
Numerical and physical instabilities in massively parallel LES of reacting flows

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Summary. LES of reacting flows is rapidly becoming mature and providing levels of precision which can not be reached with any RANS (Reynolds Averaged) technique. In addition to the multiple subgrid scale models required for such LES and to the questions raised by the required numerical accuracy of LES solvers, various issues related the reliability, mesh independence and repetitivity of LES must still be addressed, especially when LES is used on massively parallel machines. This talk discusses some of these issues: (1) the existence of non physical waves (known as ‘wiggles’ by most LES practitioners) in LES, (2) the effects of mesh size on LES of reacting flows, (3) the growth of rounding errors in LES on massively parallel machines and more generally (4) the ability to qualify a LES code as ‘bug free’ and ‘accurate’. Examples range from academic cases (minimum non-reacting turbulent channel) to applied configurations (a sector of an helicopter combustion chamber).

Key words: Combustion, Large-Eddy Simulation

1 Introduction

This paper focuses on the quality of LES in terms of mesh dependency and repetitivity, especially for reacting flows. LES codes are now routinely used to simulate combustion and more specifically to predict instabilities (mostly due to acoustics) in reacting flows [43, 23]. The fact that flames can couple with acoustics has been known for a long time [27], even though it is still not fully understood. Since acoustic waves can propagate in any direction in subsonic flows (which is the case in most combustors), they can create a feedback from any point of the flow to any other point, thereby creating multiple paths for absolute instabilities. More importantly, combustion instabilities are difficult to predict and are usually discovered at a late stage during the development of engine programmes so that they represent a significant industrial risk. These instabilities take various forms.

(1) In steady combustors like gas turbines, instabilities can lead to oscillations of all flow parameters, reaching levels which are incompatible with the normal operation of the chamber. They have been the source of multiple failures in rocket engines, as early as the Saturne or the Ariane 4 project, in aircraft engines (main chamber of

post combustion chamber), in industrial gas turbines and furnaces, etc. Fig. 1 shows an example of simulation of ‘mild’ oscillation in a gas turbine [10] where the flame position (visualized by an isosurface of temperature colored by axial velocity) pulsates at four instants of a cycle occurring at 120 Hz).

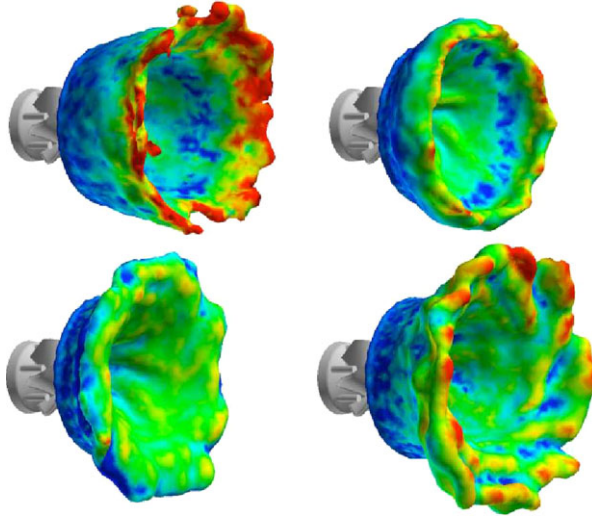


Fig. 1. Snapshots of flame position (isosurface of temperature) during one oscillation cycle at 120 Hz in an industrial gas turbine [10].

(2) In piston engines or in pulse combustors (such as the one used in German V 1 rocket during the second world war) where an external periodic motion or timing is imposed, instabilities take other forms: the most famous one is cycle-to-cycle variations. Fig. 2 shows LES results [28] in a four-valve four-stroke engine where all phases are explicitly computed (intake, compression, combustion, exhaust). Fig. 2 displays the reaction rate at exactly the same crank angle for various cycles: none of these cycles is similar. In extreme cases, certain cycles can actually not ignite or not burn at all. The source of these differences is obviously some type of instability. It can be an intrinsic bifurcation of the flow within the chamber or a coupling with the acoustic waves in the intake and exhaust pipes of the engine.

Predicting and controlling combustion instabilities is a major challenge for combustion research. Today, the most promising path is LES [23, 19, 32] something which was impossible 10 years ago with classical Reynolds Averaged Navier-Stokes methods. Evaluating the error margins associated to such LES is becoming a critical question. Multiple ‘instabilities’ are found in combustion LES. Instabilities exist in individual flame fronts and lead to the formation of cells and of various unstable modes depending on molecular transport of chemical species and heat [43, 4]. Like any shear flow, reacting flows are submitted to hydrodynamic modes [7, 13] and to vortex formation. But acoustics play the first role in reacting flows: by coupling

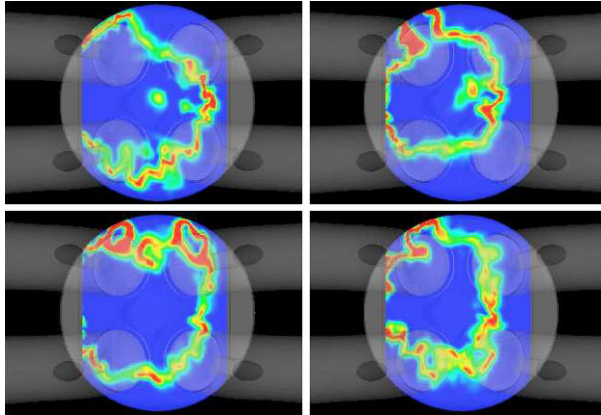


Fig. 2. Snapshots of reaction rate in a simulation of piston engine at four successive cycles for the same crank angle. None of them is the same.

with heat release, they are the source of most combustion instabilities [43, 23]. Instabilities are present in the physical problem studied but they are also present in the numerical methods used to simulate these mechanisms. Most high-fidelity numerical schemes required for Computational Fluid Dynamics exhibit low dissipation and therefore multiple non-physical instabilities (wiggles) arise which can require significant efforts to be kept under control [40, 33, 23]. Finally, CFD for reacting flows are performed today on massively parallel machines: these architectures coupled with centered schemes for turbulent flows lead to an additional type of instability linked to the growth of rounding errors and to a new type of instability where the solution depends on unexpected parameters such as the commutativity errors of addition, the initial condition or the number of processors.

All these phenomena are ‘instabilities’ even though they correspond to different mechanisms. In some cases, they can couple: for example, in LES of combustion instabilities, the first issue is to be able to control the non-physical waves due to the high-order spatial scheme as well as the rounding errors due to massively parallel computing. This paper describes numerical instabilities found in LES (Section 2), proposes an analysis of the repetitivity of LES especially on parallel machines (Section 3) and ends with a study of the influence of mesh size on the LES of a sector of a gas turbine combustion chamber (Section 4).

2 Numerical waves in LES of reacting flows

Predicting combustion instabilities requires an accurate computation of all waves mentioned in the previous section. Unfortunately, LES (like DNS and unlike RANS) can propagate other waves: these numerical waves (called Q waves [40, 33, 23]) are a significant difficulty for most high-fidelity simulations. Q waves are produced by sharp gradients, approximate initial conditions, boundary conditions, etc. They

interact with physical waves, making LES difficult and sensitive to unexpected behaviors. Knowing how Q waves interact with physics is a necessary exercise but one which is not often discussed because studying wiggles is not an exciting topic and also because most RANS codes use excessive artificial viscosity and large turbulent viscosity levels (due to turbulence models) which kill all numerical waves (they also kill all acoustic waves and hydrodynamic modes...) Methods which can compute accurately waves must use centered schemes and low turbulent viscosity levels. A convenient way to illustrate this point is to compare the various viscosities playing a role in a CFD code:

- The laminar viscosity ν is the only true flow characteristic and it defines the true Reynolds number of the flow: $Re_{real} = UL/\nu$ where U and L are a reference velocity and length of the flow respectively.
- In CFD codes, a turbulent viscosity ν_t is added through the model for turbulent fluctuations.
- Many CFD codes¹ also add an artificial viscosity ν_a or upwind (dissipative) schemes. An important dissipation is also introduced by large time steps and implicit schemes which are commonly used in RANS.

Adding two viscosities ν_t and ν_a to the true viscosity ν leads to a lower Reynolds number really seen by the code:

$$Re_{code} = UL/(\nu + \nu_t + \nu_a) \quad (1)$$

which is much smaller than Re_{real} . In RANS formulations, the turbulent viscosity introduced by models such as the $k-\epsilon$ model can reach 1000 times the physical viscosity while very high levels of artificial viscosity ν_a are used for robustness and speed. As a result, RANS results are steady: in other words, laminar. Of course, the local viscosity is tuned to match the mean characteristics of the mean turbulent flow but the turbulent character of the flow is completely lost. At the other end of the spectrum, DNS methods strive to use $\nu_a = \nu_t = 0$ so that $Re_{code} = Re_{real}$. LES formulations have to use non-zero values for ν_a and ν_t but these must be kept to very small values.

Method	Physical viscosity	Numerical viscosity	Turbulent viscosity	Capacity to propagate waves
DNS	1	0	0	excellent
LES	1	1 to 10	5 to 50	good
RANS	1	10 to 500	100 to 1000	none

Table 1. Orders of magnitude of physical, numerical and turbulent viscosity in DNS, LES and RANS codes. All values are scaled by the laminar viscosity.

¹ Certain numerical methods introduce dissipation terms which are not second order and are more difficult to compare to other viscosities: the well-known Jameson approach for example uses a fourth-order dissipation. They are not discussed here.

Table 1 shows typical levels of physical viscosity, turbulent viscosity ν_t and artificial viscosity ν_a (scaled by the laminar viscosity) reached in a combustion chamber for a standard regime. Note that viscosity affects all scales and not only the small scales. For example, acoustic waves are very strongly dissipated in a RANS code because the turbulent viscosity acts on them too. A less pleasant implication of Table 1 is that, as soon as high-fidelity methods such as DNS or LES are developed, they have to avoid large values of turbulent and artificial viscosities. This requires small mesh sizes, high-order schemes, small time steps [5, 33, 23]. These improvements unfortunately, also make these methods sensitive to numerical Q waves [34, 40, 23].

3 The growth of rounding errors in LES

The main strength of LES compared to classical Reynolds Averaged (RANS) methods is that compressible LES explicitly captures large scale unsteady motions due to turbulence and the instability modes found in reacting flows. An often ignored aspect of this feature is that LES is also submitted to a well-known feature of turbulent flows: the exponential separation of trajectories [39] implies that the flow solution exhibited by LES is very sensitive to any “small perturbations”:

- Rounding errors are an unavoidable forcing for the Navier-Stokes equations and may lead to LES variability. The study of error growth in finite precision computations is an important topic in applied mathematics [37, 3] but has found few applications in multidimensional fluid mechanics because of the complexity of the codes used in CFD.
- Initial conditions are a second source of LES results variability: these conditions are often unknown and any small change in initial conditions may trigger significant changes in the LES solution. Boundary conditions, in particular the unsteady velocity profiles imposed at inlets and outlets, can have the same effect as initial conditions but are not studied here.
- Due to its large computational resource requirements, modern LES heavily relies on parallel computing. However, in codes using domain decomposition, it is also an additional “noise” source in the Navier-Stokes equations especially at partition interfaces. Even in explicit codes, where the algorithm is independent of the number of processors, the different summation orders with which a nodal value is reconstructed at partition interfaces, may induce non-associativity errors. For example, in explicit codes on unstructured meshes using cell vertex methods [31], the residual at one node is obtained by adding the weighted residuals of the surrounding cells. In some cases, summation may yield distinct results for floating-point accumulation: the rounding errors in $(a + b) + c$ and in $a + (b + c)$ may be different [11]. After thousands of iterations, the LES result may be affected. Since these rounding errors are induced by non deterministic message arrival at partition interfaces, such behaviour may occur for any CFD code, re-

regardless of the numerical scheme and lead to results which depend on the number of processors used for the LES.²

- Even on a single processor, internal parameters of the partitioning algorithm may couple with rounding errors. For example, a different reordering of nodes using the Cuthill-McKee (CM) or the reverse Cuthill-McKee (RCM) algorithm [6, 16] may produce the same solution divergence.

LES solutions are known to have a meaning only in a statistical manner [25]: observing that the solution of a given LES/DNS at a given instant changes when the rounding errors or the initial conditions change is not really surprising. It is however a difficulty in the practical use of LES: running the same simulation on two different machines or one machine with a different number of processors or slightly different initial conditions can lead to totally different instantaneous results. For steady flows in the mean, statistics should not depend on these changes and mean profiles must be identical. However, when the objective of the LES is unsteady phenomena such as ignition or quenching in a combustor [36], knowing that results depend on these parameters is certainly a sobering thought. This section tries to address these issues and answer a simple question [35]: how does the solution produced by LES depend on the number of processors used to run the simulation? On the initial condition? On internal details of the algorithm?

The configuration is a rectangular channel computed with a fully explicit LES code [21]. The following section then gives a systematic description of the effects of rounding errors in two flows: a turbulent channel and a laminar Poiseuille flow.

3.1 Effects of the number of processors on LES

This first example is the LES of a rectangular fully developed turbulent channel of dimensions: 75x25x50 mm (Fig. 3). An homogeneous force is applied to a periodic channel flow to provide momentum; random disturbances are added to trigger transition to turbulence. There are no boundary conditions except for the walls in y direction. The Reynolds number is $Re_\tau = \delta u_\tau / \nu = 1500$, where δ is half the channel height and u_τ the friction velocity at the wall: $u_\tau = (\tau_{wall}/\rho)^{1/2}$ with τ_{wall} being the wall stress. The mesh contains 30^3 hexahedral elements, it is not refined at walls. The first grid point is at a reduced distance $y^+ = y u_\tau / \nu \approx 100$ of the wall. The sub-grid model is the Smagorinsky model and a law-of-the-wall is used at the walls [30]. The initial condition corresponds to a snapshot of the flow at a given instant, long after turbulence was initialized so that it is fully established. The computation is performed with an explicit code where domain decomposition is such that the method is perfectly equivalent on any number of processors. The Recursive Inertial Bisection (RIB) [38] algorithm is used to partition the grid and the Cuthill-McKee algorithm is the default graph reordering strategy. The scheme is the Lax-Wendroff scheme [12]. Additional tests using a third-order Taylor-Galerkin scheme [5] led to the same conclusions.

² The case of implicit codes [18, 17, 8] or in space (such as compact schemes) [15, 1, 34] is not considered here.

Table 2. Summary of turbulent LES runs (fully developed turbulent channel).

Run Id	Nbr proc	Init. cond.	Precision	Graph ordering	CFL λ
TC1	4	Fixed	Double	CM	0.7
TC2	8	Fixed	Double	CM	0.7
TC3	1	Fixed	Double	CM	0.7
TC4	1	Modif.	Double	CM	0.7
TC5	1	Fixed	Double	RCM	0.7
TC6	4	Fixed	Double	CM	0.35
TC7	8	Fixed	Double	CM	0.35
TC8	4	Fixed	Simple	CM	0.7
TC9	8	Fixed	Simple	CM	0.7
TC10	28	Fixed	Quadr.	CM	0.7
TC11	32	Fixed	Quadr.	CM	0.7

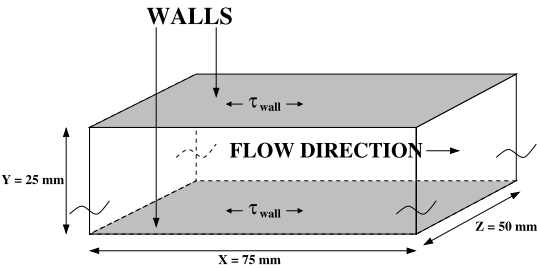


Fig. 3. Schematic of a periodic channel. The upper and lower boundaries consist of walls, all other boundaries are pairwise periodic.

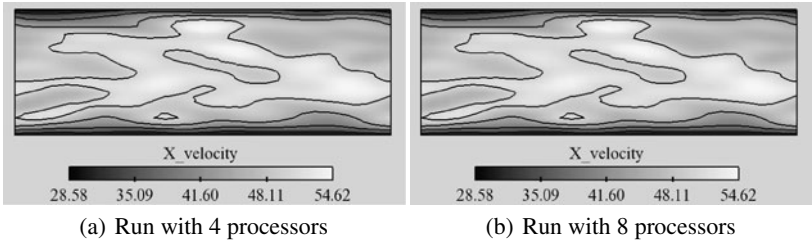


Fig. 4. Instantaneous field of axial velocity in the central plane of the channel at $t+ = 7.68$. a) run TC1 (4 processors), b) run TC2 (8 processors).

Figs. 4 and 5 show fields of axial velocity in the central plane of the channel at two instants after the initialization. Two simulations performed on respectively 4 (TC1) and 8 processors (TC2) with identical initial conditions and meshes are compared (Table 2 and 3). The instants correspond to (in wall units) $t^+ = 7.68$ and $t^+ = 26.11$ respectively where $t^+ = u_\tau t / \delta$. Obviously, the two flow fields observed at $t^+ = 7.68$ are identical. Flow fields start to diverge after $t^+ = 15$ and at $t^+ = 26.11$, the instantaneous flow fields obtained in TC1 and TC2 are totally different (Figs. 5). Even though the instantaneous flow fields are different, statistics remain the same: mean and root mean square axial velocity profiles averaged over $t^+ \approx 60$ are identical for both simulations (Figs. 6).

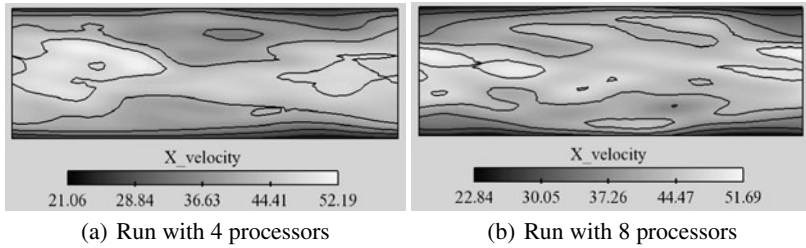


Fig. 5. Instantaneous field of axial velocity in the central plane of the channel at $t^+ = 26.11$. a) run TC1 (4 processors), b) run TC2 (8 processors).

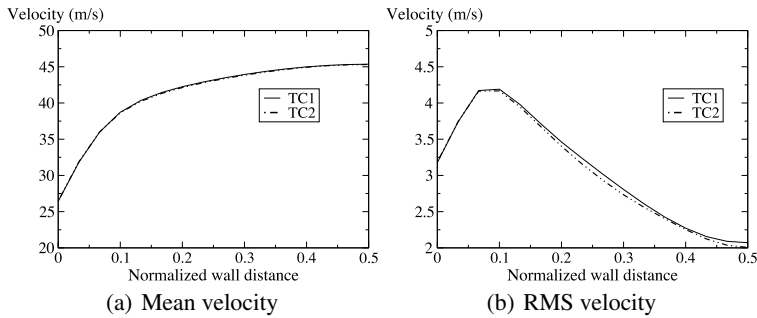


Fig. 6. Comparison of the mean (left) root mean square (right) velocity profiles for TC1 (4 processors) and TC2 (8 processors) simulations over half channel height.

3.2 Sensitivity of LES in laminar and turbulent flows

To understand how LES can produce diverging instantaneous results such as those shown above, tests were performed to investigate the effects of various aspects of the

methodology: laminar/turbulent baseline flow, number of processors, initial condition, graph ordering, time step and machine precision. The objective is to quantify differences between two LES solutions produced by a couple of simulations in Table 2 and 3. Let u_1 and u_2 be the scalar fields of two given instantaneous solutions at the same instant. A proper method to compare them is to use the iteration evolution of the following norms: N_{max} provides the maximum local velocity difference in the field between two solutions while N_{mean} yields a volumetrically averaged difference between the two solutions. Note that performing any of the LES of Table 2 twice on the same machine with the same number of processors, the same initial conditions and the same partition algorithm leads to exactly the same solution, N_{max} and N_{mean} being zero to machine accuracy. In that sense, the LES remains fully deterministic. However, this is true only if the order of operations at interfaces is not determined by the order of message arrival so that summations are always carried out in the same order. Otherwise, the randomness induced by the non-deterministic order of message arrival is enough to induce diverging solutions. The following test is to compare a turbulent channel flow studied in the previous section and a laminar flow. A three-dimensional Poiseuille flow in a pipe geometry was used as test case. The flow is laminar and the Reynolds number based on the bulk velocity and diameter is approximately 500. The boundary conditions are periodic at the inlet/outlet and no-slip at the duct walls. A constant axial pressure gradient is imposed in the entire domain.

Table 3. Summary of laminar runs (Poiseuille flow).

Run Id	Nbr proc	Init. cond.	Precision	Graph ordering	CFL λ
LP1	4	Fixed	Double	CM	0.7
LP2	8	Fixed	Double	CM	0.7

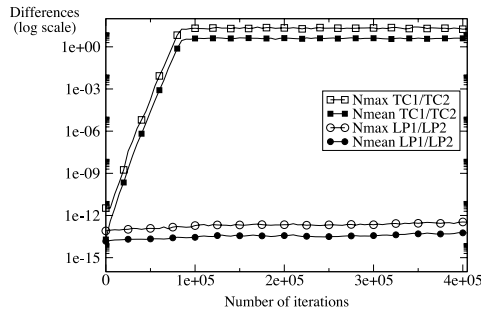


Fig. 7. Effects of turbulence. Differences between solutions: N_{max} (open symbols) and N_{mean} (closed symbols) vs iteration. Squares: differences between TC1 and TC2 (turbulent channel). Circles: differences between LP1 and LP2 (laminar flow).

Figure 7 shows the evolutions of N_{max} and N_{mean} versus iteration for runs TC1/TC2 and LP1/LP2. The only parameter tested here is a change of the number of processors. As expected from the snapshots of Figs. 4–5, the simulations are sensitive to a change in the number of processors and the solutions of TC1 and TC2 diverge rapidly leading to a maximum difference of 20 m/s and a mean difference of 3–4 m/s after 90,000 iterations. The stagnation of absolute and mean differences between TC1/TC2 simply implies that after 90,000 iterations solutions have become fully uncorrelated. On the other hand, the difference between the laminar simulations LP1 and LP2 hardly increases and levels off when reaching values of the order of 10^{-12} . This is expected since there is obviously only one stable solution for the Poiseuille flow: laminar flows do not induce exponential divergence of trajectories. This test case confirms that the turbulent character of the flow is the source of the divergence of solutions.

The basic mechanism leading to Figs. 4–5 is that the turbulent flow acts as an amplifier for rounding errors generated by the fact that the mesh is decomposed differently in TC1 and TC2. This implies a different ordering when adding the contributions to a cell residual for nodes at partition interfaces. This random noise roughly starts at machine accuracy (Fig. 7) at a few points in the flow and grows continuously if the flow is turbulent.

The previous results show that turbulence combined with a different domain decomposition is sufficient to lead to different instantaneous flow realizations. A perturbation in initial conditions has the same effect as domain decomposition as verified in runs TC3 and TC4 which are run on one processor only, thereby eliminating issues linked to parallel implementation. The only difference between TC3 and TC4 is that in TC4, the initial solution is identical to TC3 except at one random point where a 10^{-16} perturbation is applied to the streamwise velocity component. Solutions exhibited the same divergence [35]. Finally, the results of Senoner et al [35] show that the numerical scheme and the time step do not influence the growth rate of the solutions difference: for example, simulations TC6 and TC7 are performed with a time step reduced by a factor 2 compared to simulations TC1 and TC2. TC6 and TC7 are carried out on respectively 4 and 8 processors. The norms between TC6 and TC7 are similar to the other cases.

A last test to verify that the solutions divergence depends primarily on rounding errors is to perform the same computation with simple/quadruple precision instead of double precision. Simulations TC1 and TC2 were repeated using single precision in runs TC8 and TC9 (Table 2) and quadruple precision in TC10 and TC11. Results are compared to the difference between TC1 and TC2. Figure 8 shows that the solution differences for TC8/TC9 and TC10/TC11 roughly start from the respective machine accuracies (differences of 10^{-6} for single precision after one iteration, differences of 10^{-30} for quadruple precision after one iteration) and increase exponentially with the same growth rate before reaching the same difference levels for all three cases. Higher precision computations cannot prevent the exponential divergence of trajectories but only delay it.

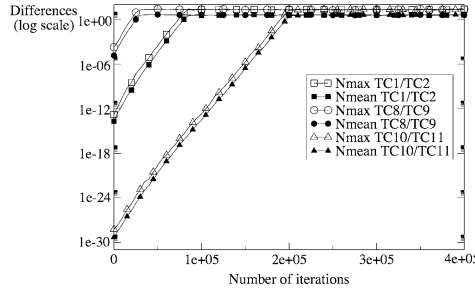


Fig. 8. Effects of machine accuracy. Differences between solutions: N_{max} (open symbols) and N_{mean} (closed symbols) vs iteration. Squares: differences between TC1 and TC2 (double precision). Circles: differences between TC8 and TC9 (single precision). Triangles: differences between TC10 and TC11 (quadruple precision).

4 Mesh effects in LES of gas turbine chamber

4.1 Objectives

The last topic discussed here is related to mesh dependency effects in LES of reacting flows. Multiple authors have underlined the importance of this point for LES [29, 25]. LES depend on mesh resolution (unlike RANS) and produce grid independent results only if the mesh is sufficiently refined. LES must then satisfy multiple properties: time-averaged values must converge, Root Mean Square (RMS) resolved values must increase when the mesh cell size decreases and the SGS turbulence level diminishes, the resolved velocity spectra must fill towards larger wave-numbers. In practice, these behaviors are expected to be controlled by the LES models, the flow Reynolds number, the grid resolution as well as the accuracy of the numerical solver (in the context of implicit filtering [29, 9, 24]). Mesh dependency analysis of non-reacting LES predictions has recently been addressed [42, 20, 26] and quality criteria have been proposed for *a posteriori* evaluation of the LES flow predictions [25, 41, 14].

For reacting flows, the computer power needed to simulate realistic geometries is so large that the grids used for LES are usually still too coarse to resolve all flow zones: multiplying the number of grid points by a significant factor to verify the effects of grid resolution on the LES results was impossible until very recent times. Very few LES of reacting flows have been devoted to mesh dependency in simple configurations [42, 20, 26] and none of them has addressed this issue in complex geometry combustors. The situation has changed in the last two years: porting LES codes on massively parallel machines in the Top 20 list has allowed a sudden increase of power for combustion computations. Speed-ups of nearly 95 percent obtained on 2 to 10 000 processors allow to address the problem of mesh dependency by performing one ‘coarse grid’ simulation with a reasonable mesh (typically 1.5 million cells) and then comparing it with an ‘intermediate grid’ simulation (8 times more cells) and finally with a ‘fine grid’ simulation (32 times more cells). In the present work, the mesh dependency of the LES predictions is studied for a helicopter combustion chamber [2].

4.2 Target configuration

The configuration (Fig. 9) corresponds to a helicopter combustion chamber where fuel is injected using an inverted cane injection system, also called pre-vaporizer. The computational domain focuses on a 36 degree section of a full annular reverse-flow combustion chamber designed by Turbomeca (Safran group). A premixed gaseous mixture of $C_{10}H_{16}$ enters the chamber through the pre-vaporizer, Fig. 9 (a) & (b). Fresh gases are consumed in the primary zone, delimited by the chamber dilution holes and the liner dome of the combustion chamber, Fig. 9 (a). To ensure full combustion, this region of the chamber is fed with air by primary jets located on the inner liner, Fig. 9 (b). Burnt gases are then cooled by dilution jets or cooling films located on the inner and outer liners as well as on the return bend of the combustion chamber. Multi-perforated plates also ensure local wall cooling in areas of the chamber shown on Fig. 9 (b).

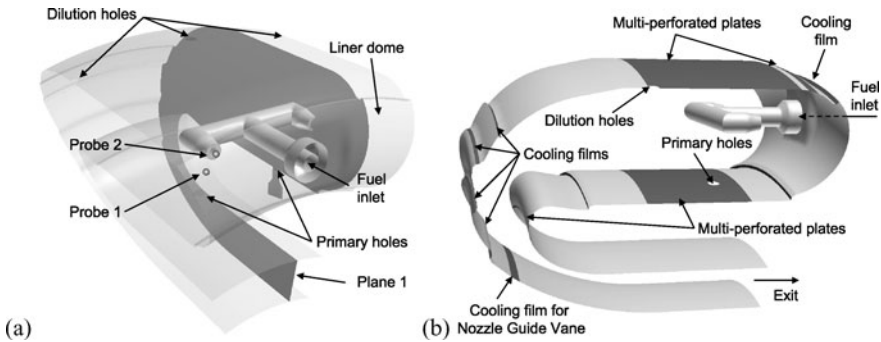


Fig. 9. Combustion chamber: (a) 3D view and (b) side view.

	'Coarse'	'Intermediate'	'Fine'
Total number of points	230,118	1,875,835	7,661,005
Total number of cells	1,242,086	10,620,245	43,949,682
Max. cell volume [m ³]	$3.12 \cdot 10^{-8}$	$8.97 \cdot 10^{-9}$	$4.05 \cdot 10^{-9}$
Min. cell volume [m ³]	$1.81 \cdot 10^{-11}$	$8.29 \cdot 10^{-12}$	$1.18 \cdot 10^{-12}$
Time step [s]	$1.52 \cdot 10^{-7}$	$0.88 \cdot 10^{-7}$	$0.49 \cdot 10^{-7}$
Averaging time [ms]	10	10	10
Number of iterations for averaging	65,790	108,695	204,082
CPU time(hours) for a 10ms LES	315	4,550	30,200

Table 4. Mesh characteristics.

The combustion regime expected in such burners mixes rich partially premixed flames in the chamber primary zone (the gases injected in the canes can be consid-

ered as premixed gases at an equivalence ratio of 3.17) and diffusion flames in the dilution region: *i.e.* RQL concept. A turbulent combustion model able to handle both regimes is therefore needed and the DTF model offers this capacity [30, 19, 36]. The meshes are refined in the primary zone, particularly in the lower part where combustion occurs, and in the regions of cooling films (Table 4). The Navier-Stokes Characteristic Boundary Conditions (NSCBC) [21, 22] are applied on boundaries to control the acoustic behavior of the system. Walls are adiabatic and are treated with a turbulent law-of-the-wall. Side boundaries of the computational domain are axi-periodic. The operating point corresponds to cruising conditions and is the same for the three grids. The cost of the three computations for the same physical time goes from 315 hours on the coarse mesh to 30,200 on the fine one.

4.3 Instantaneous flow topology and flame structure

A crucial requirement for the LES method when applied in such complex configurations is the right prediction of the combustion phenomenon. Modelling, which is needed to supply proper combustion enhancement due to lack of interactions at the unresolved scales, is paramount in that context. If improperly parameterized, a turbulent combustion model can yield different flame positions for LES computed with different mesh resolutions.

Figure 10 compares instantaneous fields of temperature for the three resolutions. The cutting plane goes through one of the pre-vaporizer outlets (Plane 1, Fig. 9) and is colored by the instantaneous field of temperature scaled by the inlet mean temperature. The observations drawn for the axial component of the velocity field also apply to Fig. 10: the temperature fields are clearly enriched with increasing grid resolution and the impact on the temperature levels seems reduced.

4.4 Mean flow results

Figure 11 shows the mean temperature field scaled by the inlet temperature. Grid resolution has an impact in various highly localized regions and some discrepancies are detected, especially in the mean temperature fields of Fig. 11. The improved mesh quality of the intermediate and fine grids makes the flow behave differently in near-wall regions where the chamber flow interacts with the flow issuing from cooling devices. For example, the thermal boundary layer created by the multi-perforated plates (Zone 1 and 3 on Fig. 11 (a)) on the intermediate mesh is thinner than the one on the coarse grid. Likewise, the penetration of the cooling film located in the upper part of the liner dome is different on the coarse grid. Despite these discrepancies, the agreement between these sets of predictions underlines mesh independence of the first moments for these calculations.

The paper of Boudier et al [2] provides more comparisons showing that velocity and temperature fields are well converged on the medium and fine grids while the reaction rate field continues to evolve when the grid is refined. This is not surprising as reaction rates are essentially subgrid scale quantities: increasing the mesh resolution allows to capture more wrinkling. However, the flame position does not change

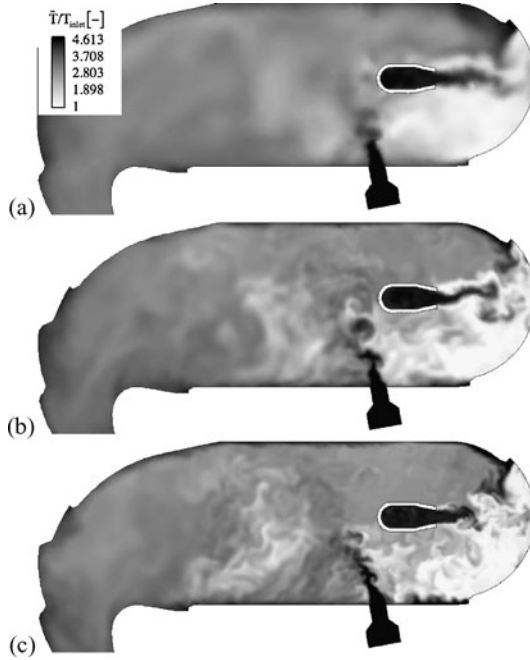


Fig. 10. Instantaneous temperature field scaled by the mean inlet temperature and obtained on (a) the coarse grid, (b) the intermediate one and (c) the fine one.

and even the acoustic activity in the chamber remains reasonably independent of the mesh.

5 Conclusions

This paper has shown that any turbulent flow computed by LES exhibits significant sensitivity to parameters such as initial solution, number of processors, message ordering. This sensitivity leads to instantaneous turbulent solutions which can be totally different while laminar flows are almost insensitive to these parameters. The divergence of solutions is due to the well known- exponential separation of trajectories in turbulent flows and to the non-deterministic rounding errors induced by different domain decompositions or different ordering of operations. More generally any change in the code lines affecting rounding errors will have the same effects. These results confirm the expected nature of LES [25] in which solutions are meaningful only in a statistical sense and instantaneous values can not be used for analysis. However, on a more practical level, they point out various difficulties to develop LES codes:

- Repeating the results of a given LES after modifying the code and verifying that instantaneous solutions have not changed is not always possible. Since any programming error will also lead to a change in instantaneous solutions, identifying

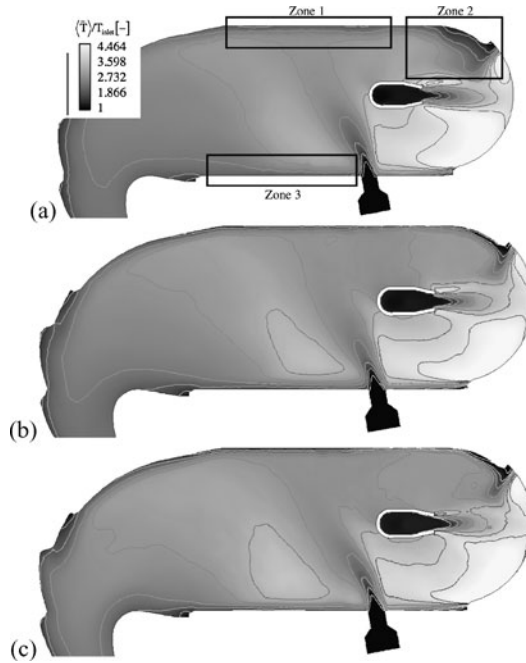


Fig. 11. Mean temperature field (scaled by the mean temperature at the pre-vaporizer inlet) obtained on (a) the coarse grid, on (b) the intermediate grid and on (c) the fine grid.

errors introduced by new lines will require a detailed analysis based on average fields (and not on instantaneous fields) and a significant loss of time.

- Verifying an LES code on a parallel machine is a difficult task: running the code on different numbers of processors will lead to different solutions and make comparisons impossible.
- Porting a LES code from one machine to another will also produce different solutions for turbulent runs, making comparison and validations of new architectures difficult.

When used on a complete reacting simulation of a sector of combustion chambers, the same conclusions are reached: instantaneous solutions can differ but the mean flow can be consistently captured with LES. The quality of the models themselves and of the numerical method accuracy was evaluated by repeating the same LES on three different meshes ranging from 1.4 million to 40 million cells and a reasonable mesh independency was observed even though more resolved wrinkling is observed when the mesh resolution is increased. More generally, these results demonstrate that the concept of “quality” in LES will require much more detailed studies and tools than what has been used up to now in Reynolds Averaged simulations. Instabilities appearing in a given LES on a given computer can have sources

which were not expected at first sight (like the number of processors). Mastering these instabilities will be an important task to get the full power of LES techniques.

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