

Assessment of Advanced SGS Models for LES Analysis of ICE Wall-Bounded Flows - Part I: Basic Test Case

Cristian Catellani, Gian Marco Bianchi, Stefania Falfari, Giulio Cazzoli, and Claudio Forte
University of Bologna

ABSTRACT

Large Eddy Simulation (LES) represents nowadays one of the most promising techniques for the evaluation of the dynamics and evolution of turbulent structures characterizing internal combustion engines (ICE). In the present paper, subdivided into two parts, the capabilities of the open-source CFD code *OpenFOAM*® v2.3.0 are assessed in order to evaluate its suitability for engine cold flow LES analyses. Firstly, the code dissipative attitude is evaluated through an inviscid vortex convection test to ensure that the levels of numerical dissipation are compatible with LES needs. Quality and completeness estimators for LES simulations are then proposed. In particular the Pope M parameter is used as a LES completeness indicator while the LSR parameter provides useful insights for calibrating the grid density. Other parameters such as the two-grid LES_{IQ} index are also discussed. Then advanced SGS models such as the dynamic WALE and the Sigma models are compared with models traditionally used for LES simulations of ICE wall-bounded flows, i.e. the dynamic Smagorinsky and the WALE models. The proposed SGS models have been implemented in the open-source CFD code *OpenFOAM*®, extending its standard capabilities. Validation of the implemented models has been performed using two different test cases: the Dellenback abrupt expansion, which is presented in part I, and the Thobois stationary flow bench, presented in part II. The results have been evaluated through comparison with experimental data and the completeness of the LES simulations has been assessed using the aforementioned quality estimators.

CITATION: Catellani, C., Bianchi, G., Falfari, S., Cazzoli, G. et al., "Assessment of Advanced SGS Models for LES Analysis of ICE Wall-Bounded Flows - Part I: Basic Test Case," *SAE Int. J. Engines* 9(1):2016, doi:10.4271/2016-01-9041.

INTRODUCTION

It is nowadays agreed that LES models will be the next generation of turbulence models for several CFD applications. This is particularly true in the field of ICE where the traditional RANS is the actual standard approach. In fact, one of the major issues with RANS modeling is its intrinsic inability to predict the unsteady flow structures characterizing ICE flows and which strongly affects complex phenomena like fuel-air mixing and cycle-to-cycle engine variability. With the advent of new engine concepts like GDI, HCCI etc. and with the continuously increasing severity of the legislation regarding pollutant emission limitations and engine efficiency, the adoption of more accurate predictive models is not an option anymore and here is where LES could make the difference over RANS.

In the RANS approach the Navier-Stokes equations are time averaged, therefore losing details on the flow turbulent fluctuations. In the LES methodology the aforementioned equations are filtered in space, directly resolving the larger scales of motion, while the smaller scales are modeled through Sub-Grid Scale (SGS) models. In this way LES provides a more physical representation of the turbulent structures being capable of reproducing the most of the unsteady flow features characterizing turbulent flows.

The continuous increase in computing power availability of the last decades has contributed to the growing interest in LES technique despite its huge computational demands when compared to RANS. This is true not only for academic research but also for industry, where LES could be a promising investigation tool for several engineering applications, amongst which ICE configurations.

The first LES applications to ICE flows dealt with simple stationary configurations: in [1] and [2] Thobois performed a systematic assessment of the LES methodology applied to a steady flow bench. The same case has been later analyzed by Brusiani [3]-[4] and Piscaglia [5], focusing on the assessment of LES quality. In [6] and [7] Keskinen tackled more realistic engine configurations demonstrating the capabilities of LES in reproducing the unsteady complex behavior of ICE flows. Realistic engine geometries have been studied by Huijnen in [8] in which the Authors have shown the superior capabilities of LES over URANS approach in resolving the inhomogeneous features of turbulence.

Other studies dealt with non-stationary cases such as the one proposed by Moureau [9] in which LES was used to study the generation and disruption of compressed tumble vortexes inside a square piston engine. Further works [10], [11], [12], [13] have demonstrated the capabilities of LES in retrieving information about

cycle-to-cycle engine variability. In a few studies [14], [15], [16] the Authors modeled also the combustion process obtaining detailed descriptions of realistic IC engine flows.

Despite the growing number of LES applications to IC engine simulation, there are, still today, some open modeling issues that must be considered.

Firstly, it must be kept in mind that for a LES simulation to be considered as such, the fraction of the resolved turbulent kinetic energy must be greater than 70 - 80% of the total turbulent kinetic energy, as highlighted by Pope in [17]. An insufficient resolution would in fact mean that the simulation is modeling a too wide fraction of the turbulent spectrum degrading the statistical characterization of the flow. To date, few Authors have taken into consideration this issue such as Piscaglia [5], Celik [18], Di Mare [19] or Brusiani [20], this latter also proposing a LES quality parameter estimator.

A second issue related to the former one concerns the numerical solution of the (filtered) Navier Stokes equations on unstructured grids, typical for IC engine applications. It is well known by literature [21] that such process tends to introduce numerical dissipation and dispersion in the solution. It is therefore of paramount importance to assess the solver dissipative behavior, evaluating its suitability for LES simulations.

Then several other aspects are important for the practicability of LES of realistic IC engine configurations. The discretization of the computational domain plays an important role in defining the filter width of (implicitly filtered) LES. In this regard the element type is an issue of major interest: despite the common acknowledgement that hexahedral elements provide less numerical diffusivity, some Authors [3], [11], [22] have successfully performed LES of ICE-related flows employing tetrahedral elements. These type of elements, among with polyhedral ones, are certainly more prone to adapt to the complexity of realistic engine geometries.

Another topic of interest is the near-wall treatment: it is well known that for the sake of LES completeness the resolution at the walls should approach $y^+ \sim 1$. This requirement is generally unfeasible for realistic cases due to the high computational costs. Some Authors like Brusiani [3], Abraham [23] and [24], have demonstrated the feasibility of near-wall modeling (i.e. the use of wall functions) for ICE cases where the focus is primarily in resolving the turbulent fluctuations in the core flow.

Again, numerical schemes and boundary condition types are active research fields. For the former there is a growing interest in higher order methods ([25]) with the pursue of an increase in both space and time resolution accuracy. However, it must be noted that nowadays most of the ICE LES applications are based on second order schemes due to their greater robustness and reliability. Then, boundary conditions in LES should be able to provide a suitable treatment for turbulence properties at domain inlets and to allow acoustic waves to properly leave the domain without reflection.

Finally SGS modeling represents a further difficulty when simulating ICE flows. They not only have to correctly model the effects of unresolved residual fluid motion but must also guarantee the proper near-wall eddy-viscosity behavior, in particular when coarse grids are adopted. Several attempts to overcome this issue have been carried out, such as the WALE model proposed by Nicoud et. al. [22] as an alternative to the classical Smagorinsky SGS model or the more commonly adopted dynamic version.

The present paper addresses the use of advanced SGS models for LES of IC engine flows. Such models, namely the "dynamic Wale" and "Sigma", proposed by Baya Toda et al. [26]-[27], are intended to be advancement of the Wale and dynamic Smagorinsky models that are today the most common choice for the aforementioned cases.

This paper is divided into three main sections. In the first one some theoretical aspects of LES modeling are recalled together with the details of the SGS models implemented in the open-source CFD code used for the present work [28]-[29]. Quality criteria for LES simulations will also be presented and discussed. In the second section the capabilities of the CFD solver in terms of level of numerical dissipation and dispersion will be assessed. This will allow to test the suitability of the code for LES analyses and will provide some guidelines for an optimal choice of discretization and numerical schemes. In the latter section of the paper the Dellenback abrupt expansion test case [30] will be used to evaluate the implemented SGS models. The results will be compared against both experimental data and numerical simulations run with "standard" SGS models. Quality assessment of the analyses will also be presented and discussed.

LES MODELLING

The Filtered Navier-Stokes Equations

The governing equations describing the motion of incompressible fluids are the Navier-Stokes (NS) equations in their incompressible formulation. In LES such equations are spatially filtered in order to retain only the larger scales of motion. Using an overbar to denote the filtering operation and adopting the Einstein notation, the filtered NS equations read:

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}^{SGS}}{\partial x_j} \quad (1)$$

and the fluid incompressibility constrain is expressed by:

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \quad (2)$$

where u , p , ρ and ν are respectively the fluid velocity, pressure, density and (molecular) kinematic viscosity. The filtered equation set (1)-(2) are formally similar to the original NS equations except for the term containing the sub-grid stresses defined as:

$$\tau_{ij}^{SGS} = \overline{u_i u_j} - \overline{u_i} \overline{u_j} \quad (3)$$

This term vanishes if the grid density is sufficiently high. In such case the filter width is small enough so that the LES tends to a DNS. Unfortunately τ_{ij}^{SGS} contains unknown terms that have to be modeled. Despite the lack of a universally accepted SGS turbulence model for LES, the eddy-viscosity assumption is, to date, the most common modeling approach. The SGS stress tensor τ_{ij}^{SGS} can be then expressed as:

$$\tau_{ij}^{SGS} - \frac{1}{3} \tau_{kk}^{SGS} \delta_{ij} = -2\nu_{SGS} \overline{S_{ij}} \quad (4)$$

where $\overline{S_{ij}}$ is the resolved rate-of-strain tensor defined as:

$$\overline{S_{ij}} = \frac{1}{2} \left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right) \quad (5)$$

With the eddy-viscosity assumption, the formulation commonly adopted for ν_{SGS} is the following:

$$\nu_{SGS} = (C_m \Delta)^2 \overline{OP}(\vec{x}, t) \quad (6)$$

where C_m is the model constant, Δ is the filter width and $\overline{OP}$ is an operator specific of each sub-grid SGS model.

In the following paragraphs the basic details of the tested SGS models will be recalled. The dynamic Smagorinsky model was already present in the *OpenFOAM*[®] libraries but it has been modified in order to compute additional quantities of interest for the current investigation, such as k_{SGS} or ε_{SGS} . All the other SGS models were not available in the libraries and they have been wholly implemented by the authors.

The Dynamic Smagorinsky SGS Model

The dynamic Smagorinsky model is based on the dynamic procedure developed by Germano [31] and subsequent improvement proposed by Lilly [32]. The model employs a second filter, the test filter $\hat{\Delta}$ larger than the initial filter Δ and usually chosen as $\hat{\Delta} = 2\Delta$. The tensor operator $\overline{OP}$ in Eq. 6 is based on the second invariant of the strain rate tensor $\overline{S_{ij}}$ of the filtered velocity field $\overline{u_i}$:

$$\overline{OP} = \sqrt{2\overline{S_{ij}}\overline{S_{ij}}} \quad (7)$$

The model constant is then dynamically evaluated from test-filtered resolved quantities:

$$C_{ds}^2 = \frac{1}{2} \frac{\langle L_{ij} M_{ij} \rangle^+}{\langle M_{ij} M_{ij} \rangle} \quad (8)$$

where L_{ij} is the Leonard stress tensor:

$$L_{ij} = \widehat{\overline{u_i u_j}} - \widehat{\overline{u_i}} \widehat{\overline{u_j}} \quad (9)$$

and

$$M_{ij} = \hat{\Delta}^2 \widehat{\overline{OP S_{ij}}} - (\hat{\Delta}^2 \widehat{\overline{OP}} \widehat{\overline{S_{ij}}}) \quad (10)$$

The superscript + in (8) means a positive clipping of all negative values to zero and the brackets $\langle \rangle$ denote a volume averaging operation adopted in order to avoid numerical instability. To be noted that in the present work homogeneous volume averaging is employed.

The WALE SGS Model

The WALE model has been developed by Nicoud and Ducros [22] and its invariant is based on the square of the velocity gradient tensor. In particular, the operator $\overline{OP}$ is based on the traceless symmetric part of the square of the velocity gradient tensor $\overline{S_{ij}^d}$, defined as

$$\overline{S_{ij}^d} = \frac{1}{2} (\overline{g_{ij}^2} - \overline{g_{ji}^2}) - \frac{1}{3} \delta_{ij} \overline{g_{kk}^2} \quad (11)$$

where $\overline{g_{ij}}$ is the velocity gradient tensor. The tensor $\overline{S_{ij}^d}$ can also be expressed as:

$$\overline{S_{ij}^d} = \overline{S_{ik}} \overline{S_{kj}} + \overline{\Omega_{ik}} \overline{\Omega_{kj}} - \frac{1}{3} \delta_{ij} [\overline{S_{mn}} \overline{S_{mn}} - \overline{\Omega_{mn}} \overline{\Omega_{mn}}] \quad (12)$$

being $\overline{S_{ij}}$ and $\overline{\Omega_{ij}}$ respectively the rate of strain and the vorticity tensors of the resolved velocity field. By construction the trace of $\overline{S_{ij}^d}$ is zero and its second invariant remains finite and proportional to $\overline{S_{ij}^d} \overline{S_{ij}^d}$. Assuming incompressibility, this latter term can be expressed as:

$$\overline{S_{ij}^d} \overline{S_{ij}^d} = \frac{1}{6} (\overline{S^2} \overline{S^2} + \overline{\Omega^2} \overline{\Omega^2}) + \frac{2}{3} \overline{S^2} \overline{\Omega^2} + 2\overline{IV_{S\Omega}} \quad (13)$$

where

$$\overline{S^2} = \overline{S_{ij} S_{ij}}, \quad \overline{\Omega^2} = \overline{\Omega_{ij} \Omega_{ij}} \quad \text{and} \quad \overline{IV_{S\Omega}} = \overline{S_{ik} S_{kj} \Omega_{jl} \Omega_{li}}$$

Thanks to the operator $\overline{S_{ij}^d} \overline{S_{ij}^d}$ the WALE model is sensitive to both strain and rotation rates. The aforementioned operator is zero in case of pure shear and this means that unlike the Smagorinsky model, the WALE model avoids producing eddy-viscosity in the case of wall-bounded laminar flows, resulting in an accurate reproduction of the laminar to turbulent transition. The tensor operator $\overline{OP}$, Eq. (6), in the WALE model reads then:

$$\overline{OP}^W = \frac{(\overline{S_{ij}^d} \overline{S_{ij}^d})^{3/2}}{(\overline{S_{ij} S_{ij}})^{5/2} + (\overline{S_{ij}^d} \overline{S_{ij}^d})^{5/4}} \quad (14)$$

The model constant has been set to $C_w = 0.575$ as an average of the values reported in [22]. When the distance from a solid wall approaches zero, the invariant (13) scales as y^2 so that the WALE operator $\overline{OP}^W$ scales as y^3 reproducing the proper behavior of the eddy-viscosity in near-wall regions.

The Dynamic WALE SGS Model

The dynamic procedure proposed by Germano [31] to develop the dynamic Smagorinsky SGS model can be applied also to the WALE model. In such case the expression (8) is replaced by:

$$C_{dw}^2 = \frac{1 < L_{ij} M_{ij}^W >^+}{2 < M_{ij}^W M_{ij}^W >} \quad (15)$$

where L_{ij} is the same as (9) and the superscript + denotes the usual positive-clipping procedure. The operator M_{ij}^W then reads:

$$M_{ij}^W = \hat{\Delta}^2 \widehat{OP^W S_{ij}} - (\Delta^2 \widehat{OP^W S_{ij}}) \quad (16)$$

As pointed out by Baya Toda et al. [26] the dynamic version of the WALE model produces too high values of the constant C_{dw} at the walls and a poor prediction of the mean velocity. The reason for this has been found by the Authors [26] who demonstrated that the dynamic procedure tends to alter the proper near-wall y^3 behavior of the model constant leading to a y^0 scaling in this region. Since the laminar viscosity is predominant in the proximity of solid boundaries, the Authors [26] concluded that there is no reason to dynamically adapt the model constant there. In order to identify the near-wall region it has been developed a sensor capable of detecting the presence of a wall with no need to have an a-priori knowledge of the geometry that can be arbitrary complex. The sensor has been named "Shear and Vortex Sensor" (SVS) and has the following formulation:

$$SVS = \frac{(\overline{S_{ij}^d S_{ij}^d})^{3/2}}{(\overline{S_{ij}^d S_{ij}^d})^{3/2} + (\overline{S_{ij} S_{ij}})^3} \quad (17)$$

The SVS invariant is bounded by 0 - 1, where the lower value corresponds to pure shear and the higher corresponds to pure rotating flows. Thanks to this property the computational domain can be ideally split into two regions: the near-wall region, identified by $SVS < 0.09$ (as proposed by the Authors [26]), where the model constant is fixed at its standard value, and a bulk region where the model constant is evaluated dynamically. The (modified) dynamic WALE SGS model can be summarized as follows:

- if $SVS < 0.09$:

$$C_{dw}^2 = \frac{1 < L_{ij} M_{ij}^W >^+}{2 < M_{ij}^W M_{ij}^W >} \quad (18)$$

- if $SVS \geq 0.09$:

$$C_{dw}^2 = 0.25 \quad (19)$$

The Sigma SGS Model

The Sigma SGS model has been recently proposed by Baya Toda et al. [27] as an upgrade of the WALE model.

In [27], the Author highlights some deficiencies of the WALE model: it can be shown that it produces nonzero eddy viscosity in simple flow configuration such as solid rotation and axisymmetric expansion or contraction, where the sub-grid scale activity should ideally be zero. The Authors developed the model in order to force the operator $\overline{OP}$ to have the following properties:

- P1: to behave as y^3 in proximity of walls.
- P2: to vanish in the case of solid body flow rotation (like the Smagorinsky model) and in the case of pure shear (like the WALE and Vreman [33] models). In general, the operator should vanish in the case of any two-dimensional flow.
- P3: to vanish where the resolved flow field is either in a pure axisymmetric or in a isotropic contraction/expansion configuration.

In the Sigma model the operator $\overline{OP}$ takes the following form:

$$\overline{OP}^\sigma = \frac{\sigma_3(\sigma_1 - \sigma_2)(\sigma_2 - \sigma_3)}{\sigma_1^2} \quad (20)$$

where σ_1, σ_2 and σ_3 are the three singular values of the velocity gradient tensor $\overline{g}_{ij}$. By definition these values are always positive and equal to the square root of the eigenvalues of the matrix $G = g'g$, which are always positive because G is symmetric semi-definite positive. Analyzing the asymptotic behavior of the singular values at walls, it can be shown that:

$$\sigma_1 = O(y^0); \sigma_2 = O(y^1); \sigma_3 = O(y^2) \quad (21)$$

Thanks to the relations (21) it is possible to verify that in Eq. (20), the product $\sigma_3(\sigma_1 - \sigma_2)(\sigma_2 - \sigma_3)$ satisfies the above mentioned properties P1, P2 and P3. The term σ_1^2 at denominator is an Authors' choice [27] in order to scale $\overline{OP}^\sigma$ to a frequency scale. The model constant is set $C_\sigma = 1.5$ as proposed in [27].

LES QUALITY

In the last decade the number of works dealing with LES of ICE flows constantly increased due to the potential this modeling approach has to offer within this field. Despite that, most of the scientific publications lack the resolution quality assessment of the simulations with some noticeable exceptions such as [3], [5], [34] and [19]. In the following paragraphs, LES quality assessment parameters are presented and discussed. It must be noted however that these represent a subset of a larger number of resolution tests available at the AVA Document Sharing Hub.

far as ICE flows are concerned, some of these tests become of limited interest because of the extra computational effort required, such as the Richardson extrapolation methods and, more in general, the two-grid estimators [18].

Fraction of Resolved Kinetic Energy - M

The amount of turbulent kinetic energy resolved by a simulation is a key aspect for evaluating LES quality. In [17] Pope defines the parameter $M(\bar{x}, t)$ as a measure of the turbulent resolution. Such parameter weights the amount of turbulent kinetic energy of the residual motion with respect to the total turbulent kinetic energy of the flow:

$$M(\bar{x}, t) = \frac{k_{sgs}(\bar{x}, t)}{k_{sgs}(\bar{x}, t) + k_{res}(\bar{x}, t)} \quad (22)$$

where $k_{res}(\bar{x}, t)$ is the resolved turbulent kinetic energy and $k_{sgs}(\bar{x}, t)$ is the residual motion turbulent kinetic energy. The value of M is bounded between 0 and 1. When $M = 1$ a RANS simulation is retrieved, while for M approaching zero, the simulation tends to a DNS. The smaller the parameter M is, the higher the resolution of the turbulent motions is. Pope suggests a threshold value of $M < 0.2$ as a reasonable resolution limit for LES.

It must be noted, however, that the parameter M alone is not sufficient to evaluate the accuracy of the simulation with respect to the actual flow since M does not account for the fraction of turbulent kinetic energy lost due to numerical dissipation. Furthermore, a high value of M at a certain point in the domain doesn't necessarily mean that in such location the grid needs refinement because the fraction of turbulent kinetic energy could be affected by the filter size in upstream locations and / or earlier in time.

A wall-bounded flow can be fully resolved only if the near-wall region is discretized with a properly refined mesh in all three directions given the three-dimensional nature of turbulence. In ICE flows such a requirement is hard to fulfill due to the huge computational effort needed. In consideration of this and trying to address feasible modeling strategies, all the turbulence models proposed in the present work make use of wall functions, if not otherwise stated.

Length Scale Resolution - LSR

The Length Scale Resolution (LSR) has been introduced by Brusiani et al. in [20] attempting to estimate the attitude of the grid to properly resolve the scales of fluid motion up to the inertial subrange. It is defined as the ratio between the actual filter size Δ and (an estimate of) the inertial subrange lower limit l_{DI} :

$$LSR(\bar{x}, t) = \frac{\Delta}{l_{DI}(\bar{x}, t)} \quad (23)$$

where $\Delta = \sqrt[3]{\Delta x \Delta y \Delta z}$ and $l_{DI} \approx 60\eta$ with η being the Kolmogorov microscale length [35]. To be noted that such an estimate of l_{DI} is based on scaling assumptions of isotropic turbulence under equilibrium conditions. In the present work the above parameters are estimated as follows:

$$\Delta = \sqrt[3]{\Delta x \Delta y \Delta z} \quad (24)$$

$$\eta(\bar{x}, t) = \nu^{3/4} \varepsilon(\bar{x}, t)^{-1/4} \quad (25)$$

$$\varepsilon(\bar{x}, t) \approx \frac{C_\varepsilon k(\bar{x}, t)^{3/2}}{\Delta} \quad (26)$$

The LSR parameter is therefore defined as the ratio between the actual filter dimension and the characteristic length of the inertial range motions. Such parameter correlates the filter dimension Δ to the fraction of resolved energy spectrum and is therefore useful to evaluate the optimality of the computational domain discretization, identifying regions that could need refinement. While having $LSR = 1$ means complete length scale resolution up to the dissipative range, accordingly to the Authors' findings [20], $LSR < 5$ is a reasonable threshold for an adequate energy resolution level at an affordable computational cost.

Viscosity Ratio - ν_{SGS}/ν

The ratio between the sub-grid viscosity ν_{SGS} and the molecular viscosity ν is representative of the degree of modeling in a LES simulation:

$$s' = \frac{\nu_{SGS}}{\nu} \quad (27)$$

Several Authors prefer to weight the amount of turbulent viscosity with respect to the effective viscosity defining the following subgrid activity parameter:

$$s'' = \frac{\nu_{SGS}}{\nu_{SGS} + \nu} \quad (28)$$

However, as Celik pointed out in [18], since $\nu_{SGS} \gg \nu$ the s'' parameter is often pretty close to unity and not really sensitive to grid resolution. For such reason in the present work the s' formulation has been used. Values of $s' < 10$ are considered sufficient to obtain an accurate LES as shown by Durbin in [36].

Two Grid Estimator - LES_{IQk}

The LES_{IQk} parameter has been proposed by Celik [18] who defined it as the ratio between the resolved turbulent kinetic energy k_{res} and the total turbulent kinetic energy $k_{tot} = k_{res} + k_{SGS} + k_{num}$:

$$LES_{IQk} = \frac{k_{res}}{k_{tot}} = \frac{k_{res}}{k_{res} + k_{SGS} + k_{num}} \quad (29)$$

When $LES_{IQk} = 0$ a RANS simulation is retrieved, while the LES simulation approaches a DNS when LES_{IQk} tends to unity. By assuming that the effective subgrid turbulent kinetic energy $k_{eff,SGS} = k_{SGS} + k_{num}$ scales with the mesh size, the Author reformulates Eq. (29) as:

$$LES_{IQk} = \frac{k_{res}}{k_{res} + a_k h^p} \quad (30)$$

where a_k is a coefficient to be determined, p is the formal order of accuracy of the numerical scheme and h is the grid size. To be noted that the formulation of this quality indicator is well suited for implicitly filtered LES, where a modification of h is directly reflected onto the filter size Δ , and, from this, onto both the numerical and SGS behaviors jointly. Denoting with superscript 1 the finer grid and with superscript 2 the coarser one, Eq. (30) can be reformulated as:

$$LES_{IQk} = \frac{k_{res}}{k_{res} + \frac{k_{res}^2 + k_{res}^1}{\alpha^p - 1} \left(\frac{h}{h_2}\right)^p} \quad (31)$$

where $\alpha = h_1/h_2 > 1$ is the grid refinement ratio. Equation 31 can be then rearranged for both grid sizes. Here the expression for the finer grid is reported:

$$LES_{IQk}^{fine} = \frac{1}{1 + \left(1 - \frac{k_{res}^1}{k_{res}^2} (\alpha^p - 1)^{-1}\right)} \quad (32)$$

In this approach the inherent difficulty of evaluating the code numerical dissipation is hidden into the parameter a_k which is computed through a Richardson's extrapolation. The extrapolation is performed with results obtained on two grids, similar in structure but with different refinement levels. Due to this last aspect, the LES_{IQk} parameter belongs to the class of two-grid estimators. The procedure is certainly computationally expensive and can lead to misleading results in practical applications as found by Di Mare [19], and this explains its scarce adoption, even in academic works. Despite these issues, this estimator has been used in the present work in order to test its capabilities in evaluating the code's numerical dissipation.

NUMERICAL DISSIPATION AND DISPERSION

It is well known by literature that numerical schemes tend to introduce numerical dissipation and dispersion on the flow field solution ([37], [21]). In explicit LES analyses, like the ones we dealt with, the dissipation of kinetic energy is provided directly as viscous dissipation or through SGS viscous dissipation, while the numerical dissipation of the code should be kept as low as possible (ideally zero). Furthermore the importance of properly resolving the time evolution of the turbulent flow structures leads to the need of minimize numerical dispersion as well. It is therefore interesting to

evaluate the attitude of *OpenFOAM*[®] towards both kinds of the aforementioned numerical errors in order to estimate its suitability for LES computations.

The adopted test case consists of a vortex convected by a uniform inviscid flow in a 2D domain as proposed by Yee et al.[38]. Supposing that there are no numerical dissipation or dispersion errors, after one or more convective times T_0 , the vortex profile remain the same as the initial (analytic) one. Similar tests employing a Taylor-Green vortex have been performed by other Authors ([39], [40] and [41]) as a method to assess code dissipation. To be noted that in the following study the dispersion error has been also evaluated as done by Brusiani et al. [20].

The computational domain, reported in Fig. 1, has been discretized using a 2.5D uniform hexahedral mesh with one cell only along z direction, accordingly to *OpenFOAM*[®] requirements for pseudo-2D analyses. Three different grid densities have been used employing 12, 24 and 48 points along the vortex radial profile, with mesh sizes of 48 x 48, 96 x 96 and 196 x 196 cells respectively. Given $D_0 = 2\pi$ meters, the initial diameter of the vortex, the domain is a square with side of $2D_0$. The domain extent has been chosen in order to minimize the effects of the boundary conditions on the solution and to allow the motion of the vortical structure for a reasonable amount of convective times (T_0).

The initial conditions for the fluid-dynamic vortex flow field were:

$$u = -\frac{\beta}{2\pi} y e^{\frac{1-x^2-y^2}{2}} \quad (33)$$

$$v = \frac{\beta}{2\pi} x e^{\frac{1-x^2-y^2}{2}} \quad (34)$$

$$p = p_0 - \frac{\beta^2}{8\pi^2} e^{(1-x^2-y^2)} \quad (35)$$

where $\beta = 5s^{-1}$ is the vortex strength and $p_0 = 101325$ Pa. A constant convective velocity U_0 of 10 m/s has been added along the x direction of the profiles in order to reproduce the convective transport process. Symmetries have been used for the top and bottom domain boundaries while periodic conditions have been applied on the other sides, as shown in Fig. 1.

The *OpenFOAM*[®] solver used is *potentialTransientFoam*, a solver which was specifically implemented during the present work for the solution of transient inviscid fluid flows. It is based on a second order backward implicit integration scheme for time advancement and employs a Bounded Central Difference scheme (BCS) for pressure and momentum equations. The PISO algorithm provides the pressure-velocity coupling. The same numerical schemes were employed in the 3D LES analyses with viscous flow solvers presented in the following section.