Computational simulation of the flow around rectangular cylinders: Effects of grid quality at wall

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When I meet God, I am going to ask him two questions: why relativity? And why turbulence? I really believe he will have an answer for the first one.

W.K. Heisenberg
Acknowledgements

The moment has arrived to write the acknowledgements. I am aware of the fact that this part will be the only section that most readers will be interested in (and I completely understand). I will try and do my best. If the language drastically changes from a sentence to the other, do not worry, for I am not going crazy but I simply thought it would help the different readers to feel more involved (that is the aim of this part after all).

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Abstract

Starting from the past decades, many engineering domains require an accurate knowledge of Fluid Dynamics problems. Possible examples are car and airfoil designing in the automotive and aeronautics fields, blood circulation through the cardiovascular system in bioengineering or the evaluation of wind turbines efficiency in the energetic field.

The first historical way to better understand a physical phenomena was to perform as much as possible experiments and to take decisions based on their results. However, sometimes the studied systems are characterized by big length or time scales and, as a consequence, experiments can be very expensive or even not possible to make. In addition to that measurement errors, if not correctly detected, can affect significantly the results.

In the sixties, in concomitance with the first calculators, a new field called Computational Fluid Dynamics (CFD) started to work side by side with experiments. The latter are not supposed to be substituted by numerical simulations, that need to be tested with experimental results, but their number can be reduced in order to decrease the costs. Even if CFD has more than half a century of history, some of its topics are still arguments of actual research. The Computational Wind Engineering (CWE) is the branch of CFD, with Civil Engineering applications, that studies the wind effect on buildings. An important test-case in the CWE community is the characterisation of the flow around rectangular, and in particular square, cylinders. As a matter of fact an important benchmark is the "Benchmark on the Aerodynamics of a Rectangular 5:1 Cylinder (BARC)". Despite being the easiest bluff body that can be thought, it is interesting due to the phenomenological complexity of the turbulent flow around it. Moreover this problem has an application into the study of wind effects on skyscrapers cross-section in Civil Engineering.

CWE computations are based on three aspects that are intrinsically linked to each other: the turbulence modelling, the interpolations schemes used for the equations discretization and the grid generation. The latter has been often neglected in literature and more focus has been addressed on the former two. For this reason, the aim of the thesis is to understand how the quality of the near wall mesh can effect the simulated results in CWE computations.
The thesis will be organized as follow:

- **Chapter 1**
  This first chapter focuses on the CWE benchmark of flows around rectangular cylinders. For this reason, the first part is devoted to the flux phenomenology around cylinders. The second part analyses some articles that are useful to understand the aim of the thesis.

- **Chapter 2**
  This chapter will discuss the equations used in CWE and their discretization. More in particular the *Navier-Stokes equations* are presented, followed by the most used *turbulence models*. Finally the classic interpolation schemes are presented.

- **Chapter 3**
  In the first part the main features of the meshes are explained. Their quality and the errors that they induce in the solution are presented. In the second part a brief review on quality indices used to measure the grid quality is discussed.

- **Chapter 4**
  In this chapter the setup of the four simulations is presented. Chapter 1 and 2 are important to understand the turbulence model and the convective schemes that have been used.
  The four near wall grids used in this thesis are illustrated and their differences discussed with a particular focus on their quality.

- **Chapter 5**
  The numerical results are compared looking at different flow fields and quantities (for example velocity and aerodynamic coefficients) in different regions like the wall and the wake. The differences between simulations are highlighted and justified in terms of grid features. When it has been possible literature reference values have been reported.

- **Chapter 6**
  Finally a brief conclusion is presented where the objective and the results of this thesis are synthesized.
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Chapter 1

Introduction and motivations on bluff cylinders applications

As expressed in the introduction, this thesis will study the effects of the grid quality on the accuracy of numerical simulations of a well known CWE test case. Before starting any discussion about equations to solve or numerical aspects, it is fundamental to understand the main features of the flow around rectangular cylinders, the scenario in which the numerical problem is settled. Gradually in the following chapters it will become clear how this knowledge plays an important role for the setting of the numerical problem.

1.1 Flux phenomenology and associated bulk parameters

A body is said to be bluff if its shape is such that the boundary layer detaches early and the wake region is broad. At the contrary, a body with an attached boundary layer along the whole surface and with a narrow wake is said to be a streamlined body. This definition is not referred on the obstacle itself but on the flow topology around it in a particular setting. As a consequence, the same body can be either bluff or streamline depending on the problems.

Parameters like the turbulence intensity, the face roughness and the angle of attack play a major or minor role in the flow features. Maybe the most important one is a physical dimensionless parameter called Reynolds number. Defining $L$ and $U$ as characteristic length and velocity, respectively, of the problem and being $\nu$ the kinematic viscosity of the fluid, then the Reynolds number reads

$$Re = \frac{UL}{\nu}.$$  (1.1)

In can be thought as the ratio between the inertial and the viscous effects on the flow. Its value varies of several orders of magnitude depending on the problem and the flow topology changes drastically with it.

Let consider the case of the circular cylinder. If its height is sufficiently bigger than the basis radius, the flow around it can be simplified to a 2D flow around a circle. Firstly, if $Re \ll 1$ the circle is streamlined and the downwind flow is symmetrical to the upwind
one. By increasing $Re$, and so the inertial effects, the upstream-downstream symmetry disappears and with $Re \approx 10$ two symmetric attached eddies appear downwind the cylinder.

![Flow behaviour around a circular cylinder with $Re << 1$ and $Re = 10$.](image)

**Figure 1.1**: Flow behaviour around a circular cylinder with $Re << 1$ and $Re = 10$. Both images come from [14].

The eddies dimension increases with the Reynolds number until, for $Re > 40$ the flow becomes unsteady, detachment occurs and the object can be classified as bluff. Finally, starting from $Re = 100$ vortex shedding occurs in the wake. A dimensionless coefficient linked to the frequency of the eddies generation is the Strouhal number defined as

$$St = \frac{f_s L}{U}$$

where $f_s$ is the frequency of the vortex shedding.

For $400 \leq Re \leq 3 \cdot 10^5$ the regime changes and it is called *sub-critical*. It is characterized by a laminar detachment that takes place earlier with higher Reynolds number and, as a consequence, the wake region becomes larger. Starting from $Re \approx 3 \cdot 10^5$ the flow behaviour changes drastically, the turbulence starts playing a fundamental role and the detachment passes from laminar to turbulent because a reattachment of the boundary layer occurs. This regime is called *Critical* and it is closely linked to the transition from laminar to turbulent regime. Finally, when the flow becomes completely turbulent, the regime is called *super-critical*.

This regimes classification is not end to itself because, depending on the regime, the behaviour *aerodynamic coefficients*, widely used in CWE, significantly vary. The two most important coefficients are called *drag coefficient* and *lift coefficient* and read

$$c_D = \frac{F_D}{\frac{1}{2} \rho U^2 l}, \quad c_L = \frac{F_L}{\frac{1}{2} \rho U^2 l}$$

where $\rho$ is the density of the fluid, $U$ is the velocity norm of the flow before the obstacle and $l$ is a reference length, for example the depth of the cylinder. $F_D$ and $F_L$, called respectively *drag* and *lift*, are the forces acting in the alongwind direction and its normal
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direction.
An analogous coefficient can be defined for the pressure
\[ c_p = \frac{p - p_\infty}{\frac{1}{2} \rho U^2} \]  
(1.4)
where \( p \) is the pressure and \( p_\infty \) is the reference pressure (the pressure is defined unless an additive value). Due to the Bernoulli’s laws, \( c_p \leq 1 \) and it is exactly equal to one in the stagnation point.

In the CWE applications the fluid is the air, with a low kinematic viscosity \( \nu = 1.45 \times 10^{-5} \, m^2 s^{-1} \), \( 5 \leq U \leq 50 \, ms^{-1} \) and \( 1 \leq L \leq 100 \, m \). Consequently the Reynolds number varies from \( 10^5 \) to \( 10^8 \) and the flow is highly turbulent and unsteady with a regime that could be sub-critical, critical or super-critical.

At the contrary of the circular cylinder where the location of the boundary layer detachment depends on the Reynolds number, in the rectangular case the presence of the upstream sharp corners leads an immediate detachment. A fundamental geometrical parameter for two-dimensional rectangular cylinders is the ratio of the alongwind dimension (Breadth) to the crosswind dimension (Depth), \( B/D \), which governs their aerodynamic behaviour. For \( B/D < 2.5 \), and so also in the square scenario, only the attachment occurs. At the contrary if \( 2.5 < B/D < 3.5 \) the reattachment is intermittent and if \( B/D > 3.5 \) the reattachment is permanent. Finally, starting from \( B/D > 6 \) more reattachments occur on the face of the cylinder. The Benchmark [1] has been chosen with \( B/D = 5 \) in order to study the case of single reattachment.

In all scenarios, in correspondence of the detached flow, in the region near to the alongwind walls there is the presence of reversed flow.

In the middle of the upwind face there is the stagnation point. Its particularity is that the flow in this point has null velocity.

At the characteristic CWE Reynold numbers, the wake of the cylinder in characterised by the creation of alternating vortexes, called Von Karman’s with opposite rotational sense at regular time intervals. The flow is therefore periodic.

Figures 1.2 and 1.3 shows the early detachment induced by the corners and the Von Karman’s vortexes in the wake for \( Re = 2.2 \times 10^4 \) in a DNS simulation [24].

Figure 1.2: Early boundary layer detachment induced by the sharp corner. The image is obtained from [24].

Figure 1.4 shows the results of three different articles that investigate the drag coefficient variation with respect the cylinder shape and the surface roughness.
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It appears that for the circular cylinder, the drag coefficient does not significantly changes in the sub-critical regime. At the contrary, entering in the critical one, its values decreases drastically until super-critical regime starts. Then, increasing the Reynolds number, the drag coefficient increases. This fact is due to the different localisation of the detachment phenomenon. In addition the presence of a rough surface anticipates the coming of the critical regime and this fact is usually exploited in the engineering applications where small values of the drag coefficients are pursued. For this reason, for flows that are naturally in sub-critical regimes with \( Re \approx 10^5 \), it can be profitable to induce super-critical regimes using rough surfaces instead of sleek ones.

Finally, it is evident that for rectangular cylinders, due to the presence of sharp corners that constrains the detachment location, the mean value of the drag coefficient does not depend on the Reynolds number.

Figure 1.3: Von Karman vortex street. The image is obtained from [24].

Figure 1.4: \( c_D \) values with respect to the Reynolds number with different \( B/D \) ratios, corners \( h/r \) curvatures (where \( h/r = 0.5 \) corresponds to the circular cylinder) and surface roughness. The curves have been extracted from [7, 8, 9].
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Figure 1.5: Different meshing approaches around the leading upper corner. From left to right, the grids are from [5, 6, 10, 11, 12].

1.2 Overview on articles about grid effects

A fundamental aspect of CWE simulations, characterized by high Reynolds numbers, is the mesh generation whose corresponds an induced errors. However this aspect is sometimes not considered.

After a quick overview on the grids used near wall for $B/D = 5$ articles, some works on the mesh effects are illustrated with relative advantages and drawbacks.

1.2.1 Review of the near wall grids for 5:1 rectangular cylinders

Since 2010, when the Benchmark of Rectangular cylinders with $B/D = 5$ [1] has been initiated, many articles have been published on this topic. In [4] a review of the first four years is made.

Figure 1.5 shows five different grid types used near the leading upper corner in different studies while Figure 1.6 presents a review of all the approaches used in literature. It appears clearly that there is not a meshing standard approach and, in addition, grids that strongly affect the results, as it will be observed in the following chapters, have been used.

From these figures, it is manifest that a study on the near wall mesh effects could be important to set a suitable standardisation that would let to reduce mesh induced errors.

1.2.2 Correlation coefficients between error and grid quality

Although the topic of mesh induced errors is not deeply investigate in literature, it would be impossible to present in few pages the whole state-of-art. For this reason it has been decided to present few works coming from aerodynamic works but also from different areas with the objective to present positive aspects that this thesis will follow but also some drawbacks that justify the present work.
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An article coming from the Fluid Dynamics of compressible flows area that is interesting for its approach is [33] that studies mesh skewness, non-orthogonality and stretching effects in a convection problem of a vortex. The idea of the article is to find quantitative correlations between grid defects and numerical errors.

Firstly, the grid induced error can be split into errors that depend on the solution and errors that depend only on the grid geometry. This fact is clear looking at the 1D convection equation

\[
\frac{\partial f}{\partial t} + U \frac{\partial f}{\partial \xi} \frac{\partial \xi}{\partial x} = 0 \quad (1.5)
\]

where \( f \) is a scalar quantity, \( U \) is the convection speed on the \( x \)-direction and \( \xi \) is a generalized coordinate. While the temporal discretization error regards the first term of (3.11), the grid error is linked to both \( \frac{\partial f}{\partial \xi} \) and \( \frac{\partial \xi}{\partial x} \). The former depends on the solution \( f \) but not the latter that is called grid transformation metric.

Then, the idea is to study the truncation error in the frequency domain using an opportune filtering operator. The main advantage of this approach is that spatial derivatives are transformed into polynomial expressions.

Given a scalar quantity \( \psi \) defined in point \( x_i \), the filtered scalar \( \hat{\psi} \) is defined as

\[
\hat{\psi}_i + \sum_{Z=-M}^{N} \alpha_Z \hat{\psi}_{i+Z} = \frac{1}{\Delta \xi} \sum_{z=-m}^{n} \alpha_z \psi_{i+z} \quad (1.6)
\]

where \( \Delta \xi \) is the spatial step for the generalized system. The spatial order of the filter depends on the choice of the filtering stencils and on the coefficients.

Let

\[
\hat{\Delta} \psi_i = \psi_i - \hat{\psi}_i, \quad (1.7)
\]

then it is possible to define the distance between original grid points and their location after the application of the filter in a 3D case where the curvilinear coordinates are \( (\xi, \eta, \zeta) \). A 2D case in shown in Figure 1.7.
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![Figure 1.7: Filtering effect on the mesh in a 2D case in [33].](image)

The grid displacement is then

$$\hat{\Delta} \xi = \sqrt{\hat{\Delta} x_i^2 + \hat{\Delta} y_i^2 + \hat{\Delta} z_i^2}. \quad (1.8)$$

Finally a grid quality metric for a three-dimensional case is defined as

$$Q = \sqrt{\left(\frac{\Delta \xi}{\Delta \xi}\right)^2 + \left(\frac{\Delta \eta}{\Delta \eta}\right)^2 + \left(\frac{\Delta \zeta}{\Delta \zeta}\right)^2} \quad (1.9)$$

where $\Delta \xi = \sqrt{x_i^2 + y_i^2 + z_i^2}$ is a local reference length that is used to normalize the index.

After that a 2D vortex convection problem is studied solving mass, momentum and energy equations. The analytical solution of the density $\rho_{exact}$ is compared to the numerical one obtained with different grids using the relative error

$$E = \frac{\rho - \rho_{exact}}{\rho_{exact}}. \quad (1.10)$$

The main idea of the article is to compute the statistical correlation between

$$Q_I = \int \int_S Q \, dxdy \quad \text{and} \quad E_I = \int \int_S |E| \, dxdy \quad (1.11)$$

in order to find out if a positive correlation is observed.

With this purpose, several grids, starting from the uniform one, are defined and the correlation coefficients are computed. Some of the cases are presented.

- **Uniform grid:** An orthogonal and non-skew grid made of squares with the same dimensions is defined as in Figure 1.8. It can be noticed that $|E| = O(10^{-6})$. This mesh will be the reference for the others that will obtained from the uniform by explicit maps.
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Figure 1.8: Uniform mesh on the left and associated error on the right.

- \textit{x-stretched grid}: A stretched mesh along the \textit{x} direction using the map

\[ x^*(\xi,\eta) = x(\xi,\eta)A_x H(x) \quad (1.12) \]

where \( x^* \) is the new \textit{x} coordinate of the grid, \( H \) represents the Heavyside function and \( A_x \) is the stretching factor. Two grids are defined with \( A_x = 1.25 \) and \( A_x = 2 \) and shown in Figure 1.9 with the respective quality indices. As expected, \( Q \) is larger for the more stretched grid and it assumes higher values in correspondence of the line \( x = 0 \) where the aspect ratio of contiguous cells is bigger than one.

Figure 1.9: \textit{x-stretching effect on the grid}. \( A_x = 1.25 \) on the left and \( A_x = 2 \) on the right.

The relative error is computed and represented in Figure 1.10. In both cases it is larger than the uniform one, as it will be for all the next scenarios. In the simulation with \( A_x = 2 \) the error affects a larger area.

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Figure 1.10: Error for \( x \)-stretching grids. \( A_x = 1.25 \) on the left and \( A_x = 2 \) on the right.

- **Grid with a line direction change:** This grid typology is obtained by defining the \( y \) coordinates as

\[
y^*(\xi, \eta) = y(\xi, \eta) + H(x)A_yx(\xi, \eta)
\]

where the constant \( A_y \) specifies the grid line gradient for \( x > 0 \).

Two grids obtained with \( A_y = 0.25 \) and \( A_y = 0.875 \) are shown with their respective quality indexes. It can be noticed that these grids are not orthogonal for positive values of \( x \).

Figure 1.11: Change of line direction effect on the grid. \( A_y = 0.25 \) on the left and \( A_y = 0.875 \) on the right.

- **Skewed grid:** A uniformly skewed grid can be generated from the uniform one using

\[
x^*(\xi, \eta) = x(\xi, \eta) + A_s y(\xi, \eta)
\]

where \( A_s \) is constant and it specifies the grid line gradient across the entire domain.
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A non-uniformly skewed grid can be defined, for example, with

\[
\begin{align*}
    x^*(\xi, \eta) &= x(\xi, \eta) + A_t \sin \left( \frac{2\pi y(\xi, \eta)}{L} \right) \\
y^*(\xi, \eta) &= y(\xi, \eta) + A_t \sin \left( \frac{2\pi x(\xi, \eta)}{L} \right)
\end{align*}
\]  
(1.15)

where, as usual, \((x, y)\) are the old coordinates and \((x^*, y^*)\) are the new ones and the coefficient \(A_t\) is linked to the skewness. Figure 1.12 represents two different meshes obtained with (1.15).

![Figure 1.12: Non-uniform skewness effect on the grid. \(A_t = 1\) on the left and \(A_t = 1.5\) on the right.](image)

For each case, several computations have been performed by changing the coefficients \(A_x, A_y, A_s, A_t\). Then the quality index and the relative error have been integrated on the domain obtaining plots like in Figure 1.13. Finally, the correlation coefficients between \(Q\) and \(|E|\) have been computed using the formula

\[
C_{QE} = \frac{< Q I E >}{[< Q^2 I > < E^2 I >]^{1/2}}
\]  
(1.16)

where \(< >\) denotes the variance operator.

The obtained values with different filtering schemes in (1.6) are shown in table 1.1.

![Table 1.1](image)

All the meshes defined starting from the uniform case present defects that can be stretching, non-orthogonality, skewness or some combination of them. It appears clearly that, qualitatively, all the meshes induces errors bigger than the optimal cases. Looking at table 1.1, it is possible to ascertain that the proposed quality index \(Q\) is well defined because it is strongly correlated to the error.

Even if the physical problem differs significantly from the one that will be analyzed in the thesis, the idea of the computation of correlation coefficients to express quantitatively the relation between grid quality and error will be used. The correlation coefficients in
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Figure 1.13: On the left, integrated quality index with different values of $A_y$ when line directions are changed. On the right $E_I$ with respect to $Q_I$.

<table>
<thead>
<tr>
<th>Grid Features</th>
<th>Explicit filter</th>
<th>Implicit filters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid spacing discontinuity</td>
<td>0.971</td>
<td>0.970</td>
</tr>
<tr>
<td>Grid direction discontinuity</td>
<td>0.955</td>
<td>0.954</td>
</tr>
<tr>
<td>Uniform skewness</td>
<td>0.427</td>
<td>0.128</td>
</tr>
<tr>
<td>Non-uniform skewness</td>
<td>0.921</td>
<td>0.921</td>
</tr>
</tbody>
</table>

Table 1.1: Correlation coefficients for each mesh obtained from the uniform one.

[33] are very high and sometimes close to one as a demonstration of the good definition of $Q$.

However, it is important to underline that, contrarily to the test case of this thesis an analytical solution is available and so the exact numerical error is computed. In addition Finite Differences are used with high-order schemes such that the grid error contributes mostly to the total error. This is not the case with FVM, that can handle also unstructured meshes at the difference of the FDM, where the spatial discretization is, at most, second order accurate. Finally the meshes are explicitly obtainable from the uniform one through an analytical expression. For unstructured grids this expression is impossible to find. In addition the meshes of the article have, usually, constant values of either skewness or non-orthogonality over all the transformed faces. Grids used in the thesis will have different values for each face.

All this features helps the correlation analysis because they let to isolate either the grid error from the others or the defects.

1.2.3 Grid refinement effects for a square cylinder

At the contrary of the previous study, [34] refers to the CWE benchmark of flow around a square cylinder. In this study the mesh induced error linked to the mesh refinement
is investigated. LES simulations for the square cylinder scenario have been performed in order to study the effect of different meshes. In particular, a structured mesh refined near the cylinder (CR), shown in Figure 1.14, is defined. Only the mesh in the $x - y$ plane is shown because the mesh over third dimension is structured and cutting the domain with a plane $z = const$ the same mesh always appears. This discussion justifies the choice of the thesis to perform 2D simulations in order to investigate the mesh quality effects.

Then, starting from CR, two more grids are obtained through unstructured refinements, the first in the wake (WR), the second both near the cylinder and in the wake (CWR). In both WR and CWR the total number of control volumes in the whole domain does not change.

By defining these three meshes, the effect of refinements in region with big values of
derivatives is studied. It is known that near wall and the wake are regions with high vorticity and deformation and, as a consequence, in both regions the mesh should be refined in order to bound the truncation error. As expected, the simulation with CWR mesh gives better results in terms of aerodynamic coefficients $c_D$ and $c_L$, in both mean and fluctuating values, pressure and velocity in the wake. It is also noticed that results with mesh WR are more accurate than the ones with CR.

This article investigates on the error associated to the mesh density, however it can be observed in Figure 1.14 looking at the mesh near the corners that grids not only change in density but also in quality. As a consequence the differences between simulated results can not be totally justified by the different grid density.

### 1.2.4 Non-orthogonality effects for a circular cylinder

The effects of mesh quality have been observed in [40]. In this article the effect of the non-orthogonality is studied in the scenario of the circular cylinder with Reynolds numbers $Re = 550$ and $Re = 3000$.

A first non-orthogonal body fitted curvilinear coordinate system mesh (NBFC grid) is defined, Figure 1.15.

Then an algorithm obtains, through a numerical quadrature of the expression of the unit vector tangent to the generalized coordinate $\xi$, new coordinates of the mesh nodes. This new nodes have the characteristic to define orthogonal grids (OBFC). Four different grids are defined, each of them with a different number of orthogonal lines, denoted by $\xi_o$, that are, respectively, $\xi_o = 5, 15, 25, 35$. This values are chosen taking into account that the total number of lines is 66 and so the percentage of orthogonal lines varies from 7.5% to 53%.

Figure 1.16 compares the numerical results obtained with NBFC and OBFC with $\xi_o = 35$. 

![Figure 1.16: OBFC vs NBFC mesh in [40] with $\xi_o = 35$.](image-url)
1. Introduction and motivations on bluff cylinders applications

(a) OBFC with $\xi_0 = 35$ and $Re = 550$.

(b) NBFC and $Re = 550$.

Figure 1.17: OBFC and NBFC results compared to experiments.

to the experimental ones. It can be observed that both simulations detect correctly the position of the main eddy core and also the separation point but, at the contrary, the recirculating zone lengths differ with the OBFC closer to the experiments. This fact is observed with both Reynolds numbers.

Finally the article reports the location in time of several points linked to the flow topology with the different meshes and different Reynolds numbers ($Re = 31, 550, 1200$). It is observed that results obtained with the non-orthogonal mesh are always farther from the experimental values than the OBFC ones. In addition, the bigger is the Reynolds number and the bigger is the error with the NBFC grid.

In conclusion, the article not only shows that non-orthogonality affects negatively the results, but also suggests that in CWE applications, where Reynolds number are bigger than the ones used in the article, the non-orthogonality error should have more impact. However, even if the simulations are based on a Finite Volume discretization, the definition of orthogonality used in this work is not the same as in [2] that will be used in this thesis and that, as it will observed, is more coherent with this discretization technique. Indeed in this paper the orthogonality refers to the angles between the lines that generates the mesh.

Moreover, the physical phenomena observed is not interesting from an engineering point of view because the analysis investigates development in early stage of the wake behind a cylinder that is impulsively started and not the stationary flow.

1.2.5 Growth factor consequences in flows around bluff bodies

Grid generation is a fundamental aspect in CFD computations as stressed in [22]. This article investigates the optimal choice of the Growth Factor (GF) such that the numerical simulation of flows around bluff bodies converges. As a matter of fact the GF, that represents the ratio between the characteristic lengths of two adjacent cells, is one of the most important error sources in the mesh generation process in addition to non-orthogonality and skewness.

Firstly the flow around a square obstacle has been studied. The three used meshes are completely orthogonal and not skewed with $GF = 1.05, 1.07, 1.1$. One of them is
1. Introduction and motivations on bluff cylinders applications

(a) Square cylinder.  (b) Rectangular cylinder.  (c) Streamlined cylinder.

Figure 1.18: Grids defined around three different bodies in [22].

represented in Figure [1.18] Some results are compared to the literature ones however the main focus is not on the errors induced by high values of the growth factor but on the occurred convergence of the simulation. For the same reason only a mesh for a rectangular cylinder and one for a streamlined body are defined and shown also in Figure [1.18] It can be easily observed that the latter is characterized by high skewness values and so its numerical effect is added to the GF one, at the contrary of the previous two cases where this error source was correctly isolated.

1.2.6 Correction terms linked to non-orthogonality and skewness in a diffusion problem

Until now, the presented articles have investigated about the error generated by the mesh by changing it and defining either finer or qualitatively better meshes. Even if [21] does not deal with a CWE application, it is interesting because it reduces the grid induced error in a Finite Volume framework by working on the correction terms defined in [2] in the discretized equation. A formal definition of the correction term will be given in the third chapter, but it is important to highlights that if this term is not considered, the numerical result can be quantitatively important.

Comparing the in-house code to ANSYS FLUENT, used in the thesis, and to OpenFOAM, the latter being open source, it has been observed that ANSYS FLUENT properly includes non-orthogonality correction term. However, when the mesh starts becoming not only non-orthogonal but also with high values of skewness, this commercial code starts having troubles obtaining solutions affected by significant errors. More in particular the 2D diffusive problem

\[ \nabla \cdot (\nabla \phi) = 0 \tag{1.17} \]

has been numerically solved with a mesh with high skewness. Figure [1.19] shows the two components of \( \nabla \phi \) obtained by the codes. It is evident that the FLUENT solution is characterized by unphysical oscillations that are induced by a wrong treatment of the skewness correction term in the equations.

Before concluding this chapter, Table [1.2] tries to synthesize the principal pros and cons of each work in order to emphasize the perspective of this thesis.
1. Introduction and motivations on bluff cylinders applications

Figure 1.19: Components of $\nabla \phi$ obtained through in-house and commercial codes in [21].

<table>
<thead>
<tr>
<th>Pros</th>
<th>Cons</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Distinction between different errors</td>
<td>• FD approach</td>
</tr>
<tr>
<td>• Engineering application</td>
<td>• Engineering application</td>
</tr>
<tr>
<td>• Studies non-orthogonality</td>
<td>• No distinction between density and</td>
</tr>
<tr>
<td>• Separates growth factor error</td>
<td>quality mesh errors</td>
</tr>
<tr>
<td>• Engineering application</td>
<td>• Engineering application</td>
</tr>
<tr>
<td>• Detects FLUENT drawbacks</td>
<td>• Ignores non-orthogonality</td>
</tr>
<tr>
<td>• Uses the same quality indicators</td>
<td>• Ignores non-orthogonality and skewness</td>
</tr>
<tr>
<td>• Engineering application</td>
<td>• Engineering application</td>
</tr>
</tbody>
</table>

Table 1.2: Synthesizing table that schematically represents advantages and drawbacks of the presented articles compared with the objective of this thesis.

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Chapter 2

Governing equations and numerical approach

CWE is based on the numerical simulation of the Navier-Stokes equations. These come from the balance laws making the hypothesis of Newtonian fluid. It is possible to define three fundamental aspects in CWE that are presented separately but that are intrinsically linked to each other:

- Turbulence model
- Equations discretization
- Grid generation

In this chapter firstly the Navier-Stokes equations will be obtained and then the first two aspects will be discussed. The third and last one will be the topic of the next chapter due to its relevance for the thesis.

2.1 Governing equations

In order to obtain the governing equations, firstly the balance laws are discussed. For the purpose of the thesis only the mass and momentum balance laws are required in order to obtain informations on pressure and velocity and so only these ones are discussed. It is important to underline that other balance laws exist, for example the energy balance is used to obtain informations on the temperature. These laws are very general and, as a matter of fact, they are the starting point for any science based on the continuum hypothesis like structural mechanics, multiphase problems and so on.

After that, it arises that the obtained system is not determined due to the fact that the unknowns are more than the equations. To overcome this difficulty it is necessary to take into account the nature of the flow and to assume a constitutive relation. In CWE it is assumed that air behaves like a Newtonian fluid.

2.1.1 Balance laws

Fluid Dynamics is based on the Continuum assumption that lets to define locally mechanical properties of the fluid. To the geometrical point with zero volume a fluid particle is
associated described by its values of density and velocity by mean of a statistical average of the molecules properties. This hypothesis is acceptable if there exists a length scale $L_2$, the particle scale, in between $L_1$ and $L_3$ such that

$$L_1 \ll L_2 \ll L_3$$

where $L_1$ and $L_3$ are the lengths of respectively microscopic and macroscopic inhomogeneities as shown in Figure 2.1. For example $L_1$ can be the molecular mean-free-path. Under this assumption it is now possible to define the density $\rho$ and the velocity $u$ fields.

![Figure 2.1: Average temperature with respect to length scales. Any fluid property like density or velocity can substitute the temperature. The figure is from [14].](image)

By defining a generic control volume $\mathcal{V}$, a finite region that contains infinitely many fluid particles, it is possible to describe mathematically how a flow quantity can change in it. A key role is played by the amount of flow property that enters or exits to the volume through the boundary $\partial\mathcal{V}$. This quantity is called flux.

1. **Mass conservation**: it is a particular case of the mass balance under the assumption that the total mass of the fluid can not change and so source terms do not exist. In this scenario the total fluid mass can change in the control volume only because of the mass flux. Usually the flux is positive if the mass goes out the volume and negative if it goes in. Indeed the mass conservation reads

$$\frac{\partial}{\partial t} \int_{\mathcal{V}} \rho \, d\mathcal{V} + \oint_{\partial\mathcal{V}} \rho (u \cdot n) \, dS = 0.$$  \hspace{1cm} (2.1)

Using the Gauss theorem, assuming fields sufficiently smooth, and because the equation is valid for any control volume $\mathcal{V}$, the local form is obtained

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0.$$  \hspace{1cm} (2.2)
2. Governing equations and numerical approach

The above equation can be simplified if the fluid is assumed to be *incompressible* and so the density \( \rho \) is constant. This hypothesis is acceptable in the CWE problems where the air speed is lower than 0.3 Mach. Then, the local mass conservation reads

\[
\nabla \cdot \mathbf{u} = 0. \tag{2.3}
\]

2. *Momentum balance:* this law says that the total momentum in the control volume can change by the effect of forces acting on the mass element. The forces can be either volumic, called also body forces, or superficial, called also stresses.

The integral form of the momentum balance is

\[
\frac{\partial}{\partial t} \int_V \rho \mathbf{u} \, dV + \oint_{\partial V} \rho \mathbf{u} \cdot \mathbf{n} \, dS - \oint_{\partial V} (\sigma \cdot \mathbf{n}) \, dS = \int_V \rho \mathbf{f}_b \, dV, \tag{2.4}
\]

where \( \sigma \) is the second order Cauchy stress tensor. The volumic forces term \( \mathbf{f}_b \), that includes for example the gravity effect, are neglected in aerodynamics.

Using the Gauss theorem like in the mass conservation law, the differential form is obtained:

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) - \nabla \cdot \sigma = 0. \tag{2.5}
\]

### 2.1.2 Constitutive relation and Navier-Stokes equations

In the tridimensional space, the derived system is made of four equations, one from the mass conservation and three from the momentum balance, but it contains nine unknowns: \( \mathbf{u} \) and six components of the symmetric tensor \( \sigma \) (the density \( \rho \) is also an unknown if the incompressibility assumption is not available). The system is therefore not closed and a constitutive relation is needed to write the Cauchy tensor as a function of the pressure, the velocity and their gradients.

For incompressible Newtonian fluids, the viscous part of the Cauchy tensor is assumed to be linear to the deformation tensor \( \mathbf{D} \) and so the constitutive relation reads

\[
\sigma_{ij} = -p\delta_{ij} + 2\mu D_{ij} = -p\delta_{ij} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{2.6}
\]

where \( p \) is the pressure that influences only the diagonal terms of the stress tensor and \( \mu \) is the *dynamical viscosity* or *molecular viscosity*.

Substituting the expression (2.6) into (2.5) and using the (2.3), the Navier-Stokes equations are obtained

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \mu \Delta \mathbf{u} = 0. \tag{2.7}
\]

The last equation can be divided by the constant density. By defining the *kinematic viscosity* \( \nu = \frac{\mu}{\rho} \), the final closed system is

\[
\begin{cases}
\nabla \cdot \mathbf{u} = 0, \\
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \nu \Delta \mathbf{u} = 0.
\end{cases} \tag{2.8}
\]
2.1.3 Initial and boundary conditions

In order to work with a well-posed differential problem, initial and boundary conditions must be imposed.

For the boundary conditions on the obstacle’s wall a usual condition is that the fluid can not pass through the obstacle. Assuming that the obstacle is fixed, this is mathematically described by the condition

\[ u \cdot n = 0 \]  \hspace{1cm} (2.9)

where \( n \) is the normal to the surface.

If the considered fluid is viscous, like the air in CWE problems, the no slip condition

\[ u = 0 \]  \hspace{1cm} (2.10)

is imposed on the wall.

The computation domain must be a bounded region and, as a consequence, non-physical boundaries are defined. Usually in the inlet the velocity field is imposed. In the outlet the normal component of the velocity field is set equal to zero and the pressure is imposed in order to define it uniquely. Indeed, from (2.8) it can be observed that the pressure field is defined unless an additive constant. Finally on the other boundaries periodic boundary conditions are imposed.

In the initial conditions, the fields \( u \) and \( p \) must be described in all the computation domain and they have to satisfy the differential system and the boundary conditions. The choice influences the number of time steps required to achieve convergence.

2.2 Turbulence models

Before starting the discussion about turbulence models and their applications in CWE, it is important to understand the main features of the turbulence.

Turbulence is a flow regime that occurs usually at high Reynolds numbers after a transition from the laminar behaviour in the system where the latter is unstable. It shows mixing properties that tend to homogenize the flow properties like momentum or temperature and for this reason it is often associated to the viscosity property.

In a turbulent regime the physical fields, that instantaneously are intrinsically tridimensional, evolve erratically in both time and space and the flow shows high vorticity.

The turbulence is a multiscale phenomenon where temporal and spatial fluctuations vary in wide time and length scales. The biggest length scale is usually denoted with \( \Lambda \) and the smallest with \( \lambda \). At each length scale \( l \in [\lambda, \Lambda] \) corresponds a Turbulent Kinetic Energy (TKE) that increases with respect to the eddy dimension and a Reynolds number defined as

\[ Re_l = \frac{lu_l}{\nu} \]  \hspace{1cm} (2.11)

where \( u_l \) is the scale of the fluctuating velocity associated to \( l \). Figure 2.2 shows the energetic distribution of the eddies.
2. Governing equations and numerical approach

While the scales are easily distinguishable in the energy domain, characterized by a continuous spectrum, in the spacial domain this is not the case because all scales are merged.

Eddies with dimension $\Lambda$ take their energy by the mean field. Then they splits into several smaller eddies, each one with a fraction of the initial energy. These eddies lie to the intermediate scales called inertial scales. This name is due to the fact that the inertial effects are dominant. As a matter of fact in a CWE scenario $Re_{\Lambda} \approx \frac{Re}{100} \gg 1$ and, as a consequence, scales smaller than $\Lambda$ can still have high inertial effects.

After that the vortexes in the inertial scales split in even smaller ones with length scales of the order of $\lambda$. This scales are called Kolmogorov scales. Finally these eddies are dissipated because the viscosity effects are important, indeed $\lambda$ is such that $Re_{\lambda} = O(1)$.

This is the motivation why a smaller scale than $\lambda$ can not be observed.

All this process is called turbulent energy cascade.

2.2.1 Direct Numerical Simulation

The Navier-Stokes equations are mathematically suitable to simulate turbulent flows. The Direct Numerical Simulation (DNS) consists on the numerical discretization of the Navier-Stokes equations without any other modelling.

Even if it is the most accurate approach, it is computationally very expensive because of the necessity to simulate all the turbulence scales and, in particular, the Kolmogorov scales.

$\lambda$ is too small to be experimentally measured, but an estimation can be obtained through a dimensional analysis. Because the Kolmogorov scales are linked to the eddies dissipation, $\lambda$, a length, has to be proportional to both the kinetic viscosity $\nu$, dimensionally $m^2/s$, and the internal energy dissipation rate $\varepsilon$, dimensionally $m^2/s^3$. With the same approach
also the time scale $t_\lambda$ can be established. The estimations are

$$\lambda \propto \left(\frac{\nu^3}{\varepsilon}\right)^\frac{1}{4} = Re^{-\frac{5}{4}}, \quad t_\lambda \propto \left(\frac{\nu}{\varepsilon}\right)^\frac{1}{2}.$$  

(2.12)

In order to obtain an accurate simulation, the spacial and time discretization must be proportional to these values. In a CWE problem with $Re = O(10^6)$, the corresponding Kolmogorov scales have $\lambda = O(10^{-7})$ m. Therefore the corresponding tridimesional mesh (the turbulence is a trigidimesional phenomenon) requires $O(10^{16})$ points and the temporal discretization must have $O(10^5)$ time steps to guarantee numerical stability. By this analysis it is clear that DNS is computationally unsustainable for industrial applications and it is used only for academic purposes in order to study the physical behaviour of turbulence.

### 2.2.2 Reynolds-Averaged Navier-Stokes

In the applications, in order to study the flow effects on structures like square cylinders in CWE, the knowledge of the mean fields are sufficient. The Reynolds-Averaged Navier-Stokes (RANS) methods are based on the splitting of the generic quantity $\varphi$, depending on space and time, at point $x_i$ in

$$\varphi(x_i, t) = \overline{\varphi}(x_i, t) + \varphi'(x_i, t)$$  

(2.13)

where $\overline{\varphi}$ is the mean component of $\varphi$ and $\varphi'$ is the fluctuating one.

In an unsteady problem the mean component is defined using an ensemble averaging operator

$$\overline{\varphi}(x_i, t) = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} \varphi_n(x_i, t)$$  

(2.14)

where $N$ is the number of members of the set of unsteady flows characterised by the same variables.

[Figure 2.3: Time averaging for unsteady flows. Image from [18].]
An important property of the averaging operator is that $\overline{\varphi} = 0$, i.e. the fluctuating component has zero mean. By applying the mean operator to the Navier-Stokes equations in (2.8), the result is

$$
\begin{align*}
\frac{\partial \overline{u}_i}{\partial x_i} &= 0 \\
\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left( \overline{u}_i \overline{u}_j + \overline{u}_i' \overline{u}_j' \right) = -\frac{1}{\rho} \frac{\partial \overline{\rho}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \nu \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) \right].
\end{align*}
$$

(2.15)

The last equation in (2.15) can be rewritten as

$$
\frac{\partial \overline{u}_i}{\partial t} + \overline{u}_j \frac{\partial \overline{u}_i}{\partial x_i} = -\frac{1}{\rho} \frac{\partial \overline{\rho}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \nu \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) \right] - \frac{\partial}{\partial x_j} \left( \overline{u}_i' \overline{u}_j' \right).
$$

(2.16)

This equation, if the last term is not considered, is formally identical to the classic equation in the Navier-Stokes system (2.8). The last term contains the divergence of the Reynolds stress tensor defined as $R_{ij} = \overline{u}_i' \overline{u}_j'$. The components of the fluctuating velocity are not statistically independent from each others and they can not be neglected.

The resulting RANS equations are not closed because in addition to the mean fields $\overline{u}$ and $\overline{p}$ also the Reynolds tensor components are unknown. It has to be observed that this tensor is symmetric.

With the aim to close the system, a first approach is to obtain exact equations for each component of the Reynolds tensor. In order to derive the equation for $R_{ij}$, it is sufficient to take equations for $u_i$ and $u_j$ in (2.8), then multiply the first one by $u_j$ and the second one by $u_i$, sum the two equations and finally applying the average operator. Even if these equations are exact, because they are obtained directly from the Navier-Stokes system, they can not be directly used because they contains terms that need to be modelled. In addition, this approach is not very used due to the computational cost to solve this system. As a matter of fact, with this approach three or six new equations, respectively in the bidimensional and tridimensional case, are coupled to the RANS equations.

A second way to find a closure to the system is to use the Boussinesq eddy-viscosity approximation based on the analogy between molecular viscosity and the turbulence mixing and dissipation properties

$$
\overline{u}_i' \overline{u}_j' = \nu_t \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right).
$$

(2.17)

$\nu_t$ is called turbulent viscosity and it is unknown.

The methods based on this approximation are called linear isotropic models. The term linear refers to the linear relation between the Reynolds tensor and the deformation tensor. The isotropic one is due to the scalar nature of the eddy viscosity $\nu_t$. Since $R$ is a tensor, it would be more appropriate to define the eddy viscosity as a tensor instead of a scalar but it would complicate the treatment.

The turbulent viscosity can be written, through a dimensional analysis, using the turbulent kinetic energy $k = \frac{1}{2} \overline{u}_i' \overline{u}_i'$ and the already defined turbulent energy dissipation rate $\epsilon$. 
2. Governing equations and numerical approach

The final relation is

\[ \nu_t = C_\mu \frac{k^2}{\varepsilon} \quad (2.18) \]

where \( C_\mu \) is a dimensionless constant.

The \( k - \varepsilon \) RANS methods add to the RANS equations, with the Boussinesq hypothesis, two differential equations for \( k \) and \( \varepsilon \).

The equation for the turbulent kinetic energy can be obtained analytically using the RANS and Navier-Stokes equations and it reads

\[
\frac{\partial k}{\partial t} + \frac{\partial (\bar{u}_j k)}{\partial x_j} = -\frac{u_i' u_j'}{\rho} \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \frac{p' u_j'}{\rho} + \frac{1}{2} u_j' u_i' + \nu \frac{\partial k}{\partial x_j} \right) - \nu \frac{\partial u_i'}{\partial x_k} \frac{\partial u_i'}{\partial x_k} + P_k - \varepsilon, \tag{2.19} \]

Equation (2.19) describes how \( k \) can evolve in time and space. Each term on the right hand side has a physical interpretation:

- \( P_k \) is always greater than zero by physical motivations and for this reason it is called \textit{Production term}. It represents the rate at which kinetic energy is transferred from the main flow to the turbulence. It can be modelled using the Boussinesq hypothesis.

- \( D_k \) is the \textit{Diffusion term}. Diffusion is induced by a pressure gradient, by \( k \) itself and by the viscosity. The first two terms need to be modelled. In particular they are modelled using the gradient assumption for which \( k \) moves from regions where it has higher values to regions with a lower one. It is expressed as

\[
\frac{p' u_j'}{\rho} + \frac{1}{2} u_j' u_i' + \nu \frac{\partial k}{\partial x_j} = -\nu \frac{\partial u_i'}{\partial x_k} \frac{\partial u_i'}{\partial x_k} \quad (2.20) \]

where \( \sigma_k \) is a coefficient.

- \( -\nu \frac{\partial u_i'}{\partial x_k} \frac{\partial u_i'}{\partial x_k} \) is the definition of the \textit{turbulent energy dissipation rate} \( \varepsilon \). This term can not be modelled and it requires a partial differential equation.

Theoretically it could be possible to deduce an exact equation for \( \varepsilon \) as made for the turbulent kinetic energy. This operation would be analytically complicated and seven different terms should be modelled. For this reason it has been preferred to write an equation formally equal to the \( k \) one, except for the factor \( \varepsilon/k \) that is used to have terms dimensionally correct.

The final equations for the \( k - \varepsilon \) model are

\[
\begin{align*}
\frac{\partial k}{\partial t} + \frac{\partial (\bar{u}_j k)}{\partial x_j} & = \frac{\partial}{\partial x_j} \left[ \left( \frac{\nu_t}{\sigma_k} + \nu \right) \frac{\partial k}{\partial x_j} \right] + P_k - \varepsilon, \\
\frac{\partial \varepsilon}{\partial t} + \frac{\partial (\bar{u}_j \varepsilon)}{\partial x_j} & = \frac{\partial}{\partial x_j} \left[ \left( \frac{\nu_t}{\sigma_\varepsilon} + \nu \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \frac{\varepsilon}{k} C_{\varepsilon 1} P_k - \frac{\varepsilon}{k} C_{\varepsilon 2} \varepsilon.
\end{align*} \tag{2.21} \]

Usual values for the coefficients in (2.21), obtained through either experiments or computational optimization, are
This $k-\varepsilon$ standard formulation (STD) has the important drawback to overestimate the turbulent viscosity. As a matter of fact, a CWE simulation with the STD $k-\varepsilon$ model can predict a steady flow in problems that are not physically steady. For this reason a modification of this model, called RNG $k-\varepsilon$, has been proposed. In this approach some constants are changed and additional terms are used in the equations for $k$ and $\varepsilon$ in order to reduce correctly $\nu_t$.

Another way to deal with this inconvenience is to define another turbulent variable, instead of $\varepsilon$, and to write for it an equation. The chosen variable is $\omega$, defined such that

$$\nu_t = \frac{k}{\omega}. \quad (2.22)$$

The RANS simulations discussed in the next chapters will always be based on RNG $k-\varepsilon$ methods and, consequently, the features of the $k-\omega$ models are not discussed in this thesis. For details, [18] is recommended.

### 2.2.3 Large Eddy Simulation

The Large Eddy Simulation, LES, is an intermediate approach situated in between the DNS approach, where all the turbulence scales are simulated, and RANS approach, where all the turbulence scales are modelled. Looking at the energetic spectrum in Figure 2.2, it appears that eddies in the energetic interval carry almost all the turbulent energy, in particular more than 95%, and it should be suitable to simulate their contribution instead of modeling it. On the other hand, the main drawback of the DNS is the high number of required grid cells due to the necessity to capture the eddies in the Kolmogorov scales. In addition, the big scales are more affected by the boundary conditions and they do not behave isotropically. For example a big eddy near the wall will be elongated on the direction parallel to wall. At the contrary small eddies do not depend on the domain geometry and so they are more universal and easier to model.

For these reasons, LES aims to simulate only the eddies in the energetic scale, that strongly influence the values of the fluctuating forces and that are complicated to physically describe, and to model the small eddies in order to reduce the computational cost.

In the energetic domain, in order to make this scales separation, it is sufficient to choose a threshold wavenumber $\kappa_l$ in the inertial range such that if $\kappa < \kappa_l$ then the scale is simulated and, at the opposite, if $\kappa > \kappa_l$ the scale is modelled. This operation is straightforward if a low pass filter $G(\kappa)$ in the wavenumber domain is defined. Then, if $\varphi$ is a spatial quantity, the simulated result will be

$$\varphi(x) = G(x) \ast \varphi(x)$$

where $G$ is the Fourier anti-transformation of the filter and $\ast$ is the convolution operator.

As mentioned previously, while the turbulence scales are distinguishable in the energy domain, this is not the case in the spatial domain where, in addition, a mesh grid is
2. Governing equations and numerical approach

defined. If a vortex is smaller that the grid dimension, it can not be detected by the simulation. This motivation drives to the definition of a filter kernel $G(x, \kappa; \Delta)$ that depends on the grid dimension $\Delta$. In order to be coherent to the physical aim to filter eddies with wavenumbers greater than $\kappa_l$, $\Delta$ must be proportional to $l$.

A practical way to distinguish the simulated scales from the modelled ones is to adopt a numerical filter. This means that the mesh plays the filtering role and the scales with length $l$ are simulated if $l > \Delta$ and they are modelled if $l < \Delta$.

The Navier-Stokes equations can be filtered obtaining

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j}(\bar{u}_i\bar{u}_j) = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \nu \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \right].$$

(2.23)

The problem with equation (2.23) is that $\bar{u}_i\bar{u}_j \neq \bar{u}_i\bar{u}_j$ and so the subgrid-scale Reynolds number

$$R_{ij}^s = \bar{u}_i\bar{u}_j - \bar{u}_i\bar{u}_j$$

needs to be modeled.

A first model was proposed by Smagorinsky [19] in 1963 and it is based on a Boussinesq-like approximation

$$R_{ij}^s = \nu^s \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right).$$

(2.25)

The subgrid viscosity is, after a dimensional analysis, $\nu^s = \varepsilon^{1/3} (C_S \Delta)^{4/3}$ where $C_S$ is a dimensionless constant. The huge problematic of the Smagorinsky model is the not universality of $C_S$ that changes depending on the flux.

In general, the closure of the filtered equations is still nowadays an important research field.

2.3 Equations discretization

In order to computationally solve (or, more accurately, approximate) the system (2.8) a spatial and a temporal discretization must be defined. In this way the infinitely-dimensional Navier-Stokes equations are approximated to a corresponding finite system. The Finite Difference Method, FDM, has been the first spatial discretization method to be used since the beginning of CFD. It is based on the derivatives approximations by differences (hence its name), obtained from Taylor’s expansions, between the variable values in mesh points. Nowadays the most used methods are the Finite Element Methods, FEM, and the Finite Volume Methods, FVM, due to their flexibility to handle unstructured meshes necessary in complex geometries. The former is based on the variational formulation of the PDEs,
the latter on the integral conservative laws. All the simulations in this thesis are based on a FVM discretization and, for this reason, only this method is discussed.

2.3.1 Finite volume method and convective schemes

FVM starts from the balance law of the generic quantity \( \varphi \) that can be a scalar, a vector or a tensor. For example, as already discussed for the governing equations, \( \varphi \) can be the density or the momentum.

The spatial domain \( V \) is divided into subdomains, called cells or control volumes, \( V_i \) with \( i = 1, \ldots, N \) and the conservation law is then written for each of them:

\[
\frac{\partial}{\partial t} \int_{V_i} \varphi \, dV = - \int_{\partial V_i} f^c \cdot n \, dS + \int_{\partial V_i} f^d \cdot n \, dS + \int_{V_i} s \, dV. \tag{2.26}
\]

Equation (2.26) expresses that the total amount of \( \varphi \) in the cell can change because there is a flux of the quantity across the boundary and because source therms can create or destroy it. After a temporal discretization, it gives a scheme to compute the mean value of \( \varphi \) in each control volume.

For simplicity, it is supposed that there is not a source term, as already done in the mass and momentum laws. The flux is divided into the convective flux, linked to the transport effect made by the velocity field, and the diffusive flux, linked to the gradient of \( \varphi \).

\( V_i \) are chosen as polygons in 2D and polyhedra in 3D and, for this reason, the flux term integral in (2.26) can be expressed as the sum of integrals over the \( n \) faces of \( V_i \). Denoting by \( f \) a generic flux that can be either convective or diffusive, then

\[
\int_{\partial V_i} f \cdot n \, dS = \sum_{S=1}^{n} \int_{S} f \cdot n \, dS \approx \sum_{S=1}^{n} S \cdot f_S(\varphi_S) =: \sum_{S=1}^{n} S \cdot f_S \tag{2.27}
\]

where the surface integral has been approximated. \( S = |S|n \) and \( f_S \) is the flux in the face center.

The formula (2.27) presents the main problematic of the FVM formulation. In order to compute the flux terms, the knowledge of \( \varphi \) in the middle of the face \( S \) is required but the FVM gives information only about the average of \( \varphi \) in the cells. As a consequence in the past decades, many convective schemes have been proposed to reconstruct the value on the faces starting from the cell averages.

The most important convective schemes are now discussed. For sake of simplicity they will be presented in the monodimensional case. The complication induced by a bidimentional problem will be discussed in the next chapter about grid induced errors.

Let consider the configuration reported in Figure 2.4. The different convective schemes aim to build the value \( \varphi_e \) using the cell averages of the near cells. For this reason, the capital letter subscript denotes the average over the cell and not the value in the cell center.

For simplicity, it is assumed that the velocity is constant equal to \( a \) and the convective flux can be written as

\[
f^c = a \varphi.
\]
2. Governing equations and numerical approach

Figure 2.4: 1D domain where capital letters refer to the cells. \( e \) is the face between cell P and cell E.

1. **Central Differencing Scheme (CDS)**
   The value at the face is obtained through a linear interpolation between the two averages over the cells that share the face:

   \[
   \varphi_e = \lambda_P \varphi_P + \lambda_E \varphi_E
   \]  
   \[(2.28)\]

   where the coefficients

   \[
   \lambda_P = \frac{x_e - x_P}{x_E - x_P}, \quad \lambda_E = \frac{x_E - x_e}{x_E - x_P}
   \]  
   \[(2.29)\]

   weight with respect to the distance of the face to the cell centers. The condition \( \lambda_P + \lambda_E = 1 \) is always satisfied.

   While this scheme is stable for the diffusive flux, it is unstable and creates unphysical oscillations when used for the convective flux. This behaviour can be physically explained: while the diffusive flux is linked to the gradient and tends to average \( \varphi \) like a linear interpolation makes, the nature of the convective flux is connected to the velocity field and, as a consequence, a scheme that does not take into account the velocity fails in its reconstruction.

2. **Upwind Differencing Scheme (UDS)**
   The value at the face is set to be equal to the upwind cell value, i.e.

   \[
   \varphi_e = \begin{cases} 
   \varphi_P & \text{if } a > 0, \\
   \varphi_E & \text{if } a < 0.
   \end{cases}
   \]  
   \[(2.30)\]

   Using this definition the link between the convective flux and the velocity is kept. As a matter of fact this scheme is stable even if it is only first order accurate.

3. **Quadratic Upwind Interpolation for Convective Kinematics (QUICK)**
   This scheme, firstly proposed in [20] in 1979, takes into account the velocity but it uses three interpolation points to increase the spatial accuracy.

   The face value is

   \[
   \varphi_e = \begin{cases} 
   \frac{1}{3} \varphi_E + \frac{5}{6} \varphi_P - \frac{1}{6} \varphi_W & \text{if } a > 0, \\
   \frac{1}{3} \varphi_P + \frac{5}{6} \varphi_E - \frac{1}{6} \varphi_{EE} & \text{if } a < 0.
   \end{cases}
   \]  
   \[(2.31)\]
2. Governing equations and numerical approach

Several other convective schemes exist but they are all based on the idea of taking the information upwind like in the UDS and QUICK cases. They differ on the number of interpolation points and on the coefficients. It has to be observed that, in a multidimensional scenario with the non-linear Navier-Stokes equations, it becomes more difficult to define if a cell is upwind or downwind and for this reason schemes with a small number of interpolation points, like the QUICK one, are used.

2.3.2 Time discretization

The time discretization methods are usually divided into explicit methods and implicit methods.

Let consider the equation

$$\frac{\partial \varphi}{\partial t} + \mathcal{L}(\varphi) = 0 \quad (2.32)$$

where the operator $\mathcal{L}$ represent a linear operator that does not involve time derivations.

Let define a time discretization with time steps $t^i$ with $i = 1, ..., n$ with constant step size $\Delta t$.

The explicit and implicit first order methods compute $\varphi$ for $t = t^{n+1}$, denoted by $\varphi^{n+1}$, using its value at the previous time step.

1. First order explicit

The equation (2.32) is discretized as

$$\frac{\varphi^{n+1} - \varphi^n}{\Delta t} + \mathcal{L}(\varphi^n) = 0.$$

Consequently, $\varphi^{n+1}$ can be immediately obtained:

$$\varphi^{n+1} = \varphi^n - \Delta t \mathcal{L}(\varphi^n) \quad (2.33)$$

2. First order implicit

The equation (2.32) is discretized as

$$\frac{\varphi^{n+1} - \varphi^n}{\Delta t} + \mathcal{L}(\varphi^{n+1}) = 0.$$

At the contrary of the explicit case, in order to obtain $\varphi^{n+1}$, a linear system must be solved:

$$\varphi^{n+1} + \Delta t \mathcal{L}(\varphi^{n+1}) = \varphi^n. \quad (2.34)$$

Apparently, the explicit method seems to be a better choice because it does not require the resolution of a linear system that, at least, is strongly sparse due to the fact that a cell exchange fluxes only with its neighbors.

Actually, the implicit case has the huge advantage to be unconditionally stable. This means that this numerical scheme converges for any value of $\Delta t$. Of course, the bigger is the time step and the less accurate is the solution but convergence is guaranteed. At the contrary, the explicit scheme is unconditionally unstable. This means that the time step $\Delta t$ must be chosen small enough, depending on the spatial volume sizes, to obtain
a convergence of the scheme. If the temporal step is bigger than the threshold value, the scheme diverges. This drawback is particularly problematic in grid refinement studies and in problems with different volume sizes where the time step must be selected to fit with the smallest one.

For example, in case of the transport equation with $\mathcal{L}(\varphi) = a\varphi$, it is well known that the Courant-Friedrichs-Lewy (CFL) conditions yield: the explicit scheme is stable if and only if

$$\frac{a \Delta t}{\Delta x} < 1. \quad (2.35)$$

Before ending this chapter it is important to observe that the Navier-Stokes momentum equations cannot be classified in the (2.32) framework because of the presence of the non-linear convective term $u \cdot \nabla u$. In order to overcome this problematic, in the codes, inside the temporal loop there is an inner loop associated to the non-linearity that linearise the problem at each step.
Chapter 3

Computational grids

Any CWE simulation is based on three different aspects: turbulence models, interpolation rules, more in particular convective schemes, and finally the mesh generation. The latter is discussed separately in this chapter due to its central role in the thesis but it is important to observe that the previous mentioned aspects are equally important. Each of them generates errors that are added together. If one of these errors is orders of magnitude bigger then the others, the numerical solution will not be accurate even if the other two aspects have been dealt suitably. Lastly, this three components are not independent to each other. At the contrary they are mutually linked. For example the LES turbulence model is based on the grid elements size.

In this chapter firstly some terminology will be introduced and the general mesh categories are presented. Then the errors induced by the mesh and the grid quality are discussed. Finally, some usual mesh quality indicators are defined.

3.1 Mesh classification

The mesh is a partition of the computational domain into cells that are the basis of the FVM discretization. The more are these cells and the more accurate is, in general, the numerical solution and the more expensive is the simulation.

3.1.1 Structured and unstructured meshes

Depending on the way the cells are created and stored in memory three different classes can be defined:

- **Structured grids**
  They are characterized by cells that are disposed with a regular pattern that can be observed looking at their connectivity. This peculiarity lets to store in memory the informations such that it results easier the research of a particular cell. Another important aspect of this meshes is that, if the cells are efficiently numbered, the sparse linear system associated to the discretization is band with a small bandwidth. For such systems, very efficient solvers have been developed.
  Unfortunately, the generation of structured domains becomes hard, if not even
impossible, in presence of complicated geometries or computational domains. In addition, usually it can not be made by mesh generator algorithms, that are coded to handle any type of geometries.

- **Unstructured grids**
  The opposite scenario is represented by the unstructured grids. Their main advantages are that they can be generated by meshing algorithms and they can used in industrial applications with complex geometries. On the other hand, the cells connectivity is not linked to their memory storage and the search of a particular cell can be difficult or even impossible. Moreover the associate linear system needs a reordering to obtain a band system. This can be performed efficiently with, for example, a reversed Cuthill-McKee algorithm [27] based on graph theory but it is, nevertheless, quite expensive.

- **Hybrid grids**
  The computational domain can be split in several regions. If in some of them the mesh is structured and in the others the mesh is unstructured, then the grid is called hybrid.
  This approach is the more flexible because it allows to create an unstructured mesh in most of the domain except for limited areas that, however, are important for the flux features (for example the boundary layer or the wake region) in which a structured mesh can be defined.

It is important to observe that the structured/unstructured classification does not involve neither the concept of mesh quality nor the cells shape but only of connectivity pattern. An unstructured mesh can be qualitatively better (in the next section the meaning of this expression will be clarified) than a structured one or vice versa. In addition structured and unstructured grids both can be made of, for example, triangles as in Figure 3.1.

![Structured and unstructured meshes](image)

**Figure 3.1**: Structured and unstructured meshes with the same cells shape.

Other classifications exist. A mesh is said to be **uniform** if all the cells have the same size. In the contrary case it is called **non-uniform**. The former are not used in the CWE
problems and the reason will be cleared in the next section. This fact justify the wide use of implicit schemes for the spatial discretization: in non-uniform meshes the time step must be chosen looking at the smallest cell, increasing hugely the number of required time steps.

Finally a grid can be body-fitted or boundary-fitted. In the first case the cells faces orientation follows the direction of the obstacle walls. This mesh type is also denoted by o-type. Examples can be the last two meshes around rectangular cylinders in 1.6 or around the streamlined body in 1.18. In the boundary-fitted one the faces orientation is given by the computation domain boundaries. Body-fitted meshes are often used in aerodynamic of stream-line bodies because the wake region is narrow.

In general the choice of the mesh typology plays a key role in the computation. Firstly it influences the number of control volumes. The more they are and the bigger is the computational cost. Then, it influences the cells quality and so the accuracy, as it will be observed in the following part of this chapter.

3.2 Mesh induced errors and mesh quality

Errors induced by the mesh can have different causes. It has been decided to divide them in errors due to the cells size and errors due to the cells quality.

3.2.1 Errors linked to the truncation error

An important quantity that is widely used to study the accuracy of a discretization method is the local truncation error. For simplicity only the case of convective schemes is discussed. As mentioned in the previous chapter, the exact flux that satisfy the exact differential equation is not known and so it has to be numerically reconstructed using a convective scheme. Then the numerical solution of the FVM satisfy the discretized scheme with the numerical flux and not the exact flux. The local truncation error is the error committed by using the cell averages of the exact problem into the numerical schemes with the numerical flux, divided by the cell size $\Delta x$ because it is the local error. The local truncation error of a convective scheme can be expressed, in a 1D problem (in 2D and 3D scenarios the truncation error can be defined for each direction), as

$$\tau(\Delta x) = \alpha (\Delta x)^p \frac{\partial^{p+1} \varphi}{\partial x^{p+1}}$$

where $\alpha$ is a constant coefficient and $\Delta x$ is the cell size. $p$ is called order of accuracy of the scheme. If a convective scheme interpolates exactly a polynomial of degree $d$, then the scheme has order $p = d + 1$. For this reason in the previous chapter the UDS, that interpolates exactly a polynomial of degree zero, has been classified as a first order accurate convective scheme.

Finally, the order of the derivative determines the typology of the error. It can be proven through a Fourier analysis that derivatives of even order enhance diffusive errors. At the opposite, derivatives of odd order cause dispersive errors.
Looking at (3.1), it immediately appears that the grid resolution affects the accuracy because the smaller is \( \Delta x \) and the smaller is \( \tau(\Delta x) \).

Moreover, the truncation error is proportional also to the spatial derivative of \( \varphi \). As a consequence, in a uniform mesh with spatial step \( \Delta x \) regions characterized by bigger gradients are more affected by errors. The solution to this problem, in order to have a local truncation error uniform all over the grid, is to reduce the cells size \( \Delta x \) in correspondence of the zones where the gradient of \( \varphi \) is higher. For this reason non-uniform meshes are used in CWE where, for example, the flow has high vorticity and so big velocity gradients. It seems that the problem of having a uniform truncation error has been solved by defining smaller cells where \( \varphi \) changes quickly in space. The intrinsic problem of this solution is that \( \varphi \) is the unknown of the problem and, in fact, the aim of the simulation is to approximate it. How could be possible to refine the mesh \textit{a priori} in some regions depending on the gradient of \( \varphi \) if this one is known only \textit{a posteriori}?

The answer to this problem is that the non-knowledge of \( \varphi \) can be partially overcome by a physical familiarity with the problem that has to be simulated. The mesh is usually refined where a priori it is known that the flux will be characterized by high changes as in the boundary layer, near wall regions with high curvature (in case of bluff bodies near the corners) and in the wake, all featured by high gradients of the velocity and pressure fields.

3.2.2 Mesh quality and errors induced by low-quality grids

In addition to the mesh elements size, an important role is also played by the quality of the cells. This is intrinsic of each cell and it depends on neither the cell size nor the cell position in the domain. Poor-quality meshes can generate higher errors than ones induced by coarser grids highly qualitative. For this reason techniques that improve the quality of the grid can be fundamental to increase the accuracy of the solution without increasing the computational cost.

Three different quality indicators are presented. For each of them the induced error is investigated. The first one can be discussed for the 1D case and consequently the same notation of the previous section, described in Figure 2.4, is used. At the contrary, for the last two the notation will follow Figure 3.2 because they are intrinsically linked to at least 2D problems where sometimes it is difficult, if even impossible, to determine the North, South, East, West neighbours of a cell.

1. \textbf{Aspect ratio}

The aspect ratio, or equivalently growth factor, is the ratio of characteristic lengths of adjacent cells. Ideally, neighbour cells should have the same size and the ratio should be equal to one. This feature increases the order of accuracy of the interpolation schemes. For example in the CDS scheme, used for the interpolation of the gradient in the diffusive flux, the first derivative is discretized as

\[
\left( \frac{\partial \varphi}{\partial x} \right)_e = \frac{\varphi_E - \varphi_P}{x_E - x_P} + \frac{(x_e - x_P)^2 - (x_E - x_e)^2}{2(x_E - x_P)} \left( \frac{\partial^2 \varphi}{\partial x^2} \right)_e + o((x_E - x_P)^2). \tag{3.2}
\]

If the grid is uniform then the coefficient before the second derivative cancels out
and the order is two, otherwise it is one.

2. Orthogonality

The orthogonality is associated to the angle $\theta_{I-II}$ between the line that connects the cells centers of two adjacent control volumes and the normal vector to the face shared among them. If the angles are equal to zero, the grid is called orthogonal, otherwise it is called non-orthogonal.

By definition, given firstly in [2], this property refers to the face shared by two control volumes and not to a single cell. For this reason the orthogonality is always satisfied in 1D meshes where the faces reduce to nodes.

The effect of the non-orthogonality can be studied starting from the relation (2.27) applied to the diffusive flux

$$\nabla \cdot (\nu \nabla \varphi) \approx \sum_{f=1}^{n} \nu \mathbf{F} \cdot (\nabla \varphi)_f.$$  (3.3)

Let define $\mathbf{d}$ as the vector that connects the cells centers $I$ to $II$ one. Two cases are possible:

- orthogonality ($\mathbf{F}_{I-II} \parallel \mathbf{d}$)

  Then $(\nabla \varphi)_{f_{I-II}}$ can be reconstructed directly by using a CDS scheme as

  $$\mathbf{F}_{I-II} \cdot (\nabla \varphi)_{f_{I-II}} \approx F_{I-II} \frac{\varphi_{II} - \varphi_I}{d}.$$  (3.4)

- non-orthogonality ($\mathbf{F}_{I-II} \not\parallel \mathbf{d}$)

  Then the vector $\mathbf{F}_{I-II}$ can be split as $\mathbf{F}_{I-II} = \Delta + \mathbf{k}$ where

  $$\Delta = \frac{\mathbf{d} \cdot \mathbf{F}_{I-II}}{||\mathbf{d}||} \mathbf{d}.$$  (3.5)

  Using the definition of $\Delta$ in (3.5), it follows that $\Delta \parallel \mathbf{d}$ and $\mathbf{k} \perp \mathbf{d}$. So

  $$\mathbf{F}_{I-II} \cdot (\nabla \varphi)_{f_{I-II}} = \Delta \cdot (\nabla \varphi)_{f_{I-II}} + \mathbf{k} \cdot (\nabla \varphi)_{f_{I-II}}.$$  (3.6)

  The first term in the right hand side of (3.6) can be discretized as before with a CDS interpolation scheme

  $$\Delta \cdot (\nabla \varphi)_{f_{I-II}} \approx \Delta \frac{\varphi_{II} - \varphi_I}{d}$$  (3.7)

  and the second term can be approximated as a linear combination of the gradients of $\varphi$ in points $I$ and $II$

  $$\mathbf{k} \cdot (\nabla \varphi)_{f_{I-II}} \approx \mathbf{k} \cdot (\lambda (\nabla \varphi)_I + (1 - \lambda)(\nabla \varphi)_{II}).$$  (3.8)
3. Computational grids

λ depends on the orthogonal distance between I and the face $F_{I-II}$. $(\nabla \varphi)_{I,II}$ can be obtained using the Gauss theorem

$$\int_{V_i} \nabla \varphi \, dV = \oint_{\partial V_i} \varphi \, n \, dS \approx \sum_{f=1}^{n} S_f \varphi_f$$  \hspace{1cm} (3.9)

with $i = I, II$ and, consequently,

$$(\nabla \varphi)_i \approx \frac{1}{|V_i|} \sum_{f=1}^{n} S_f \varphi_f$$  \hspace{1cm} (3.10)

where $\varphi_f$ are reconstructed with a CDS.

If the correction term (3.8) is not taken into account, then the scheme accuracy decreases from second to first order and the associated error can significantly affect the solution.

In [2] a first approach have been proposed based on (3.10). ANSYS FLUENT commercial code, used for the resolution of the flow around the square cylinder in next chapters, uses an appropriate correction term as observed in [21].

3. Skewness

Skewness is defined as the distance between the face center $f_{I-II}$ and the intersection $f^S_{I-II}$ between the face and the line that connects the two cells centers. As in the non-orthogonal case, this characteristic has not meaning for a 1D grid.

The associated error is caused by the wrong location of the reconstructed value. As a matter of fact, in order to obtain a second order CDS, the equation (2.27) is based on the reconstruction of the flux in the face center. At the contrary, using a centered interpolation scheme, the flux is reconstructed on the line between I and II, more precisely in $f^S_{I-II}$.

Let study the effect on the convective flux defined as

$$\nabla \cdot (\rho u \varphi).$$  \hspace{1cm} (3.11)

In case of high quality mesh without skewness, the numerical convective flux is defined as

$$F^c = \sum_{f=1}^{n} \rho S \cdot (u \varphi)_f.$$  \hspace{1cm} (3.12)

$\rho$ is considered constant because of the incompressibility assumption.

At the contrary, the numerical result obtained with a linear interpolation with a skewed face is

$$F_{sk}^c = \sum_{f=1}^{n} \rho S \cdot (u \varphi)_{fs}.$$  \hspace{1cm} (3.13)

The error associated to the wrong position for the interpolation of $\varphi$ is then defined as

$$E_{sk}^c = \sum_{f=1}^{n} \rho S \cdot (u \delta \varphi)_f, \quad \text{where} \quad \delta \varphi_{f_{I-II}} = s \cdot (\nabla \varphi)_{f_{I-II}}$$  \hspace{1cm} (3.14)
with \( \mathbf{s} = \mathbf{x}_{f_{I-II}} - \mathbf{x}_{f_{I-II}}' \).

In has to be observed that the error definition in (3.14) is not the difference between \( F^c \) and \( F^c_{sk} \) because, in this case, the error induced by a wrong interpolation of the velocity field should taken into account. At the contrary, this error definition is helpful to study the error generated only by \( \varphi \).

If \( \mu_{sk} \) is defined as

\[
\mu_{sk} = \rho \mathbf{u}_{f_{I-II}} \cdot \mathbf{s}
\]

that is dimensionally a viscosity, then it is immediate to observe, using the Gauss theorem, that the skewness enhances a diffusive error

\[
E^c_{sk} = \nabla \cdot (\mu_{sk} \nabla \varphi).
\]

As expected, the bigger is the skewness and the bigger is \( \mu_{sk} \) and, as a consequence, the associated error.

If, for example, a UDS scheme is used to reconstruct the velocity field, the skewness error is relevant for highly skewed grids with \( ||\mathbf{s}|| \approx ||\mathbf{d}|| \).

Figure 3.2 compares also the optimal case of a orthogonal and not skewed face to the non-orthogonal and skewed ones.

It has been described how mesh features as non-orthogonality and skewness can affect negatively on the accuracy of the simulation. It is important to observe that there is a strong link between mesh characteristics and interpolation schemes. This relation drove the research on the reduction of errors due to non-orthogonality and skewness in two different directions:
1. adding corrective terms in the interpolation schemes that take into account poor-quality meshes and that cancels out with orthogonal and not-skewed faces. This approach has been partially discussed;

2. generating qualitatively better meshing algorithms or algorithms that, given a specific mesh, change the location or the connectivity of determined cells in order to improve the quality.

### 3.3 Other mesh quality indices

It is known that the mesh quality, and not only cells dimensions, affects the accuracy of the solution. Three main characteristics have been detected: the grid stretching, the non-orthogonality and the skewness.

A natural idea is to define some quantities, referred to the grid, that can indicate a priori the quality of the mesh. The natural choice with a Finite Volume approach would be to use directly the indicators associated to the faces defined in the previous section. However, often and mostly in commercial codes different indicators are used. These are not unique and universal. Usually each of them refers to only one of the mesh defects and it is defined for particular control volumes shapes.

#### 3.3.1 Commercial codes indicators

Different usual indicators, defined in commercial codes, are presented. Some of them are defined only for 2D meshes.

If \( r \) and \( R \) are the radii of the, respectively, inscribed and circumscribed circles of a triangular volume, then
\[
Q_{AR} = \frac{1}{2} \frac{R}{r} \geq 1
\]

is called *aspect ratio*. \( Q_{AR} = 1 \) only for equilateral triangles. Because a mesh made of equilateral triangle is orthogonal, this indicator can be interpreted as a measure of the orthogonality.

\( Q_{AR} \) has the drawback to be defined only for triangles. Another quantity, more general, that an be useful to investigate the orthogonality is the *edge ratio*
\[
Q_{ER} = \frac{\max(s_1, s_2, \ldots, s_n)}{\min(s_1, s_2, \ldots, s_n)} \geq 1
\]

where \( s_i \) with \( i = 1, \ldots, n \) are the edges lengths. This quantity is exactly equal to one for equilateral triangles and for squares. It has to be noticed that \( Q_{ER} \) is not able to optimally detect the orthogonality. As a matter of fact, a mesh made of identical rectangles in orthogonal and not skew but \( Q_{ER} > 1 \).

The *equiangle skewness* is defined as
\[
Q_{EAS} = \max\left(\frac{\theta_{\max} - \theta_{eq}}{180 - \theta_{eq}}, \frac{\theta_{eq} - \theta_{\min}}{\theta_{eq}}\right)
\]

(3.19)
where $\theta_{eq}$ is the angle such that all the angles are equal (for example $\theta_{eq} = 60^\circ$ for triangles and $\theta_{eq} = 90^\circ$ for quadrilaterals). It holds $0 \leq Q_{EAS} \leq 1$ and it can be related to the skewness.

![Diagram](image)

(a) Aspect ratio  
(b) Equiangle skewness

Figure 3.3: Geometrical meaning of the aspect ratio and equiangle skewness.

The cell squishiness is calculated from the dot products of each vector pointing from the centroid of a cell toward the center of each of its faces $\mathbf{r}$, and the corresponding face area vector $\mathbf{S}_f$ as

$$Q_{CS} = \max_f \left\{ 1 - \frac{\mathbf{r} \cdot \mathbf{S}_f}{||\mathbf{r}|| \ ||\mathbf{S}_f||} \right\}. \quad (3.20)$$

Hence, the worst cells have this index close to one.

The last two indexes are defined in Fluent.

### 3.3.2 Indices based on Taylor expansions

The principal drawbacks of the above indicators are the non-universality and the restriction to 2D case.

In [28] universal indicators are defined and successively in [29] those quantities are defined also for 3D meshes.

Both articles are based on a cell-vertex FV discretization, i.e. the variables are defined on the nodes of the mesh and not on the cells centers. For this reason the gradient of the velocity, directly linked to the fluxes, is reconstructed on the nodes and not on the faces. Even with this difference, the indicators are defined starting from considerations that can be transposed in a cell FV approach.
Let denote with $\nabla^h u$ the approximation of $\nabla u$ obtained by using the quadrature rule (2.27) where the flux is substituted by the velocity gradient. The Truncation Error (TE) is defined as

$$E(x, y) = \nabla^h u - \nabla u.$$  

(3.21)

Then in the expression for TE, $u^h$, the numerical velocity, is substituted with its Taylor expansion. After this operation, the truncation error along the direction $i = x, y$ reads

$$E^i = e^i_{x} x u^i_{x} + e^i_{y} y u^i_{y} + e^i_{xy} x y u^i_{xy} + e^i_{xx} x x u^i_{xx} + e^i_{yy} y y u^i_{yy} \ldots$$  

(3.22)

where $u^i_j$ is the derivative along the $j$-th direction of the $i$-th component of the velocity field. The coefficients of the expansion are called error coefficients (EC). Their expression have been determined using the symbolic mathematics capability of Matlab. After having proved that the EC associated to the first derivatives are equal to zero if the numerical discretization is consistent, geometrical considerations are made to link the remaining EC to the stretching, the non-orthogonality and the skewness, Figure 3.5.

Figure 3.4: Cell-vertex FV approach in [28]. The dark surface is called medial dual area.

Figure 3.5: Images used in [28] to highlights cell features to the truncation error.
Since, effectively, the ECs increase if the mesh defects are more marked, the following coefficients are defined

\[ Q^i = \frac{e^{i}_{xx} + e^{i}_{xy} + e^{i}_{yy}}{L^i} \]  

(3.23)

where \( L^i \) is a local characteristic length along direction \( i \) used to normalize the coefficient.

Finally the sum of the two coefficients is defined and the final indicator

\[ Q = Q^x + Q^y \]  

(3.24)

is obtained.

A more accurate coefficient can be defined if also the ECs linked to the third derivatives are used.

The extension to the 3D case presented in [29] is simply based on 3D Taylor expansions.

The indicators presented in this section aim to provide a priori check on the mesh quality. The first indexes are not universal but they are defined on the most used cell geometries. At the contrary, the last one can be defined or any 2D or 3D cell.

The main drawback of all these indicators is the lack of exact correlations with non-orthogonality and skewness. As a matter of fact, each index is computed for each cell but non-orthogonality and skewness are involved in the fluxes interpolation and they are defined for each face.
3. Computational grids
Chapter 4

B/D = 1 application: simulation setup

In this chapter the settings of the numerical simulations considered in this thesis are described. First of all, the numerical approach is presented. Then, starting from the informations that can be extrapolated from FLUENT, the quality of the four different grids that have been used are discussed. More in particular, the four meshes differ only in the near wall region. In this way the effects of the grid in a small region, that however is very important for the simulation, can be investigated looking at the simulated flux. This discussion will be the topic of the next chapter.

4.1 Simulation settings

A RANS 2D approach has been chosen because it is able to correctly capture the detachment phenomena without having the computational cost that would require a 3D LES turbulence model. More in particular a RNG \( k - \varepsilon \) model is used.

The Reynolds number is set to be equal to \( Re = 2.2 \cdot 10^4 \), a reference value in the CWE literature.

The problem has been set to be dimensionless, i.e. the physical properties are equal to

\[
\rho = 1, \quad B = D = 1, \quad U_\infty = 1, \quad \mu = \frac{1}{Re} = 4.54 \cdot 10^{-5}
\]

where the dynamic viscosity depends on the Reynolds number.

As already observed in the governing equations chapter, the simulations must be performed in a bounded domain whose dimension can not be determined by physical considerations because the problem in settled in an unbounded region. If the domain is too small, the boundary conditions influence the results inducing errors. For this reason several studies in wind engineering investigates on the distance that boundaries should have from the obstacle as reported for example in [30]. Figure 4.1 synthesises the domain size in the simulations of this thesis.

As it can be observed, the computational domain has been divided into several subdomains. This choice let to define different meshing strategies in FLUENT for each region. In this way the mesh can have a higher density where the flow is characterized by high
4. \[ \frac{B}{D} = 1 \] application: simulation setup

Figure 4.1: Computational domain.

Figure 4.2: Mesh definition in the domain. The meshes used in this thesis differ only in the near wall region.

gradients values such as near wall and in the wake. Figure 4.2 shows the mesh used in a particular simulation of this thesis. It can be easily observed that the mesh is not uniform but finer where it is required.

Possible choices of boundary conditions have been discussed in Chapter 1. Table 4.1 shows the boundary conditions used in the simulations.

In order to discretize and solve this problem, the following numerical methods and solver options have been imposed:

- **Solver**: Pressure-Based.

- **Pressure-Velocity coupling**: PISO.

- **Spatial discretization**
  - **Gradient**: Least Squares Cell Based.
  - **Pressure**: Second Order.
  - **Momentum**: QUICK.
4. **B/D = 1 application: simulation setup**

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Boundary condition</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cylinder’s walls</td>
<td>No slip</td>
<td>( \mathbf{u} = 0 ) on the wall.</td>
</tr>
<tr>
<td>Inlet</td>
<td>Velocity inlet</td>
<td>( u_x = U = 1 ) at the inlet. Turbulent intensity and length scale are, respectively, set to 2% and 0.5</td>
</tr>
<tr>
<td>Lateral</td>
<td>Symmetry and Periodic</td>
<td>Within periodic type, we impose a translational motion.</td>
</tr>
<tr>
<td>Outlet</td>
<td>Pressure outlet</td>
<td>Dirichlet conditions: ( p_{rel} = 0 ) and ( u_y = 0 ). In addition, turbulence intensity and length scale are equal to those defined in the inlet boundary condition.</td>
</tr>
</tbody>
</table>

Table 4.1: Boundary conditions

- **Turbulent Kinetic Energy**: QUICK.
- **Turbulent Dissipation Rate**: QUICK.

**Transient Formulation**: Second Order Implicit (Euler method).

Finally, the residuals define the convergence ratio. Normally, to avoid errors induced by the solver, these values, one for each variable of the problem, are small enough, in this case 0.001.

4.2 **Near wall meshes**

This thesis will compare the results obtained from four different simulations that differ only by the definition of the grid near wall. The same grids, shown in Figure 4.3, were defined and used in the thesis \[42\]. Their main characteristics are now presented.

1. **High quality grid (High-q)**
   - This grid is structured, orthogonal and not-skewed. For this reason it is a high quality mesh and it represents the best scenario.

2. **Low quality grid (Low-q)**
   - Also this mesh is structured but, as it will be deeper observed in the next section, it is not orthogonal and it has skewed faces. For this reason it is a low quality mesh. It can be also classified as a \( \alpha \)-type-like mesh.

3. **Hybrid grid**
   - This mesh is characterized by the presence of both structured and unstructured
4. B/D = 1 application: simulation setup

4. Downwind Low quality grid (DW Low-q)

This mesh is equal to the High-q one in the upwind region and to the Low-q in the downwind region.

It is interesting to investigate about the cells number of each grid near wall. In the High-q case, this region is divided into eight squares whose edges are split into 24 segments of equal size. As a consequence this grid consists of 4608 cells. The Low-q grid is divided in four trapezoidal regions with opposite edges split into respectively 72 and 24 parts. It implies that this near wall region is divided into 6912 cells. The structure of the DW Low-q grid is such that it has a cells number that is the average of the two previous cases, in particular 5760. Finally the number of cells of the hybrid grid can not be computed a priori because a meshing algorithm is used in the corners regions. It results that the near wall region is formed by 3889 cells.

So it appears that these four grids have a different cells number and it could appear reasonable that Low-q results would be more accurate, followed in order by DW Low-q, High-q and Hybrid. However the results that will be presented in the following chapter will show a completely different behaviour. The differences are consequently also linked to the mesh quality and not only to the size of the mesh elements.

4.3 Meshes quality

FLUENT defines some quality indicators. These refer to the cells and they are partially linked to mesh defects presented in the past chapters. In [42], these indexes have been used to find a correlation with the error.

At the contrary, in this thesis, the non-orthogonality and the skewness are computed and directly used. This choice is justified by the expression of the grid errors linked to the interpolation schemes on faces. It seems more natural to study the faces features because the error is induced by the face characteristics.

Figure 4.3: Different near wall grids used in this thesis.
The main problematic with this approach when the software FLUENT is used is that the faces informations are not available and must be separately computed.

### 4.3.1 How the indicators have been obtained

Once the simulation is completed, it is possible to export the results into txt files. This feature is convenient if it is advisable to post-process on a different software. In this thesis all the processing has been performed with MATLAB.

Following the steps File -> Export -> Solution Data it is possible to select all the necessary variables, including the spatial coordinates of cells and nodes. FVM is based on the cell center localisation of the variable, so it is natural to export the variables in these points. By the way, it is possible to obtain the values located at the nodes (it can be useful for coupled fluid-structure problems where the structure solver is based on Finite Element Method) where these values are obtained through a linear interpolation from the cells values.

The main drawback with this set-up is that faces informations are not available. In addition, the FLUENT mesh file msh is encrypted and, as a consequence, the mesh connectivity can not be obtained. In general, a grid is not uniquely defined if only the cells centers and the nodes coordinates are known. The mesh is determined once it is established which nodes belongs to each cell.

On the other hand, in order to compute non-orthogonality and skewness, it is necessary to know the nodes of each face. The objective is to build all these face informations with the data available in FLUENT.

For the High-q, Low-q and DW Low-q grids this operation is almost straightforward because of the structure of these meshes. As a consequence, the cells and the nodes were stored in ASCII files following a deterministic pattern. This feature lets to define a priori which nodes are the extremes of the face.

For the hybrid grid the situation is much more complicated because the square regions near the cylinder’s corners are unstructured. As a consequence it is impossible to exploit some storing pattern. In order to avoid the manual insertion of each face, operation that would have required a huge amount of time (the cells are 968 and the nodes are 1036 in the considered region), an algorithm coded in MATLAB has been used. Even if this algorithm does not work correctly with any grid, due to the fact that many grids could be generated with the same cells centers and nodes, it has been observed that it generates correctly the faces for the hybrid mesh. This is mostly due to the fact that the cells are not very stretched and the angles are not far from the ideal value.

Finally it has to be observed that this grid contains mostly quadrangular cells but also some triangular ones. Fortunately, FLUENT has a field that let to understand the number of edges of the cell.

The algorithm is structured as follows:

1. iterate over the cells;
2. find the closest node and save it;

3. store the direction that links this node to the cell center;

4. find the second closest node. Store it only if the direction node-cell center is not close to the one of first search. This operation is done by looking at the angle between the two directions and by comparing it to a threshold value $\alpha$. $\alpha_t$ for triangular cells is smaller than $\alpha_q$ for quadrangular cells;

5. iterate in the same way until three or four nodes, depending on the number of nodes for the cell, have been found. For each new node, the new direction must be compared to all the previous ones.

So, the idea is to find for each cell its nodes. This is done by searching the closest nodes taking into account the directions nodes-center in order to avoid, for example, that the cell center is outside the nodes convex region. The threshold values have been tuned and set to $\alpha_t = 40^\circ$ and $\alpha_q = 45^\circ$.

For each cell, it has been decided to look for the closest nodes and not the closest cells because problems rise with cells on the boundary of the region. Indeed, a cell has a fixed number of nodes (three or four depending of the cell but this number is known a priori) while the adjacent cells number can vary. For example a quadrangular cell can have, in the selected region, only three or even two neighbours if it is located on the boundary. Once the nodes are associated to the cells, it is sufficient to find which cells share exactly two nodes and to define the new face.

Finally, for both structured and unstructured grids, the skewness and the non-orthogonality are computed.

For the skewness computation, a linear system is solved to find the intersection between the face and the line connecting the two cells center. The distance $s$ between the face center and the intersection is then divided by the length of the face $F$ divided by 2

$$sk = \frac{s}{F/2}$$ (4.2)
in order to have a dimensionless quantity. The coefficient 2 has been chosen in order to have a physical interpretation of $sk$. Indeed, the skewness is linked to the distance from the middle point of the edge and so $sk = 1$, i.e. $s = F/2$, means that the intersection point is over one of the edge vertices.

Also the non-orthogonality, linked to the angle $\theta$ between the face direction and the line that connects the two cells centers, is normalized

$$orth = \frac{\theta}{90^\circ}.$$  \hfill (4.3)

In this way, its value is always such that $orth \leq 1$.

### 4.3.2 Comparison between grids

Being non-orthogonality and skewness computed, some detailed analysis on the meshes quality could be made. For sake of simplicity only the downwind region is considered.

- **High-$q$ grid**
  As expected, the High-$q$ grid is orthogonal and not-skewed. In addition, all the cells have same size and so there are not stretching effects.
  The computed values are zero or, sometimes, very close to zero due to numerical effects. As a matter of fact, the biggest value of the skewness is $O(10^{-7})$.

- **Low-$q$ and DW Low-$q$**
  Figure 4.5 shows the values of non-orthogonality and skewness. The values have been plotted using the `scatter` command in MATLAB. Each black dot is centred on the mid point of the corresponding face. The radius is proportional to the value of non-orthogonality and skewness. For a better visualization, the former have been multiplied by a factor 10, the latter by 50.
It can be observed that the orthogonality increases when faces approach to the diagonal of equation \( y = 0.5 - x \). While the cells center under the diagonal form lines with almost constant \( y \)-value, the vertical faces become more inclined near the diagonal. An analogous consideration can be made above the diagonal and this fact justify the non-orthogonal behaviour. It has to be noticed that faces exactly on the diagonal have values that are negligible, in particular \( \text{orth} = O(10^{-6}) \).

The opposite behaviour characterizes the skewness that is small in the whole domain except for the faces on the diagonal. The largest value outside the diagonal is \( O(10^{-3}) \) while on the diagonal the largest value is 0.4884. Figure 4.6 represents three consecutive cells in the diagonal region in order to highlights the reason of the above behaviour of non-orthogonality and skewness. The shared faces are blue while the lines connecting two cell centers are red. It can be observed that the intersection is located in the face’s middle point (in black) for the under diagonal cells but they are not orthogonal. The scenario is opposite for the face located on the diagonal where the intersection is far from the middle point but there is orthogonality.

Figure 4.6: Three consecutive cells in the diagonal region.

- Hybrid grid

Figure 4.7 shows the values of non-orthogonality and skewness. The multiplicative factors used for the dots size are the same of the previous case.

In the structured uniform regions these values are zero like for High-q grid. At the contrary, this is not the case in the unstructured region. Because of the unstructured nature of the grid, non-orthogonality and skewness does not show particular patterns.

It appears immediately that the non-orthogonality affects principally the structured non-cartesian grids while the hybrid one has more faces with significant skewness values.

Table 4.2 highlights the main differences that have been discussed. The field \( \# \text{ faces} > 0.1 \) counts how many faces have the considered quantity bigger than 0.1.
4. B/D = 1 application: simulation setup

Figure 4.7: Faces non-orthogonality and skewness in the hybrid grid.

![Orthogonality absolute value](image1)
![Skewness](image2)

(a) Non-orthogonality  
(b) Skewness

Table 4.2: Non-orthogonality and skewness values in the downwind region for meshes Low-q and Hybrid.

<table>
<thead>
<tr>
<th></th>
<th>max</th>
<th># faces &gt; 0.1</th>
<th>mean</th>
<th>median</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hybrid orth</td>
<td>0.2857</td>
<td>131</td>
<td>0.0223</td>
<td>0</td>
</tr>
<tr>
<td>Low-q orth</td>
<td>0.4955</td>
<td>2810</td>
<td>0.2778</td>
<td>0.2952</td>
</tr>
<tr>
<td>Hybrid sk</td>
<td>0.5532</td>
<td>139</td>
<td>0.0241</td>
<td>9.36e-7</td>
</tr>
<tr>
<td>Low-q sk</td>
<td>0.4884</td>
<td>24</td>
<td>0.0061</td>
<td>0.0047</td>
</tr>
</tbody>
</table>

For the hybrid mesh, the prevalence of faces in the structured region implies that its orthogonality median value is zero. At the contrary 2810 faces over 3360 (84%) of the Low-q meshes have a value greater than 0.1 and consequently the median value is 0.2952. Skewness differences are also remarked: the number of faces in the hybrid mesh with values larger than 0.1 is higher than the Low-q one that coincides exactly with the faces on the diagonal of equation $y = 0.5 - x$. In addition, the mean value in the first case is four times the second.
4. $B/D = 1$ application: simulation setup
Chapter 5

B/D = 1 application: simulation results

In this chapter the results of the four different simulations are illustrated. The flow around square cylinder with $Re = 2.2 \cdot 10^4$ is periodic. For all the simulations, the time span has been divided into 20 phases. As a consequence a field that refers to a single phase is said to be instantaneous while one obtained through an averaging process of the 20 instantaneous fields is said to be time-averaged or a mean field. It has been decided to present the results starting principally from the behaviour of the instantaneous fields in extended domains, continuing with time averaged flow fields in order to understand the differences of the simulated flows. After this operation, some standard bulk and time-averaged quantities like the aerodynamic coefficients are compared to literature results in order to better test the results.

5.1 Flux phenomenology and vorticity field

All the simulations are characterized by a periodic flow. This fact implies that the lift coefficient $c_L$ is periodic and not constant in time. An interesting quantity that is usually used in literature to understand the flux topology in the vorticity magnitude

$$|\omega| = \left| \frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y} \right|$$

because it highlights regions with rotational flow. Figure 5.1 represents the vorticity magnitude when the $c_L$ coefficient has its higher value and when it is equal to zero and it is decreasing. It can be observed that the flow detaches at the two leading corners, regions with high values on vorticity magnitude. Along the alongwind faces the flow is reversed. The sizes of the reversed flow regions depend on the phase in the period. Finally in the wake there are alternated vortexes.

It is already clear that the Low-q simulation behaves in a completely different way. Even if the flow is periodic, the vorticity magnitude is drastically underestimated (the color scale is equal for all the 8 flow field representations) because of the poor grid quality. At the contrary, it looks like the other three cases are very similar.
5. B/D = 1 application: simulation results

The differences between the simulations can be observed also looking at the time-averaged flow. To show it, in Figure 5.2 curves obtained fitting the vorticity magnitude isocontours are represented. While three curves are very similar, the Low-q one has a completely different shape that is more elongated coherently with the plots in Figure 5.1 for the instantaneous fields.

This observed discrepancies between the Low-q results and the others will always be manifest in each analysis.

5.2 Velocity field along 1D domains

In the past chapter, it has been observed, through Figure 4.5 that the diagonals of equation \( y = x - 0.5 \) and \( y = 0.5 - x \) are particularly important for the structured non-orthogonal mesh because of the high values of the skewness. For this reason the behaviour of the time-averaged field \( u_x \) is investigated in these lines and in another one
in between where all the grids are orthogonal and not-skewed. In order to compare the results and to represent their faces quality, the fields are interpolated on the faces centers coordinates of the Low-q grid. All the informations are shown in Figure 5.3.

In domain $l_1$ not only the Low-q $u_x$ profile differs from the others that are mutually overlapping but also the monotony changes. The lower quality of the unstructured upwind corner with respect to the structured case does not play a relevant role in this domain. It can be also observed that, in average, the skewness near the diagonal of the hybrid grid is lower that the Low-q one. Domain $l_2$ does not present faces defects but the Low-q profile still differs considerably from the others. This is due to the fact that errors generated in the upwinding regions (like in $l_1$) are transported from the flow. Moreover the High-q and DW Low-q profile are not distinguishable from each other even if, starting from $l_2$, the latter is a bad quality mesh. It can be explained by the fact that the simulated problem is convective-dominant and so the error generated by the mesh does not travel in the downwind direction. Another important consideration is that from simulation Low-q the flow is not reversed near wall at the contrary of the other simulations that, correctly, expect a recirculation region. Finally the Low-q free flow velocity, the region where $\partial u_x/\partial y \approx 0$, is lower than

Figure 5.3: 1D domains in (a). $u_x$, skewness and non orthogonality in (b).
the others.
In $l_3$ differences between High-$q$ horizontal velocity profile and the others can be detected in the shear layer, i.e. the region where the velocity is increasing, while the asymptotic free outer flow velocity is the same for all the simulations. Also in this case the Low-$q$ simulation does not capture the presence of reversed flow.

As a conclusion, the Low-$q$ simulation gives completely different horizontal velocity profiles that are not in accordance with the phenomenology of the flow that contemplates, for example, reversed flow near wall. The error, furthermore, is generated in regions with a bad mesh quality and it propagates following the wind direction and so differences emerge even in region with high mesh quality like in domain $l_2$. Moreover, for the same reason, the error committed in $l_3$ by DW Low-$q$ is much smaller than the Low-$q$ one even if the two meshes coincide in this 1D domain.

### 5.3 Determination of the separation point

An important physical phenomenon that occurs in high Reynolds number flows around square cylinders is the detachment of the boundary layer and it is the reason why this body is denoted by the adjective bluff.

In the previous section, while studying $u_x$ in 1D domains, it has been observed that the Low-$q$ simulation does not expect, wrongly, retrograde flow near wall. This fact would suggest that in this scenario the flow does not detach or, at least, that the detachment point is wrongly placed.

Firstly Figure 5.4 shows the isocontours $u_x = 0$ near the cylinder region for each time-averaged simulation. It suggests that, except for the Low-$q$ grid, detachment occurs at the leading corner where the three isocontours start (more precisely from the first cell after the corner). In between the isocontours and the wall there is reversal flow while outside $u_x$ is positive. These three isocontours start becoming distinguishable from each other from $x \approx 0.7$, coherently with the results observed in the past section. Big differences are evident in the wake where the DW Low-$q$ isocontour is located before the High-$q$ and the Hybrid ones. In terms of mean flow, this informations means that the two symmetrical vortices (one for $y > 0$ and one for $y < 0$) behind the cylinder are smaller when a DW Low-$q$ is used. As a consequence, while this grid seems to not significantly affect the results for $0 \leq x \leq 1$, it affects the results in the wake. At the contrary the hybrid mesh seems to be accurate both along the wall and in the wake.

The Low-$q$ isocontour needs a separate discussion. It starts for $x \approx 0.7$ suggesting that in this simulation the boundary layer separation occurs in this point and not in the leading corner. As a consequence there is not reversal flow until this point, as already detected observing $u_x$ on domain $l_2$ in the previous section. Finally this isocontour is particularly elongated and it ends for $x \approx 2.75$ instead of $x \approx 1.8$ like in the reference High-$q$ case.

Another quantity that can be used to investigate the detachment is the wall shear stress $\tau_s$ that depends, for a Newtonian fluid, on the derivative of the tangential velocity with respect to the normal to the wall direction. This quantity, defined on the curvilinear coordinate, is positive when the tangential flow has the same direction of the curvilinear
coordinate direction, it is negative when the flow is reversal and it is equal to zero for inflection points.

Figure 5.5 shows the wall shear stress, after being adimensionalised, compared to the results in [34]. It has to be observed that, surprisingly, the thesis results obtained through a RANS computation are qualitatively but also quantitatively in agreement with the data from [34] obtained, at the contrary, with a LES simulation. Only the Low-q curve is completely different with the extremal values that are, in absolute value, hugely bigger than the others. For Newtonian fluids the shear stress is associated to the viscosity and so the diffusive effect of the Low-q grid plays an important role for this higher values. However in almost all the region that corresponds to the alongwind face ($0.5 \leq s/D \leq 1.5$) the stress in negative in all simulations, probably due to the recirculation region, except for the Low-q one where the shear stress is negligible as the literature result highlights. After that the DW Low-q grid influences the results in the second corner where the wall shear stress behaviour is similar, even if damped, to the Low-q one in the leading corner. At the contrary, Hybrid and High-q meshes gives overlapping results. For all the thesis simulations, the peaks are predicted slightly, respectively, before and after the reference results for the positive and negative cases in the near corners regions. This fact is not surprising because they corresponds to the closest nodes in the grid to the corner one and so it would be impossible to predict the peaks nearer to the corners. As a matter of fact, in the Low-q case for $s/D = 0.5$, so in correspondence of the leading square corner, this transition zone from positive to negative values is thinner because the mesh has more nodes. Finally, it can be observed that all curves start to the zero value because $s/D = 0$ corresponds to the stagnation point that is an inflection point.

The investigation of the wall shear stress has highlighted the diffusive behaviour of a bad
5. B/D = 1 application: simulation results

Figure 5.5: Wall shear stress along the curvilinear coordinate for all the simulations compared to [34]. $s/D = 0$ corresponds to the stagnation point, $s/D = 0.5$ to the leading corner and $s/D = 1.5$ to the second corner.

quality mesh. This effect, that also appeared looking at the instantaneous vorticity fields in Section 5.1 will appear also in the analysis of results in following sections.

5.4 Pressure distribution

The pressure coefficient $c_p$ is an important coefficient in CWE that is defined as in [14]. It is usually represented with respect to the curvilinear coordinate $s/D$ where $s = 0$ corresponds to the stagnation point.

Figure 5.6 displays the mean and the Root Mean Square (RMS) of the pressure coefficients and it compares them to other numerical and experimental data. All the results are such that $\bar{c}_p = 1$ and $c_{prms} = 0$ for $s/D = 0$ as expected from the definition of the pressure coefficient. This check is usually used to verify the correctness of the simulation.

The mean $c_p$ curves, except for the Low-q curve, are completely in accordance to the literature results. Low-q overshoots the mean $c_p$ for $x < 0.6$ and then overestimates it.

For the RMS pressure coefficients, the reference values are not close to each other because, in general, the fluctuating component of a coefficient is more difficult to measure experimentally or it is more affected by errors in the simulations than its mean part. However it is evident that High-q and Hybrid grids have very similar RMS results that agree with the literature ones especially before the leading corner ($x < 0.5$) where also the DW Low-q coincides. The latter seems to be overestimated starting from the leading
5. B/D = 1 application: simulation results

Figure 5.6: Mean pressure coefficients (a) and Root Mean Square (RMS) pressure coefficient (b).

corner. Finally the Low-q curve is completely underestimated and unrealistic compared to the literature results.

5.5 Wake flow

The wake region is usually important to observe because of the propagation of alternating vortexes with opposite rotational velocity. A wrong description of them can affect drastically the results. Figure 5.7 shows the mean horizontal velocity along the line of equation $y = 0$ in the wake starting from the downwind face ($x/D = 1$). The velocity profiles are compared to the ones from simulations with a LES turbulence model such as in [34] and from experimental works such as [36, 35].

First of all, the results start from $u_x = 0$ due to the wall boundary condition. Then for $x \approx 1.5$ the Low-q starts to differ from the other curves. The region with negative velocity is much more extended in this case as it has been observed in Section 5.3 meaning that the reversed flow region is bigger.

Finally the velocities of the free stream far from the cylinder in the wake are very similar for High-q, Hybrid and DW Low-q cases and they are in accordance to the LES 3D value. On the other hand the Low-q value, around $u_x = 0.8$, seems to be underestimated even if it agrees with the experimental value Durao.

5.6 Aerodynamic coefficients

The aerodynamic coefficients defined in (1.3) are widely used in CWE to estimate the forces acting on the cylinder. They are bulk parameters obtained through an integration in space all over the cylinder boundary. Both $c_D$ and $c_L$ are periodic and, because of the symmetry of the problem, physically it holds $\bar{c}_L = 0$. As a consequence, usually in literature the mean drag coefficient $\bar{c}_D$, the maximum value of the fluctuating part of the
5. B/D = 1 application: simulation results

Figure 5.7: $u_x$ in the wake region. The results are compared to Lyn [36], Durao [35], Trias [24], Cao [34] and other literature values.

The aerodynamic coefficients are always drastically underestimated in the Low-q simulation. This fact can be explained by the diffusive error type that is generated by a low quality mesh. Indeed the forces acting on the square are obtained through an integration of the stress Cauchy tensor that involves velocity gradients that are underestimates because of the mesh diffusion. On the other hand, the values from High-q, Hybrid and DW Low-q are comparable and almost in accordance with the literature results. Again, the DW Low-q values are slightly different from the two others. Contrary to the aerodynamic coefficients, the Strouhal number is bigger for the DW Low-q simulation. It can be another confirmation of the tendency of the results to be "more steady".

5.7 Comparison between turbulence viscosity and skewness induced viscosity

The results presented until now in this chapter highlight the big differences between the Low-q fields and the others and, sometimes, also between the DW Low-q results compared to both Hybrid and High-q ones, even if these differences are smaller. The four simulations are identical regarding the turbulence model and interpolation schemes. In addition, the meshes have the same structure except for the near wall region. As a consequence the differences have to be the by-product of the mesh-induced errors.
linked to its bad quality as discussed in Section 3.2. In that section the diffusive nature of the error associated to the skewness has been determined and the explicit formula (3.16) associates the skewness to an equivalent kinematic viscosity \( \nu_{sk} \) (obtained from the molecular one in (3.15) dividing by the density \( \rho \)). This fact is coherent with the previous analyses where some results could be directly explained through the diffusive behaviour of the mesh.

It is also important to underline that in addition to the physical kinematic viscosity there is also the turbulent viscosity \( \nu_t \) defined in (2.18) from the \( k-\varepsilon \) turbulence model. Consequently it is natural to define an effective Reynolds number as

\[
Re_{eff} = \frac{UD}{\nu + \nu_t + \nu_{num}}
\]  (5.1)

that determines the flow that appears looking at the simulation results.
While \( \nu \) is a physical property of the fluid and \( \nu_t \) is artificially defined to substitute the diffusive effect of the non-simulated Kolmogorov scales, the numerical viscosity is nothing more than the consequences of chosen interpolation schemes and of the mesh quality, that are not neither linked to the physics nor to the mathematical modelisation of the problem. In addition to that, the numerical viscosity can not be determined exactly and it is impossible to distinguish its effects from the others due to \( \nu \) and \( \nu_t \). However, it is possible to express the contribution of the skewness-induced viscosity. For this reason Figure 5.9 represents on the left the ratio \( \nu_t/\nu \) and on the right \( \nu_{sk}/\nu \) for all the grids. They are plotted separately because both \( \nu_t \) and \( \nu_{sk} \) depends on space-depend variables like \( u, k, \varepsilon \) and so it has been decided to compare them to the constant quantity \( \nu \). The plot of \( \nu_{sk}/\nu \) for the High-q simulation is not reported because this ratio is identically equal to zero because the grid is not skewed. The color range is set to be equal for all
the seven subplots such that the results are easier to compare.

![Figure 5.9: Ratio between turbulent viscosity and kinematic viscosity on the left. Ratio between the viscosity induced by the skewness and the kinematic viscosity on the right.](image)

Firstly the skewness-induced viscosity is locally generated only in limited regions corresponding to the locations of the skewed faces. At the contrary the turbulent viscosity is a field defined everywhere in the domain.

Looking to the $\nu_t/\nu$ plots, it appears that the ratio has high values with a maximum of the order of 350 and so it is fundamental to determine the effective Reynolds number. This ratio is lower for the Low-$q$ simulation. It can be explained looking at the system \[ 2.21 \] for $k$ and $\varepsilon$ where both the production terms are underestimated because of the numerical viscosity. Consequently, the mesh induces a diffusive viscosity that influences also the values of the turbulence viscosity.

The ratio $\nu_{sk}/\nu$ usually has lower values but, where the faces are highly skewed, it assumes values around 200, with a maximum of 290 for the Hybrid computation, that are comparable to the $\nu_t/\nu$ ones. Moreover, the skewness viscosity is generated in regions where $\nu_t/\nu$ is small and so the skewness effect becomes dominant. In the Low-$q$ case, the two diagonal contributions are not equal because $\nu_{sk}$ depends not only on the skewness but also on the velocity that differs in these two regions.

After this considerations it is possible to assert that a bad quality mesh with highly skewed faces has a diffusive effect on the simulated flow that can be thought as an addi-
tional viscosity term in the expression of the effective Reynolds number. This non-physical diffusion affects significantly the aerodynamic coefficients, the vorticity magnitude, the shear stress and the other fields.

Even if this additional diffusion changes significantly the simulated results, the flow from the Low-\(q\) simulation is nevertheless characterized by the vortex shedding. This fact that seems to be positive can become a huge drawback because it is more difficult to notice big quantitative errors in a simulation that is qualitatively correct.

5.8 Correlation coefficients between mesh quality and simulated error

Grids with a bad quality and in particular with high skewness generates errors that have a diffusive nature. Following the idea presented in Section 1.2.2, the objective is seeking a correlation between a grid quality indicator and the committed error.

In this scenario, at the opposite of [33], an analytical solution is not available and so the error in computed using the High-\(q\) computation as reference. This choice is caused by the fact that its results are closer to the literature ones and because it is not affected by mesh errors induced by non-orthogonality and skewness in the near wall region.

From now on, a quantity that refers to the High-\(q\) simulation will be denoted by the subscript \(Hq\), one that refers to the Low-\(q\) with the subscript \(Lq\), one to the Hybrid with the subscript \(Hyb\) and finally one that is from the DW Low-\(q\) simulation will be denoted with the subscript \(DWLq\).

It is known that diffusion dumps the gradients of the fields. As a consequence, it has been decided to choose as error quantity the field

\[
err_i := \frac{\|\nabla u\|_{Hq} - \|\nabla u\|_i}{\|\nabla u\|_{Hq}}, \quad \text{with} \quad i = Lq, Hyb, DWLq. \tag{5.2}
\]

where \(\|\nabla u\|\) is the saturation product of the velocity gradient with itself defined as

\[
\|\nabla u\| = \left(\frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j}\right)^{1/2}.
\]

Of course this relative error has not been defined for the High-\(q\) computation otherwise it would be identically zero and it would not have any relevance in the analysis. The main idea behind the definition (5.2) is that a mesh with high skewness underestimates \(\|\nabla u\|_i\) because of its viscous effect and so the numerical diffusivity should be detectable obtaining positive values of \(err_i\).

After having defined an error metric, the next step is to determine a mesh quality index. In Section 3.2 the errors of grid stretching, non-orthogonality and skewness have been presented. The former does not affect the simulations near wall because the cells have the same dimensions. At the contrary the meshes, with the exception of the High-\(q\) one, are, at least in some regions, non-orthogonal and skewed. Consequently it seems appropriate to define two different mesh quality indices associated to the two aspects.
5. **B/D = 1 application: simulation results**

<table>
<thead>
<tr>
<th>domain</th>
<th>grid</th>
<th>$c_{\text{orth}}$</th>
<th>$p_{\text{orth}}$</th>
<th>$c_{\text{sk}}$</th>
<th>$p_{\text{sk}}$</th>
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<td>0.9840</td>
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<td>0.8753</td>
<td>0.1394</td>
<td>0.5158</td>
</tr>
</tbody>
</table>

Table 5.1: Correlation coefficients and associated probability of the test hypothesis in the domain $l_2$.

Being the High-q grid completely orthogonal and not skew, the mesh quality indices are defined as

$$sk_i := sk_i - sk_{Hq} = sk_i, \quad orth_i := orth_i - orth_{Hq} = orth_i \quad \text{with} \quad i = Lq, Hyb, DWLq \quad (5.3)$$

where the expression of $sk$ and $orth$ are (4.2) and (4.3) respectively.

Before starting the analysis, the expected behaviour is to find a positive correlation on the grids between $err$ and, at least, $sk$ whose diffusive nature has analytically been shown in (3.16). Indeed the bigger is the skewness and the more dumped should be the velocity gradient and the bigger should be $err$.

To each coefficient a probability $p$ that tests the hypothesis of correlation is associated. In particular, if $p > 0.05$ the correlation hypothesis should be rejected.

The correlation coefficients $c_{sk}$ and $c_{orth}$ have been computed on the 1D domains $l_2$ and $l_3$ shown in Figure 5.3 in Section 5.2 and they are reported in Table 5.1. In order to compare the results in the same region, $sk_{Hyb}$ and $orth_{Hyb}$ are obtained through a linear interpolation in the coordinates of the Low-q faces center.

It has been investigated only for grids that differs from the High-q one in the selected domain otherwise $sk$ and $orth$ would be identically equal to zero because the meshes are equal.

First of all it can be observed that in most of the cases there is not correlation. This consideration is highlighted by both the values of the coefficients close to zero and by the high values of $p$. The non-orthogonality coefficients have been computed even if in these domains the faces are almost orthogonal and, most importantly, orthogonality is almost constant over the faces and so without the required variance to obtain a meaningful correlation. This justify the results linked to the orthogonality coefficient. At the contrary the skewness not only is relevant but it varies significantly as it can be also observed in Figure 5.3.

Looking at $c_{sk}$ for the Low-q grid two opposite results are obtained. In both cases the $p_{sk}$ is small enough to let suppose a correlation between the error and the skewness, however this correlation in negative in $l_2$ and positive in $l_3$. Another important observation is that the two values of $c_{sk}$ for Low-q are comparable in terms of absolute value with the one in $l_2$ that is bigger than the $l_3$ one. However, the maximum value of $sk_{Lq}$ in $l_2$ is 0.006 while the lowest one in $l_3$ is 0.16, 27 times higher.
After this observations, it can be concluded that correlation coefficients are not adequate to capture the diffusion effect of the mesh, effect that has been obtained from analytical considerations and that has been detected all along the observation of the simulations results.

The real drawback of this mathematical tool is its local behaviour. Indeed, the correlation is computed looking at the value of \( \text{err} \) and either \( \text{sk} \) or \( \text{orth} \) in the faces centers. In the other hand the problem is driven by the convection effect and consequently the diffusion effect should be analysed in a non-local way as made in the previous sections. This fact is clear looking at Figure 5.3 where the \( u_x \) profiles in \( l_1 \) and \( l_3 \) are shown. Even if \( l_1 \) and \( l_3 \) have exactly the same faces properties, because of their symmetry, the fields are completely different. The difference is partially due to the physical flux phenomenology that changes from the upwinding corner, where detachment occurs, to the downwinding one and also partially to the convection of the error that propagates transported by the wind. As a matter of fact, passing through the first diagonal, the flux is affected by the diffusion effect of the skewness and, in a second moment, the same flow is influenced by the second diagonal diffusive effect. Nevertheless the correlation coefficient acts like if there was not flux history. In the same way particles in regions with a good quality mesh could have been already affected by upwinding diffusion induced by skewed faces while, computing the correlation coefficients, the skewness in considered equal to zero.
5. $B/D = 1$ application: simulation results
Chapter 6

Conclusions

Computational Fluid Dynamics (CFD) is highly used in academic and industrial applications. In particular Computational Wind Engineering (CWE) investigates the wind effects on civil structures like bridges and skyscrapers. For this reason the geometrically easier benchmark of flow past rectangular cylinders is widely studied. In this scenario the flow is highly turbulent and characterized by high Reynolds numbers with vortex shedding in the wake.

CFD computations are based on three fundamental aspects: the turbulence model, the interpolation schemes and the mesh generation. While the first, primarily, and the second have been widely discussed in literature in the past decades, the last aspect has been neglected.

The thesis firstly presents a literature review on meshes, then some errors induced by the mesh linked principally to the non-orthogonality and the skewness have been discussed. The near wall grid effect has been investigated in the well known CWE test case of flow around a square cylinder. With this purpose, four different simulations that differs only by the near wall grids have been performed.

Firstly the characteristics and the quality of the meshes are discussed and then the results are compared.

It has been highlighted that the structured non-orthogonal and skewed simulation is widely affected by diffusion-like grid errors even if it provides a qualitatively correct flow pattern in the wake region. About this problematic Professor Ferziger said:

"the greatest disaster one can encounter in computation [...] are results that are simultaneously good enough to be believable but bad enough to cause troubles."

No partial safety factor in structural engineering can secure the design face to an underestimation of the fluctuating lift almost equal to a factor 10 like the one obtained with the non-orthogonal and skewed near wall mesh.

On the other hand both the hybrid and the structured downwind non-orthogonal grids give results quantitatively comparable to the reference case. However, the former seems to be slightly better while the second generates errors in the wake.

Finally a correlation between the error and the mesh quality has been sought through the usage of correlation coefficients. However it has been observed that this mathematical
tool is not suitable for this problem due to the convective dominance of the problem.

In future, the same type of analysis should be proposed for the rectangular case $B/D = 5$. This case is much more complex because of the reattachment of the boundary layer. A different turbulence model must be used and the grid cannot be as simple and with a low number of cells near wall as in the square case. In this consolidated benchmark there is not a settled standard on the near wall grids. As a matter of fact in literature different meshes have been used, sometimes non-orthogonal and skewed, that can dangerously affect the results.
Bibliography


[38] ANSYS FLUENT 12.0 User’s Guide.


