INDICATORS FOR THE QUALITY ASSESSMENT OF THE GRID RESOLUTION

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ABSTRACT

The choice of the grid resolution in thermo-fluid dynamics simulations is to be made as a balance between the quality of the results and the computational effort. When quick results are needed, coarse resolutions are often used, but in some cases this could be detrimental for the reliability of the numerical results. However, it is well known that reducing the size of the mesh affects dramatically the overall simulation time.

Several approaches can be used to ensure that the mesh size is appropriate to reproduce the fire and smoke dynamics for a given scenario with suitable computational effort and make reliable predictions.

The first and most used approach consists of limiting the ratio between the characteristic fire diameter $D^*$ and the grid size $dx$ inside a range based on a series of experimental tests reported in literature. This approach is generally used as a first step in order to define a tentative grid resolution for the given model.

Other approaches consist of checking if some indicators are included in a literature-based range once the simulation has run. For example, the dimensionless parameter $y^+$ is a measure of how well the near-wall field is solved and can be effectively useful when the roughness of the walls affects the overall flow field. The measure of turbulence resolution (MTR), instead, is a quantity related to the resolved i.e. calculated turbulent kinetic energy and gives an idea of how detailed the turbulence effects are accounted in the model.

These indicators are certainly a significant source of information regarding the quality of the model as well as the need of local refinement. However, they are not a guarantee for the achievement of convergent results of the quantity of interest (e.g. temperature, visibility, FED) which from the engineering point view are as valuable as the quality assessment of the model.

In the paper, the traditional indicators are reviewed from a theoretical point of view and the Pearson’s coefficient is introduced as an attempt to add other statistical correlation principles. The purpose is to couple mesh quality metrics with a global convergence check of the quantity of interest of the fire safety analysis, driven also by aspects of conservativeness and computational cost. An application to a case study is also provided and shows pros and cons of the indicators.

KEYWORDS:

quality metrics, correlation, sensitivity analysis, grid optimization, turbulence, LES, fire compartments

NOMENCLATURE LISTING

- $D^*$: characteristic fire diameter (m)
- $dx$: grid size (m)
- $K_{SGS}$: modeled turbulence kinetic energy (subgrid)
- $K_{LES}$: resolved turbulence kinetic energy
- $MTR$: measure of turbulence resolution
- $y^+$: viscous wall units
- $c_p$: specific heat (J mol$^{-1}$ K$^{-1}$)
- $u_f$: friction velocity (m/s)
- $q_i$: quantity of interest
- $T_\infty$: ambient temperature (K)
- $\tau_w$: viscous stress
- $\delta_n$: wall-normal cell dimension (m)
- $\delta_v$: local viscous length scale (m)
- $\mu$: Viscosity (kg m$^{-1}$ s$^{-1}$)
- $\rho_\infty$: Ambient density (kg/m$^3$)
- $Q$: total heat release rate

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INTRODUCTION

The choice of the grid size in thermo-fluid dynamics simulations is to be made as a balance between the quality of the results and the computational effort. When quick results are needed, coarse resolutions are often used, but in some cases this could be detrimental for the reliability of the numerical results. However, it is well known that reducing the size of the mesh affects dramatically the overall simulation time. For instance, considering cubic cells, if the side of each cell is reduced by a factor of two, the simulation time will increase of approximately 16 times (2^3 for each axis and 2 for the time step, in order to satisfy the CFL condition).

From the point of view of a fire practitioner, the main interest is to spend the least computational effort and provide reliable results in terms of output quantities e.g. temperature, radiative heat flux gas, visibility, FED, etc. This is not necessarily a guarantee for accurate results if comparisons are made with experimental tests, given the unavoidable limitations of the turbulence modeling [1]. However, considering that CFD allows for the most detailed description of fire and smoke phenomena, it might expect that a high accuracy from the simulation and reliable predictions for design purpose is achieved.

Today, the fire design of different types of buildings relies more and more on the fire safety engineering and the use of advanced modeling of fire is rocketing, also thanks to a renewed attention and openness of the fire authorities. FDS is currently the most used software for fire simulations for a wide variety of civil applications [2]. It works under the Low-Mach approximation, valid for the typical range of pressure showed during fire scenarios, and the turbulence formulation is a LES (Large Eddy Simulation) with implicit filtering. With this approach, a set of filtered equations is obtained from the complete Navier-Stokes equations, and as FDS adopts an implicit filter (filter ~ grid size) we know from the very beginning the results are affected by the grid resolution, as the governing equations are. Pope [3] identified in the adaptive LES the only way to make LES formulation complete e.g. free from flow-dependent specifications [4]. This can be theoretically obtained by adapting step by step the grid size (e.g. the filter) in order to maintain the level of turbulence resolution below the required tolerance and ensure in the whole domain the same accuracy and reliability of the results. However, this is not generally practiced in fire simulations and therefore a quality assessment must explicitly be carried out to check the correctness of the model and a balance among accuracy, conservative results and computing time.

METRICS FOR QUALITY ASSESSMENT

A review of some indicators helpful for the definition of the grid resolution is conducted. Some of them, e.g. rule of thumb, can be considered \textit{a priori} methods, because they are applied to build the first tentative grid layout for the given model, with no information on the results. Others are instead applied \textit{a posteriori}, e.g. MTR, once the results of the simulation are available and one can check the quality of the grid resolution.

Rule of thumb

The first and most used method consists of limiting the ratio between the characteristic fire diameter $D^*$ and the grid size $dx$ inside a range of 4-16 [2]. The characteristic fire diameter should be thought one of the many possible length scales that need to be resolved to capture accurately the fire and turbulence phenomena. It can be expressed via the relation (1) where $Q$ is the total heat release of the fire, $\rho_\infty$ is the ambient density, $c_p$ is the ambient specific heat, $T_\infty$ the ambient temperature and $g$ is gravity.

$$D^* = \left(\frac{\hat{Q}}{\rho_\infty c_p T_\infty g D^2}\right)^{\frac{1}{2}}$$

In many instances, $D^*$ is comparable to the physical diameter of the fire, in which case, $Q^*$ is on the order of 1. The $\hat{Q}^*$ represent the square root of the Froude number and has been given by the following relation (2):

$$\hat{Q}^* = \frac{\hat{Q}}{\rho_\infty c_p T_\infty g D^2}$$

Since the formula (1) has derived from the formula (2) that defines $\hat{Q}^*$, it is important to define an optimum value for the engineering applications. Cox and Kumar [5] define that the dimensionless HRR ($\hat{Q}^*$) should be in the range of 0.3 to 2.5 for natural fires in buildings. The above mentioned range of the ratio $D^*/dx$ comes from the test series reported in NUREG 1824 [6] and therefore it is the range that worked well for those examined cases. Thus, this does not necessarily imply that the range is suitable for our model, considering the geometrical characteristics as well as the fire size and the ventilation conditions.

Near wall resolution $y^+$
A method to check the quality of the grid resolution near the wall is to limit $y^+$ in the range 30-1000 [2]. Similarly, Cox and Kumar [5] suggested that $y^+$ must be greater than 400 to capture the main physical features of the flow. The value of $y^+$ is calculated as reported in (3), as a half of the ratio (since the velocity lives at the cell face center) between the wall-normal cell dimension $\delta_y$ and the local viscous length scale, $\delta_v$. In addition, $\tau_w$ is the viscous stress evaluated at the wall and $u_e$ is the friction velocity.

$$y^+ = \frac{1}{2} \frac{\delta_y}{\delta_v}; \delta v = \frac{\mu}{\rho \delta v}; u_e = \sqrt{\frac{\tau_w}{\rho}}$$

This parameter $y^+$ is a measure of how well the near-wall field is solved and can be effectively useful when the roughness of the walls affects the overall flow field. The $y^+$ can be extrapolated from FDS as a boundary file or as a punctual device and the lowest is, the higher the resolution of the near wall field is.

### Measure of turbulence resolution

The MTR is a quantity related to the resolved turbulent kinetic energy and gives a measure of the resolved turbulence in the domain. It is expressed as the ratio between the subgrid turbulent kinetic energy $K_{SGS}$ and the total energy (sum of $K_{SGS}$ and the solved energy $K_{LES}$) as in (4). By definition, MTR is always included between 0 (all solved) and 1 (all modeled) and satisfactory values should not exceed 0.2 for LES [3]. However, this threshold has been calculated in case of isotropic turbulence conditions, which are certainly not reached near the fire source or every time there is a strongly prevalent component of the velocity.

$$MTR = \frac{K_{SGS}}{K_{SGS} + K_{LES}}$$

Considering FDS, $K_{SGS}$ can be obtained as an output quantity at a given point, while $K_{LES}$ can be calculated by post-processing the three components of the velocity, considering mean values and fluctuations according to the equation (5) where $\bar{u}_i$ is the component $i$ of the velocity and $\langle \bar{u}_i \rangle$ is its mean.

$$TKE = \frac{1}{2}(\bar{u}_i - \langle \bar{u}_i \rangle)(\bar{u}_i - \langle \bar{u}_i \rangle)$$

The MTR can be evaluated in the time range of interest e.g. when the flow field is rather stable.

### THE NEED OF ADDITIONAL QUALITY INDICATORS

The methods described above are a valuable source of information for the quality of our grid resolution and the need of local refinement; nevertheless, in some cases they are not helpful to achieve a high quality configuration of the mesh. Two typical situations are identified:
- although the MTR is below the 0.2 threshold, by varying the grid resolution, the output quantities keep changing significantly (according to the tolerance required by the user);
- near the fire source and high gradient zones where the flow field is highly anisotropic it is not possible to achieve MTR lower than 0.2 i.e. MTR is not reduced with refinement. At the same time, however, there is no indication in literature on a different threshold that could be used to compare with and one could be forced to make predictions even if the results keeps changing and are affected by uncertainties.

Additional indicators taking into account directly the output quantities are reviewed below.

### Pearson’s Coefficient

Correlation coefficients are used in statistics to measure how strong a relationship is between two variables. There are several types of correlation coefficients: Pearson’s coefficient is a correlation commonly used in linear regression [7]. It is possible to use the Pearson coefficient ($r$) to quantify the correlation (linear dependence) between two variables $X$ and $Y$, where $\bar{X}$ and $\bar{Y}$ are the mean values of the samples.

$$r = \frac{\sum_{i=1}^{n}(X_i-\bar{X})(Y_i-\bar{Y})}{\sum_{i=1}^{n}(X_i-\bar{X})^2\sqrt{(Y_i-\bar{Y})^2}}$$

As reported in the Fig. 1, the value of this coefficient are included in the range of -1 to +1. A value of 1 implies that a linear equation describes the relationship between $X$ and $Y$ perfectly, whereas a value of 0 implies that there is no linear correlation between the variables [7]. This Pearson’s Coefficient (later called PC) could be used, during the sensitivity analysis, to assess the X-Y correlation where X and Y are the time-averaged values of the output quantities $q_i$ (e.g. temperature, visibility, etc.) of the same fire scenario, but at different grid resolutions. The advantage of using such an indicator is that the correlation is checked directly on the $q_i$, therefore it could give an additional information compared to MTR and $y^+$, which instead are ultimately the basis for local mesh refinement. By adjusting the grid resolution, the $q_i$ is expected to converge to a stable trend and the PC to increase (0.75 is recommended as a good value [8]).
Mean error

The mean error (ME) calculation can be coupled with the PC. For example, one may assure that although the PC is below the recommended value of 0.75, the mean error between the time-averaged trends is decreasing, implying that we are moving towards a stable prediction of the $q_i$. This calculation should be thought as an additional information for convergence of the model. The limitation of using ME is that it is not reliable when small values of the $q_i$ are compared (large relative error, not representative of the overall model error).

TENTATIVE APPROACH

A tentative approach is reported in the Fig. 2 and commented on below. The drawback of the approach is that as a minimum three different configurations for the given simulation must be considered. The advantage is that it extends the zone where MTR is significantly higher than 0.2. A similar application can be done using $y^+$ instead of MTR (in case one is interested in near wall prediction).

- Step 1. Define the objective of the analysis e.g. the fire size, the quantities of interest $q_i$ and specifically the tolerance accepted when refining the mesh (e.g. 10 %, 20 % etc.);
- Step 2. Rule of thumb is applied for the choice of the grid resolution (coarse, medium and fine);
- Step 3. MTR (and/or $y^+$) is calculated in the domain;
- Step 4. If MTR is lower than 0.2 and the $q_i$ from the coarse or the medium resolutions are conservative with respect to the $q_i$ of the fine resolution, one may consider the highest cell size for
making prediction (on the safe side with less computation cost). If the conservative \( q_i \) is that of finest grid, other indicators should be used:

- Step 5. Calculation of the PC for the \( q_i \). If by refining the grid the correlation increases (higher PC), this implies that the time-averaged trends of the \( q_i \) are not diverging;
- Step 6. Although the PC is not increasing with the grid refinement, the finest grid can be considered as acceptable if the PC 2-3 is higher than 0.75 (recommended value for good correlation).
- Step 7. In case of weak correlation (< 0.75), it may be verified that there is no increment in the ME. Otherwise, an additional refinement is needed (grid 4).

**CASE STUDY**

The approach previously described is applied to a simple geometry (building size 20 m x 10 m x 3 m), lateral ventilation openings along the 10 m walls and central position of the fire (burner surface 2x1 m²). Table 1 shows that each one of the two scenario typologies have a different Heat Release Rate i.e. 2 MW and 4 MW, which is constant during the whole simulation. Three different grid resolutions are analyzed (50 cm, 25 cm, 10 cm). Furthermore, Table 1 shows the values of \( D^*/dx \) used for the initial calibration of the grid resolution. It is worth mentioning that both simulations consider value of \( Q^* \) that are inside the above mentioned range [6]. Specifically, the 4 MW case study has a \( Q^* \) of 1.1 whereas, in the 2 MW, it is 0.56.

| Grid spacing (cm) | \( D^*/dx \)  |
|-------------------|----------------|
|                   | HRR: 2 MW | HRR: 4 MW |
| 50                | 2.5       | 3.4       |
| 25                | 5.1       | 6.7       |
| 10                | 12.7      | 16.8      |

Table 1. Case studies performed and values of \( D^*/dx \)

The MTR has been evaluated according to the equations (4)-(5) by post-processing the velocity components outputs in order to obtain TKE. The devices have been placed at two different heights from the ground i.e. 1 m and 2 m, and at different distances from the burner along the x and y axes (passing through the center of the compartment, where the burner is placed). Table 2 shows that, refining the grid, the MTR decreases below the threshold 0.2 recommended by Pope [3]. As previously commented, it is important to choose the mesh to capture the main physical features of the flow ensuring that the near-wall nodes satisfy the criterion \( y^+ >400 \). In the 4 MW case the \( y^+ \) reaches approximately values of 700, but it decreases by refining the grid up to 200 (grid spacing 10 cm), ensuring a satisfactory behavior in the near wall region (the results are only commented for lack of space).

Table 2. MTR along x and y direction for 2 and 4 MW cases
Table 3 shows instead the temperature values (time-averaged every 10 s) for different grid spacing and allows an overall assessment of conservativeness supporting the choice of the mesh, which normally accompanies the proper quality assessment of the model from practical engineering perspective. In this way, with a single graph and a unique value of PC we have an indication on which mesh is the best for our case without the need of plotting the trends of the output quantities at given points. In the 4 MW case, the correlation increases by refining the grid in agreement with the increment of the PC (from 0.88 to 0.9), so there is a convergence of the qi. From this analysis, the 25 cm grid seems a reasonable choice for the simulation, because it provides higher (therefore, on the safe side) values compared to the 10 cm resolution but far less computational time. Nevertheless, depending on the aim of the fire safety analysis, it should be evaluated if the differences in the results are appreciable and hence if it is the case to refine the grid further.

### Table 3. 4 MW fire at z = 2 m (average of significant points)

| Temperature - Grid spacing 50 cm vs 25 cm | Temperature - Grid spacing 25 cm vs 10 cm |
|------------------------------------------|------------------------------------------|
| PEARSON COEFFICIENT = 0.88               | PEARSON COEFFICIENT = 0.90                |

**CONCLUSIONS**

To wrap up, the following conclusions can be drawn.

- The traditional approaches used to assess the quality of the grid resolution are straightforward from the theoretical point of view and are generally a valid source of information in the assessment of our model. However, for fire conditions they can sometimes give poor information (e.g. when MTR is greater than 0.2, most of the times with high HRR and near the fire source).
- Additional possible indicators are identified e.g. the PC which can be used to analyze directly the qi of different grid resolutions and check if, by refining the mesh, a global convergence has been reached for our model in the qi, allowing us to make engineering predictions.
- The case study shows a possible use of the indicators reviewed and highlights that the PC is in agreement with the rule of thumb, y+ and MTR (25 cm medium resolution is on the safe side). It is worth to notice that for more complex geometries and boundary conditions, higher HRR, etc. in which the traditional indicators might give no meaningful information in some region of the model, the PC may be even more helpful from a practical point of view as it is directly related to output quantities.

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