

Department of Aerospace Science and Technology Doctoral Programme In Aerospace Engineering

Analysis of a novel hybrid RANS/LES technique based on Reynolds stress tensor reconstruction

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2016 - XXVIII cycle

Keywords: Large Eddy Simulation, Hybrid RANS/LES methods, Turbulence, Discontinuous Galerkin

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Printed in Italy

There were two roads out of Ashton, a new one which was paved, and an older one that wasn't. People didn't use the old road anymore, and it had developed the reputation of being haunted. Well, Since I had no intention of ever returning to Ashton, this seemed as good a time as any to find out what lay down that old road.

Edward Bloom, Big Fish (2003)

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Abstract

In the context of hybrid RANS/LES methods, a promising framework is represented by the hybrid filter approach proposed by Germano in 2004. The filter, \mathcal{H} , is composed by the LES filter \mathcal{F} and the statistical operator RANS \mathcal{E} : $\mathcal{H} = k\mathcal{F} + (1-k)\mathcal{E}$, where k is a blending factor which varies from 0 (pure RANS) to 1 (pure LES). Applying this filter to the Navier-Stokes equations it is possible to obtain a new set of formally correct hybrid equations. The hybrid filter has been studied and analysed, and a new approach for the Reynolds stress tensor has been proposed. This term that is usually modelled by means of an explicit RANS model, here it is reconstructed, exploiting the properties of the hybrid filter, from the LES subgrid stress tensor and the resolved velocity field. As a consequence, no explicit RANS model, and then no additional equations, are required. This results in a very simple and cheap hybrid method, in which the RANS contribution is used to integrate, and not to substitute, LES in the context of coarse grid. The methodology has been studied using FEMilaro, a gnu license software originally developed at the mathematics department of Politecnico di Milano, and improved during this work. The space discretization of the hybrid filtered equations has been obtained by means of the discontinuous Galerkin (DG) finite element method. The approach has been initially tested with constant and uniform blending factor k for the turbulent channel flow testcase, obtaining a general improvement of pure LES results. The simulations have highlighted also a clear dependence between k and the quantity of turbulent energy modelled and resolved. In order to set a different value of RANS contribution in the different parts of the domain, also a space dependent blending factor has been considered. This modification makes the equations very complex because of the additional terms related to the non commutativity of k and space derivatives. In order to obtain a simple and applicable formulation a piecewise constant blending factor has been used. In fact, keeping the blending factor constant in the element, the additional terms related to the space derivatives go to zero. Moreover, the discontinuity between two consecutive elements are treated with the standard numerical fluxes of the DG approach used for the space discretization. Numerical simulations have been performed for the turbulent channel flow testcase and for periodic hill flow, showing a significant improvement of the pure LES for the first testcase. On the other hand, no significant benefits have been obtained for the periodic hill flow, probably this is related to the difficulty of determining an appropriate blending factor function for a more complex geometry. However, the results obtained confirm that the hybrid filter with RANS reconstruction approach can be a promising technique for turbulence modelling. In fact, it can reasonably be expected that, introducing the right value of the blending factor, the methodology analysed can be suitable for improve accuracy of the turbulence description for coarse grid. Therefore, future work will be focused on the research of a reliable criterion for the choice of the optimal value of the blending factor, element by element. Sommario

Nel contesto dei metodi ibridi RANS/LES un approccio molto promettente è rappresentato dal filtro ibrido proposto da Germano nel 2004. Il filtro (\mathcal{H}) è composto dal filtro LES (\mathcal{F}) e dall'operatore statistico RANS (\mathcal{E}): $\mathcal{H} = k\mathcal{F} + (1-k)\mathcal{E}$; dove k rappresenta un peso che varia tra 0 (pura RANS) e 1 (pura LES). Applicando il filtro ibrido alle equazioni di Navier- Stokes è possibile ottenere un nuovo sistema di equazioni filtrate formalmente corrette. Il filtro ibrido è stato studiato e analizzato, ed un nuovo approccio per il calcolo del tensore degli sforzi di Reynolds è stato proposto. Questo termine è generalmente modellato utilizzando un modello RANS. Nell'approccio utilizzato in questa tesi invece il termine viene ricostruito a partire dallo sforzo sotto griglia LES e dal campo di velocità risolto, sfruttando le proprietà del filtro ibrido. Di conseguenza il modello RANS non è più necessario, risparmiando le relative equazioni e ottenendo una metodologia semplice ed economica. Il metodo è stato analizzato utilizzando il software FEMilaro, sviluppato dal dipartimento di Matematica del Politecnico di Milano e arricchito nel corso di questa tesi. La discretizzazione spaziale è ottenuta utilizzando l'approccio degli elementi finiti di tipo Discontinuous Galerkin (DG). Il nuovo approccio è stato inizialmente testato utilizzando un peso k costante ed uniforme per il canale piano turbolento, ottenendo un generale miglioramento dei risultati ottenuti con la simulazione LES. Le simulazioni hanno anche mostrato una chiara dipendenza tra il peso k ed il rapporto tra energia turbolenta risolta e modellata. Al fine di impostare un diverso valore del contributo RANS nelle diverse aree del dominio è stato anche analizzato il caso di un fattore di peso dipendente dallo spazio. Questa dipendenza rende le equazioni molto più complesse, a causa della comparsa di termini aggiuntivi legati alla non commutatività tra la derivata spaziale e il filtro ibrido. Per ottenere una formulazione più semplice ed applicabile è stato utilizzato un peso costante a tratti. In questo modo, mantenendo il peso costante all'interno degli elementi, i termini aggiuntivi si annullano mentre le discontinuità tra gli elementi sono trattate utilizzando i normali flussi numeri che caratterizzano il metodo DG utilizzato per la discretizzazione spaziale. Le simulazioni numeriche sono state effettuate per il canale piano e per il flusso tra colline periodiche, ottenendo per il primo caso un netto miglioramento rispetto alla pura LES. Per quanto riguarda le colline periodiche invece non sono stati ottenuti significativi vantaggi, probabilmente a causa della difficile scelta di un peso ottimale. Tuttavia i risultati confermano che la metodologia può rappresentare una promettente strategia per la modellazione numerica di flussi turbolenti. Infatti può essere ragionevolmente supposto che, utilizzando il giusto peso, sia possibile migliorare l'accuratezza delle simulazioni numeriche su griglie troppo lasche per una pura LES. Gli sviluppi futuri saranno quindi concentrati sull'elaborazione di una strategia per l'ottenimento di un fattore di peso ottimale per ogni elemento del dominio di calcolo.

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Chapter 1

Introduction

In this chapter an introduction about the topic of hybrid RANS/LES methods is presented. The first section concerns a brief history of fluid dynamics from the origins to the computational fluid dynamics. This part is mainly based on [1],[2] and the purpose is to provide an historical background for the computational fluid dynamics (CFD), summarizing the most important steps that led to the formulation of Navier-Stokes equations and after to their modelling. After the general introduction about the history of fluid science, the framework of the hybrid RANS/LES methods with the different models and strategies is described in details. Finally, the motivation and the outline of this work is presented.

1.1 Historical notes

1.1.1 From the origins to the Navier-Stokes equations

As the great part of science and our culture, also fluid dynamics traces its roots to the Greeks. In fact, even tough some fluid knowledges and hydraulic techniques were known and applied for irrigation and sailing since prehistoric age, Aristoteles (384-322 BC) laid the foundations for modern science introducing the concept of continuum and fluid resistance. Moreover, also the first quantitative result is due to a Greek scientist, Archimedes (287 - 212 BC), who studied the fluid statics and the pressure. He understood that in fluid the pressure is linearly proportional to the depth, and that each point of wetted surface is subjected to same force. His famous principle: "Any object, wholly or partially immersed in a fluid, is buoyed up by a force equal to the weight of the fluid displaced by the object" can be considered the first quantitative result in fluid physics. Moreover, he also grasped the effect of the pressure gradient, supposing that a fluid moves from high pressure to low pressure zone.

After Archimedes we have to wait more than 1500 years to have other improvements in fluid dynamics. In fact, Romans built a lot of complex aqueduct but did not achieve scientific results and no results was achieved also during the middle ages. With Leonardo da Vinci (1452 - 1519) starts a new era for fluid dynamics. His interest in fluids, and most specifically in aerodynamics, grow up with his fascination with flight. He observed the birds' flight and draw a lot of flight machines, *ornithopter*, with the purpose to imitate the birds and the bats giving to the men the possibility of flying. Obviously, he never succeeded, and he probably neither really tried to build such machines. However, his contribution to fluid dynamics is more related to his observation of rivers and channels. First of all, he understood that for the the conservation of mass the product between the flow velocity and the conduct area have to be constant. He also observed and draw the vortical structure in separated flow. Moreover he understood the principle which is in the basis of the modern wind tunnel: "The same force as is made by the thing against the air, is made by the air against the thing".

In the following century the fluid dynamics research was mainly dedicated to reduce the drag for the ship, especially for military purpose. A huge develop from theoretical point of view started in the seventeenth century with Isaac Newton (1642-1727) who studied the law of motion and dedicated the second book of his *Principia* (1687) to fluids. His main purpose was to study the resistance, in particular he found a contradiction between Kepler statements, that affirmed that planet's motion was lacking of dissipative phenomena, and the Descartes assumption according to which the space was filled with matter. As was already clear, also from

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experience, a body moving in a fluid it is subject to a resistance force. Newton studied this force and found out that it was proportional to the flow density, the body reference surface, i.e. the circle built on the diameter for a planet, and, most important the square of the velocity. This important result, obtained theoretically by Newton, was already known thanks to the experiments performed by Mariotte and Huygens. Some conflicts about the credits of this finding still remain, in fact Mariotte published the results before, in the 1673, but Huygens, who accused Mariotte of plagiarism, obtained the same results some years before. Anyway, what really matters is that up to this point scientists, including also Galileo, believed that aerodynamics force was simply proportional to the velocity. The reasons were also for philosophical: why in a perfect world could exit a non linear relationship between force and velocity?

Nevertheless, the most important improvements for fluid dynamics arrived in the 18th century. At the beginning of this century, in the University of Basel in Swiss, a thirteen years old boy called Leonard Euler (1707-1783) starts his studies under the supervision of the professor Johann Bernoulli (1667 - 1748), the father of Daniel Bernoulli (1700 - 1782). Euler, in particular, and Daniel Bernoulli lay the foundation for modern fluid dynamics. Daniel Bernoulli was the first one to use the term hydrodynamics in his most famous works called Hydrodinamica, and his name is strictly linked to the famous principle: $P_1 + \frac{1}{2}\rho v_1^2 = P_2 + \frac{1}{2}\rho v_2^2$; even tough he just stated that the pressure decreases as the velocity increases. The first one who really formalized the *Bernoulli principle* was Euler. Euler was a very brilliant scientist and he produced a huge amount of articles, despite he become blind in the middle of his career. His most important work from fluid dynamics point of view, are the governing equations for inviscid flow, which now are known as *Euler equations*. Those equations represents a landmark for fluid dynamics, in fact they are still a valid model to describes some fluid phenomena.

In order to have a complete model we just need to add another ingredient to the Euler equations: viscosity. Two scientists did that during the 19th century, their names were Louis Marie Henri Navier (1785 - 1836) and George Gabriel Stokes (1819 - 1903). Navier and Stokes worked independently and with totally different approach. Navier was a civil engineer and he was famous as bridge builder, he wrote firstly the complete governing equations for fluids including the friction in 1833, even tough he did not understand the role of shear stress. In fact, he add the correct term to the Euler equation in order to take into account some generic molecular forces. On the counter part, Stokes was a great mathematician and physicist, professor at Cambridge university where he held the Lucasian Chair, the same held by Newton two century before, until his death. Stokes did not know the works of Navier and derived correctly the modern Navier-Stokes equation in 1845. He started from the concept of internal shear stress and, differently from Navier, he considered the constant that multiply the second derivative of the velocity as the viscosity coefficient. Nevertheless, there is also a third scientist who worked at the Navier-Stokes equations. He knew the results obtained by Navier but he understood also their physical meaning, so he correctly derived the equations two years before Stokes. This scientist is Adhémar Jean Claude Barré de Saint-Venant (1793-1886) but his name is now associated only to the stress analysis and shallow waters equations.

From physical point of view, Navier–Stokes equations probably represent the goal of fluid dynamics and no modifications have been applied since 1845.

Nevertheless, after having derived the governing equations the challenge is moved to how to use it and how to integrate them. Navier–Stokes equations are non linear and only for very particular conditions it is possible to find an analytical solution. Moreover, these few solutions are unstable and they presents strong discrepancy with respect to the real flow observed in the experiments.

This behaviour was clear since the birth of Navier–Stokes equations. As noted by Darrigol [3], in 1840's Stokes already suspected that these differences were related to instability phenomena. In the same years, Saint-Venant explicitly spoke about *tumultuous* character of the fluid motion, about forty years before the 1883, year of the well-known experiment in which Osborne Reynolds (1842-1912) showed the transition from laminar to turbulent regime in the pipe flow.

A great part of the fluid dynamics research between the second half of

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nineteenth century and the twenties century has been dedicated to find a good way to apply and simplify Navier–Stokes and Euler equations in order to obtain realistic results also for turbulent flow.

In these years several simplified theories and models to compute aerodynamics load were developed. Probably the most important researches in this fields have been carried out by Ludwig Prandtl (1875 - 1953), who described the boundary layer and studied the stall phenomena.

However, especially looking at our days, the main important idea is probably due to Reynolds. In 1895, noting the similarity with kinetic gas theory, he proposed to apply a statistical approach to the fluid equations. His intuition consisted in averaging the Navier–Stokes equations, obtaining a new set of equations, now called Reynolds-Averaged Navier Stokes (RANS) equations. RANS equations are characterized by a new, unknown term the *Reynolds stress* tensor, which need to be modelled. Nevertheless, RANS equations was not applicable at the beginning of 20^{th} . This approach will become very popular only several decades later, when the computers drastically transformed the approach to fluid dynamics.

1.1.2 The computer era: The birth of Computational Fluid Dynamics

In the second half of 20th, science, and more in general our life, has drastically changed. The computers become rapidly faster and cheaper, for fluid dynamics point of view this means the beginning of new era. Let us consider that in 1922 Lewis Fry Richardson in the book "Weather Prediction" [4] supposed to predict the weather using a "computer" consisting in 64000 humans working together in a theatre. Less then forty years later, the first computations using linear potential began available. In the following decades the computational capability of computers rapidly grow up, and began sufficient to compute Euler equations (1980) and finally, in the nineties, also RANS began feasible for industrial and research application.

But, there is not only Euler and RANS equations. In the 1963, Smagorinsky [5] firstly proposed a novel mathematical model for fluid equations. The main purpose was related to the meteorology, in particular the aim was to predict the atmospheric currents. The approach was based on filtering the Navier-Stokes equations, to the end of resolving only the large eddies and using a model for the remaining, smaller, ones. Therefore, this new methodology provide an instantaneous representation of the flow field and it is capable of describing turbulent fluctuations. This approach is now known as Large Eddy Simulation (LES).

From practical point of view, the difference with respect to RANS is that the LES model concerned only the smaller scales that can be supposed more *universal*, i.e. less dependent to the external characteristic of flow. Therefore, the LES models can be simpler with respect to the RANS ones, requiring less calibration constants and equations. On the other hand, the need of resolving the large eddy strongly increase the grid accuracy required, leading to a huge increase of the computational cost.

In the last thirty year, numerical simulations of fluid phenomena have been widely performed both from industry and research applications. For this reason the development of RANS and LES models has been one of the most studied topic in fluid science.

As discussed in the previous section, RANS approach was formulated at the end of 19^{th} century, therefore several models were proposed. The great part of the models is based on the concept of eddy viscosity and in particular to the well known Boussinesq hypothesis. This hypothesis states that the Reynolds stress tensor is proportional to the mean strain rate tensor by the eddy viscosity coefficient. Thanks to Boussinesq assumption the problem begin finding the correct value for the eddy viscosity.

A huge amount of eddy viscosity models have been proposed in the last decades: the simpler algebraic, or zero-equations, models like Cebeci-Smith [6] or Baldwin-Lomax [7], the one equation models like the classical Prandtl mixing layer model or the Spalart-Allmaras model [8] and finally the two equations models like $k - \epsilon$ [9], $k - \omega$ [10] and $k - \omega SST$ [11].

Besides the eddy viscority models there is another important categories RANS model: Reynolds stress equation model (RSM) or second moment closure model [12]. In these methods the computations of the Reynolds stress tensor is obtained solving an equation for each component of the unknown tensor.

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Due to the greater simplicity of the model, the variety of LES models is more limited. The most classical model is the Smagorinsky model [5], which is a zero equations model based on the Boussinesq hypothesis. The eddy viscosity depends on a static and uniform coefficient known as Smagorinsky coefficient. The most significant improvement has been obtained introducing a dynamic procedure for the computation of the local value of the Smagorinsky coefficient [13], [14], which then can vary in time and space. The dynamic procedure allow also to have negative values of eddy viscosity that enables the back-scatter, i.e. the energy transfer from the small scales to the large scales, improving the accuracy of the model.

1.2 Hybrid RANS/LES methods

1.2.1 Why Hybrid RANS/LES Methods?

Both from industrial and research point of view, very often is required a good description of turbulent flows and their unsteady features, such as forces and vortical structures. This requirement have to take into account a practical and very important limitation: the computational cost.

As previously discussed, the LES is able to represents an instantaneous picture of the flow, ensuring good accuracy, but it is very demanding in term of cost. Therefore, although the huge improvements in computer science, is still far from being applicable for complex geometries. In a famous paper of 2000 [15] Spalart stated that an LES simulation for a complete wing will be unfeasable until the 2045. In a well resolved LES in fact, we have to model a great part of turbulent kinetic energy, at least the 80% of the total amount, according to the literature [16], this leads to the need of a very fine grid, that in certain condition can be comparable to the ones required by a DNS. Moreover, even tough with a smaller coefficient, similarly to DNS also LES depends on the Reynolds number [17]. As highlighted by Gopalan [18], in a fully resolved LES simulation of a wall bounded flow, the number of the grid points scales with the Reynolds number as $N \sim Re^{1.76}$, while for RANS the dependency concerns only the wall normal direction and the number of grid points scales as $N \sim lnRe$. Nevertheless, we remark that

RANS can only provide a description of the mean quantities.

Therefore, we can identify a sort of chiasmus: LES is sufficiently detailed but too expensive, RANS is sufficiently cheap but too superficial. For these reasons, seems natural trying to combine the two approach, obtaining hybrid RANS/LES methods.

1.2.2 Framework

The first question to be answered is: how to combine a time dependent approach like LES with a statistical one like RANS? This issue is not a trivial question. First of all, we should notice that in the field of hybrid methods we almost always refer to *unsteady*–RANS (URANS), in which the solution is time dependent [19],[20]. The fundamental assumption for URANS is a clear scale separation, i.e. the temporal scales of turbulence have to be sufficiently smaller of scales of the flow analysed, for a review we refer to [21]. Moreover, as higlighted by [22], even tough RANS and LES have a very different basis, they are very similar from structural point of view. Let see the RANS and LES momentum equation for incompressible flow, for RANS we have:

$$\partial_t \langle u_i \rangle_{\mathcal{E}} + \partial_{x_j} \left(\langle u_i \rangle_{\mathcal{E}} \langle u_j \rangle_{\mathcal{E}} \right) + \partial_i \langle p \rangle_{\mathcal{E}} = \partial_{x_j} \left(\nu \partial_{x_j} \langle u_i \rangle_{\mathcal{E}} \right) - \tau_{ij}^{\mathcal{E}}, \tag{1.1}$$

whereas for LES we have:

$$\partial_t \langle u_i \rangle_{\mathcal{F}} + \partial_{x_j} \left(\langle u_i \rangle_{\mathcal{F}} \langle u_j \rangle_{\mathcal{F}} \right) + \partial_i \langle p \rangle_{\mathcal{F}} = \partial_{x_j} \left(\nu \partial_{x_j} \langle u_i \rangle_{\mathcal{F}} \right) - \tau_{ij}^{\mathcal{F}}.$$
 (1.2)

where $\langle \rangle$ are used to represent quantities filtered $_{\mathcal{F}}$, averaged $_{\mathcal{E}}$ or hybridfiltered. The two equations have different unknowns, $\langle u_i \rangle_{\mathcal{E}}$ and $\langle u_i \rangle_{\mathcal{F}}$, but are formally identical and the only difference is related to the stress tensor τ_{ij} which represents the Reynolds stress for RANS and the subgrid stress tensor for LES. Therefore, in principle, changing this term we can move from a RANS to LES, this concept is known as *implicit filtering* and is fundamental for most of hybrid models. In this context the distinction between RANS and LES is not always clear. A fundamental characteristic of LES is the presence of a filter that depends to the step size of the computational grid. According to [22] this dependencies is fundamental to identify

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an proper LES, in RANS in fact we have dependencies only on geometric features like wall distance and physical quantities.

The DES and the unified methods

One of the first and probably the most famous hybrid model, the Detached Eddy Simulation (DES)[23], exploits the idea of implicit filtering. The DES in fact is based on the Spalart-Allmaras turbulence model [8]. The model consists in an empirical transport equation for the quantity $\tilde{\nu}$:

$$\partial_t \widetilde{\nu} + \langle u_i \rangle_{\mathcal{E}} \partial_{x_i} \widetilde{\nu} = c_{b1} \widetilde{S} \widetilde{\nu} + \frac{1}{\sigma} \left[\partial_{x_i} \left((\nu + \widetilde{\nu}) \right) \partial_{x_i} \widetilde{\nu} + c_{b2} \left(\partial_{x_i} \widetilde{\nu} \right)^2 \right] - c_{w1} f_w \left(\frac{\widetilde{\nu}}{d} \right)^2.$$
(1.3)

 $\tilde{\nu}$ is then linked to the turbulent viscosity used to model Reynolds stress tensor by the relation $\tilde{\nu} = \nu_t / f_{\nu 1} (y^+)$. In order to switch to an LES model Spalart and Allmaras introduced a modification on the last terms of eq. 1.3, substituting the wall distance d with an explicit function of the grid step size. Therefore, in the final model the equation is the same in the whole domain and the original length scale d is replaced by

$$\widetilde{d} = \min(d, C_{DES}\Delta) \tag{1.4}$$

where C_{DES} is a constant and Δ was originally defined as the maximum grid size in the three direction: $\Delta = max(\Delta_x, \Delta_y, \Delta_z)$.

From eq. 1.4, we can see that close to wall where the d is minimum the model turns to RANS, while where the distance from the wall is grater then $C_{DES}\Delta$ a pure LES simulation is performed. Therefore, in DES "the boundary layer is treated by RANS, and regions of massive separation are treated with LES" [24]. From theoretical point of view RANS is used as a wall model for LES, this concept was firstly proposed by Schumann [25] and extended in [26], while examples of applications can be found also in [27].

The main problem related to DES is represented by the presence of *grey areas* between LES and RANS. In fact, in the RANS area the velocity

fluctuations are strongly limited and their kinetic energy is obtained by modelling. On the contrary, in LES, where the modelled part is just the 20% of the total amount of energy, the solution exhibit strong fluctuations that need to be resolved. After the transition to LES we can incur in a situation in which modelled stresses are reduced without a correct compensation by the resolved ones. This phenomena has been defined as *modelled stress depletion* [28] and results in a lack of energy and momentum transfer between LES and RANS. This can produce a log-layer characterized by unphysichal eddies and streaks whose dimensions is dependent to the grid size [29] [30].

In general, problems at the interface between RANS and LES are very common in hybrid methods, Piomelli et Al. [31] showed that a possible strategies to fix these problems can be represented by introducing a *backscatter* model consisting in an artificial forcing term in the interface region.

In the specific of DES this problems is mainly related to a too early transition to LES. As explained by [28] in fact, for certain grids a small step size could lead to $C_{DES}\Delta < d$, see eq. 1.4, also in the boundary layer where we would need to use RANS.

In order to fix this flaw, the same authors proposed a new version of DES called DDES, i.e. *Delayed Detached Eddy Simulation* [28]. In this new method the eq. 1.4 is modified in

$$\widetilde{d} = d - f_d max(0, d - C_{DES}\Delta).$$
(1.5)

Where f_d is a function designed to avoid a too early transition to LES, ensuring that the boundary region is treated by RANS.

In the review provided by Frölich and Von Terzi [22], methods like DES and DDES are classified as *unified* methods. The main characteristic of this typology is that the unknown is a generic hybrid quantity, e.g. the velocity $\langle u_i \rangle_{\mathcal{H}}$, and the following equation is solved for the whole domain:

$$\partial_t \langle u_i \rangle_{\mathcal{H}} + \partial_{x_j} \left(\langle u_i \rangle_{\mathcal{H}} \langle u_j \rangle_{\mathcal{H}} \right) + \partial_i \langle p \rangle_{\mathcal{H}} = \partial_{x_j} \left(\nu \partial_{x_j} \langle u_i \rangle_{\mathcal{H}} \right) - \tau_{ij}^{\mathcal{H}}.$$
(1.6)

In the context of unified methods, different strategies exist to determine the term $\tau_{ij}^{\mathcal{H}}$. For example it is possible to introduce a clear interface between RANS and LES area and then put respectively $\tau_{ij}^{\mathcal{H}} = \tau_{ij}^{\mathcal{E}}$ or $\tau_{ij}^{\mathcal{H}} = \tau_{ij}^{\mathcal{E}}$. The interface can be fixed and constant, hard interface (e.g. DES), or depending step by step on the solution, soft interface (e.g. DDES). This class of unified methods is the most popular, and DES and DDES are implemented in almost every commercial CFD software. Therefore interfacing methods have been applied in a wide range of applications: from the study of the flow over a delta wing [32] to the analysis of the slipstream of a train [33], but also in mixing process simulation [34], heat transfer problems [35] and several other studies.

However it is also possible to move from RANS to LES in a smooth manner, this the case of the *blending* models. Here there is no more a distinction between RANS and LES, but $\tau_{ij}^{\mathcal{H}}$ it is the result of linear combination between the RANS model $\tau_{ij}^{\mathcal{E}}$ and the LES ones $\tau_{ij}^{\mathcal{F}}$. One of the first attempt to obtain a blending model can be found in [29].

The idea is similar to the shear-stress transport model [11]. This RANS turbulence model, known as $k - \omega SST$, is combination of $k - \omega$ model near to the walls and $k - \epsilon$ away. In fact, in order to transform the $k - \omega SST$ RANS model to an hybrid method we can maintain the same formalism substituting the $k - \epsilon$ model with an LES model [36],[37].

In a blending model a critical point is represented by the choice of the correct blending factor. The issue is not trivial, especially considering that, differently from the method with interface, here RANS is not used simply as wall model but could coexist with LES in a wider area of the domain. Usually the blending factor is related to the distance from the wall distance and to the grid size [38], but could be also computed using a dynamic procedure [39].

Although it presents significant differences with respect to the methods described above, Frölich and Von Terzi considered also the FSM (*Flow Simulation Methodology*) methods [40], [41],[42] as a unified-blending model. In fact, in FSM methods LES is not explicitly modelled and the hybrid method is obtained by damping the RANS model:

$$\tau_{ij}^{\mathcal{H}} = f_{\Delta}(\frac{\Delta}{l_K})\tau_{ij}^{\mathcal{E}}.$$
(1.7)

The f_{Δ} depends on the grid size Δ and a characteristic local length scale of turbulence, for example the Kolmogorov length-scale. Therefore, f_{Δ} is space and time dependent and varies from 1, pure RANS, to 0 removing the model, i.e. DNS, where $\Delta \approx l_K$.

Segregated methods

Another possibility to obtain an hybrid method is simply to divide a priori the domain in RANS and LES area, we called these methods segregated. It is worth noting that this approach is completely different from a unified model with hard or soft interface: here different equations are solved in the different regions and, most important, the solution continuity at the interfaces is lost. Doing that it is possible to save cost applying LES only in certain areas. Moreover, at least in principle, we can combine a real stationary RANS simulation with a completely unsteady LES.

This approach is very suitable for the cases in which totally different flow conditions are present in the domain. For example, in [43] a segregated approach has been used to model the flow in a gas turbine engine, using a RANS solver for the turbine and an LES solver for the flow in the combustor which is characterized by complex phenomena like detached flows, chemical reactions and heat release.

The main problem for this approach is to allow exchange of informations between the RANS and LES regions, therefore the coupling conditions become of fundamental importance. Obtaining boundary condition for RANS is relatively easy, in fact it is possible to evaluate RANS variable just averaging the LES solution. The point here is to avoid problems of reflections in the LES domain. The problem become harder when boundary conditions for LES are needed, because the unsteady fluctuations have to be reconstructed starting from the mean flow computed by means of RANS simulation. This situations become critical when the flow is directed from the RANS region toward the LES region.

The two most common approaches are the vortex method [44] [45], [46] and the *enrichment* technique [47].

In the vortex method, similarly to what already seen for the grey areas in

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the unified methods [31], a velocity perturbation is added to the mean flow, but in this case the perturbations is obtained by means of series of vortex. As stated by [48] the advantage is that the velocity field is temporally and spatially correlated. Moreover, it takes into account the anisotropy of the flow in the near-wall region, leading to a more realistic representation of turbulence with respect to the ones obtained adding a random perturbation.

Concerning the enrichment technique, the boundary conditions for LES are obtained reconstructing the LES solution in some ghost nodes in RANS region and vice versa. For an example of application we remand to [49], where the flow over an airfoil at Mach=0.16, near to stall conditions has been studied. A generalization of enrichment procedure, based on convective boundary conditions for velocity, have been proposed in [50]. In this method no calibration constant are required, and a study of the pressure coupling condition for incompressible case is performed.

Besides these techniques several other approaches have been studied in the literature. For example in [43] the fluctuation obtained by means a previous LES computation are added to RANS field, in [51] was suggested to use a random turbulence generator, in [52] a review of the existing coupling technique and a method based on turbulent viscosity reconstruction are proposed. This last approach has been successfully applied to the study of shock wave - boundary layer interaction [53].

Second generation URANS

Recently, hybrid methods are evolving from the original concept of wall modelling LES, i.e. an LES simulation in which RANS is used to model the flow near to the wall. Several new hybrid methods are seen no more as the coupling of two different approaches like RANS and LES, but as intermediate approaches more similar to an evolution of the unsteady RANS. Frölich and Von Terzi collected these methods in a third category of hybrid methods, called 2^{nd} generation URANS. The difference between this category and the previous ones is that there is no more an explicit dependencies from the grid size, therefore we can not strictly speak of LES methods. Nevertheless, 2^{nd} G-URANS aims to resolve a significant part of turbulent fluctuations simply reducing the modelled contribution. In order to do that, a possibility is to introduce a damping factor for the original Reynolds stress tensor, similarly to what happens in the FSM methods. This is the strategy applied in the PANS, i.e. *Partially Averaged Navier-Stokes*, model [54]. PANS method is based on a constant damping factor, prescribed *a priori* and depending only on the amount of energy that we want to resolve without involving the grid resolution, this is the difference with respect to FSM approach, see eq.1.7.

The PANS has been widely applied for cavitation problems [55],[56],[57]. Recently, comparisons with LES and URANS using the cavity flow as testcases [58], [59] have been published. For the case considered the main flow statistics obtained with PANS are comparable to the ones obtained with URANS, probably as a consequence of the limited range of turbulence scales exhibited by the flow. Nevertheless, PANS approach seems to improve URANS results regarding the description of the flow structures. A similar very approach is represented by PITM, i.e. *Partially Integrated Transport Model*, [60], a RANS based model in which a dissipation equation is used to obtain the length scale of subgrid turbulence.

Scale-Adaptive Simulation (SAS) [61] is another relevant 2^{nd} G-URANS method. SAS model is based on the k-kL model [62], a transport equation for the quantity kL where L is an integral length scale of turbulence and k is the turbulent kinetic energy. Menter et Al. introduced the Karman length-scale into the turbulence scale equation, obtaining a dynamic model capable of resolving turbulent fluctuations and to switching to a standard RANS simulation in the regions of stable flow. For an overview of SAS methods we remand to [63]. This approach has been successfully applied in many testcases improving the URANS results [64], in particular seems to suitable for massive separated flow [65].

Filtering approach

In addition to the categories analysed by Frölich and Von Terzi, we can add a fourth strategy, represented by the hybrid filter methods. In these methods the equations are derived applying the hybrid filter directly to

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the Navier-Stokes equations. Doing that, is possible to obtain a new set of exact equations which already contain RANS and LES terms.

In the literature we can find two example: the additive filter proposed by Germano in 2004 [66] and the spatial filter proposed by Hamba in 2011 [67]. The latter is defined as

$$\langle u_i \rangle_{\mathcal{H}} = \int d\mathbf{x}' G(\mathbf{x} - \mathbf{x}, \Delta) u_i(\mathbf{x}')$$
 (1.8)

where G is the filter operator, but the filter width Δ is now a function of the position, independent of the grid spacing. Therefore, where Δ has the same size of grid spacing a pure LES is obtained, while, if Δ increase the simulation move toward a RANS, until reaching a pure RANS simulation in the limit of $\Delta \rightarrow \infty$.

Hamba analysed in particular the effect of the extra terms that appear as a consequence of the non-commutativity between the filter and the space and time derivative. In his study shows that the extra terms are active in the transition area between RANS and LES, allowing the energy and momentum transfer. Therefore, extra terms act similar to the stochastic forcing terms added in the unified methods [31], but in this case they are not artificial.

The Germano hybrid filter is based on the weighted sum of the LES filter with the statistical operator RANS, and is the one analysed in this work. Up to now, Rajamani and Kim [68] for incompressible flow and Sanchez-Rocha and Menon [69], [70] for compressible flow, studied this approach focusing the attention on the role of the extra terms. The Germano hybrid filter will be described in detail in the following chapter.

In general, the strength of the filtering approaches rely on the reduction of empiricism: once the filter is defined the LES/RANS coupling is obtained mathematically without further assumptions. On the other hand, the drawback is that the equations are not simply to be implemented, and modelling all the additional terms is not trivial. Despite some promising results, these problems have restricted the applications of this strategy only to academic research.

1.3 Motivation of the work and outline

The purpose of this work is to analyse the Germano additive filter [66], in order to understand the perspectives of the technique for complex simulations and practical applications. In particular, we investigate an innovative approach that exploit the numerical properties of the hybrid filter, leading to a method in which no explicit RANS model is needed. The procedure, called *RANS-reconstruction*, allows to reconstruct the Reynolds stress tensor from the resolved velocity field and the LES sub-grid stress tensor [71].

In this framework we are no more oriented to a classical wall modelling LES, i.e. an hybrid approach in which RANS is simply used as a wall model, but to an LES simulation in which the RANS contribution is used to model part of the energy unresolved for the low grid resolution.

In the following chapter the Germano hybrid filter will be presented. In chapter 3 the numerical approach based on the Discontinuous Galerkin finite element method is introduced and the LES modelling is described in details. RANS-reconstruction procedure and the hybrid methodology studied is presented in chapter 4, while the numerical results obtained with new formulation are reported in chapter 5.

Finally, in the chapter 6 concluding remarks and future perspectives are reported.

Chapter 2

Hybrid filter approach

In this chapter the hybrid filter approach proposed by Germano [66] is described. The definition of hybrid filter, its properties and the related hybrid filtered equations are shown in the first section, while in the second section a resume of the studies already conducted by Rajamani and Kim [68] and Sanchez-Rocha and Menon [69], [70] is presented.

2.1 Germano's hybrid filter

In 2004 Germano [66] proposed a new approach for hybrid RANS/LES methods. He introduced an hybrid additive filter, obtained combining a statistical operator RANS with an LES filter. The hybrid filter is given by

$$\mathcal{H} = k\mathcal{F} + (1-k)\mathcal{E},\tag{2.1}$$

where k is a blending factor and \mathcal{F} and \mathcal{E} are respectively the LES filter and the statistical RANS operator. The blending factor, in general, can vary between 1, resulting in a pure LES, to 0 yielding a pure RANS.

The assumptions made by Germano are:

$$\mathcal{EH} = \mathcal{E}, \qquad \mathcal{EF} = \mathcal{E}, \qquad \mathcal{F}\frac{\partial}{\partial x} = \frac{\partial}{\partial x}\mathcal{F}.$$
 (2.2)

Notice that (2.2) is the standard assumption of commutativity between filtering and differentiation for LES models. Such an assumptions is not strictly satisfied by the operator \mathcal{F} that will considered here. However, we will ignore the resulting error, as it is often done in LES modelling, when a non-uniform filter is used [72]. Nevertheless, the non commutative terms can not be ignored for the hybrid filter. In fact, we observe that it does not commute with space and time derivatives

$$\mathcal{H}\frac{\partial}{\partial x} = \frac{\partial}{\partial x}\mathcal{H} - \frac{\partial k}{\partial x}\left(\mathcal{F} - \mathcal{E}\right) \quad , \quad \mathcal{H}\frac{\partial}{\partial t} = \frac{\partial}{\partial t}\mathcal{H} - \frac{\partial k}{\partial t}\left(\mathcal{F} - \mathcal{E}\right).$$
(2.3)

Therefore, additional terms appear in the hybrid equations if the blending factor is space or time dependent.

The definition of the hybrid filter 2.1, together with the assumptions 2.2, leads to the following relations:

$$\langle u_i \rangle_{\mathcal{E}} = \langle \langle u_i \rangle_{\mathcal{H}} \rangle_{\mathcal{E}} \tag{2.4}$$

$$\langle u_i \rangle_{\mathcal{F}} = \frac{\langle u_i \rangle_{\mathcal{H}} - (1-k) \langle u_i \rangle_{\mathcal{E}}}{k}$$
(2.5)

where $\langle \rangle_{\mathcal{E}}$ means RANS average, while $\langle \rangle_{\mathcal{H}}$ and $\langle \rangle_{\mathcal{F}}$ stand for respectively the hybrid and the LES filter operator. Starting from the incompressible Navier-Stokes equations

$$\frac{\partial}{\partial x_j} u_j = 0 \tag{2.6}$$

$$\frac{\partial}{\partial t}u_i + \frac{\partial}{\partial x_j}(u_i u_j) + \frac{\partial}{\partial x_i}p - \nu \frac{\partial^2 u_i}{\partial x_j^2} = 0, \qquad (2.7)$$

applying the hybrid filter 2.1, and assuming a time-invariant blending

2.1. GERMANO'S HYBRID FILTER

factor k, we obtain a new set of hybrid filtered equations

$$\frac{\partial}{\partial x_{j}} \langle u_{j} \rangle_{\mathcal{H}} = \frac{\partial}{\partial x_{j}} k \left(\langle u_{j} \rangle_{\mathcal{F}} - \langle u_{j} \rangle_{\mathcal{E}} \right) \tag{2.8}$$

$$\frac{\partial}{\partial t} \langle u_{i} \rangle_{\mathcal{H}} + \frac{\partial}{\partial x_{j}} \left(\langle u_{i} \rangle_{\mathcal{H}} \langle u_{j} \rangle_{\mathcal{H}} \right) + \frac{\partial}{\partial x_{i}} \langle p \rangle_{\mathcal{H}} - \nu \frac{\partial^{2} \langle u_{i} \rangle_{\mathcal{H}}}{\partial x_{j}^{2}} =$$

$$\frac{\partial}{\partial x_{i}} k \left(\langle p \rangle_{\mathcal{F}} - \langle p \rangle_{\mathcal{E}} \right) + \frac{\partial}{\partial x_{i}} \left(\langle u_{i} u_{j} \rangle_{\mathcal{F}} - \langle u_{i} u_{j} \rangle_{\mathcal{E}} \right)$$

$$- 2\nu \frac{\partial}{\partial x_{i}} k \frac{\partial}{\partial x_{j}} \left(\langle u_{i} \rangle_{\mathcal{F}} - \langle u_{i} \rangle_{\mathcal{E}} \right) - \nu \frac{\partial^{2} k}{\partial x_{j}^{2}} \left(\langle u_{i} \rangle_{\mathcal{F}} - \langle u_{i} \rangle_{\mathcal{E}} \right)$$

$$- \frac{\partial}{\partial x_{j}} \tau^{\mathcal{H}} (u_{i}, u_{j}), \tag{2.9}$$

where the term $\tau^{\mathcal{H}}(u_i, u_j) = \langle u_i u_j \rangle_{\mathcal{H}} - \langle u_i \rangle_{\mathcal{H}} \langle u_j \rangle_{\mathcal{H}}$ is the hybrid turbulent stress term, which is given by

$$\tau^{\mathcal{H}}(u_i, u_j) = k\tau^{\mathcal{F}}(u_i, u_j) + (1 - k)\tau^{\mathcal{E}}(u_i, u_j) + k(1 - k)(\langle u_i \rangle_{\mathcal{F}} - \langle u_i \rangle_{\mathcal{E}})(\langle u_j \rangle_{\mathcal{F}} - \langle u_j \rangle_{\mathcal{E}}).$$
(2.10)

In 2.10, $\tau^{\mathcal{F}}(u_i, u_j) = \langle u_i u_j \rangle_{\mathcal{F}} - \langle u_i \rangle_{\mathcal{F}} \langle u_j \rangle_{\mathcal{F}}$ represents the LES subgrid stress tensor, $\tau^{\mathcal{E}}(u_i, u_j) = \langle u_i u_j \rangle_{\mathcal{E}} - \langle u_i \rangle_{\mathcal{E}} \langle u_j \rangle_{\mathcal{E}}$ is the Reynolds stress tensor and $k(1-k)(\langle u_i \rangle_{\mathcal{F}} - \langle u_i \rangle_{\mathcal{E}})(\langle u_j \rangle_{\mathcal{F}} - \langle u_j \rangle_{\mathcal{E}})$ is an additional stress terms related to the additivity of the filter[66], usually known as *Germano* stress. It is worth to notice that this last term explicitly couples RANS and LES velocity and does not appear in the traditional blending models [29],[36], [39]. In fact, the Germano stress, together with the extra terms, represents a peculiarity of the hybrid method herein studied.

As highlighted Rajamani and Kim [68], from the continuity equation 2.8 we can see that the velocity is no more divergence free. This look strange, in fact can leads to a fail in the mass conservation. However, the same authors show that the equation is divergence free on the average:

$$\langle \frac{\partial}{\partial x_j} \langle u_j \rangle_{\mathcal{H}} \rangle_{\mathcal{E}} = \langle \frac{\partial k}{\partial x_j} \left(\langle u_j \rangle_{\mathcal{F}} - \langle u_j \rangle_{\mathcal{E}} \right) \rangle_{\mathcal{E}} \frac{\partial}{\partial x_j} \langle \langle u_j \rangle_{\mathcal{H}} \rangle_{\mathcal{E}} = \frac{\partial k}{\partial x_j} \left(\langle \langle u_j \rangle_{\mathcal{F}} \rangle_{\mathcal{E}} - \langle \langle u_j \rangle_{\mathcal{E}} \rangle_{\mathcal{E}} \right)$$
(2.11)
$$\frac{\partial}{\partial x_j} \langle u_j \rangle_{\mathcal{E}} = 0.$$

The *rhs* of continuity equations can be ignored in LES or RANS area, as well as the region in which the k is constant, but become relevant in the case of a smooth transition between RANS and LES [68].

A relevant aspect of the hybrid filter approach is that it make up a general framework, in which the subgrid and the Reynolds stress tensor in 2.10, can be modelled using respectively any LES and RANS turbulence model. More than that, the stresses can be also reconstructed from a precedent numerical simulation, using experimental data or, concerning the RANS term, reconstructed implicitly from LES model and resolved quantities exploiting the hybrid filter properties, as we will see in the chapter 5.

2.2 Early results

Rajamani and Kim [68] studied the hybrid filter approach for the incompressible case. In particular they analysed the role of the Germano stress and of the additional terms related to the non commutativity, which will be referred to as extra terms (HT).

They demonstrated that the contribution of HT and Germano stress is very relevant in the transition area. In particular, by means of an *a priori* test, they showed that the absence of the Germano stress led to significant errors in the total shear profile, and that HT can reach the 33% of the total amount of the *rhs* of the momentum equation 2.9.

In the numerical simulations of the turbulent channel flow, no super streaks nor velocity discrepancies have been observed in the log layer for DDES, obtaining results similar to the ones obtained by Piomelli[31] with a stochastic and artificial forcing term.

Sanchez-Rocha & Menon [69], [70] generalized the approach to the compressible Naveir-Stokes equation

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_j}(\rho u_j) = 0 \tag{2.12}$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) + \frac{\partial}{\partial x_i}p - \frac{\partial}{\partial x_j}\sigma_{ij} = 0$$
(2.13)

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_j}(\rho E u_j) = \frac{\partial}{\partial x_j}\left((\sigma_{ij} - p\delta_{ij})u_i + \kappa \frac{\partial T}{\partial x_j}\right)$$
(2.14)

in which

$$p = \rho RT$$
, $\rho E = \rho C_v T + \frac{1}{2} \rho u_k u_k$ (2.15)

$$\sigma_{ij} = \mu \left(\mathcal{S}_{ij} - \frac{1}{3} \mathcal{S}_{kk} \delta_{ij} \right) \quad , \quad \mathcal{S}_{ij} = \frac{\partial u_i}{\partial x_i} + \frac{\partial u_j}{\partial x_j} \tag{2.16}$$

where μ is the dynamic viscosity, E is the total energy, κ is the heat conductivity, T is the temperature and R is the ideal gas constant.

In order to obtain the filtered equations for compressible flow we define also the Favre hybrid filter for a generic variable ψ

$$\{\psi\}_{\mathcal{H}} = \frac{\langle \rho \psi \rangle_{\mathcal{H}}}{\langle \rho \rangle_{\mathcal{H}}}.$$
(2.17)

and the following second order central moments:

$$\langle \tau(a,b) \rangle_x = \langle \rho \rangle_x \left(\{ab\}_x - \{a\}_x \{b\}_x \right)$$
(2.18)

$$\langle \chi(a,b) \rangle_x = \{ab\}_x - \{a\}_x \langle b \rangle_x \tag{2.19}$$

$$\langle \zeta(a,b) \rangle_x = \{ab\}_x - \{a\}_x \{b\}_x, \tag{2.20}$$

where x stands for \mathcal{E}, \mathcal{H} or \mathcal{F} , 2.18 is equivalent to the one already seen for the momentum equation for the incompressible case, and 2.19 and 2.20 are related to the energy equations. Exploiting the Favre filter 2.17 and the definition of the hybrid filter 2.1, the second order central moments are given by

$$\langle \tau(a,b) \rangle_{\mathcal{H}} = (1-k) \langle \tau \rangle_{\mathcal{E}} + (k) \langle \tau \rangle_{\mathcal{F}} +$$

$$\langle \rho \rangle_{\mathcal{H}} \left[\frac{\langle \rho \rangle_{\mathcal{E}}}{\langle \rho \rangle_{\mathcal{H}}} \{a\}_{\mathcal{E}} \{b\}_{\mathcal{E}} (1-k) \left(1 - (1-k) \frac{\langle \rho \rangle_{\mathcal{E}}}{\langle \rho \rangle_{\mathcal{H}}} \right) - k(1-k) \frac{\langle \rho \rangle_{\mathcal{E}} \langle \rho \rangle_{\mathcal{F}}}{\langle \rho \rangle_{\mathcal{H}}} \{a\}_{\mathcal{E}} \{b\}_{\mathcal{F}} \right] +$$

$$\langle \rho \rangle_{\mathcal{H}} \left[\frac{\langle \rho \rangle_{\mathcal{F}}}{\langle \rho \rangle_{\mathcal{H}}} \{a\}_{\mathcal{F}} \{b\}_{\mathcal{F}} k \left(1 - k \frac{\langle \rho \rangle_{\mathcal{F}}}{\langle \rho \rangle_{\mathcal{H}}} \right) - k(1-k) \frac{\langle \rho \rangle_{\mathcal{E}} \langle \rho \rangle_{\mathcal{F}}}{\langle \rho \rangle_{\mathcal{H}}} \{a\}_{\mathcal{F}} \{b\}_{\mathcal{E}} \right]$$

$$(2.21)$$

$$\langle \chi(a,b) \rangle_{\mathcal{H}} = (1-k) \langle \chi \rangle_{\mathcal{E}} + k \langle \chi \rangle_{\mathcal{F}} +$$

$$\left[\{a\}_{\mathcal{E}} \langle b \rangle_{\mathcal{E}} (1-k) \left(1 - (1-k) \frac{\langle \rho \rangle_{\mathcal{E}}}{\langle \rho \rangle_{\mathcal{H}}} \right) - k(1-k) \frac{\langle \rho \rangle_{\mathcal{E}}}{\langle \rho \rangle_{\mathcal{H}}} \{a\}_{\mathcal{E}} \langle b \rangle_{\mathcal{F}} \right] +$$

$$\left[\{a\}_{\mathcal{F}} \langle b \rangle_{\mathcal{F}} k \left(1 - k \frac{\langle \rho \rangle_{\mathcal{F}}}{\langle \rho \rangle_{\mathcal{H}}} \right) - k(1-k) \frac{\langle \rho \rangle_{\mathcal{F}}}{\langle \rho \rangle_{\mathcal{H}}} \{a\}_{\mathcal{F}} \langle b \rangle_{\mathcal{E}} \right]$$

$$(2.22)$$

$$\begin{split} \langle \zeta(a,b) \rangle_{\mathcal{H}} &= (1-k) \langle \zeta \rangle_{\mathcal{E}} + k \langle \zeta \rangle_{\mathcal{F}} + \tag{2.23} \\ & \left[\{a\}_{\mathcal{E}} \{b\}_{\mathcal{E}} (1-k) \left(1 - (1-k) \frac{\langle \rho \rangle_{\mathcal{E}}^2}{\langle \rho \rangle_{\mathcal{H}}^2} \right) - k(1-k) \frac{\langle \rho \rangle_{\mathcal{E}} \langle \rho \rangle_{\mathcal{F}}}{\langle \rho \rangle_{\mathcal{H}}} \{a\}_{\mathcal{E}} \{b\}_{\mathcal{F}} \right] + \\ & \left[\{a\}_{\mathcal{F}} \{b\}_{\mathcal{F}} k \left(1 - k \frac{\langle \rho \rangle_{\mathcal{F}}^2}{\langle \rho \rangle_{\mathcal{H}}^2} \right) - k(1-k) \frac{\langle \rho \rangle_{\mathcal{E}} \langle \rho \rangle_{\mathcal{F}}}{\langle \rho \rangle_{\mathcal{H}}} \{a\}_{\mathcal{F}} \{b\}_{\mathcal{E}} \right]. \end{split}$$

Therefore, applying the hybrid filter to the compressible Navier–Stokes equations we finally obtain the new set of hybrid equations [69]:

$$\frac{\partial \langle \rho \rangle_{\mathcal{H}}}{\partial t} + \frac{\partial}{\partial x_j} (\langle \rho \rangle_{\mathcal{H}} \{ u_j \}_{\mathcal{H}}) = \mathcal{HT}_{\rho}$$
(2.24)

$$\frac{\partial \langle \rho \rangle_{\mathcal{H}} \{u_i\}_{\mathcal{H}}}{\partial t} + \frac{\partial}{\partial x_j} \left(\langle \rho \rangle_{\mathcal{H}} \{u_i\}_{\mathcal{H}} \{u_j\}_{\mathcal{H}} + \langle p \rangle_{\mathcal{H}} \delta_{ij} - \{\sigma_{ij}\}_{\mathcal{H}} + \tau^{\mathcal{H}}(u_i, u_j) \right) = \mathcal{HT}_{\rho u_j}$$
(2.25)

$$\frac{\partial \langle \rho E \rangle_{\mathcal{H}}}{\partial t} + \frac{\partial}{\partial x_j} \left(\langle \rho \rangle_{\mathcal{H}} \{ E \}_{\mathcal{H}} \{ u_j \}_{\mathcal{H}} + \langle p \rangle_{\mathcal{H}} - \langle \kappa \rangle_{\mathcal{H}} \frac{\partial \{T\}_{\mathcal{H}}}{\partial x_j} - \{ \sigma_{ij} \}_{\mathcal{H}} \{ u_j \}_{\mathcal{H}} \right. \\ \left. + \tau^{\mathcal{H}}(E, u_j) + \chi^{\mathcal{H}}(u_j, p) - \chi^{\mathcal{H}}(\frac{\partial T}{\partial x_j}, \kappa - \zeta^{\mathcal{H}}(\sigma_{ij, u_i})) \right) = \mathcal{HT}_{\rho E}$$

$$(2.26)$$

2.2. EARLY RESULTS

where \mathcal{HT}_{ρ} , $\mathcal{HT}_{\rho u_j}$ and $\mathcal{HT}_{\rho E}$ represent the extra terms related to the non commutativity between hybrid filter and time and space derivatives:

$$\mathcal{HT}_{\rho} = \frac{\partial k}{\partial x_{j}} \left(\langle \rho \rangle_{\mathcal{F}} \{ u_{j} \}_{\mathcal{F}} - \langle \rho \rangle_{\mathcal{E}} \{ u_{j} \}_{\mathcal{E}} \right) + \frac{\partial k}{\partial t} \left(\langle \rho \rangle_{\mathcal{F}} - \langle \rho \rangle_{\mathcal{E}} \right)$$
(2.27)

$$\mathcal{HT}_{\rho u_j} =$$

$$\frac{\partial k}{\partial x_{j}} \left(\langle \rho \rangle_{\mathcal{F}} \{ u_{i} \}_{\mathcal{F}} \{ u_{j} \}_{\mathcal{F}} - \langle \rho \rangle_{\mathcal{E}} \{ u_{i} \}_{\mathcal{E}} \{ u_{j} \}_{\mathcal{E}} + \tau^{\mathcal{F}}(u_{i}, u_{j}) - \tau^{\mathcal{E}}(u_{i}, u_{j}) \right. \\
\left. + (\langle p \rangle_{\mathcal{F}} - \langle p \rangle_{\mathcal{E}}) \delta_{ij} - (\{ \sigma ij \}_{\mathcal{F}} - \{ \sigma ij \}_{\mathcal{E}}) - \frac{\partial}{\partial x_{j}} \left(\frac{\partial k}{\partial x_{j}} (\langle \mu \rangle_{\mathcal{F}} \{ u_{i} \}_{\mathcal{F}} - \langle \mu \rangle_{\mathcal{E}} \{ u_{i} \}_{\mathcal{E}}) \right. \\
\left. + \frac{\partial k}{\partial x_{i}} (\langle \mu \rangle_{\mathcal{F}} \{ u_{j} \}_{\mathcal{F}} - \langle \mu \rangle_{\mathcal{E}} \{ u_{j} \}_{\mathcal{E}}) - \frac{2}{3} \frac{\partial k}{\partial x_{k}} (\langle \mu \rangle_{\mathcal{F}} \{ u_{k} \}_{\mathcal{F}} - \langle \mu \rangle_{\mathcal{E}} \{ u_{k} \}_{\mathcal{E}}) \right) \\
\left. + \frac{\partial k}{\partial t} (\langle \rho \rangle_{\mathcal{F}} \{ u_{i} \}_{\mathcal{F}} - \langle \rho \rangle_{\mathcal{E}} \{ u_{i} \}_{\mathcal{E}}) \right) \tag{2.28}$$

 $\mathcal{HT}_{\rho E} =$

$$\frac{\partial k}{\partial x_{k}} \left(\langle \rho \rangle_{\mathcal{F}} \{ u_{j} \}_{\mathcal{F}} \{ E \}_{\mathcal{F}} - \langle \rho \rangle_{\mathcal{E}} \{ u_{j} \}_{\mathcal{E}} \{ E \}_{\mathcal{E}} + \tau^{\mathcal{F}}(E, u_{j}) - \tau^{\mathcal{E}}(E, u_{j}) + \left\{ u_{j} \}_{\mathcal{F}} \langle p \rangle_{\mathcal{F}} - \{ u_{j} \}_{\mathcal{E}} \langle p \rangle_{\mathcal{E}} + \chi^{\mathcal{F}}(u_{j}, p) - \chi^{\mathcal{E}}(u_{j}, p) - \langle \kappa \rangle_{\mathcal{F}} \frac{\partial \{T\}_{\mathcal{F}}}{\partial x_{j}} + \langle \kappa \rangle_{\mathcal{E}} \frac{\partial \{T\}_{\mathcal{E}}}{\partial x_{j}} - \chi^{\mathcal{F}}(\frac{\partial T}{\partial x_{j}}, \kappa) + \chi^{\mathcal{E}}(\frac{\partial T}{\partial x_{j}}, \kappa) - \{ \sigma_{ij} \}_{\mathcal{F}} \{ u_{i} \}_{\mathcal{F}} + \{ \sigma_{ij} \}_{\mathcal{E}} \{ u_{i} \}_{\mathcal{E}} - \zeta^{\mathcal{F}}(\sigma_{ij}, u_{i}) + \zeta^{\mathcal{E}}(\sigma_{ij}, u_{i}) \right) + \frac{\partial k}{\partial t} (\langle \rho \rangle_{\mathcal{F}} \{ E \}_{\mathcal{F}} - \langle \rho \rangle_{\mathcal{E}} \{ E \}_{\mathcal{E}}) \qquad (2.29)$$

Eq. 2.24,2.25,2.26 represent the most general equations. Sanchez-Rocha and Menon in [69] focused they attention on the effect of the extra terms related to non commutativity between hybrid filter and space derivative. They perform several simulations of a channel flow with different blending factor, avoiding the time dependences and then zeroing the $\frac{\partial k}{\partial t}$ in eq.2.27, 2.28 and 2.28. The remaining extra terms *a posteriori* from previous LES simulations. The results confirmed the importance of the extra terms in avoiding unphysical phenomena in the transition area. The authors stressed the concept performing also a simulation with a step function of the blending factor which led to a zonal simulation with no transition area between LES a RANS. In this case the extra terms are zero and anomalous phenomena peaks of velocity normal gradient in the buffer layer has been shown.

However, it is clear that eq. 2.24,2.25,2.26 are very difficult to be applied, and the modelling of every extra terms is a very challenging problems. As a consequence, further hypothesis are required in order to make hybrid filter approach suitable for applications also for compressible flow. For example, in [70] Sanchez–Rocha & Menon proposed a first order approximation of the extra terms, confirming the results obtained in the previous work.

Chapter 3

Numerical Approach and LES modelling

In this section the numerical approach is described. In particular, we focused the attention on the Discontinuous Galerkin (DG) finite element method used for the space discretization and on the LES modelling. Three different LES subgrid models have been considered and described: the standard Smagorinsky model 3.3.1, the dynamic model 3.3.2 and finally the anisotropic dynamic model3.3.3. In the last section 3.4, the numerical simulations performed in order to validate the models, and then to decide the best one to be used in the hybrid method, are shown. The main subject and the numerical results presented in this chapter has been published in [73].

3.1 Why Discontinous Galerkin?

The Discontinuous Galerkin finite element method can be seen as an intelligent combination of the finite element and the finite volume methods [74]. This approach in fact, as a classical finite element methods, allows an high order accuracy and h-p adaptivity, i.e. the possibility of increase the quality of the approximation both changing the size of the element or the order of the polynomial basis functions.

Nevertheless, similarly to the finite volume method, the solution is discontinuous and the coupling between is obtained by means of arbitrary numerical fluxes. As a results, we have a very simple and local mass matrix, which leads to a good scalability and parallelizability, very important for the huge amount of degree of freedoms that are typical of CFD problems.

Moreover, in the specific of LES simulations, a further advantage is the possibility of defining a filter simply by projecting the solution on a lower order polynomial space. This turns to be very useful for the dynamic procedure [13], in which different filtering levels are required, and is coherent with the Variational Multiscale (VMS) framework introduced in [75], and applied for LES of incompressible flows in [76], [77], [78] (see also the review in [79]).

In the last years the interest in DG approach for fluids problems is arising, we can found many examples from RANS simulation [80], [81], to LES. In this context, example of DG-VMS approach can be found in [82], [83] and [73], or in the work performed by *Renac et Al.* [84] with the *Aghora* software. The same high order DG approach has been successfully used also for DNS simulation [85].

3.2 Model Equations

We start considering the compressible Navier-Stokes equations in dimensionless form

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_j}(\rho u_j) = 0 \tag{3.1}$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) + \frac{1}{\gamma Ma^2} \frac{\partial}{\partial i} p - \frac{1}{Re} \frac{\partial}{\partial x_j} \sigma_{ij} = \rho f_i$$
(3.2)

$$\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x_j}(\rho h u_j) - \frac{\gamma M a^2}{R e} \frac{\partial}{\partial x_j}(u_i \sigma_{ij}) + \frac{1}{\kappa R e P r} \frac{\partial q}{\partial x_j} = \gamma M a^2 \rho f_j u_j, \qquad (3.3)$$

where ρ , **u** and *e* respectively represent the density, velocity and specific total energy, *p* is the pressure, **f** is a generic forcing term, *h* is the specific enthalpy defined by $\rho h = \rho e + p$ and σ and *q* are the diffusive momentum and heat fluxes. $\gamma = c_p/c_v$ is the ratio between the specific heats at constant pressure and volume respectively. The Mach number *Ma*, the Reynolds number *Re* and the Prandtl number *Pr* are defined as

$$Ma = \frac{V_r}{\left(\gamma RT_r\right)^{1/2}}, \qquad Re = \frac{\rho_r V_r L_r}{\mu_r}, \qquad Pr = \frac{c_p}{\kappa}$$
(3.4)
3.2. MODEL EQUATIONS

where the subscript $_r$ indicates a reference quantities, R is the ideal gas constant $R = c_p - c_v$ and $\kappa = R/c_p$.

The set of equations 3.1-3.3 is completed with the state equations of ideal gas, which is dimensionless form is simply

$$p = \rho T, \tag{3.5}$$

Introducing the specific internal energy e_i :

$$e = e_{\mathbf{i}} + \frac{\gamma M a^2}{2} u_k u_k, \tag{3.6}$$

it is possible to express the temperature T in terms of the velocity and the specific total energy

$$T = \frac{\kappa}{1 - \kappa} e_{\rm i}.\tag{3.7}$$

Finally, the diffusive momentum and the heat flux are given by:

$$\sigma_{ij} = \mu \mathcal{S}_{ij}^d, \qquad q_i = -\mu \frac{\partial}{\partial i} T, \qquad (3.8)$$

with $S_{ij} = \frac{\partial}{\partial j}u_i + \frac{\partial}{\partial i}u_j$ and $S_{ij}^d = S_{ij} - \frac{1}{3}S_{kk}\delta_{ij}$.

In accordance with the Sutherland's hypothesis [86] the dynamic viscosity μ is assumed to depend only on the temperature

$$\mu(T) = T^{\alpha}.\tag{3.9}$$

with $\alpha = 0.7$.

3.2.1 Filtering and discretization

The LES equations are obtained applying to the Navier-Stokes equations an appropriate filter operator $\langle \cdot \rangle$, which is characterized by a spatial scale Δ . Considering that in this chapter hybrid and RANS operator do not appear, for sake of simplicity we will consider implicit the subscript $_{\mathcal{F}}$ to indicate the LES filter. As already explained, in a correct LES simulation this length scales has to be related to the grid step size. Our approach exploits the DG method used for the discretization, resulting in a Δ that depends on local element size and on the degree of the polynomial basis function used in each element. As a result, the Δ is a piecewise constant function in space.

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In order to avoid subgrid terms arising in the continuity equation we define the Favre average $\{\cdot\}$:

$$\langle \rho u_i \rangle = \langle \rho \rangle \{ u_i \}, \qquad \langle \rho e \rangle = \langle \rho \rangle \{ e \}.$$
 (3.10)

Similarly, for the internal energy and the enthalpy we have

$$\langle \rho e_{\mathbf{i}} \rangle = \langle \rho \rangle \{ e_{\mathbf{i}} \}, \qquad \langle \rho h \rangle = \langle \rho \rangle \{ h \} = \langle \rho \rangle \{ e \} + \langle p \rangle,$$

as well as for the temperature, which, according to state equations (3.5), yields

$$\langle \rho T \rangle = \langle \rho \rangle \{T\} = \langle p \rangle.$$
 (3.11)

Finally the relationship between the temperature and the specific total energy (3.6) becomes

$$\langle \rho \rangle \{e\} = \langle \rho \rangle \{e_{\mathbf{i}}\} + \frac{\gamma M a^2}{2} \left(\langle \rho \rangle \{u_k\} \{u_k\} + \tau_{kk} \right), \qquad \langle \rho \rangle \{e_{\mathbf{i}}\} = \frac{1 - \kappa}{\kappa} \langle \rho \rangle \{T\},$$
(3.12)

where

$$\tau_{ij} = \langle \rho u_i u_j \rangle - \langle \rho \rangle \{ u_i \} \{ u_j \}.$$
(3.13)

In order to obtain the filtered version of (3.1-3.3), we just need to define the filtered counterpart of the diffusive fluxes (3.8)

$$\{\sigma_{ij}\} = \mu(T)\{\mathcal{S}_{ij}\}^d, \qquad \{q_i\} = -\mu(T)\frac{\partial}{\partial i}\{T\}, \qquad (3.14)$$

where $\{S_{ij}\} = \frac{\partial}{\partial j} \{u_i\} + \frac{\partial}{\partial i} \{u_j\}$ and $\{S_{ij}\}^d = \{S_{ij}\} - \frac{1}{3} \{S_{kk}\} \delta_{ij}$.

Therefore, neglecting the commutation error of the filter operator with respect to space and time differentiation, the filtered equations are given by

$$\begin{aligned} \frac{\partial}{\partial t} \langle \rho \rangle &+ \frac{\partial}{\partial j} (\langle \rho \rangle \{u_j\}) = 0 \end{aligned} \tag{3.15} \\ \frac{\partial}{\partial t} (\langle \rho \rangle \{u_i\}) &+ \frac{\partial}{\partial j} (\langle \rho \rangle \{u_i\} \{u_j\}) + \frac{1}{\gamma Ma^2} \frac{\partial}{\partial i} \langle p \rangle - \frac{1}{Re} \frac{\partial}{\partial j} \{\sigma_{ij}\} + \langle \rho \rangle f_i \\ &= -\frac{\partial}{\partial j} \tau_{ij} - \frac{\partial}{\partial j} \epsilon_{ij}^{\text{sgs}} \tag{3.16} \\ \frac{\partial}{\partial t} (\langle \rho \rangle \{e\}) &+ \frac{\partial}{\partial j} (\langle \rho \rangle \{h\} \{u_j\}) - \frac{\gamma Ma^2}{Re} \frac{\partial}{\partial j} (\{u_i\} \{\sigma_{ij}\}) + \frac{1}{\kappa RePr} \frac{\partial}{\partial j} \{q_j\} \\ &= -\frac{\partial}{\partial j} (\rho hu_j)^{\text{sgs}} + \frac{\gamma Ma^2}{Re} \frac{\partial}{\partial j} \phi_j^{\text{sgs}} - \frac{1}{\kappa RePr} \frac{\partial}{\partial j} \theta_j^{\text{sgs}} + \gamma Ma^2 \langle \rho \rangle f_j \{u_j\}, \end{aligned}$$

where

$$\epsilon_{ij}^{\text{sgs}} = \langle \sigma \rangle_{ij} - \{ \sigma_{ij} \}, \qquad (\rho h u_i)^{\text{sgs}} = \langle \rho h u_i \rangle - \langle \rho \rangle \{ h \} \{ u_i \}, \phi_j^{\text{sgs}} = \langle u_i \sigma_{ij} \rangle - \{ u_i \} \{ \sigma_{ij} \}, \quad \theta_i^{\text{sgs}} = \langle q \rangle_i - \{ q_i \}.$$

$$(3.18)$$

Coherently with [87] and [88] and on the fact that

 $\langle \sigma \rangle_{ij} \approx \{ \sigma_{ij} \}, \qquad \langle q \rangle_i \approx \{ q_i \}$ (3.19)

we neglect the term $\frac{\partial}{\partial j} \phi_j^{\text{sgs}}$, as well as $\epsilon_{ij}^{\text{sgs}}$ and θ_j^{sgs} . Concerning the subgrid enthalpy flux, we proceed as follows. First of all, notice that using (3.5) and (3.6), as well as their filtered counterparts (3.11) and (3.12), we have

$$\rho h = \frac{1}{\kappa} \rho T + \frac{\gamma M a^2}{2} \rho u_k u_k, \qquad \langle \rho \rangle \{h\} = \frac{1}{\kappa} \langle \rho \rangle \{T\} + \frac{\gamma M a^2}{2} \left(\langle \rho \rangle \{u_k\} \{u_k\} + \tau_{kk} \right).$$

Introducing now the subgrid heat and turbulent diffusion fluxes

$$Q_i^{\text{sgs}} = \langle \rho u_i T \rangle - \langle \rho \rangle \{ u_i \} \{ T \} = \langle \rho \rangle \left(\{ u_i T \} - \{ u_i \} \{ T \} \right)$$

$$J_i^{\text{sgs}} = \langle \rho u_i u_k u_k \rangle - \langle \rho \rangle \{ u_i \} \{ u_k \} \{ u_k \} = \langle \rho \rangle \{ u_i u_k u_k \} - \langle \rho \rangle \{ u_i \} \{ u_k \} \{ u_k \}$$
(3.20a)
$$(3.20a)$$

we have

$$(\rho h u_i)^{\text{sgs}} = \frac{1}{\kappa} Q_i^{\text{sgs}} + \frac{\gamma M a^2}{2} \left(J_i^{\text{sgs}} - \tau_{kk} \{ u_i \} \right).$$
(3.21)

(3.17)

Notice that, introducing the generalized central moments $\tau(u_i, u_j, u_k)$ as in [89], with

$$\tau(u_i, u_j, u_k) = \langle \rho \rangle \{u_i u_j u_k\} - \{u_i\} \tau_{jk} - \{u_j\} \tau_{ik} - \{u_k\} \tau_{ij} - \langle \rho \rangle \{u_i\} \{u_k\}, \quad (3.22)$$

 J_i^{sgs} in (3.20b) can be rewritten as

$$J_i^{\text{sgs}} = \tau(u_i, u_k, u_k) + 2\{u_k\}\tau_{ik} + \{u_i\}\tau_{kk}.$$
(3.23)

Summarizing, given the above approximations and definitions, the filtered equations (3.15-3.17) become

$$\frac{\partial}{\partial t} \langle \rho \rangle + \frac{\partial}{\partial j} (\langle \rho \rangle \{u_j\}) = 0$$

$$\frac{\partial}{\partial t} \langle \rho \rangle \{u_j\} + \frac{\partial}{\partial t} \langle \rho \rangle \{u_j\} \langle u_j \rangle + \frac{1}{2} \frac{\partial}{\partial t} \langle \rho \rangle - \frac{1}{2} \frac{\partial}{\partial t} \{\sigma_{ij}\} = -\frac{\partial}{\partial t} \tau_{ij} + \langle \rho \rangle f_{ij}$$
(3.24)

$$\frac{\partial}{\partial t}\left(\langle\rho\rangle\{u_i\}\right) + \frac{\partial}{\partial j}\left(\langle\rho\rangle\{u_i\}\{u_j\}\right) + \frac{1}{\gamma Ma^2}\frac{\partial}{\partial i}\langle\rho\rangle - \frac{1}{Re}\frac{\partial}{\partial j}\{\sigma_{ij}\} = -\frac{\partial}{\partial j}\tau_{ij} + \langle\rho\rangle f_i$$
(3.25)

$$\frac{\partial}{\partial t} \left(\langle \rho \rangle \{e\} \right) + \frac{\partial}{\partial j} \left(\langle \rho \rangle \{h\} \{u_j\} \right) - \frac{\gamma M a^2}{Re} \frac{\partial}{\partial j} \left(\{u_i\} \{\sigma_{ij}\} \right) + \frac{1}{\kappa RePr} \frac{\partial}{\partial j} \{q_j\} \\ = -\frac{1}{\kappa} \frac{\partial}{\partial j} Q_j^{\text{sgs}} - \frac{\gamma M a^2}{2} \frac{\partial}{\partial j} \left(J_j^{\text{sgs}} - \tau_{kk} \{u_j\} \right) + \gamma M a^2 \langle \rho \rangle f_j \{u_j\}.$$
(3.26)

The filtered equations (3.24-3.26) are then discretized in space by means of DG finite element method. The DG approach here employed is analogous to that described in [90] and relies on the so called Local Discontinuous Galerkin (LDG) method, see e.g. [91], [92], [93], [94], for the approximation of the second order viscous terms. The procedure herein described is the same available in [73], for the details we refer to [95].

In the LDG method, equations (3.24-3.26) are rewritten introducing an auxiliary variable \mathcal{G} , so that

$$\frac{\partial}{\partial t} \mathbf{U} + \nabla \cdot \mathbf{F}^{c}(\mathbf{U}) - \nabla \cdot \mathbf{F}^{v}(\mathbf{U}, \mathcal{G}) + \nabla \cdot \mathbf{F}^{sgs}(\mathbf{U}, \mathcal{G}) = \mathbf{S}$$

$$\mathcal{G} - \nabla \varphi = 0, \qquad (3.27)$$

where $\mathbf{U} = [\langle \rho \rangle, \langle \rho \rangle \{ \mathbf{u} \}^T, \langle \rho \rangle e^T]^T$ and $\boldsymbol{\varphi} = [\{U\}, \{T\}]^T$ collects the variables whose gradients are required for flux computations, i.e. velocity and temperature.

The fluxes $\mathbf{F}^{c}, \mathbf{F}^{v}, \mathbf{F}^{sgs}$, respectively *convective*, *viscous* and *sub-grid*, ans the source term \mathbf{S} are given by

$$\mathbf{F}^{c} = \begin{bmatrix} \langle \rho \rangle \{ \mathbf{u} \} \\ \langle \rho \rangle \{ \mathbf{u} \} \otimes \{ \mathbf{u} \} + \frac{1}{\gamma M a^{2}} \overline{p} \mathcal{I} \\ \langle \rho \rangle \widetilde{h} \{ \mathbf{u} \} \end{bmatrix}, \mathbf{F}^{v} = \begin{bmatrix} 0 \\ \frac{1}{Re} \widetilde{\sigma} \\ \frac{\gamma M a^{2}}{Re} \{ \mathbf{u} \}^{T} \widetilde{\sigma} - \frac{1}{\kappa RePr} \widetilde{\mathbf{q}} \end{bmatrix}$$

and

$$\mathbf{F}^{\text{sgs}} = \begin{bmatrix} 0 \\ \tau \\ \frac{1}{\kappa} \mathbf{Q}^{\text{sgs}} + \frac{\gamma M a^2}{2} \left(\mathbf{J}^{\text{sgs}} - \tau_{kk} \{ \mathbf{u} \} \right) \end{bmatrix}, \mathbf{S} = \begin{bmatrix} 0 \\ \langle \rho \rangle \mathbf{f} \\ \gamma M a^2 \langle \rho \rangle \mathbf{f} \cdot \{ \mathbf{u} \} \end{bmatrix}$$

where τ , \mathbf{Q}^{sgs} and \mathbf{J}^{sgs} will be obtained by means of a subgrid models. It is worth noting that this structure is absolutely general and, according to the concept of *implicit* filtering [96], is the same used also for the hybrid RANS/LES method.

The discretization is then obtained using the classical method of lines, therefore we start from space discretization and then we use a time integrator to advance in time. In this case a fourth order, five stage, Strongly Stability Preserving Runge–Kutta method (SSPRK) [97] has been used.

As usual, to obtain the DG discretization, we consider a tessellation \mathcal{T}_h of the computational domain Ω into non-overlapping tetrahedral elements K.

Introducing the finite element space of the polynomial functions of degree at most q on the element K, which is defined as:

$$\mathcal{V}_h = \left\{ v_h \in L^2(\Omega) : v_h |_K \in \mathbf{P}^q(K), \, \forall K \in \mathcal{T}_h \right\}$$
(3.28)

the DG formulation for problem (3.27) will be: find the solution $(\mathbf{U}_h, \boldsymbol{\mathcal{G}}_h) \in ((\mathcal{V}_h)^5, (\mathcal{V}_h)^{4\times 3})$ such that, $\forall K \in \mathcal{T}_h, \forall v_h \in \mathcal{V}_h, \forall \mathbf{r}_h \in (\mathcal{V}_h)^3$,

$$\frac{d}{dt} \int_{K} \mathbf{U}_{h} v_{h} d\mathbf{x} - \int_{K} \mathbf{F}(\mathbf{U}_{h}, \boldsymbol{\mathcal{G}}_{h}) \cdot \nabla v_{h} d\mathbf{x} + \int_{\partial K} \widehat{\mathbf{F}}(\mathbf{U}_{h}, \boldsymbol{\mathcal{G}}_{h}) \cdot \mathbf{n}_{\partial K} v_{h} d\sigma = \int_{K} \mathbf{S} v_{h} d\mathbf{x}, \qquad (3.29a)$$
$$\int_{K} \boldsymbol{\mathcal{G}}_{h} \cdot \mathbf{r}_{h} d\mathbf{x} + \int_{K} \boldsymbol{\varphi}_{h} \nabla \cdot \mathbf{r}_{h} d\mathbf{x} - \int_{\partial K} \widehat{\boldsymbol{\varphi}} \mathbf{n}_{\partial K} \cdot \mathbf{r}_{h} d\sigma = 0, \qquad (3.29b)$$

where $\mathbf{U}_h = [\rho_h, \rho_h \mathbf{u}_h, \rho_h e_h]^T, \boldsymbol{\varphi}_h = [\mathbf{U}_h, T_h]^T, \mathbf{n}_{\partial K}$ represents the outward normal on ∂K and the terms $\hat{\mathbf{F}}$ and $\hat{\boldsymbol{\varphi}}$ are the numerical fluxes. These terms represent the only connection between adjacent elements, which would be otherwise uncoupled. The numerical fluxes are needed to solve the ambiguity of double valued functions at the interface between adjacent elements and to weakly impose the boundary conditions on $\partial \Omega$. There are different ways to define the numerical fluxes [90], in this work we use the *Rusanov* flux for $\hat{\mathbf{F}}$ and the centered flux for $\hat{\boldsymbol{\varphi}}$.

The solution and the test functions are defined in terms of orthogonal basis functions, this is a quite natural choice considering that in DG there are no constraints related to the continuity; this approach is commonly defined as modal DG. We also mention that all the integrals are evaluated by means of the quadrature formulae reported in [98]. In order to have a correct evaluation for the products, we have used formulae which are exact for polynomial of degree up to 2q.

Let us consider now the definition of the filter operators $\langle \cdot \rangle$ with the associated Favre decompositions. We follow the guidelines proposed in [99], [100], [83], defining the filter operators in terms of some L^2 projectors. Given a subspace $\mathcal{V} \subset L^2(\Omega)$, let $\Pi_{\mathcal{V}} : L^2(\Omega) \to \mathcal{V}$ be the associated projector defined by

$$\int_{\Omega} \Pi_{\mathcal{V}} u \, v \, d\mathbf{x} = \int_{\Omega} u \, v \, d\mathbf{x}, \qquad \forall u, v \in \mathcal{V},$$

where the integrals are evaluated with the same quadrature rule used in (3.29). For $v \in L^2(\Omega)$, the filter $\langle \cdot \rangle$ is now defined by

$$\langle v \rangle = \Pi_{\mathcal{V}_h} v, \tag{3.30}$$

or equivalently $\overline{v} \in \mathcal{V}_h$ such that

$$\int_{K} \langle v \rangle v_h \, d\mathbf{x} = \int_{K} v v_h \, d\mathbf{x} \qquad \forall K \in \mathcal{T}_h, \quad \forall v_h \in \mathcal{V}_h.$$
(3.31)

Notice that the application of this filter is built in the discretization process and equivalent to it. Therefore, once the discretization of equations (3.27) has been performed, only the filtered quantities are computed by the model.

We also remark that these filters do not commute with the differentiation operators. As previously discussed, according to a not uncommon practice in LES modelling [101]. An analysis of the terms resulting from non zero commutators between differential operators and projection filters is presented in [83].

3.3 Subgrid models

3.3.1 Smagorinsky model

Originally proposed by Smagorinsky in 1963 [5], the classical Smagorinsky model is the first and probably the most famous LES model. This model, as well as the following, exploits the eddy viscosity hypothesis and the deviatoric part of the subgrid stress tensor τ_{ij} is modelled as

$$\tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} = -\frac{1}{Re} \langle \rho \rangle \nu^{\text{sgs}} \{ \mathcal{S}_{ij} \}^d.$$
(3.32)

 ν^{sgs} is the turbulent viscosity and is given by

$$\nu^{\text{sgs}} = \operatorname{Re} C_S^2 \Delta^2 |\{\mathcal{S}\}| f_D \tag{3.33}$$

where $C_S = 0.1$ is the Smagorinsky constant, $|\{S\}|^2 = \frac{1}{2}\{S_{ij}\}\{S_{ij}\}, \Delta$ is the filter scale and f_D is Van Driest damping function [102]. This function is applied in order to zeroing the eddy viscosity at the wall and to reduce the scale Δ according to the smaller size of turbulent structures close to the wall [101]. In (3.33) is defined as

$$f_D(y^+) = 1 - \exp\left(-y^+/A\right),$$
 (3.34)

where A is a constant, hereinafter the value A = 25 is employed, and $y^+ = \frac{\rho_r u_\tau^d d_{\text{wall}}^d}{\mu_r}$, with d_{wall}^d denoting the (dimensional) distance from the wall and u_τ^d the (dimensional) friction velocity.

We also notice that the Reynolds number has been included in the definition of ν^{sgs} so that the corresponding dimensional viscosity can be obtained as $\nu^{\text{sgs,d}} = \frac{\mu_r}{\rho_r} \nu^{\text{sgs}}$.

In accordance with [103], for this model the isotropic part of the subgrid stress tensor is not explicitly modelled, in fact, by defining a modified pressure gradient, it can be included into the pressure contribution. In alternative it is possible to follow the guidelines given in [104], according to that, the τ_{kk} is then modelled as

$$\tau_{kk} = C_I \langle \rho \rangle \Delta^2 |\{\mathcal{S}\}|^2. \tag{3.35}$$

The subgrid temperature flux (3.20a) is assumed to be proportional to the resolved temperature gradient and is modelled with the eddy viscosity model

$$Q_i^{\rm sgs} = -\frac{Pr}{Pr^{\rm sgs}} \langle \rho \rangle \nu^{\rm sgs} \frac{\partial}{\partial x_i} \{T\}, \qquad (3.36)$$

where Pr^{sgs} is a subgrid Prandtl number. Notice that the corresponding dimensional flux is $Q_i^{\text{sgs,d}} = q_r Q_i^{\text{sgs}}[105]$.

Finally, the turbulent diffusion J_i^{sgs} , in analogy with RANS models, the term $\tau(u_i, u_j, u_k)$ in (3.23) is neglected [106], yielding

$$J_i^{\text{sgs}} \approx 2\{u_k\}\tau_{ik} + \{u_i\}\tau_{kk}.$$
(3.37)

3.3.2 Dynamic model

A great improvement of the Smagorinsky model has been obtained with the dynamic procedure proposed by Germano in 1991 [13] and improved by Lilly [14]. In this approach, the coefficients C_S and C_I of the Smagorinsky model are no more constant and chosen *a priori* for the whole domain, but are dynamically computed from the resolved field.

The deviatoric part of the subgrid stress tensor is very similar to the (3.32)

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = -\langle \rho \rangle C_S \Delta^2 |\{\mathcal{S}\}|\{\mathcal{S}_{ij}\}^d.$$
(3.38)

It is worth to notice that we do not need any more to use a damping function to correct results in the wall region [13]. Moreover, differently from classical Smagorinsky model the coefficient is now C_S and no more C_S^2 . Thanks to the dynamic procedure in fact, C_S can assume also negative values, leading to a positive work done by the subgrid stresses on the mean flow. This phenomena is known as *backscatter*, and is an important improvement with respect to the Smagorinsky model which is dissipative by construction. Nevertheless, the positive total dissipation is ensured using a limiting factor.

In order to compute dynamically the coefficients C_S and C_I , we need to introduce test filter operator $\langle \cdot \rangle$. The test filter is simply obtained by projecting the solution on a new finite element space, characterized by a lower order of the polynomial basis functions. Similarly to (3.28), we can define it as

$$\widehat{\mathcal{V}_h} = \left\{ v_h \in L^2(\Omega) : v_h|_K \in \mathbf{P}^{\widehat{q}(K)}, \, \forall K \in \mathcal{T}_h \right\},\tag{3.39}$$

with $0 < \hat{q} < q$. Therefore, with the same approach used for the LES filter (3.30), the test filter is defined as:

$$\langle v \rangle = \Pi_{\mathcal{V}_h} v, \tag{3.40}$$

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The test filter is also associated to a Favre filter, denoted by $\check{\cdot}$, through the Favre decomposition, for a generic variable ϕ , we have

$$\widehat{\rho\phi} = \widehat{\rho}\breve{\phi}. \tag{3.41}$$

Applying the test filter to the momentum equation (3.2) and proceeding as before we arrive at

$$\frac{\partial}{\partial t} \left(\hat{\rho} \check{u}_i \right) + \frac{\partial}{\partial x_j} \left(\hat{\rho} \check{u}_i \check{u}_j \right) + \frac{1}{\gamma M a^2} \frac{\partial}{\partial x_i} \hat{p} - \frac{1}{Re} \frac{\partial}{\partial x_j} \hat{\sigma}_{ij} \\
= -\frac{\partial}{\partial x_i} \left(\hat{\tau}_{ij} + \mathcal{L}_{ij} \right)$$
(3.42a)

where

$$\mathcal{L}_{ij} = \langle \rho \rangle \widehat{\{u_i\}} \{u_j\} - \widehat{\langle \rho \rangle} \{\check{u_i}\} \{\check{u_j}\}$$
(3.43)

is the Leonard stress tensor. Assuming now that model (3.38) can be used to represent the right-hand-side of (3.42a) implies

$$\widehat{\tau}_{ij}^d + \mathcal{L}_{ij}^d = -\langle \widehat{\rho} \rangle \widehat{\Delta}^2 | \{ \check{\mathcal{S}} \} | C_S \{ \check{\mathcal{S}} \}^d_{rs}.$$
(3.44)

Substituting (3.38) for τ^d_{ij} and applying a least square approach [14] provides the required expression

$$C_S = \frac{\mathcal{L}_{ij}^d \mathcal{R}_{ij}}{\mathcal{R}_{kl} \mathcal{R}_{kl}},\tag{3.45}$$

where

$$\mathcal{R}_{kl} = \langle \rho \rangle \Delta^2 \widehat{|\{\mathcal{S}\}|} \{\mathcal{S}\}_{kl}^d - \langle \widehat{\rho} \rangle \widehat{\Delta}^2 |\{\breve{\mathcal{S}}\}| \{\breve{\mathcal{S}}\}_{kl}^d.$$
(3.46)

The dynamic procedure is also applied to the isotropic components of the subgrid stress tensor

$$\tau_{kk} = C_I \langle \rho \rangle \Delta^2 |\{\mathcal{S}\}|^2. \tag{3.47}$$

where the C_I coefficient is determined by

$$C_I = \frac{\mathcal{L}_{kk}}{\langle \widehat{\rho} \rangle \widehat{\Delta}^2 |\{\check{\mathcal{S}}\}|^2 - \langle \rho \rangle \widehat{\Delta^2} |\{\check{\mathcal{S}}\}|^2}$$
(3.48)

Let us now consider the subgrid stress terms in the energy equation, namely \mathbf{Q}^{sgs} and \mathbf{J}^{sgs} . According to [95] and [73] we treat both of them within the same

dynamic framework used for the subgrid stresses. Concerning the subgrid heat flux, we let

$$Q_i^{\text{sgs}} = -\langle \rho \rangle \Delta^2 | \{ \mathcal{S} \} | C_Q \frac{\partial}{\partial x_i} \{ T \}, \qquad (3.49)$$

where the coefficient C_Q can be computed locally by the dynamic procedure. To this aim, we define the temperature Leonard flux

$$\mathcal{L}_{i}^{Q} = \langle \rho \rangle \widehat{\{u_{i}\}} \{T\} - \widehat{\langle \rho \rangle} \{ \overset{\smile}{u_{i}} \} \{ \overset{\smile}{T} \}, \qquad (3.50)$$

we apply the test filter to the energy equation and we observe that, thanks to the similarity hypothesis, model (3.49) should be also applied in the resulting equation, so that

$$\widehat{Q}_{i}^{\text{sgs}} + \mathcal{L}_{i}^{Q} = -\langle \widehat{\rho} \rangle \widehat{\Delta}^{2} | \{ \breve{S} \} | C_{Q} \frac{\partial}{\partial x_{i}} \{ \breve{T} \}.$$
(3.51)

Substituting (3.49) for \hat{Q}_i^{sgs} , applying the least squares method yields

$$C_Q = \frac{\mathcal{L}_i^Q \mathcal{R}_i^Q}{\mathcal{R}_k^Q \mathcal{R}_k^Q},\tag{3.52}$$

where

$$\mathcal{R}_{i}^{Q} = \langle \rho \rangle \Delta^{2} |\{\mathcal{S}\}| \frac{\partial}{\partial x_{i}} \{T\} - \langle \widehat{\rho} \rangle \widehat{\Delta}^{2} |\{\breve{\mathcal{S}}\}| \frac{\partial}{\partial x_{i}} \{\breve{T}\}.$$
(3.53)

For the dynamic procedure we do not neglect the term $\tau(u_i, u_k, u_k)$ in (3.23), but instead adopt a scale similarity model as in [87] where such term is approximated as a subgrid kinetic energy flux

$$\tau(u_i, u_k, u_k) \approx \langle \rho \rangle \{ u_i u_k u_k \} - \langle \rho \rangle \{ u_i \} \{ u_k u_k \}.$$
(3.54)

In analogy with the other subgrid terms, we modelled $\tau(u_i, u_k, u_k)$ as a function of the gradient of the resolved kinetic energy, letting

$$\tau(u_i, u_k, u_k) = -\langle \rho \rangle \Delta^2 |\{\mathcal{S}\}| C_J \frac{\partial}{\partial x_i} \left(\frac{1}{2} \{u_k\}\{u_k\}\right).$$
(3.55)

Introducing the kinetic energy Leonard flux

$$\mathcal{L}_{i}^{J} = \langle \rho \rangle \{ \widehat{u_{i}} \} \{ u_{k} \} - \langle \widehat{\rho} \rangle \{ \widetilde{u_{i}} \} \{ \widetilde{u_{k}} \} \{ \widetilde{u_{k}} \}$$
(3.56)

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and proceeding exactly as for the previous terms we arrive at

$$C_J = \frac{\mathcal{L}_i^J \mathcal{R}_i^J}{\mathcal{R}_k^J \mathcal{R}_k^J},\tag{3.57}$$

where

$$\mathcal{R}_{i}^{J} = \langle \rho \rangle \Delta^{2} | \{\mathcal{S}\} | \widehat{\frac{\partial}{\partial x_{i}}} \left(\frac{1}{2} \{ u_{k} \} \{ u_{k} \} \right) - \langle \widehat{\rho} \rangle \widehat{\Delta}^{2} | \{ \breve{\mathcal{S}} \} | \frac{\partial}{\partial x_{i}} \left(\frac{1}{2} \{ \breve{u}_{k} \} \{ \breve{u}_{k} \} \right).$$
(3.58)

To avoid numerical instabilities, all the model coefficients are assumed to be averaged over each element, while they are not averaged in time.

3.3.3 Anisotropic dynamic model

The dynamic procedure described in the previous section leads to an isotropic subgrid viscosity. For this reason there are some limitations such as the alignment of the subgrid flux tensors with the gradients of the corresponding quantities. To overcome these problems Abbà et Al. proposed an anisotropic extension of the dynamic procedure [107]. The approach has been the extended to the compressible flow in [95] and [73].

Also in this model the subgrid stress tensor τ_{ij} is assumed proportional to the strain rate tensor, but in this case the proportionality is through a fourth order symmetric tensor as follows

$$\tau_{ij} = -\langle \rho \rangle \Delta^2 | \{ \mathcal{S} \} | \mathcal{B}_{ijrs} \{ \mathcal{S}_{rs} \}.$$
(3.59)

To compute dynamically the tensor \mathcal{B}_{ijrs} , we observe that a generic, symmetric fourth order tensor can be represented as

$$\mathcal{B}_{ijrs} = \sum_{\alpha,\beta=1}^{3} \mathcal{C}_{\alpha\beta} a_{i\alpha} a_{j\beta} a_{r\alpha} a_{s\beta}, \qquad (3.60)$$

where a_{ij} is a rotation tensor, i.e. an orthogonal matrix with positive determinant, and $C_{\alpha\beta}$ is a second order, symmetric tensor. Therefore (3.60) represents a generalization of the orthogonal diagonalization for symmetric second order tensors. According to that we can define the following algorithm:

1. choose a rotation tensor a_{ij}

- 2. compute the six components of $C_{\alpha\beta}$ by means of the classical dynamic procedure
- 3. define \mathcal{B}_{ijrs} using (3.60), thereby completely determining the subgrid flux (3.59).

The rotation tensor a_{ij} can be chosen arbitrarily, and in principle can be any rotation tensor, possibly varying in space and time. The values of the components $C_{\alpha\beta}$ depend on the choice of a_{ij} , resulting in general in different subgrid fluxes. Many different choices have been proposed in the past, essentially trying to identify at each position three directions intrinsically related to the flow configuration; examples are a vorticity aligned basis, the eigenvectors of the velocity strain rate, or the eigenvectors of the Leonard stresses [108], [107], [109]. However, the numerical results do not seem to exhibit a strong dependency on the choice of a_{ij} , for this reason we simply set $a_{ij} = \delta_{ij}$.

Following the same assumption already done for the dynamic model, we can write:

$$\widehat{\tau}_{ij} + \mathcal{L}_{ij} = -\langle \widehat{\rho} \rangle \widehat{\Delta}^2 | \{ \check{\mathcal{S}} \} | \mathcal{B}_{ijrs} \{ \check{\mathcal{S}} \}_{rs}.$$
(3.61)

Now, multiplying (3.61) by $a_{i\alpha}a_{j\beta}$ and summing over i, j, using the orthogonality of the rotation tensor,

$$a_{i\alpha}a_{j\beta}\left(\widehat{\tau}_{ij}+\mathcal{L}_{ij}\right)=-\langle\widehat{\rho}\rangle\widehat{\Delta}^{2}|\{\breve{\mathcal{S}}\}|\mathcal{C}_{\alpha\beta}a_{r\alpha}a_{s\beta}\{\breve{\mathcal{S}}\}_{rs},$$

substituting (3.59) for τ_{ij} and solving for $\mathcal{C}_{\alpha\beta}$ provide the required expression

$$\mathcal{C}_{\alpha\beta} = \frac{a_{i\alpha}\mathcal{L}_{ij}a_{j\beta}}{a_{r\alpha}a_{s\beta}\left(\langle\rho\rangle\Delta^{\widehat{2}}|\{\widehat{\mathcal{S}}\}|\{\mathcal{S}_{rs}\} - \widehat{\langle\rho\rangle}\widehat{\Delta}^{2}|\{\check{\mathcal{S}}\}|\{\check{\mathcal{S}}\}_{rs}\right)}.$$
(3.62)

Assuming now $a_{ij} = \delta_{ij}$ we immediately have

$$\mathcal{C}_{ij} = \frac{\mathcal{L}_{ij}}{\left(\langle \rho \rangle \Delta^2 | \{ \mathcal{S} \} | \{ \mathcal{S}_{ij} \} - \langle \widehat{\rho} \rangle \widehat{\Delta}^2 | \{ \breve{\mathcal{S}} \} | \{ \breve{\mathcal{S}} \}_{ij} \right)}$$
(3.63)

and

$$\tau_{ij} = -\langle \rho \rangle \Delta^2 | \{ \mathcal{S} \} | \mathcal{C}_{ij} \{ \mathcal{S}_{ij} \}, \qquad (3.64)$$

where no summation over repeated indices is implied in the above formula. In this model the deviatoric and isotropic parts of the subgrid stress tensor are modelled together, without splitting the two contributions. Similarly to the dynamic model,

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the coefficients C_{ij} are averaged over each element and a limiting coefficient is introduced to ensure positive total dissipation.

The procedure for the computation of the subgrid heat flux is very similar, we start defining

$$Q_i^{\text{sgs}} = -\langle \rho \rangle \Delta^2 | \{ \mathcal{S} \} | \mathcal{B}_{ir}^Q \partial_r \{ T \}, \qquad (3.65)$$

where \mathcal{B}_{ir}^Q is a symmetric tensor. Assuming that \mathcal{B}_{ir}^Q is diagonal in the reference defined by the rotation tensor *a* we have

$$\mathcal{B}_{ir}^Q = \sum_{\alpha=1}^3 \mathcal{C}_{\alpha}^Q a_{i\alpha} a_{r\alpha}, \qquad (3.66)$$

where the three coefficients C^Q_{α} can be computed locally by the dynamic procedure. As usual, model (3.65) should be also applied to model the rhs of the test filtered energy equation:

$$\widehat{Q}_{i}^{\text{sgs}} + \mathcal{L}_{i}^{Q} = -\widehat{\langle \rho \rangle} \widehat{\Delta}^{2} | \{ \check{\mathcal{S}} \} | \mathcal{B}_{ir}^{Q} \partial_{r} \{ \check{T} \}.$$
(3.67)

Substituting (3.65) and (3.66) for \hat{Q}_i^{sgs} , multiplying by $a_{i\alpha}$, summing over *i* and solving for \mathcal{C}_{α} yields

$$\mathcal{C}^{Q}_{\alpha} = \frac{a_{i\alpha}\mathcal{L}^{Q}_{i}}{a_{r\alpha}\left(\langle\rho\rangle\Delta^{2}\widehat{|\{\mathcal{S}\}|\partial_{r}\{T\}} - \widehat{\langle\rho\rangle}\widehat{\Delta}^{2}|\{\breve{\mathcal{S}}\}|\partial_{r}\{\breve{T}\}\right)}.$$
(3.68)

The same procedure is also applied to model the subgrid kinetic energy flux

$$\tau(u_i, u_k, u_k) \approx \langle \rho \rangle \{ u_i u_k u_k \} - \langle \rho \rangle \{ u_i \} \{ u_k u_k \}.$$
(3.69)

Coherently with the other subgrid terms, we define the symmetric tensor \mathcal{B}_{ir}^{J}

$$\mathcal{B}_{ir}^J = \sum_{\alpha=1}^3 \mathcal{C}_{\alpha}^J a_{i\alpha} a_{r\alpha}, \qquad (3.70)$$

letting

$$\tau(u_i, u_k, u_k) = -\langle \rho \rangle \Delta^2 |\{\mathcal{S}\}| \mathcal{B}_{ir}^J \partial_r \left(\frac{1}{2} \{u_k\}\{u_k\}\right).$$
(3.71)

Proceeding exactly as for the previous terms we arrive at

$$\mathcal{C}^{J}_{\alpha} = a_{i\alpha} \mathcal{L}^{J}_{i} / \mathcal{M}_{\alpha}, \qquad (3.72)$$

where

$$\mathcal{M}_{\alpha} = a_{r\alpha} \left(\langle \rho \rangle \Delta^2 | \{ \mathcal{S} \} | \widehat{\partial_r \left(\frac{1}{2} \{ u_k \} \{ u_k \} \right)} - \langle \widehat{\rho} \rangle \widehat{\Delta}^2 | \{ \check{\mathcal{S}} \} | \partial_r \left(\frac{1}{2} \{ \check{u}_k \} \{ \check{u}_k \} \right) \right).$$

	Moser et Al	Present
Ma		0.2
$Re_{\rm b}$		2800
L_x	4π	2π
L_z	$\frac{4}{3}\pi$	$\frac{4}{3}\pi$
Δ_x^+	17.7	23
$\Delta_z +$	5.9	10
$\Delta_{y_{min}}^+ / \Delta_{y_{max}}^+$	0.05/4.4	0.65/7.9

Table 3.1: Grid and simulation parameters

3.4 Numerical Results

All the simulations performed hereinafter are realized using the finite element toolkit FEMilaro [110], a FORTRAN/MPI library, available under GPL license. The software has been improved and partly developed during this thesis, in particular concerning the implementation and the optimization of the LES and the hybrid RANS/LES modelling.

3.4.1 Turbulent channel flow

The first test case considered for the numerical simulations is the turbulent channel flow at Ma =0.2 with a skin friction Reynolds numbers: $Re_{\tau} = 180$. The results were compared to DNS data obtained by the incompressible numerical simulation of Moser et al. (MKM) [111].

The computational domain size, in dimensionless units, is $2\pi \times 2 \times 4/3\pi$, representing respectively L_x , L_y and L_z . We use x for streamwise direction, y for normal direction and z for spanwise direction. No-slip, isothermal boundary conditions have been prescribed at the wall $(y = \pm 1)$, while periodic conditions have been applied for the remaining directions.

The structured mesh used is composed by $N_x = 8$, $N_y = 16$, $N_z = 12$ hexahedra in the x, y, z directions, each hexahedra is then divided into $N_t = 6$ tetrahedral elements. The grid is uniform in x and z directions, while, to increase the resolution near the wall, in the normal direction (y) the planes that define the hexahedra are given by:

$$y_j = -\frac{\tanh\left(\omega\left(1 - 2j/N_y\right)\right)}{\tanh\left(\omega\right)} \qquad j = 0, \dots, N_y, \tag{3.73}$$

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where the parameter ω is set fixing the position of the first element.

Mesh resolution can be estimated using the following formula:

$$\Delta_i = \frac{H_i}{\sqrt[3]{N_t N_q}} \qquad i = x, y, z, \tag{3.74}$$

where H_i represents a characteristic element size and N_q is the number of degrees of freedom for each finite element, in this case employing 4^{th} degree basis functions we have $N_q = 35$. Multiplying (3.74) by Re_{τ} , i.e. the skin friction Reynolds number, we obtain the grid spacing estimation in wall units, Δ_i^+ , reported in Table 3.4.1.

In order to maintain a constant mass flux along the channel a body force in streamwise direction has been added. This forcing term $f_x(t)$ can be considered as a PI controller term [112]. In fact is composed by a proportional terms, which depends on the difference between the mass flux calculated at each time step Q(t) and the prescribed value Q_0 , and an integral terms, which allows to avoid the accumulation of the errors:

$$f_x(t) = -\frac{1}{\rho_{\rm b}} \left[\alpha_1 \left(Q(t) - Q_0 \right) + \alpha_2 \int_0^t \left(Q(s) - Q_0 \right) ds \right], \tag{3.75}$$

the constants α_1 and α_2 are respectively 0.1 and 0.2.

The results obtained with this forcing terms are good, and therefore no derivative terms have been considered.

All the considered numerical simulations start from a laminar Poiseille profile. The turbulence is obtained adding a perturbation to the velocity in the x direction. This random perturbation is computed from a fixed number of iteration of logistic map: $\xi^{k+1} = 3.999\xi^{(k)}(1 - \xi^{(k)})$. As a result, we can obtain a definition of the random perturbation which allows the repeatability of the results. After the statistical steady turbulent regime was reached, the simulations were continued enough to have a well verified time invariance for the mean profiles. In the simulations herein shown the sample used for statistics computation is ate least 60 non-dimensional time units.

The statistics are computed averaging the solution, both in space and time, on a set of fixed planes, parallel to the wall. For a generic quantity φ we have:

$$<\varphi>(|y|) = \frac{1}{2TL_xL_z} \int_{t_f}^{t_f-T} \int_0^{L_x} \int_0^{L_z} \left(\varphi(t,x,-|y|,z) + \varphi(t,x,|y|,z)\right) \, dz \, dx \, dt.$$
(3.76)

where T is the time used for statistics computation.



Figure 3.1: Streamline velocity u, mean profiles: *(left)* cartesian representation , *(right)* logarithmic representation

	$ au_{ m w}$	Re_{τ}	u_{τ}/U_b
DNS	11.21	178	0.06357
Anis. dyn.	10.38	171	0.0608
Iso. dyn.	10.62	172	0.0614
Smag.	9.98	167	0.0596

Table 3.2: Mean flow quantities for the numerical experiments at Mach= 0.2. The results obtained with anisotropic dynamic, isotropic dynamic and classical Smagorinsky model are compared with DNS results obtained by Moser *et Al.*[111].



Figure 3.2: Velocity root mean square (rms) profiles and shear stress tensor, from the left: streamwise velocity u rms, normal velocity v rms, spanwise velocity w rms and shear stress tensor τ_{uv} . The LES results are compared to the DNS data.

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The numerical results show significant differences between Smagorinsky and two dynamic models. In particular, the comparison with DNS data highlights a globally better performance of the dynamics models with respect to Smagorinsky. Concerning the mean velocity (Fig.3.1) the Smagorinsky one shows an underestimation in the buffer region, this is probably related to the dissipative nature of the Smagorinsky model. This is confirmed by Table 3.4.1 in which the mean value of τ_w , Re_{τ} and u_{τ} are reported. The differences become greater in the velocity root mean square profiles and in the shear stress (Fig.3.2). Here both the dynamic models well represent the streamwise flutuations, and only a small underprediction is observed for normal and spanwise directions. On the other hand, Smagorinsky always overestimates the fluctuations in the center of the channel, especially for the streamwise component where the overestimation reaches also the buffer region. Moreover, the fluctuations are underestimated in near the wall for spanwise and normal direction.

This behaviour is confirmed also by the shear stress (Fig.3.2(d)), here Smagorinsky does not present the correct trend at the wall and the shear stress is considerably overestimated.

Therefore, the results highlight that the dynamic models perform better then the classical Smagorinsky model. Moreover, the computational cost is quite similar:using the same configuration and machine, the average wall clock times per time step needed by the isotropic and anisotropic dynamic models were 26% and 34% larger, respectively, than that of the Smagorinsky model.

3.4.2 Periodic hill flow

To evaluate the performance of the implemented subgrid scale models in a more complex setting, in which e.g. separation and reattachment arise and a less trivial geometry is considered, turbulent channel flow over a periodic hill has been simulated. First studied in [113], the periodic hill flow has become an important test case for CFD and in particular for RANS and LES simulations that has been discussed in a number of ERCOFTAC workshops [114], [115], [116]. Despite the apparently simple geometry, the periodic hill test case presents some challenging feature, like the massive flow separation from a curved surface, the high sensitivity of the reattachment point location to the separation and the strong acceleration of the flow. Most of the results in the published literature refers to the incompressible case [117], [118], while a compressible simulation can be found in [119]. Here we employ the modified geometry defined in [120]. For this test, only the performance of the dynamic models has been assessed, considering the generally inferior



Figure 3.3: Periodic hill geometry: $L_x = 9.0h$, $L_z = 4.5h$, $L_y = 3.036h$

performance of the simpler Smagorinsky model in the previous plane channel test case.

The computational domain (Fig. 3.3) is a periodic plane channel constricted by two hills of the height h of about one third of the total channel, placed respectively at the inflow and at the outflow. Domain dimensions are: $L_x = 9.0h$ for streamwise direction, $L_z = 4.5h$ for spanwise direction and $L_y = 3.036h$ for the height.

The Mach number is still Ma = 0.2, while the Reynolds number is Re = 2800.

A structured hexahedral mesh, where each hexahedron is divided into 6 tetrahedra, is used to resolve the boundary layer close to the hill profile, while a fully unstructured, three-dimensional mesh is used in the bulk region. The total number of elements is 16662. For the structured, boundary layer mesh, we have $N_z = 12$ elements in the spanwise direction, which, using basis functions of degree q = 4, leads to a $\Delta z/h \simeq 0.062$. In order to accurately describe the hill shape, the streamwise resolution varies from $\Delta x/h \simeq 0.062$ between the two hills to $\Delta x/h \simeq 0.023$ at the top of the hill. The mesh is refined in the normal direction to reach $\Delta y/h \simeq 0.0032$ at the bottom wall, whereas, in order to reduce the computational cost, no mesh refinement has been applied close to the upper wall.

Figure 3.4 shows a two dimensional section of the mesh, the dotted lines indicate the position of the point sections in which the statistics are evaluated.

The no-slip and isothermal wall boundary conditions are imposed at both upper and lower surfaces. Cyclic boundary conditions are imposed in the streamwise and spanwise directions where the flow is assumed to be periodic. As in the chan-



Figure 3.4: Section in the (x - y) plane of the mesh used for the periodic hill simulations; the dotted lines at x/h = 0.5, 2, 4, 6 denote the positions of the mean profiles displayed in the following figures.

nel flow simulation, a varying in time driving force is applied to keep constant mass flow.

A first view of the results is provided in Figure 3.5, in which the averaged values of the streamwise velocity component are displayed along the channel, as computed using the anisotropic dynamic model. The two dimensional representation has been obtained averaging the solution both in time and in space, over the spanwise direction. The figure highlights the flow separation after the first hill and the following reattachment, showing a qualitative agreement with the DNS results reported in the literature. The performances of the two LES model have been studied analysing the velocities and turbulent stress profiles averaged over the spanwise direction and time at the four different positions indicated in Figure 3.4. More specifically, the four positions are: x/h = 0.5, just after the separation; x/h = 2, at the beginning of the flat floor, is inside the main recirculation bubble; x/h = 4 just before the reattachment; and the last one x/h = 6 is located in the reattached flow region. The results obtained have been compared to the DNS data provided by Breuer [117].

The mean streamwise velocity profiles (Fig. 3.6), for both the dynamic models, show an excellent agreement with DNS results. Some discrepancies are presented in the mean normal velocity profiles in Figure 3.7. Here, the dynamic isotropic model presents a better agreement with the DNS with respect to the anisotropic model.

On the other hand, the anisotropic model describes better the turbulent stresses (Figure 3.8-3.10), even tough the positions of the peaks in all the profiles and the shape of the shear layer are well captured by both dynamic models.



Figure 3.5: Averaged streamwise velocity representation with isolines in the period hill flow test case obtained using the anisotropic dynamic model. The average is both in time and space.

Therefore, from these results, it is hard to understand which models is more suitable for LES modelling in the hybrid method. Nevertheless, we have observed a greater robustness of the anisotropic model, especially in the simulations performed at higher Mach [73]. For this reason, the LES subgrid stress tensor in the hybrid stress tensor (2.10), will be modelled using the anisotropic dynamic model.



Figure 3.6: Mean streamwise velocity profiles in the periodic hill flow test case at different locations along the channel;; (a): x/h = 0.5; (b): x/h = 2; (c): x/h = 4; (d): x/h = 6.



Figure 3.7: Mean normal velocity profiles in the periodic hill flow test case at different locations along the channel; (a): x/h = 0.5; (b): x/h = 2; (c): x/h = 4; (d): x/h = 6.



Figure 3.8: Turbulent stresses profiles in the periodic hill flow test case, streamwise component at different locations along the channel; (a): x/h = 0.5; (b): x/h = 2; (c): x/h = 4; (d): x/h = 6. The profiles are obtained considering both the resolved and the modelled contributions.



Figure 3.9: Turbulent stresses profiles in the periodic hill flow test case, normal component at different locations along the channel; (a): x/h = 0.5; (b): x/h = 2; (c): x/h = 4; (d): x/h = 6. The profiles are obtained considering both the resolved and the modelled contributions.



Figure 3.10: Turbulent stresses profiles in the periodic hill flow test case, shear stress component at different locations along the channel; (a): x/h = 0.5; (b): x/h = 2; (c): x/h = 4; (d): x/h = 6. The profiles are obtained considering both the resolved and the modelled contributions.

Chapter 4

Hybrid methodology

In this chapter the hybrid methodology here studied and developed is presented. In the first section we introduce the hybrid equations and the modelling approach for subgrid terms in momentum and energy equations, while, in the second section, we present the RANS reconstruction used to obtain the Reynolds stress tensor without using an explicit RANS model.

4.1 Model equations

Let us start from the Navier Stokes compressible equations (3.1)-(3.2). Applying the hybrid filter (2.1) and considering the the same hypothesis of the LES, we obtain a set of equations very similar to (3.24)-(3.26):

$$\begin{aligned} \frac{\partial}{\partial t} \langle \rho \rangle_{\mathcal{H}} &+ \frac{\partial}{\partial j} (\langle \rho \rangle_{\mathcal{H}} \{ u_j \}_{\mathcal{H}}) = HT_{\rho} \end{aligned} \tag{4.1} \\ \frac{\partial}{\partial t} (\langle \rho \rangle_{\mathcal{H}} \{ u_i \}_{\mathcal{H}}) &+ \frac{\partial}{\partial j} (\langle \rho \rangle_{\mathcal{H}} \{ u_i \}_{\mathcal{H}} \{ u_j \}_{\mathcal{H}}) + \frac{1}{\gamma Ma^2} \frac{\partial}{\partial i} \langle p \rangle_{\mathcal{H}} - \frac{1}{Re} \frac{\partial}{\partial j} \{ \sigma_{ij} \}_{\mathcal{H}} = \\ &- \frac{\partial}{\partial j} \tau_{ij}^{\mathcal{H}} + \langle \rho \rangle_{\mathcal{H}} f_i + HT_m \end{aligned} \tag{4.2} \\ \frac{\partial}{\partial t} (\langle \rho \rangle_{\mathcal{H}} \{ e \}_{\mathcal{H}}) &+ \frac{\partial}{\partial j} (\langle \rho \rangle_{\mathcal{H}} \{ h \}_{\mathcal{H}} \{ u_j \}_{\mathcal{H}}) - \frac{\gamma Ma^2}{Re} \frac{\partial}{\partial j} (\{ u_i \}_{\mathcal{H}} \{ \sigma_{ij} \}_{\mathcal{H}}) + \\ &+ \frac{1}{\kappa RePr} \frac{\partial}{\partial j} \{ q_j \}_{\mathcal{H}} = -\frac{1}{\kappa} \frac{\partial}{\partial j} Q_j^{\mathcal{H}} - \frac{\gamma Ma^2}{2} \frac{\partial}{\partial j} (J_j^{\mathcal{H}} - \tau_{kk}^{\mathcal{H}} \{ u_j \}_{\mathcal{H}}) + \\ &+ \gamma Ma^2 \langle \rho \rangle_{\mathcal{H}} f_j \{ u_j \}_{\mathcal{H}} + HT_e. \end{aligned}$$

where all the terms are the same already defined for (3.1)-(3.2).

The difference is related to the additional terms HT that depends on the noncommutativity between hybrid filter and space and time derivatives. In fact, these terms, which are usually neglected in LES simulations, have to be considered in hybrid simulations, as shown by [68], [69] and [70] and as already discussed in chapter 2.

4.1.1 Momentum equation

Here we will consider only a nearly incompressible flow. Therefore, the sub-grid stress tensor $\tau_{ij}^{\mathcal{H}}$ in (4.2) can be approximated as:

$$\tau_{ij}^{\mathcal{H}}(\rho, u_i, u_j) \approx \langle \rho \rangle_{\mathcal{H}} \tau_{ij\,inc}^{\mathcal{H}}(u_i, u_j) \,. \tag{4.4}$$

where the term $\tau_{ij\ inc}^{\mathcal{H}}$ is the hybrid incompressible subgrid stress tensor already defined in (2.10):

$$\tau^{\mathcal{H}}(u_i, u_j) = k\tau^{\mathcal{F}}(u_i, u_j) + (1 - k)\tau^{\mathcal{E}}(u_i, u_j) + k(1 - k)(\langle u_i \rangle_{\mathcal{F}} - \langle u_i \rangle_{\mathcal{E}})(\langle u_j \rangle_{\mathcal{F}} - \langle u_j \rangle_{\mathcal{E}}).$$
(4.5)

This formulation is useful to understand one of the strengths of hybrid filter approach: in fact, as already mentioned in chapter 2, the last term, i.e. the

4.1. MODEL EQUATIONS

Germano stress, explicitly couples LES and RANS velocity making the transition between RANS and LES smoother and reducing interface problems. Anyway, in order to obtain a more suitable formulation, we can substitute the filtered velocity $\langle u \rangle_{\mathcal{F}}$

$$\langle u_i \rangle_{\mathcal{F}} = \frac{\langle u_i \rangle_{\mathcal{H}} - (1-k) \langle u_i \rangle_{\mathcal{E}}}{k}, \qquad (4.6)$$

in 4.5, obtaining:

$$\tau^{\mathcal{H}}(u_i, u_j) = k\tau^{\mathcal{F}}(u_i, u_j) + (1 - k)\tau^{\mathcal{E}}(u_i, u_j) + \frac{1 - k}{k} (\langle u_i \rangle_{\mathcal{H}} - \langle u_i \rangle_{\mathcal{E}}) (\langle u_j \rangle_{\mathcal{H}} - \langle u_j \rangle_{\mathcal{E}}).$$
(4.7)

Doing that the subgrid stress tensor depends on the resolved velocity instead of the LES velocity that needs to be reconstructed.

We remark that (4.7) is absolutely general, and $\tau^{\mathcal{F}}(u_i, u_j)$ and $\tau^{\mathcal{E}}(u_i, u_j)$, can be modelled using respectively any LES and RANS model.

As discussed in the previous chapter, we have chosen the anisotropic dynamic model presented in [107] as LES model. Concerning the Reynolds stress tensor $\tau^{\mathcal{E}}(u_i, u_j)$, in addition to the explicit modelling by means of a RANS model we have also other alternatives: for example we can obtain it by using DNS/LES data or from experimental results, but we can also reconstruct it implicitly exploiting the hybrid filter. The latter is the approach herein proposed and tested, the procedure called *RANS reconstruction* will be described in 4.2.

4.1.2 Energy equation

As shown in chapter 2, the application of the hybrid filter to energy equation leads to several additional terms, making modelling very costly and difficult. To avoid this problem here a different approach has been adopted.

Following the guidelines given by Lenormand [121] and Knight [106] for the LES approximation of energy equation, the sub-grid stress tensor can be reduced to two contributions: heat flux (Q) and turbulent diffusion(J).

Extending these assumptions to the dynamic-anisotropic model, we have

$$\vartheta_j = Q_j + J_j \approx \bar{\rho} \Delta^2 |S| C_j^Q \partial_j T + \bar{\rho} \Delta^2 |S| C_j^J u_k \partial_j u_k - \tau_{jk}^F u_k - \frac{1}{2} u_j \tau_{kk}^F, \quad (4.8)$$

where S represents the rate of strain tensor, and coefficient C^q and C^J are computed using a dynamic procedure.

In the proposed hybrid formulation, the first two terms are the same of LES, while in the latter ones the $\tau^{\mathcal{F}}$ is substituted by $\tau^{\mathcal{H}}$, the same calculated for momentum balance by means of (4.14).

Thanks to this correction, hybrid terms enter into the energy equation modifying the turbulent diffusion. Considering the simplicity of the implementation and that it does not require any computational overhead, this seems to be a good compromise, especially at the low Mach number.

Notice that the resulting method turns out to be rather general; in fact, it can be extended to any LES model in which sub-grid turbulent diffusion is modelled starting from the Knight proposal [106]

$$J_j \approx \tau_{jk} u_k - \frac{1}{2} u_j \tau_{kk} \tag{4.9}$$

4.2 RANS reconstruction

The Reynolds stress tensor $\tau^{\mathcal{E}}(u_i, u_j)$ can be written as

$$\tau^{\mathcal{E}}(u_{i}, u_{j}) = \langle u_{i}u_{j}\rangle_{\mathcal{E}} - \langle u_{i}\rangle_{\mathcal{E}}\langle u_{j}\rangle_{\mathcal{E}} =$$

$$= \langle \langle u_{i}u_{j}\rangle_{\mathcal{H}}\rangle_{\mathcal{E}} - \langle \langle u_{i}\rangle_{\mathcal{H}}\rangle_{\mathcal{E}}\langle \langle u_{j}\rangle_{\mathcal{H}}\rangle_{\mathcal{E}} +$$

$$\langle \langle u_{i}\rangle_{\mathcal{H}}\langle u_{j}\rangle_{\mathcal{H}}\rangle_{\mathcal{E}} - \langle \langle u_{i}\rangle_{\mathcal{H}}\langle u_{j}\rangle_{\mathcal{H}}\rangle_{\mathcal{E}} =$$

$$= \langle \tau^{\mathcal{H}}(u_{i}, u_{j})\rangle_{\mathcal{E}} + \tau^{\mathcal{E}}(\langle u_{i}\rangle_{\mathcal{H}}, \langle u_{j}\rangle_{\mathcal{H}})$$
(4.10)

where, splitting velocity at \mathcal{H} level in average and fluctuating part, $\langle \mathbf{u} \rangle_{\mathcal{H}} = \langle \langle \mathbf{u} \rangle_{\mathcal{H}} \rangle_{\mathcal{E}} + \langle \mathbf{u} \rangle'_{\mathcal{H}}$, the latter term becomes:

$$\tau^{\mathcal{E}}(\langle u_i \rangle_{\mathcal{H}}, \langle u_j \rangle_{\mathcal{H}}) =$$

$$= \langle (\langle \langle u_i \rangle_{\mathcal{H}} \rangle_{\mathcal{E}} + \langle u_i \rangle_{\mathcal{H}}')(\langle \langle u_i \rangle_{\mathcal{H}} \rangle_{\mathcal{E}} + \langle u_i \rangle_{\mathcal{H}}')\rangle_{\mathcal{E}} - \langle \langle u_i \rangle_{\mathcal{H}} \rangle_{\mathcal{E}} \langle \langle u_j \rangle_{\mathcal{H}} \rangle_{\mathcal{E}} =$$

$$= \langle (\langle u_i \rangle_{\mathcal{H}} - \langle u_i \rangle_{\mathcal{E}})(\langle u_j \rangle_{\mathcal{H}} - \langle u_j \rangle_{\mathcal{E}})\rangle_{\mathcal{E}}.$$
(4.11)

Substituting the hybrid stress tensor definition (4.7) in (4.10) one obtains

4.2. RANS RECONSTRUCTION

$$\tau^{\mathcal{E}}(u_i, u_j) = k \langle \tau^{\mathcal{F}}(u_i, u_j) \rangle_{\mathcal{E}} + (1 - k) \tau^{\mathcal{E}}(u_i, u_j) +$$

$$\frac{1 - k}{k} \langle (\langle u_i \rangle_{\mathcal{H}} - \langle u_i \rangle_{\mathcal{E}}) (\langle u_j \rangle_{\mathcal{H}} - \langle u_j \rangle_{\mathcal{E}}) \rangle_{\mathcal{E}} +$$

$$\tau^{\mathcal{E}}(\langle u_i \rangle_{\mathcal{H}}, \langle u_j \rangle_{\mathcal{H}}).$$
(4.12)

Using now relation (4.11), the Reynolds stress tensor becomes:

$$\tau^{\mathcal{E}}(u_i, u_j) = \langle \tau^{\mathcal{F}}(u_i, u_j) \rangle_{\mathcal{E}} + \frac{1}{k^2} \tau^{\mathcal{E}}(\langle u_i \rangle_{\mathcal{H}}, \langle u_j \rangle_{\mathcal{H}}).$$
(4.13)

Inserting relation (4.13) in (4.7), we can finally obtain the expression of $\tau^{\mathcal{H}}(u_i, u_j)$, namely

$$\tau^{\mathcal{H}}(u_{i}, u_{j}) = k\tau^{\mathcal{F}}(u_{i}, u_{j}) + (1-k)\langle \tau^{\mathcal{F}}(u_{i}, u_{j})\rangle_{\mathcal{E}} + \frac{1-k}{k^{2}}\tau^{\mathcal{E}}(\langle u_{i}\rangle_{\mathcal{H}}, \langle u_{j}\rangle_{\mathcal{H}}) + \frac{1-k}{k}(\langle u_{i}\rangle_{\mathcal{H}} - \langle u_{i}\rangle_{\mathcal{E}})(\langle u_{j}\rangle_{\mathcal{H}} - \langle u_{j}\rangle_{\mathcal{E}}).$$

$$(4.14)$$

Therefore, we have obtained a very simple formulation with the great advantage to avoid the need of an explicit RANS model, and then without introducing the related additional equations. In this formulation we just need to compute some average quantities, from computational point of view this operations are not so demanding and different strategies can be applied. For example we can use a pure time average, with a fixed time interval or a running time average, or we can also use an hybrid space and time average in order to reduce the initialization of the average quantities.

The main drawback is related to the term $\frac{1}{k^2}$ in (4.13). In fact, this term leads to an ill conditioned problem for low values of k. In fact, although at least in principle, considering (4.6), a lower limit for k should be set also in the traditional approach (i.e. using an explicit RANS model), the square term k^2 at the denominator leads to a greater value for this limit.

As we increase k we move to LES, and then we have to solve a greater number of turbulent scales. As a consequence, this drawback make impossible a classical wall-modelling LES approach. However, the simplicity of the formulation obtained leads to a very small additional cost related to the computation of the hybrid terms. Therefore, in our opinion, this approach can be suitable to integrate the LES in the context of *coarse* grid, i.e. for a grid that is too coarse for a well resolved LES, but anyway finer then a RANS grid.

Chapter 5

Numerical Results

In this section the results of the numerical simulations performed with the hybrid methodology introduced in chapter 4 are presented. In the first section we consider the constant blending factor case, we compare the hybrid results with the pure LES simulation and we analysis the effect of the blending factor. In the second section we introduce a space dependent blending factor and we show the results obtained for the turbulent channel flow and the periodic hill flow testcases.

5.1 Constant blending factor

As already discussed above, the non-commutativity of the hybrid filter with the derivatives leads to several additional terms HT in the governing equations. In order to perform a preliminary study, in this first part we will use a constant and uniform value of the blending factor.

Clearly, this configuration is not optimal, in fact the number of turbulent scales resolved in the domain is not constant and then the RANS contribution should increase where the number of scales resolved decreases and vice versa. However, this analysis is useful to understand the capability and the potentiality of the methodology, and also to analyse the effect of the different blending factors.

Therefore, all the additional terms, which depend on the k derivatives, are equal to zero. We remark that this is not an approximation: we do not neglect any terms, but on the basis of this assumption the additional terms are simply zero.

5.1.1 Turbulent channel flow

The test case considered for these numerical simulations is the turbulent channel flow at Ma =0.2 with two different skin friction Reynolds numbers: $Re_{\tau} = 180,395$. The results were compared to DNS data obtained by the incompressible numerical simulation of Moser et al. (MKM) [111].

Three different values of blending factor k for the hybrid method have been tested: k = 0.5, k = 0.75 and k = 1.0, i.e. pure LES. As previously mentioned, the anisotropic dynamic model [107] has been used as LES model.

The computational domain is the same of the LES shown in section 3.4.1, so in dimensionless units, is $2\pi \times 2 \times 4/3\pi$. Also the boundary conditions are the same: no-slip, isothermal boundary conditions have been prescribed at the wall $(y = \pm 1)$ and periodic conditions have been applied for the remaining directions.

The same grid has been used, for both the skin friction Reynolds numbers, this results in two different space resolutions: a finer one for the lower Reynolds number $Re_{\tau} = 180$, and a coarser for the higher $Re_{\tau} = 395$. In general, the mesh is coarser then the one used in section 3.4.1 for $Re_{\tau} = 180$, and is composed by $N_x = 6$, $N_y = 12$, $N_z = 10$ hexahedra that are divided into $N_t = 6$ tetrahedral elements. The grid is uniform in x and z directions, while, to increase the resolution near the wall, in the normal direction (y) the planes that define the hexahedra are given by:

$$y_j = -\frac{\tanh\left(\omega\left(1 - 2j/N_y\right)\right)}{\tanh\left(\omega\right)} \qquad j = 0, \dots, N_y, \tag{5.1}$$

where the parameter ω is set fixing the position of the first element.

The grid parameters and the dimension details are reported in Table 5.1.1.

For the lower Reynolds number the resolution is near to the ones required to a well resolved LES [122], whereas for $Re_{\tau} = 395$ the grid is too coarse for such simulation.

The initial conditions and the statistics computation procedure are the same of 3.4.1, as well as the body force added to maintain a constant mass flux along the channel.

Mean velocity profiles (Fig. 5.1) do not show significant differences for the cases considered. As expected, the results are close to the DNS data for $Re_{\tau} = 180$ and are poor for the simulations at $Re_{\tau} = 395$, in which the resolution decrease.

Figures 5.3-5.5 show the velocity r.m.s. profiles. In general the simulations overestimate the peak in streamwise direction and, on the counterpart, underestimate the whole profile in normal and spanwise direction. Although the results

	$Re_{\tau} = 180$		$Re_{\tau} = 395$	
	Moser et Al	Present	Moser et Al	Present
Ma		0.2		0.2
$Re_{\rm b}$		2800		6880
L_x	4π	2π	4π	2π
L_z	$\frac{4}{3}\pi$	$\frac{4}{3}\pi$	$\frac{4}{3}\pi$	$\frac{4}{3}\pi$
Δ_x^+	17.7	31.68	10.0	69.5
$\Delta_z +$	5.9	12.8	6.5	28.1
$\Delta^+_{y_{min}}/\Delta^+_{y_{max}}$	0.05/4.4	0.65/11.52	0.03/6.5	1.4/25.28

Table 5.1: Hybrid method simulations with constant blending factor for the turbulent channel flow testcase: grid and simulations parameters.

obtained are quite similar, the hybrid method with k = 0.75 gives the better results for $Re_{\tau} = 180$, whereas for $Re_{\tau} = 395$ the better results are the ones obtained with the lower value of the blending factor. This trend is confirmed also by the shear stress profiles (Fig. 5.6). Therefore, considering that k = 1.0 is a pure LES, the results show that using an appropriate value of the blending factor it is possible to improve the LES results.

Clearly, this is only a feasibility study for the methodology and further analysis are required. Nevertheless, these simulations suggest that the hybrid method with the reconstruction of the Reynolds stress tensor can be a valid technique to integrate the LES when the grid resolution is too coarse to resolve the appropriate quantities of turbulent scales. Moreover, the increase of computational cost for the hybrid method with respect to the pure LES is negligible, in fact only algebraic operations are added.

Finally, it is interesting to notice that, differently from what expected, the results obtained with k = 0.75 are not in general closer to pure LES, i.e. k = 1, then the ones obtained with k = 0.50. This highlights the complexity of the interaction between LES and RANS field and in particular the not trivial dependence of the simulations with respect the choice of the parameter k.

5.1.2 Analysis of blending factor's effect

The blending factor strongly impacts on the amount of the quantities resolved and modelled. As shown by Figure 5.7 for the shear stress and by Figure 5.8 for the turbulent kinetic energy, the resolved part is the most important in pure LES. As the blending factor decreases, k = 0.75, the resolved part decreases and



Figure 5.1: Velocity mean profile, streamwise direction : (*left*) $Re_{\tau} = 180$, (*right*) $Re_{\tau} = 395$.



Figure 5.2: Velocity mean profile, logarithmic rappresentation, streamwise direction : (*left*) $Re_{\tau} = 180$, (*right*) $Re_{\tau} = 395$.


Figure 5.3: Velocity r.m.s. profile, streamwise direction : (*left*) $Re_{\tau} = 180$, (*right*) $Re_{\tau} = 395$.



Figure 5.4: Velocity r.m.s. profile, normal direction : (*left*) $Re_{\tau} = 180$, (*right*) $Re_{\tau} = 395$.



Figure 5.5: Velocity r.m.s. profile, spanwise direction: (*left*) $Re_{\tau} = 180$, (*right*) $Re_{\tau} = 395$.



Figure 5.6: Shear stress profile, τ_{uv} : (left) $Re_{\tau} = 180$, (right) $Re_{\tau} = 395$. The resolved and modelled stress contribution are plotted together.

modelled one increases. Finally, for k = 0.5, the modelled contribution becomes greater than the resolved one. Therefore, at least theoretically, the blending factor permits a direct control of the resolved kinetic energy. As stressed by Pope [123], the ratio between the turbulent kinetic energy of the resolved motion and the total turbulent energy could be a conceptually simple measure of the turbulence resolution in a LES simulation, and moreover this kind of criterion seems to be very suitable in the hybrid RANS/LES framework [124]. This ratio for the DNS is one, everything is resolved, and for RANS is zero, everything is modelled. Usually for LES this ratio is near to one, or presumed as that, at least as indicated by the postprocessing procedures that usually do not consider the subgrid contributions. A basic question is the following: is it really possible to perform LES simulations with a resolution ratio of 0.7, or of 0.5, or less? This point is very important not only theoretically, but also as regards the hybrid RANS/LES methods, that try to join zonally RANS and LES computations. From the results shown in Figure 5.7-5.8, we can see that, in our new reconstruction method, the ratio between resolved and modelled energy scales approximately as k^2 . This seems reasonable, in fact if we define a resolution factor R_F for a pure LES as

$$R_F = \frac{\tau^{\mathcal{E}}(\langle u_i \rangle_{\mathcal{F}}, \langle u_i \rangle_{\mathcal{F}})}{\tau^{\mathcal{E}}(u_i, u_i)}, \qquad (5.2)$$

and an equivalent one R_H for a generic hybrid RANS/LES filter,

$$R_H = \frac{\tau^{\mathcal{E}}(\langle u_i \rangle_{\mathcal{H}}, \langle u_i \rangle_{\mathcal{H}})}{\tau^{\mathcal{E}}(u_i, u_i)}.$$
(5.3)

Substituting the \mathcal{H} - filtered velocity definition $\langle u \rangle_{\mathcal{H}}$: $\langle u \rangle_{\mathcal{H}} = k \langle u \rangle_{\mathcal{F}} + (1 - k) \langle u \rangle_{\mathcal{E}}$ in (5.3), and remembering that

$$\tau^{\mathcal{E}}(\langle u_i \rangle_{\mathcal{H}}, \langle u_i \rangle_{\mathcal{H}}) = \langle \langle u_i \rangle_{\mathcal{H}} \langle u_i \rangle_{\mathcal{H}} \rangle_{\mathcal{E}} - \langle \langle u_i \rangle_{\mathcal{H}} \rangle_{\mathcal{E}} \langle \langle u_i \rangle_{\mathcal{H}} \rangle_{\mathcal{E}},$$

it is easy to verify that $R_H \sim k^2 R_F$. Therefore, considering that for a well resolved LES $R_F \sim 1$, we have that $R_H \approx k^2$.

5.2 Space dependent blending factor

In the previous section we have seen that the results obtained with a fixed value blending factor are close and in part better then the ones obtained with k = 1.0, i.e. pure LES. Therefore, it can reasonably be expected that introducing a variable



Figure 5.7: Comparison between resolved (continuous line) and modelled (dashed line) contributions to the shear stress τ_{uv} : (left) $Re_{\tau} = 180$, (right) $Re_{\tau} = 395$.



Figure 5.8: Comparison between resolved (continuous line) and modelled (dashed line) contributions to the turbulent kinetic energy tke: (left) $Re_{\tau} = 180$, (right) $Re_{\tau} = 395$.

blending factor the methodology analysed can be suitable for improve accuracy of the turbulence description for coarse grid.

In fact, as discussed above, the value of k should be related to the accuracy of the mesh, and in particular to its capability to resolve a certain number of turbulent scales. A variable blending factor can be useful to set the optimal value of RANS reconstruction contribution in every part of the domain.

On the other hand, we have seen that using a variable blending factor makes the equations very complex because of the additional terms.

A possible solution is to use a piecewise constant function of k. In fact, if we keep the blending factor constant in the element, the additional terms will be equal to zero and the discontinuity between two consecutive elements do not represent a problem considering the DG approach used for the space discretization. This approach seems to be a good compromise in order to obtain a simple formulation, suitable for applications. The approach is similar to the one presented [69], where a zonal RANS/LES formulation has been tested using a discontinuous blending factor equal to zero in RANS zone and equal to one in the LES zone. However, here the numerical method is different and, most important, the transition is smoother and starts from mixed RANS/LES area.

5.2.1 Turbulent channel flow

The first testcase analysed is the turbulent channel flow, the grid and the parameter are the same described in 5.1.1.

As customary for hybrid methods we consider a wall distance y dependent blending factor. k depends to y according to the following parabolic law:

$$k(y) = \begin{cases} -0.617y^2 + 1.111y + 0.5, & \text{for } y < 0.9\\ 1, & \text{for } y \ge 0.9. \end{cases}$$

the lower value is equal to k = 0.5 at the wall, and we recover a pure LES simulation in the center of the channel. Figure 5.9 show the blending factor values along the channel, the value of k in each elements is obtained fro $k(y_{\rm b})$, where $y_{\rm b}$ represents the distance from the wall to the barycenter of the element.

The grids and the parameters of the simulation are the same of the section 5.1.1, and are still compared with the DNS data provide by [111] and with pure LES results.

The mean velocity profiles (Fig. 5.10, 5.11) show a good agreement for $Re_{\tau} =$ 180, here both the hybrid method and the pure LES well describe the streamwise



Figure 5.9: Blending factor function k(y) for the turbulent channel flow testcase.

component of the velocity. Nevertheless, in the logarithmic representation the hybrid methods show a better fit. The results get worse for $Re_{\tau} = 395$ in which the velocity is overestimated in buffer layer and underestimated in center of the channel.

Greater differences are shown in the rms profiles (Fig. 5.12-5.14). Here the hybrid method shows significant benefits with respect to the pure LES for every component of the velocity. The better results are the ones obtained for the spanwise component, but in general the profiles are closer to DNS especially near to the wall, i.e. where RANS reconstruction contribution is greater. The better behaviour of hybrid method is also confirmed by the shear stress profiles (Fig. 5.15). As already done for the constant blending factor results, it is also interesting to analyse the separated contribution of the modelled and resolved contribution for the shear stress shown in Figure 5.16. As we can see the modelled contribution is prevalent near to the wall, where k is smaller, and decrease as the k increases, reaching very low values near to the centerline.

Therefore the obtained with a very simple function of k are in very good agreement with the DNS results. Probably better results could have been obtained with a different function, in particular for the simulation with $Re_{\tau} = 395$ where the same function used for $Re_{\tau} = 180$ has been used, even tough the mesh accuracy is very different, and then a greater contribution of RANS reconstruction could have been useful to integrate the resolved contribution.



Figure 5.10: Velocity mean profile, streamwise direction : (*left*) $Re_{\tau} = 180$, (*right*) $Re_{\tau} = 395$.



Figure 5.11: Velocity mean profile, logarithmic representation, streamwise direction : (*left*) $Re_{\tau} = 180$, (*right*) $Re_{\tau} = 395$.



Figure 5.12: Velocity r.m.s. profile, streamwise direction : (*left*) $Re_{\tau} = 180$, (*right*) $Re_{\tau} = 395$.



Figure 5.13: Velocity r.m.s. profile, normal direction : (*left*) $Re_{\tau} = 180$, (*right*) $Re_{\tau} = 395$.



Figure 5.14: Velocity r.m.s. profile, spanwise direction : (*left*) $Re_{\tau} = 180$, (*right*) $Re_{\tau} = 395$.



Figure 5.15: Shear stress profile, τ_{uv} : (*left*) $Re_{\tau} = 180$, (*right*) $Re_{\tau} = 395$. Modelled and resolved contribution are plotted together.



Figure 5.16: Comparison between resolved (continuous line) and modelled (dashed line) contributions to the shear stress τ_{uv} : (left) $Re_{\tau} = 180$, (right) $Re_{\tau} = 395$.

5.2.2 Periodic hill flow

As we have done for LES in 3.4.2, also for the hybrid method it is important to test the method in a more geometrically complex testcase like the periodic hill flow. The geometry of the testcase is the same described in 3.4.2. In this case the geometry of the channel changes along the streamwise direction and therefore is more difficult to determine the blending factor. In general, from our tests, we have obtained better results using a k = k(x, y) instead of using blending factor dependent only with the wall distance. More specifically, better results have been obtained increasing the RANS contribution in recirculation area. The blending factor used for the numerical simulations is represented in (Fig. 5.17) and is based on parabolic law starting from k = 0.7 at the wall and is damped in order to reach the lowest value for x/h = 2.5, i.e. approximately at the center of the separated flow.

The grid is coarser than the ones used in 3.4.2, and the total number of elements is now 14756, with a reduction of the ~ 12% with respect to the previous one. The structured boundary layer mesh, is still composed by $N_z = 12$ elements in the spanwise direction that, using the same basis functions of degree q = 4, leads to a $\Delta z/h \simeq 0.062$. The streamwise resolution varies from $\Delta x/h \simeq 0.09$ between the two hills to $\Delta x/h \simeq 0.031$ at the top of the hill. As usual, the mesh is refined in the normal direction and the resolutions is $\Delta y/h \simeq 0.006$ at the bottom wall.



Figure 5.17: 2D representation of the blending factor k(x, y) for the periodic hill flow.

Also in this case no mesh refinement has been applied close to the upper wall.

The statistics are computed for the same positions of section 3.4.2: x/h = 0.5, 2, 4, 6. The streamwise mean velocity profiles (Fig. 5.18) do not show significant differences except for x/h = 4, in which the hybrid method performs slightly better then LES, and for x/h = 6. The normal mean velocity component (Fig.5.19) shows a greater sensitivity, at the beginning of the first hill x/h = 0.5, and also for x/h = 4, LES is in excellent agreement with DNS, while in the separated region x/h = 2 the hybrid method is closer to the DNS.

In general, the results obtained with LES and hybrid method for the mean flow are quite similar. Greater differences appear for the stress profiles (Fig.5.20 - 5.22). Here LES performs slightly better then hybrid method especially for τ_{uu} (Fig.5.20) and τ_{vv} (Fig.5.21), while for shear stress profiles (Fig.5.15) the performances are more similar.

Therefore, the good results obtained for the turbulent channel flow are not confirmed for the periodic hill flow. Probably this can be related to the difficult choice of the blending factor: the massive separated region and the variability of the reattachment point location make the choice of the blending factor very difficult. Moreover, a time variable blending factor would pose serious theoretical problems, not only related to the noncommutativity between k and hybrid filter that could be resolved adding additional terms, but also for the noncommutativity between k and the RANS operator. In fact, as is customary in the applications the RANS average is based on time, more specifically in this work on a running time average has been used. Therefore the choice of the optimal blending factor is still an open problem.



Figure 5.18: Mean streamwise velocity profiles in the periodic hill flow test case at different locations along the channel; (a): x/h = 0.5; (b): x/h = 2; (c): x/h = 4; (d): x/h = 6.



Figure 5.19: Mean normal velocity profiles in the periodic hill flow test case at different locations along the channel; (a): x/h = 0.5; (b): x/h = 2; (c): x/h = 4; (d): x/h = 6.



Figure 5.20: Turbulent stresses profiles in the periodic hill flow test case, streamwise component at different locations along the channel; (a): x/h = 0.5; (b): x/h = 2; (c): x/h = 4; (d): x/h = 6. The profiles are obtained considering both the resolved and the modelled contributions.



Figure 5.21: Turbulent stresses profiles in the periodic hill flow test case, normal component at different locations along the channel; (a): x/h = 0.5; (b): x/h = 2; (c): x/h = 4; (d): x/h = 6. The profiles are obtained considering both the resolved and the modelled contributions.



Figure 5.22: Turbulent stresses profiles in the periodic hill flow test case, shear stress component at different locations along the channel; (a): x/h = 0.5; (b): x/h = 2; (c): x/h = 4; (d): x/h = 6. The profiles are obtained considering both the resolved and the modelled contributions.

Chapter 6

Concluding remarks and perspectives

A novel procedure for the computation of RANS stress have been studied and tested for the hybrid filter approach proposed by Germano. This procedure, called RANS reconstruction, exploits the mathematical properties of the hybrid filter and allows to reconstruct the Reynolds stress tensor without using an explicit RANS model.

The RANS/LES method has been implemented using a variational multiscale approach combined to a DG-FEM space discretization. The methodology have been tested for LES considering three different subgrid models: the classical Smagorinsky model, the dynamic isotropic model and, finally, its anisotropic extension. The last one has been chosen as LES model for hybrid RANS/LES simulation.

The hybrid method have been tested for the turbulent channel flow and periodic hill flow testcases, in near incompressible condition (Mach = 0.2) and using both fixed and space-dependent blending factors.

More specifically, in order to analyse the role this parameter, three different constant blending factors have been considered for the turbulent channel simulations: k = 0.75, k = 0.50 and k = 1.0, i.e. pure LES, and two Reynolds numbers, $Re_{\tau} = 180,395$. The results highlighted the importance of the blending factor to determine the ratio between energy resolved and modelled. Moreover, the profiles obtained with k = 0.75 and k = 0.50, are close and in part better then the ones obtained with k = 1.0, i.e. pure LES.

After having performed the simulations with constant values, also the space dependent blending factors have been considered. In order to avoid additional terms, a piecewise constant function of wall distance has been chosen. This is made possible The simulations for the channel flow show a very good performance of the hybrid method, which improves the the results obtained with pure LES, both for $Re_{\tau} = 180$ and $Re_{\tau} = 395$. The same results have not been obtained for the more complex periodic hill flow. Here the hybrid method is able to provide a good representation of the flow features, but do not improve the results obtained with pure LES. This can be related to a not optimal choice of the blending factor that for this flow is not trivial.

In our opinion, considering the simplicity and the very small additional cost, the hybrid filter approach with Reynolds stress reconstruction can be a very promising approach for turbulence modelling. The open problem is how to choose the correct value of the blending factor, and therefore the future works will be focused on this point.

In fact, from the results obtained, it can reasonably be expected that, once an optimal strategy for choosing the right blending factor will be developed, the methodology analysed will be suitable to improve accuracy of the turbulence description, in particular considering simulation with grids coarser than the ones required by a well resolved LES.

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Acknowledgements

Ultima pagina. Anche questa volta ho finito, tardi, all'ultimo giorno, ma ho finito. Le ultime righe di questa tesi sono dedicate alle persone che mi hanno aiutato ad arrivare a questo punto e che hanno contributo a rendere questi tre anni un' esperienza positiva da un punto di vista professionale e soprattutto umano.

La prima persona a cui sento di dover dire grazie è la Prof. Antonella Abbà: per la sua competenza, per tutto il tempo che mi ha dedicato e per la fiducia che mi ha sempre dimostrato, anche quando le correnti non volevano saperne di diventare turbolente, quando non riuscivo ad ottenere altro che NaN e quando, spesso, i risultati sembravano contraddirsi e non avere alcun senso.

Quattro anni fa di questi tempi stavo preparando l'esame di turbolenza e per la prima volta studiavo la LES e la procedura dinamica. Allora di certo non immaginavo che di lì a poco avrei avuto la fortuna di lavorare con il Prof. Massimo Germano. Un grazie enorme va a lui, che non solo con la sua intuizione ha dato il via al progetto, ma che ha anche collaborato attivamente alla sua realizzazione, dimostrandosi sempre disponibile e non facendo mai mancare il suo incoraggiamento.

Una parte considerevole del mio dottorato è stata dedicata a cercare di tradurre in fortran modelli ed equazioni, lottando con problemi teorici, segmentation fault e bug vari. Se, in molti casi, sono riuscito a venirne a capo, lo devo soprattutto a Marco Restelli e alla sua infinita pazienza e conoscenza.

Vorrei inoltre ringraziare il Prof. Alberto Guardone, grazie al quale ho potuto iniziare questo percorso.

Una delle cose che mi mancheranno di più di questi tre anni saranno i dialoghi, spesso surreali, in pausa pranzo e più in generale il rapporto con i miei compagni di avventura. Un grazie speciale va alle due persone che hanno condiviso con me non solo i tre anni di dottorato, ma anche i cinque della laurea: Barbara, senza la quale probabilmente sarei stato sbranato dai coyote sulla Dead Valley o mi sarei perso per Praga o Pilsen o, più probabilmente, sarei stato cacciato dal dottorato per non aver rispettato qualche scadenza, e Andrea, socio fidato in molti progetti che non hanno avuto il successo sperato, ma a cui ci siamo dedicati con la nostra massima devozione. Grazie poi ai miei compagni di tavolo Francesca e Fabio, e grazie a Mirco, Paolo, Claudio, Alessandro, Riccardo, Federica, Valentina, Matteo e tutte quelle persone con cui ho avuto il piacere di parlare e di condividere una parte di questa esperienza.

Quest'ultima pagina segna anche la fine del mio percorso di studi. Oggi tornando a casa dal lavoro, il mio primo *vero* lavoro, mi è tornata in mente una foto del mio primo giorno di scuola: facevo la verticale, o almeno ci provavo, davanti al cancello di casa, avevo il grembiule blu e la cartella dei Power Rangers. Sono passati vent'anni. Al di là di ogni parola, grazie a chi c'era quel giorno e, in un modo o nell'altro, c'è ancora.

Buonanotte