

VERIFICATION AND VALIDATION CONSIDERATIONS REGARDING THE QUALIFICATION OF NUMERICAL SCHEMES FOR LES FOR DILUTION PROBLEMS

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Abstract

The Large Eddy Simulation (LES) concept is, since a long time, considered as a very promising candidate for “advanced thermalhydraulic modelling”. However, limited CPU resources and very long related elapsed time have restricted its extensive use for industrial purposes in general and for Nuclear Reactor Safety (NRS) issues. The increased CPU resources have significantly improved its potential. The picture today is that, even if some particular turbulent flows (for examples high Reynolds number near wall dominated flows) still compel to mix the LES approaches with other approaches derived from Reynolds Average (RANS) models, “perhaps the most compelling case for LES can be made for momentum, heat and mass transfer in free shear flows at high Reynolds numbers” (from Pope (2004)). Under these basic conditions there are strong suggestions to make use of LES for dilution problems. Extensive verification and validation attempts towards this objective as well as for industrial applications (Bieder et al. (2006 and 2007)) have already been performed for the Trio_U¹ code. This paper proposes a short overview of what has been done, what can be related to the so-called Best Practice Guidelines (BPG (2007)) in this work and tends to answer specific issues of the LES validation for dilution issues.

1 INTRODUCTION

The modelling issues coming along with the use and the validation of LES for Boron dilution problems are numerous and cannot be totally treated through this paper. We therefore have focused on the test and selection of the convection scheme. The results of a LES are known to be very sensitive to this parameter and the Boron concentration calculated at the core inlet is mainly the result of the Boron convection and the related turbulent diffusion.

The selection of the numerical scheme is part of the numerous recommendations coming along with the use of LES for simulation on NRS issues (BPG (2007)). “Low diffusive schemes” are said to be mandatory for LES of turbulent flows since upwinding compromises accuracy (Garnier et al. (1999) as well as Mittal and Moin (1997)) in the meaning that the numerical dissipation may spuriously interact and eventually hide the molecular and sub-grid viscosity effects. Some works associate this property with the search for quadratic quantities conservation at a discrete level which is an interesting property as far as the kinetic energy conservation is concerned (see Ducros et al. (2000) for schemes related to structured meshes and Mahesh et al. (2004) for unstructured meshes). However, models based on numerical dissipation coming along with upwinding are very attractive to use since they may behave well and are already available in all CFD codes: this approach refers to Monotonic Integrated Large Eddy Simulation (MILES, see: Fureby et al.(2005)). The use of such schemes may show robustness advantages but there seems to be a large consensus to prefer the previous mentioned low dissipative schemes when there are available.

Recent works focus on the treatment of scalar advection and suggest that the best compromise for LES is to make use of centred schemes for momentum transport and high order regularizing schemes for scalar transport (see: Chatelain et al. (2004)) for a proposal for structured meshes). Among the

¹ <http://www-trio-u.cea.fr>

reported reasons for this choice are the previous kinetic energy conservation for the momentum equation and the search for a compromise between the required positivity of the convection scheme for the scalar, which is mandatory to keep the scalar between physical bounds and the fact that a too large numerical diffusion may, as for the momentum, spuriously interact with the turbulent diffusion at the cut of level. We also have to bear in mind that it is the scalar extremum (in fact the minimum Boron concentration) that is scrutinized at the core inlet in the particular case of the Boron dilution problem. A particular attention has therefore to be paid to the meaning of “extrema” in the LES framework and what are the main sensitive parameters that influence directly these values.

In addition, using CFD for industrial purposes leads to the treatment of arbitrary complex geometries, what generally requires the use of unstructured meshes. Logically, the verification and validation (V&V) processes should be conducted in the spirit that the used mesh should exhibit the same features as the ones encountered in the eventual applications. This means that V & V tests should in particular take into account strong meshing anisotropy and cell size variations if such events are to be part of the industrial model application.

After a brief recall of LES features, the paper gives a short overview of what has been done for the validation of the LES scheme of the Trio_U code for free shear flows and summarises an application of LES for dilution problems. A short analysis of what can be seen as conform to the BPG, as well as what can be pointed out as non-conform is proposed. Some related questions are then addressed and discussed:

- What is the meaning of a filtered minimum value in the LES framework?
- Is it possible to define a “BPG” to approve a numerical scheme?
- How is the choice of a given mesh and discretisation element determinant for the simulation result?

The paper finally concludes with some recommendations which are based on the posed questions.

2 SELECTED LES FEATURES WHICH ARE IMPORTANT FOR DILUTION MODELLING

The first question, as also posed in Pope (2004), is: “Is LES the right approach?” In accordance with Pope, we are convinced that considering the whole spectra of turbulent flows, it is now valuable to have a large range of approaches to study turbulent flows and therefore that there are models “adapted to given issues”. However, there is a larger and larger successful field of LES applications, mainly due to the increasing power of computers and the ongoing work of scientific community.

So let’s first stress some advantages brought up with the LES underlying concepts. To simplify, one has to consider the result of any LES on a mesh of local size h as the filtered counterpart \overline{u}_i at a filter scale Δ of the full resolved field u_i . The basic decomposition coming along reads $u_i = \overline{u}_i + u_i^{sgs}$ where the filtered field may be considered as resulting from a convolution product on u_i : Sagaut (2003). The range of motion scales of size above the filter size is explicitly resolved. The influence of the unresolved scales on the resolved ones is modelled either through the application of SubGrid Scale (SGS) eddy viscosity models or through numerical treatments, or by a combination of both. This leads to potentially consider Δ as different from h . The topic of the impact of the ratio of Δ/h on the solution is rather complex and, in any case, not solved to date. According to Pope (2004), the global picture now suggests to discard between:

- Pure physical LES (the unresolved motion is explicitly physically modelled with negligible numerical errors),
- Physical LES (the unresolved motion is explicitly physically modelled but where numerical errors are tolerated within the resolved scales) and
- Numerical LES (the description of the resolved field \overline{u}_i depends on the numerical method, which is typically the case of MILES).

Dealing with industrial flows involving complex geometries yields in using most of the time unstructured meshes and numerical schemes of limited order. The treatment of these problems with scheme of limited numerical diffusion generally leads to consider that the resulting effective filter is so that Δ is close to h , i.e. that the resulting LES is close to “physical LES” in the Pope’s classification. Nevertheless, independent of the real classification of the LES approaches, the LES concept leads to some very interesting and common features we recall here:

- In the limiting case when Δ is going to zero, $\overline{u_i}$ represents the complete field u_i . Improved results are thus expected every time the mesh is refined, which tend towards the DNS result for moderate Reynolds number cases.
- Depending of the selected modelling, the influence of the unresolved motion is treated through a mix of physical models and the numerical treatment. These scales are close the homogeneous isotropic turbulence, i.e. statistically isotropic and universal. One can consider the resulting modelling to be universal, which is a clear strength of LES approaches over RANS modelling.

Since the dominant phenomena for Boron dilution events are related to the mixing, where the turbulent transport is directly affected by the large energy containing scales, it is tempting to consider LES as a very promising tool to deal with Dilution issues, provided a proper V & V process is followed.

3 BORON DILUTION TREATED BY LES CALCULATION

In the first CFD4NRS conference, a procedure to qualify the CFD code Trio_U for predictive full scale reactor applications has been presented: Bieder and Graffard (2006). In this case, a plug of pure water is transported into the lower plenum under natural convection conditions. Calculations under nominal conditions are under way. The structures in the lower plenum are shown on Fig. 1 as well as an example of the Boron concentration 80 seconds after the onset of natural convection.

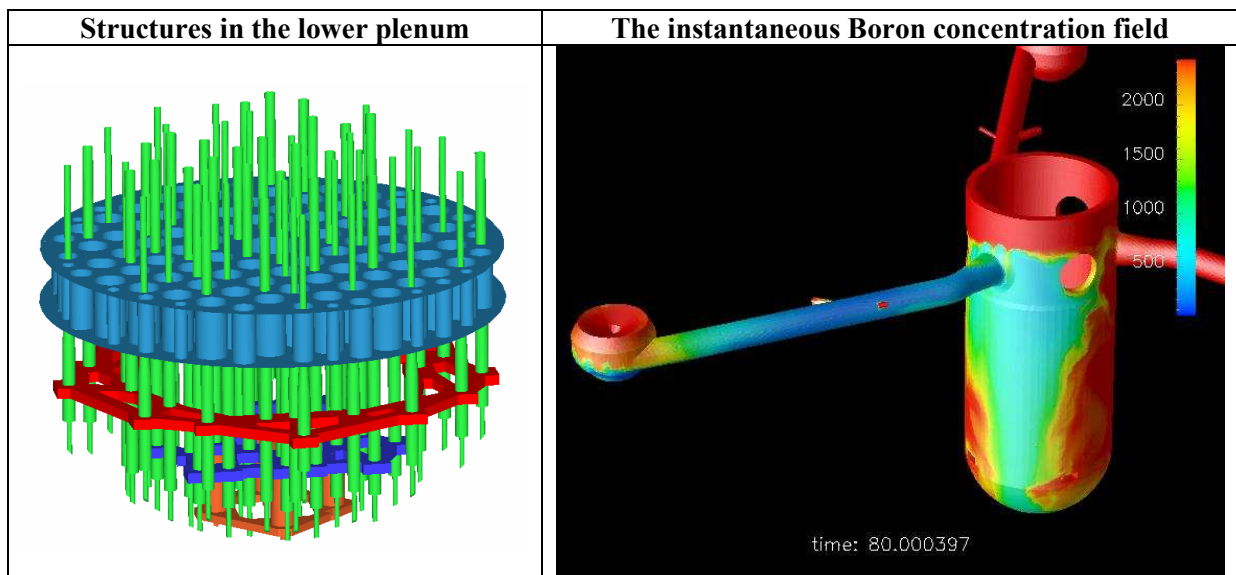


Fig. 1: Structures of the lower plenum and Boron concentration field

Such complex geometry can hardly be discretized on conform hexagonal structured meshes. Thus the numerical schemes of Trio_U are based on tetrahedral meshes. These elements allow avoiding non-conforming meshes and large mesh anisotropies in physically important regions. The corresponding meshing of the lower plenum is given in Fig. 2, where, for nominal mass flow conditions, an example of an instantaneous velocity field in the lower plenum is added (vectors and norm of the velocity in colors)

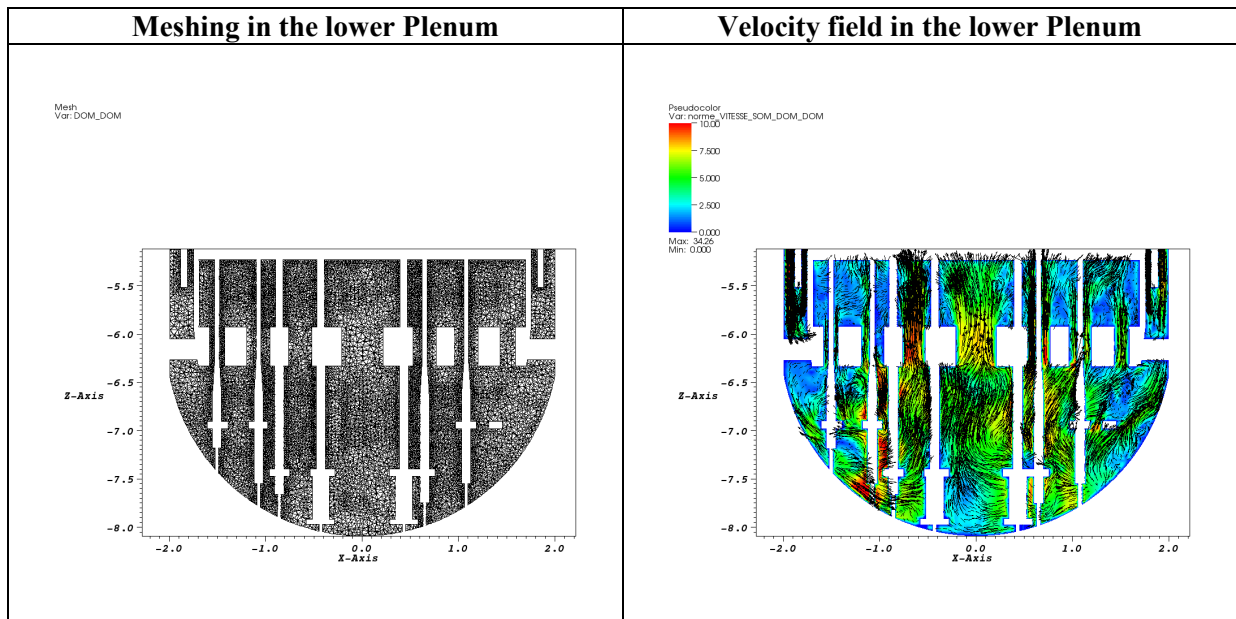


Fig. 2: Example of a tetrahedral meshing and a velocity field in the mover plenum

The qualification of Trio_U for Boron dilution is the third step in a quality assurance procedure which includes the code verification (test of the code on single effect test cases and analytical solutions) and the code validation (integral test of the code on complex experiments including multiple physical phenomena). The qualification is then a test strategy, which guarantees the correct prediction of target quantities for an engineering problem. The flowchart for the qualification of Trio_U for predictive full scale reactor calculations is shown below on Fig. 3. The applicative calculations of the real reactor cases are “limited” to predictivity due to the lack of published data of full scale experiments.

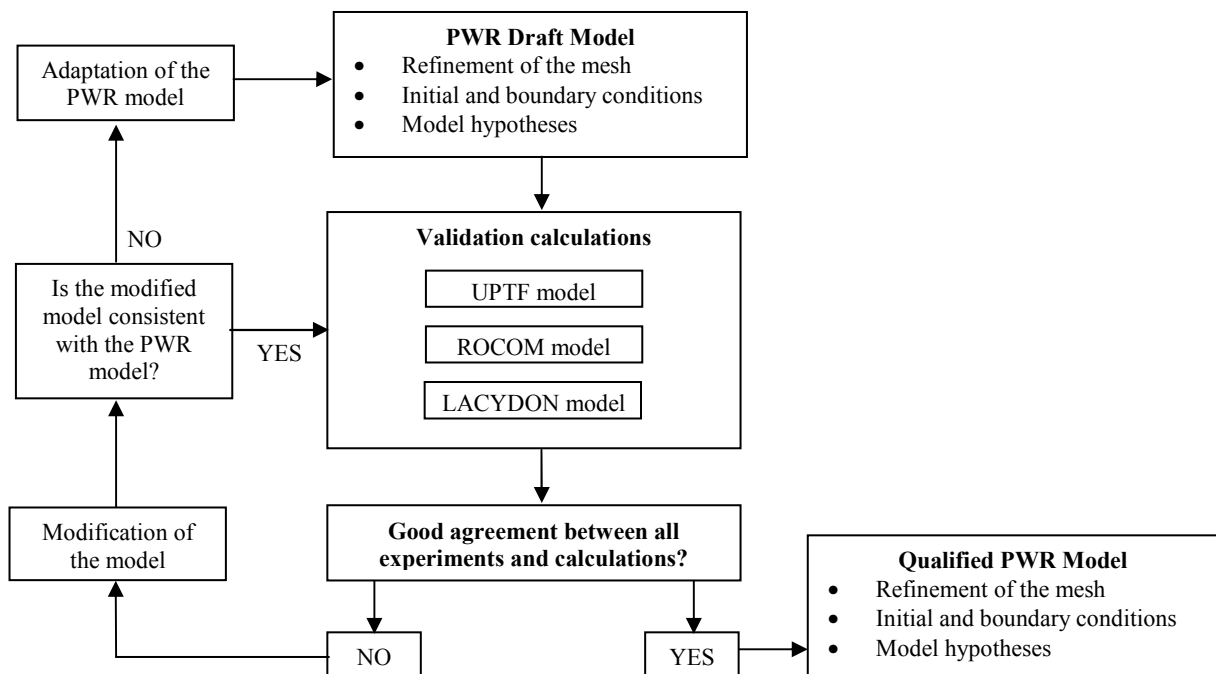


Fig. 3: Flowchart of a procedure to qualify a code for predictive PWR calculations

When following this procedure, it is important to note, that the predictive calculation is based on the same modeling hypothesis as the validation calculations. The validation on UPTF, ROCOM (Höhne et al. (2004)) and LACYDON experiments (Bieder and Graffard (2006)) is performed on integral effects

as the distribution of scalars at the core inlet. In this context, the meshing has been successively refined in order to catch the large scale energy containing scales. Then, the integral results are no more mesh dependent. When looking to the flow field in Fig. 2, these large scales are in the order of 0.2m to 1m, which are well resolved by a meshing with h of about 2cm. However, due to the limitation of the total mesh number, some mixing phenomena must be modeled, as e.g. the mixing in the wake of obstacles, where the scales may be of the order of some cm. The present resolution ensures that the main structures of the flow responsible for mixing are captured by the mesh. Further details on the numerical scheme behavior will show that this description is close to the Pope's "physical LES". These results confirm Pope's intuition (Pope (2004)) for "compelling cases" of momentum driven flows for mixing phenomena. In this case, some Best Practice Guidelines (BPG (2007)) recommendations have been followed:

- Concerning the mesh design: the 3D meshes do not contain large growth factor between adjacent elements and contains a "sufficient" enough number of elements to solve the most kinetic energy containing eddies, while describing the main flow gradients.
- A purely explicit time marching method has been adopted, which guaranty the correct time integration of moving eddies.

However, we have to stress some "distances" with the BPG, as well as some open induced questions which will be discussed.

- What is the knowledge of extrema treatment in the LES framework and what are the most sensitive parameters that are linked with extrema values?
- As previously mentioned, it is said, that LES "should be used in conjunction with non-diffusive high order (energy conserving, centred) schemes for space discretization". The choice is more open for MILES modelling where more numerical diffusion is present. The question is how to qualify a given numerical scheme with respect to these features and should the "good properties" for a scheme be the same for both, momentum and scalar transport?
- The underlying spirit of the BPG leads readers to make use (if possible) of a pure, orthogonal hexahedral mesh (at least to avoid tetrahedral meshes) for both numerical and CPU reasons. What are the consequences of the use of a pure tetrahedral grid?

4 WHAT MEANS A MAXIMUM (OR MINIMUM) VALUE IN THE LES FRAMEWORK AND WHAT IS THEIR RELATION WITH NRS ISSUES?

Let us consider the following scale separation $\phi = \bar{\phi} + \phi^{sgs}$ as resulting from the application of a convolution product on the scalar ϕ . Let's take a scalar field as $\phi(x) = \sin(\omega x)$ and apply a box filter between $[x - \Delta; x + \Delta]$ to evaluate $\bar{\phi}$. The ratio $\bar{\phi}/\phi$ depends on $\sin(\omega\Delta)/\omega\Delta$. Considering a more complex signal containing a range of scales up to the smallest scale η , the dependence of the ratio $\bar{\phi}/\phi$ may be then investigated in terms of η/Δ . Under these conditions, whatever the properties of the numerical scheme are (see below), there would not be any "strict" mesh convergence as long as the global approach links directly the mesh and the filter sizes (i.e. $\Delta = \Delta(h)$). Moreover, a brief analysis of $\bar{\phi}/\phi$ suggests that the maximum and minimum values of $\bar{\phi}$ are all the more "reduced" as the ratio of η/Δ is reduced. Applying this on reactor safety issues means that filtering the continuous field ϕ will result in a field with reduced maxima and minima, what is against any intuitive "conservatism" rules. Beyond this intuitive analysis, the real impact of this potential "biased evaluation of minimum" for NRS should be investigated. Indeed, since local conservation of Boron is ensured by most of the numerical schemes, "local biased minimum values" will end in "little too diffuse concentration defects", which is of no consequences if the size of this "diffused" spot is small enough. However, three types of improvements seem possible:

- A clearer dependency between the extrema of $\bar{\phi}$ and the ratio η/Δ should be investigated. If such a dependency may be modelled, in a form like $\max\|\phi - \bar{\phi}\| \leq fct(\eta/\Delta)$, then the local evaluation of the Kolmogorov's scale η will allow to provide a more precise evaluation of local extrema,
- A local refinement of the mesh in areas where the extrema are expected will reduce their under prediction. Such a refinement is particularly easy to implement when using tetrahedral meshes.
- The modelling should be validated not only against average quantities, but also against extrema.

Nevertheless, whatever the CFD code capabilities are to produce a locally fine mesh or to reconstruct an interval for a given extremum of $\bar{\phi}$, this only makes sense if there is a strong confidence in the original $\bar{\phi}$ value. This partially results from transport capabilities of convection scheme. This will be addressed in the next paragraph.

5 HOW TO DEFINE A “BPG” APPROVED NUMERICAL SCHEME AND WHAT ARE THE LINKS WITH THE NRS ISSUE?

An intend of review of existing LES methods that pay attention to discrete energy conservation for unstructured grid is provided in Mahesh, Constantinescu and Moin (2005), that presents a proposal for such a scheme in the frame of finite volume (FV) methods. The method used in Trio_U relies on a finite volume/finite element (FV/FE) numerical scheme and offer possibilities to switch between pure FE and mixed FE/FV formulations. The variables are computed as a combination of base functions that are assigned to each element, depending on the nodal values: the discretization is based on a staggered positioning: P1-non-conforming for the velocity and P0/P1 for the pressure (Bieder et al. (2007)). This discretization method yields a strong velocity/pressure coupling, while ensuring global conservation of the transported quantities (momentum and scalar in our case). For momentum and scalar transport, the user has the choice between several convection schemes of second order, which go from purely centred, over the “centred stabilized scheme” presented in Kuzmin and Turek (2004) to standard 2nd order upwind scheme of MUSCL type. Details for the numerical methods can be found in Heib (2003).

5.1 The momentum transportation

The kinetic energy conservation at a discrete level can be ensured through the finite element approach, provided that a centred scheme and its antisymmetric counterpart are used.

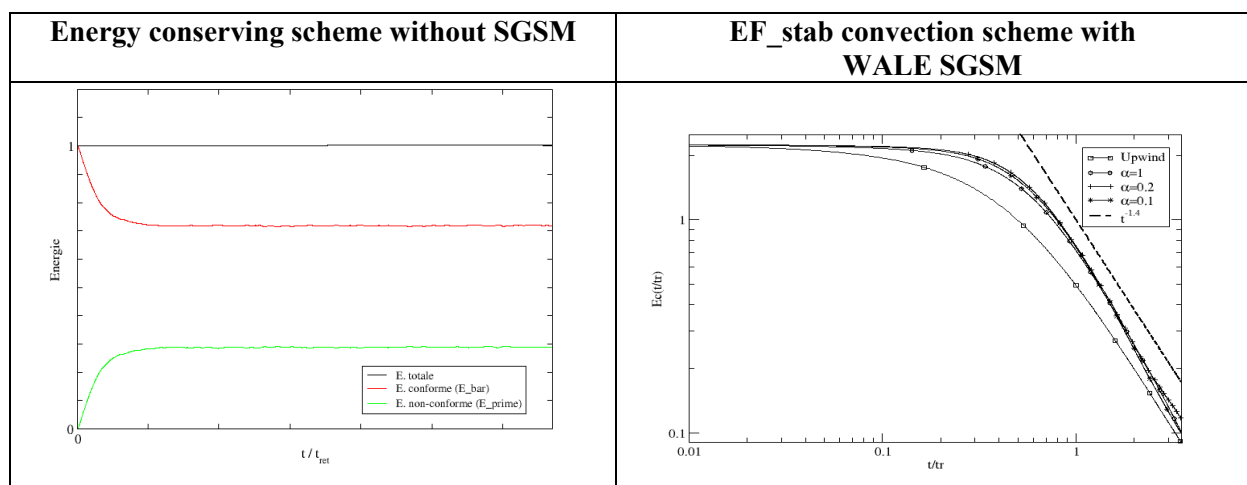


Fig. 4: Kinetic energy time evolution for a free decaying isotropic turbulence

This is shown in Fig. 4 for the case of the computation of a freely decaying isotropic turbulence in a periodic cube of $32*32*32$ hexahedra, where each hexahedron is cut into 6 tetrahedral cells. The simulation is performed without any SGS model (SGSM).

Even if this scheme provides interesting results for configurations close to academic concerns, its use for arbitrary complex geometries of applications in the nuclear field encounters some lack of robustness and, as mentioned above, it is worth to add some stabilizing procedures. Considering the momentum equation

$$\frac{\partial \bar{U}}{\partial t} + \bar{U} \bar{\nabla} \cdot \bar{U} = \bar{\nabla} \cdot (\nu (\bar{\nabla} \bar{U} + \bar{\nabla}^T \bar{U})) - \bar{\nabla} \cdot \left(\frac{P}{\rho} \right) + \beta (T - T_0) \bar{g}, \quad (1)$$

the centred stabilized scheme used in Trio_U to discretize the convection term $[\bar{U} \bar{\nabla} \cdot \bar{U}]$ can be considered as a blending between a purely centred part and a mix of diffusion/anti diffusion terms:

$$[\bar{U} \bar{\nabla} \cdot \bar{U}]_{centred} + \alpha \left[(\Delta \|\bar{U}\|) \bar{\nabla} \cdot (\bar{\nabla} \bar{U}) \right]_{diffusion} + SL(\bar{U}) (\Delta \|\bar{U}\|) \bar{\nabla} \cdot (\bar{\nabla} \bar{U})_{antidiffusion} \quad (2)$$

The origin of this scheme is discussed in the two papers of Küzmin and Turek (2004). Our formulation (called EF_stab) offers the possibility of combining a centred scheme with the stabilizing effects of upwind decentring, depending on the parameters α et SL:

- If α is zero, a pure centred scheme is activated.
- The slope limiter $SL(\bar{U})$ automatically deactivates the anti-diffusive term what yields an upwind scheme in regions of high gradients. In Trio_U, usually, the SUPERBEE limiter is used.
- The parameter α further weights the reduction of the decentring part of the scheme.

Values of $\alpha = 1.0$; 0.2 and 0.1 have been tested extensively. In order to evaluate the quality of the scheme, let us consider first the kinetic energy time evolution for a free decaying isotropic turbulence in the periodic cube of $32*32*32$ cells hexahedral cells, each cell cut into 6 tetrahedrons. Fig. 4 shows the temporal kinetic energy decrease for several values of α in conjunction with a standard SGSM (WALE model from Nicoud and Ducros (1999)), together with the $t^{-1.4}$ reference slope. As expected, the UPWIND scheme shows a particular trend to dissipate the kinetic energy more than the others, whereas no clear discrepancies can be exhibited for the others. Similar picture (not shown) of a simulation with no SGS model will more or less leads to the same conclusions, suggesting that, once one has injected some non linear stabilizing process in the scheme, the diffusion is enough to extract kinetic energy and acts as a SGS model, at least for this global measure of kinetic energy.

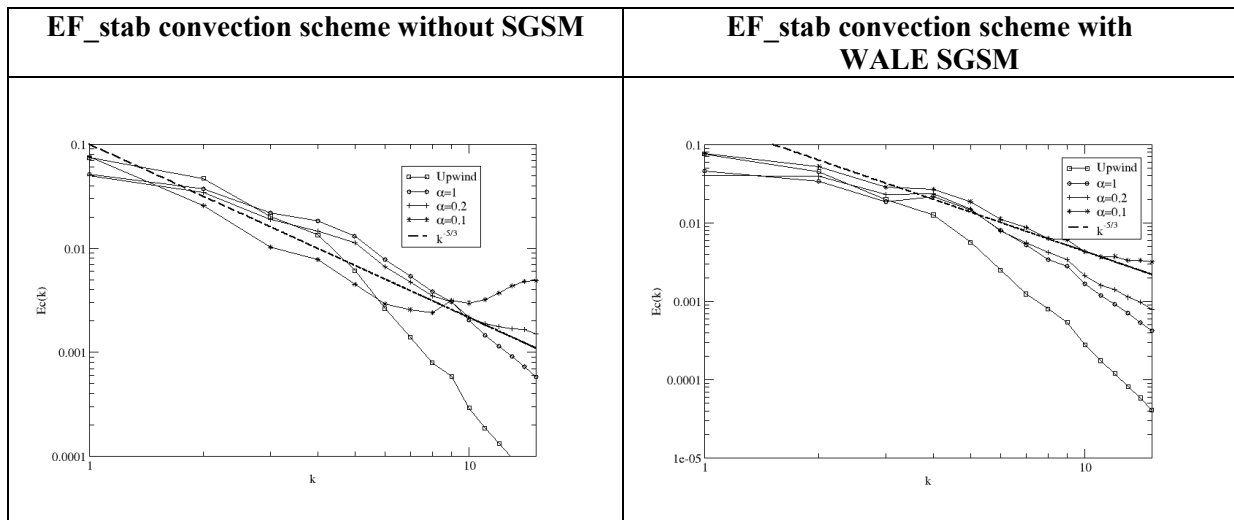


Fig. 5: Kinetic energy spectra after six turn over cycles for a free decaying isotropic turbulence

For a more profound test of the scheme, Fig. 5 shows the kinetic energy spectra at about 6 turns over times for simulations without (left) and with WALE SGS (right), together with the reference $k^{-5/3}$ slope. For low values of α the slope at small scales is controlled by the SGS modelling, the whole modelling assuring the turbulent spectrum to follow a more or less constant slope up to the cut-off scale. This suggests considering Δ/h to be of the order of one. Hence, the whole modelling corresponds to “physical LES” in the Pope’s classification, which is close to an optimal compromise.

5.2 The scalar transportation

The first measure of the quality of a scheme for scalar transport concerns its capacity to fulfil the requirement of physical bounds respect, a property related to the positivity of the scheme. A former publication (Chatelain et al. (2004)) shows that centred schemes were not able to keep the scalar into the physical bounds, even in the case of completely developed turbulence, where sharp gradients are not attended. The paper therefore suggests that a compromise is to be searched for a regularizing scheme that is not too diffusive for the scalar transport. Defining such a compromise for unstructured data is not straightforward, and it can be shown that some reputed TVD schemes exhibit not strictly TVD behaviour when dealing with arbitrary flows on arbitrary mesh. The proposed test consists in the convection of a scalar spot (values between 0 and 1) in the main diagonal of a cube. A perspective view of the meshing as well as a typical result of the scalar concentration is given in Fig. 6 for stationary conditions.

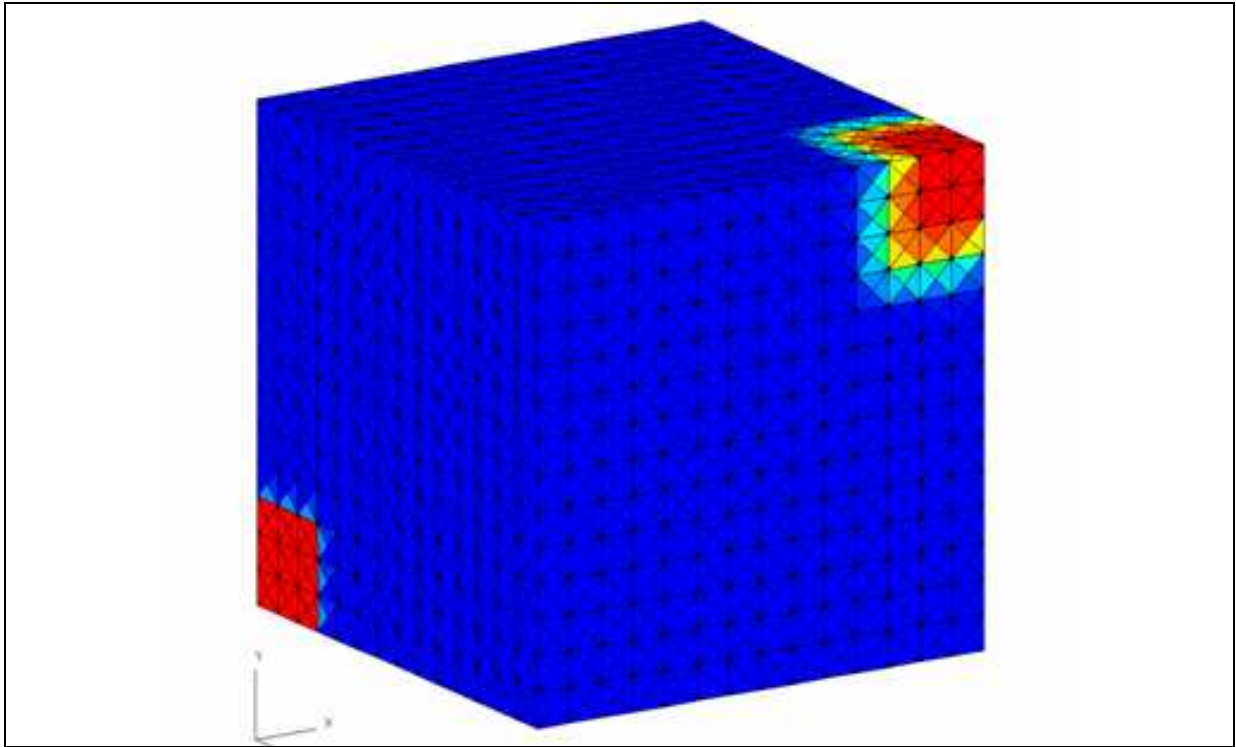


Fig. 6: Transport of a scalar along a cube diagonal.

Three schemes available in Trio_U are compared in Fig. 7, where the concentration fields in the diagonal cut plane are shown. The first order UPWIND scheme is positive but very diffusive. Our implementation of the MUSCL scheme with the limiters “van Leer” and “minmod” (Kuzmin and Turek (2004)) shows limited but reproductive out of bounds values. It should be stressed that other implementations of the same limiters may modify the compromise between “respects of the physical bounds” and “diffusive features” and lead to a strictly positive but more diffusive MUSCL scheme, which confirms a strong dependency on the implemented limiters. The centred stabilized scheme EF_stab with $\alpha=1$ respects the bounds and gives not too diffusive “physically correct” results.

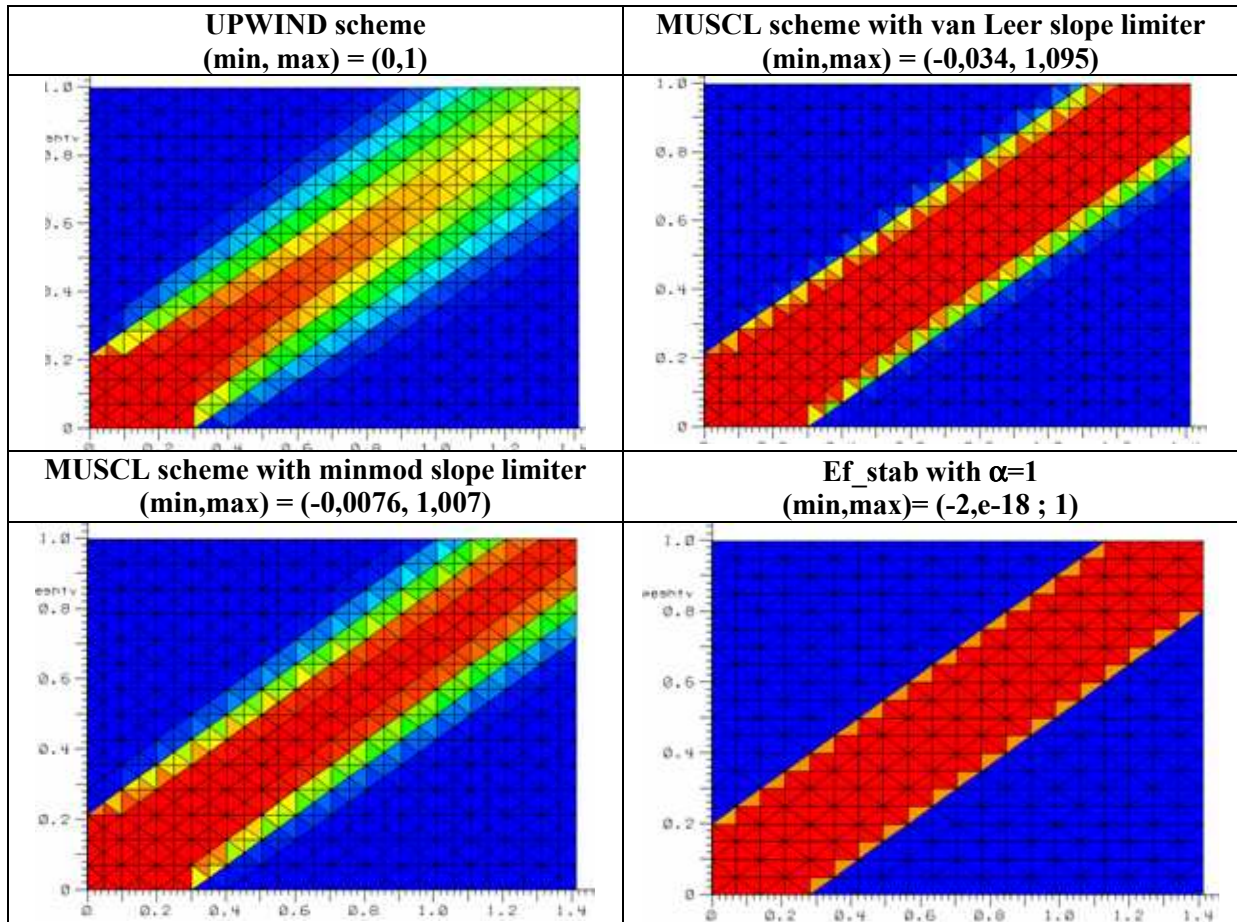


Fig. 7: Transport of a scalar along a cube diagonal (diagonal cut plane)

These transport features have also been tested in the case of the scalar (temperature) transport in a freely decaying isotropic turbulence where the initial conditions consist in a scalar spot that exhibits contact discontinuities. The temporal evolution of the extrema (maximum and minimum temperature) is show on Fig. 8. Overshoots for the MUSCL scheme and high dissipation for the UPWIND scheme are detected.

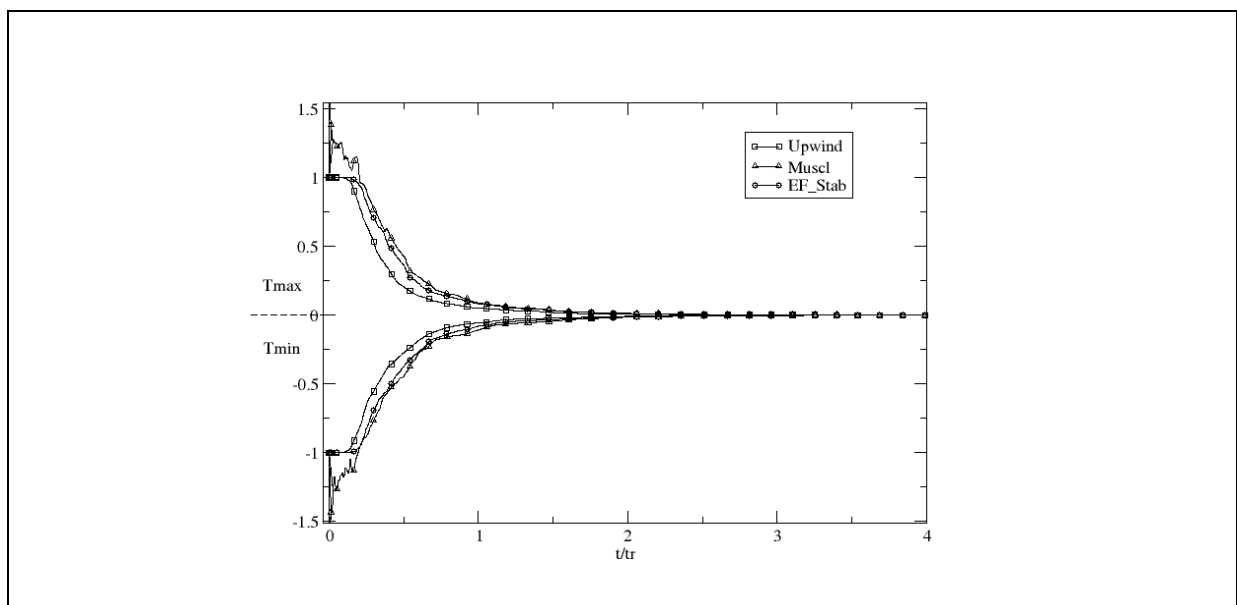


Fig. 8: Time evolution of the scalar extrema during a freely decaying isotropic turbulence

From a NRS point of view, it is clear that the less diffusive scheme that respects physical constraints has to be chosen since the application of too diffusive schemes will reduce the occurrence and intensity of extrema. For the Boron dilution problem this results in an under prediction of the probability of low concentrations concurrency as well as in a poor evaluation of the area with low concentration values.

As a conclusion and regarding the state of the art for LES modelling, our best compromise leads to make use of stabilized scheme for both momentum and scalar convection. For the momentum equation, the stabilizing procedure is tuned so that the global modelling is of “physical LES” according to Pope’s classification, whereas the positivity of the scheme is strictly applied for the scalar transport.

6 HOW TO DECIDE IF TETRAHEDRONS OR HEXAHEDRONS ARE THE BEST CHOICE FOR INDUSTRIAL APPLICATIONS?

The role which plays the local mesh size and the convection scheme on the evaluation of extrema of the field $\bar{\phi}$ has been discussed. Both are related to the used meshing. Generally, Best Practice Guidelines (BPG (2007)) recommend the use (if possible) of a pure, orthogonal hexahedral mesh and at least to avoid tetrahedral meshes. Is this recommendation always a good choice?

Since only tetrahedral meshes have been tested for LES in the Boron dilution problem with Trio_U, there is not enough information to really discard between hexahedral or tetrahedral elements. The flow in the lower plenum of a vessel does not exhibit any main preferential directions and therefore the validation should take this fact into account. We further stress three interesting features coming along with tetrahedral scheme:

- Tetrahedral meshes are much easier to generate. In NRS analysis, often $\frac{3}{4}$ of the required man power is related to mesh generation. A simplification in this field would dramatically reduce the costs for CFD calculations.
- Local mesh refinement techniques can be easily considered in tetrahedral grid. Such a local mesh refinement is necessary for a correct determination of extrema.
- Recent numerical developments as presented in this paper show that good convection schemes are also available for tetrahedral meshes.

7 RECOMMENDATIONS AND CONCLUSIONS

A LES classification in the spirit of Pope (2004) has been recalled. This classification suggests that the optimal LES methodology relies on “physical LES” which supposes a filter to local mesh element size of about 1. Before applying such an LES on an industrial basis, we propose simple tests to check the behaviour of the used LES modelling and suggest for these applications the acceptance of little amount of numerical stabilization. The proposed test simulates the freely decaying isotropic turbulence in a periodic box

For the scalar transport we first have underlined the role played by the LES filter of the extrema of a LES field. We then have focused on the scalar transport scheme features to underline the difficulty to get a real 3D TVD scheme for arbitrary tetrahedral mesh with little dissipative features. We have proposed such a scheme and show that the modelling results from a compromise between “numerical diffusion” and “respects of physical bounds”. We have proposed to measure this compromise with tests against an isotropic freely decaying turbulence including passive scalar transport, and against more standard scalar spot transport cases in non trivial mesh directions.

As stressed in the BPG (2007), mesh convergence can not be followed in general for LES. In practice this means that we are satisfied with the convergence to DNS that comes along with “physical LES” as define here. Even if this can be seen as an acceptable LES feature with regards to resolved variables when looking at their average values (for variables as well as for higher moments), it should be looked with care to the convergence to scalar extrema.

The use of tetrahedral element is presented here as a clear advantage in terms of meshing capability. The numerical scheme is of FE type, which does not lead to compel with orthogonality constraints concerning grid angles. Under these conditions and considering the present qualification, using this

type of scheme and modelling leads to the conclusion that there are no real reasons to prefer other types of elements for this application.

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