ON THE USE OF (U)RANS AND LES APPROACHES FOR TURBULENT INCOMPRESSIBLE SINGLE PHASE FLOWS IN NUCLEAR ENGINEERING APPLICATIONS

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ABSTRACT

The present paper gives some ideas and guidelines one should keep in mind while running (U)RANS or LES computations. The paper starts with (U)RANS approaches, advocating the use of Reynolds Stress Models for complex flows and recommending further work on modeling of turbulent heat fluxes, which remains today too basic in industry. The superiority of wall resolved models vs. wall modeled in RANS is recalled and the use of adaptive wall treatment is suggested. The concept of Unsteady RANS is finally questioned.
Then, important issues around LES are raised. The mesh refinement criteria are recalled for wall resolved LES and the use of a wall models addressed. The production of DNS and wall resolved LES for flow understanding and RANS validation is encouraged.

KEYWORDS
LES, (U)RANS, Nuclear engineering, Wall resolved, Wall modeled

1 INTRODUCTION

(Unsteady) Reynolds Averaged Navier Stokes ((U)RANS) and Large Eddy Simulation (LES) approaches are today widely used in nuclear engineering applications for predicting the dynamics and heat transfer of turbulent flows. Both approaches exist since a long time and will remain useful for understanding several industrial configurations for several decades, playing different roles.
The present overview is restricted, for the sake of clarity, to (U)RANS and LES for configurations in which the flow is incompressible and single phase as we consider that a lot of work is still required for this type of flow and for these two approaches. This article is in the continuity of an invited lecture [1] at Turbulence Heat and Mass Transfer conference 6. In this contribution, the authors insisted on the importance of RANS approaches in general and in Reynolds Stress Models (RSMs) in particular without forgetting the role of LES.

DES, SAS, ... turbulence modeling approaches are out the scope of the present article. Verification and Validation (V&V), which is a necessary procedure to check the correct numerical solution of the equations and the ability of a model to predict standard flows is a prerequisite but will not be addressed. Neither can Uncertainty Quantification (UQ) but the hundreds of simulations required for the latter make fine LES unaffordable, incompatible, with UQ. The statements given in the following largely assume the use a finite volume approach as this is the most common discretization used in nuclear engineering. Regarding heat transfer, nothing particular will be said for very low Prandtl numbers and one assumes values around 1 which is the case in Pressure Water Reactors (PWR). Finally, as turbulence modeling is full of acronyms, the author does his best to reduce them and to recall them, at least for the first use.

On the one hand, steady and unsteady RANS turbulence models are frequently used in nuclear engineering applications as they are more affordable than finer approaches. While looking at the literature, it is obvious that the users are more inclined to use Linear Eddy Viscosity Models (LEVMs), especially stable and widely known/recommended ones such as the Realizable k-ε, the k-ω SST, ... This is legitimate, but are they the best models to be used in NURETH related configurations? Why is our use of RSMs is so marginal? Wall resolved models, often called Low Reynolds Number models (LRN) exist for both Eddy Viscosity Models (EVMs) and RSMs. These models are still rarely used due to their cost. Is it possible today to avoid the use of wall functions/boundary layer modeling, at least in some applications? While performing heat transfer computations, as several computations are done using LEVMs, almost all the contributions use a Simple Gradient Diffusion Hypothesis (SGDH) which utilizes the concept of the turbulent Prandtl number. Limitations of such assumptions will be shown later. Is the concept of wall functions/modeling really avoidable, in particular for large computational domains or very high Reynolds numbers? One can find several contributions using an Unsteady RANS when LES is difficult to carry out or unaffordable and when quantifying the unsteadiness is needed such as in Fluid Structure Interaction or thermal fatigue issues. Is the spectral content of a URANS computation always meaningful?

On the other hand, LES is becoming more and more utilized thanks to the growth of High Performance Computing (HPC) resources (speed, memory, storage). The present article focuses on standard use of LES using sub-grid scale eddy viscosity concept as it is the one widely used in industry. What are the space discretization criteria that make us confident in a LES simulation? Due to standard limitations in computational resources, wall modeled LES using wall functions or even hybrid RANS/LES approaches are still the solution to tackle high Reynolds numbers. Is this approach realistic?

Finally, few words are said about HPC projections in the near future as this is one of the major evolutions that one may expect, in particular for LES.

2 (U)RANS APPROACHES

2.1 Regarding the Use of LEVMs vs. RSMs

Linear Eddy Viscosity Models might be very useful, even combined with wall functions, in order to obtain reliable global quantities such as pressure drops, mass flow rates, averaged Nusselt numbers... Many examples exist in the literature showing that these approaches are sufficient to reasonably predict these kinds of quantities, or even more local ones, such as mean velocity or mean temperature profiles.
[2] and the related special session in NURETH 16 give an overview of a benchmark organized by EPRI where several models have been used to predict the flow through a fuel assembly. LEVMs seem sufficient to predict the pressure drop through a grid with mixing vanes (see [3]). However, [4] shows that the utilized RSM (SSG [5] model), on the same configuration, is very sensitive to the discretization scheme and produces good results with an accurate numerical scheme. Thus, the RSMs are much more sensitive to the discretization errors than the EVMs and should be used with special care. One can find in the literature conclusions such as "The Reynolds Stress Model gives poor results compared to the k-ε"! As the latter is just the trace of the first one, this is not intellectually speaking satisfactory. Something must be wrong with the use of the model (numerical approach, inlet boundary conditions ...).
Furthermore, many of those using RSMs in the literature rarely give details about the specific model used. One may find sentences such as "The RSM has been tested ...". On the contrary, when they use an EVM, the precise version of the model is given; standard k-ε [6], Realizable k-ε [7], k-ω SST [8]... There are several RSMs in the literature; among them the LRR [9] and the SSG [5], with several variants that may affect the constants or some terms in the Reynolds stresses and dissipation equations (see [10]). There are also numerous test cases and publications and even a whole book [11] demonstrating the necessity of resorting to RSMs when body forces (buoyancy, rotation, swirl) induce specific anisotropy to the stress

which is then no longer aligned on the mean velocity gradient. These remarks show that, on the one hand, RSMs (or users of RSMs) are probably not mature enough in an industrial context and, on the other hand, they need to be used more often in order to obtain a wealth of feedback similar to the one existing for EVMs.

[12] focuses on the importance of turbulence modeling to predict swirling flows. The case shown in Figure 1 clearly emphasizes the inability of EVMs, even advanced ones such as the v^2f (here the $\varphi = v^2/f$ - model introduced by [13]), to predict the circumferential flow in a vortex tube. The test-case is taken from Escudier et al. [14] (see Figure 1 top). The swirl is globally created in the large cylinder then goes inside the small one. Even at high small to large tube diameter ratios, EVMs are unable to correctly predict the flow structure (see Figure 1 bottom). However, the Reynolds Stress Model (SSG model here) and the LES predict the flow rather well. Note that for small diameter ratios, only LES is able to predict the vortex breakdown phenomenon which appears. The ability of LES to predict such flows has been already shown by Derksen [15] and is confirmed here. This kind of example shows that when rotating or secondary flows play a major role, such as the flow through mixing grids or in the hot legs of a PWR upper plenum, a second moment closure (RSM) should be used by default in order to capture the anisotropy of turbulence and, hence, obtain satisfactory local quantities.
A last argument used sometimes to justify the use of an EVM instead of a RSM is the cost of this latter. As for incompressible solvers, the pressure correction step in much more expensive than solving transport equations, this is in the author's opinion an argument out of date.

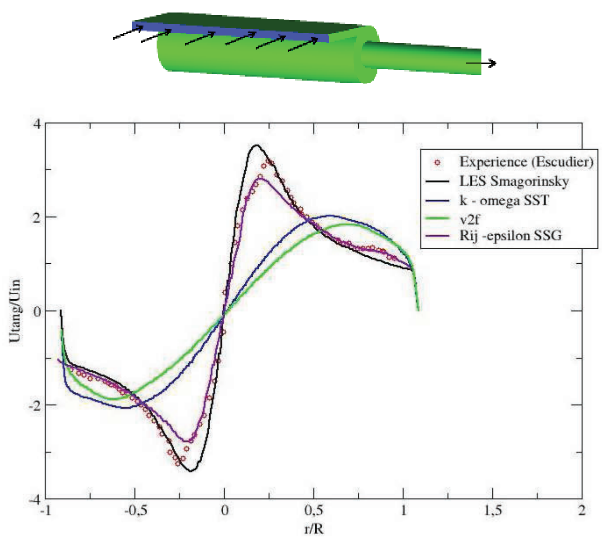

Figure 1. Top: Confined Vortex Tube Geometry, bottom: Tangential velocity in the large pipe.

2.2 Wall Resolved vs. Wall Modeled RANS Approaches

Using a wall resolved RANS model (often called in specialized literature Low Reynolds Number (LRN) models) is obviously better than using a wall modeled one. If one uses the same wall resolved RANS model (such as the k-ω SST, the k-ε from Launder and Sharma [16], the v^2f [17] or one of its more robust versions), as a basis, one can't expect obtaining better results with a wall model either with an algebraic approach (so called "wall functions" approach [18]) or even with a numerical one (solving 1D differential equations at the near wall cell [19]). Thus, when it is possible, the calculation should be done with a wall resolved model, fulfilling the requirement $y^+<1$ everywhere, where y^+ is the non-dimensional distance to the wall of the first computational cell based on the friction velocity and the kinematic viscosity. Of course, a grid refinement study has to carried out in order to obtain a numerically convergent result. This is possible if the Reynolds number is moderate to high (depending on the definition of the Reynolds number, this gives Reynolds numbers going from 10^4 to 10^7).

However, even if the case can be, theoretically speaking, computed using a wall resolved RANS model, the complexity of the geometry may lead, depending on the meshing strategy, to regions where it is impossible to refine and thus which need a wall treatment. Solutions to mix wall resolved and wall modeled regions, called "adaptive wall treatment" in a single mesh are being developed [20]. A mesh cut downstream a mixing grid in a fuel assembly is shown in Figure 2. The meshing strategy uses here a block-structured method. One can see the trace of the dimples and springs and the variations in the refinement obtained around a rod. This shows the importance of developing adaptive wall treatments, either with wall functions or a 1D numerical approaches, departing from a wall resolved model; see two other examples in [21] and [22] departing from an EVM and a RSM, respectively.

Wall modeled approaches might give satisfactory results in some configurations, in particular for predicting global quantities. This is not always true, that is why a grid sensitivity study is recommended whenever one uses this kind of approaches. An example is given in Figure 3. Several computations (not all shown here but the reader can refer to [23] and [24]) have been performed for the flow through a square edged orifice plate at a Reynolds number equal to 25 000, based on the bulk velocity in the upstream pipe. The target value is either the discharge coefficient or the pressure loss through the contraction. Both values exhibit the same behavior. Figure 3 shows the pressure loss coefficient measured 2 D upstream of the centre of the orifice plate and 6 D downstream. EVMs, not shown here, exhibit similar mesh sensitivity as the wall modeled RSM utilized here (the SSG of [5]). The ISO correlation estimate represented in the figure gives an idea of the target value (however, only the behavior of the numerical results is important here). The present wall resolved RANS approach uses the Elliptic Blending (EB) concept [25] with SSG Reynolds Stress Model (note that the same concept exists for EVMs, see [26]). This model is inspired from elliptic relaxation for the six components of the Reynolds stresses but using only one elliptic equation to model the wall damping instead of six, one for each Reynolds stress as initially suggested in [27]. The wall modeled RSM is based on the SSG approach with standard wall functions. Figure 3 shows the pressure loss across the orifice as a function of the refinement. Note here that the characteristic mesh size in the abscissa is representative of the stream-wise refinement and is not the wall normal one. Two different meshes are used for the wall modeled approach. For the coarsest refinement of Mesh2, the non-dimensional wall distance y^+ is approximately 55 upstream of the orifice and increases up to $y^+\approx150$ where the flow reattaches. For the finest refinement of Mesh2, $y^+\approx22$ upstream of the orifice and $y^+\approx60$ where the flow reattaches. The non-dimensional wall distances for the refinements of Mesh1 lie within the range of those of Mesh2. The corresponding values for the coarsest mesh of the wall resolved model are $y+\approx 1$ upstream of the orifice and $\mathrm{y}+\approx 2$ where the flow reattaches. The refinement ratio between two successive meshes is 1.3 and is applied equally in the stream-wise, radial and azimuthal directions. More details are available in [23]. As one can notice, the wall resolved model results are grid independent, whereas wall modeled approach based on the same homogeneous model (SSG model far from the walls), exhibits a strong sensitivity to the mesh refinement. In the present case, if one uses intermediate refinements (corresponding here to y^+ around 40 in the upstream pipe), the results seem very accurate but this is obtained by chance. Only the wall modeled approach based on an advanced concept such as the elliptic blending is able to predict a pressure drop not very sensitive to the mesh refinement and within 5% of the ISO correlation value (this one is confirmed by a wall resolved LES [24].

The last examples show the systematic and logical superiority of wall resolved or Low Reynolds Numbers approaches compared to wall modeling ones (algebraic or numerical wall treatment). However, wall resolved approaches will remain impossible for decades to use systematically either for very large computational domains (a whole nuclear vessel for example) or for very large Reynolds numbers (such as in the hot legs of a 1300 MWe where the Reynolds number is of the order of 10^8). In these cases, the use of specific near wall treatments will remain mandatory for many years.

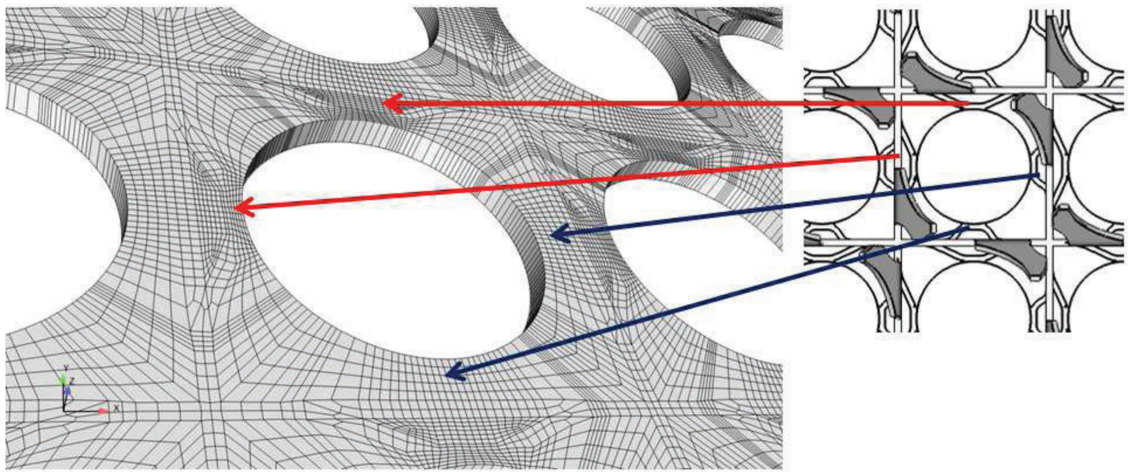

Figure 2. Mesh cut downstream a grid with mixing vanes.

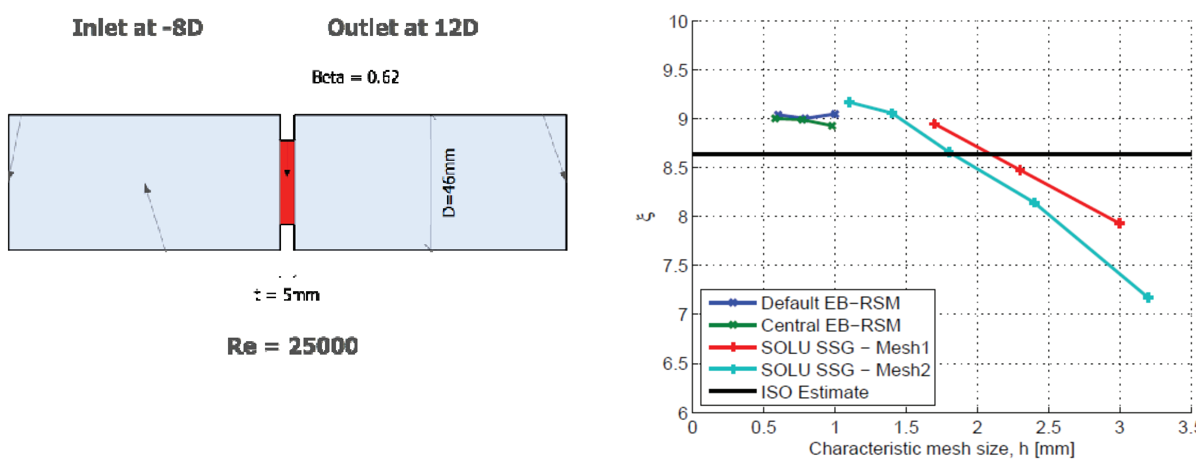

Figure 3. Left: Computational domain for the square edged circular orifice plate, Right: Pressure loss across the orifice versus mesh refinement.

2.3 Heat Transfer Predictions with RANS Approaches

2.3.1 With Eddy Viscosity Models

As a majority of industrial contributions still use EVMs and particularly, LEVMs, one starts by these models. It is impressive to see the number of users who still utilize the Simple Gradient Diffusion Hypothesis (SGDH) approach even with buoyancy effects. It is possible with an EVM to increase models' capabilities by introducing more sophisticated models [28] such as the Generalized Gradient Diffusion Hypothesis (GGDH), the AFM (Algebraic Flux Model) which can take into account buoyancy effects, or even more advanced models based on transport equations for the turbulent heat fluxes. The little interest for modeling the turbulent heat fluxes has several reasons. First, the lack of experimental or Direct Numerical Simulation data compared to the ones available for the dynamics. The lack of experimental data can be explained by the difficulties one may face to carry out such experiments and the inherent financial cost. Some valuable DNS data have been made available for turbulent flows with heat transfer ([29], [30] among others) but much more efforts are still needed in particular for conjugate heat transfer cases. For the latter, DNS data is rare, with the exception of [31] and the ongoing work [32], whereas with current DNS codes and resources, the scientific community could easily be more prolific in this area.

The next example is often studied as coolant flows in the cores of current gas-cooled nuclear reactors which contain ascending vertical flows in a large number of parallel passages [33]. The flow going upwards in a vertical heated pipe is the analogous academic test case. The flow properties are considered constant and the Boussinesq approximation is used. While increasing buoyancy, the flow experiences a re-laminarization. This transition, which may occur in other situations and which dramatically affects heat transfer, may be found in other industrial configurations. Both [34] and [33] studied this flow with EVMs and Figure 4 gives a fair illustration of the results. They concluded that several EVMs fail in predicting the mixed convection regime. One may notice in particular that the widely used k-ω SST exhibits good results for low and high buoyancy parameter values but totally fails in predicting the transitional regime. Note that the computations have been carried out with two different codes (see Figure 4). More recent models such as the ones based on elliptic relaxation concepts tend to better predict such flows as they include wall normal velocity and turbulent length-scale characteristics (φ=v^2/f model results in [33]). Introducing more physics in the EVMs seems then necessary to better predict heat transfer phenomena.

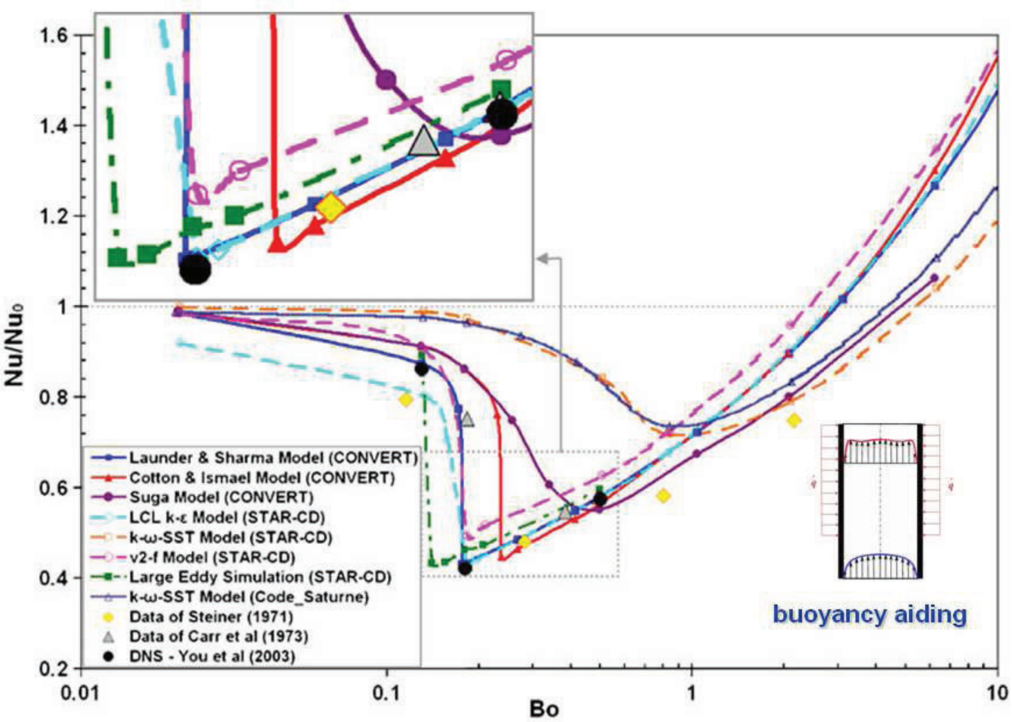

Figure 4. Ratio of mixed-to-forced convection Nusselt number as a function of the buoyancy parameter by several RANS models, LES and DNS for an ascending mixed convection flow [33].

2.3.2 Going beyond Eddy Viscosity Models

Another way to enrich the physics is to use a RSM combined with an advanced treatment for the turbulent heat fluxes using at least an AFM or if possible a Differential Flux Model (see [35] among others) in which transport equations are solved for the turbulent fluxes. Several authors already introduced these approaches but these are still far from mainstream. Recently [36] used the AFM in conjunction with the EB-RSM (Elliptic Blending-Reynolds Stress Model). Figure 5 shows the results obtained for the temperature variance in the turbulent channel flow at a Reynolds number based on the friction velocity of 150 in the forced convection regime (DNS data from [37]). These profiles show a progressive enhancement of the temperature variance as the model is enriched (from SGDH to DFM, then, from EB-GGDH to EB-DFM [38]).

Other more complex flows such as the one in a heated cavity and a PWR upper plenum and its hot legs confirm the need of advanced models, at least algebraic ones.

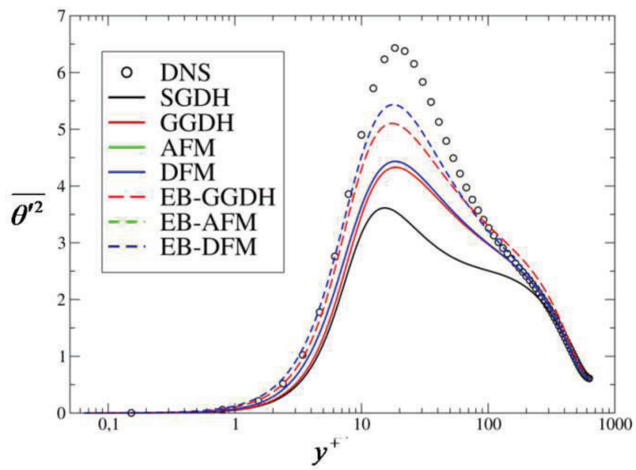

Figure 5. Temperature variance, forced convection, channel flow, Re_τ=640, Pr=0.71, comparisons to DNS data from [37].

2.4 On Unsteady RANS

RANS equations in their unsteady form (so called URANS) are widely used when unsteadiness is needed. Their use in fuel bundle configurations is widespread in particular while aiming at predicting gap instabilities [39], [40]. The approach is attractive since DNS or even LES are still impossible to carry out with standard computational resources at the core Reynolds numbers [41]. First, as it has been reported in [41], one should be very cautious about the interpretation of the regular coherent structures predicted in URANS. The question raised hereafter is about the meaning of unsteadiness with URANS. The following example shows that if one observes unsteadiness with URANS on a given mesh, it might disappear while refining the mesh and in this case what started out as URANS ends up as a steady state RANS. Of course, the instability of the following case has nothing to do with gap instability but shows that a popular case which has been considered for a long time as a URANS case, in particular with RSMs, is actually a RANS one and no unsteadiness should be expected. [42] computed the 2D backward facing step flow and proved that the unsteadiness of the vortex shedding decreases while refining the mesh by using a wall resolved RSM. They also showed that 3D computations give a steady converged solution. Figure 6 shows the maximum value of the ratio resolved energy/total energy as a function of the stream-wise location while progressively refining the mesh (from mesh 7 to 11, mesh 12 giving a steady solution). This example clearly campaigns for verifying the evolution of the resolved energy while performing mesh sensitivity/convergence studies (the latter being a standard requirement for all RANS computations).

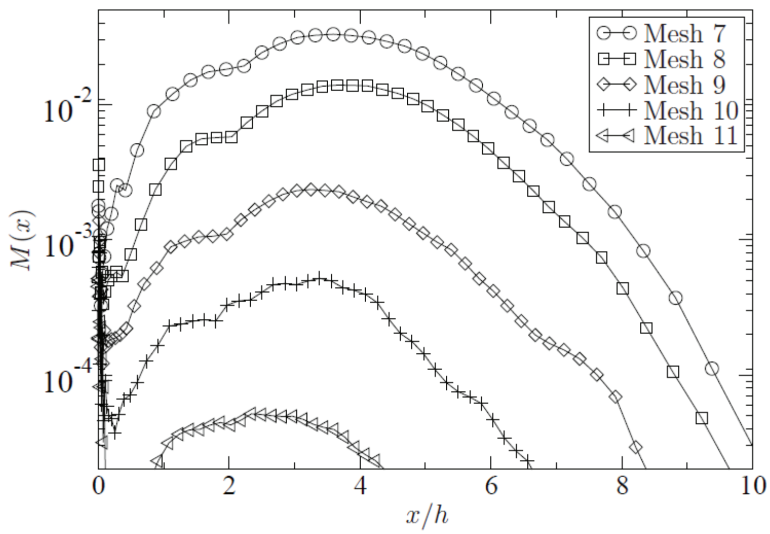

Figure 6. Maximum *resolved energy/total energy* ratio as a function of the stream-wise location for successive mesh refinements. Mesh 12, finest, gives a steady solution. Image taken from [42].

3 LES APPROACHES

3.1 Quasi-DNS and Wall Resolved LES

More and more wall resolved LES are found in the literature (see for example [43]). These computations are sometimes called Quasi-DNS [44] or even DNS [45] providing valuable data, such as Reynolds Stresses budgets or turbulent heat fluxes [46], for RANS modeling. However, in the author's opinion, the nomenclature is not adequate as in numerous examples the discretization is only second order in space or less as sometimes a bounded central differencing scheme is introduced for the convection term. Rhie and Chow interpolation in the pressure correction step is utilized with the collocated arrangement and introduces additional numerical error. These computations should rather be called wall-resolved LES or very fine LES. With the growth of computing power and thanks to advanced numerical techniques, proper DNS computations for complex flows, higher Reynolds numbers and even more complex geometries are today available (see for example [47], [48] among others) and there is a hope that this will continue in the future.

3.2 Wall Resolved LES Space Refinement Requirements

Still several communications dealing with wall resolved LES insist on the refinement in the wall normal direction ($\Delta y^+<1$) but not on the stream-wise and span-wise ones. It is commonly admitted today that for a turbulent channel flow and using a second order discretization scheme, one has to respect the two additional criteria; $\Delta x^+<40$ and $\Delta z^+<20$, where x and z are the stream-wise and span-wise coordinates, respectively. Figure 7 gives an illustration of the results one may obtain while only refining in the wall normal direction without taking care of the other directions (here Δx^+ and Δz^+ go from 100 to 1000). With this computation, the predicted shear stress is too important due to artificial streaks that appear at the wall.

The computation using wall functions (the same refinement in x and z directions) but a first computational point that satisfies $30<\Delta y^{+}<100$ gives better results.

However, the wall refinement is not the only criteria. One has ideally to check whether the computational cells are all in the inertial sub-range, let's say of the order of the Taylor-micro length scale. One may perform a precursor RANS computation which gives of course reasonable results. This computation can give an estimate of the Taylor micro-scale and the LES mesh can then be created (one should take care of locations where the flow exhibits too low turbulent Reynolds numbers). A posteriori checks should also be performed in order to check whether the turbulent kinetic energy is reasonably resolved. [14] showed this kind of a posteriori estimations by computing an estimate of the sub-grid scale dissipation rate and turbulent kinetic energy (see Figure 8). If the estimated sub-grid scale turbulent kinetic energy is everywhere lower than 5% of the total turbulent kinetic energy, one can consider that the Large Eddy Simulation is fine enough.

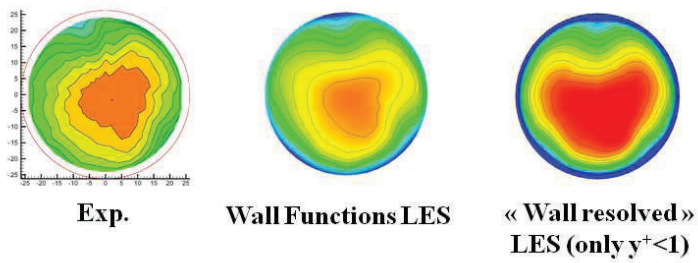

Figure 7. Mean stream-wise velocity component downstream a T-junction.

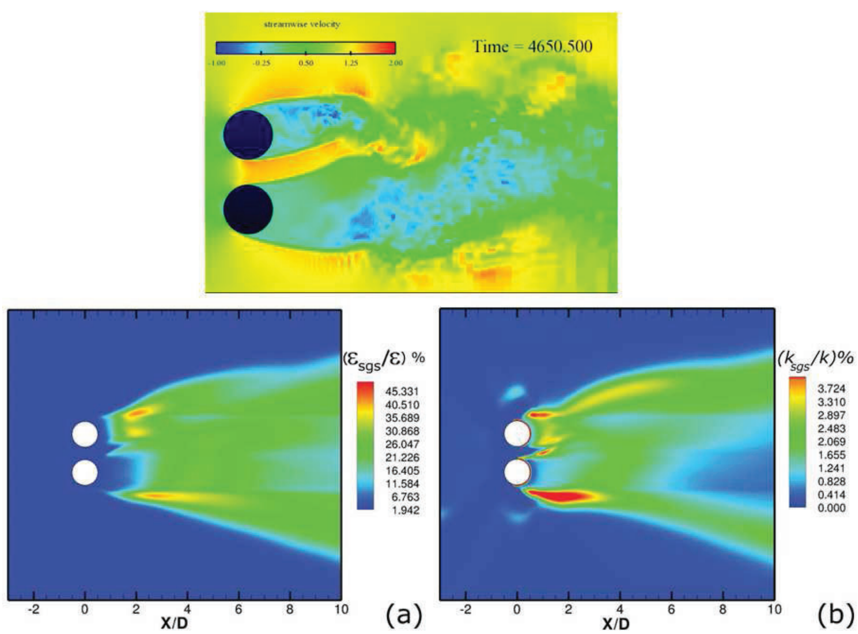

Figure 8. The flow around two side-by-side cylinders at subcritical Reynolds numbers – estimates of the sub-grid scale dissipation rate and sub-grid scale kinetic energy.

3.3 Wall Modeling in LES?

As it has been shown in Figure 7, wall modeled LES might give correct mean values. However, its use is still subject to discussion and objections (see [49]). This approach, which often uses wall functions concepts, is a very first step of hybrid RANS/LES technique (using a log profile for example). Considering the complexity of the flow dynamics in the near wall region, there is rather weak correlation between an instantaneous velocity at a given distance from the wall and the instantaneous shear-stress under it and only long time averaged values are well rendered, by construction. This approach is thus a priori not recommended for unsteady problems such as thermal fatigue or Fluid Structure Interaction.

However, in order to deal with realistic Reynolds numbers, one can test this approach and check whether the low frequencies predicted at the first computational cell are sufficient for the studied problem. Figure 9 gives an example taken from [49] in which the objective is to compute the pressure load along a rod bundle in a typical fuel assembly at Re=40000, based on the hydraulic diameter and the bulk velocity. The pressure load has been used combined to a beam equation to predict the displacements obtained along the central rod and the qualitative results correspond to what is observed in reality (few microns). However, this computation can't be considered as validated and the methodology has to be confronted to experimental data (or why not DNS data with the available computing power today).

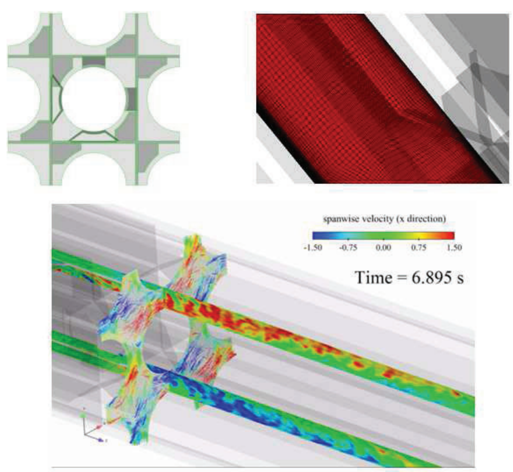

Figure 9. Flow through a mixing grid at Re=40000. Top left: cut of the computational domain (2x2 periodic bundle), top right: hexahedral mesh (8 million cells), bottom: snapshot of the instantaneous cross-stream velocity.

3.3. TOWARDS VERY LARGE COMPUTATIONS?

Several CFD codes are showing very efficient scalability on very large computers, among them: *Code_Saturne* open source EDF CFD tool [51], [51]. This code is based on a collocated finite volume approach. Figure 10 gives a tentative road-map of the computation sizes that would be used (this is valid for both RANS and LES approaches). One should first distinguish between standard computations (or “production computations”) and “Big” computations (could be named “Research computations”). Of course, the objective of these two kinds of simulations is not the same.

Standard computations are today around 10 million cells for a duration of a couple of weeks. Some computations reach the order of 100 million cells in nuclear engineering but are still rare (simulating the whole nuclear vessel for example). The factor that can be gained for this kind of computations in the next five years is not large. A factor of 10 would be very good, considering that standard users will have standard HPC machines with a limited access to the cores and a limited storage memory. It is possible to enhance this projection by enhancing pre and post-processing tools and access to supercomputers.

“Big computations” will probably continue to grow to reach up to few hundred billion cells or even more with durations of few months. Those who carry out these computations have access to exceptional resources and are rather performing computations using LES or DNS on relatively simple geometries.
One should consider also the physical time needed. In the example shown in Figure 9, the physical time needed to obtain an exploitable pressure load led to run the computation over almost one year on a BlueGene/P with 1024 cores (much more time was needed to predict pressure load than statistics). In addition, one of the objectives is to increase the Reynolds number. Let’s take the example of DNS in a homogeneous isotropic turbulence. If the time step is of the order of the Kolmogorov time scale, increasing the turbulent Reynolds number by a factor of 100 will reduced the time step by a factor of 10 which will make the computation naturally longer. This effect should be less dramatic in LES but there will be also an increase of the needed computational time.

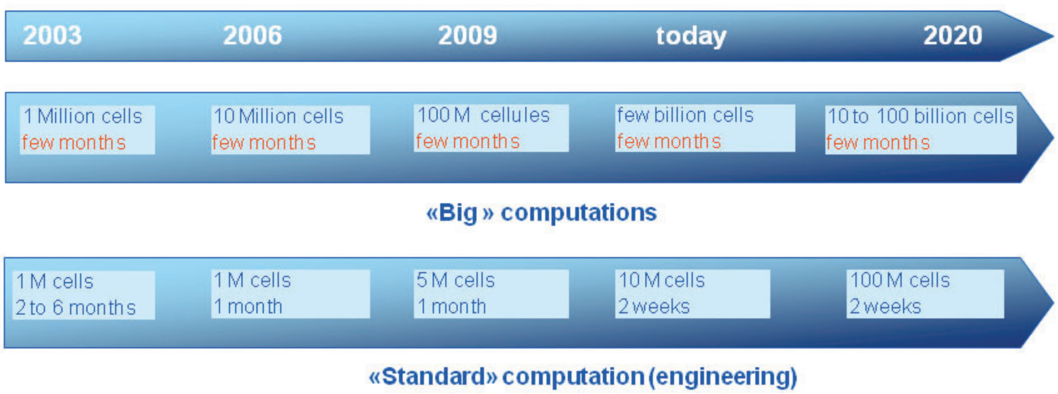

Figure 10. Tentative roadmap of HPC computations using *Code_Saturne*

4 CONCLUSIONS AND PERSPECTIVES

The present paper gives some ideas and guidance one should keep in mind while running (U)RANS or LES computations. Here are the major ones concerning both approaches:

- LEVMs can produce satisfactory results in particular while dealing with global quantities,
- If the flow exhibits anisotropic turbulence due to rotating or secondary flows, one should rather use a RSM, in particular to obtain local quantities,
- Wall resolved RANS simulations are clearly superior to wall modeled ones,
- Predicted unsteadiness from (U)RANS simulations should be treated with caution as they might be highly dependent on numerical parameters.,
- Wall refinement is not the only important issue for a wall resolved LES, the cell sizes far from the wall should be small enough to be in the inertial zone and some a posterior tests can be performed to check the quality of the computation,

Some perspective can be also drawn:

- RSMs and advanced models for turbulent heat fluxes still need much more development, feedback and dissemination,
- Adaptive wall treatment for RANS in order to deal with very large Reynolds numbers can replace more standard approaches,
- More DNS and very fine LES should be carried out in the future, in particular on complex geometries, to contribute to fluid flow understanding and to (U)RANS validation,
- Wall modeling in LES will remain questionable,
- The physical time needed for DNS and LES will increase in the future leading to longer computations,
- More efforts (pre-post processing, access to bigger resources) need to be made to increase the size of "standard" computations.

5 ACKNOWLEDGMENTS

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