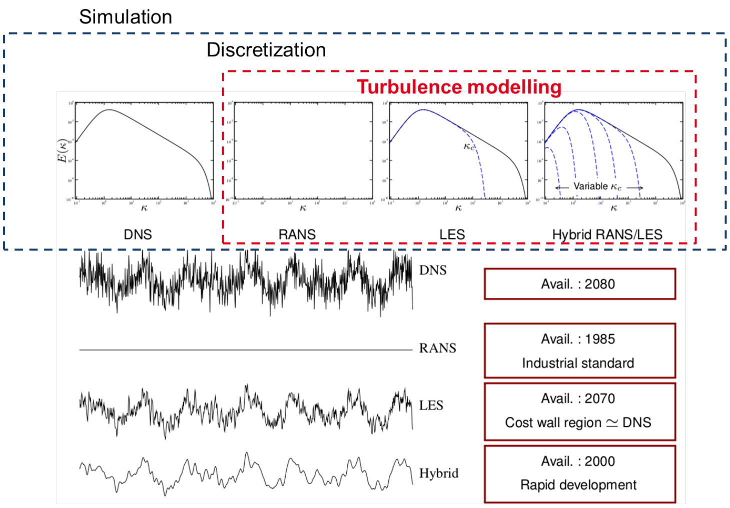

Figure 1. A schematic view of the different nested steps for turbulent flow simulation: from DNS to hybrid RANS-LES. The approximate dates at which the different approaches are or will be routinely used in the industry are indicated in the boxes on the right (extrapolations based on the present rate of increase in computer performances).

3.1.2. *Computational fluid mechanics: high order discretization on unstructured meshes and efficient methods of solution*

All the methods considered in the project are mesh-based methods: the computational domain is divided into cells, that have an elementary shape: triangles and quadrangles in two dimensions, and tetrahedra, hexahedra, pyramids, and prisms in three dimensions. If the cells are only regular hexahedra, the mesh is said to be structured. Otherwise, it is said to be unstructured. If the mesh is composed of more than one sort of elementary shape, the mesh is said to be hybrid. In the project, the numerical strategy is based on discontinuous Galerkin methods. These methods were introduced by Reed and Hill [43] and first studied by Lesaint and Raviart [39]. The extension to the Euler system with explicit time integration was mainly led by Shu, Cockburn and their collaborators. The steps of time integration and slope limiting were similar to high order ENO schemes, whereas specific constraints given by the finite element nature of the scheme were progressively solved, for scalar conservation laws [28], [27], one dimensional systems [26], multidimensional scalar conservation laws [25], and multidimensional systems [29]. For the same system, we can also cite the work of [31], [36], which is slightly different: the stabilization is made by adding a nonlinear term, and the time integration is implicit. Contrary to continuous Galerkin methods, the discretization of diffusive operators is not straightforward. This is due to the discontinuous approximation space, which does not fit well with the space function in which the diffusive system is well posed. A first stabilization was proposed by Arnold [18]. The first application of discontinuous Galerkin methods to Navier-Stokes equations was proposed in [23] by mean of a mixed formulation. Actually, this first attempt led to a non compact computation stencil, and was later proved to be not stable. A compactness improvement was made in [24], which was later analyzed, and proved to be stable in a more unified framework [19]. The combination with the $k - \omega$ RANS model was made in [22]. As far as Navier Stokes equations are concerned, we can also cite the work of [34], in which the stabilization is closer to the one of [19], the work of [40] on local time stepping, or the first use of discontinuous Galerkin methods for direct numerical simulation of a turbulent channel flow done in [30]. Discontinuous Galerkin methods are so popular because:

- They can be developed for any order of approximation.
- The computational stencil of one given cell is limited to the cells with which it has a common face. This stencil does not depend on the order of approximation. This is a pro, compared for example with high order finite volumes, which require as more and more neighbors as the order increases.
- They can be developed for any kind of mesh, structured, unstructured, but also for aggregated grids [21]. This is a pro compared not only with finite differences schemes, which can be developed only on structured meshes, but also compared with continuous finite elements methods, for which the definition of the approximation basis is not clear on aggregated elements.
- p-adaptivity is easier than with continuous finite elements, because neighboring elements having a different order are only weakly coupled.
- Upwinding is as natural as for finite volumes methods, which is a benefit for hyperbolic problems.
- As the formulation is weak, boundary conditions are naturally weakly formulated. This is a benefit compared with strong formulations, for example point centered formulation when a point is at the intersection of two kinds of boundary conditions.

For concluding this section, there already exist numerical schemes based on the discontinuous Galerkin method which proved to be efficient for computing compressible viscous flows. Nevertheless, there remain many things to be improved, which include: efficient shock capturing methods for supersonic flows, high order discretization of curved boundaries, low Mach number behavior of these schemes and combination with second-moment RANS models.Another drawback of the discontinuous Galerkin methods is that they can be computationally costly, due to the accurate representation of the solution calling for a particular care of implementation for being efficient. We believe that this cost can be balanced by the strong memory locality of the method, which is an asset for porting on emerging many-core architectures.

3.1.3. Experimental fluid mechanics: a relevant tool for physical modeling and simulation development

With the considerable and constant development of computer performance, many people were thinking at the turn of the 21st century that in the short term, CFD would replace experiments considered as too costly and not flexible enough. Simply flipping through scientific journals such as Journal of Fluid Mechanics, Combustion of Flame, Physics of Fluids or Journal of Computational Physics or through websites such that of Ercoftac [7] is sufficient to convince oneself that the recourse to experiments to provide either a quantitative description of complex phenomena or reference values for the assessment of the predictive capabilities of the physical modeling and of the related simulations is still necessary. The major change that can be noted though concerns the content of the interaction between experiments and CFD (understood in the broad sense). Indeed, LES or DNS assessment calls for the experimental determination of time and space turbulent scales as well as time resolved measurements and determination of single or multi-point statistical properties of the velocity field. Thus, the team methodology incorporates from the very beginning an experimental component that is operated in strong interaction with the physical modeling and the simulation activities.

[7] http://www.ercoftac.org

3.2. Research directions

3.2.1. Boundary conditions

3.2.1.1. Generating synthetic turbulence

A crucial point for any multi-scale simulation able to locally switch (in space or time) from a coarse level of turbulence description to a more refined one, is the enrichment of the solution by fluctuations as physically meaningful as possible. Basically, this issue is an extension of the problem of the generation of realistic inlet boundary conditions in DNS or LES of subsonic turbulent flows. In that respect, the method of anisotropic linear forcing (ALF) we have developed in collaboration with EDF proved very encouraging, by its efficiency, its generality and simplicity of implementation. So, it seems natural, on the one hand, to extend this approach to the compressible framework and then implement it in AeroSol. On the other hand, we shall concentrate (in cooperation with EDF R&D in Chatou in the framework of a just-started CIFRE PhD) on the theoretical link between the local variations of the scale's description of turbulence (e.g. a sudden variations in the size of the time filter) and the intensity of the ALF forcing transiently applied to help in the development of missing scales of fluctuations.

3.2.1.2. Stable and non reflecting boundary conditions

In aerodynamics, and especially for subsonic computations, handling inlet and outlet boundary conditions is a difficult issue. A lot of work has already been done for second order schemes for Navier Stokes equations, see [42], [45] and the huge number of papers citing it. On the one hand, we believe that strong improvements are necessary with higher order schemes: indeed, the less dissipative the scheme is, the worse impact have the spurious reflections. For this, we will first concentrate on the linearized Navier-Stokes system, and analyze the boundary condition imposition in a discontinuous Galerkin framework with a similar approach as in [33]. We will also try to extend the work of [46], which deals with Euler equations, to the Navier Stokes equations.

3.2.2. Turbulence models and model agility

3.2.2.1. Extension of zero Mach models to the compressible system

We shall develop in parallel our multi-scale turbulence modeling and the related adaptive numerical methods of AeroSol. Without prejudice to methods that will be on the podium in the future, a first step in this direction will be to extend to a compressible framework the continuous hybrid temporal RANS/LES models we have developed up to now in a Mach zero context.

3.2.2.2. Study of wall flows with and without mass or heat transfer at the wall: determination and validation of relevant criteria for hybrid turbulence models

In the targeted application domains, the turbulence/wall interaction and the heat transfer at the fluid-solid interfaces are physical phenomena whose numerical prediction is at the heart of the concerns of our industrial partners. For instance, for a jet engine manufacturer, being able to properly design the configuration of the cooling of the walls of its engine combustion chamber in the presence of thermoacoustic instabilities is based on the proper identification and a thorough understanding of the major mechanisms that drive the dynamics of the parietal transfers. For our part, we will gradually use all our analysis and experimentation tools to actively participate in the improvement of the collective knowledge on such kind of transfers. The flow configurations dealt with by the beginning of the project will be those of subsonic single phase impacting jets or JICF with the possible presence of an interacting acoustic wave. The conjugate heat transfer at the wall will be also progressively tackled. The existing criteria of switching of the hybrid RANS/LES model will be tested on those flow configurations in order to determine their domain of validity. In parallel, the hydrodynamic instability modes of the JICF will be studied experimentally and theoretically (in cooperation with the SIAME laboratory) in order to determine if it is possible to drive a change of instability regime (e.g. from absolute to convective) and so propose challenging flow conditions that would be relevant for the setting-up of an hybrid LES/DNS approach aimed at supplementing the hybrid RANS/LES one.

3.2.2.3. Improvement of turbulence models

The production and the subsequent use of DNS (AeroSol library) and experimental (bench MAVERIC) databases dedicated to the improvement of the physical models will be an important part of our activity. In that respect, our present capability of producing in-situ experimental data for simulation validation and flow analysis is clearly a strongly differentiating mark of our project. It is on the improvement of the hybrid RANS/LES approach that will focus most of our initial efforts of analysis of the DNS and experimental data as soon as they will become available. This method has a decisive advantage over all other hybrid RANS/LES approaches since it relies on a well defined time filtering formalism. This greatly facilitates the proper extraction from the databases of the various terms appearing in the relevant flux balances obtained at the different scales involved (e.g. from RANS to LES). But we would not be comprehensive in that matter if we were not questioning the relevance of any simulation-experiment comparisons. In other words, a central issue will also be to answer positively the following question: will we be comparing the same quantities between simulations and experiment? From an experimental point of view, the questions to be raised will be, among others, the possible difference in resolution between the experiment and the simulations, the similar location of the measurement points and simulation points, the acceptable level of random error associated to the necessary finite number of samples. In that respect, the recourse to uncertainty quantification techniques will be advantageously considered.

3.2.3. Development of an efficient implicit high-order compressible solver scalable on new architectures

As the flows we wish to simulate may be very computationally demanding, we will maintain our efforts in the development of AeroSol in the following directions:

- Efficient implementation of the discontinuous Galerkin method.
- Implicit methods based on Jacobian-Free-Newton-Krylov methods and multigrid.
- Porting on heterogeneous architectures.
- Implementation of models.

3.2.3.1. Efficient implementation of the discontinuous Galerkin method

In high order discontinuous Galerkin methods, the unknown vector is composed of a concatenation of the unknowns in the cells of the mesh. An explicit residual computation is composed of three loops: an integration loop on the cells, for which computations in two different cells are independent, an integration loop on boundary faces, in which computations depend on data of one cell and on the boundary conditions, and an integration loop on the interior faces, in which computations depend on data of the two neighboring cells. Each of these loops are composed of three steps: the first step consists in interpolating data at the quadrature points, the second step in computing a nonlinear flux at the quadrature points (the physical flux for the cell loop, an upwind flux for interior faces or a flux adapted to the kind of boundary condition for boundary faces), and the third step consists in projecting the nonlinear flux on the degrees of freedom.

In this research direction, we propose to exploit the strong memory locality of the method (i.e., the fact that all the unknowns of a cell are stocked contiguously). This formulation can reduce the linear steps of the method (interpolation on the quadrature points and projection on the degrees of freedom) to simple matrix-matrix product which can be optimized. For the nonlinear steps, composed of the computation of the physical flux on the cells and of the numerical flux on the faces, we will try to exploit vectorization.

3.2.3.2. Implicit methods based on Jacobian-Free-Newton-Krylov methods and multigrid

For our computations of the IMPACT-AE project, we use an explicit time stepping. The time stepping is limited by the CFL condition, and in our flow, the time step is limited by the acoustic wave velocity. As the Mach number of the flow we simulate in IMPACT-AE is low, the acoustic time restriction is much lower than the turbulent time scale, which is driven by the velocity of the flow. We hope to have a better efficiency by using time implicit methods, for using a time step driven by the velocity of the flow.

Using implicit time stepping in compressible flows in particularly difficult, because the system is fully nonlinear, so that the nonlinear solving theoretically requires to build many times the Jacobian. Our experience in implicit methods is that the building of a Jacobian is very costly, especially in three dimensions and in a high order framework, because the optimization of the memory usage is very difficult. That is why we propose to use Jacobian free implementation, based on [38]. This method consists in solving the linear steps of the Newton method by a Krylov method, which requires Jacobian-vector product. The smart idea of this method is to replace this product by an approximation based on a difference of residual, therefore avoiding any Jacobian computation. Nevertheless, Krylov methods are known to converge slowly, especially for the compressible system when the Mach number is low, because the system is ill-conditioned. In order to precondition, we propose to use an aggregation-based multigrid method, which consists in using the same numerical method on coarser meshes obtained by aggregation of the initial mesh. This choice is driven by the fact that multigrid methods are the only one to scale linearly [47], [48] with the number of unknowns in term of number of operations, and that this preconditioning does not require any Jacobian computation.

Beyond the technical aspects of the multigrid approach, which will be challenging to implement, we are also interested in the design of an efficient aggregation. This often means to perform an aggregation based on criteria (anisotropy of the problem, for example) [41]. For this, we propose to extend the scalar analysis of [49] to a linearized version of the Euler and Navier-Stokes equations, and try to deduce an optimal strategy for anisotropic aggregation, based on the local characteristics of the flow. Note that discontinuous Galerkin methods are particularly well suited to h-p aggregation, as this kind of methods can be defined on any shape [21].

3.2.3.3. Porting on heterogeneous architectures

Until the beginning of the 2000s, the computing capacities have been improved by interconnecting an increasing number of more and more powerful computing nodes. The computing capacity of each node was increased by improving the clock speed, the number of cores per processor, the introduction of a separate and dedicated memory bus per processor, but also the instruction level parallelism, and the size of the memory cache. Even if the number of transistors kept on growing up, the clock speed improvement has flattened since the mid 2000s [44]. Already in 2003, [35] pointed out the difficulties for efficiently using the biggest clusters: "While these super-clusters have theoretical peak performance applications is far from the peak. Salinas, one of the 2002 Gordon Bell Awards was able to sustain 1.16 Tflops on ASCI White (less than 10% of peak)." From the current multi-core architectures, the trend is now to use many-core accelerators. The idea behind many-core is to use an accelerator composed of a lot of relatively slow and simplified cores for executing the most simple parts of the algorithm. The larger the part of the code executed on the accelerator, the faster the code may become. In this task, we will work on the heterogeneous aspects of computation. These heterogeneities are intrinsic to our computations and have two sources. The first one is the use of hybrid meshes, which are necessary for using a local structured mesh in a boundary layer. As the different cell shapes (pyramids, hexahedra, prisms and tetrahedra) do not have the same number of degrees of freedom, nor the same number of quadrature points, the execution time on one face or one cell depends on its shape. The second source of heterogeneity are the boundary conditions. Depending on the kind of boundary conditions, user defined boundary values might be needed, which induces a different computational cost. Heterogeneities are typically what may decrease efficiency in parallel if the workload is not well balanced between the cores. Note that heterogeneities were not dealt with in what we consider as one of the most advanced work on discontinuous Galerkin on GPU [37], as only straight simplicial cell shapes were addressed. For managing at best our heterogeneous computations on heterogeneous architectures, we propose to use the execution runtime StarPU [20]. For this, the discontinuous Galerkin algorithm will be reformulated in term of a graph of tasks. The previous tasks on the memory management will be useful for that. The linear steps of the discontinuous Galerkin methods require also memory transfers, and one task of the project will consist in determining the optimal task granularity for this step, i.e. the number of cells or face integrations to be sent in parallel on the accelerator. On top of that, the question of which device is the most appropriate to tackle such kind of tasks will be discussed.

Last, we point out that the combination of shared-memory and distributed-memory parallel programming models is better suited than only the distributed-memory one for multigrid, because in a hybrid version, a wider part of the mesh shares the same memory, therefore allowing for a coarser aggregation.

The consortium will benefit from a particularly stimulating environment in the Inria Bordeaux Sud Ouest center around high performance computing, which is one of the strategic axis of the center.

3.2.3.4. Implementation of turbulence models in AeroSol and validation

We will gradually insert models developed in research direction 3.2.2.1 in the AeroSol library in which we develop methods for the DNS of compressible turbulent flows at low Mach number. Indeed, thanks to its formalism of temporal filtering, the HTLES approach offers a theoretical framework characterized by a continuous transition from RANS to DNS, even for complex flow configurations (e.g. without directions of spatial homogeneity). As for the discontinuous Galerkin method available presently in AeroSol, it is the best suited and versatile method able to meet the requirements of accuracy, stability and cost related to the local (varying) level of resolution of the turbulent flow at hand, regardless of its configuration complexity. The first step in this direction was taken in 2017 during the internship of Axelle Perraud, who has implemented a turbulence model (k-ω-SST) in the Aerosol library.

3.2.4. Validation of the simulations: test flow configurations

To supplement whenever necessary the test flow configuration of MAVERIC and apart from configurations that could emerge in the course of the project, the following configurations for which either experimental data, simulation data or both have been published will be used whenever relevant for benchmarking the quality of our agile computations:

- The impinging turbulent jet (simulations).
- The ORACLES two-channel dump combustor developed in the European projects LES4LPP and MOLECULES.
- The non reactive single-phase PRECCINSTA burner (monophasic swirler), a configuration that has been extensively calculated in particular with the AVBP and Yales2 codes.
- The LEMCOTEC configuration (monophasic swirler + effusion cooling).
- The ONERA MERCATO two-phase injector configuration provided the question of confidentiality of the data is not an obstacle.
- Rotating turbulent flows with wall interaction and heat transfer.
- Turbulent flows with buoyancy.

4. Application Domains

4.1. Aeroengines

Cagire is presently involved in studies mainly related with two subcomponents of the combustion chamber of aeroengines:

- The combustion chamber wall: the modelling, the simulation and the experimentation of the flow around a multiperforated plate representative of a real combustion chamber wall are the three axes we have been developing during the recent period. The continuous improvement of our in-house test facility Maveric is also an important ingredient to produce our own experimental validation data for isothermal flows. For non-isothermal flows, our participation in the EU funded program Soprano will be giving us access to non-isothermal data produced by Onera.
- The fuel nozzle: the impact of small geometrical variations related to the fabrication process on the pressure losses of the injector is being studied for a generic geometry provided by our industrial partner AD Industrie. RANS based simulations are intended to help designing some critical components of the fuel nozzle. A project is currently written to answer a call of the Nouvelle Aquitaine region, with the objective of extending this study to hybrid RANS/LES methods.

4.2. Power stations

R. Manceau has established a long term collaboration (4 CIFRE PhD theses in the past, 2 ongoing) with the R & D center of EDF of Chatou, for the development of refined turbulence models in the in-house CFD code of EDF, Code_Saturne :

- The prediction of heat transfer in fluid and solid components is of major importance in power stations, in particular, nuclear power plants. Either for the thermohydraulics of the plenum or in the study of accidental scenarii, among others, the accurate estimation of wall heat transfer, mean temperatures and temperature fluctuations are necessary for the evaluation of relevant thermal and mechanical design criteria. The PhD thesis (CIFRE EDF) of G. Mangeon is dedicated to the development of relevant RANS models for these industrial applications.
- Moreover, the prediction of unsteady hydrodynamic loadings is a key point for operating and for safety studies of PWR power plants. Currently, the static loading is correctly predicted by RANS computations but when the flow is transient (as, for instance, in Reactor Coolant Pumps, due to rotor/stator interactions, or during operating transients) or in the presence of large, energetic, coherent structures in the external flow region, the RANS approach is not sufficient, whereas LES is still too costly for a wide use in industry. This issue constitutes the starting point of the just-started PhD thesis (CIFRE EDF) of Vladimir Duffal.

4.3. Automotive propulsion

- The engine (underhood) compartment is a key component of vehicle design, in which the temperature is monitored to ensure the effectiveness and safety of the vehicle, and participates in 5 to 8% of the total drag and CO2 emissions. Dimensioning is an aerodynamic and aerothermal compromise, validated on a succession of road stages at constant speed and stopped phases (red lights, tolls, traffic jam). Although CFD is routinely used for forced convection, state-of-the-art turbulence models are not able to reproduce flows dominated by natural convection during stopped phases, with a Rayleigh number of the order of 10^{10}, such that the design still relies on costly, full-scale, wind tunnel experiments. This technical barrier must be lifted, since the ambition of the PSA group is to reach a *full digital design of their vehicles in the 2025 horizon*, i.e., to almost entirely rely on CFD. This issue is the focus of the ongoing PhD thesis (CIFRE PSA) of S. Jameel, supervised by R. Manceau, and also a part of the ANR project MONACO_2025 described in section 9.2.2.
- The Power & Vehicles Division of IFPEN co-develops the CFD code CONVERGE to simulate the internal flow in a spark-ignition engine, in order to provide the automotive industry with tools to optimize the design of combustion engines. The RANS method, widely used in the industry, is not sufficiently reliable for quantitative predictions, and is only used as a tool to qualitatively compare different geometries. On the other hand, LES provides more detailed and accurate information, but at the price of a CPU cost unafordable for daily use in the industry. Therefore, IFPEN aims at developing the hybrid RANS/LES methodology, in order to combine the strengths of the two approaches. The just-started PhD thesis of Hassan Afailal, co-supervised by Rémi Manceau, is focused on this issue.

5. Highlights of the Year

5.1. ANR MONACO_2025

The MONACO_2025 proposal has been selected by ANR. In addition to Cagire, the consortium of this project, coordinated by [RM], consists in an academic partner, the institute PPrime of Poitiers, and two industrial partners, PSA and EDF. It is focused on the the development of a CFD methodology for transient, buoyancy-affected turbulent flows, that are crucial for the two industrial partners. This project built up on the long-term collaboration with EDF, and the more recent collaboration with PSA through a master internship and the CIFRE PhD thesis of Saad Jameel.

5.2. First implementation of a turbulence model in AeroSol

In the long-term strategy of the CAGIRE team, the development of agile simulation, a first step towards auto-adaptive RANS/LES methods was made this summer during the internship of Axelle Perraud. This step consisted in the implementation in AeroSol of a first near-wall resolving turbulence model. Before focusing on innovative RANS and hybrid RANS/LES methods developed in CAGIRE, it was chosen to implement the standard, well-established k-ω RANS model, in order to make possible a straightforward validation in comparison with other CFD codes.

6. New Software and Platforms

6.1. AeroSol

KEYWORD: Finite element modelling
FUNCTIONAL DESCRIPTION: The AeroSol software is a high order finite element library written in C++. The code has been designed so as to allow for efficient computations, with continuous and discontinuous finite elements methods on hybrid and possibly curvilinear meshes. The work of the team CARDAMOM (previously Bacchus) is focused on continuous finite elements methods, while the team Cagire is focused on discontinuous Galerkin methods. However, everything is done for sharing the largest part of code we can. More precisely, classes concerning IO, finite elements, quadrature, geometry, time iteration, linear solver, models and interface with PaMPA are used by both of the teams. This modularity is achieved by mean of template abstraction for keeping good performances. The distribution of the unknowns is made with the software PaMPA , developed within the team TADAAM (and previously in Bacchus) and the team Castor.
NEWS OF THE YEAR: The following points have been developed in the code

*A postprocessing in the high order GMSH format has been added

*On the Uhaina part, the work has been focused on the entropy viscosity approach for shock limiting, and on the positivity preserving limiters for ensuring positive water height

*On the dealing of low Mach problems -Multidimensional numerical flux accurate for the computation of steady and unsteady low Mach flows. -Test cases at low Mach

*A method for penalizing rigid bodies instead of meshing it has been developed within the postdoc of Marco Lorini. The model was implemented, an improvement of time schemes for steady problems was done. The method has been tested with 2d and 3d tests: bump, flow around a cylinder. These tests allowed to fix bugs, especially for wall boundary conditions. The coupling with adaptation tools has began.

*The library has benefited from the HPCLib Inria Hub, which aims at improving the development environment of HPC libraries within the Bordeaux Sud Ouest Centre. Within this project, a static analysis of the library based on sonarqube has been performed.

*A wiki for gathering the documentation of the different test cases has begun.

- Participants: Benjamin Lux, Damien Genet, Dragan Amenga Mbengoue, Hamza Belkhayat Zougari, Mario Ricchiuto, Maxime Mogé, Simon Delmas and Vincent Perrier
- Contact: Vincent Perrier

7. New Results

7.1. Development of an accurate and stable finite volume scheme for simulating low Mach number flows with or without acoustic waves

Starting from the Roe scheme and various low Mach fixes for the barotropic Euler PDE's system and using a 2-scale asymptotic analysis of the (semi)-discrete system, a new Roe based scheme is derived whose set of dissipative terms is chosen in order to ensure both accuracy, stability and checkerboard free behaviour. A paper on this topic is being finalized.

7.2. Analysis of liquid sheet flowing under gravity

In the framework of an informal cooperation with Y. Le Guer and K. El Omari who are supervising the PhD thesis of A. Kacem, we have been involved in the experimental and the numerical study of liquid sheets falling under gravity [14]. The various flow regimes have been characterized in terms of the relevant dimensionless numbers (Weber, Reynolds, Ohnesorge) with a particular emphazis on the regimes leading to the appearance fo holes within the liquid sheet. A journal paper has been submitted mid-2017 and is presently under revision.

7.3. First order hyperbolic formulation of dissipative systems

In the framework of the leave of Vincent Perrier at National institute of Aerospace, a general framework for defining first order formulation of nonlinear dissipative systems equipped with an entropy has been developed. The numerical methods for discretizing this type of system are still in development.

7.4. Improvement of turbulent heat flux modelling for buoyant flows

Several modifications were introduced in the Elliptic Blending Differential Flux Model (EB-DFM) to account for the influence of wall blockage on the turbulent heat flux. These modifications are introduced in order to reproduce, in association with the most recent version of the EB-RSM, the full range of regimes, from forced to natural convection, without any case-specific modification. The interest of the new model is demonstrated using analytical arguments, a priori tests and computations in channel flows in the different convection regimes, as well as in a differentially heated cavity. This work is published in *Int. J. Heat Fluid Flow* [10].

7.5. Modelling of turbulent flows with strong variations of the physical properties

The effects of a strong transverse temperature gradient, very common in industrial applications, on a turbulent Poiseuille flow were studied numerically using RANS models, in order to determine the closure level necessary to reproduce the influence of variations of the physical properties, for a wide range of wall-temperature ratios. Eddy-viscosity models prove able to correctly reproduce the asymmetry of the flow and the tendency toward relaminarization close to the hot wall, which are mainly due to the strong variations of the molecular viscosity. Discrepancies in the predictions of the different closure levels only appear for the highest temperature ratios. A journal paper is under revision for publication in *Int. J. Heat Fluid Flow*.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

EDF: "Advanced modelling of heat transfer for industrial configurations with or without accounting of the solid wall", contract associated to the PhD thesis of Gaëtan Mangeon

EDF: "Hybrid RANS/LES modelling for unsteady loadings in turbulent flows", contract associated to the PhD thesis of Vladimir Duffal

IFPEN: "3D simulation of non-reactive internal aerodynamics of spark-ignition engines using an hybrid RANS/LES method", contract associated to the PhD thesis of Hassan Al Afailal

PSA: ""Turbulence modelling in the mixed and natural convection regimes in the context of automotive applications", contract associated to the PhD thesis of Saad Jameel.

8.2. Bilateral Grants with Industry

EDF (Cifre PhD grant): "Advanced modelling of heat transfer for industrial configurations with or without accounting of the solid wall", PhD student: Gaëtan Mangeon

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PSA (Cifre PhD grant): "Turbulence modelling in the mixed and natural convection regimes in the context of automotive applications", PhD student: Saad Jameel.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. Predicting head losses in aeronautical fuel injectors

This is a 3-year programme, started mid-2015 and funded by Conseil Régional d'Aquitaine (2014 Call) and two small-size companies, AD Industrie (Gurmençon, France) and GDTECH (Bordes, France). The objective is to investigate the possibility of using advanced RANS or hybrid RANS-LES approaches to better predict the pressure losses in aeronautical fuel nozzles. [PB,RM]

9.1.2. SEIGLE

SEIGLE means "Simulation Expérimentation pour l'Interaction de Gouttes Liquides avec un Ecoulement fortement compressible". It is a 3-year program which has started since October 2017 and was funded by Régional Nouvelle-Aquitaine, ISAE-ENSMA, CESTA and Inria. The interest of understanding aerodynamic mechanisms and liquid drops atomization is explained by the field of applications where they play a key role, specially in the new propulsion technologies through detonation in the aerospace as well as in the securities field. The SEIGLE project was articulated around a triptych experimentation, modeling and simulation. An experimental database will be constituted. It will rely on a newly installed facility (Pprime), similar to a supersonic gust wind tunnel/ hypersonic from a gaseous detonation tube at high pressure. This will allow to test modeling approaches (Pprime / CEA) and numerical simulation (Inria / CEA) with high order schemes for multiphasic compressible flows, suitable for processing shock waves in two-phase media [VP, JJ].

9.2. National Initiatives

9.2.1. GIS Success

We are members of the CNRS GIS Success (Groupement d'Intérêt Scientifique) organised around two of the major CFD codes employed by the Safran group, namely AVBP and Yales 2. No scientific activity has been devoted around those codes during 2017 but Yales2 has been installed and tested on one of our workstation to prepare some planned scientific activity to come in 2018 in the field of low Mach flows and low Reynolds flows simulations [PB].

9.2.2. ANR MONACO_2025 [RM]

The ambition of the MONACO_2025 project, coordinated by Rémi Manceau, is to join the efforts made in *two different industrial sectors* in order to tackle the industrial simulation of transient, turbulent flows affected by buoyancy effects. It brings together two academic partners, the project-team Cagire hosted by the university of Pau, and the institute Pprime of the CNRS/ENSMA/university of Poitiers (PPRIME), and R&D departments of two industrial partners, the PSA group and the EDF group, who are major players of the automobile and energy production sectors, respectively.

- The main **scientific objective** of the project is to make a breakthrough in *the unresolved issue* of the modelling of turbulence/buoyancy interactions in transient situations, within the continuous hybrid RANS/LES paradigm, which consists in preserving a computational cost compatible with industrial needs by relying on statistical approaches where a fine-grained description of the turbulent dynamics is not necessary. The transient cavity flow experiments acquired during MONACO_2025 will provide the partners and the scientific community with *an unrivalled source of knowledge* of the physical mechanisms that must be accounted for in turbulence models.
- The main **industrial objective** is *to make available computational methodologies* to address dimensioning, reliability and security issues in buoyancy-affected transient flows. It is to be emphasized that such problems are *not tackled using CFD at present in the industry*. At the end of MONACO_2025, a panel of methodologies, ranging from simple URANS to sophisticated hybrid model based on improved RANS models, will be evaluated in transient situations, against the dedicated cavity flow experiments and a real car underhood configuration. This final benchmark exercise will form *a decision-making tool* for the industrial partners, and will thus pave the way towards high-performance design of low-emission vehicles and highly secure power plants. In particular, the project is in line with the *Full Digital 2025 ambition*, e.g., the declared ambition of the PSA group to migrate, within the next decade, to a design cycle of new vehicles nearly entirely based on CAE (computer aided engineering), without recourse to expensive full-scale experiments.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

9.3.1.1. SOPRANO

Participants: Rémi Manceau, Pascal Bruel, [Post doc starting in 2018].

Topic: MG-1.2-2015 - Enhancing resource efficiency of aviation

Project acronym: SOPRANO

Project title: Soot Processes and Radiation in Aeronautical inNOvative combustors

Duration: 01/09/2016 - 31/08/2020

Coordinator: SAFRAN

Other partners:

- France: CNRS, CERFACS, INSA Rouen, SAFRAN SA, Snecma SAS, Turbomeca SA.
- Germany: DLR, GE-DE Gmbh, KIT, MTU, RRD,
- Italy: GE AVIO SRL, University of Florence
- United Kingdom: Rolls Royce PLC, Imperial College of Science, Technology and Medecine, Loughborough University.

Abstract: For decades, most of the aviation research activities have been focused on the reduction of noise and NOx and CO2 emissions. However, emissions from aircraft gas turbine engines of non-volatile PM, consisting primarily of soot particles, are of international concern today. Despite the lack of knowledge toward soot formation processes and characterization in terms of mass and size, engine manufacturers have now to deal with both gas and particles emissions. Furthermore, heat transfer understanding, that is also influenced by soot radiation, is an important matter for the improvement of the combustor's durability, as the key point when dealing with low-emissions combustor architectures is to adjust the air flow split between the injection system and the combustor's walls. The SOPRANO initiative consequently aims at providing new elements of knowledge, analysis and improved design tools, opening the way to: • Alternative designs of combustion systems for future aircrafts that will enter into service after 2025 capable of simultaneously reducing gaseous pollutants and particles, • Improved liner lifetime assessment methods. Therefore, the SOPRANO project will deliver more accurate experimental and numerical methodologies for predicting the soot emissions in academic or semi-technical combustion systems. This will contribute to enhance the comprehension of soot particles formation and their impact on heat transfer through radiation. In parallel, the durability of cooling liner materials, related to the walls air flow rate, will be addressed by heat transfer measurements and predictions. Finally, the expected contribution of SOPRANO is to apply these developments in order to determine the main promising concepts, in the framework of current low-NOx technologies, able to control the emitted soot particles in terms of mass and size over a large range of operating conditions without compromising combustor's liner durability and performance toward NOx emissions.

In the SOPRANO project, our objective is to complement the experimental (ONERA) and LES (CERFACS) work by RANS computations of the flow around a multiperforated plate, in order to build a database making possible a parametric study of mass, momentum and heat transfer through the plate and the development of multi-parameter-dependent equivalent boundary conditions. Our activity is due to start in September 2018.

9.4. International Initiatives

9.4.1. Informal International Partners

- Collaboration with Alireza Mazaheri, from NASA Langley Research Center on the first order formulation of the compressible Navier-Stokes system (2-month leave of V. Perrier at National Institute of Aerospace, Hampton, VA).
- Collaboration with E. Dick (University of Ghent, Belgium) and Y. Moguen (UPPA) on the determination of the best splitting of variables for handling low Mach flows with a pressure-energy based coupling. [PB]
- Collaboration with A. Beketaeva and A. Naïmanova (Institute of Mathematics, Almaty, Kazakhstan) related to the simulations of a supersonic jet in crossflow configuration. Contacts were also made with Axel Vincent from Onera Palaiseau in order to have access to recent experimental data on supersonic combustion.The low-Mach preconditioning of an in-house ENO based compressible flow solver was also adressed. [PB] (10-day stay in Almaty).
- Collaboration with P. Correia (University of Evora, Portugal) related to the development of enhanced boundary conditions for the simulations of Mach zero flows with the artificial compressibility method. [PB] (5-day stay in Evora).
- Collaboration with S. Lardeau (Siemens Industry Software Computational Dynamics, Nuremberg, Germany) on the EB-RSM model and hybrid RANS/LES model for industrial applications. [RM]

9.5. International Research Visitors

9.5.1. Visits of International Scientists

- Prof. Sergio Elaskar (Conicet and University National of Cordoba, Argentina) visited LMAP-Cagire for a 1-week stay from August 28 to September 1, 2017.
- Prof. Ezequiel Del Rio (Polytechnic University of Madrid) visited LMAP-Cagire for a 4-day stay from August 21 to August 31, 2017. The objective of these two simultaneous visits was to determine the possibility of generating data on the Maveric test facility to validate the intermittency model (mapping) jointly developed by S. Elaskar and E. Del Rio.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Member of the Organizing Committees

- Member [RM] of the steering committee of the Special Interest Group "Turbulence Modelling" (SIG-15) of ERCOFTAC (European Research COmmittee for Flow, Turbulence and Combustion) that organizes a series of international workshops dedicated to cross-comparisons of the results of turbulence models and experimental/DNS databases.

10.1.2. Scientific Events Selection

10.1.2.1. Member of the Conference Program Committees

- Intl Symp. Turbulence, Heat and Mass Transfer [RM]
- Intl. Symp. Engineering Turbulence Modelling and Measurement [RM]
- ASME 2018 Fluids Engineering Division Summer Meeting (FEDSM) [RM]

10.1.2.2. Reviewer

This year, the team members have reviewed (3) contributions for the following conferences:

- ASME-GT Turbo Expo 2018 (Oslo, Norway) (1) [PB]
- FVCA 2017 (Lille, France) (1) [JJ]
- REEE 2017 (Fez, Marocco) (1) [PB]

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

- Visualization of Mechanical Processes [PB]
- Advisory Board of International Journal of Heat and Fluid Flow [RM]
- Advisory Board of Flow, Turbulence and Combustion [RM]

10.1.3.2. Reviewer - Reviewing Activities

During 2017, the team members reviewed (13) papers for the following journals:

- Combustion and Flame (3) [PB]
- Compte Rendus Mécanique (1) [PB]
- Energy and Buildings (1) [PB]
- International Journal of Fluid Mechanics Research (1) [PB]
- International Journal of Heat and Fluid Flow (2) [RM]
- Journal of Petroleum Science and Engineering (1) [PB]
- Mathematics and Computers in Simulation (1) [RM]
- Nuclear Eng Design (2) [RM]
- Physics of fluids (1) [RM]

10.1.4. Research Administration

- Co-responsible of seventh day of welcoming new recruits at Institut Henri Poincaré on January [JJ]
- Co-responsible of the organisation of the LMAP seminar [8] [JJ]
- Member of the LMAP council [PB]
- Member of the IPRA scientific council [RM]

[8] http://lma-umr5142.univ-pau.fr/fr/activites-scientifiques/seminaires/seminaires-math-et-applications.html

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Master : "Maths 2: Data analysis", 68h25, M1 - Génie Pétrolier, Université de Pau et des Pays de l'Adour, Pau, France. [JJ]

Master : "Finite volume for hyperbolic systems and compressible fluid mechanics", 26h25, M2 - MMS, Université de Pau et des Pays de l'Adour, Pau, France. [JJ]

Master : "Finite volume for hyperbolic systems and compressible fluid mechanics", 24h75, M2 - MMS, Université de Pau et des Pays de l'Adour, Pau, France. [VP]

Master : "Turbulence modelling" (in English), 27h30, M2 - International Master program Turbulence, Université de Poitiers/Ecole centrale de Lille, France. [RM]

Eng. 3 : "Industrial codes for CFD" (in English), 12h30, 3rd year of engineering school (M2), ENSMA, Poitiers, France. [RM]

Eng. 3 : "Advanced physics–Turbulence modelling for CFD", 16h, 3rd year of engineering school (M2), ENSGTI, France. [RM]

10.2.2. Supervision

PhD in progress: Gaetan Mangeon, "Modelisation avancée des transferts thermiques pour les configurations industrielles avec et sans prise en compte de la paroi solide", 2017 Supervisor: [RM].

PhD in progress: Saad Jamel, "Modélisation de la turbulence en régimes de convection mixte et naturelle dans un contexte automobile", 2017, Supervisor: [RM].

PhD,in progress: Al Hassan Afailal, "Simulation numérique tridimensionnelle de l'aérodynamique interne non réactive des moteurs à allumage commandé par une méthode hybride RANS/LES", 2017 Supervisor: [RM].

PhD, in progress: Vladimir Duffal, "Hybrid RANS/LES modelling for unsteady loadings in turbulent flows", 2017, Supervisor [RM]

10.2.3. Juries

The participation in the following thesis juries is noted ("referee" in a French doctoral thesis jury is more or less equivalent to an external opponent in an Anglo-Saxon like PhD jury):

PhD: Océane Lambert «Solutions architecturées par fabrication additive pour le refroidissement de parois de chambres de combustion» Communauté Université Grenoble Alpes, France, 17 October 2017. Supervisors: R. Dendeviel - C. Davoine. [PB, referee]

10.3. Popularization

- «Forum des Métiers» organized by "Collège Pierre Emmanuel", Pau (64), France, 18 May 2017. A stand was manned during one day with the objective of explaining the activity of researcher to an audience of middle school students. [PB]

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Publications of the year

Articles in International Peer-Reviewed Journals

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