Large Eddy Simulations of Turbulent Reacting Flows in Real Burners: the Status and Challenges

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Abstract. Turbulence is a recurrent and recognised challenge for which the scientific community has not been able to provide reliable methodologies necessary for the predictions in complex industrial applications. In fact and throughout the past century, that challenge has been identified as a million dollar achievement simply because of the tremendous impact such a contribution would have on existing industrial processes. Among all industries, the gas-turbine companies are probably the most receptive to any new contributions in the field of turbulent reacting flows because of the upcoming new regulations and the existing pressure linked to petroleum consumption and pollutant emissions. From a purely scientific point of view, the treatment of combustion and turbulence yields additional difficulties. However, and because of the advent of Highly Parallel Computers (HPC) providing teraflop capabilities, the fully unsteady, temporally and spatially dependent approach that is Large Eddy Simulations (LES) provides new insights and promises when dealing with these industrial applications. In this document, state-of-the-art LES for complex flows is presented along necessary developments and potential challenges that are needed to improve LES in order to yield an efficient and reliable tool for the prediction of real industrial turbulent reacting flows.

1. Introduction

As of today, understanding and predicting simple turbulent reacting flows (or more generally turbulent flows) remains a great challenge for researchers and current developments heavily rely on computer codes. Major progresses hence depend on the available computing power and the development of new architectures. It not only impacts fundamental work but also industry which uses numerical tools developed by engineers and scientists. With the recent developments of High Performance Computing (HPC) facilities[1], teraflop capabilities have been reached and the symbolic pentaflop machine seems within reach. Off course, such a computer power increase opens new perspectives to the scientific community and should change the way industry currently addresses turbulent reacting flows.

Currently, three numerical approaches coexist in the field of turbulent flows. The first approach, named Direct Numerical Simulations (DNS) [1; 2], aims at improving the scientific understanding of turbulence and its coupling with various physical phenomena as encountered in real applications. Among the subjects involving turbulence and investigated by DNS, one

[1] Refer to the TOP 500 list issued on June 2008 and ranking all worldwide super-computing systems: http://www.top500.org/lists/2008/06#top10.

notes: combustion [3–14] (fuel consumption and pollutant emissions), multi-phase flows [15–20], radiation [21–23], primary and secondary break-up of liquid sheets [24–27], thermo-acoustic instabilities [28; 29], aero-acoustics [30–33] etc. With DNS, physicists simulate the governing equations with as much accuracy as possible for ideal/simple configurations. The limit is essentially linked to the computing power available. The highly detailed results are then usually probed to improve the understanding of the physics involved [34–36]. Such databases are also exploited to provide inputs or models for the other set of numerical methods which have less stringent computer costs. Note that DNS is a tool aimed at fundamental issues and ongoing researches also benefit from the new computing facilities as illustrated in recent progresses [1; 2]. The models constructed from DNS, experimental or theoretical investigations ease the simulation of more complex and realistic flows within industry which uses other numerical methods. The most achieved approach and routinely used in industry is probably RAS (Reynolds Average Simulations) and was mainly developed in the seventies [37–39]. In RAS, one only looks for an estimate of the turbulent flow behaviour: *i.e.* the mean solution. With this tool, only the mean quantities (in the sense of time or ensemble average) are available and all the effects of turbulence on the mean field are modelled. Although computer effective, this approach heavily relies on the models supplied by the scientists. Their range of applicability is theoretically restricted to statistically stationary flows although industry currently uses RAS beyond this limit to dimension new industrial systems. Here again, the increase of computing power offers an efficient turn-over time which allows to gauge new design points before industrial validation of the final design on expensive experimental test facilities. In order to extend the domain of validity of the numerical tools, especially in the industrial context, a third approach is currently being developed. This new numerical method, called Large Eddy Simulations (LES) [40; 41], introduces the notion of scale separation which filters out the high frequency flow structures and retain only the large scale motions which usually depend on the geometry considered. With this separation of scales, the computing effort is increased when compared to RAS while remaining largely below the inferred computer costs of DNS. The models, still needed with LES, are nonetheless more universal and more physics is naturally imbedded in the simulations. Indeed, LES offer access to a spatially and temporally dependent flow description, a particularly valuable information in complex configurations. As such and despite the fact that LES are still under development, it opens new perspectives, especially in the industrial context where transient physical phenomena a known to be critical.

The development of LES for an extensive use by industry at the design stages needs to meet several requirements. Among the important issues, code management and scalability are of the foremost importance since these applications aim at running on HPC architectures to bring response times within the industrial requirements or to tackle ever more complex geometries. Systematic model and code validations are necessary to guarantee predictability of the LES tool. In the following document, a brief state-of-the-art for LES of turbulent reacting flows in complex configurations is first proposed in section 2. Issues about modelling, code implementation, validation procedures and scalability are then discussed in sections 3, 4 and 5 respectively. Potential perspectives and closing remarks are given in section 6.

2. LES of turbulent reacting flows in complex geometries: a brief status

Current HPC facilities provide enough computing power to demonstrate the capacity of advanced LES codes in addressing complex industrial configurations. Although still at the state of demonstration, these simulations [42–45], Fig. 1, are usually produced in a specific context where everything is eased to produce the results. Among the necessary conditions usually met for the computations shown on Fig. 1, one notes the implication of four types of personnel:

- the experts, usually scientists with a strong background on modelling issues specific to the physics simulated by LES,

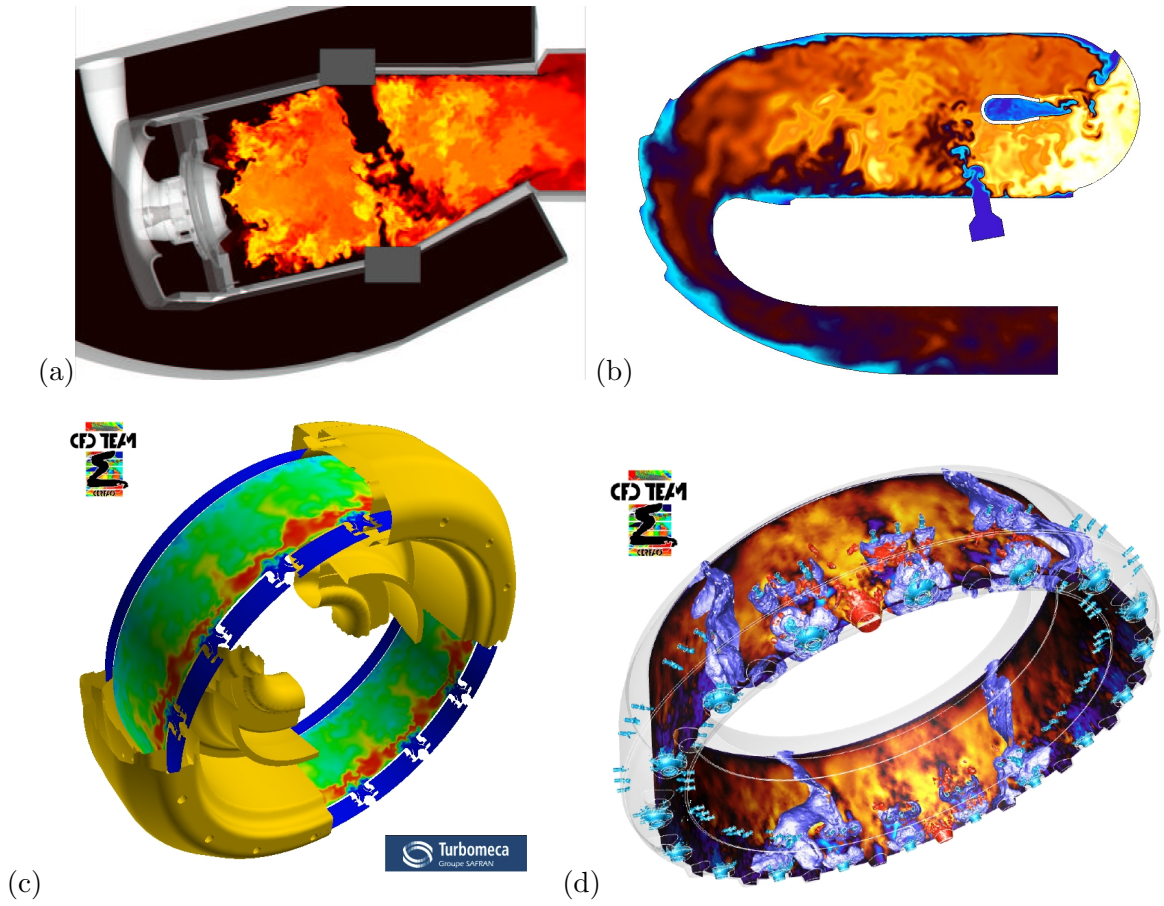

Figure 1. Instantaneous views of state-of-the-art LES applied to real aero-engine combustion chambers: (a) Pratt & Whitney single sector burner [42], (b) a single sector Turbomeca helicopter chamber [43], (c) a full Turbomeca chamber [44] and (d) an ignition sequence in a full annular combustion chamber of Turbomeca [45]. All views provide information on the temperature distribution in the burner at one given instant and as obtained by LES.

- the computer scientists with a strong background on programming, HPC and involved in the development of the code devised to produce the simulation,
- the computer scientists with a strong background on hardware and HPC who usually works for the computing centre or computer manufacturer hosting the computation,
- the engineers from aero-engine company which provides the real application to be simulated by LES.

The final requirement that may be necessary and which usually dimensions the size and the type of the problem targeted, is the accessibility to the computing facility or more importantly the access to a large number of processors. For example, the fully transient LES of the ignition phase for a complete helicopter gas-turbine combustion chamber citeBoileau:2008, Fig. 1 (d), was achieved thanks to a dedicated access to the top 19 Bull machine (Tera-10 Nova-Scale 5160) from the CEA computing facility located in France as well as the top 24 IBM (blue-Gene/P) architecture located in Rochester, USA, top 13 Barcelona Super-computing Centre (Blade Centre JS21) IBM, Spain, and top 7 Oak Ridge National Centre (Cray XT3/XT4) Cray,

USA[2]. Note also that the other results shown on Fig. 1 (a) & (b), only treat a single sector of the full annular combustor and do not necessitate such dedicated accesses. Furthermore and with the increasing number of ever larger HPC centres (INCITE), full annular chamber computations will rapidly exit the realm of "opportunity" or the need for specific "challenges". It is also interesting to underline that although all of the reported advanced LES results aimed at being purely demonstrative, the acquired knowledge yield important scientific contributions with several journal publications in the field of turbulence and combustion. This interesting consequence further emphasises the importance of such pioneering works for industry but also for the scientific community.

Such computations, although demonstrative and scientifically valorised, should however be viewed as a first step toward the full industrial use of LES. Most of the results are obtained for fully gaseous LES when real engines operate on liquid fuels and chemistry models are simple. In fact, a lot of the fundamental physics present in the real engine combustion chamber is still not understood or modelled in such computations. Technological aspects introduced by the manufacturer to specifically address cooling of the chamber walls for example are open issues which only start to be dealt and modelled by LES experts [46–48]. Note also that the validation of these LES simulations in a rigourous scientific way remains a challenge since experimental measurements are scarce for such real burners. Finally, issues specific to the LES approach, its analysis and the handling of the huge amount of data generated by such codes[3] are basic questions that need to be addressed to fully capitalise on the information generated by LES in the industrial context. Although most likely incomplete, part of these questions are presented and discussed in the following section and prior to a discussion on future developments and potential perspectives for HPC LES applications.

3. Specific issues related to advanced LES in complex geometries: the challenges

LES for reactive multi-species mixtures involves the spatial filtering operation, Fig. 2, which reduces for spatially, temporally invariant and localised filter functions [49; 50], to:

$$\widetilde{f(\mathbf{x},t)} = \frac{1}{\overline{\rho(\mathbf{x},t)}} \int_{-\infty}^{+\infty} \rho(\mathbf{x}',t)\, f(\mathbf{x}',t)\, G(\mathbf{x}'-\mathbf{x})\, d\mathbf{x}', \tag{1}$$

where G denotes the filter function and $\widetilde{f(\mathbf{x},t)}$ is the Favre filtered value of the variable $f(\mathbf{x},t)$ [51]. Note that the quantities of interest have spatial, $\mathbf{x}$ (a three component vector for full $3D$ applications) and a temporal, t, dependencies.

In the mathematical description of gaseous turbulent flows with chemical reactions and species transport, the primary variables are the species volumic mass fractions $\rho_\alpha(\mathbf{x},t)$, the velocity vector $u_i(\mathbf{x},t)$, the total energy $E(\mathbf{x},t) \equiv e_s + 1/2\ u_i u_i$, and the density $\rho(\mathbf{x},t) = \sum_{\alpha=1}^{N} \rho_\alpha(\mathbf{x},t)$. Note that $\rho_\alpha(\mathbf{x},t)$ is linked to the species mass fractions $Y_\alpha(\mathbf{x},t)$ and for a mixture of N species, mass conservation imposes: $\sum_{\alpha=1}^{N} Y_\alpha(\mathbf{x},t) = 1$.

The fluid follows the ideal gas law, $p = \rho\, r\, T$ and $e_s = \int_0^T C_p\, dT - p/\rho$, where e_s is the mixture sensible energy, T the temperature, $C_p = \sum_{\alpha=1}^{N} C_{p,\alpha}\, Y_\alpha$ the fluid heat capacity at constant pressure and r is the mixture gas constant, which varies with composition and is obtained by $r = \frac{R}{W} = R \sum_{\alpha=1}^{N} \frac{Y_\alpha}{W_\alpha}$, where $R = 8.314\ \mathtt{kg\,m^2/(s^2K)}$ and W_α is the molecular weight of the species α. The viscous stress tensor, the heat diffusion vector and the species molecular transport use classical gradient approaches. The fluid viscosity follows Sutherland's law, the heat diffusion coefficient follows Fourier's law, and the species diffusion coefficients are

[2] Classification based on the November 2007 Top 500 list.

[3] One snapshot for the instantaneous field of full annular combustor weights about 1.4 Gbytes and a temporal evolution of the main flow structures usually necessitates 4 million iterations.

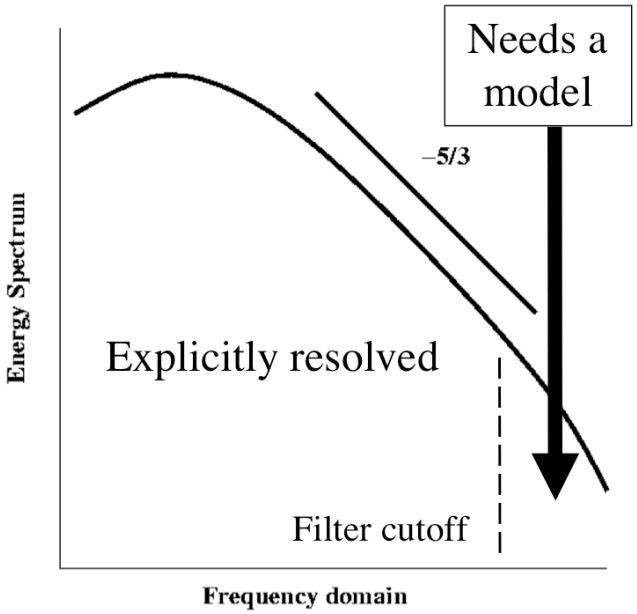

Figure 2. Schematic representation of the LES concept based on the typical energy spectrum of the velocity field for a large Reynolds number, homogeneous, isotropic turbulent flow [52; 53].

obtained using a constant species Schmidt number and diffusion velocity corrections for mass conservation [34].

As presented above (and only in the context of pure gaseous flows), the mathematical system to be solved is represented by to five highly coupled partial differential equations to which you need to add N species transport equations. The resulting number of dependent variables for which one looks for a fully $3D$ and time dependent solution is $N + 5$.

3.1. Modelling the unclosed terms

The application of the filtering operation to the instantaneous set of transport equations with chemical reactions yields the LES equations, which need modelling for the system to be closed [36; 40]. The new unknowns in the momentum transport equation and also called the Sub-Grid-Scale (SGS) turbulent velocity tensor is usually addressed through the concept of SGS turbulent viscosity model and the Boussinesq assumption [35; 54–57]. The SGS species flux (SGS mixing of the individual species which appear in the species transport equations), and the SGS energy flux (energy transport equation), are respectively modelled by use of the species SGS turbulent diffusivity along with a turbulent Schmidt number [58–61]. The eddy diffusivity is also used along with a turbulent Prandtl number [58–61]. Note that the performance of the models can be improved through the use of a dynamic formulation [56; 62–65] or more advanced type of closures [66–72].

When dealing with reacting flows, LES is faced with another set of unclosed terms issued by the highly non-linear expressions involved in the chemical kinetics that represents the production and consumption rates of the various species involved in the chemical reaction. Again, the lack of information below the filter length scale needs to be modelled to properly mimic the interaction between combustion and turbulence. Such models are crucial since combustion usually happens below the filter length scale and a direct use of the filtered mean field (species concentrations for example) to approximate combustion results in erroneous predictions [34; 35].

Many turbulent/combustion models have been developed to perform LES of turbulent reacting flows [66; 67; 70; 71; 73–78]. The major drawback for these models stems from the fact that they are usually derived for specific combustion regimes: *i.e.* fully premixed, partially-premixed or diffusion regimes [59]. Off course when dealing with industrial burners, most of the current designs never operate with a given regime of combustion but often exhibit all of the three regimes. Extensive use of these closures in an industrial context needs therefore a lot of caution and exhaustive validations.

3.2. Chemical kinetic schemes

Another open issue lies in the modelling of the chemical kinetics [60]. Indeed, and it still remains a large area of investigation for chemists, aeronautical fuels and air combustion usually involves thousands of chemical compounds and hundreds of chemical reactions. As such and when known, a detailed kinetic model usually contains too many species to be solved by LES or DNS, Fig. 3. The induced computer cost would be, in this context, prohibitive and out of reach with today's technologies. Alternative solutions are common, two of which being: kinetic reduction until a limited number of species [60; 79] is obtained to allow the computation, Fig. 3, or use of tabulated approaches [80; 81] coupled to a progress variable and a Zeldovic'h conserved scalar transport equations to parameterize the combustion table [82]. The induced limitation appears in the need for new kinetic models or tables when the operating point to be simulated is changed: *i.e.* pressure and temperature dependencies of the different rates of productions are lost with these approaches and intermediate species (mostly involved in pollutant) are usually miss represented which also influences the flame dynamics. Another shortcoming of such approaches is the overall lack of generality of the constructed kinetic or table which will not cover ignition phases, the entire range of premixed and/or diffusion flames.

Detailed kinetics of H_2/O_2

9 species, 38 reactions

Nb	Reaction	B	b	E
1	$H_2 + O_2 \rightleftharpoons 2OH$	1.70E+13	0.000	47780
2	$OH + H_2 \rightleftharpoons H_2O + H$	1.17E+09	1.300	3626
3	$H + O_2 \rightleftharpoons OH + O$	2.00E+14	0.000	16800
4	$O + H_2 \rightleftharpoons OH + H$	1.80E+10	1.000	8826
5[a]	$H + O_2 + M \rightleftharpoons HO_2 + M$	2.10E+18	-1.000	0.
6	$H + O_2 + O_2 \rightleftharpoons HO_2 + O_2$	6.70E+19	-1.420	0.
7	$H + O_2 + N_2 \rightleftharpoons HO_2 + N_2$	6.70E+19	-1.420	0.
8	$OH + HO_2 \rightleftharpoons H_2O + O_2$	5.00E+13	0.000	1000.
9	$H + HO_2 \rightleftharpoons 2OH$	2.50E+14	0.000	1900.
10	$O + HO_2 \rightleftharpoons O_2 + OH$	4.80E+13	0.000	1000.
11	$2OH \rightleftharpoons O + H_2O$	6.00E+18	1.300	0.
12[b]	$H_2 + M \rightleftharpoons H + H + M$	2.23E+12	0.500	92600
13	$O_2 + M \rightleftharpoons O + O + M$	1.85E+11	0.500	95560
14[c]	$H + OH + M \rightleftharpoons H_2O + M$	7.50E+23	-2.600	0.
15	$H + HO_2 \rightleftharpoons H_2 + O_2$	2.50E+13	0.000	700.
16	$HO_2 + HO_2 \rightleftharpoons H_2O_2 + O_2$	2.00E+12	0.000	O.
17	$H_2O_2 + M \rightleftharpoons OH + OH + M$	1.30E+17	0.000	45500
18	$H_2O_2 + H \rightleftharpoons HO_2 + H$	1.60E+12	0.000	3800
19	$H_2O_2 + OH \rightleftharpoons H_2O + HO_2$	1.00E+13	0.000	1800

Reduced kinetics of H_2/O_2

Baurle, 2003: 6 species, 7 reactions

Nb	Reaction	B	b	E
1	$H_2 + O_2 \rightleftharpoons 2OH$	1.70E+13	0.000	48050
2	$OH + H_2 \rightleftharpoons H_2O + H$	2.20E+13	0.000	5155
3	$H + O_2 \rightleftharpoons OH + O$	1.20E+17	- 0.910	16530
4	$O + H_2 \rightleftharpoons OH + H$	5.06E+04	2.670	6293
5[a]	$2\,OH \rightleftharpoons H_2O + O$	6.300+12	0.000	1090
6	$H+OH+M \rightleftharpoons H_2O + M$	2.21E+22	- 2.000	0
7	$H+H+M \rightleftharpoons H_2 + M$	7.30+17	-1.000	0

3 species, 1 reaction

Nb	Reaction	B	b	E
1	$H_2 + 1/2\,O_2 \rightarrow H_2O$	2.56E+13	0.000	40000

Figure 3. Typical detailed versus reduced kinetic schemes for the combustion of H_2-O_2.

3.3. Multi-phase flows

As shown by the numerous examples published in the last years [34; 43; 45; 73; 74; 83–91], LES is very accurate in complex turbulent gaseous flows. This mainly results from the explicit and direct computation of the largest scale structures of the flow, which are the most difficult to model and contain a significant part of the physics controlling the flame. The introduction of a dispersed liquid fuel raises two kinds of problems:

- The physics of a liquid fuel spray is very complex and is not yet fully understood [46]. The atomisation process of a liquid fuel jet [92–96], the turbulent dispersion of the resulting droplets [97–101], their interaction with walls [102; 103], their evaporation and combustion [24] are phenomena occurring for LES at the sub-grid scale and therefore requiring accurate modelling.
- The numerical implementation of two-phase flow in LES remains a challenge. The equations for both gaseous and dispersed phases must be solved together at each time step in a strongly coupled manner. This differs again from classical RAS where both phases can be solved in a weakly coupled procedure, bringing first the gas flow to convergence, then calculating the associated dispersed phase and iterating until convergence of both phases.

Attempts to extend RAS formulation to LES of two-phase combustion may be found in [86; 104; 105]. They are all based on a Euler-Lagrange (EL) description of the dispersed phase in which the flow is solved using an Eulerian method and the particles are tracked with a Lagrangian approach. An alternative is the Euler-Euler (EE) description, also called two-fluid approach, in which both the gas and the dispersed phases are solved using an Eulerian formulation. Both strategies have advantages and shortcomings which are further emphasised in the LES context.

Following the individual trajectory of millions of droplets created by standard injectors implies computer resources that are still far beyond the capacities of computers available today and even in the coming years. To overcome this issue the stochastic Lagrangian approach is usually introduced, where each particle is only a "numerical" particle, representing in fact a statistically homogeneous group of real particles. This reduces the number of particles to compute but implies modelling for these parcels of particles [106]. Another difficult point is that the topology of the flow in dense zones (like near the injectors) differs from a cloud of droplets and a Lagrangian description may not be adapted in these specific regions. The EE description requires an initial modelling effort much larger than in the EL method [15] and faces difficulties in handling droplet clouds with extended size distributions [107]. Moreover the resulting set of equations is numerically difficult to handle and requires special care [108].

In the context of LES, just like for the gas phase, modelling issue appears for two-phase flow simulations, either in the EL or EE formulation. The closure problem is here linked to the SGS contribution to the turbulent droplet dispersion. This problem has already been addressed in [109] but is still an open question.

3.4. Numerics

The modelling problems being specifically addressed by LES, a remaining issue discussed here and often disregarded in the context of complex configuration simulations deals with the numerical scheme implemented in the computer code. Indeed once closed, the system of governing LES transport equations needs to be solved numerically to yield a numerical approximations of the $N + 5$ flow variables. The conventional strategy which is common to any Computational Fluid Dynamics (CFD) code, aims at representing the non-linear mathematical operators by introducing linear discrete operators to ease the temporal integration given an initial solution. Because of the geometrical complexity of target configurations, the scheme should cope with unstructured and/or hybrid meshes. For this specific reason, the finite-volume numerical approach [111] is often retained for CFD codes. Developments and researches on the

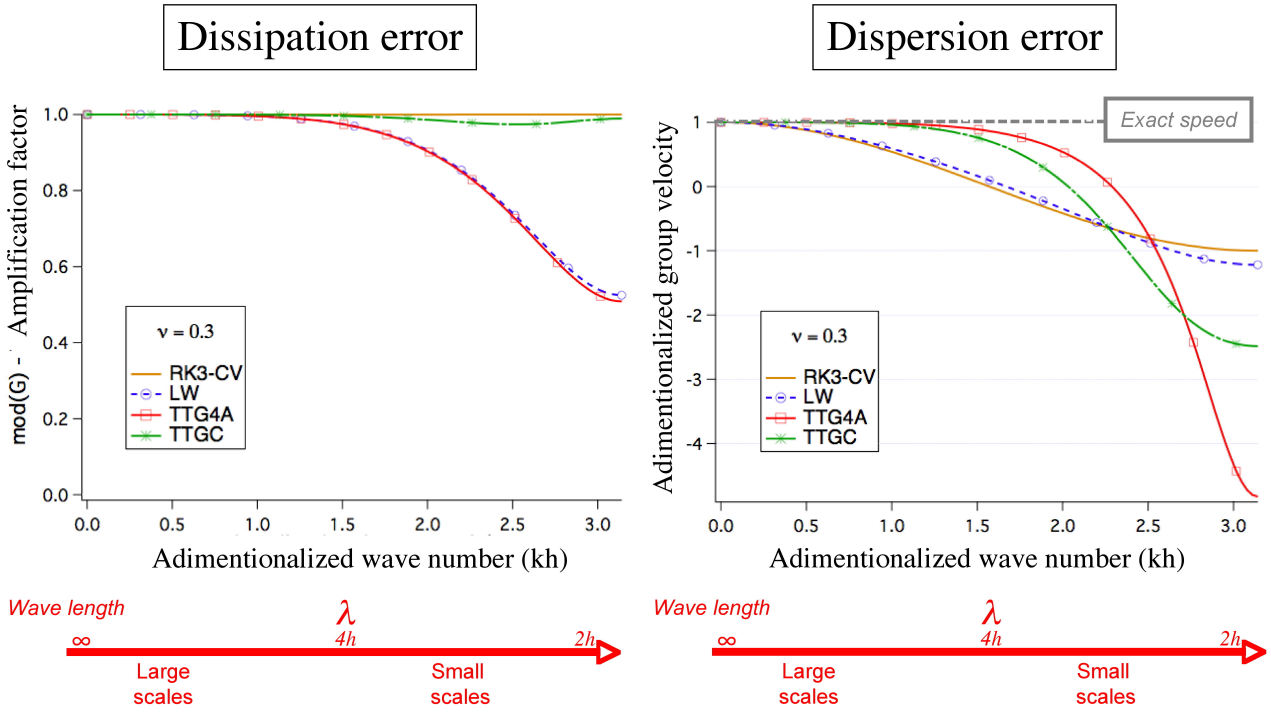

Figure 4. Dissipation and dispersion errors as functions of the wave number and as introduced by conventional numerical schemes used in LES on unstructured meshes: extracted from [110]

finite-element approaches [111] for CFD exist but do not seem to be used in advanced LES codes as discussed here. The difficulty is then to derive generic high order temporal and spatial discrete operators with a decent computer overhead and various cell topologies.

Off course the restriction of the governing equations onto a discrete set of cells and operations introduces errors. These truncation errors (in time and space) will impact the numerical prediction and the approximation will differ from the exact solution. For LES, the approach looks for spatially and temporally dependent flow solutions over a range of wavelengths that cover the characteristic size of the geometry all the way to the smallest grid cell. To be accurate, the LES information linked to these wavelengths need to be correctly propagated in space and in time. Numeric cannot guarantee such constraints especially over such a large range of wave-lengths. In fact and depending on the approach retained, the properties of the schemes are function of the local mesh size to the wave-length ratio: *i.e.* the number of grid nodes per wave-length. The errors introduced by numeric on a problem of convection are of two folds, Fig. 4:

- Dissipation errors: the simple convection problem the initial solution is simply convected in space at the fixed convective velocity. With numerical scheme based on the notion of up- or down-winding, that property is not guaranteed and the initial solution is diffused [112]. This lack of conservation is referred to as a dissipative error and results in the regular decrease of the maximum value as the solution advances in time.
- Dispersion errors: an additional effect introduced by some numerical scheme is a wave dependent convection velocity. It is traduce by wavelengths that are convected at different velocities and as a function of the wavelength to the grid point number ratio as depicted on Fig. 4. The initial solution is then deformed as time evolves with in some circumstances

some information travelling upstream.

The last numerical issue stems from numeric is the well-known Courant-Friedrichs-Lewis (CFL) stability criterion [111] which guarantees the overall stability of the integration. That is to say that the round-off errors or the noise artificially introduced by the discretization will not be amplified by the scheme only if the CFL is respected. Likewise in the context of diffusion dominated physics, schemes are stable under the Fourier criterion [111]. All of these behaviours are usually known issues. However and due to the specific context of LES, these spurious oscillations need to be controlled or at least quantified to properly assess a given SGS model or computer code. In that respect, the coupling and interactions between numeric and models are still not understood by the LES community although recent researches illustrate the impact on LES, its reliability and the understanding of the method [113; 114].

4. LES validation

The previous discussion clearly highlights the need for extensive and comprehensive validation procedures of LES: *i.e.* the physics, the models, the numeric... Such validations are necessary for newly developed LES codes and prior to their application on industrial applications, Fig. 1. As a matter of fact, all of the recent complex geometry LES results are obtained by research codes with years of development and multiple validations often published in scientific journals.

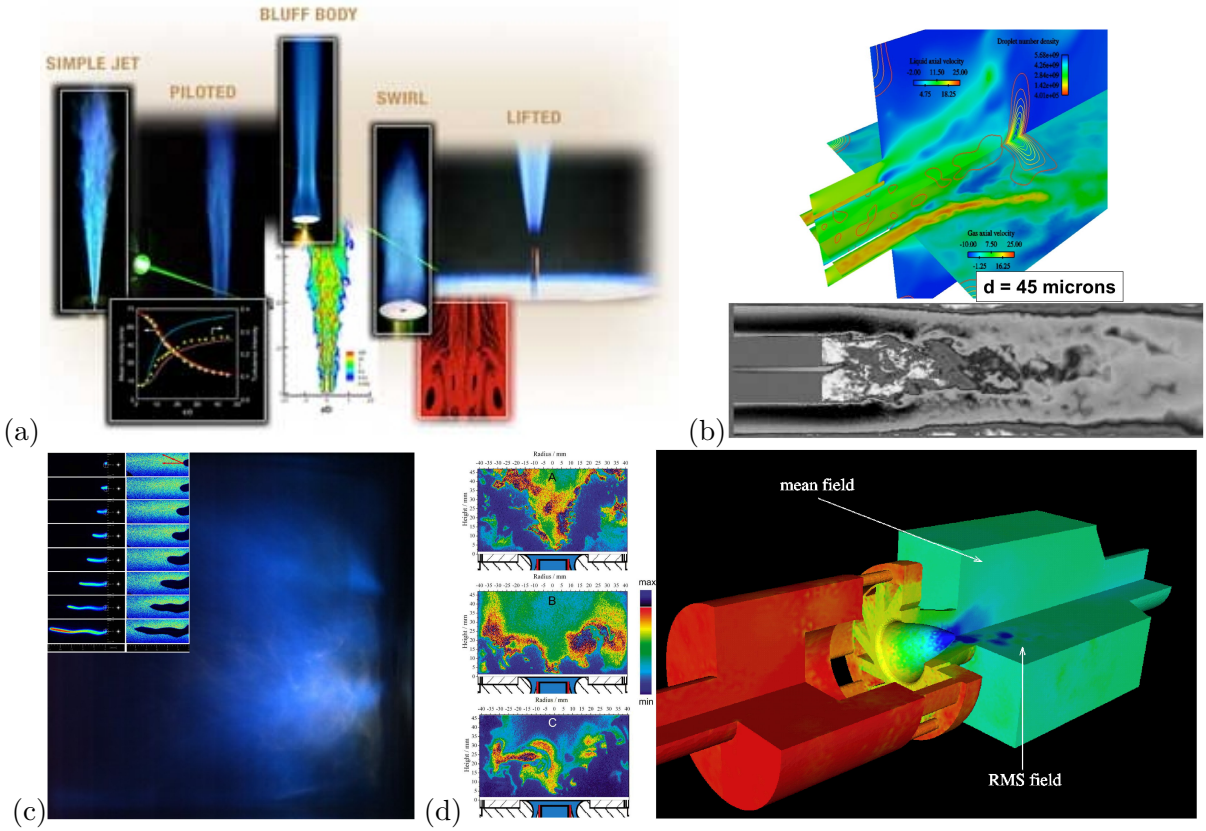

Figure 5. (a) Turbulent Non-premixed Flames[5] (TNF): community covering measurement techniques and numerical validations with combustion. (b) Sommerfeld and Hercules experiments [115] provide data for multiple phase flows. (c) Ignition experiments with fully transient diagnostics [116] and (d) the Preccinsta burner [117] designed for thermo-acoustic instabilities.

From a modelling point of view, LES models should in principle degenerate when the grid resolution meets the DNS context. Likewise, for large filter sizes, RAS type of predictions are expected [34; 35]. For multiple-phase and reacting LES, modelling appears at different levels. The initial modelling of the physics as prescribed by a EL / EE approach or for premixed / diffusion flames does not ease the process. Once the development context fixed, the filtering process of LES is introduced and the new closure problem appear. Simple analytical test cases are of great help to validate the implemented models and numeric as found in complex codes. *A priori* and *a posteriori* validations of models against DNS predictions are also largely recommended [35; 36] although the Reynolds number dependency of DNS somehow limits a direct extrapolation of the diagnostic to complex industrial flows.

Detailed experiments in increasingly complex configurations are also necessary. However and contrarily to the RAS context, these experiments require well controlled physics, accurate boundary condition description and when possible access to time series for an accurate validation of LES code. Such benchmark test cases, Fig. 5, are of valuable scientific interest and greatly impact the LES community with a large number of combustion scientists involved. They also constitute an interesting and stimulating research environment especially with the increased difficulty that is unsteadiness. Furthermore the steady increase in difficulty of these benchmark test facilities need to be sustained with more and more physics to be addressed. Statistically stationary turbulent flows are usually first targeted: free and confined jets, re-circulating flows, swirl flows... Fully transient flows, such as ignition sequences, start only to be addressed by experimentalists and already raise interesting issues if to be simulated with LES [116].

5. Parallelization and code scalability

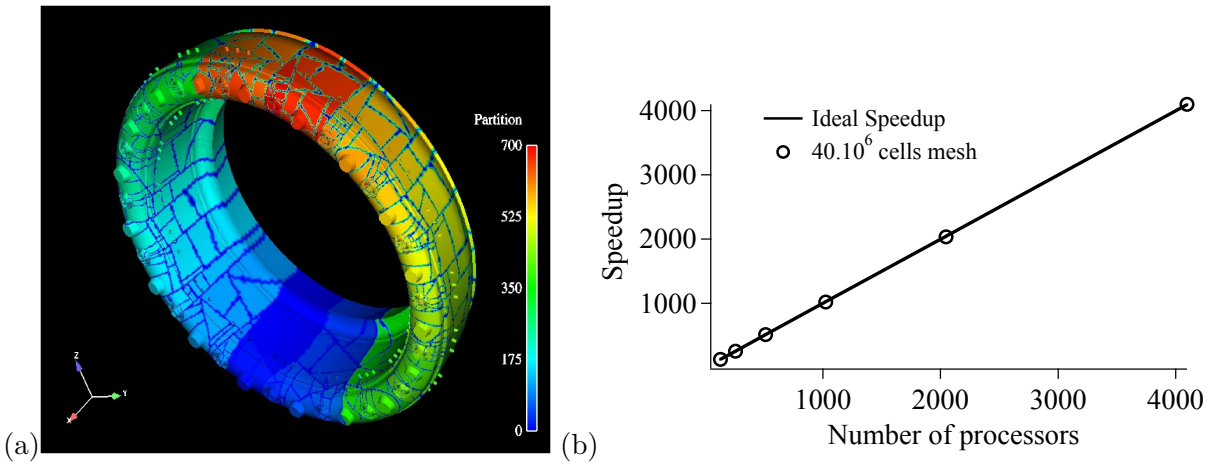

Figure 6. Domain partitioning strategy as implemented for an advanced LES code: (a) view of all the sub-domains assigned to each processor (one colour corresponds to one part of the domain computed by one processor, blue lines corresponds to surfaces where processors need to exchange information) and (b) scalability test on a HPC system as obtained by the LES code.

Usual validation of LES codes are obtained on scientific applications with increasing complexity and for which the computing effort does not necessarily justify state-of-the-art HPC. In some circumstances however, these computer codes and models need to be thought with an extended range of use and potential end-users in the industrial realm. With this in mind, several new constraints appear. The first one belongs to computing sciences and deals with scalability of the computer application, Fig. 6(b): *i.e.* the ability to efficiently take advantage of a large

number of processors by reducing the number of operations per processor while increasing the number of operations performed in parallel. With scalability, not only is the wall-clock time potentially reduced (the time the end-user has to wait before to have a solution to his problem) but it also provides increased computer memory which allows to tackle large problems.

Contrarily to scientific burners, industry usually treats large and complex geometries for which LES require much larger number of grid nodes and cells. Deploying such grids on a HPC systems ultimately necessitates a large number of processors. CFD codes and their algorithmic are heavily impacted by such a use. Scientific choices are also of importance and should ease scalability. The final aims of the retained strategy are for these computer codes:

- to minimise the time devoted to communications inferred by the dissemination among the processors of pieces of the geometry and which induces the exchange of information between processors with common interfaces,
- to maximise the time devoted to the integration of the mathematical system by each processor.

For LES, it is easy to show that only domain partitioning is efficient on large grids because task parallelization would require the communication of very large three-dimensional data sets at each iteration between all processors. Load balancing among the processors is thus the first issue that provides scalability. With partioning, the first objective is thus to partition a grid in sub-domains which will guarantee a uniform computational effort throughout the processors despite the fact that they will treat different parts of the mathematical problem. Note that depending on the physics, partioning may need to be reinitialised as the computation proceeds as recently developed.

Reduced communications also goes with the choice of the numerical scheme and partly explains why finite-volume is preferred to finite-difference for example [111]. In the former, interfaces between processors reduce to cell faces, Fig. 6(a), and only the fluxes and/or face nodal values are to be communicated from one processor to the next. For the latter more information is exchanged since some overlap of the different sub-domains is needed. These duplicated cells guarantee coherence of the solutions at the processor interfaces and induce message sizes that scale with the number of points in the overlap region. Note that in the case of high order schemes, as preferred for LES, the nodes in the overlapping region is large.

The nature of the differential equations used to model the physics is also of importance. For instance, flow dynamics may be addressed in the context of the compressible / incompressible Navier-Stokes equations. The incompressible system needs to find a solution for the pressure field that is obtained by solving a Poisson equation which follows a logarithmic scalability law as the number of grid points increases. The main advantage of that formulation comes from the stability criterion which relies on the convective velocity. The compressible formalism requires a CFL condition based on the convective plus acoustic speeds (smaller time steps). Scalability of the problem is however linear with the number of grid points. Explicit / implicit numerical schemes are other issues that need to be carefully addressed for efficient HPC codes.

Finally and specifically for two-phase flow applications, two methods may be used for LES: (1) task parallelization in which certain processors compute the gas flow and others compute the droplets flow and (2) domain partitioning in which droplets are computed together with the gas flow on geometrical sub-domains mapped on parallel processors. With (2) droplets must be exchanged between processors when leaving a sub-domain to enter an adjacent domain. However, codes based on domain partitioning are difficult to optimise on massively parallel architectures when droplets are clustered in one part of the domain (typically, near the fuel injectors). Moreover, the distribution of droplets may change during the computation: for a gas turbine re-ignition sequence, for example, the chamber is filled with droplets when the ignition begins thus ensuring an almost uniform droplet distribution; these droplets then evaporate rapidly during

the computation, leaving droplets only in the near injector regions. To preserve a high parallel efficiency on thousands of processors, dynamic load-balancing strategies are required that re-decompose the domain during the computation itself. Finally the computer implementation of the EL approach is not well-suited to parallel computers: since two different solvers must be coupled, the complexity of the implementation on a parallel computer if improperly done will increase drastically compared to a single-phase code. The EE approach has the important advantage to be straightforward to implement in a numerical tool, and immediately efficient as it allows the use of the same parallel algorithm than for the gas phase [118].

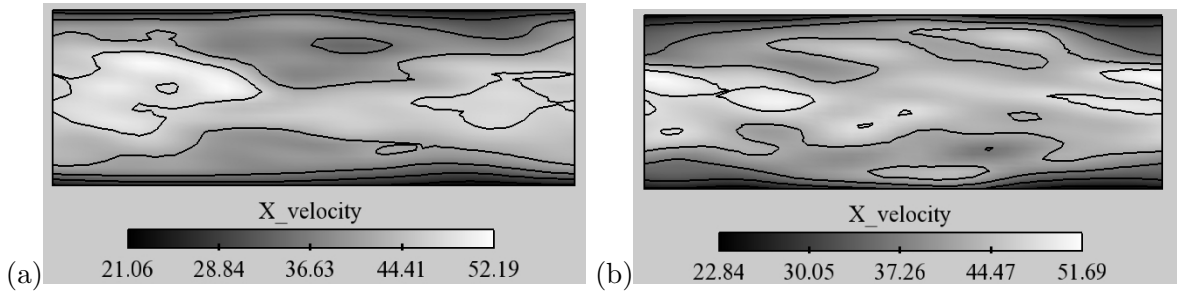

Figure 7. Instantaneous LES snapshots in the mid-channel width showing the axial velocity component in a periodic turbulent channel flow computed using (a) four processors and (b) eight processors. For this test case, initial conditions, mesh resolution, time step... are identical and the flow fields are obtained after the same number of iterations [119; 120].

HPC LES codes involve huge computer programming skills and stat-of-the-art codes are usually the result of numerous collaborations at the various stages of it developments. Parallel applications bring new issues such as error propagation and impact on LES predictions as illustrated on Fig. 7. Indeed, partioning is inevitably linked to the number of processors to be used and that number may not be fixed. Sub-domains will thus differ as the number of processors varies. Likewise, message ordering among the processors and at interfaces is impossible so that commutativity errors and round-off errors will differ [119; 120] potentially resulting in different instantaneous LES snapshots. Finally, LES is intimately linked to the grid resolution and LES realisations will differ as the mesh resolution is increased, Fig. 8, further complicating the validation of the LES approach.

6. Conclusions and perspectives

Large Eddy Simulation is a fully unsteady spatially dependent numerical approach with high potential when applied to industrial flow applications. Current state-of-the-art fully turbulent and reacting use of LES obtained thank to new HPC facilities produce convincing results for aeronautical engines despite the numerous physical issues that are not accounted for in these simulations. Such pioneering results open new research perspectives and applications not only for the LES community but the entire scientific community that is dealing with combustion. With the benefit from these new computing centres, CFD research should expand and new subject linked to fluid mechanics and its coupling to other physical phenomena should appear: radiation, heat transfer, combustion instability, detailed chemistry, multi-phase flows... Fundamental applications also benefiting from HPC such as Direct Numerical Simulations should also help in tackling more and more complex applications with LES. Finally, it is noted that frontier simulations stimulate the scientific community and propagates to the experimentalists with the development of leading edge diagnostics addressing unsteady flow behaviours.

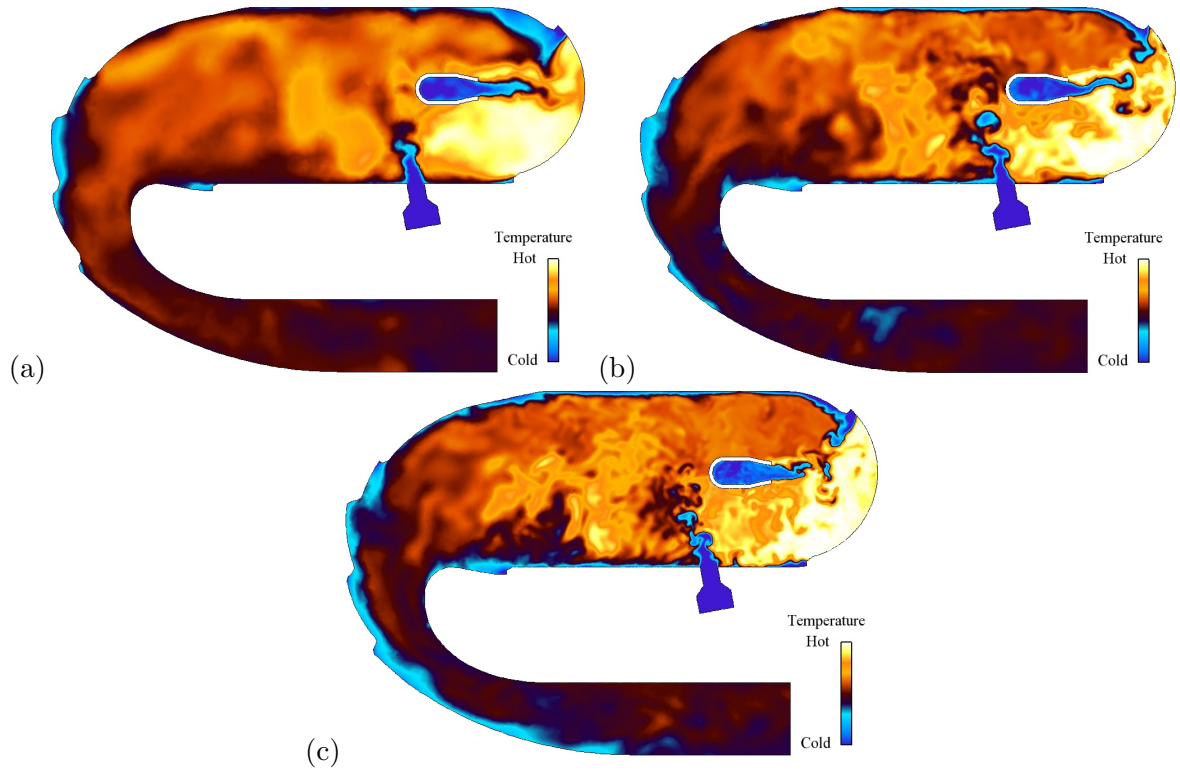

Figure 8. Instantaneous views of the temperature field as obtained by three LES of the same helicopter chamber with different grid resolution [121]: (a) $1,242,086$, (b) $10,620,245$ and (c) $43,949,682$ tetrahedrons.

From a pure computational point of view, application of LES in an industrial context raises new issues that will need to be addressed. Data management and diagnostic will need to adjust to ever bigger databases produced by LES. Code scalability and efficiency will need to be investigated thoughtfully. Finally, in-depth analysis of grid resolution, errors propagation and interactions, repetitivity of LES predictions with parallel computing raises new questions that will need to addressed prior extensive use of LES by industry.

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