QUALITY CRITERIA FOR LARGE EDDY SIMULATION

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Abstract

CFD is often employed in industry as an alternative to experimental investigations. As a trade-off between the costs involved and accuracy obtained by using DNS and RANS methods, LES is increasingly being used. However, LES results depend heavily on various factors including the grid, the numerical method employed, the boundary conditions and the statistical sampling and convergence criteria. Further, no well-established quality control guidelines are currently available.

The current project aims to provide a set of best practice guidelines for LES, with emphasis on a priori determination of the ‘sufficient’ grid density.

This first year report presents an introduction to turbulence analysis and a literature review of numerical simulation. The review includes the current methods of quality control and error estimation. Further, the inter-relations of the different turbulence lengthscales and their physical significance have been researched. Some preliminary grid-building guidelines are proposed and successfully tested for plane parallel channel flow test case. These preliminary guidelines are now to be tested and refined by employing different flow configurations. Preliminary RANS results for the next test case, that of concentric jets, have also been presented.
Chapter 1

Introduction

Most natural and industrial flows are turbulent in nature. Of the three most widespread numerical methods of predicting turbulence; namely Direct Numerical Simulation (DNS), Large Eddy Simulation (LES) and Reynolds Averaged Navier Stokes (RANS); RANS methods are most commonly used in an industrial context.

By definition, the RANS approach has an inherent disadvantage in that it only resolves the mean flow, averaging out the turbulent fluctuations. Despite this drawback, RANS methods have been successfully employed in industry for over three decades and have been the subject of extensive development in this same period. However, more recently, industrial design and analysis has started to depend increasingly on Computational Fluid Dynamics (CFD), and in many cases, additional information about the instantaneous nature of the flow is required.

The turbulent fluctuations in the flow are usually resolved by employing either DNS or LES.

The basic principle of LES is to resolve all the energy carrying ‘large eddies’, while the dissipative ‘small eddies’ are modelled. In terms of computational requirements and time, LES occupies an intermediate position be-
tween DNS and RANS. Recent advances in computational technology have made LES more viable and affordable for industrial studies of turbulence.

Over the past decade, more and more and more attention is being paid to the reliability of using LES for the analysis of turbulent flows. However, at present, it is yet to replace RANS as the most widely used industrial approach for the prediction of turbulence.

One factor for the prevalence of RANS is undoubtedly the existence of a wealth of guidelines and quality control measures which by far outweigh the consensus of advice for users of LES. Furthermore, the accuracy of LES results depends very strongly on the grid employed and for wall bounded flows, a very fine near wall grid resolution is imperative. The majority of industrial flows are wall bounded to some extent. In case of conformal (structured) grids, the fine near wall grid resolution is usually extended into the inner regions of the domain, resulting in an extremely fine grid. Often, such a fine grid is unaffordable within industrial constraints and coarser grids are employed, resulting in bad quality predictions.

The purpose of this study is to provide a set of guidelines for an \textit{a priori} determination of a non-conformal (unstructured) grid resolution for LES so as to offer economies in the grid size and computational expense, relative to a fully structured mesh, without compromising the inherent ‘quality’, or accuracy, of the prediction.

\section{Turbulent flows}

Turbulent flows can be commonly observed in numerous natural and industrial cases. However, a precise definition is somewhat difficult and all that can be done is a listing of some of its characteristics \cite{Tennekes1972}.
The most significant characteristic of all turbulent flows is the associated irregularity or randomness. Consequently, a deterministic approach to the study of turbulence is impossible, and statistical methods have to be relied on [Tennekes and Lumley, 1972].

For engineering applications, the diffusivity of turbulence is an important factor. The diffusivity leads to rapid mixing, thereby increasing transfer rates of momentum, heat and mass through the flow domain. For example, turbulence can delay boundary layer separation on aerofoils at large angles of attack, increase heat transfer rates, provide resistance to flow in ducts, increase momentum transfer between currents, and so on.

Turbulent flows always occur at a Large Reynolds number, and often originate as the instability of laminar flows with increasing Reynolds numbers.

Turbulent flows are rotational and three dimensional. They are characterised by high levels of fluctuating vorticity. An important vorticity-maintenance mechanism is ‘vortex stretching’, not exhibited by two dimensional flows, and hence turbulent fluctuations are essentially three dimensional vorticity fluctuations.

All turbulent flows are inherently dissipative. Dissipation is the deformation work of the viscous stresses which increases the internal energy at the expense of the kinetic energy of the turbulence. To make up for this loss, turbulent flows require a continuous supply of energy, failing which, the turbulence decays rapidly.

Turbulence is a continuum phenomenon governed by the equations of fluid mechanics. Even the smallest scales in any turbulent flow are much larger than any molecular lengthscale.

Finally, turbulence is a flow feature, and not a fluid feature. If the Reynolds number is high enough, most turbulent dynamics is the same, i-
respective of the fluid, whether liquid or gaseous.

1.2 The study of turbulent flows

From the point of view of industrial applications, turbulent flows are immensely important in many diverse fields ranging from meteorology and aeronautics to biophysics and medicine. Consequently, it is important to understand the phenomenon of turbulence and correctly predict its effects.

Turbulent flows have been investigated for well over a century now [Tennekes and Lumley, 1972]. However, there does not exist one general approach to the study and solution of turbulent flow problems. A number of techniques have been employed to predict turbulence and its properties.

The studies of turbulence can be broadly classified into three categories [Pope, 2000]. Discovery or experimental (or simulation) studies are aimed at providing qualitative or quantitative information about the flow under study. Modelling or theoretical studies are aimed at developing tractable mathematical models to accurately predict turbulent flow properties. Control studies typically involve experimental as well as theoretical work aimed at manipulating turbulence in a beneficial way.

Accurate quantitative predictions of turbulence are impossible without relying on empirical data. Statistical studies of the equations of fluid flow always lead to the closure problem: more unknowns than equations. In order to make the number of equations equal to the number of unknowns, assumptions are imperative.

There are numerous theories pertaining to such assumptions. The phenomenological theories make crucial assumptions in early stages of the analysis. Very formal and sophisticated theories also need rather arbitrary postulates. Further, all these theories involve rigorous mathematical complexities
and hence a listing of these theories and their description is not attempted here.

1.3 The separation of scales in turbulent flows

As a first step in the study of turbulent flows, a distinction has to be made between small-scale turbulence and large-scale motion.

At high Reynolds numbers, there exists a separation of lengthscales wherein large-scale motion is strongly influenced by the geometry of the flow domain while the small-scale motion is almost entirely independent of the geometry. This range of lengthscales is limited at the large-scale end by the overall dimensions of the flow field and at the small-scale end by the diffusive action of molecular viscosity.

Turbulent transport and mixing is controlled by the large-scale motion or large eddies, which are of a size comparable to the overall dimensions of the flow field. Consequently, the relevant lengthscale for the analysis of the interaction of the turbulence and the mean flow, is the flow dimension.

The small lengthscales are limited at the smallest end by the diffusive action of the molecular viscosity. These small scales become progressively smaller with increasing Reynolds number.

Two consequential themes concerning these small lengthscales in turbulence are the energy cascade and the Kolmogorov hypothesis [Pope, 2000] which are discussed at a later stage in this report.
Chapter 2

Literature Review

2.1 Numerical Analysis of Turbulence

In the past half century, the numerical analysis of turbulence has seen a phenomenal amount of research and development. This field of study has been applied in a range of areas; various branches of engineering, pure and applied sciences and medicine. An important factor in the growth and success of numerical analysis is attributable to the rapid growth and increased accessibility of computational power.

In the area of fluid dynamics, the various numerical and computational methods of analysis developed over the years are collectively termed as methods in *Computational Fluid Dynamics* (CFD). The most common modern CFD methods for turbulent flows are broadly classified as *Direct Numerical Simulation* (DNS), *Large Eddy Simulation* (LES) and *Reynolds Averaged Navier Stokes* (RANS) methods.
2.1.1 The Navier-Stokes Equations

The general equations for fluid flow are known as the Navier-Stokes equations, which comprise the conservation of mass (continuity) equation and the conservation of momentum equations.

For an incompressible Newtonian fluid, these can be written as

\[
\nabla \cdot U = 0 \\
\frac{\partial U}{\partial t} + (U \nabla) \cdot U = -\frac{1}{\rho} \nabla p + \nu \nabla^2 U
\]  

(2.1)

where \( U \) is the fluid velocity at a point in the flow domain, \( p \) is the pressure of the fluid, \( \rho \) is the fluid density and \( \nu \) is the kinematic viscosity, related to the dynamic viscosity \( \mu \) by the relation \( \nu = \frac{\mu}{\rho} \).

According to whether the viscous (\( \nu \nabla^2 U \)) or inertial ((\( U \nabla \)) \cdot U) forces are predominant, the fluid flow is said to be either laminar or turbulent respectively. In 1883, Osborne Reynolds discovered a non-dimensional number, known today as the Reynolds number, which can be used to quantitatively define the point at which the flow ‘transitions’ from laminar to turbulent conditions, or vice versa. It is defined as:

\[
Re = \frac{UL}{\nu}
\]

(2.2)

where \( U \) is the fluid velocity, \( l \) is the characteristic length of the flow domain and \( \nu \) is the kinematic viscosity.

This number limits the transition between the laminar and turbulent flow regimes and its actual numerical value differs according to flow configuration. At \( Re \) lower than the transition limit, the viscous stresses damp out small perturbations, if indeed there are any, thereby restraining the flow from becoming turbulent. However, once the transition \( Re \) is crossed, the viscous stresses become insufficient relative to the inertial perturbations in the flow, which then amplify; at this point the flow is said to become fully turbulent.
Turbulent flow is characterised by, among other properties, the existence of a wide range of lengthscales. The energy transfer across these various scales is perhaps the most important feature of turbulence.

### 2.1.2 Direct Numerical Simulation

Direct Numerical Simulation (DNS) is, in a way, the most straightforward approach to CFD. DNS involves the direct solution of the flow field from the Navier Stokes equations without employing neither averaging nor modelling. Consequently, it is, by definition, the most accurate method of numerically studying turbulent flows. DNS results are considered on par with, if not superior to, experimental evidence, and may offer a practical, non-invasive alternative to experimentation in some cases.

The principle factor affecting the accuracy of this solution is the numerical method employed and the major drawback of this method is the excessive amount of computational capacity and high order of numerical method required for high accuracy. In order to ensure that all the features of turbulence are predicted correctly, a large computational domain and a very dense grid are often imperative. The extent of the domain depends on the integral lengthscale, i.e. the distance beyond which the self correlations of the velocity components cease to exist. The number of grid points depends on the flow Reynolds number (Re). With increasing Re, the ratio of the integral lengthscale to the smallest lengthscale in the flow increases. To ensure quality, the grid must be able to capture these smallest scales of motion. Consequently, DNS is computationally expensive and not well suited to complex engineering flows of industrial interest.

The great value of DNS is its capacity to provide a high resolution snapshot of the flow field. Consequently, it is an invaluable tool in the study of
the physics of turbulence.

2.1.3 Reynolds Averaged Navier Stokes

The Reynolds Averaged Navier Stokes (RANS) method employs time averaging of the main flow field in such a way that all the contribution of fluctuating components are grouped into the so called “Reynolds stresses” which must be modelled directly. A turbulence model is required to approximate the values of the Reynolds stresses so as to close the Navier-Stokes equations.

RANS performs well in boundary layers and requires considerably less computing resources than DNS or LES. However, it is often shown to give mixed results when applied to flows involving more than a single dominant lengthscale.

The dimensions of the flow field are limited to the dimensions of the geometry, for e.g. in case of a two dimensional geometry, only a two dimensional flow field solution can be obtained.

2.1.4 Large Eddy Simulation

Large Eddy Simulation involves the extraction of the small-scale motion from the main velocity field by spatial filtering. The Navier Stokes equations are solved for the main flow field (or large eddies) while the smallest eddies are modelled. The grid density or filter width defines the portion of the flow which is to be modelled; i.e. if a dense grid is used with LES, the modelled component is less and a DNS solution is approached.

However, LES does require more computing resources as compared to RANS and is not yet applicable to all engineering problems.
2.1.5 RANS-LES coupling

The RANS approach is the most widely used computational method in industry. However, the limitations of RANS have, over the last decade, resulted in an increased focus upon the capabilities of LES. Consequently, various attempts have been made to combine the best features of both RANS and LES approaches in so called hybrid, or RANS-LES, methods.

Hybrid methods apply RANS in the boundary layers and LES in other parts of the flow field. Consequently, a coarser mesh than that required by LES may be employed in the boundary layer, and an improved description of the separated flow regions than that generally offered by RANS can be obtained. However, one problem with such methods, requiring the coupling of RANS and LES, is that the excessive damping induced by RANS models may inadvertently affect the LES result. In addition, the time averaging employed by RANS neglects the turbulent fluctuations, which cannot be easily reintroduced for the region of the domain to be calculated using LES.

2.2 Turbulence modelling

The resolution of all the turbulent structures, down to the smallest scales, is possible only with DNS. However, it is computationally expensive and practically limited to low Reynolds number flows as previously discussed. Consequently, it is not a practical option for engineering problems. For complex engineering flows, realistic alternatives are RANS and LES. Both these techniques often require some turbulence modelling. The accuracy of the result is thereby limited by the accuracy of the underlying turbulence model. The performance of the turbulence model and the resulting ability of the technique to predict turbulent flow, is most often evaluated by comparing
the modelled results with experimental or DNS data. For the predictions to be reliable and accurate, procedures for determining the numerical uncertainty and errors in modelling and numerical methods are required. While such procedures are well researched and documented in the RANS context, the task seems to provide many challenges for LES.

In LES, the large energy carrying lengthscales of turbulence are resolved completely and the small structures are modelled. The separation of these large and small scales is performed by applying a low-pass filter to the Navier-Stokes equations and the effect of the small-scale turbulence on the resolved scales is modelled using a sub-grid scale (SGS) model.

The SGS model commonly employs information from the smallest resolved scales as the basis for modelling the stresses of the unresolved scales. Consequently, it is imperative that the resolved lengthscales are captured accurately by the numerical scheme. This, in turn, requires that the numerical error of the scheme is sufficiently small and hence, high order numerical schemes are necessary [Gullbrand, 2001].

The SGS model is an integral component of the LES calculations and is therefore an influential factor in the accuracy of the predictions. In contrast to expectations, in some cases, the classical (standard) Smagorinsky model performs better than the dynamic Smagorinsky model [Chen et al., 2005, Meneveau, 2005]. Therefore, it is evident that there is a need of experimental and numerical work to assess the performance of LES and the underlying SGS models in complex engineering flows.

Lately, there is growing interest in the scientific community to look into quality assessment for LES, hitherto a pretty much untrodden area. The advances in construction of SGS models for LES of a range of engineering flows encompass improvements not only in numerical solution but also in the
process representations for accurate system definition. However, there is still
little agreement on the systematic assessment and reporting of the credibility
of the simulations.

2.3 Quality and Reliability of Numerical Simulation

The numerical analysis of fluid flow has been a well reviewed subject for al-
most a century. However, it is only in the last decade that a lot of concern
about the reliability of numerical simulation has been cited. Available liter-
ature can be classified as targeting different aspects of numerical simulation.
The relevant aspects for the current study are quality and reliability in CFD,
formal policies on numerical uncertainty in general, and with particular re-
gard to LES, the grid resolution, accuracy limitations and error estimation.

CFD techniques commonly used to predict turbulent flow properties are
inherently susceptible to modelling and numerical errors. As CFD is brought
into widespread use, it is important to limit these errors in solution without
an excessive increase in computational cost. It is therefore necessary to
calculate a prior assessment of the quality of the particular CFD technique
employed.

CFD has now more or less become a standard tool for fluid flow investiga-
tions, however a quality assessment of the results is often unavailable, partic-
ularly for LES. Quality control in CFD can be implemented with guidelines
for calculation with sufficient accuracy and reporting results with sufficient
information to judge the result quality [Sorensen and Nielsen, 2003].

RANS methods are widely used in industry, chiefly because of their speed,
and lower sensitivity to numerical and grid issues. Methods of assessing
quality of results obtained from RANS simulations are well established.
However, RANS methods can yeild erroneous results for certain flow geometries. Furthermore they do not provide an instantaneous time history of the flow, which may be required to correctly model flow features such as combustion or acoustics. LES can offer more accuracy in such scenarios, providing not only the full time history of the flow, but also resolving small scale, energetic eddies.

However, an estimation of the quality of LES results is less readily defined as compared to that for RANS results. One of the reasons for this is that LES results are very sensitive to the grid resolution and the numerical method employed. The grid resolution affects not only the numerical discretization error but also the subgrid scale (SGS) model contribution. Further, these quantities are coupled, thereby adding to the complexity of assessment [Klein, 2005, Celik et al., 2005].

The increase in number of LES applications dictates the requirement for imposing quality criteria for such investigations. Conscientious documentation is necessary to ensure high quality of results, failing which, poorly executed methods may cause large deviations in the predictions and a subsequent deterioration of quality. This study aims to provide a criterion involving the determination of grid refinement prior to actual simulation. An attempt is made to dictate the optimal meshing from an estimation of the turbulent lengthscales.

### 2.4 Policy statements on numerical uncertainty

Beginning with the ASME Journal of Fluids Engineering in 1986, a number of journals have adopted explicit policies on numerical uncertainty.

The Journal of Fluids Engineering has since expanded its original policy, while other journals have adopted their own [Board, 1994, AIAA, 1994,
Gresho and Taylor, 1994]. This topic has been the subject of debate for several symposia of the ASME, resulting in a series of special publications [Celik and Freitas, 1990, Celik et al., 1993, Johnson and Hughes, 1995]. Most of these policy statements dictate the requirements imperative for the acceptance of computational results. These requirements typically include, among other less stringent criteria, the following.

1. A precise description of the basic features of the numerical method, including a formal assessment of the order of the truncation errors in the individual terms in the governing equations.

2. An accuracy of at least the second order in space for nodes in the interior of the computational grid, in order to avoid the devastating effect of numerical diffusion on the solution accuracy in first order methods.

3. An assessment of the inherent or explicit artificial viscosity or diffusivity and an explanation of the efforts to minimize the same.

4. A systematic evaluation of the truncation error and accuracy and the confirmation of grid independence and convergence of the solution by presenting solutions over a range of significantly different grid resolutions.

5. Use of error estimates based on methods such as the Richardson extrapolation or techniques in adaptive grid methods.

6. A precise explanation of stopping criteria and estimation of corresponding convergence error for iterative calculations.

8. A complete explanation of the accuracy and method of implementation of boundary and initial conditions as the overall accuracy of a simulation is strongly affected by the same.

9. Citation of existing code in easily available references.

10. A demonstration of accuracy by using appropriate analytical or well-established numerical benchmark solutions.

11. A validation of the solution by comparison with reliable experimental results as long as the experimental uncertainty is established.

Given the phenomenal increase in CFD related publications and the numerous significant advancements in computational techniques and computer technology, the quality-control measures are revised time and again. Each revision formulates a more detailed policy to further improve the quality of publications and provides guidelines for calculation and reporting of error estimates in simulations. The underlying perspective is that CFD studies will eventually aim to predict the outcomes of physical events for which experimentally verified data is unavailable.

The European Research Community On Flow, Turbulence and Combustion (ERCOFTAC) in the nineteen nineties produced a considerable conversion of views on the need for quality-control measures. First and foremost, the end-users were universally supportive of an initiative on quality and trust, which was considered both timely and valuable. Secondly, there was a strong desire for code vendor participation. Although the code vendors were less certain of the need, they were willing to participate in order to cater to the end-user’s wants. It was generally agreed that the production of CFD application procedures was a sound objective. At the same time, it was recognised
that this objective was ambitious and could not be attained without a concurrent proposal for channelling sufficient resources towards it. With this in mind, the Special Interest Group (SIG) on Quality and Trust in the Industrial Application of Computational Fluid Dynamics was formally inaugurated in October 1997.

This SIG sought to produce CFD Application Guidance Procedures to inform users how to perform quality assessments for a range of industrial flows and how to interpret the results with trust. A step-wise approach was undertaken and the following key tasks were involved therein.

1. Construction of a categorisation of the fundamental flows underlying industrial applications.

2. Identification of well studied cases covering the categorisation.

3. Establishing a quality set of CFD computations for each test case.

4. Assembling best practices and application guidelines for each test case.

5. Issuing CFD application guidance procedures.

In spite of all these efforts, no standard method for evaluating numerical uncertainty is currently accepted by the CFD community. However, the aforementioned guidelines or policy statements for accuracy of numerical computations do provide techniques for the same. Estimation of the error is, for most nontrivial fluid flow problems, an \textit{a posteriori} estimation. Systematic grid-convergence studies are the most common, most straightforward and arguably the most reliable technique for the quantification of numerical uncertainty.
2.5 Grid resolution for LES

In general, LES results are in better agreement with experimental evidence compared to RANS if a sufficiently fine grid is employed. However, without a prior knowledge of flow characteristics, it is difficult to ascertain the ‘sufficient’ resolution. As claimed by Celik [Celik, 2005:1], ‘a good LES is almost a DNS’, i.e. for correct resolution of wall layers and prediction of transition, LES requires an extremely fine grid.

It was pointed out by Speziale [Speziale, 1998] that a good LES, as the grid resolution tends to the smallest scales, i.e. the Kolmogorov scales, tends to DNS. As a consequence, grid independence cannot really exist in LES as a grid-independent LES is actually a DNS and therefore the ‘systematic grid-convergence’ studies offer no great benefit. The LES philosophy loses its meaning if it achieves grid independence and the advantage of LES being more economical than DNS on account of resolving only the most energetic eddies, is lost [Celik et al., 2005]. Physical phenomena, including mixing and combustion depend strongly on the intensity of turbulent fluctuations and the convection of these fluctuations, exhibited as turbulent dissipation; the accurate prediction of turbulent statistics becomes important. This makes quality assessment measures imperative for LES in engineering applications.

In the nineteen nineties, a number of attempts were made at reducing the computational requirements of LES for wall bounded flows. Most of these were attempts at manipulating the grid such that all the near-wall eddies could be resolved without having a large number of grid points in the outer layers. In wall bounded flows, the near wall flow structures are extremely small when compared to the overall flow dimensions. However, these small structures play a very important part in the turbulent boundary layer dynamics and therefore need to be well resolved.
In typical mean flow computations, the large mean velocity gradients are resolved using grid stretching in the wall-normal direction. In turbulence simulations, however, a fine near-wall mesh is also required in the direction parallel to the wall. This fine resolution was normally extended into the outer layers. This was not really necessary and consequently, the attempts at lowering computation cost by modifying the grid employed were largely successful.

A popular method of reducing the number of outer layer grid points was to use zonal embedded grids [Kallinderis, 1992, Rai and Moin, 1993, Kravchenko et al., 1996]. This approach involves construction of several regions or zones such that the mesh spacing decreases from zone to zone as the wall is approached as shown in figure 2.1. Grid-stretching in one direction can be combined with zonal embedding in the other two. Kravchenko et al [Kravchenko et al., 1996] found that the results thus obtained showed
good agreement with previously published numerical as well as experimental results for same flow conditions. The calculations required a fraction of the CPU time required for single zone grid calculation with same near-wall grid density. In addition, the memory requirements were significantly reduced.

An interesting, yet perhaps unsurprising, finding is that errors from modelling and numerical method can have opposite signs in some flow regimes, which results in better performance with coarser grids, while keeping the filter size in the SGS model unchanged [Geurts and Frohlich, 2002]. As yet more factors are changed, the possibility of achieving this kind of ‘fluke’ result is again increased. Klein [2005] performed systematic grid and model variation in order to separate the influence of the numerical error and the contribution from the model term. Three simulations, one each for standard, modified model and coarse grid, are recommended to be performed. Also, all results for characteristic quantities are required to be reported, together with the modelling and numerical errors calculated from the simulation results. The results may then be accepted if they satisfy the original simulation. If not, the whole procedure is to be repeated on a finer grid. Comparison of the three simulations gives significant information on the resolution quality and the performance of the SGS model for the flow.

Undeniably, the quantification of accuracy for LES is an arduous task, requiring strict quality control measures and focused resources.

### 2.6 Error estimation and accuracy limitations for LES

The verification of LES calculations is difficult due to the fact that both the SGS model contribution and the numerical discretisation errors are functions of the grid resolution. The prediction of accuracy limitations in large eddy
CHAPTER 2. LITERATURE REVIEW

simulation has been attempted since the late nineteen nineties [Kravchenko and Moin, 1997, Geurts and Frohlich, 2002]. It has been addressed by Celik et al. [2005] through formulation of an index termed LES IQ, the LES index of quality. Other studies by Klein [2005], Geurts [2005], Meyers et al. [2003] and Celik [2005:2] have also attempted an estimation of the errors in LES calculations.

The following taxonomy for obtaining error estimates [Roache, 1998, Klein, 2005] has been employed for RANS simulations, but are also applicable to LES.

1. Additional solutions of the governing equations on other grids
   
   *Grid refinement/coarsening*

2. Additional solutions of the governing equations on the same grid
   
   *Higher/lower order accuracy solutions*

3. Auxiliary PDE solutions on the same grid
   
   *Solution of an error equation*

4. Auxiliary algebraic evaluations on the same grid; surrogate estimators
   
   *Non-conservation of higher order moments, grid adaptation methods, convergence of higher order quadratures, etc.*

The grids employed in LES of turbulent flows are just fine enough to resolve the important large flow structures. The numerical discretisation errors on such grids can have considerable effects on the simulation results. These numerical errors can be attributed to either truncation or aliasing. The truncation errors result from the numerical evaluation of the derivatives, while the aliasing errors result from the evaluation of nonlinear terms on a discrete grid [Kravchenko and Moin, 1997]. Unlike truncation errors, aliasing errors
can be removed from some simulations, and a method of controlling them is available in the Fourier space [Orszag, 1971]. However, complete de-aliasing is computationally expensive and difficult, particularly in complex engineering geometries. It is important only if the aliasing errors are comparable to the truncation errors. A strange phenomenon often discussed in spectral simulation literature is that aliasing errors are destructive for some forms of nonlinear terms but apparently harmless for others [Kravchenko and Moin, 1997].

Most of the modelling strategies motivated by the intricacies of turbulence are aimed at reliably predicting primary flow phenomena, while reducing the complexity of the underlying dynamical system. These inherently conflicting requirements are expressed in LES by capturing the flow features on one hand and coarsening the grid on the other [Geurts and Frohlich, 2002]. This is achieved by subgrid modelling and spatial filtering. The accuracy of the simulation is therefore limited by the numerical contamination of smaller retained flow structures, in addition to the quality of the subgrid parameterization.

Klein and Freitag [2005, 2006] attempted the assessment of LES quality in the context of implicit filtering. Single-grid estimators for turbulent kinetic energy were investigated a priori as well as a posteriori. The results indicated that the estimation of the unresolved turbulent kinetic energy could range from being far too optimistic to too pessimistic depending on the model and geometry combination employed. Certain approaches fail to take into account the numerical dissipation which is often comparable to the SGS dissipation. Further, complexities arise from the different models for estimating the SGS turbulent kinetic energy and the fact that it can be higher than the true turbulent kinetic energy.
Celik et al [2005] proposed various indices of quality measures, termed LES\_IQ and recommended one LES\_IQ based on the Richardson extrapolation concept. They claimed that if eighty percent of the kinetic energy is resolved, then the simulation results are reliable. The method was applied to a number of cases and the calculated LES\_IQ results were compared with the relative total experimental and DNS errors (IQ\_EX and IQ\_DNS respectively). Further, it was postulated that in practical LES applications, the numerical dissipation will always be a significant part of the overall dissipation and hence must be accounted for in any assessment of the quality of LES.

In recent years, the grid resolution for LES computations has been made the centre of discussion in many papers that are attempting to provide a sensitive way to measure the quality of the LES predictions[Celik et al., 2005, Klein, 2005, Jordan, 2005]. However, this has not been found to be a straightforward task due to the influence of the numerical dissipation that must be accounted for in the analysis. Thus, some assumptions had to be introduced regarding the global order of the numerical error as well as the scaling of the error like a power with grid refinements. Even with these approximations, the method suggested by Klein [2005] for example, request a strict minimum of three LES runs for the same case to be able to obtain any meaningful LES results.

The present work expands towards an alternative method which can be used with any commercial or research CFD code to provide guidance for building a proper grid for LES computations, eventually using a precursor RANS simulation.
2.7 Guidelines for designing grids

The Ercoftac Best Practice Guidelines [2000] lists the errors and uncertainties involved in any computational analysis and provides guidelines for minimising the same. This list, though not exhaustive, is intended to offer rules of advice covering about eighty percent of the problems likely to be encountered in order that most common pitfalls in CFD simulations are avoided. For the present work, the guidelines with regard to grid design are particularly important.

The geometry of the flow domain is represented by the computational grid. An adequate representation of the geometrical and expected flow features is imperative and, for structured grids, may be captured by two approaches - regular grids and body-fitted grids.

Regular grids are structured grids incorporating the complete flow domain with extraneous regions cut away. Curved surfaces are represented by a series of steps with two ends on the actual geometrical surface or by a series of flat faces with irregular boundary cells.

Body-fitted grids are designed to follow the domain surface and the interior is built up to satisfy the geometrical constraints of the boundary.

Grid points in a structured grid are addressed by a triplet of indices and connectivity is straightforward. Cells edges form a continuous lines between opposite block faces. The cells are all hexahedral.

Unstructured meshed are assembled cell by cell without consideration of edge line continuity. Connectivity information needs to be explicitly stored and cell faces may or may not match. Special cases of unstructured grids include block structured grids, chimera grids and hybrid grids.

Simulation accuracy usually increases with increase in the grid density. Other factors influencing the quality of a mesh include the shape of the cells
(aspect ratio, skewness, warp angle, etc) and the spatial distribution of cell sizes.

Among the Ercoftac Best Practice Guidelines [2000] the following are particularly relevant to the present work.

1. Selection of a mesh global topology to help satisfy the specific code’s requirements with regard to skewness, aspect ratio and expansion ratios.

2.Extent of the computational domain to be chosen to capture relevant flow and geometrical features. If required, the sensitivity of the calculation to the choice of computational domain to be examined.

3. Assessment of the geometrical features that can be omitted. In areas requiring fine local detail, considering local grid refinement. Grid refinement, when employed, additional grid points should lie on the original geometry and not simply be a linear interpolation of more grid points on the original coarse grid.

4. Highly obstructed zones or fine detail of obstructions, if any, to be accounted for by the use of distributed losses or porosity.

5. Highly skewed cells to be avoided. For hexahedral cells or prisms the grid lines should be optimised in such a way that the included angles are approximately 90 degrees. Tetrahedra should tend to have their four angles equal.

6. Highly warped cells, that is cells with large deviations from co-planar faces to be avoided. Warp angles (measured between the surface normals of triangular parts of the faces) greater than 75 degrees can lead to serious convergence problems and deterioration in the results.
7. Non-orthogonal cells near boundaries to be avoided. This requirement is stronger than the requirement for the non-orthogonal cells away from the boundaries.

8. Tetrahedral elements to be avoided in boundary layers. Prismatic or hexahedral cells to be preferred because of their regular shape and ability to adjust in accordance with the near-wall turbulence model requirements.

9. High aspect ratios to be avoided in important regions of the flow domain but may be large in non-critical regions. This restriction may be relaxed near walls.

10. Specific code requirements for cell mesh stretching or expansion ratios to be observed. The change in mesh spacing should be continuous and mesh size discontinuities are to be avoided, particularly in regions of large changes.

11. Automatic grid adaptation techniques offered by some codes to be noted, as they might not always improve the grid quality (skewness, aspect ratio).

12. Critical regions with high flow gradients or with large changes (such as shocks, high shear, significant changes in geometry or where suggested by error estimators) to have a finer and a more regular mesh in comparison with non critical regions. Local mesh refinement to be employed in these regions in accordance with the selected turbulence wall modelling.

13. When using periodic boundary conditions, high geometric precision of the periodic grid interface to be ensured.
14. Arbitrary mesh coupling, non-matching cell faces, grid refinement interfaces or extended changes of element types to be avoided in the critical regions of high flow gradients.

15. Assumptions made when setting up the grid with regard to critical regions of high flow gradients and large changes to be checked with the result of the computation and grid points to be rearranged if found to be necessary.

16. Grid dependency study to be employed to analyse the suitability of the mesh and to give an estimate of the numerical error in the simulation.
Chapter 3

Turbulence Lengthscales

At high Reynolds numbers, the dynamics of the flow is characterized by the existence of a wide range of lengthscales. Surprisingly, there exists no clear lengthscale criterion distinguishing the small-scale turbulence and the large scale motions. Such a demarkation is of utmost importance in LES with the underlying principle of correctly resolving all large scale motion and modelling only the small scale turbulence.

One of the aims of the current study is to determine such a lengthscale criterion that would also enable an *a priori* determination of the required grid width. As a first step, a discussion of important mathematical relations encountered in the current study is presented.

3.1 Energy cascade and Kolmogorov hypothesis

The energy cascade idea proposed by Richardson [1922] is that kinetic energy enters the turbulence only at its largest scales of motion by the production mechanism and is then transferred to smaller and smaller scales by inviscid action [Pope, 2000].

The first concept in this view of the energy cascade is that turbulence
can be considered as a set of eddies of varying sizes. Eddies of size $l$ have a characteristic velocity $u(l)$ and timescale $\tau(l) \equiv l/u(l)$.

According to Richardson large eddies, of size $l_0$ comparable to the overall flow dimension $L$, are unstable and break up, transferring their energy to slightly smaller eddies. These smaller eddies undergo a similar break-up and transfer their energy to still smaller eddies. Such an energy cascade continues until the Reynolds number $Re(l) \equiv u(l)l/\nu$ is small enough for the eddy to be stable. At this stage, the molecular viscosity is effective in dissipating the kinetic energy.

Kolmogorov [1941] added to Richardson’s viewpoint and quantified the picture, particularly by identifying the *Kolmogorov scales*. The small-scale motion tends to have small time scales and hence, this motion can be assumed to be statistically independent of the relatively slow large-scale turbulence and mean flow. Consequently, the small-scale motion depends only on the rate at which it is supplied with energy from the mean flow and the kinematic viscosity. Further, the rate of energy supply to the small-scale motion being the same as the rate of dissipation of large-scale energy. The net rate of change of small-scale energy is therefore related to the time scale of the large-scale flow and is small when compared to the rate of energy dissipation [Tennekes and Lumley, 1972]. This is the basis for Kolmogorov’s *universal equilibrium theory* of small scale turbulence.

Kolmogorov’s hypothesis of local isotropy states that

“at sufficiently high Reynolds number, the small-scale turbulent motions ($l \ll l_0$) are statistically isotropic” [Pope, 2000].

The directional information of the large-scales as well as the information of the geometry of the large eddies is lost as the energy passes down the cascade. Consequently, the statistics of the small-scale motion are universal.
in every high-Reynolds number turbulent flow.

At this stage, it is convenient to introduce a lengthscale $l_{EI}$ such that the relation $l \ll l_0$ can be written as $l < l_{EI}$.

Kolmogorov’s first similarity hypothesis states that

“in every turbulent flow at sufficiently high Reynolds number, the statistics of the small-scale motions ($l < l_{EI}$) have a universal form that is uniquely determined by the viscosity $\nu$ and rate of energy dissipation $\varepsilon$” [Pope, 2000].

The size range $l < l_{EI}$ is termed as the universal equilibrium range.

With the parameters $\nu$ and $\varepsilon$, it is possible to obtain unique length, velocity and time scales, which are now called the Kolmogorov microscales and are given by the following relations.

Kolmogorov microscale of length,

$$\eta \equiv \left(\frac{\nu^3}{\varepsilon}\right)^{1/4} \quad (3.1)$$

Kolmogorov microscale of velocity,

$$u_\nu \equiv (\varepsilon \nu)^{1/4} \quad (3.2)$$

Kolmogorov microscale of time,

$$\tau_\nu \equiv \left(\frac{\nu}{\varepsilon}\right)^{1/2} \quad (3.3)$$

Kolmogorov’s second similarity hypothesis states that

“in every turbulent flow at sufficiently high Reynolds number, the statistics of the motions of scale $l$ in the range $l_0 \gg l \gg \eta$ have a universal form that is uniquely determined by $\varepsilon$, independent of $\nu$” [Pope, 2000].

Introducing a lengthscale $l_{DI}$ such that the relation $l_0 \gg l \gg \eta$ in the above hypothesis can be written as $l_{EI} > l > l_{DI}$, it can be observed that this lengthscale $l_{DI}$ splits the universal equilibrium range ($l < l_{EI}$) into two
Figure 3.1: The ranges and subranges of scales in a turbulent flow.

Figure 3.2: Schematic representation of the energy cascade.
subranges. These are termed as the inertial subrange \( l_{EI} > l > l_{DI} \) and the dissipation range \( l < l_{DI} \).

Figures 3.1 shows the various lengthscales and ranges. As the names imply, the inertial subrange involves motion determined by inertial effects, viscous effects being negligible and the dissipation range involves motion experiencing essentially all the viscous dissipation. Figure 3.2 sketches the energy cascade involving successive transfer of energy from larger eddies eddies to smaller eddies.

### 3.2 The two-point correlation

The two-point, one-time autocovariance is the simplest statistic containing information on the spatial structure of any random field and is often referred to as the two-point correlation.

For a turbulent field \( U(x, t) \), the two-point correlation is defined as

\[
R_{ij}(r, x) \equiv \langle u_i(x, t)u_j(x + r, t) \rangle
\]  

(3.4)

This correlation function is an indication of the effect of one point in the field on another point in the same field. With particular regard to turbulence, this can be thought of as an estimate of the relation between neighbouring velocity fluctuations.

In case of homogeneous isotropic turbulence (HIT), the two-point correlation \( R_{ij}(r, x) \) is independent of \( x \) and hence can be represented as \( R_{ij}(r) \).

A consequence of isotropy is that \( R_{ij} \) can be expressed in terms of two scalar functions \( f(r, t) \) and \( g(r, t) \) as

\[
R_{ij}(r, x) = u'^2 (g(r)\delta_{ij} + [f(r) - g(r)] \frac{r_i r_j}{r^2})
\]  

(3.5)

For co-ordinate directions \( x_i \) with unit vector \( e_i \) and the relation \( r = e_i r_i \),
this equation yields
\[
\frac{R_{11}}{u'^2} = f(r) = \frac{< u_1(x + e_1 r, t) u_1(x, t) >}{u_1^2}
\]
\[
\frac{R_{22}}{u'^2} = g(r) = \frac{< u_2(x + e_1 r, t) u_2(x, t) >}{u_2^2}
\]
\[
R_{33} = R_{22} \quad \text{and} \quad R_{ij} = 0, \text{ for all } i \neq j
\] (3.6)

The functions \( f \) and \( g \) are termed as the longitudinal and transverse autocorrelations respectively.

Further, the continuity equation implies that
\[
\frac{\partial R_{ij}}{\partial r_j} = 0
\] (3.7)

Therefore, 3.5 leads to
\[
g(r, t) = f(r) + \frac{1}{2} r \frac{\partial}{\partial r} f(r)
\]
\[
= \frac{1}{2} (f(r) + \frac{\partial}{\partial r} [rf(r)])
\] (3.8)

which implies that in isotropic turbulence, the two-point correlation \( R_{ij}(r) \) is completely determined by the longitudinal autocorrelation function \( f(r) \).

The longitudinal and transverse autocorrelation functions can be employed as a basis for defining longitudinal and transverse lengthscales. Two such lengthscales of importance are the integral lengthscales and the Taylor microscales.

### 3.3 Integral lengthscales

From the two-point correlation, a number of integral scales can be defined. For example, for the \( x_i \) co-ordinate direction with unit vector \( e_i \), the Integral scale \( L_{ii} \) is defined as
\[
L_{ii}(x) \equiv \frac{1}{R_{ii}(0, x)} \int_0^\infty R_{ii}(e_i r, x) dr
\] (3.9)
The longitudinal integral scale is obtained by the integration of the longitudinal autocorrelation and is defined as

\[ L_{11} \equiv \int_0^\infty f(r)dr \] (3.10)

Similarly, the transverse integral scale is

\[ L_{22} \equiv \int_0^\infty g(r)dr \] (3.11)

3.8, 3.10 and 3.11 imply that, for isotropic turbulence, the transverse integral scale, \( L_{22} \) is half the longitudinal integral scale \( L_{11} \).

### 3.4 Taylor microscales

The second important lengthscale defined from the autocorrelation functions is the Taylor microscale \( \lambda \). The longitudinal and transverse scales are defined as

\[ \lambda_{11}(t) = \left[ -\frac{1}{2} f''(0, t) \right]^{-1/2} = \sqrt{\frac{2u'^2}{< \left( \frac{\partial u_1}{\partial x_1} \right)^2 >}} \] (3.12)

\[ \lambda_{22}(t) = \left[ -\frac{1}{2} g''(0, t) \right]^{-1/2} = \sqrt{\frac{2u'^2}{< \left( \frac{\partial u_2}{\partial x_2} \right)^2 >}} \] (3.13)

For homogeneous isotropic turbulence, the Taylor microscales are given by

\[ \lambda_{ii} = \sqrt{\frac{15}{\varepsilon}} \frac{< u_i u_i >}{\nu} \] (3.14)

Also, the transverse and longitudinal taylor microscales are related as

\[ \lambda_{11} = \sqrt{2} \lambda_{22} \] (3.15)
3.5 Velocity spectra

In case of homogeneous isotropic turbulence, the two-point correlation $R_{ij}(r)$ can be expressed in terms of a *wavenumber spectrum*.

Consider the spatial Fourier mode

$$e^{i\kappa \cdot x} = \cos(\kappa \cdot x) + i \sin(\kappa \cdot x) \quad (3.16)$$

This function varies sinusoidally in the direction of the wavenumber vector $\kappa$ with wavelength $l = 2\pi/|\kappa|$.

The velocity spectrum tensor $\Phi_{ij}(\kappa)$ is defined as the Fourier transform of the two-point correlation

$$\Phi_{ij}(\kappa) = \frac{1}{(2\pi)^3} \int \int \int_{-\infty}^{\infty} e^{-i\kappa \cdot r} R_{ij}(r) dr \quad (3.17)$$

where $d\boldsymbol{r}$ is written for $dr_1dr_2dr_3$.

Consequently, the two-point correlation can be obtained from the velocity spectrum tensor by employing the inverse Fourier transform as

$$R_{ij}(r) = \int \int \int_{-\infty}^{\infty} e^{i\kappa \cdot r} \Phi_{ij}(\kappa) d\kappa \quad (3.18)$$

where $d\boldsymbol{\kappa}$ is written for $d\kappa_1d\kappa_2d\kappa_3$.

For $r = 0$, from equations 3.4 and 3.18, we have the relation

$$R_{ij}(0) = <u_iu_j> = \int \int \int_{-\infty}^{\infty} \Phi_{ij}(\kappa) d\kappa \quad (3.19)$$

Consequently, $\Phi_{ij}(\kappa)$ represents the contribution of the velocity modes with wavenumber $\kappa$ to the autocovariance $<u_iu_j>$.

The two-point correlation as well as the velocity spectrum function contain two different kinds of directional information. The dependence of $R_{ij}(r)$ and $\Phi_{ij}(\kappa)$ on $r$ and $\kappa$ respectively give the direction in physical space of the
Fourier mode, while the components of $R_{ij}$ and $\Phi_{ij}$ (the subscripts $i$ and $j$) give the directions of the velocities.

The two-point correlation and the velocity spectrum function can therefore be represented as $R_{ij,k}$ and $\Phi_{ij,k}$ respectively, where the index $k$ represents the direction in physical space.

A third part of the information is the lengthscale of the mode given by $l = \frac{2\pi}{|\kappa|}$.

Further, information regarding the velocity derivatives is contained in $\Phi_{ij}$. This can be extracted, among other methods, by the relation

$$< \frac{\delta u_i}{\delta x_k} \frac{\delta u_j}{\delta x_l} > = \int \int \int_{-\infty}^{\infty} \kappa_k \kappa_l \Phi_{ij}(\kappa) d\kappa$$

(3.20)

The dissipation rate is therefore given by

$$\varepsilon = \int \int \int_{-\infty}^{\infty} 2\nu \kappa^2 \frac{1}{2} \Phi_{ii}(\kappa) d\kappa$$

(3.21)

### 3.6 Energy spectrum

In comparison to the great deal of information contained in $\Phi_{ij}$, a more simple yet less complete description is provided by the *energy spectrum function* $E(\kappa)$ given by

$$E(\kappa) \equiv \int \int \int_{-\infty}^{\infty} \frac{1}{2} \Phi_{ii}(\kappa) \delta(|\kappa| - \kappa) d\kappa$$

(3.22)

This may be viewed as a non directional representation of the velocity spectrum tensor $\Phi_{ij}(\kappa)$ and is a very important quantity for qualitative discussions.

Integration of 3.22 over all scalar wave numbers $\kappa$ yeilds the turbulent kinetic energy,

$$k = \int_{0}^{\infty} E(\kappa) d\kappa = \frac{1}{2} R_{ii}(0, t) = \frac{1}{2} <u_i u_i>$$

(3.23)
Consequently, $E(\kappa) d\kappa$ represents the contribution of all modes with $|\kappa|$ in the range $\kappa \leq |\kappa| \leq \kappa + d\kappa$ to the total turbulent kinetic energy $k$.

Motions of lengthscale $l$ correspond to wavenumber $\kappa = 2\pi/l$ and the energy in the wavenumber range $(\kappa_a, \kappa_b)$ is given by

$$k_{(\kappa_a, \kappa_b)} = \int_{\kappa_a}^{\kappa_b} E(\kappa) d\kappa$$ (3.24)

The dissipation of the turbulent kinetic energy is defined as

$$\varepsilon = 2\nu <s_{ij}s_{ij}>$$ (3.25)

where $s_{ij}$ is the fluctuating rate of strain given by

$$s_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$ (3.26)

Further, the pseudo dissipation $\tilde{\varepsilon}$ is defined as

$$\tilde{\varepsilon} = \nu < \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} >$$ (3.27)

and is related to the total dissipation $\varepsilon$ as

$$\tilde{\varepsilon} = \varepsilon - \nu \frac{\partial <u_iu_j>}{\partial x_i \partial x_j}$$ (3.28)

For almost all practical flow situations, the second term is at most a few percent of the true dissipation and hence the dissipation is usually approximated as being equal to the pseudo dissipation.

The total dissipation can be obtained from the energy spectrum by the relation

$$\varepsilon = \int_{0}^{\infty} 2\nu \kappa^2 E(\kappa) d\kappa$$ (3.29)
3.7 Turbulent energy lengthscale

Based on RANS results, from the predicted turbulent kinetic energy and its dissipation, it is possible to obtain, by dimensional analysis, the energy carrying eddies scale or the turbulent energy lengthscale $L_{RM,i}$ as

$$L_{RM,i} \equiv A \frac{< u_i u_i >^{3/2}}{\varepsilon}$$  \hspace{1cm} (3.30)

The subscript “RM” for “RANS model” indicates that the lengthscale is estimated from a RANS model. This lengthscale characterises the size of the energy carrying large eddies and for homogeneous isotropic turbulence, with the constant $A$ taken close to unity [Kang et al., 2003], gives an indication of the true integral scale.

The turbulence Reynolds number based on $L_{RM}$ is therefore

$$Re_L \equiv \frac{k^{1/2} L_{turb}}{\nu} = \frac{k^2}{\varepsilon \nu}$$  \hspace{1cm} (3.31)

The following relations can now be deduced

$$\lambda_{22} = \sqrt{10} L_{RM} Re_L^{-1/2}$$  \hspace{1cm} (3.32)
$$\eta = L_{RM} Re_L^{-3/4}$$  \hspace{1cm} (3.33)
$$\lambda_{22} = \sqrt{10} \eta^{2/3} L_{RM}^{1/3}$$  \hspace{1cm} (3.34)

Consequently, for high $Re$, $\lambda_{22}$ is between $\eta$ and $L_{RM}$.

3.8 Taylor’s hypothesis

*Taylor’s hypothesis* [Taylor, 1938], or the *frozen-turbulence approximation*, is the approximation of spatial correlations by temporal correlations. Such approximations are important, chiefly for experimental determination of spatial correlations, which would otherwise require measurements of the two-point correlation $R_{ij}(r)$ for all $r$. 
One such technique is the ‘flying hot wire’ technique which involves moving a single hot-wire probe rapidly through the turbulent field at a constant velocity $V$ along a straight line parallel to direction $x_1$ with unit vector $e_1$. If the location of the probe at time $t = 0$ is $x_0$ then at time $t$, its location is

$$X(t) \equiv x_0 + e_1 V t$$

and the velocity that it measures $U^{(m)}(t)$ is

$$U^{(m)}(t) = U(X(t), t) - e_1 V$$

The two-point two-time autocovariance or the temporal autocovariance obtained from the measured velocity $U^{(m)}(t)$ is

$$R^{(m)}_{ij}(s) \equiv \langle [U_i^{(m)}(t) - \langle U_i^{(m)}(t) \rangle][U_j^{(m)}(t + s) - \langle U_j^{(m)}(t + s) \rangle] \rangle$$

$$= \langle u_i(X(t), t)u_j(X(t + s), t + s) \rangle$$

$$= \langle u_i(X(t), t)u_j(X(t) + e_1 r_1, t + r_1/V) \rangle$$

(3.37)

where $r_1 = V s$ is the distance that the probe travels in time $s$.

For a turbulent field that is statistically homogeneous in the $x_1$ direction, the hypothetical limit of the probe speed $V$ tending to infinity yields the following relation.

$$R^{(m)}_{ij}(s) = \langle u_i(x_0 + e_1 V t, 0)u_j(x_0 + e_1 V t + e_1 r_1, 0) \rangle$$

$$= \langle u_i(x_0, 0)u_j(x_0 + e_1 r_1, 0) \rangle$$

$$= R_{ij}(e_1 r_1, x_0, 0)$$

(3.38)

Consequently, the temporal autocovariance yields the spatial autocovariance at $(x_0, 0)$. For practical cases of a finite probe velocity $V$, it is clearly an approximation, improving with increasing $V$.

In statistically stationary flows, wherein the turbulence intensity $u'$ is small when compared to the mean velocity $\langle U \rangle$ in the $x_1$ direction, a
single stationary probe is used. For such a measurement, in the frame of reference moving with the mean velocity $< U >$, the probe velocity is $e_1 V = - < U > = -e_1 < U_1 >$. The flying hot wire analysis can therefore be applied with $r_1 = - < U_1 > s$.

The accuracy of this approximation depends not only on the flow properties, but also on the quantity being measured. On one hand, in grid turbulence with $u'/ < U_1 > \ll 1$ it is quite accurate, facilitating higher order corrections [Lumley, 1965] while in free shear flows, while on the other, it has been experimentally shown to fail in free shear flows [Tong and Warhaft, 1995].

### 3.9 One-dimensional spectra

Most experimental data on turbulent spectra come from stationary hot wire measurements. The quantities deduced from such measurements using the Taylor’s hypothesis are of the form

\[
R_{11}(e_1 r_1) = < u_1^2 > f(r_1) \tag{3.39}
\]

\[
R_{22}(e_1 r_1) = < u_2^2 > g(r_1) \tag{3.40}
\]

The one-dimensional spectra $E_{ij}(\kappa_1)$ are defined as twice the one-dimensional Fourier transform of the autocorrelation $R_{ij}(e_1 r_1)$.

Mathematically,

\[
E_{ij}(\kappa_1) \equiv \frac{1}{\pi} \int_{-\infty}^{\infty} R_{ij}(e_1 r_1) e^{-i\kappa_1 r_1} dr_1 \tag{3.41}
\]
3.10 Kolmogorov spectra

According to Kolmogorov’s hypothesis, the high wavenumber portion of the velocity spectra in any turbulent flow at a sufficiently high Reynolds number adopts particular universal forms.

Thus, from the first similarity hypothesis, the velocity statistics pertaining to the universal equilibrium range have a universal form uniquely determined by $\varepsilon$ and $\nu$. Thus, for $\kappa > \kappa_E I$, $E(\kappa)$ is a universal function of $\kappa$, $\varepsilon$ and $\nu$.

A simple dimensional analysis yields $E(\kappa)$ in terms of $\varepsilon$ and $\nu$ as

$$E(\kappa) = (\varepsilon \nu^5)^{1/4} \varphi(\kappa \eta)$$

$$= u_\eta^2 \eta \varphi(\kappa \eta)$$  \hspace{1cm} (3.42)

where $\varphi(\kappa \eta)$ is a universal non-dimensional function termed as the Kolmogorov spectrum function.

If, $\varepsilon$ and $\kappa$ are used to non-dimensionalize $E(\kappa)$, we have the relation

$$E(\kappa) = \varepsilon^{2/3} \kappa^{-5/3} \Psi(\kappa \eta)$$  \hspace{1cm} (3.43)

where $\Psi(\kappa, \eta)$ is called the compensated Kolmogorov spectrum function.

These universal functions are related as

$$\Psi(\kappa \eta) = (\kappa \eta)^{5/3} \varphi(\kappa \eta)$$  \hspace{1cm} (3.44)

From the second similarity hypothesis, in the inertial subrange $E(\kappa)$ has a universal form uniquely determined by $\varepsilon$ and is independent of $\nu$. This implies, from 3.43, that in the inertial subrange, $\Psi(\kappa \eta)$ is independent of $\nu$ and hence equal to a constant $C$. 
Thus, the energy spectrum function in the inertial subrange is

\[ E(\kappa) = C \varepsilon^{2/3} \kappa^{-5/3} \] (3.45)

which is the famous Kolmogorov $-5/3$ spectrum and $C$ is the universal Kolmogorov constant. Experimental data suggest the value $C = 1.5$.

Further, it can be shown that the one-dimensional spectra are given by

\[ E_{11}(\kappa_1) = C_1 \varepsilon^{2/3} \kappa_1^{-5/3} \] (3.46)

\[ E_{22}(\kappa_1) = C'_1 \varepsilon^{2/3} \kappa_1^{-5/3} \] (3.47)

where

\[ C_1 = \frac{18}{55} C \] (3.48)

\[ C'_1 = \frac{4}{3} C_1 = \frac{24}{55} C \] (3.49)

### 3.11 Lengthscales and spectra

At this stage, it is deemed necessary to have an idea of the physical interpretation of the various lengthscales, in particular the Integral lengthscale and the Taylor microscale. The Kolmogorov lengthscale $\eta$ is the characteristic lengthscale of the smallest eddies in the turbulent field.

The Taylor microscale does not have a clear physical interpretation. Its approximate position on turbulent energy spectra seems to indicate that it lies at the dissipation region end of the inertial subrange. This can be assessed by considering a model spectrum and evaluating the Taylor microscale for the same.
A model energy spectrum for homogeneous isotropic turbulence can be defined as

\[ E(\kappa) = A \left( \frac{\kappa}{\kappa_I} \right)^2 \quad \text{for} \quad \kappa < \kappa_I \]

\[ = A \left( \frac{\kappa}{\kappa_I} \right)^{-5/3} \quad \text{for} \quad \kappa > \kappa_I \]  

(3.50)

Figure 3.3 displays this model spectrum and the position of the integral lengthscale and Taylor microscale on the same.
Figure 3.4: Integral lengthscale and Taylor microscale on a one-dimensional model energy spectrum.

Figure 3.4 shows the integral lengthscale and Taylor microscale along with a model one-dimensional energy spectrum defined as

\[
E_{ii} = \begin{cases} 
1.1A - \frac{17A}{22} \left( \frac{\kappa_i}{\kappa_I} \right)^2 + A \left( \frac{\kappa_i}{\kappa_I} \right)^{2\log\frac{\kappa_i}{\kappa_I}} & \text{for } \kappa_i < \kappa_I \\
\frac{18A}{55} \left( \frac{\kappa_i}{\kappa_I} \right)^{-5/3} & \text{for } \kappa_i > \kappa_I 
\end{cases}
\]  

(3.51)
Further, Figure 3.5 displays the longitudinal one-dimensional energy spectra at two stations (20 and 48) in homogeneous isotropic turbulence obtained from the experiment of Kang et al. [2003] at Reynolds number $Re_\tau = 720$. Added on the figure are the integral scale and the Taylor microscale computed from equations 3.9 and 3.14 which are valid in homogeneous isotropic turbulence and hence agreement comes as no surprise.

It maybe observed from the three figures, quite obviously so, that while the integral scales are positioned at the top limit of the inertial range (notice the $-5/3$ slope), the Taylor scales are located almost two decades lower, at a more or less optimum position that can be well suited for defining a grid size for this flow.
Thus, if it is possible to prove that these observations are extendable to non-homogeneous turbulence, then the Taylor scales would be the ideal parameter to define the grid resolution for LES computations.

In fact, the Taylor microscale is a combination of the turbulent energy lengthscale and the Kolmogorov scale as \( \lambda \sim L_{RM}^{1/3} \eta^{2/3} \) so \( \lambda / \eta / L_{RM} \sim (\eta / L_{RM})^{2/3} \). Consequenlty, an LES based on the Taylor microscale would become over-resolved at higher Reynolds numbers; and a bound on the filter scale such as \( \Delta = max(\lambda, L_{RM}/10) \) could be recommended.
Chapter 4
Turbulent Channel Flow

4.1 Non-homogeneous turbulence

It has been demonstrated [Belmabrouk and Michard, 1998] that, for small separations, the shape of the correlation function can still be approximated by

\[ R_{ii}(r, x) = 1 - \frac{r^2}{\lambda_{ii}^2(x)} + ... \]  (4.1)

This implies that even in shear flows it is still possible to estimate the Taylor microscales using equations (3.12) and (3.13) which may be computed either from the one-dimensional spectra or by fitting the two-point correlations with a parabola over a certain interval \([0, r_{max}].\)

Alternatively, they may be approximated by the HIT derived formula

\[ \lambda_{RM,i} = \sqrt{15 \frac{\langle u_i u_i \rangle}{\varepsilon} \nu} \]  (4.2)

This relation can be extended outside homogeneous isotropic turbulence by assuming a relation between componentiality (velocity components) and directionality (lengthscale direction) which, though not obvious in general, is reasonable for near wall flows. Again, the subscript “RM” indicates that an estimate could be provided by a RANS model; more precisely a low Reynolds Stress transport model if an accurate representation of anisotropy is required.
4.2 Lengthscales in turbulent channel flow

For plain channel flow, the internal flow notations are specified as: 1 $\sim x$ for streamwise; 2 $\sim y$ for wall normal and 3 $\sim z$ for spanwise directions.

Results for turbulent channel flow from direct numerical simulations performed at Reynolds numbers ranging from $Re_\tau = 150$ to 720\cite{Iwamoto2002, Hu2001} were employed to extract velocity and energy spectra, two point correlations and consequently the different turbulent lengthscales.

In figures 4.1 and 4.2, the Taylor microscales are displayed along with the one-dimensional spectra at two dimensionless distances from the wall. It is clear from the figures that the Taylor microscales indicate isotropy at $y^+ = 320$ but not at $y^+ = 5$. It is no longer possible to identify an inertial range like in the HIT test case. It may be observed from the figures however, that near the wall region is dominated by anisotropic structures up to the Kolmogorov scales, while in the log-layer the flow becomes more isotropic. The Taylor microscales exhibit the same behaviour. It can therefore be reasonably stated that away from the wall, the Taylor microscales should be able to dictate an isotropic grid that is well suited for LES. Near the wall however, in order that the anisotropy of the structures be correctly captured, the computation should ideally switch to a DNS.

Longitudinal lengthscales are divided by 2 or $\sqrt{2}$ for integral and Taylor scales in subsequent graphs.

Figure 4.3 shows the integral lengthscales as defined from integral of the two point correlation, and extracted from the THTLab database\cite{Iwamoto2002}. Effectively, the integrations have been stopped when the correlation
Figure 4.1: Streamwise energy spectra from DNS computations at $Re_\tau = 720$.

Figure 4.2: Spanwise energy spectra from DNS computations at $Re_\tau = 720$. 
is lower than 10% to avoid spurious effects of periodicity conditions in the simulations. As could be expected, the streamwise correlations \((k = 1)\) show the overwhelming influence of streaks up to \(y^+ = 100\). For this Re, note that the scales at the wall \((y^+ = 0)\) are roughly the same as those in the core of the flow \((80\) wall units\). The spanwise correlation \((k = 3)\) on the other hand, show an initially linear growth \((\text{roughly scaling with the Von Karman mixing length 0.41})\), starting from a wall value of about 20 viscous units. Hence for a well resolved near wall layer one must have \(Dx^+ \ll 80\) and \(Dz^+ \ll 20\), which is empirical practice. At the centre, the scatter between components is larger compared to our expectation of isotropic turbulence, but this may be attributed to the fact that large scales require larger statistical samples. However, the streamwise and spanwise scales are coming together. Figure 4.4 now shows the turbulent energy scales as could be obtained from a RANS model \((\text{a perfect model, as DNS data is used as input to the formula})\). Scaling the mesh steps with these scales is not appropriate as they obviously start from zero, but also decrease at the centre, except the wall normal component which has a monotonic growth and better differentiates between the Log layer and core of the channel \((\text{this is in fact one of the assets of Durbin’s } v^2 - f \text{ model})\).

The scales for the high Reynolds number \((Re_\tau = 720)\) are plotted in Figure 4.5 as a function of the normalized wall distance. It is interesting to notice that the transverse Taylor microscales vary similarly to the Kolmogorov scales. In agreement with the above observations, both scales show a large variation and anisotropy near to the wall \((\text{up to } y^+ = 30, \text{ in dotted lines in the figure})\), then almost a linear variation in the log-layer region. The transverse Taylor scales in the three directions are almost identical in that region which is a sign of isotropy. The integral scale computed as \(L_i = u_i^3/\varepsilon_{ii}\)
Figure 4.3: Integral lengthscales for $Re_\tau = 395$ from DNS

Figure 4.4: Energy lengthscales for $Re_\tau = 395$ from DNS
is nearly 10 times larger in the log-layer. Furthermore, it does not seem to follow the same linear variation.

The streamwise Taylor microscales \( k = 1 \), when divided by \( \sqrt{2} \), seem to indicate that a streamwise filter of \( \Delta_1^+ = 35 \) to 55 viscous units should be sufficient to capture the wall normal velocity fluctuations \( i = 2 \) which demand the finest resolution.

It is interesting to notice that the transverse Taylor microscales \( k = 3 \) vary similarly to ten times the Kolmogorov scales even up to the centre (for this Re). Both scales show a large variation and anisotropy near to the wall (up to \( y^+ = 30 \)), then almost a linear variation, making it difficult to distinguish the log-layer region from the core region of the channel. The one-tenth of estimated integral lengthscale as estimated from \( L_{RM,i} \) was expected to dominate in the central region, but \( Re_\tau = 720 \) is still too low for this to happen. Near the wall \( L_{RM,i}/10 \) decreases very rapidly compared to the Kolmogorov or transverse Taylor scales. The latter suggest \( \Delta_3^+ = 15 \) at the wall to 45 at the centre which is in line with empirical knowledge. The estimated Taylor scale \( \lambda_{RM,i} \) is quite close to the actual one for \( i = 1 \) and 3, but shows an overestimation for the wall normal velocity. It also has the disadvantage of going to zero at the wall. Finally the “anisotropic” Kolmogorov scale is of course isotropic for \( y^+ > 50 \), but is singular at the wall for \( i = 2 \), and is thus not worth pursuing.

From literature it is possible to find that the maximum grid size that is used for DNS is about 5 times the Kolmogorov scales everywhere. Thus, it can be argued that computations using grids based on these scales are still within the limits of the LES approach. To conclude one may recommend an unstructured mesh such that \( \Delta_1 = max(min(\lambda_{11,l}, \lambda_{22,l}, \lambda_{33,l}), L_{RM}/10) \) and \( \Delta_3 = max(min(\lambda_{11,3}, \lambda_{22,3}, \lambda_{33,3}), L_{RM}/10) \), but with \( \lambda_{i,j,k} = max(\lambda_{RM,k}, \eta/5) \)
Figure 4.5: Comparison between different lengthscales for the channel flow test case at $Re_\tau = 720$. 
when the Taylor microscale needs to be guessed from a RANS model. No
two point correlation data is available for the wall normal lengthscales, so an
estimate $\Delta_2 = \max(\min(\lambda_{22,1}, \lambda_{22,2}, \lambda_{22,3}), L_{RM}/10)$ is used.

In practice the one-dimensional spectra are not always available, how-
ever, based on the above observations, it is possible to compute the Taylor
microscales as a function of the Kolmogorov scales (a constant for each direc-
tion is relatively easy to obtain and calibrate at different Reynolds numbers).
In particular, the value 10 seems to be appropriate for the normal and span-
wise directions. From literature it is possible to find that the maximum grid
size that is used for DNS is about 5 times the Kolmogorov scales everywhere.
Thus, it can be argued that computations using grids based on these scales
are still within the limits of the LES approach.

4.3 Lengthscales in high Reynolds channel flows

For high Reynolds number flows for which reliable DNS or fine LES results are
not available, it is imperative to use RANS results to predict the turbulence
lengthscales.

In order to gain an insight into the variation of these lengthscales with in-
creasing Reynolds number, channel flows at $Re_\tau$ ranging from 2000 to 10000
are simulated using the $k-\varepsilon$ model. The simulations are performed using
\texttt{Code_Saturne}. \texttt{Code_Saturne} is an in-house code developed by Electricite
De France (EDF) and distributed freely. It is designed to solve the Navier-
Stokes equations for a range of geometries: 2D, 2D axisymmetric and 3D
flows. It can be used to simulate flows that are steady or unsteady, compress-
able ot incompressible, laminar ot turbulent, isothermal or non-isothermal.
A finite volume discretisation is employed and number of mesh formats are
supported. It is possible to use hybrid meshes as also meshes with hanging
nodes.

*Code Saturne* is composed of two main elements: the Preprocessor and the Kernel. The Preprocessor handles mesh data reading from a number of file formats (including, among others, universal IDEAs, CGNS 2.0, EnSight 6, Gmsh, Comet-Design and Gambit Neutral), mesh pasting, domain decomposition for parallel computations and definition of periodic boundary conditions, both translational and rotational. The Kernel module is the numerical solver.

The channel flow $k - \varepsilon$ simulations are performed using a simple mesh. A domain size of $(0.1, 2.0, 0.1)$ is employed with periodic conditions in the streamwise and spanwise directions.

The integral lengthscale and Taylor microscale are calculated as

$$L_{RM} \equiv \frac{k^{3/2}}{\varepsilon} \tag{4.3}$$

and

$$\lambda_{RM} \equiv \sqrt{10 \frac{k\nu}{\varepsilon}} \tag{4.4}$$

Figures 4.6 and 4.7 show the variation of the mean velocity and the turbulent kinetic energy across the channel as obtained from the performed $k - \varepsilon$ simulation along with the profiles obtained in a DNS study of the same case [Hoyas and Jimenez, 2006]. It can be observed that the RANS simulation with the $k - \varepsilon$ modelling results in an overprediction of turbulence and therefore a flatter velocity profile resulting in underprediction of the mean velocity.

Figure 4.8 shows the dissipation profile obtained while the turbulent energy lengthscale and the Taylor microscale as calculated from equations 4.3
Figure 4.6: Velocity profiles obtained from $k - \varepsilon$ simulation in comparison with DNS velocity profiles [Hoyas and Jimenez, 2006] for $Re_{\tau} = 2000$.

Figure 4.7: Turbulent energy profiles obtained from $k - \varepsilon$ simulation in comparison with DNS velocity profiles [Hoyas and Jimenez, 2006] for $Re_{\tau} = 2000$.  

and 4.4 are shown in Figures 4.9 and 4.10.
Figures 4.11 to 4.15 show similar results for $Re_\tau = 6000$.

$k - \varepsilon$ simulations over the range $Re_\tau = 2000$ to $Re_\tau = 10000$ have facilitated a direct comparison of how the turbulent energy lengthscale and the Taylor microscale scale with $Re_\tau$.

Figure 4.16 shows that the turbulent energy lengthscale $L_{RM}$ is indeed limited by the size of the domain and is virtually independent of the Reynolds number.

Figure 4.17 shows how the increasing Reynolds number affects the Taylor microscale. As is expected, the Taylor microscale decreases with increasing Reynolds number.

More importantly, from Figure 4.18, showing the Taylor microscales as non-dimensionalized using the $Re_\tau$, it can be seen that the Taylor microscales grow almost linearly with $Re_\tau$ at least for the range of $Re_\tau$ in the current study.
CHAPTER 4. TURBULENT CHANNEL FLOW

Figure 4.9: Variation of turbulent energy lengthscale across channel at $Re_\tau = 2000$.

Figure 4.10: Variation of Taylor microscale across channel at $Re_\tau = 2000$. 
Figure 4.11: Velocity profile across channel for $Re_\tau = 6000$.

Figure 4.12: Turbulent energy profile across channel for $Re_\tau = 6000$. 
Figure 4.13: Dissipation profile across channel for $Re_\tau = 6000$.

Figure 4.14: Variation of turbulent energy lengthscale across channel at $Re_\tau = 6000$. 
Figure 4.15: Variation of Taylor microscale across channel at $Re_\tau = 6000$.

Figure 4.16: Variation of turbulent energy lengthscale with $Re_\tau$. 
Figure 4.17: Variation of Taylor microscale with $Re_{\tau}$.

Figure 4.18: Variation of the normalized Taylor microscale with $Re_{\tau}$.
CHAPTER 4. TURBULENT CHANNEL FLOW

Table 4.1: Number of cells in the three directions of the domain

<table>
<thead>
<tr>
<th></th>
<th>(N_x)</th>
<th>(N_y)</th>
<th>(N_z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LES</td>
<td>68 to 200</td>
<td>46</td>
<td>42 to 100</td>
</tr>
<tr>
<td>DNS</td>
<td>256</td>
<td>193</td>
<td>192</td>
</tr>
</tbody>
</table>

4.4 LES grid based on Taylor microscales

Based on the above analysis, a grid has been generated for a plane channel at \(Re_\tau = 395\) using the transverse Taylor microscales. The grid density is summarized in Table 4.1 in comparison of a DNS grid used by Moser et al[1999] and figure 4.19 illustrates the anisotropic cell distribution in the three directions of the domain with a total of 443,272 cells. The commercial code Star-CD has been used for the present simulations. The computations have been carried out using the classical Smagorinsky model with Vandriest damping function.

4.5 LES results

Figure 4.20 illustrates the obtained results in comparison with results from DNS and LES employing structured grids. A remarkable feature is that over-prediction of the mean velocity and streamwise component of fluctuating velocity, usually encountered in LES, are not very pronounced in this simulation. However, some under-prediction of the wall normal and fluctuating velocities occurs, chiefly in the centre of the channel. The velocity profile results very closely follow DNS results and therefore, the attempt of building an LES grid based on the Taylor microscale has been very successful.

The dissipation profiles obtained (figure 4.21), while illustrating an improvement over those obtained by structured grid LES, do not approximate closely the DNS results, especially in the centre of the channel. The peaks
Figure 4.19: Grid built for channel flow using Taylor microscales.

Figure 4.20: LES results obtained with the grid generated using Taylor scales (LES Taylor) in comparison with an LES using structured grid (LES STRUC).
Figure 4.21: Effects of the grid resolution on the dissipation profiles. Symbols, DNS; dashed lines, LES with structured grid and line, LES with grid generated using Taylor scales.
are captured well, but the channel centre discrepancy seems to be linked to the under-predicted fluctuating velocities in that zone. Due to the fact that the energy dissipation rate is associated with eddies of the order of the Kolmogorov scales; a very fine grid is required for it to be correctly captured [Baggett et al., 1997]. More points are required in the buffer layer to capture the rapid variation of the dissipation in that region.
Chapter 5
Conclusions

An unstructured grid following the spanwise Taylor microscales in the streamwise, wall normal and spanwise directions gives good agreement of the LES results with those obtained from DNS.

The most important features of this grid, differentiating it from all earlier empirical meshes, are the almost cubical geometry of the cells and the fineness in the spanwise direction. Empirical LES grids, currently very widely used, have a very fine (approximately four times finer) wall normal resolution and a coarse (about twice as coarse) streamwise resolution as compared to a grid based on the Taylor microscales.

The cubical nature of the grid enables the flow vorticity to be effectively captured. Consequently, the turbulent mixing is well taken into account and near wall fluid acceleration is restricted. The results seem to indicate that the spanwise mesh resolution is very consequential in correctly resolving turbulence in channel flows.

The prescribed criteria now need to be tested in different configurations such as jets and separating flows.
The aim of the current project is an *a priori* determination of an unstructured mesh for LES in such a way that the grid density is ‘sufficient’. In the first year, the different turbulence lengthscales and their inter-relations have been researched. A completely unstructured grid based on the Taylor microscales has been found to give good prediction of the mean velocity and Reynolds stresses for plane channel flow.

However, in plane channel flow, at the Reynolds numbers considered in this study, a very wide range of lengthscales has not been observed. Further, the grid based on the Taylor microscales was very coarse as compared to typical empirical LES grids from similar computations.

As the present investigation was in progress, a paper by Meyers and Sagaut [2007] showed that a very coarse DNS can predict mean profiles surprisingly well, for very specific cell size distributions, but depends strongly on the wall normal resolution and Reynolds number. The convergence behaviour is not monotonic and the contribution of the subgrid scale model quality to the perceived simulation quality may be negligible.

Nevertheless the present unstructured grid has been build on physically meaningful lengthscales rather than trial and error.
CHAPTER 6. FUTURE WORK

The present work relied on DNS results for the extraction of the Taylor microscales. The next step is to extract the lengthscales from a presursor RANS simulation. Different test cases will be investigated before attempting to simulate an industrial flow.

A framework for the intended plan is shown in figure 6.1.

6.1 Test case 1: Confined jet

The first test case is selected as a confined coaxial turbulent jet. This test case has been widely researched, both experimentally [Champagne and Wygnanski, 1971, Habib and Whitelaw, 1979, Ahmed and Nejad, 1990] and numerically [Habib and Whitelaw, 1979, Akselvoll and Moin, 1996, Apte et al., 2003]. The geometry, as shown in Figure 6.2, resembles that of a coaxial jet combustor and so an insight into the phenomena in the same, particularly with regard to turbulent mixing, can be gained.

In his PhD thesis, Berrouk [2007] recommends the co-axial jet as a test case for numerical simulation. He performed a RANS simulation with the same parameters as the experiment of Ishima et. al. [1999] and found
Figure 6.2: Coaxial confined jet

descrepancies between the RANS and experimental results. Riber [2007] employed the test case for a detailed study the behaviour of LES models and their underlying mechanisms.

6.1.1 Preliminary RANS results

As a first step, in order to provide realistic inlet conditions, regular meshes for a pipe and an annulus (Figures 6.3 and 6.4) have been built. $k - \varepsilon$
Table 6.1: Data of experimental work [Ishima et al., 1999]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Combustor length</td>
<td>$L = 1.5\text{m}$</td>
</tr>
<tr>
<td>Inner jet radius</td>
<td>$R_1 = 0.01\text{m}$</td>
</tr>
<tr>
<td>Inner jet maximal velocity</td>
<td>$U_1 = 4\text{m/s}$</td>
</tr>
<tr>
<td>Inner jet Reynolds number</td>
<td>$Re_1 \approx 5200$</td>
</tr>
<tr>
<td>Flow rate in inner jet</td>
<td>$F_{f,j} = 1.27\text{g/s}$</td>
</tr>
<tr>
<td>Annulus inner radius</td>
<td>$R_2 = 0.075\text{m}$</td>
</tr>
<tr>
<td>Annulus outer radius</td>
<td>$R_3 = 0.150\text{m}$</td>
</tr>
<tr>
<td>Annular flow maximal velocity</td>
<td>$U_2 = 6\text{m/s}$</td>
</tr>
<tr>
<td>Annular flow Reynolds number</td>
<td>$Re_2 \approx 30000$</td>
</tr>
<tr>
<td>Flow rate in annular flow</td>
<td>$F_{f,a} = 261\text{g/s}$</td>
</tr>
</tbody>
</table>

Figure 6.3: RANS mesh for inner pipe.

and $k - \omega$ (SST) models have been employed to predict the flow conditions which are then used to prescribe inlet conditions to the final simulation of the concentric jets.

Figure 6.5 shows the profiles as obtained using the two RANS models. The simulations are set to give the same mass flow rate as that for the experimental data used for comparison. It is found that the maximal velocity observed in the experiment is not correctly predicted by either models.

A block-structured mesh for a wedge shaped domain (wedge angle $10^\circ$) has been built as a control grid and preliminary RANS simulations are em-
CHAPTER 6. FUTURE WORK

Figure 6.4: RANS mesh for annulus.

Figure 6.5: Inlet velocity conditions as obtained from $k - \varepsilon$ and $k - \omega$ (SST) models.
The \( k - \omega \) (SST) model is employed to predict the flow and initial conditions are prescribed from the results of the aforementioned pipe and annulus simulations.

Figure 6.7 shows the fluid velocity and figures 6.8 and 6.9 show the details of the two stagnation points that divide the flow into three distinct regions and the intermediate recirculation zone.

Figure 6.10, 6.11 and 6.12 show the current results in comparison to those employed to extract the integral lengthscale, based on which an LES grid could be built. Figure 6.6 shows the orientation of the blocks and Table 6.2 enlists the mesh refinement for each block.

Table 6.2: Mesh refinement details for block structured grid.

<table>
<thead>
<tr>
<th>Block</th>
<th>( x_{\text{min}} )</th>
<th>( x_{\text{max}} )</th>
<th>( N_x )</th>
<th>( z_{\text{min}} )</th>
<th>( z_{\text{max}} )</th>
<th>( N_z )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Block 1</td>
<td>0</td>
<td>10</td>
<td>40</td>
<td>0</td>
<td>1500</td>
<td>500</td>
</tr>
<tr>
<td>Block 2</td>
<td>10</td>
<td>75</td>
<td>260</td>
<td>0</td>
<td>500</td>
<td>125</td>
</tr>
<tr>
<td>Block 3</td>
<td>75</td>
<td>150</td>
<td>300</td>
<td>0</td>
<td>500</td>
<td>125</td>
</tr>
<tr>
<td>Block 4</td>
<td>10</td>
<td>100</td>
<td>200</td>
<td>500</td>
<td>1500</td>
<td>125</td>
</tr>
<tr>
<td>Block 5</td>
<td>100</td>
<td>150</td>
<td>50</td>
<td>500</td>
<td>1500</td>
<td>125</td>
</tr>
</tbody>
</table>
CHAPTER 6. FUTURE WORK

Figure 6.7: Fluid velocity (m/s) in the domain.

Figure 6.8: Zoom on fluid velocity (m/s) near inlet showing stagnation points.
available from the simulations of Berrouk [2007] and Riber [2007].

The variation of the turbulent energy $k$ and the turbulent dissipation $\varepsilon$ calculated from the $k - \omega$ simulation as $\varepsilon = c_\mu k \omega$ with $c_\mu = 0.09$ across the flow domain are shown in figures 6.13 and 6.14.

The turbulent energy and turbulent dissipation facilitate the estimation of the integral lengthscale as $k^{1.5} \varepsilon^{-1}$. Figure 6.15 shows the variation of this estimated integral lengthscale. It can be seen that it varies from nearly zero in some regions to more than 100 mm (or 66% of the combustor radius) in some other regions. This observation implies that an unstructured grid with very high range of cell dimensions could be employed to predict the flow.

Figure 6.16 shows the three grids employed by Riber [2007] in comparison with the obtained integral lengthscale variation in the domain. A grid based on the lengthscale criteria would be different from the grids shown, chiefly as the shear layer of the annular jet can be seen to extend to a considerable distance from the inlet.
CHAPTER 6. FUTURE WORK

Figure 6.10: Velocity distribution obtained with the current simulation (a) in comparison to that of Berrouk [2007] (b).
Figure 6.11: Axial fluid velocity profile obtained (a) in comparison to that of Berrouk [2007] (b).
Figure 6.12: Axial velocity as obtained with the current simulation result (a) in comparison to that of Riber [2007] (b). The black lines indicate the isocontours of zero axial velocity.
CHAPTER 6. FUTURE WORK

Figure 6.13: Turbulent energy ($m^2/s^2$).

Figure 6.14: Turbulent dissipation ($m^2/s^3$).
6.1.2 Further work

The same control grid will be used along with Reynolds Stress model in order and the integral scale will be similarly extracted. The results will be compared to those available from experimental data in order to estimate the reliability of the RANS results.

An LES grid will be made according to the RANS predicted length scales and compared to that prescribed from available experimental data, to get an estimate of the uncertainty involved in extracting the required length scale from RANS results. This will form the basis of a set of guidelines to build an LES mesh from RANS results.

A coarse LES on the control grid will enable a comparison with results obtained with LES employing the grid based on the prescribed length scale.
Figure 6.16: Grids employed by Riber [2007] in comparison to the variation of the integral lengthscale in the domain.
6.2 Test case 2: Cylinder in cross flow

The second test case is selected as a cylinder in cross flow, again a widely researched test case. It is a classic fluid mechanics problem involving vortex shedding, as outlined in figure 6.17.

Again, an approach similar to that for the confined jet test case will be employed. The set of guidelines will be followed to build an LES mesh from a precursor RANS calculation. LES results will then be analysed and the guidelines will be modified if required.

6.3 Industrial test case

Based on the experience of the two test cases, solution of an industrial flow problem will be attempted. The exact problem specification and set up is yet to be planned. The set of guidelines from the two test cases will be followed and its industrial viability will be confirmed.
Bibliography


