Grid Adaptation for Large Eddy Simulation Using Feature-Based and Goal-Oriented Error Estimators

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Abstract

Grid adaptation for Large Eddy Simulation (LES) is a non-trivial problem. The challenge of error estimation for grid adaptation in LES relies on two aspects. First, the source of error in LES shows the inherent coupling of the modeling and numerical errors, and the numerical dissipation plays an important contribution to the total error in LES through an effective modeled turbulent kinetic energy (TKE) and is difficult to estimate. Second, LES equations represent a chaotic system for which many promising error estimators cannot be applied, including the traditional goal-oriented error estimator due to the tremendous computational and storage costs as well as the instability of the adjoint system for long time backward time integration. In this thesis, solutions are proposed for both above-mentioned problems.

In the first part of the thesis, the sources of error in LES are studied in detail. Following the work of Schranner et al. [89], a novel approach to estimate the numerical dissipation of the turbulent kinetic energy (TKE-based approach) equations is proposed. The presented approach allows the computation of the local numerical dissipation for arbitrary curvilinear grids through a post-processing procedure. This method, as well as empirical and kinetic-energy-based [13, 97] approaches (KE-based approach), are employed to estimate the inherent numerical TKE. We incorporate the numerical TKE to evaluate an effective eddy viscosity, an effective Kolmogorov length scale, and an effective TKE to build a family of Index Quality (IQ) based error estimators. The proposed IQ based estimators are then assessed and utilized to show their effectiveness through an application of grid adaptation for the periodic hill test case and transitional flow over the SD 7003
airfoil. Numerical results are validated through a comparison against reference LES and experimental data. Flow over the adapted grids appears better able to capture pertinent flow features and integrated functions, such as the lift and drag coefficients.

In the second part of the thesis, we propose two approximation methods to derive a single-solve adjoint system for statistically steady chaotic problems. The first approximation leads to an adjoint system based on the time-averaged Jacobian and the sensitivity of the functional; while, the second approximation is based on converting the LES flow solution to a Reynolds-averaged Navier-Stokes (RANS)-type steady flow solution, on which the steady adjoint approach could be applied. The approaches are further applied to derive an adjoint-based error estimator for LES. The error estimator was validated using the SD7003 airfoil case. Tests were carried out for two different Reynolds numbers and angles of attack on coarse, fine, and adapted grids. Numerical results were validated through a comparison against reference LES and experimental data and it was shown that the adjoint-based adapted grids lead to fast convergence of the prediction of the functional as well as the capture of pertinent flow structures compared to feature-based and manually adapted grids.
L’adaptation de maillage pour la simulation de grands tourbillons (LES) est un problème non trivial. Le défi de l’estimation des erreurs pour l’adaptation de maillage dans LES repose sur deux aspects. Premièrement, la source d’erreur dans LES inclut le couplage inhérent de l’erreur de modélisation et de l’erreur numérique, et la dissipation numérique joue une contribution importante à l’erreur totale dans LES puisqu’elle change l’énergie cinétique turbulente capturée (TKE) et son impact est difficile à estimer. Deuxièmement, les équations LES représentent un système chaotique pour lequel de nombreux estimateurs d’erreur prometteurs ne peuvent pas être appliqués, y compris l’estimateur d’erreur traditionnel basé sur un objectif, également appelé l’estimateur d’erreur basé sur l’adjoint, en raison des coûts de calcul et de mémoire énorme ainsi que de l’instabilité du système adjoint pour une intégration dans le temps en arrière à long terme. Dans cette thèse, des solutions sont proposées pour les deux problèmes mentionnés ci-dessus.

Dans la première partie de la thèse, les sources d’erreur en LES sont étudiées en détail. Suite aux travaux de Schranner et al. [89], une nouvelle approche pour estimer la dissipation numérique des équations d’énergie cinétique turbulente (l’approche basée sur TKE) est proposée. L’approche présentée permet le calcul de la dissipation numérique locale pour des maillages curvilinéaires arbitraires à travers une procédure de post-traitement. Cette méthode, ainsi que l’approche empirique et l’approche basée sur l’énergie cinétique [13, 97] (l’approche basée sur KE), sont utilisées pour estimer la TKE numérique inhérente. Nous incorporons le TKE numérique pour évaluer une viscosité de tourbillon effectif, une échelle de longueur de Kolmogorov effectif et une TKE effectif pour construire une famille
d’estimateurs d’erreur basés sur un index de qualité (IQ). Les estimateurs proposés basés sur le IQ sont ensuite évalués et utilisés pour montrer leur efficacité via une application de l’adaptation de maillage pour le cas de test de colline périodique et l’écoulement de transition sur le profil aérodynamique SD 7003. Les résultats numériques sont validés par une comparaison avec les données expérimentales et numériques de références. Les maillages adaptés sont capables de mieux capturer les caractéristiques d’écoulement pertinentes et les fonctions intégrées, telles que les coefficients de portance et de traînée.

Dans la deuxième partie de la thèse, nous proposons deux méthodes d’approximation pour dériver un système adjoint à résolution unique pour des problèmes chaotiques statistiquement stables. La première approximation conduit à un système adjoint basé sur le Jacobien moyen en temps et la sensibilité de la fonctionnelle; tandis que la deuxième approximation est basée sur la conversion de la solution d’écoulement instable LES en une solution d’écoulement stable de type RANS, sur laquelle l’approche adjointe régulière pourrait être appliquée. Les approches sont ensuite appliquées pour dériver un estimateur d’erreur basé sur l’adjoint pour LES. L’estimateur d’erreur est utilisé sur l’écoulement de transition sur le profil aérodynamique SD 7003. Des tests ont été réalisés pour deux nombres de Reynolds et deux angles d’attaque différents sur le maillage grossière, fine et les maillages adaptés. Les résultats numériques sont validés par une comparaison avec les données expérimentales et numériques de références. Il est démontré que les maillages adaptés basées sur l’adjoint conduisent à une convergence rapide de la prédiction de la fonctionnelle ainsi qu’à la capture des structures d’écoulement pertinentes comparé aux maillages adaptés basées sur les caractéristiques ou adaptées manuellement.
Nomenclature

Scalars

(′) Fluctuation value
(−) Time-averaged value
(−') Resolved value with filtering operation
α Angle of attack
Δn+ Dimensionless wall distance
Δt Time step
Δ Filter size
εn Numerical dissipation
η Kolmogorov length scale
γ Specific heat ratio
μ Dynamic viscosity coefficient
ν Kinematic viscosity
νt Eddy viscosity
ω Time frequency
$\Omega_H$  Coarse grid

$\Omega_h$  Fine grid

$\rho$  Density

$C_d$  Drag coefficient

$C_l$  Lift coefficient

$C_p$  Pressure coefficient

$E$  Specific total energy

$e$  Specific internal energy

$h$  Grid cell size

$IQ$  Index Quality error estimator

$J$  Objective function

$k$  Turbulent kinetic energy

$k_t$  Thermal conductivity coefficient

$k_{mod}$  Modeled turbulent kinetic energy

$k_{num}$  Numerical turbulent kinetic energy

$k_{res}$  Resolved turbulent kinetic energy

$p$  Pressure

$Pr$  Prandtl number

$Re$  Reynolds number

$u$  Velocity
Vectors and Matrices

$\psi$  Adjoint solution vector

$F_d$  Artificial dissipation flux vector in physical space

$f_d$  Discretized artificial dissipation flux vector

$F_V$  Viscous flux vector in physical space

$f_V$  Discretized viscous flux vector

$F$  Convective flux vector in physical space

$f$  Discretized convective flux vector

$I$  Identity matrix

$I_h^H$  Coarse to fine prolongation operator

$k$  Spatial wave number vector

$R$  Steady residual vector

$R^*$  Unsteady residual vector

$u_h^H$  Flow solution projected from coarse to fine grid

$u_H$  Flow solution on coarse grid

$u_h$  Flow solution on fine grid

$u$  Velocity vector

$W$  Conservative state variable vector
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Chapter 1

Introduction

There are multitude of approaches in CFD to model and capture turbulence. Direct Numerical Simulation (DNS), for example, resolves all scales down to the grid scale. However, since the range increases rapidly with Reynolds number, the computational cost of DNS limits its current application to low-Reynolds number flows over flat-plate type geometries, precluding industrially relevant problems. In industry, the Reynolds-averaged Navier-Stokes (RANS) method is the default approach to modeling turbulent flow. By using the Reynolds decomposition, the RANS method provides an approximation to the time-averaged solutions and models the influence of all scales of turbulence motion. Despite its widespread use in industry, RANS often fails to capture unsteady flow physics accurately such as transitional flows and turbulent smooth-body separation. This is due in large part to the lack of a clear separation of scales between the time scales associated with the mean flow variation and the turbulent fluctuations.

Large Eddy Simulation (LES) has thus emerged as an alternative approach to provide a compromise between computational expense and the extent to which scales are resolved. In LES, a filter is employed for the state variables in space in order to separate the large and small scales. The unsteady large scales are captured while the unresolved small scales are modeled. Two filtering processes, namely implicit and explicit filtering, have been developed by the CFD community in the past two decades. When using an
integral-based finite-volume discretization, if a built-in filter (commonly of the grid cell size [25]) is implicitly applied [25, 61] with no explicit implementation of a filtering process, then the approach is deemed implicit filtering. Unlike implicit filtering, explicit filtering techniques are applied directly to the Navier-Stokes (NS) equation or only on the non-linear terms as an independent filter, whose width is fixed manually throughout the grid and decoupled with the grid cell size. As a consequence, a grid independent LES is achieved. The advantages and disadvantages of both techniques have been exclusively studied [8, 10, 24, 25, 61, 104] and is not the main focus of this thesis. To date implicit filtering has generally been adopted by commercial CFD softwares for industrial problems thanks to its flexibility and simplicity.

Although LES is less computationally expensive compared to DNS, as the Reynolds number of the flow increases, the range of scales to be resolved also increase, which is especially true in the near-wall region where the length scales are much smaller than the boundary layer thickness ($\eta \ll \delta$, typically $\delta^3 \sim 2500\Delta_x\Delta_y\Delta_z$ for wall-resolved LES [18]). The immense size of the grid is far beyond the computational capacity of present high-performance computers (HPC). Hence it is crucial to wisely refine the computational grid in critical regions in order to minimize error as well as to keep the computational cost affordable. Manual grid generation of complex geometries is typically a very time-consuming process and does not guarantee efficient use of computational resources, nor can it ensure that the final grid would be adequate [28]. Automatic grid adaptation provides a data-driven approach to efficiently target the most critical regions for optimal use of the computational resource.

The potential for industrial application of automatic grid adaptation for LES is significant. Recent years have seen an increase in the implementation of hybrid LES/RANS approaches in commercial software for industrial cases such as detached eddy simulation (DES) [95, 96], the partially averaged Navier-Stokes (PANS) method [40], and the scale adaptive simulation (SAS) [67]. With the continuous development of affordable computational power and the availability of massively parallel computing architecture, LES will
eventually become the main computational analysis tool for practical engineering problems in the foreseeable future. However, the architecture of LES models demands mesh generation and CFD engineers to understand thoroughly the flow physics, especially the various length scales involved in the numerical and physical models, such that LES users without significant experience and knowledge cannot obtain results with the level of solution fidelity that can be expected. Automatic grid adaptation for LES will allow future CFD users with little experience to perform LES simulations using reasonable and ready-to-use grids.

The automatic grid adaptation process is typically based on an error estimator, which is essential in the adaptation process since it targets the regions to refine or to coarsen. However, it is not obvious how to evaluate the local error in LES, as both grid resolution and model accuracy play an equally important role nor are the sources of error in LES mutually exclusive.

1.1 Sources of Error in LES

LES intends to resolve the large scales while models the small via an SGS model. Large-scale motions contain a majority of the kinetic energy and are important in the dynamics of the flow, while small scales are isotropic in nature and comprise a small aspect of the turbulent kinetic energy. A commonly accepted concept [17,38,111] to define the total error is to split the error in LES into a numerical error, $\epsilon_{\text{num}}$, defined as the difference between a fine and coarse grid LES, and a modeling error, $\epsilon_{\text{mod}}$ which represents the departure of the fine grid LES from a filtered [17] or unfiltered [68] DNS result. Assuming that the errors arising from the filtering and the numerical discretization are unrelated, we can represent the total error for an arbitrary variable $u$ as,

$$\epsilon_{\text{tot}} = \epsilon_{\text{num}} + \epsilon_{\text{mod}} = u_{\text{DNS}} - u_{\text{LES}},$$

(1.1)
Figure 1.1: Statistic $Q^m$ versus length scale $l$, $Q^m_0$ is the DNS limit as $\Delta$ tends to zero and $Q^m_I$ is the intermediate asymptote.

where $\epsilon_{\text{num}} = u_{\text{fine LES}} - u_{\text{LES}}$ and $\epsilon_{\text{mod}} = u_{\text{DNS}} - u_{\text{fine LES}}$. In the context of explicit filtering, through the definitions of the filtering width and the grid size, the two error contributions can be dissociated to achieve grid independent solutions. As is shown by Pope [78], the ratio between the grid cell size and the filter width $r = h/\Delta$ is an indicator of the amount of numerical error to modeling error. For every model used, there exists an “optimal” value of $h$, in terms of accuracy and computational cost. It is preferred that the filter width $\Delta$ should be set in the inertial subrange so that the SGS model could be uniformly designed only using the filter width $\Delta$ as the length scale. Pope [78] proposed a conceptual way to evaluate the quality of LES based on the filter width. Assume that we intentionally form a statistic $Q$ of the velocity field $U(X,t)$, which has contributions from both the energy-containing and dissipative ranges but has little change in the inertial subrange (between $l_{DI}$ and $l_{EI}$ in Fig. 1.1), such that $Q$ shows an intermediate asymptote when drawn against the length scale as shown in Fig. 1.1. LES is able to estimate $Q$ by an approximation $Q^m$ with the filtered equation. Clearly, the approximate statistic $Q^m$ depends on the filter width $\Delta$. For an optimal LES, whose filter width $\Delta$ is in the inertial
subrange, the approximate statistic $Q^m$ should catch the intermediate asymptote of $Q$ and is locally independent of $\Delta$. Pope proposed to change $\Delta$ locally and examine if the captured $Q^m$ changes with $\Delta$ to verify if $\Delta$ is well set into the inertial subrange. However, this criterion is difficult to verify since: first, the construction of such a statistic is not obvious; second, the local change of $\Delta$ and the relaunch of the same simulation is very time consuming; third, for cases with moderate Reynolds numbers the range for the intermediate asymptote is unclear; fourth and the most important, in the widely used implicit filtering, the common practice of using the grid size within the SGS model strongly couples the numerical and modeling errors and renders grid independence intractable, such that the study of $Q^m$ versus $\Delta$ independent of $h$ is impossible. Pope [78] proposed an alternate criterion widely accepted in the community, that a “good” LES approach should resolve at least 80% of the total turbulent kinetic energy. Hence the capture of sufficient turbulent kinetic energy is an important criterion for mesh adaptation for LES. In implicit filtered LES, the filter width $\Delta$ is directly controlled by the grid cell size $h$, and grid refinement not only leads to a reduction of the truncation error in the numerical discretization and the capture of smaller scales but modifies the inherent dissipation of the SGS model. If we are to further organize the sub-contributors to the numerical error into dissipation, dispersion, and aliasing; then the primary contributor is dissipation, as noted by Celik et al. [17], as it alters the apparent Reynolds number of the flow. The assessment of the loss of the captured TKE due to modeling error and numerical dissipation is essential for designing a proper feature-based error estimator for implicitly filtered LES.

### 1.2 Error Estimators in Computational Fluid Dynamics

In this section we focus on the discussion of existing error estimators in CFD from a broad class of approaches. Generally, error estimators for flow simulations fall within three classes: feature- [31, 54, 56, 57, 83, 114], residual- [16, 76] and output-based error estimators [43, 82, 106–108].
Feature-based estimators detect large solution gradients or related variables in the flow field and assume that regions with large and diverse flow features contain a larger fraction of numerical errors, among which the jump indicator \[63\] is the simplest, which associates large errors with the jump of variables such as the Mach number, density or entropy within an element or along an edge. More advanced feature-based estimators involve more sophisticated flow variables, such as the local resolved velocity magnitude \[99\] and percentage of local resolved TKE \[14, 53\], and have been successfully applied for LES \[31, 54, 56, 57, 83, 114\]. Since the error estimation is generally based on post-processing of the flow solution, the approach is advantageous for its portability and low computational cost and it could be easily extended to arbitrary flow solvers. However, the performance of the approach depends on the design of the “feature-based indicator”; where, it has been shown to be case-dependant \[2,59\]. In the case of LES, the construction of a proper flow feature as an error indicator is more challenging than its RANS counterpart since it demands proper consideration of both modeling and numerical errors. Generally, the approach is proven to be less effective for complex cases \[59\]. First, the assumption that regions of important flow features are related to large errors is not always true \[59\], and this procedure may even lead to incorrect results \[106\] for some cases. Second, a feature-based approach would refine in regions that may not contribute towards an accurate integral quantity and hence would require greater computational resources compared to an output-based approach \[2, 59, 75\]. For instance, it is observed in our numerical tests as demonstrated in this thesis that the wake region of an airfoil case could be overly refined due to high turbulence, but may only lead to limited improvement in the total drag estimation.

Residual-based indicators identify regions of the flow where the solution does not satisfy the governing PDEs at a given tolerance by quantifying the norm of the residual. The approach is generally based on truncation error (TE) estimation. One example of a residual estimation approach is Richardson extrapolation methods \[16,76\], which provide for an accurate estimation when the grid size is within the asymptotic range (when the
grids are sufficiently fine). However, it becomes inaccurate if the studied grids are not adequately fine. In addition, the approach requires the computation of an approximated solution on multiple levels of grids, thus it does not offer a cost effective way for three-dimensional industrial applications. Another more practical residual-based approach is based on $\tau$-estimation [8] as it does not require the solution on a secondary grid, where the local truncation error $\tau$ on a coarse grid is approximated using a fine-to-coarse operator, which projects the fine grid solution and residual to the coarse grid. The projected solution and residual are then used to estimate the local truncation error through a defect correction approach [29, 30]. The technique is closely linked to the forcing term in the full approximation storage (FAS) approach of the multigrid technique [8, 66]. Another single-grid residual-based approach to evaluate the truncation error is based on the error transport equation (ETE) [15, 92], which provides for a more accurate estimation by taking into account the transport of truncation error through the computational domain. This residual-based error estimator is generally inexpensive and effective for simple and low-dimensional flows but does not perform well for three-dimensional flows [33, 47, 116].

Today the most popular approach is the output-based adaptation, which is based on the duality concept, where an adjoint of the primal differential equations is formulated. The solution of the dual problem provides the sensitivity information of a functional output, such as the lift or drag coefficient, on the primal solution. The local error is then a dot product of the dual solution and the residual of the flow or primal solution. The dual-weighted residual provides the ability to target cells that not necessarily have high residuals but those that have a direct influence on the desired output. Since specific key outputs are targeted for grid adaptation and error estimators are derived for the outputs, the approach has generated much interest within the industrial community. It originates from optimal control theory and was first used in aerospace for aerodynamic design optimization by Jameson [48] for inviscid compressible flow. The approach was further extended for viscous compressible flow by Jameson et al. [50] and for incompressible turbulent viscous flows by Cowles and Martinelli [21]. Becker and Rannacher [4] outlined

However, the extension of the adjoint-based approach for unsteady flows is much more challenging than its steady counterparts. The exact adjoint-based error estimation approach was derived for unsteady flows [64,70–72], but the method relies on storing the flow solution either on a storage device or the compute-node’s memory at each time step and the adjoint solver retrieves the unsteady flow solution and performs a backward integration in time. The primary disadvantage of this procedure is the large storage requirements for the unsteady flow solutions and the large computational cost due to the evaluation of the unsteady adjoint equations at each time step. Belme [5,6] proposed an output-based adaptation approach for unsteady flows based on performing internal iterations within the time sub-intervals. The approach solves the unsteady flow in the entire time interval, inside of which a certain number of checkpoints are set where the flow information is stored. Then the spatial error is evaluated through the solution of the unsteady adjoint equations at the specified checkpoints and an adapted grid is produced at each time interval. The method was tested for both inviscid and viscous flows. However, the approach still relies on backward integration in time for solving adjoint equations and is computationally costly. In an attempt to include both the grid size and the time step within the adaptation process, Luo and Fidkowski [62] proposed an output-based space-time adaptation approach for unsteady flows which regards the temporal domain as an additional dimension and adapts the grid size and the time step for the complete simulation. The approach was demonstrated on a two-dimensional convection-diffusion-reaction problem and a two-dimensional flow over an airfoil.
1.3 Error Estimators for Large Eddy Simulation

In this section, we focus on the application of the existing feature- and adjoint-based error estimators for LES. Most of the existing [31, 46, 54, 56, 57, 83, 114] LES error estimators are based on a feature-based error estimation depending on the construction of a parameter to estimate local errors, of which the strengths and drawbacks are discussed in the current section. An attempt to apply the adjoint-based error estimation on a chaotic system is also briefly discussed.

1.3.1 Feature-based error estimator

Designing a proper feature-based error estimator is not straightforward for LES, since it relies on constructing a local error indicator to quantify both sources of error mentioned in section 1.1. The challenge of separating numerical from modeling errors further confounds the problem in creating a general framework to develop error estimators. Existing error estimators and grid adaptation procedures for RANS solvers could serve as references [46] but cannot be directly applied to LES due to the nature of the turbulence model. Despite the number of publications devoted to the assessment of LES quality [31, 54, 56, 57, 83, 114], few of them could be directly applied to grid adaptation for practical LES applications, due to the following limitations:

1. Different from RANS, where the grid size mainly affects the discretization error; in LES, both modeling and numerical errors are implicitly dependent on each other and are non-trivial to estimate;

2. LES is intrinsically unsteady and chaotic, such that the error estimators should include some averaging process in space and/or time;

3. Different from detail LES quality assessment, grid convergence or sensitivity study which depend on multiple level grid solutions, error estimation for LES grid adaptation should only allow for single-grid estimators for practical reasons.
Geurts and Frohlich proposed the activity parameter [37] for LES quality assessment based on the estimation of turbulent and viscous dissipation. Celik et al. [14, 17] introduced a family of Index Qualities for LES error estimation, based on the effective Kolmogorov scale $\eta_{\text{eff}}$ or the eddy viscosity $\nu_{\text{eff}}$ which incorporates the contribution from the SGS model and the numerical dissipation. The estimator was extended using the proportion of resolved to total TKE based on Pope’s suggestion [77] that a “good” LES approach should resolve at least 80% of the total TKE. Instead of using the proportion of resolved TKE, Antepara et al. [1] used the residual velocity magnitude (without scaling) as an error indicator. In the approaches above, there is at least one parameter [114] which requires an estimation based on empirical equations. For instance, the Index Quality of Celik et al. [14, 17] relies on an empirical estimation of the numerical TKE for single grid estimators. In addition, the Index Quality based on $\eta_{\text{eff}}$ and $\nu_{\text{eff}}$ call for proper tuning of coefficients to shape the Index Quality curve such that a value of 0.8 corresponds to a sufficient LES grid. Lastly, in [1], grid refinement was initiated when the local residual velocity magnitude reaches a threshold that depends on a user-defined averaging function and case-dependent constants.

To avoid the use of empirical equations to estimate the amount of numerical dissipation, multiple grid estimates were introduced, where Celik and Karatekin [16] proposed a Richardson extrapolation-based approach. Klein [56] extended the Richardson extrapolation method of [16] using multiple grids to evaluate the Index Quality, where he assumed that both modeling and numerical errors for implicit filtering can be combined and represented as a unique function of grid size. The multiple grid Index Quality approach was further extended in [31, 114] to separate the modeling and numerical errors, in addition to the coupling error through systematic independent grid refinements and model variations. However neither single nor multiple grid estimators provided for a directional approach to adapt the filter or the grid size. Toosi and Larsson [99–101] proposed a small energy density indicator depending on the residual velocity magnitude which included directional information. A second anisotropic test filter [99] is then applied in the post-
processing stage to estimate the directional error to study the solution sensitivity to a change in filter size. However, the approach is based on the assumption that the application of a larger test filter in post-processing is similar to the application of a larger filter during LES.

The quality of the error estimator hinges on an appropriate estimation of the inherent discretization and modeling errors, regardless of the LES approach. At present, multiple grid estimators do not offer a cost effective approach to provide an accurate estimate of both the modeling and numerical errors. The development of an efficient single-grid estimator relies on the study of crucial flow features to quantify the impact of numerical dissipation. Domaradzki et al. [26] proposed an approach to evaluate the numerical dissipation of kinetic energy in implicit LES in spectral space. The evolution of kinetic energy is crucial for accurate simulations of flow [49], where there is an energy cascade between the different eddy scales. Currently, kinetic energy preserving schemes [49, 89] have contributed towards this objective; however, the rationale proposed by Domaradzki et al. [26] still allows for a quantification and perhaps further refines the estimate of numerical dissipation present in the flow. The approach was extended to the physical space by Schranner et al. [89], where the authors employed the numerical dissipation of the kinetic energy equation as an LES quality assessment criterion and presented results for the Taylor-Green vortex. Castiglioni and Domaradzki [12] confirmed the findings of [89] for a realistic flow over a NACA0012 airfoil at a Mach number of 0.4 and Reynolds number 50,000. However, the authors [12] highlighted a limitation of the approach, where negative numerical dissipation was observed in regions of laminar flow with weak velocity gradients. Nevertheless, Cadieux et al. [11] further promoted the approach for explicit LES and Sun and Domaradzki [97] for adaptive implicit filtering; where the authors performed adaptive grid refinement using a block-based ratio of the numerical and physical dissipation rates as a criterion.
1.3.2 Adjoint-based error estimator

Adjoint-based grid adaptation has established itself [43, 82, 84] as the preeminent approach for RANS simulations over complex geometries. Its strength lies in its ability to adapt grids to improve the accuracy of integrated functions such as the lift or drag coefficient over an aerodynamic surface. However, existing adjoint-based approaches have encountered challenges for LES. The following are some of the primary obstacles:

1. LES requires very large computational grids and small time steps, thus the storage and computational costs for the backward integration in time required to solve the adjoint system of equations become intractable;

2. LES is intrinsically chaotic and the unsteady adjoint equations for chaotic systems have been demonstrated to diverge exponentially for long-time integration [101, 113].

A possible way to overcome the above-mentioned challenges is to propose a single-solve adjoint system based on the solution of time-averaged flow variables statistics. The idea presents the following advantages: first, it avoids the storage and backward time integration through a single solve process; and second, the temporal averaging removes the transient behavior and hence implicitly smooths the solution and allows for a stable adjoint system of equations. An attempt to follow the idea and extend the adjoint method for chaotic systems using a single solve adjoint equation was proposed by Larsson [58]. The author derives an adjoint system based on the time-averaged and fluctuation terms, yielding two single adjoint systems of equations. Instead of the standard approach to compute the local error estimate using an inner product of the dual solution and the residual at a finer grid level, Larsson [58] introduces a residual model to establish a relationship between the grid spacing and the local error sources; where the latter represents the difference of the fine and coarse grid residuals of the time-averaged and variance equations. The promising approach was applied to a one-dimensional Kuramoto-Sivashinsky...
equation; however, the extension to the three dimensional Navier-Stokes equation is not straightforward.

1.4 Motivations and Contributions

The primary objective of this thesis is to develop novel reliable and practical feature-based and adjoint-based error estimators for grid adaptation for LES with the in-house code SYN3D of the Computational Aerodynamics Group at McGill University. The research objective can be realized through three phases.

In the first phase, the work focuses on introducing an appropriate data structure within the code to allow for an efficient means to adapt the computational grid. The introduction of new control volumes through the splitting of existing cells will require a new entry into the data structure. Here, we choose to use an octree data structure for its efficient use of memory. Moreover, the splitting of the control volume introduces subfaces where cells may share a face with more than a single adjacent control volume.

In the second phase, the research will focus on developing a feature-based error estimator for LES. The work extends [11, 89, 97] to evaluate the numerical dissipation of the turbulent kinetic energy (TKE) equation and employ it within a posteriori single-grid error estimators of Celik et al. [17]. Our extension differs from the original approach in four aspects. First, instead of using the numerical dissipation as the error estimator, we further develop the method to fit within the framework of Index Quality through the derivation of the numerical TKE. Second, unlike the block-based evaluation approach in [97], we employ cell-based error estimation and provide a direct indication of the local truncation error. Third, instead of the kinetic energy equation, we utilize the turbulent kinetic energy equation to estimate the numerical TKE. Fourth, we engage an automatic grid adaptation approach. The proposed error estimators are easily implemented within a post-processing procedure without modifying the underlying flow solver. Our aim is to focus on developing cost effective single grid estimators, provide a comprehensive assess-
ment of them, and demonstrate the effectiveness through a single grid adaptation cycle. A conventional mesh adaptation approach that repeatedly adapts the grid is currently infeasible for LES, and hence our objective is to present an approach where an acceptable but not sufficient grid is improved in a single cycle. Thus our contributions during this phase are:

- First, a novel error estimator that appropriately evaluates the total error, which includes contributions from both numerical and modeling errors in LES for a given grid, especially focusing on the impact of numerical dissipation.

- Second, a comparison of several error estimators on the performance of estimating the grid quality for LES.

- Third, a proposal for a complete pipeline for LES grid adaptation and demonstration of the effectiveness of the LES error estimator in providing significant improvement in engineering interest.

For the last phase, the research will focus on developing a practical approximate adjoint-based error estimator for LES grid adaptation. Our aim is to focus on developing cost effective adjoint-based single grid estimators, provide a complete framework of the approach, and demonstrate the effectiveness through a single grid adaptation cycle. Similar to the second phase, we aim at presenting an approach where an acceptable but not sufficient grid is improved within a single cycle. We focus on statistically steady LES solutions and our contributions during the current phase include:

- First, the proposition of a reliable and practical approximation method to perform a single adjoint solve for statistically steady flows.

- Second, the development of an adjoint-based error estimator for LES based on the approximate adjoint solution.
Third, perform an adjoint-based grid adaptation for LES applications based on the proposed error estimators and compare it against feature-based and manually refined grids.

1.5 Thesis organization

The thesis is organized as follows. Chapter 2 details the methodology for flow simulations; where, section 2.1 describes the governing equations and section 2.2 presents the LES techniques. The flow solver information is detailed in section 2.3, including the numerical schemes and the data structure for grid adaptation. Chapter 3 presents the methodology for feature-based error estimation. The concept for Index Quality is first presented in section 3.1, which serves as the basis for our proposed feature-based error estimator. The novel proposed $IQ_k$-based (feature-based) error estimator is presented in 3.2. Chapter 4 discusses the proposed adjoint-based error estimator for LES. The traditional unsteady adjoint error estimator is derived in section 4.1 with two different approaches. Section 4.2 and 4.3 further show two novel approximation approaches that lead to fast and stable single solve adjoint systems. Section 4.4 details the implementation of the adjoint-based error estimator. Chapter 5 shows the numerical validation of error estimators through a complete cycle of grid adaptation using both feature- and adjoint-based error estimators via the periodic hill and SD7003 airfoil test cases. Lastly, Chapter 6 provides the conclusions and future work.
Chapter 2

Methodology for Flow Simulation

This chapter presents the mathematical models and main features of the flow solver employed in this research. Section 2.1 presents the fundamental governing equations. Section 2.2 details the filtering operation and other techniques employed within the LES framework. Section 2.3 presents the flow solver and the implementation details for grid adaptation; where, subsection 2.3.1 introduces the octree data structure, and subsection 2.3.2 details the evaluation of the convective and viscous fluxes, while subsection 2.3.3 introduces the artificial dissipation flux. Finally subsection 2.3.4 presents the temporal integration.

2.1 Governing equation

The fundamental equations for three-dimensional viscous compressible flow are described by the Navier-Stokes equations, coupled with the continuity and energy equations. When written in the conservative form using Einstein notation we have

$$\frac{\partial W}{\partial t} + \frac{\partial F_i}{\partial x_i} - \frac{\partial F_{vi}}{\partial x_i} = 0,$$

(2.1)
where $W$ is the state variable vector, $F_i$ presents the convective flux and $F_{vi}$ is the viscous flux,

$$W = \begin{bmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho E \end{bmatrix}, \quad F_i = \begin{bmatrix} \rho u_i \\ \rho u_1 u_i + \rho \delta_{i1} \\ \rho u_2 u_i + \rho \delta_{i2} \\ \rho u_3 u_i + \rho \delta_{i3} \\ \rho E u_i + pu_i \end{bmatrix}, \quad F_{vi} = \begin{bmatrix} 0 \\ \tau_{ij} \delta_{i1} \\ \tau_{ij} \delta_{i2} \\ \tau_{ij} \delta_{i3} \\ u_j \tau_{ij} + k_t \frac{\partial T}{\partial x_i} \end{bmatrix},$$

where $\rho, p, T$ and $E$ are the density, pressure, temperature and specific total energy; while, $k_t$ is the thermal conductivity coefficient, $\delta_{ij}$ is the Kronecker delta function, and lastly, $\tau_{ij}$ is the viscous stress tensor. For a Newtonian fluid, $\tau_{ij}$ could be written as

$$\tau_{ij} = \mu \left[ \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \right] \delta_{ij},$$

where $\mu$ is the dynamic viscosity coefficient and $\lambda$ is the bulk viscosity coefficient. Following Stokes’ hypothesis that $\lambda = 2\mu/3$, we can obtain the expression

$$\tau_{ij} = \mu \left[ \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \right] \delta_{ij}.$$  

The ideal gas law is employed to relate the pressure to the density and temperature,

$$p = \rho RT,$$

where $R$ is the specific gas constant. The specific internal energy $e$ can be calculated from

$$e = \frac{1}{\gamma - 1} \frac{p}{\rho},$$
where $\gamma$ is the specific heat ratio and has been taken to be 1.4 for this work. The specific total energy $E$ is the sum of the internal energy and the kinetic energy,

$$E = e + \frac{|u|^2}{2}, \quad (2.7)$$

where $|u|^2$ is the $L^2$ norm of velocity vector, $|u|^2 = u_1^2 + u_2^2 + u_3^2$. Eq. 2.6 and 2.7 lead to an alternative form of the equation of state

$$p = (\gamma - 1)\rho \left[ E - \frac{|u|^2}{2} \right], \quad (2.8)$$

based on which the pressure is derived from the conservative variables. The thermal conductivity coefficient $k_t$ is obtained from

$$k_t = \frac{c_p \mu}{Pr}, \quad (2.9)$$

where $\mu$ is the dynamic viscosity coefficient, $c_p$ is the specific heat capacity and $Pr$ is the Prandtl number.

### 2.2 Filtering and LES

The objective of LES is to employ a spatial filter on the governing equations of motion to separate the large from the small scales and then integrate the spatially filtered governing equations to resolve the largest scales of the flow; while modeling the smaller scales with an appropriate turbulence model.

#### 2.2.1 Filtering Operations

The filtering operation is represented mathematically in physical space as a convolution integral with the kernel function, $G$. The resolved part, $\tilde{\phi}(x, t)$, of a space-time variable
Table 2.1: Three classical filters in one-dimensional space.

<table>
<thead>
<tr>
<th>Filter</th>
<th>Kernel in physical space</th>
<th>Kernel in spectral space</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top-hat</td>
<td>( G(x - r, \Delta) = \begin{cases} \frac{1}{\Delta} &amp; \text{if }</td>
<td>x - r</td>
</tr>
<tr>
<td>Gaussian</td>
<td>( G(x - r, \Delta) = \left( \frac{\sigma}{\Delta^2} \right)^{1/2} \exp\left(-\frac{\sigma(x-r)^2}{\Delta^2}\right) )</td>
<td>( \hat{G}(k) = e^{-\left(k^2\Delta^2/4\sigma\right)} )</td>
</tr>
<tr>
<td>Sharp cutoff</td>
<td>( G(x - r, \Delta) = \frac{\sin(k_c(x-r))}{k_c(x-r)} ), with ( k_c = \pi/\Delta )</td>
<td>( \hat{G}(k) = \begin{cases} 1 &amp; \text{if }</td>
</tr>
</tbody>
</table>

\( \phi(x, t) \) is defined as

\[
\tilde{\phi}(x, t) = \iint G(x - r, \Delta) \phi(r, t) dr \equiv G \ast \phi.
\] (2.10)

We can further study the filtering operation in the spectral space. Based on convolution theorem [79,86], the Fourier transform of a convolution of two functions is the scalar product of their Fourier transforms. The spectrum of the filtered quantity \( \tilde{\phi}(k, \omega) \) of \( \tilde{\phi}(x, t) \) is obtained by the multiplication of the spectrum \( \hat{\phi}(k, \omega) \) of \( \phi(x, t) \) and the transfer function \( \hat{G}(k, \omega) \) of \( G(x, t) \):

\[
\tilde{\phi}(k, \omega) = \hat{\phi}(k, \omega) \hat{G}(k, \omega),
\] (2.11)

where \( k \) is the spatial wave number and \( \omega \) is the time frequency. Three particular convolution filters are often employed and discussed, including the top-hat filter, the Gaussian filter, and the sharp cutoff filter. Their one-dimensional spatial kernel functions are presented in Table 2.1. The filter behavior in physical (kernel function \( G(x) \)) and spectral spaces (kernel function \( \hat{G}(k/k_c) \)) are illustrated in Fig. 2.1. It can be observed that the top-hat filter has a compact support in the physical space, while the sharp cutoff filter has a compact support in the spectral space. The Gaussian filter is non-local in both the spectral and physical spaces. An example of the energy spectrum with and without filtering operations is presented in Fig. 2.2, which demonstrates the difference in the energy spectral behavior in the high wave number region. For LES, the sharp cutoff filter has an advantage in that it perfectly separates the resolved from the modeled part [77]. If the cutoff wave number \( k_c \) is appropriately chosen then the filtered part only contains
Figure 2.1: Kernel function in physical ($G(x)$ on the left) and spectral ($\hat{G}(k/k_c)$ on the right) space of common filters: (a) Top-hat; (b) Gaussian; (c) Sharp cutoff.
isotropic fluctuations and can be perfectly modeled. In reality, the design of the sharp cutoff filter for arbitrary schemes and grid types is a non-trivial task, but the aim should be to separate the scales as clearly as possible.

### 2.2.2 Explicit and Implicit filtering

The filter applied in LES can be either explicit or implicit. The procedure for explicit filtering (for details see [61]) is similar to that of the filtering process for image and signal processing. Generally, governing equations are solved directly on the grid and then the solution or its terms are filtered at each time step. The filter could be applied either to the entire governing equation or only to the non-linear terms, where the latter may introduce high-frequency content but results [8, 24, 61] have demonstrated minimal differences between the approaches. The explicit filtering technique allows active control of the ratio $r = h/\Delta$ between the grid spacing and the filter width, which leads to a control of the ratio between the numerical and modeling error. In practice the explicit filter could be realized in either an analytical [24, 103] or a discrete [24, 45, 61, 65, 86, 103, 105] form. The
use of discrete filters is more common due to a lower computational cost [105]. The general construction rule of explicit discrete filters for homogeneous flow fields was given by Gullbrand [42]. Vasilyev et al. [105] proposed a set of rules for constructing linear discrete filters and a general theory for sharp cut-off filters. However, the linear discrete filter demands a transformation from non-uniform physical grids to uniform computational space, which restricts its application to structured meshes. Other advanced filter construction approaches for unstructured mesh [19, 45, 65, 73] or with high-order features [19, 65] have been proposed. In practice, the implementation of high-order explicit filters on unstructured grids introduces additional challenges compared to structured grids, and the filtering procedure for inhomogeneous flows is not as well-established, such that its application to complex geometries still remains an open question. To this date, explicit filtering techniques are not generally adopted by commercial CFD softwares and are generally not employed for the simulation of complex turbulent flows.

The implicit filtering technique makes use of the computational grids or numerical scheme to implicitly apply a low-pass filter to the governing equations. Initiated by Smagorinsky [94] and Lilly [60] (for more details see [25]), it is shown in [25] that for any integral-based flux reconstruction, one attains an approximation of the top-hat filter kernel. The induced shape and width of the filter are directly controlled by the grid cell size. The implicit filtering technique is widely used thanks to its flexibility and simplicity. In addition, the technique takes full advantage of the numerical grid resolution, where the captured scale is determined by the grid cell size. However, there are disadvantages when compared to explicit filtering. First, there are difficulties in distinguishing between numerical and modeling errors, since the filter width is associated with the local grid cell size and hence the results are dependent on the grid resolution. Second, the presence of aliasing errors, where non-linear terms of the Navier-Stokes equations generate high-frequency components, which alias back as resolved lower frequency solutions and presents themselves as fictitious stresses [61]. Third, the influence of the commutation error, which arises due to the commutation process between the filtering and the differ-
ential operation. The error must be maintained at the same scale as the truncation error of the numerical scheme [61]; however, implicit filters do not ensure direct control of the commutation error.

The advantages and disadvantages of both filtering techniques have been exclusively studied [8, 10, 24, 25, 61, 104] and will not be further discussed. The focus of the current thesis is on the error estimation for implicitly filtered LES, since to date implicit filtering has generally been prevalent for commercial CFD softwares for industrial problems.

2.2.3 SGS Model

For LES to correctly resolve the flow, sub-filtered terms in the Navier-Stokes equation need to be modeled by a subgrid-scale (SGS) model. Alternatively, one could employ an implicit Large Eddy Simulation (ILES) approach, where the numerical scheme itself acts as a dissipation mechanism and hence no SGS model is explicitly included. However, in this work, we chose to include an explicit SGS model since the use of a model would allow us to better distinguish the difference between numerical and modeling errors. The efficacy of the ILES approach and comparisons against classical explicit and implicit filtering techniques with SGS models have been extensively studied and the reader is advised to consult one of the following articles [7, 36, 41, 110, 112].

It should be mentioned that most of the existing work in LES, including the development of SGS models, are devoted to incompressible flows [85], but is often applied directly to low Mach number compressible flows [35] without additional modifications. We employed a wall-adapting local eddy-viscosity turbulence model [74] as the SGS model. Using Einstein notation, the final form of the governing equations for LES can be obtained,

\[
\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial \tilde{u}_i \tilde{u}_j}{\partial x_j} = - \frac{1}{\rho} \frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial \tilde{\tau}_{ij}}{\partial x_j} - \frac{\partial \tilde{\tau}_{ij}^{SGS}}{\partial x_j},
\]

(2.12)

where \(\tilde{u}_i, \tilde{p}, \tilde{T}\) and \(\tilde{\tau}_{ij}\) are the filtered velocity, pressure, temperature and stress tensor, under the filtering operation discussed in section 2.2.1, where the kernel function \(G\) is a
top-hat function and the filter size is assumed to be equal to or proportional to the grid space $h$. The subgrid scale stress tensor is employed to model the unclosed sub-filtered part

$$\tau_{ij}^{SGS} = \tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j.$$  \hfill (2.13)

When an eddy viscosity model is employed, the Boussinesq hypothesis is applied to the subgrid scale stress tensor with the introduction of an eddy viscosity, $\nu_t$,

$$\tau_{ij}^{SGS} = -\nu_t \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right).$$ \hfill (2.14)

A Wall-Adapting Local Eddy-viscosity (WALE) model [74] is adopted for the current research with the following expression for the eddy viscosity

$$\nu_t = \Delta_s^2 \frac{(S^d_{ij} S^d_{ij})^{3/2}}{(S_{ij} \tilde{S}_{ij})^{5/2} + (S^d_{ij} S^d_{ij})^{5/4}},$$ \hfill (2.15)

where

$$\Delta_s = C_w V^{1/3},$$
$$S^d_{ij} = \frac{1}{2} (\tilde{g}^2_{ij} + \tilde{g}^2_{ji}) - \frac{1}{3} \delta_{ij} \tilde{g}^2_{kk},$$
$$\tilde{g}_{ij} = \frac{\partial \tilde{u}_i}{\partial x_j},$$ \hfill (2.16)
$$\tilde{g}^2_{ij} = \tilde{g}_{kk} \tilde{g}_{kj},$$
$$\tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right),$$

and the constant $C_w = 0.325$. The model is based on the commonly held believe that the turbulent eddy viscosity is assumed to be proportional to the resolved velocity gradients and hence the impact of the unresolved scales are to dissipate the larger resolved scales.
2.3 Discretization and Flow Solver

SYN3D is a finite-volume based multi-block structured flow solver developed at the Computational Aerodynamics Group at McGill University. The flow solver is designed for three-dimensional Navier-Stokes equations with the inclusion of various turbulence models including RANS, LES, and hybrid RANS/LES models. Parallelization is enabled through a Message Passing Interface (MPI) standard. The governing equations can be rewritten over the computational domain in semi-discrete form as,

\[ V \frac{\partial W}{\partial t} + R(W) = 0, \]  

(2.17)

where \( V \) is the cell volume and \( R(W) \) is the residual, which is a function of the state variable \( W \), of which the definition is given in Eq. 2.2,

\[ W = [\rho, \rho u_1, \rho u_2, \rho u_3, \rho E]^T. \]  

(2.18)

Note that for implicitly filtered LES, the solved state variable is the filtered value after the application of the built-in filter as discussed in subsection 2.2.2. The residual term \( R(W) \) contains both the convective and dissipative as well as artificial dissipation flux gradients. We employ a cell-centered finite volume method with an artificial dissipation scheme [51] based on a blend of second-and fourth-order differences which result from the sum of additional first-and third-order fluxes. Using the \( i, j, k \) coordinates system and the \( \pm \frac{1}{2} \) notation to indicate the quantity defined at a flux face, the discrete form for the residual at cell \((i, j, k)\) is written as

\[ R(W)_{i,j,k} = f_{i+\frac{1}{2},j,k} - f_{i-\frac{1}{2},j,k} + f_{i,j+\frac{1}{2},k} - f_{i,j-\frac{1}{2},k} + f_{i,j,k+\frac{1}{2}} - f_{i,j,k-\frac{1}{2}} \]
\[ - f_{v,i+\frac{1}{2},j,k} + f_{v,i-\frac{1}{2},j,k} - f_{v,i,j+\frac{1}{2},k} + f_{v,i,j-\frac{1}{2},k} - f_{v,i,j,k+\frac{1}{2}} + f_{v,i,j,k-\frac{1}{2}} \]
\[ - f_{d,i+\frac{1}{2},j,k} + f_{d,i-\frac{1}{2},j,k} - f_{d,i,j+\frac{1}{2},k} + f_{d,i,j-\frac{1}{2},k} - f_{d,i,j,k+\frac{1}{2}} + f_{d,i,j,k-\frac{1}{2}}, \]  

(2.19)
where $f_c, f_v, f_d$ are the convective, viscous and artificial dissipation fluxes at the six faces of cell $(i, j, k)$ and are further elaborated in subsections 2.3.2 and 2.3.3.

### 2.3.1 Octree data structure

In order to achieve grid adaptation, a cell-based octree data structure [55] is incorporated within SYN3D. The data structure keeps the origin $(i, j, k)$ coordinates of the most coarse level (the lowest level) grid cells. The high level cells are appended to the system when coarse cells are targeted for refinement. An additional indexing system is introduced for all level of cells where each cell is identified by a single integer ID. When a parent cell is flagged for refinement, eight children cells are generated and a continuous sequence of memory is allocated, such that only the pointer to the first child is stored in the parent cell. The following information is stored in each cell with cell ID $i$ for the data structure:

- level of the cell in the tree $level[i]$;
- pointer to the parent cell $parent[i]$;
- pointer to the first child $child[i]$;
- pointers to 6 neighbor cells $n[i]$.

We show a two-dimensional illustration of the current data structure in Fig. 2.3 as an example. The coarsest cells (or root cells, e.g. cell 1, 2, or 3) have a level of 0. When identifying the neighbor for a given cell, the system prioritizes the cells on the same level (e.g. left neighbor of cell 15 in Fig. 2.3). If no cells at the same level are found in the neighboring cell, the lower level cell will be regarded as the neighbor (e.g. right neighbor of cell 16 in Fig. 2.3). The identified neighbor cell pointer array (length of 6) is stored inside the current cell. In the code we use an ordering rule for the neighbor cell pointer array as explained here: For cell $i$, $n[i]$ is a list of 6 neighboring cells sharing faces with the cell $i$, identified by $face_{i,n[i]_1...6}$; where

- $face_{i,n[i]_1}$ vs. $face_{i,n[i]_2}$;
Figure 2.3: Illustration of octree structure in two dimensional space.

- $\text{face}_{i,n[i]_3}$ vs. $\text{face}_{i,n[i]_4}$;

- $\text{face}_{i,n[i]_5}$ vs. $\text{face}_{i,n[i]_6}$

are the opposite faces of the hexahedron cell. With the introduction of the octree data structure, Eq. 2.19 becomes

$$R(W)_i = f_{\text{face}_{i,n[i]_2}} - f_{\text{face}_{i,n[i]_1}} + f_{\text{face}_{i,n[i]_4}} - f_{\text{face}_{i,n[i]_3}} + f_{\text{face}_{i,n[i]_6}} - f_{\text{face}_{i,n[i]_5}}$$

$$-f_{v,\text{face}_{i,n[i]_2}} + f_{v,\text{face}_{i,n[i]_1}} - f_{v,\text{face}_{i,n[i]_4}} + f_{v,\text{face}_{i,n[i]_3}} - f_{v,\text{face}_{i,n[i]_6}} + f_{v,\text{face}_{i,n[i]_5}}$$

$$-f_{d,\text{face}_{i,n[i]_2}} + f_{d,\text{face}_{i,n[i]_1}} - f_{d,\text{face}_{i,n[i]_4}} + f_{d,\text{face}_{i,n[i]_3}} - f_{d,\text{face}_{i,n[i]_6}} + f_{d,\text{face}_{i,n[i]_5}}$$

(2.20)

Given a list of refined cells from the error estimator, the parent, child, and neighbor pointers are automatically generated and the ranks are rebalanced for parallel efficiency. In the current flow solver, only geometry variables exist on face and vertices while all flow variables are cell-center based.
2.3.2 Convective and Viscous Fluxes

The cell-centered flow variables are viewed as cell averages and arithmetic averaging is used to approximate the convective and viscous fluxes at the cell boundaries. Thus, the convective and viscous flux at a face has equal contributions from the two cells sharing the face. Both convective and viscous fluxes are evaluated using the metrics of the shared face and state variables based on cell center values. For example, the discrete formulation of the convective and viscous flux on face $f_{a\text{c}\text{e}}_{\text{idx}, n[\text{idx}]_1}$ is written as

$$f_{f_{a\text{c}\text{e}}_{\text{idx}, n[\text{idx}]_1}} = \frac{1}{2} (S_{f_{a\text{c}\text{e}}_{\text{idx}, n[\text{idx}]_1}} F_{\text{idx},i} + S_{f_{a\text{c}\text{e}}_{\text{idx}, n[\text{idx}]_1}} F_{\text{n[\text{idx}]_1,i}}),$$  \hspace{1cm} (2.21)

$$f_{v_{f_{a\text{c}\text{e}}_{\text{idx}, n[\text{idx}]_1}}} = \frac{1}{2} (S_{f_{a\text{c}\text{e}}_{\text{idx}, n[\text{idx}]_1}} F_{v_{\text{idx},i}} + S_{f_{a\text{c}\text{e}}_{\text{idx}, n[\text{idx}]_1}} F_{v_{\text{n[\text{idx}]_1,i}}}),$$

where $F_{\text{idx},i}$, $F_{v_{\text{idx},i}}$, $F_{v_{\text{idx},i}}$ and $F_{v_{\text{n[\text{idx}]_1,i}}}$ are convective and viscous flux contributions from the two neighboring cells, $\text{idx}$ and $n[\text{idx}]_1$, which share the same face $f_{a\text{c}\text{e}}_{\text{idx}, n[\text{idx}]_1}$. Refering to Eq 2.2, we can obtain the expression for the convective and viscous flux vectors for cell $\text{idx}$ as,

$$F_{\text{idx},i} = \begin{bmatrix} (\rho u_1)_{\text{idx}} \\ (\rho u_1)_{\text{idx}} u_{\text{idx},i} + p_{\text{idx}} \delta_{i1} \\ (\rho u_2)_{\text{idx}} u_{\text{idx},i} + p_{\text{idx}} \delta_{i2} \\ (\rho u_3)_{\text{idx}} u_{\text{idx},i} + p_{\text{idx}} \delta_{i3} \\ (\rho E)_{\text{idx}} u_{\text{idx},i} + p_{\text{idx}} u_{\text{idx},i} \end{bmatrix},$$

$$F_{v_{\text{idx},i}} = \begin{bmatrix} 0 \\ \tau_{\text{idx},ij} \delta_{i1} \\ \tau_{\text{idx},ij} \delta_{i2} \\ \tau_{\text{idx},ij} \delta_{i3} \\ u_{\text{idx},j} \tau_{\text{idx},ij} + (k_T \frac{\partial T}{\partial x_i})_{\text{idx}} \end{bmatrix},$$  \hspace{1cm} (2.22)

where $u_{\text{idx},i}$ is the $i$-th dimensional velocity stored at the center of cell $\text{idx}$. The same formula is applied to the other five faces of a cell at $f_{a\text{c}\text{e}}_{\text{idx}, n[\text{idx}]_2,..,6}$ and the scheme leads to a seven-point stencil for the entire convective and viscous flux contribution to the residual of a particular cell. It should be mentioned that as specified in subsection 2.3.1, in the current data structure the defined neighboring cells are always on the same or on a lower level compared to the current cell $\text{idx}$ which stores the pointer $n[i]$. When updating the residual of the current cell $\text{idx}$ on a face, where the neighboring cell is identified with the
same level while having children cells on a higher level, the current face is not updated at the current moment, instead, the flux contribution are calculated from the higher level children cells first and aggregated to obtain the flux contribution to the current cell $idx$.

### 2.3.3 Artificial dissipation

The artificial dissipation scheme used within this project is a blend of adaptive second- and fourth-order differences which result from the sum of additional first- and third-order fluxes. We have employed a scalar dissipation scheme first introduced by Jameson, Schmidt and Turkel [51]. Based on our octree data structure, the discrete formulation of the artificial dissipation flux on $f_{ace idx, n[dx]1}$ is written as

$$f_{d, face idx, n[dx]1} = f_{d, face idx, n[dx]1}^{(2)} + f_{d, face idx, n[dx]1}^{(4)},$$

(2.23)

where

$$f_{d, face idx, n[dx]1}^{(2)} = \nu_{f ace idx, n[dx]1}^{(2)} \Lambda_{f ace idx, n[dx]1} (u_{n[dx]1} - u_{idx}),$$

$$f_{d, face idx, n[dx]1}^{(4)} = \nu_{f ace idx, n[dx]1}^{(4)} \Lambda_{f ace idx, n[dx]1} (u_{n[dx]1} - 3u_{n[dx]1} + 3u_{idx} - u_{n[dx]2}),$$

(2.24)

and the same formula is applied to the other five faces of a cell at $f_{ace idx, n[dx]2...6}$. $\Lambda_{f ace idx, n[dx]1}$ is the spectral radius term while $\nu_{f ace idx, n[dx]1}^{(2)}$ and $\nu_{f ace idx, n[dx]1}^{(4)}$ act as low- and high-order pressure sensors,

$$\nu_{f ace idx, n[dx]1}^{(2)} = \epsilon^{(2)} \max(\sigma_{idx}, \sigma_{n[dx]1}),$$

$$\nu_{f ace idx, n[dx]1}^{(4)} = \max(0, \epsilon^{(4)} - \nu_{f ace idx, n[dx]1}^{(2)}),$$

(2.25)

where

$$\sigma_{idx} = \frac{|p_{n[dx]1} - p_{idx} + p_{n[dx]2}|}{p_{n[dx]1} + p_{idx} + p_{n[dx]2}},$$

(2.26)

and $\epsilon^{(2)}$ and $\epsilon^{(4)}$ are adjustable constants which control the amount of second- and fourth-order artificial dissipation.
Following [52], we used the Isotropic Decaying Turbulence (DIT) [20] test case to properly tune the values of $\epsilon^{(2)}$ and $\epsilon^{(4)}$ for LES in our flow solver. The geometry and an instantaneous velocity contour for the DIT case is shown in Fig. 2.4. The non-dimensional length of the sides is $2\pi$ for all three dimensions. A divergence-free velocity field is used as the initial condition and periodic boundary conditions are used in all directions. The case is widely used as a simple case for turbulence model validation. Its isotropicity and periodicity make it an ideal test case for the initial validation and tuning of constants in a numerical scheme or in a turbulence model. The velocity spectra from both measurement data and numerical data are available at non-dimensional time $T = 42, 98$ and $171$.

As is discussed in subsection 2.2.2, the artificial dissipation directly determines the built-in filter applied to the equations. Following the concept of LES, the ideal numerical dissipation should not contaminate the capture of large scales in the low wave number region, but only dissipate small scales in the high wave number region (as mentioned at the end of subsection 2.2.1), which could be modeled by the SGS model discussed in subsection 2.2.3. Different combinations of $\epsilon^{(2)}$ and $\epsilon^{(4)}$ have been tested and the energy spectra at $T = 98$ are compared and shown in Fig. 2.5. Although the value pairs ($\epsilon^{(2)} = 0.3$, $\epsilon^{(4)} = 0.0$) and ($\epsilon^{(2)} = 0.5$, $\epsilon^{(4)} = 0.0$) seem to capture the energy spectrum, the total removal of the fourth-order dissipation leads to high frequency oscillations and can cause numerical instability for cases with a more complex geometry, as observed for the problems attempted in this thesis. We observe that with a value of $\epsilon^{(2)} = 0.7$ and $\epsilon^{(4)} = 0.04$, the scheme is able to sufficiently resolve the large scales and show a rather sharp drop when the wave number increases to a certain value (at $k \approx 10^2$); while, ensuring stability for the aforementioned cases. The pair of values lead to a clear separation of captured and filtered scales at the cutoff length (at $k_c \approx 10^2$) and thus are adopted for the remaining flow simulations in the current study.
2.3.4 Temporal integration

Time integration is achieved by using a five-stage Runge-Kutta (RK5) method [51]. Multistage schemes advance the solution in a number of stages between the current time $n$
Table 2.2: Coefficient for five-stage Runge-Kutta scheme.

<table>
<thead>
<tr>
<th>stage</th>
<th>α</th>
<th>β</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.25</td>
<td>1.0</td>
</tr>
<tr>
<td>2</td>
<td>0.1667</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>0.375</td>
<td>0.56</td>
</tr>
<tr>
<td>4</td>
<td>0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>5</td>
<td>1.0</td>
<td>0.44</td>
</tr>
</tbody>
</table>

and the next time level $n + 1$,

\[
W^0 = W^n
\]

\[
W^k = W^0 - \alpha_k \Delta t R(W^{k-1}) \quad \text{for} \ k = 1, 2, \cdots, m
\]

\[
W^{n+1} = W^m,
\]

where $m$ is the total number of stages and the residual $R(W^{k-1})$ is evaluated with the solution $W^{k-1}$ of the previous stage. The residual at each stage is defined as,

\[
R^k = R^k_c + R^k_d
\]

where

\[
R^k_c = R_c(W^k),
\]

\[
R^k_d = \beta_k R_d(W^k) + (1 - \beta_k) R_d(W^{k-1}),
\]

where $R^k_c$ includes the contributions from the convective flux and $R^k_d$ includes the contributions from the viscous and artificial dissipations. In this work, the stage coefficients $\alpha$ and $\beta$ used for the five-stage Runge-Kutta scheme is shown in Table. 2.2.

Additional adaptations are implemented for the octree data structure. While each cell update is based on a five-stage Runge-Kutta method mentioned above, the time advancement updates in the whole computational domain are performed for all levels of cells recursively. The time integration follows the process proposed in [55], where the time steps in fine cells (higher level cells) are automatically reduced from that of the parent.
Figure 2.6: Illustration of coarse-fine cell interface update.

cell,

$$\Delta t(l) = 2^{-l} \Delta t,$$

where $\Delta t$ is the time step on the root cell and $l$ the level of the current cell. Assuming the flux evaluation and time advancement procedures using RK5 at level $l$ to be $A(l)$, the operation at level $l$ is

$$O(l) = \begin{cases} O(l+1)O(l+1)A(l); & \text{if } l < l_{\text{max}}; \\ A(l); & \text{if } l = l_{\text{max}}, \end{cases}$$

where $l_{\text{max}}$ is the maximum level of cells among all the descendants of the current root cell.

A two dimensional illustration of the cell update procedure is shown in Fig. 2.3. Suppose the current time $t$ and time step for root/coarsest cell (Cell 1 and Cell 2 in Fig. 2.3) is $\Delta t$. Time advancement updates of the system is executed through two steps: first, flux F1 through F4 are evaluated and fine cells (Cell 11 through 14) are updated with time advancement of $\Delta t/2$; second, flux F1 through F4 are evaluated and Cell 11 through 14, along with Cell 2 are updated at $t + \Delta t$. Cell 1 information is also updated through an averaging of state variables of its children cells (Cell 11 through 14).

The data structure is validated through various in-house benchmark test cases. Fig. 2.7 shows an example of our validation using the ONERA M6 wing [87]. Two refined grids
Figure 2.7: Onera M6 Wing grid (slice view at spanwise location $Z = 0.26b$) generated using octree data structure: (a) coarse, $l_{\text{max}} = 0$; (b) one-level refinement, $l_{\text{max}} = 1$; (c) two-level refinement, $l_{\text{max}} = 2$.

Figure 2.8: $x$-momentum contour for flow over 3D Onera M6 Wing at spanwise location $Z = 0.26b$ with different refinement level: (a) coarse, $l_{\text{max}} = 0$; (b) one-level refinement, $l_{\text{max}} = 1$; (c) two-level refinement, $l_{\text{max}} = 2$.

are generated based on the octree data structure. We target the first eight layers of cells from the wing surface for the first level refinement (as shown in Fig. 2.7 (b)) and the first four layers are further refined with second level cells (as shown in Fig. 2.7 (c)). Fig. 2.8 and 2.9 show the $x$-momentum and pressure contours near the leading edge of the wing at spanwise location $Z = 0.26b$. The pressure coefficient on the wing surface is illustrated in Fig. 2.10 where the pressure distribution converges as the grid is refined. This verifies the implementation of the grid adaptation.
Figure 2.9: Pressure contour for flow over 3D Onera M6 Wing at spanwise location $Z = 0.26b$ with different refinement levels: (a) coarse, $l_{max} = 0$; (b) one-level refinement, $l_{max} = 1$; (c) two-level refinement, $l_{max} = 2$.

Figure 2.10: Pressure coefficient $C_p$ on wing surface at spanwise location $Z = 0.26b$. 
Chapter 3

Methodology for Feature-Based Error Estimation

This chapter studies in detail and extends a family of feature-based error estimators for LES. Section 3.1 presents the existing Index Quality error estimators and details how the effect of numerical dissipation (or numerical TKE) is taken into consideration for the error estimator to quantify both the modeling and numerical errors in LES. Section 3.2 revisits the evaluation of numerical TKE, where in subsection 3.2.1 an approach proposed by Schranner et al. [89] is extended and applied to the Index Quality error estimator. In subsection 3.2.2, a novel approach for the evaluation of the numerical TKE is proposed and presented in the framework of Index Quality error estimators for LES.

3.1 Index Quality family

Index of Quality is a family of error estimators for LES which allows for single-grid error estimation [14] and this concept is adopted in our grid adaptation process. In this section the formulas and the implementation of three classical Index of Quality error estimators are presented.
3.1.1 Index Quality $IQ_\nu$

The Index Quality based on effective eddy viscosity takes the form of

$$IQ_\nu = \frac{1}{1 + \alpha_\nu \left( \frac{\nu_{\text{eff}}}{\nu} \right)^n},$$

(3.1)

where the eddy viscosity $\nu_{\text{eff}}$ incorporates the contribution from the SGS model and the numerical dissipation. The implementation of $IQ_\nu$ can be directly fulfilled by using

$$\nu_{\text{eff}} = \nu_{\text{num}} + \nu_{\text{sgs}},$$

(3.2)

where $\nu_{\text{num}}$ is estimated from

$$\nu_{\text{num}} = \text{sgn}(k_{\text{num}}) C_\nu \Delta \sqrt{\text{abs}(k_{\text{num}})},$$

(3.3)

by analogy to the SGS model formula [115], while $k_{\text{num}}$ is an estimate of the numerical TKE due to numerical dissipation inherent in the discretization of the governing equations. The inclusion of the numerical TKE was proposed by Celik et al. [17] with an empirical formula which will be discussed in section 3.1.4. In section 3.2 we extend the estimator to two novel versions depending on the approach to evaluate $k_{\text{num}}$. The $IQ_\nu$ estimator will target regions where either the SGS eddy viscosity or the numerical eddy viscosity is large compared to the kinematic viscosity $\nu$.

3.1.2 Index Quality $IQ_\eta$

The Index Quality based on the effective Kolmogorov scale is defined as,

$$IQ_\eta = \frac{1}{1 + \alpha_\eta \left( h_{\text{eff}} \right)^m},$$

(3.4)
where the effective Kolmogorov length scale $\eta_{\text{eff}}$ is defined by

$$\eta_{\text{eff}} = \left(\frac{\nu^3}{\epsilon}\right)^{1/4}. \quad (3.5)$$

The dissipation $\epsilon$ is estimated from

$$S = \left(\frac{\epsilon}{\nu_{\text{eff}}}\right)^{1/2}, \quad (3.6)$$

where $S = \sqrt{2S_{ij}S_{ij}}$ is the square root of the double inner product of the mean strain rate tensor $S_{ij}$ and the effective eddy viscosity, $\nu_{\text{eff}}$ is evaluated from Eq. 3.2. Lastly, the grid cell length scale $h$ is given by $h = V^{1/3}$, where $V$ is the volume of the cell and $\alpha_\eta$ and $m$ are empirical constants. The estimator targets regions where the grid size $h$ is large compared to the effective Kolmogorov length scale. The estimator is related to $IQ_\nu$ by involving the same effective eddy viscosity $\nu_{\text{eff}}$, while the $IQ_\eta$ estimator mainly targets regions where the grid cell size is not sufficiently small to resolve flow structures on the scale of the effective Kolmogorov length scale.

### 3.1.3 Index Quality $IQ_k$

The Index Quality was extended using the proportion of resolved to total TKE,

$$IQ_k = \frac{k_{\text{res}}}{k_{\text{res}} + k_{\text{eff}}}, \quad (3.7)$$

where the resolved TKE, $k_{\text{res}}$, is obtained by adding the contribution from the diagonal terms in the Reynolds stress tensor, obtained by subtracting the instantaneous flow field from the time-averaged solution,

$$k_{\text{res}} = \frac{1}{2} \sum_{i=1}^{3} u_i'u_i'. \quad (3.8)$$
with $u'_i = u_i - \bar{u}_i$, where $u_i$ and $\bar{u}_i$ are the instantaneous and time-averaged velocities. For a single-grid approach, $k_{\text{eff}}$ is the sum of the modeled TKE, $k_{\text{sgs}}$, and numerical TKE, $k_{\text{num}}$. The modeled TKE can be derived from the SGS eddy viscosity using the formula

$$k_{\text{sgs}} = \left( \frac{\nu_{\text{sgs}}}{C_{\nu} \Delta} \right)^2. \quad (3.9)$$

The evaluation of $k_{\text{num}}$ is nontrivial and the classical approach relies on an empirical formula [17]. We proposed different formulas for the derivation of $k_{\text{num}}$ which will be presented in section 3.2. The estimator targets regions where an insufficient percentage of TKE is resolved by the flow solver.

The above mentioned Index Quality error estimators follow the same conception and the constants in each formula are tuned [17] such that the value of all IQ-based error estimators are in a comparable range. However, the estimators focus on different scales within the flow field. $IQ_{\nu}$ focuses on the effective eddy viscosity, thus the product of a velocity and length scale in the dissipative range. $IQ_{\eta}$ focuses on the Kolmogorov length scale and the indicator is related to $IQ_{\nu}$ with the inclusion of the local strain rate, $s$, as an additional factor, such that the $IQ_{\eta}$ estimator also targets regions with high strain rate (e.g. the turbulent mixing layer and boundary layer). $IQ_k$ focuses on the resolution of TKE. An empirical laminar flow correction factor proposed by Celik et al. [17] was applied for all three IQ estimators to avoid an incorrect estimation in near wall regions, where the molecular viscosity is much higher than the eddy viscosity. The correction factor is defined as

$$f_{\text{lam}} = 0.5(1 + \tanh(\beta(Re_{\text{tr}}^{0.5} - C_{\text{sl}} Re_{\text{tr-crt}}^{0.5}))), \quad (3.10)$$

where $\beta$ and $C_{\text{sl}}$ are empirical constants and $Re_{\text{tr-crt}}$ is the critical Reynolds number for transitional flow. This scaling function tends to zero smoothly as it approaches the wall. The turbulence Reynolds number $Re_{\text{tr}}$ is defined as

$$Re_{\text{tr}} = \frac{\left( \frac{2}{3} k_{\text{tot}} \right)^{1/2}}{\bar{u}_e f}, \quad (3.11)$$
where

\[ k_{\text{tot}} = k_{\text{res}} + k_{\text{sgs}} + k_{\text{num}}, \]  \hspace{1cm} (3.12)

and the integral length scale \( l \) is estimated by

\[ l = \frac{k_{\text{tot}}^{1/2}}{\epsilon}, \]  \hspace{1cm} (3.13)

with the help of Eq. 3.6.

### 3.1.4 Empirical Evaluation of the Numerical TKE

All of the above formulas depend on an estimation of numerical TKE, \( k_{\text{num}} \); however, its assessment is nontrivial for single-grid simulations. Considering that \( k_{\text{sgs}} \) and \( k_{\text{num}} \) are related to the length scale \( \Delta \) and \( h \) respectively, Celik et al. [17] proposed a direct way of evaluating \( k_{\text{num}} \) on a single-grid by assuming a linear relationship between \( k_{\text{num}} \) and \( k_{\text{sgs}} \), and the coefficient reflects the ratio of \( h/\Delta \),

\[ k_{\text{num}} = C_n \left( \frac{h}{\Delta} \right)^2 k_{\text{sgs}}. \]  \hspace{1cm} (3.14)

In the case of implicit filtering, the filter size is directly related to the grid size, such that the only parameter to tune is \( C_n \), which is properly tuned following [52]. Although the uniform turbulence may show a linear relation between \( k_{\text{sgs}} \) and \( k_{\text{num}} \), the linear assumption has two primary drawbacks because of the nature of the error even if the coefficient \( C_n \) is tuned:

- The SGS model primarily contributes to the modeled TKE in the high wave number region while the numerical dissipation contributes to the numerical TKE in a much wider wave number range.
• When approaching the wall, the modeled TKE tends to zero, while clearly $k_{num}$ is expected to be non-zero. Therefore $k_{sgs}$ should not serve as an indicator to estimate $k_{num}$ in the near-wall region.

An alternative way to study the impact of numerical dissipation is through the framework proposed by Schranner et al. [11, 89]. The method estimates the numerical dissipation in the kinetic energy equation and further derives the numerical eddy viscosity, $\nu_{num}$. The application to LES was performed without [89] and with [11] an explicit SGS model. The extension of this approach to estimate the numerical TKE forms the fundamental contribution of this research and is presented in the following section.

3.2 Evaluation of Numerical TKE

In this section, we focus on two novel approaches to estimate the numerical TKE. As previously mentioned in subsection 2.2.3, we focus on low Mach number flows which have been reported to yield sufficiently accurate results by compressible flow solvers for LES [22, 23], and hence we introduce the incompressible flow assumption during the derivation of the error estimators. We introduce this assumption for the primary reason that the derivation of the transport equations for kinetic and turbulent kinetic energy is tractable. Starting from the LES governing equation, we detail the procedure of [11] to estimate the numerical eddy viscosity, $\nu_{num}$, and extend the approach to evaluate the numerical TKE, $k_{num}$, in section 3.2.1. In section 3.2.2 we present an alternative novel approach to estimate the numerical TKE. Two evaluation methods are implemented in the Index Quality, leading to two novel error estimator families for LES.
3.2.1 Evaluation from Kinetic Energy Numerical Dissipation (KE-based approach)

Following the procedure described by Schranner et al. [89], we present briefly the derivation of the numerical dissipation of kinetic energy, or KE numerical dissipation for short. The transport equation for the kinetic energy $e_{\text{kin}}$ is formed by separating the transport equation for internal energy from the conservation of total energy. To simplify our notation, we choose to omit the filter symbol ($\tilde{}$) and assume all variables obtained in the following sections are LES resolved values. Assuming incompressible flow condition, the final form can be defined as,

$$\frac{\partial e_{\text{kin}}}{\partial t} + \frac{\partial (u_i e_{\text{kin}})}{\partial x_i} = -\frac{u_i}{\rho} \frac{\partial p}{\partial x_i} + u_j \frac{\partial [2(\nu + \nu_t)S_{ij}]}{\partial x_i}, \quad (3.15)$$

where $\nu_t$ is the subgrid-scale eddy viscosity, and

$$S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right). \quad (3.16)$$

We then employ the same numerical scheme that was used to discretize the Navier-Stokes solver to discretize the transport of kinetic energy to estimate $e_{\text{kin}}$. In the following equation, the left-hand-side represents the discretization of Eq. 3.15; while the non-zero right-hand-side provides the estimate of the numerical dissipation of kinetic energy $\epsilon_n$,

$$\left( \frac{\partial e_{\text{kin}}}{\partial t} \right)_d + (NS)_d e_{\text{kin}} = \left( \frac{\partial e_{\text{kin}}}{\partial t} \right) + (NS)_{e_{\text{kin}}} + \epsilon_n, \quad (3.17)$$

where $(NS)_d$ is the discretized Navier–Stokes operator. Schranner et al. [89] employed both high-order and second-order finite volume schemes and demonstrated that although a high-order scheme is preferred to minimize the numerical errors, the method could be applied to second-order schemes and the difference was minimal. Castiglioni et al. [12, 13] and Cadieux et al. [11] confirmed that using the same discretization order as in the
flow solver provided for sufficient accuracy for various test cases. The residual $\epsilon_n$ serves as an estimate of the numerical dissipation of kinetic energy. The residual is largely a function of the truncation error of the numerical scheme and includes both dissipative and dispersive errors. For the purposes of this work where $\epsilon_n$ will be employed towards a grid adaptation indicator, an accurate approximate is not as critical as a consistent trend in the distribution of the numerical dissipation. Next, we rewrite Eq. 3.17 for the finite volume framework employed in this work as,

$$\quad -\epsilon_n = e_{\text{kin},t} + F_{e_{\text{kin}}} + F_{ac} + F_{\nu} + \epsilon_{\nu},$$  

(3.18)

where the right-hand-side includes the total time-rate of change of kinetic energy:

- $e_{\text{kin},t} = \frac{\partial e_{\text{kin}}}{\partial t}$,

- $F_{e_{\text{kin}}} = \frac{\partial (u_j e_{\text{kin}})}{\partial x_j}$,

- $F_{ac} = \frac{1}{\rho} \frac{\partial (\rho u_i)}{\partial x_i}$,

- $F_{\nu} = -2 \frac{\partial [(\nu + \nu_t) S_{ij} u_j]}{\partial x_j}$,

- $\epsilon_{\nu} = 2(\nu + \nu_t) S_{ij} \frac{\partial u_i}{\partial x_j}$.

The first term on the right-hand-side, $e_{\text{kin},t}$ denotes the time rate of change of kinetic energy within the control volume, which we calculate using a second-order central difference using $e_{\text{kin}}$ at the $t_{n-1}$ and $t_{n+1}$ time steps. The term averages to be zero for a statistically steady regime. The following term on the right-hand-side, $F_{e_{\text{kin}}}$ represents the convective flux term and tracks the net rate of change of kinetic energy through the control volume. The term $F_{ac}$ represents the acoustic flux driven by pressure work. The viscous flux, $F_{\nu}$, represents the transport of kinetic energy by Reynolds stresses; while, $\epsilon_{\nu}$ is the kinetic energy dissipation term. Each cell is treated as a control volume and flux terms are evaluated on each cell surface.

In order to achieve a local cell-based error estimation, Eq. 3.18 is evaluated locally in each computational cell, providing local $\epsilon_n$ values. Eq. 3.18 is then evaluated at each
time interval \( n \Delta t \) (in the order of \( 0.05 h_{ref}/v_{ref} \) where \( h_{ref} \) and \( v_{ref} \) are the reference length and velocity scales and \( n \) is the time interval period), which lead to time and spanwise averaged values of \( \bar{\epsilon}_n \). Following the concept proposed in [88], a temporal and spatial along the \( z \) (spanwise) averaged numerical eddy viscosity \( \nu_{num} \) is estimated by analogy to the formula for the viscous dissipation term,

\[
\bar{\epsilon}_n = 2 \nu_{num} S_{ij} \frac{\partial u_i}{\partial x_j},
\]

such that

\[
\nu_{num} = \frac{1}{2} \frac{\bar{\epsilon}_n}{S_{ij} \frac{\partial u_i}{\partial x_j}}.
\]

A temporal and spanwise averaged numerical TKE, \( k_{num} \), is estimated from \( \nu_{num} \) through Eq. 3.3. The process of \( \epsilon_n \) evaluation is similar to the residual evaluation procedure in the flow solver. The implementation of the approach could easily be carried out for an arbitrary flow solver. However, the approach shows two drawbacks when applied for grid adaptation for LES:

- Due to the nature of the term, the dissipation \( \epsilon_n \) is always positive; the unsteady term \( \epsilon_{kin,t} \) tends to zero after time-averaging for a statistically steady case, while the flux terms, \( F_{kin} \), \( F_{ac} \) and \( F_{\nu} \), have the possibility of showing negative values, such that the total numerical dissipation could result in negative values in certain regions where the dissipative effect is negligible compared to the convective effect. For example, \( F_{kin} \) and \( F_{ac} \) could become the leading terms in both steady or laminar regions with high mean flow velocities and low turbulent intensities as well as low-velocity gradients; where it leads to negative numerical dissipation [12]. Therefore in practice, we only consider positive values of the numerical dissipation,

\[
\bar{\epsilon}_{n,pos} = \max(\bar{\epsilon}, 0),
\]
to avoid steady or laminar regions with negative values from being targeted for grid refinement. Since the motivation is to approximate the truncation error, an alternate procedure would be to take the absolute value of the numerical dissipation. However, in practice, we observed that laminar regions with large convective acceleration yielded larger $\epsilon_n$ values. Since our objective is to perform grid adaptation in turbulent regions of the flow, Eq. 3.21 proved to be the more appropriate choice.

- The current approach is focused on the kinetic energy numerical dissipation which incorporates both mean flow kinetic energy and turbulent kinetic energy numerical dissipations, where both parts contribute to the evaluation of $\nu_{\text{num}}$. However, the concept of the $IQ_k$ error estimator is based on the percentage of captured turbulent kinetic energy instead of the kinetic energy, thus ideally $IQ_k$ should only be formulated based on the numerical dissipation of the turbulent kinetic energy.

3.2.2 Evaluation from the Turbulent Kinetic Energy Numerical Dissipation (TKE-based approach)

In this subsection, we present the novel aspect of this work. We believe that the most appropriate way to estimate numerical TKE, or the amount of turbulent kinetic energy dissipated by the discretization error, is to extend the approach of [89] to the transport equation for the resolved TKE in the flow solver. A generalization of Eq. 3.17 for the turbulent kinetic energy equation can be expressed as,

$$\left( \frac{\partial k}{\partial t} \right)_d + (NS)_d k = \left( \frac{\partial k}{\partial t} \right) + (NS)k + \epsilon_n.$$  \hspace{1cm} (3.22)

In LES, Eq. 3.22 refers to the resolved TKE evolution and $\epsilon_n$ estimates the influence of numerical dissipation on the resolved TKE, or TKE numerical dissipation. Since most of the SGS model is based on eddy viscosity, we focus on the derivation of the discretized resolved turbulent kinetic energy equation for LES with the inclusion of $\nu_t$. Since we aim
to achieve a posteriori error estimators through a post-processing approach, as employed for the numerical dissipation of kinetic energy we engage the same numerical discretization as the flow solver to assess the TKE numerical dissipation. We begin by expressing the instantaneous momentum equation for LES,

$$\frac{\partial u_i}{\partial t} + u_k \frac{\partial u_i}{\partial x_k} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_k} \left[ (\nu + \nu_t) \frac{\partial u_i}{\partial x_k} \right], \quad (3.23)$$

where the instantaneous resolved velocity $u_i$ could be decomposed into a mean and fluctuation part,

$$u_i = \bar{u}_i + u'_i, \quad (3.24)$$

where the mean part is the time-averaging over the entire simulation period,

$$\bar{u}_i = \frac{1}{T} \int_T u_i dt, \quad (3.25)$$

and the time-averaged resolved momentum equation for incompressible LES leads to

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_k \frac{\partial \bar{u}_i}{\partial x_k} + \frac{\partial}{\partial x_k} \left[ \bar{u}'_i \frac{\partial \bar{u}_i}{\partial x_k} \right] - \frac{\partial}{\partial x_k} \left[ \bar{u}'_k \frac{\partial \bar{u}_i}{\partial x_k} \right] = -\frac{1}{\rho} \frac{\partial p'}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_k^2} + \nu_t \frac{\partial^2 \bar{u}_i}{\partial x_k \partial x_k} + \nu'_t \frac{\partial^2 \bar{u}_i}{\partial x_k^2} + \frac{\partial}{\partial x_k} \left[ \bar{u}'_k \frac{\partial \bar{u}_i}{\partial x_k} \right] + \frac{\partial}{\partial x_k} \left[ \bar{u}'_i \frac{\partial \bar{u}_i}{\partial x_k} \right] - \frac{\partial}{\partial x_k} \left[ \bar{u}'_i \frac{\partial \bar{u}_i}{\partial x_k} \right]. \quad (3.26)$$

We can subtract Eq. 3.23 by Eq. 3.26 to acquire the instantaneous fluctuation equation

$$\frac{\partial u'_i}{\partial t} + \bar{u}_k \frac{\partial u'_i}{\partial x_k} + u'_k \frac{\partial \bar{u}_i}{\partial x_k} + u'_k \frac{\partial \bar{u}_i}{\partial x_k} - \frac{\partial}{\partial x_k} \left[ \bar{u}'_k \frac{\partial u'_i}{\partial x_k} \right] = -\frac{1}{\rho} \frac{\partial p'}{\partial x_i} + \nu \frac{\partial^2 u'_i}{\partial x_k^2} + \nu_t \frac{\partial^2 \bar{u}_i}{\partial x_k \partial x_k} + \nu'_t \frac{\partial^2 \bar{u}_i}{\partial x_k \partial x_k} - \frac{\partial}{\partial x_k} \left[ \bar{u}'_i \frac{\partial u'_i}{\partial x_k} \right] \quad (3.27)$$
Next we premultiply Eq. 3.27 by $u_j'$,

$$
\begin{align*}
&u_j' \frac{\partial u_i'}{\partial t} + u_j' \frac{\partial u_j'}{\partial x_k} + u_j' u_k' \frac{\partial u_i'}{\partial x_k} + u_j' u_k' \frac{\partial u_i'}{\partial x_k} - u_j' \frac{\partial}{\partial x_k} u_i' u_k' = \\
&- \frac{u_j' \partial u_i'}{\rho \partial x_i} + \nu u_j' \frac{\partial^2 u_i'}{\partial x_k \partial x_k} + \nu u_j' \frac{\partial^2 u_i'}{\partial x_k \partial x_k} + \nu u_j' \frac{\partial^2 u_i'}{\partial x_k \partial x_k} + \nu u_j' \frac{\partial^2 u_i'}{\partial x_k \partial x_k} - u_j' \frac{\partial^2 u_i'}{\partial x_k \partial x_k} \tag{3.28}
\end{align*}
$$

Switching $i$ and $j$ in Eq. 3.28 and adding itself to Eq. 3.28 yields,

$$
\begin{align*}
&\frac{\partial u_i'u_j'}{\partial t} - \frac{u_k'}{\rho} \frac{\partial u_i'}{\partial x_k} + \frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k} + \frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k} + \frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k} - \frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k} \\
&= - \frac{u_i' \partial u_j'}{\rho \partial x_i} - \frac{u_j' \partial u_i'}{\rho \partial x_i} + \nu u_i' \frac{\partial^2 u_j'}{\partial x_k \partial x_k} + \nu u_j' \frac{\partial^2 u_i'}{\partial x_k \partial x_k} + \nu \frac{\partial^2 u_j'}{\partial x_k \partial x_k} - \nu \frac{\partial^2 u_i'}{\partial x_k \partial x_k}
\end{align*}
$$

$$
\begin{align*}
&= - \frac{1}{\rho} (u_i' \frac{\partial u_j'}{\partial x_k} + u_j' \frac{\partial u_i'}{\partial x_k}) + \nu \frac{\partial^2 u_i'u_j'}{\partial x_k \partial x_k} - 2 \nu \frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k} + \nu \frac{\partial^2 u_i'u_j'}{\partial x_k \partial x_k} - 2 \nu \frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k} \\
&\quad + \nu \frac{\partial^2 u_i'u_j'}{\partial x_k \partial x_k} - 2 \nu \frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k} + \nu \frac{\partial^2 u_i'u_j'}{\partial x_k \partial x_k} - \nu \frac{\partial^2 u_i'u_j'}{\partial x_k \partial x_k} - \nu \frac{\partial^2 u_i'u_j'}{\partial x_k \partial x_k} \\
\end{align*}
$$

disappear when averaging in time

$$
\begin{align*}
&+ \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} \\
&\quad + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} \\
&\quad + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} \\
\end{align*}
$$

disappear when averaging in time

$$
\begin{align*}
&\quad + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} \\
\end{align*}
$$

disappear when averaging in time

$$
\begin{align*}
&\quad + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} \\
\end{align*}
$$

disappear when averaging in time

$$
\begin{align*}
&\quad + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} + \frac{\partial \tilde{p}_i \partial u_i'u_j'}{\partial x_k} \\
\end{align*}
$$

(3.29)
which is the transport equation for the Reynolds stress tensor $\tau_{ij}' = u'_i u'_j$. We now average Eq. 3.29

\[
\frac{\partial u'_i u'_j}{\partial t} + \bar{u}_k \frac{\partial u'_i u'_j}{\partial x_k} + u'_i u'_k \frac{\partial \bar{u}_j}{\partial x_k} + u'_j u'_k \frac{\partial \bar{u}_i}{\partial x_k} + \frac{\partial}{\partial x_k} u'_i u'_j u'_k = \\
- \frac{1}{\rho} (u'_i \frac{\partial p'}{\partial x_i}) + (\nu + \nu_t) \frac{\partial^2 u'_i u'_j}{\partial x_k \partial x_k} - 2(\nu + \nu_t) \frac{\partial u'_i}{\partial x_k} \frac{\partial u'_j}{\partial x_k} + \bar{\nu}' u'_i \frac{\partial^2 \bar{u}_j}{\partial x_k \partial x_k} + \nu'_j \frac{\partial^2 \bar{u}_i}{\partial x_k \partial x_k} \\
+ \frac{\partial \nu_t}{\partial x_k} \frac{\partial u'_i u'_j}{\partial x_k} + u'_i \frac{\partial \bar{u}_j}{\partial x_k} + u'_j \frac{\partial \bar{u}_i}{\partial x_k},
\]

(3.30)

The contraction operation to the Reynolds stress tensor leads to the definition of TKE,

\[\text{contr}(\tau_{ij}') = \delta_{ij} \tau_{ij}' = u'_i u'_i\]  

(3.31)

using Einstein summation convention. We are able to apply the contraction operation to Eq. 3.30 to obtain the equation for the TKE budget,

\[
\frac{\partial \frac{1}{2} u'_i u'_i}{\partial t} + \bar{u}_k \frac{\partial \frac{1}{2} u'_i u'_i}{\partial x_k} + u'_i u'_k \frac{\partial \bar{u}_i}{\partial x_k} + \frac{\partial}{\partial x_k} \frac{1}{2} u'_i u'_i u'_k = \\
- \frac{1}{\rho} (u'_i \frac{\partial p'}{\partial x_i}) + (\nu + \nu_t) \frac{\partial^2 \frac{1}{2} u'_i u'_i}{\partial x_k \partial x_k} - (\nu + \nu_t) \frac{\partial u'_i}{\partial x_k} \frac{\partial u'_i}{\partial x_k} + \bar{\nu}' u'_i \frac{\partial^2 \bar{u}_i}{\partial x_k \partial x_k} + \nu'_i \frac{\partial^2 \bar{u}_i}{\partial x_k \partial x_k} \\
+ \frac{\partial \nu_t}{\partial x_k} \frac{\partial \frac{1}{2} u'_i u'_i}{\partial x_k} + u'_i \frac{\partial \bar{u}_i}{\partial x_k},
\]

(3.32)

which can be re-written as the time-averaged resolved TKE equation:

\[
\frac{\partial \bar{k}}{\partial t} + \bar{u}_k \frac{\partial \bar{k}}{\partial x_k} + u'_i u'_k \frac{\partial \bar{u}_i}{\partial x_k} + \frac{\partial}{\partial x_k} \frac{1}{2} u'_i u'_i u'_k = \\
- \frac{1}{\rho} (u'_i \frac{\partial p'}{\partial x_i}) + (\nu + \nu_t) \frac{\partial^2 \frac{1}{2} u'_i u'_i}{\partial x_k \partial x_k} - (\nu + \nu_t) \frac{\partial u'_i}{\partial x_k} \frac{\partial u'_i}{\partial x_k} + \bar{\nu}' u'_i \frac{\partial^2 \bar{u}_i}{\partial x_k \partial x_k} + \nu'_i \frac{\partial^2 \bar{u}_i}{\partial x_k \partial x_k} \\
+ \frac{\partial \nu_t}{\partial x_k} \frac{\partial \frac{1}{2} u'_i u'_i}{\partial x_k} + u'_i \frac{\partial \bar{u}_i}{\partial x_k},
\]

(3.33)
such that at each time step,

\[
\frac{\partial k}{\partial t} + \bar{u}_j \frac{\partial k}{\partial x_j} + u'_i u'_j \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial}{\partial x_j} k u'_j =
\]

\[- \frac{u'_i (p'\frac{\partial}{\partial x_i}) + (\nu + \nu_t) \frac{\partial^2 k}{\partial x_j \partial x_j} - (\nu + \nu_t) \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_j}{\partial x_j} + \nu'_i u'_j \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} \]

\[\frac{\partial k}{\partial x_j} \frac{\partial k}{\partial x_j} + u'_i \frac{\partial u'_i}{\partial x_j} + \text{first-order fluctuation terms},\]

where all first-order fluctuation terms vanish once time averaging is applied, thus are not needed to be considered. Eq. 3.34 can be further re-written as

\[
\frac{\partial k}{\partial t} + \frac{\partial}{\partial x_j} (k u_j + \frac{u'_i p'}{\rho}) = k \frac{\partial u'_i}{\partial x_j} \frac{\partial}{\partial x_j} \frac{\partial}{\partial x_j} - \frac{\partial}{\partial x_j} - (\nu + \nu_t) \frac{\partial^2 k}{\partial x_j \partial x_j} \]

\[- \frac{\partial}{\partial x_j} - (\nu + \nu_t) \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_j}{\partial x_j} + \nu'_i u'_j \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} \]

\[\frac{\partial k}{\partial x_j} \frac{\partial k}{\partial x_j} + u'_i \frac{\partial u'_i}{\partial x_j} + \text{first-order fluctuation terms}.\]

Using the same technique as the previous subsection, we express the numerical dissipation of resolved TKE as the discretization of all the terms of Eq. 3.35 in the flow solver,

\[- \epsilon_n = (\frac{\partial k}{\partial t})_d + (NS)_d k \]

\[-\]

\[-\]
\[ k_t = \frac{\partial k}{\partial t}, \]

\[ F_k = \frac{\partial}{\partial x_j}(k u_j), \]

\[ F_{ac} = \frac{\partial}{\partial x_j}\left(\frac{u'_i p'}{\rho}\right), \]

\[ F_\nu = -(\nu + \nu_t) \frac{\partial^2 k}{\partial x_j \partial x_j}, \]

\[ P = u'_i u'_j \frac{\partial u_i}{\partial x_j}, \]

\[ \epsilon_\nu = (\nu + \nu_t) \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_i}{\partial x_j}, \]

\[ \epsilon_{\text{interact}} = -\nu'_i u'_j \frac{\partial^2 u_i}{\partial x_j \partial x_j} - \frac{\partial \nu_t}{\partial x_j} \frac{\partial k}{\partial x_j} - u'_i \frac{\partial u'_i}{\partial x_j} \frac{\partial u_i}{\partial x_j}. \]

The first term on the right-hand-side \( k_t \) is the time rate of change of TKE within the control volume, which averages to zero for a statistically steady flow. The temporal derivative is approximated using the turbulent kinetic energy data from the simulations at time steps \( t_{n-1} \) and \( t_{n+1} \); \( F_k \) is the convection of TKE; \( F_{ac} \) is the transport of TKE by pressure fluctuation; and \( F_\nu \) represents the turbulent and viscous transport of TKE, which exhibits a diffusive property. \( P \) is the turbulent production of TKE from the interaction between the mean flow and the fluctuation; while, \( \epsilon_\nu \) is the dissipation term and \( \epsilon_{\text{interact}} \) are the interactive terms which primarily display a dissipative behaviour. We adopted a cell-based approach where flux terms are evaluated on all cell surfaces. The numerical dissipation, \( \epsilon_n \) is then evaluated at each time interval \( n \Delta t \) (in the order of 0.05\( h_{\text{ref}}/u_{\text{ref}} \) where \( h_{\text{ref}} \) and \( u_{\text{ref}} \) are the reference length and velocity scales and \( n \) is the time interval period), and averaged in the temporal and spanwise directions, resulting in \( \bar{\epsilon}_n \). The dissipated TKE due to the existence of numerical error, or numerical TKE \( k_{\text{num}} \), is then estimated using a local length scale \( l_{\text{scale}} \) and velocity scale \( u_{\text{scale}} \),

\[ k_{\text{num}} = \bar{\epsilon}_n \frac{l_{\text{scale}}}{u_{\text{scale}}}. \]
Considering that the numerical dissipation occurs at the scale of the cell size $h$ and the velocity fluctuation scale, we employ

$$l_{\text{scale}} = V_{\frac{1}{3}}, \quad \text{and}$$

$$u_{\text{scale}} = |u'| = \sqrt{\frac{2}{3}k_{\text{res}}},$$

where $V$ is the local cell volume and $k_{\text{res}}$ is the local resolved TKE.

We can then finally evaluate the Index Qualities. This is accomplished through three possible approaches to evaluate $k_{\text{num}}$ (empirical, KE-based, and TKE-based) and subsequently the Index Quality error estimators to derive $IQ_{\nu,\eta,k}$; an empirical approach which leads to $IQ_{\nu,\eta,k-\text{emp}}$, the KE-based approach on the evaluation of KE numerical dissipation deemed $IQ_{\nu,\eta,k-\text{ke}}$ and the evaluation of TKE numerical dissipation using the TKE-based approach designated as $IQ_{\nu,\eta,k-\text{tke}}$. 

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Chapter 4

Methodology for Adjoint-Based Error Estimator

In this chapter, we focus on proposing a practical adjoint-based error estimator for LES grid adaptation. Section 4.1 presents the traditional adjoint-based error estimation for unsteady flows. After defining the optimization problem we use two different approaches to derive the unsteady adjoint system, shown in subsection 4.1.1 and subsection 4.1.2 respectively. In sections 4.2 and 4.3, we propose two viable approximations, which lead to two different single-solve adjoint systems for error estimation for LES grid adaptation.

4.1 Unsteady adjoint-based error estimator

Consider an initial LES solution on a coarse grid $\Omega_H$. We are then interested in estimating an integrated quantity, $\bar{J}(u(t))$,

$$\bar{J}(u(t)) = \frac{1}{T} \int_0^T J(u(t), t) \, dt + J_T(u(T)),$$

(4.1)

where $u(t)$ is the solution to a system of partial differential equations at time level $t$ that governs the flow. The first term represents a time-averaged functional, while $J_T$ is a function of the solution at the final time, $T$. For example, the integrated functional could
represent the temporal history of the drag coefficient over an aircraft wing. Through a
discretization of the governing equations, the integrated quantity can be approximated
on the coarse grid as \( \bar{J}_H(u_H) \), where \( u_H \) is the solution to the discretized system. Now
consider a fine grid, \( \Omega_h \) and define \( \bar{J}_h(u_h) \) as the discretized integrated function on the
fine grid.

Our objective is to acquire an estimate of \( \bar{J}_h(u_h) \) without ever solving on the fine grid.
We begin by performing a Taylor series expansion of the objective function on the fine
solution at time step \( n \), \( J_h(u_{h,n}) \), with respect to the functional based on the coarse grid
solution projected to the fine grid \( J_h(u_{H,h,n}) \),

\[
J_h(u_{h,n}) = J_h(u_{H,h,n}) + \frac{\partial J_h}{\partial u_h} \bigg|_{u_{h,n}} (u_{h,n} - u_{H,h,n}) + \cdots,
\]

(4.2)

where \( u_{H,h,n} \) represents the coarse grid solution \( u_{H,n} \) projected to the fine grid through a
prolongation operator,

\[
u_{h,n}^H = \mathbf{I}_h^H u_{H,n}.
\]

For this work we are only concerned with an objective function based on a time-
averaged target functional, and as such the discrete form of Eq. 4.1 using a constant time
step yields,

\[
\bar{J}_h(u) = \frac{1}{T} \sum_{n=1}^{N} J_h(u_{h,n}) \Delta t, \tag{4.3}
\]

where \( T = N \Delta t \) is the total time period of the averaging while \( N \) is the total number of
discrete time steps. Thus, the Taylor expansion of the time-averaged objective function is
obtained by introducing Eq. 4.2 into Eq. 4.3,

\[
J_h(u) = \frac{1}{T} \sum_{n=1}^{N} J_h(u_{H,h,n}) \Delta t + \frac{1}{T} \sum_{n=1}^{N} \frac{\partial J_h}{\partial u_h} \bigg|_{u_{h,n}} (u_{h,n} - u_{H,h,n}) \Delta t + \cdots. \tag{4.4}
\]

Given an error vector \( (u_{h,n} - u_{h,n}^H) \), we can approximate the functional on the fine
grid. To acquire such an error vector, we next introduce the governing equations in semi-
discrete form for each control volume for the fine grid $\Omega_h$ as,

$$V \frac{d u_h}{dt} + R(u_h) = 0,$$

where $V$ is the volume of the control volume and $R(u_h)$ represents the residual resulting from the spatial discretization. If we are to discretize the temporal derivative with an Euler time stepping scheme, then the unsteady nonlinear residual operator can be represented as,

$$R^*(u_{h,n}, u_{h,n-1}) = u_{h,n} - u_{h,n-1} + R_h(u_{h,n}) = 0,$$  \hfill (4.5)

where $R_h(u_{h,n})$ is the nonlinear residual operator representing only the divergence of the fluxes at the $n$-th time level. A Taylor series expansion of the instantaneous unsteady nonlinear residual $R^*_h(u_{h,n}, u_{h,n-1})$ at the $n$-th time step about the coarse grid solution yields,

$$R^*_h(u_{h,n}, u_{h,n-1}) = R^*_h(u_{H,h,n}, u_{H,h,n-1}) + \left. \frac{\partial R^*_h}{\partial u_{h,n}} \right|_{u_{H,h,n}} (u_{h,n} - u_{H,h,n})$$

$$+ \left. \frac{\partial R^*_h}{\partial u_{h,n-1}} \right|_{u_{H,h,n-1}} (u_{h,n-1} - u_{H,h,n-1}) + \cdots.$$  \hfill (4.6)

The linearization bears two first-order derivatives or Jacobians since the nonlinear residual is a function of solutions at the $n$-th and $(n-1)$-th time levels. The Jacobian $\left. \frac{\partial R^*_h}{\partial u_{h,n}} \right|_{u_{H,h,n}}$ of the fine grid system of equations is evaluated using the projection of the coarse-grid solution, $u_{H,h,n}$; while, $\left. \frac{\partial R^*_h}{\partial u_{h,n-1}} \right|_{u_{H,h,n-1}}$ employs $u_{H,h,n-1}$.

With the decomposition in Eq. 4.5, the derivatives of the unsteady residual leads to

$$\frac{\partial R^*_h}{\partial u_{h,n}} = \frac{\partial R_h}{\partial u_{h}} + \frac{I}{\Delta t} \quad \text{and,}$$

$$\frac{\partial R^*_h}{\partial u_{h,n-1}} = -\frac{I}{\Delta t}.$$  \hfill (4.7)
Now let us decompose $R_h^*(u_{h,n}, u_{h,n-1})$ following Eq. 4.5 and substitute it into Eq. 4.6,

$$
R_h^*(u_{h,n}, u_{h,n-1}) = R_h^*(u_{h,n-1}^H, u_{h,n-1}^H) + \frac{\partial R_h^*}{\partial u_{h,n}}(u_{h,n} - u_{h,n}^H) \\
+ \frac{\partial R_h^*}{\partial u_{h,n-1}}(u_{h,n-1} - u_{h,n-1}^H) \\
= R_h^*(u_{h,n-1}^H, u_{h,n-1}^H) + \left( \frac{\partial R_h^*}{\partial u_{h,n}} \right)(u_{h,n} - u_{h,n}^H) \\
- \frac{I}{\Delta t}(u_{h,n-1} - u_{h,n-1}^H) + \cdots
$$

(4.8)

### 4.1.1 Classical derivation

Now that we have the expressions of the discretized time-averaged functional (Eq. 4.3) and discretized instantaneous unsteady residual (Eq. 4.8), we can build up the unsteady optimization problem in a discrete form. We are looking to optimize a time-averaged objective function $\bar{J}_h(u_h)$ of engineering interest under the constraint that the unsteady flow residual $R_h^*(u_{h,n}, u_{h,n-1})$ equals to zero,

$$
\min_{u_h} \bar{J}_h(u_h),
$$

subject to: $R_h^*(u_{h,n}, u_{h,n-1}) = 0.$

(4.9)

Note that, the time step $n$ could be discretized as well and represented as $n_H$, where the subscript $H$ here denotes a coarse discretization in the temporal domain. However, in this work we are only interested in adapting the spatial grid and will leave the temporal grid as is. An extension of the described approach to account for the temporal discretization will be part of future work.
We can premultiply Eq. 4.8 by a Lagrangian multiplier, or the adjoint solution, \( \psi^T_{h,n} \) for each time step and obtain

\[
\psi^T_{h,n} R^*_h(u_{h,n}, u_{h,n-1}) = \psi^T_{h,n} R^*_h(u^H_{h,n}, u^H_{h,n-1}) + \psi^T_{h,n} \left( \frac{\partial R_h}{\partial u_h} \bigg|_{u^H_{h,n}} + \frac{I}{\Delta t} \right) (u_{h,n} - u^H_{h,n})
\]

\[ - \psi^T_{h,n} \frac{I}{\Delta t} (u_{h,n-1} - u^H_{h,n-1}) + \ldots \tag{4.10} \]

Under the constraint that \( R^*_h(u_{h,n}, u_{h,n-1}) = 0 \), Eq. 4.10 could be rewritten as

\[
- \psi^T_{h,n} R^*_h(u^H_{h,n}, u^H_{h,n-1}) = \psi^T_{h,n} \left( \frac{\partial R_h}{\partial u_h} \bigg|_{u^H_{h,n}} + \frac{I}{\Delta t} \right) (u_{h,n} - u^H_{h,n})
\]

\[ - \psi^T_{h,n} \frac{I}{\Delta t} (u_{h,n-1} - u^H_{h,n-1}) + \ldots \tag{4.11} \]

We can then perform a time averaging of \( \psi^T_{h,n} R^*_h(u^H_{h,n}, u^H_{h,n-1}) \) over the time period \( T \). Using a constant time step \( \Delta t \) and the discrete form, the time-averaging of Eq. 4.11 yields,

\[
- \frac{1}{T} \sum_n \psi^T_{h,n} R^*_h(u^H_{h,n}, u^H_{h,n-1}) \Delta t = \frac{1}{T} \sum_n \psi^T_{h,n} \left( \frac{\partial R_h}{\partial u_h} \bigg|_{u^H_{h,n}} + \frac{I}{\Delta t} \right) (u_{h,n} - u^H_{h,n}) \Delta t
\]

\[ - \frac{1}{T} \sum_n \psi^T_{h,n} \frac{I}{\Delta t} (u_{h,n-1} - u^H_{h,n-1}) \Delta t + \ldots \tag{4.12} \]

Note that Eq. 4.12 presents a time-averaged equation over long time period \( T \) for statistically steady state flows. The index in the last term on the right-hand-side of Eq. 4.12 can be altered (shifted by 1) such that

\[
- \frac{1}{T} \sum_n \psi^T_{h,n} \frac{I}{\Delta t} (u_{h,n-1} - u^H_{h,n-1}) \Delta t + \frac{1}{T} \sum_n \psi^T_{h,n+1} \frac{I}{\Delta t} (u_{h,n} - u^H_{h,n}) \Delta t. \tag{4.13} \]
Thus Eq. 4.12 can be further simplified such that we can isolate the factor \((u_{h,n} - u_{h,n}^H)\) on the right-hand-side of the equation,

\[
-\frac{1}{T} \sum_n \psi_{h,n}^T R_h^* (u_{h,n}^H, u_{h,n}^H - 1) \Delta t = \frac{1}{T} \sum_n \psi_{h,n}^T \frac{\partial R_h}{\partial u_h} \bigg|_{u_{h,n}^H} + \frac{I}{\Delta t} (u_{h,n} - u_{h,n}^H) \Delta t \\
- \frac{1}{T} \sum_n \psi_{h,n+1}^T \frac{I}{\Delta t} (u_{h,n} - u_{h,n}^H) \Delta t + \cdots \\
\approx \frac{1}{T} \sum_n \left[ \psi_{h,n}^T \frac{\partial R_h}{\partial u_h} \bigg|_{u_{h,n}^H} + \psi_{h,n}^T \frac{I}{\Delta t} - \psi_{h,n+1}^T \frac{I}{\Delta t} \right] (u_{h,n} - u_{h,n}^H) \Delta t.
\]

(4.14)

The error vector \((u_{h,n} - u_{h,n}^H)\) is the difference between the fine grid solution \(u_{h,n}\) and the projected flow solution from the coarse to the fine grid \(u_{h,n}^H\). Since the fine grid solution \(u_{h,n}\) is an unknown value and the choice of the adjoint solution \(\psi_{h,n}^T\) is arbitrary, then we can propose an unsteady adjoint equation to remove the need to evaluate the error vector \((u_{h,n} - u_{h,n}^H)\). We thus introduce an equation to substitute the second term on the right-hand-side of Eq. 4.4 by the right-hand-side of Eq. 4.14,

\[
\frac{1}{T} \sum_{n=1}^{N} \frac{\partial J_h}{\partial u_h} \bigg|_{u_{h,n}^H} (u_{h,n} - u_{h,n}^H) \Delta t = \frac{1}{T} \sum_n \left[ \psi_{h,n}^T \frac{\partial R_h}{\partial u_h} \bigg|_{u_{h,n}^H} + \psi_{h,n}^T \frac{I}{\Delta t} - \psi_{h,n+1}^T \frac{I}{\Delta t} \right] (u_{h,n} - u_{h,n}^H) \Delta t.
\]

(4.15)

After further simplification the unsteady adjoint formulation leads to

\[
\frac{1}{n} \sum_n \left[ \frac{\partial J_h}{\partial u_h} \bigg|_{u_{h,n}^H} - \psi_{h,n}^T \frac{\partial R_h}{\partial u_h} \bigg|_{u_{h,n}^H} - \psi_{h,n}^T \frac{I}{\Delta t} + \psi_{h,n+1}^T \frac{I}{\Delta t} \right] (u_{h,n} - u_{h,n}^H) = 0.
\]

(4.16)

We have thus established an adjoint system for unsteady flows. Since the choice of \(\psi_{h,n}^T\) is arbitrary in Eq. 4.14, we can force the adjoint solution \(\psi_{h,n}^T\) at time step \(n\) to satisfy the unsteady adjoint equation,

\[
\frac{\partial J_h}{\partial u_h} \bigg|_{u_{h,n}^H} - \psi_{h,n}^T \frac{\partial R_h}{\partial u_h} \bigg|_{u_{h,n}^H} - \psi_{h,n}^T \frac{I}{\Delta t} + \psi_{h,n+1}^T \frac{I}{\Delta t} = 0.
\]

(4.17)
It is shown that in order to solve the adjoint solution $\psi_{h,n}^T$ at time step $n$, we require the flow solution at the $n$-th time step, $u_{h,n}^H$, and the adjoint solution at time step $n+1$, $\psi_{h,n+1}^T$. This illustrates the fact that the unsteady adjoint equation depends on a backward time integration. With all $N$ unsteady adjoint equations at each time step satisfied, we can substitute the second term on the right-hand-side of Eq. 4.4 and finally derive the estimate of the objective function on the fine grid, $\Omega_h$ as

$$ \bar{J}_h(u_h) \approx \bar{J}_h(u_h^H) - \frac{1}{N} \sum_{n=1}^{N} \psi_{h,n}^T R_h^*(u_{h,n}^H, u_{h,n-1}^H). $$

(4.18)
4.1.2 Alternate derivation

In this subsection we offer an alternate approach to derive the unsteady adjoint equation for the purpose of grid adaptation. The approach is more in line with that used by the goal-oriented grid adaptation research community as opposed to the classical approach presented in the previous subsection that is employed by the adjoint-based shape optimization community. The alternate approach highlights the propagation of the error from the initial to the final time steps as well as some of the shortcomings of the adjoint approach in terms of the computational and storage cost.

We now refer back to Eq. 4.8 that demonstrates that the Taylor series expansion of the unsteady nonlinear residual is a function of the error in the solution at time levels \(n\) and \(n-1\). Therefore the error in the solution at time level \(n\) is an implicit function of the unsteady nonlinear residual at time levels \(n+1\) and \(n\). To yield a close-form expression for the error requires a system of equations representing the Taylor series expansions at all time levels, as expressed in the following system of equations,

\[
\begin{bmatrix}
\frac{\partial R^*_h}{\partial u_{h,1}} u_{h,1}^H \\
\frac{1}{\Delta t} \left[ \frac{1}{\Delta t} + \frac{\partial R^*_h}{\partial u_{h,2}} \right] u_{h,2}^H \\
\vdots \\
\frac{1}{\Delta t} \left[ \frac{1}{\Delta t} + \frac{\partial R^*_h}{\partial u_{h,n}} \right] u_{h,n}^H \\
\frac{1}{\Delta t} \left[ \frac{1}{\Delta t} + \frac{\partial R^*_h}{\partial u_{h,N}} \right] u_{h,N}^H
\end{bmatrix}
= \begin{bmatrix}
u_{h,1} - u_{h,1}^H \\
u_{h,1} - u_{h,1}^H \\
\vdots \\
u_{h,n} - u_{h,n}^H \\
u_{h,n} - u_{h,n}^H
\end{bmatrix}
= \begin{bmatrix}
R^*_h(u_{h,1}) \\
R^*_h(u_{h,2}, u_{h,1}) \\
\vdots \\
R^*_h(u_{h,n}, u_{h,n-1}) \\
R^*_h(u_{h,N}, u_{h,N-1})
\end{bmatrix}
\]

The matrix in Eq. 4.19 forms a lower-triangular system and therefore can be solved through a forward sweep. At time level \(n = 1\) we solve for a steady state solution; thus, the error at the first time level yields,

\[
u_{h,1} - u_{h,1}^H \approx -\left[ \frac{\partial R^*_h}{\partial u_{h,1}} \right]^{-1} R^*_h(u_{h,1}) \approx -\left[ \frac{\partial R^*_h}{\partial u_{h,1}} \right]^{-1} R^*_h(u_{h,1}),
\]  

(4.20)
and at the second time level, we can express the error as,

\[
\mathbf{u}_{h,2} - \mathbf{u}^H_{h,2} \approx \left[ \frac{\mathbf{I}}{\Delta t} + \frac{\partial \mathbf{R}^*_h}{\partial \mathbf{u}_{h,2}} \right]^{-1} \left[ -\mathbf{R}^*_h(\mathbf{u}_{h,2}, \mathbf{u}^H_{h,1}) + \frac{\mathbf{I}}{\Delta t} (\mathbf{u}_{h,1} - \mathbf{u}^H_{h,1}) \right]
\]

\[
\approx \left[ \frac{\mathbf{I}}{\Delta t} + \frac{\partial \mathbf{R}^*_h}{\partial \mathbf{u}_{h,2}} \right]^{-1} \left[ -\mathbf{R}^*_h(\mathbf{u}_{h,2}, \mathbf{u}^H_{h,1}) - \frac{\mathbf{I}}{\Delta t} \left[ \frac{\partial \mathbf{R}^*_h}{\partial \mathbf{u}_{h,1}} \right] \right]^{-1} \mathbf{R}_h(\mathbf{u}^H_{h,1}) \]

\[
\approx -\mathbf{G}^{-1}_{h,2} \mathbf{R}^*_h(\mathbf{u}^H_{h,2}, \mathbf{u}^H_{h,1}) - \mathbf{G}^{-1}_{h,2} \left[ \frac{\partial \mathbf{R}^*_h}{\partial \mathbf{u}_{h,1}} \right] \mathbf{R}_h(\mathbf{u}_{h,1})
\]

(4.21)

where \( \mathbf{G}_{h,n} \) denotes the diagonal block matrix from Eq. 4.19. As expected the error at the final time level \( N \) is a function of the unsteady residuals of all previous time levels and hence,

\[
\mathbf{u}_{h,n} - \mathbf{u}^H_{h,n} \approx -\sum_{i=n}^{1} \left( \frac{\mathbf{I}}{\Delta t} \right)^{n-i} \left[ \prod_{k=n}^{i} \mathbf{G}^{-1}_{h,k} \right] \mathbf{R}^*_h i.
\]

(4.22)

We can now revisit the Taylor series expansion of the functional from Eq. 4.4 and introduce the expression for the error at each time level,

\[
\tilde{J}_h(\mathbf{u}_h) = \tilde{J}_h(\mathbf{u}^H_h) + \frac{1}{N} \sum_{n=1}^{N} \frac{\partial J_h}{\partial \mathbf{u}_h} \bigg|_{\mathbf{u}^H_{h,n}} (\mathbf{u}_{h,n} - \mathbf{u}^H_{h,n}) + \cdots
\]

\[
= \tilde{J}_h(\mathbf{u}^H_h) + \frac{1}{N} \left[ \frac{\partial J_h}{\partial \mathbf{u}_h} \bigg|_{\mathbf{u}^H_{h,N}} (\mathbf{u}_{h,N} - \mathbf{u}^H_{h,N}) + \frac{\partial J_h}{\partial \mathbf{u}_h} \bigg|_{\mathbf{u}^H_{h,N-1}} (\mathbf{u}_{h,N-1} - \mathbf{u}^H_{h,N-1}) + \cdots \right.
\]

\[
\left. \cdots + \frac{\partial J_h}{\partial \mathbf{u}_h} \bigg|_{\mathbf{u}^H_{h,1}} (\mathbf{u}_{h,1} - \mathbf{u}^H_{h,1}) \right]
\]

\[
= \tilde{J}_h(\mathbf{u}^H_h) + \frac{1}{N} \left[ \sum_{n=1}^{N} \frac{\partial J_h}{\partial \mathbf{u}_h} \bigg|_{\mathbf{u}^H_{h,n}} \left\{ -\sum_{i=n}^{1} \left( \frac{\mathbf{I}}{\Delta t} \right)^{n-i} \left[ \prod_{k=n}^{i} \mathbf{G}^{-1}_{h,k} \right] \mathbf{R}^*_h \right\} \right]
\]

(4.23)
Next we expand both the summation and product expressions from the second term of Eq. 4.23 and introduce the adjoint state $\lambda_{h,n}$,

$$
\left. \frac{\partial J_h}{\partial u_h} \right|_{u_{h,N}^H} \left[ - \sum_{i=N}^{1} \left( \frac{1}{\Delta t} \right)^{N-i} \left[ \prod_{k=N}^{i} G_{h,k}^{-1} \right] R_{h,i}^* \right] = - \left. \frac{\partial J_h}{\partial u_h} \right|_{u_{h,N}^H} \left\{ \left( \frac{1}{\Delta t} \right)^{N-N} \left[ \prod_{k=N}^{N} G_{h,k}^{-1} \right] R_{h,N}^* \right\} + \left. \frac{\partial J_h}{\partial u_h} \right|_{u_{h,N}^H} \left\{ \left( \frac{1}{\Delta t} \right)^{N-1} \left[ \prod_{k=N}^{N-1} G_{h,k}^{-1} \right] R_{h,N-1}^* \right\} + \left. \frac{\partial J_h}{\partial u_h} \right|_{u_{h,N}^H} \left\{ \left( \frac{1}{\Delta t} \right)^{N-2} \left[ \prod_{k=N}^{N-2} G_{h,k}^{-1} \right] R_{h,N-2}^* \right\} + \cdots \\
= - \left. \frac{\partial J_h}{\partial u_h} \right|_{u_{h,N}^H} \left\{ G_{h,N}^{-1} R_{h,N}^* \right\} + \left. \frac{\partial J_h}{\partial u_h} \right|_{u_{h,N}^H} \left\{ G_{h,N}^{-1} G_{h,N-1}^{-1} R_{h,N-1}^* \right\} + \cdots \\
= - \left. \frac{\partial J_h}{\partial u_h} \right|_{u_{h,N}^H} \left\{ G_{h,N}^{-1} R_{h,N}^* \right\} + \left. \frac{\partial J_h}{\partial u_h} \right|_{u_{h,N}^H} \left\{ G_{h,N}^{-1} G_{h,N-1}^{-1} R_{h,N-1}^* \right\} + \cdots \\
= \left. \frac{\partial J_h}{\partial u_h} \right|_{u_{h,N}^H} \left\{ G_{h,N}^{-1} R_{h,N}^* \right\} + \left. \frac{\partial J_h}{\partial u_h} \right|_{u_{h,N}^H} \left\{ G_{h,N}^{-1} G_{h,N-1}^{-1} R_{h,N-1}^* \right\} + \cdots \\
(4.24)
$$

The above formulation represents the dual-weighted residual term that is synonymous with goal-oriented error indicators with the presences of contributions from each time step. An interesting characteristic of Eq. 4.24 is the need to solve for the adjoint state at time level, $N$ before seeking the solution at $N-1$. We can express the adjoint equation at time level $N-1$ between the braces as,

$$
\left( \frac{1}{\Delta t} \right)^T \lambda_{h,N}^T G_{h,N-1}^{-1} + \left. \frac{\partial J_h}{\partial u_h} \right|_{u_{h,N-1}^H} G_{h,N-1}^{-1} = \lambda_{h,N-1}^T \\
(4.25)
$$

$$
G_{h,N-1}^T \lambda_{h,N-1} = \left[ \left. \frac{\partial J_h}{\partial u_h} \right|_{u_{h,N-1}^H} \right]^T + \left( \frac{1}{\Delta t} \right)^T \lambda_{h,N}. \\
(4.26)
$$
We can finally represent the estimate of the objective function on the fine grid, $\Omega_h$ as

$$\bar{J}_h(u_h) \approx \bar{J}_h(u_{Hh}^H) - \frac{1}{N} \sum_{n=1}^{N} \psi_{h,n}^T R_h^* (u_{h,n}^H, u_{h,n-1}^H).$$

(4.27)

This leads to the same formula as the classical derivation approach (in subsection 4.1.1), as shown in Eq. 4.18. Note that Eq. 4.27 requires the solution of the adjoint on the fine grid. An alternate approach that is typically adopted by the research community is to replace the adjoint state on the fine grid by an interpolated coarse-grid adjoint, $\psi_{h,n}^H = I_h^H \psi_{H,n}$. The Jacobian of the governing equation and the sensitivity of the objective function to the state are replaced with their counterparts on the coarse grid. This yields an error estimate that is void of the need to evaluate neither the primal nor the dual on the fine grid but accrues an error due to the interpolation of the coarse-grid adjoint. Therefore the error estimator can be recast as

$$- \frac{1}{N} \sum_{n=1}^{N} \psi_{h,n}^T R_h^* (u_{h,n}^H, u_{h,n-1}^H) = - \frac{1}{N} \sum_{n=1}^{N} \left[ \psi_{h,n}^H \bigg|_{u_{h,n}^H} \right]^T R_h^* (u_{h,n}^H, u_{h,n-1}^H)$$

$$+ \frac{1}{N} \sum_{n} \left[ \psi_{h,n}^H \bigg|_{u_{h,n}^H} - \psi_{h,n} \right]^T R_h^* (u_{h,n}^H, u_{h,n-1}^H).$$

(4.28)

In practice, we can only evaluate the computable correction [106] as the error estimator for grid adaptation. However, the evaluation of the computable correction relies on solving the unsteady adjoint at each time step following Eq. 4.26, which contributes greatly to both computational memory and cost. The exact algorithm requires the storage of flow solutions of the total $N$ time steps and requires $N$ adjoint linear solves. In addition, the adjoint solver for chaotic flows has proven to be unstable [113].
4.2 Approximation 1

To avoid the need to solve an unsteady adjoint due to both the computational cost and potential instability, we seek for an alternate approach to compute the error vector $u_{h,n} - u_{h,n}^H$. A possible approximation is to revisit the Taylor expansion of the time-averaged objective function from Eq. 4.4 and introduce a linearization such that the error vector can be expressed as the sum of a mean and fluctuation component,

$$ u_{h,n} - u_{h,n}^H = (u_h - u_h^H) + (u_{h,n} - u_{h,n}^H)' $$  \hspace{1cm} (4.29)

Substitution of the linearization into the Taylor expansion of Eq. 4.4 yields the following form of the expression,

$$ \bar{J}_h(u_h) = \bar{J}_h(u_h^H) + \frac{\partial J_h}{\partial u_h} \bigg|_{u_h^H} (u_h - u_h^H) + \cdots $$  \hspace{1cm} (4.30)

To complete the derivation, an expression for the mean error over the time period can be obtained by first time-averaging Eq. 4.8,

$$ \bar{R}_h^*(u_h) = \bar{R}_h^*(u_h^H) + \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H} \frac{I}{\Delta t} (u_{h,n} - u_{h,n}^H) - \frac{I}{\Delta t} (u_{h,n-1} - u_{h,n-1}^H) + \cdots $$  \hspace{1cm} (4.31)

where the temporal derivative terms vanish for statistically steady state flows. Likewise, the sum of the unsteady terms on the right-hand-side, $\frac{I}{\Delta t} (u_{h,n} - u_{h,n}^H) - \frac{I}{\Delta t} (u_{h,n-1} - u_{h,n-1}^H)$, will tend to zero if the statistically steady state flow is averaged over a long time period.

Following a similar linearization of the error vector (Eq. 4.29), the Jacobian can be expressed in a similar approach and be decomposed into a mean and fluctuation component.
as,
\[
\frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H, n} = \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H, n} + \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H, n} \quad (4.32)
\]

where
\[
\frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H, n} = \frac{1}{T} \sum_n \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H, n} \Delta t
\]
\[
\frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H, n} = \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H, n} - \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H}.
\]

With such a decomposition, we can further decompose the term \( \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H} (u_h - u_H^H) \) and perform the time-averaging, which leads to
\[
\frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H} (u_h - u_H^H) = \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H} (u_h - u_H^H) + \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H} (u_h - u_H^H) \quad (4.34)
\]
\[
\frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H} (u_h - u_H^H) = \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H} (u_h - u_H^H) + \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H} (u_h - u_H^H) \quad (4.35)
\]

If we are to assume that the first term on the right-hand-side of Eq. 4.34 dominates over the second term, the time-averaging of Eq. 4.31 reduces to
\[
\bar{R}_h(u_h) = \bar{R}_h(u_h^H) + \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H} (u_h - u_H^H) \quad (4.35)
\]
\[
\approx \bar{R}_h(u_h^H) + \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H} (u_h - u_H^H).
\]

If we are to assume \( \bar{R}_h(u_h) = 0 \), we can derive a version of the mean error vector as,
\[
(u_h - u_H^H) \approx \left( \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H} \right)^{-1} \bar{R}_h(u_h^H) \quad (4.36)
\]
Subsequent substitution into Eq. 4.30 yields the following single adjoint equation,

$$\frac{\partial J_h}{\partial u_h} \bigg|_{u_h^H} - \psi_h^T \frac{\partial R_h}{\partial u_h} \bigg|_{u_h^H} = 0,$$

where $\psi_h^T$ depends on a single solve and an expression for the corrected objective function is obtained,

$$J_h(u_h) \approx J_h(u_h^H) - \psi_h^T \overline{R}_h(u_h^H) \approx J_h(u_h^H) - \psi_h^T \overline{R}_h(u_h^H),$$

where the unsteady residual $\overline{R}_h(u_h^H)$ is replaced by steady residual $\overline{R}_h(u_h^H)$ for statistically steady flow. The implementation of the approach requires the storage of the time-averaged Jacobian and the sensitivity of the functional, both of which can be accumulated during the forward time integration. At the completion of the flow calculation, a single linear solve of the adjoint is obtained and corresponding local error estimates.

### 4.3 Approximation 2

An alternate approximation is to convert the unsteady flow solution obtained by LES to a RANS-type steady flow solution. The proposal here is not to develop a turbulence model for the RANS equation to resolve the flow but to approximate the LES solution and allow existing RANS-based adjoint solvers to provide dual-weighted residuals for the purpose of grid adaptation. For LES to correctly resolve the flow, sub-filtered terms in the Navier-Stokes equation need to be modeled by a subgrid-scale (SGS) model. When employing an eddy viscosity model, a time dependent viscosity $\nu_{t,LES}$ is included and the governing momentum and energy equations can be obtained,

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} [2(\nu + \nu_{t,LES})S_{ij}],$$
where $u_i$ is the instantaneous velocity solved by LES and

$$S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad (4.40)$$

for incompressible flow. Time-averaging of Eq. 4.39 leads to

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + 2\nu \frac{\partial \bar{S}_{ij}}{\partial x_j} \left[ 2\bar{\nu}_{LES} \bar{S}_{ij} + 2\nu'_{LES} S'_{ij} \right] \quad (4.41)$$

with $u_i = \bar{u}_i + u'_i$ where $\bar{u}_i$ is the time-averaged velocity and $u'_i$ is the velocity fluctuation and $S_{ij} = \bar{S}_{ij} + S'_{ij}$. As is generally recognized for LES, a low-pass filter is implicitly applied to each flow variable in the governing equation, of which the kernel function depends on the numerical scheme of the flow solver (generally a top-hat filter for the type of finite-volume scheme used in the current flow solver). Here we make the assumption that the application of an implicit filter has little effect on the time-averaged velocity value,

$$\bar{u}_i = \tilde{\bar{u}}_i, \quad (4.42)$$

where $\tilde{\bar{u}}_i$ is the filtered velocity in LES. Recalling the governing equation for RANS,

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ 2(\nu + \nu_{RANS}) \bar{S}_{ij} \right], \quad (4.43)$$

and comparing the disparate terms from Eq. 4.39 and Eq. 4.43, we arrive at the following formulation for the RANS momentum transfer due to turbulent fluctuations,

$$2\nu_{RANS} \bar{S}_{ij} \approx 2\bar{\nu}_{LES} \bar{S}_{ij} + 2\nu'_{LES} S'_{ij} - \bar{u}'_i \bar{u}'_j, \quad (4.44)$$

such that

$$\nu_{RANS} \approx \frac{1}{2} \left[ 2\bar{\nu}_{LES} \bar{S}_{ij} + 2\nu'_{LES} S'_{ij} - \bar{u}'_i \bar{u}'_j \right] / \bar{S}_{ij}, \quad (4.45)$$
With the conversion of LES to a RANS flow solution using the aforementioned approximation in Eq. 4.45, we can apply a steady adjoint approach to obtain the adjoint solution $\psi^T_h$. Further assuming that

$$R_h(u_h^H) \propto \frac{1}{T} \sum_n R_h(u_{h,n}^H) \Delta t = R_h(u_h^H), \quad (4.46)$$

the error estimation could finally be performed for an LES flow solution.

### 4.4 Implementation of error estimator

Fig. 4.1 shows the implementation pipeline for error estimation based on two approximations. The process begins by writing the coarse grid solution $u_h^H$ to disk for the final set of predetermined set of flow-through periods. For approximation 1, upon the completion of all time periods, the first step is to retrieve the coarse grid solution, $u_h^H$ and
perform a projection on a uniformly refined fine grid, $\Omega_h$ leading to $u_h^H$. We then evaluate the residual $R_h(u_h^H)$ based on the projected solution $u_h^H$ and subsequently the flow Jacobian $\frac{\partial R_h}{\partial u_h^H} \bigg|_{u_h^H}$ and the sensitivity of the functional, $\frac{\partial J_h}{\partial u_h} \bigg|_{u_h^H}$ on the fine grid based on the projected flow solution, $u_h^H$. The linearization is based on automatic differentiation using the Tapenade [44] software. Since we require the time-averaged Jacobian and sensitivity of the functional to solve the dual problem, we continue with the retrieval of the coarse grid solution at the following time step and evaluate the projected fine grid solution $u_h^H$, the residual $R_h(u_h^H)$, as well as Jacobian and the sensitivity of the functional to form the time-averaged $\frac{\partial J_h}{\partial u_h} \bigg|_{u_h^H}$, and $R_h(u_h^H)$. The second to last step sees the solution to the dual problem. Here we employ a GMRES to solve Eq. 4.37 using the PETSc package [3] with an ILU(0) preconditioner. Once the adjoint solution is acquired we perform the final step to evaluate the cell-based error estimator based on Eq. 4.38. The local errors are then sorted before refinement is performed.

The process is somewhat similar for Approximation 2, of which the most important step is the conversion of the LES flow solution to a RANS flow solution. First, the LES flow solution data $u_H$ at each time step is retrieved for the evaluation of the time-averaged quantities, including time-averaged velocity $\bar{u}_i$ and time-averaged stress tensor $\bar{S}_{ij}$ referring to Eq. 4.43 and 4.44. The calculation is realized through a serial loading of the pre-stored instantaneous LES flow solutions from disk into memory. Second, the fluctuation quantities $u'_i$ and $S'_{ij}$ for each time step are computed and stored locally using the instantaneous flow solution and the calculated time-averaged values. Third, an additional serial loading of the fluctuation quantities is performed to calculate the time-averaged quantities appearing on the right-hand-side of Eq. 4.44 (e.g. $\bar{\nu}_{tLES} S'_{ij}$ and $\bar{u}'_i u'_j$). We subsequently assemble the terms appearing in Eq. 4.44 and evaluate the RANS eddy viscosity $\nu_{tRANS}$. The complete converted RANS solution is then fully recovered. Fourth, we evaluate the linear adjoint system $\psi_H$ on the coarse grid based on the time-averaged RANS flow solution with PETSc-GMRES [3]. The coarse grid adjoint solution $\psi_H$ is then projected to the fine grid to obtain $\psi_h^H$. The cell-based error estimation is finally evaluated.
Chapter 5

Numerical Results

In this chapter, we validate the proposed feature- and adjoint-based error estimators through various numerical test cases (shown in Table 5.1). Section 5.1 validates the $IQ_k$-based (feature-based) error estimator through the periodic hill case and the SD7003 airfoil case. Section 5.2 shows the numerical validation for the proposed adjoint-based error estimator using the SD7003 case under three different flow conditions. All numerical validations are based on one complete grid adaptation cycle and the simulation results on the adapted grids are compared with experimental and reference numerical data.

5.1 $IQ_k$-based grid adaptation

In this section, the proposed feature-based error estimator is validated via the periodic hill and SD7003 airfoil test cases. The proposed methods for numerical TKE estimation

<table>
<thead>
<tr>
<th>Error estimator</th>
<th>Test cases</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feature ($IQ_k$)-based</td>
<td>Periodic hill</td>
</tr>
<tr>
<td></td>
<td>SD7003, $\alpha = 8^\circ$, $Re = 60,000$</td>
</tr>
<tr>
<td>Adjoint-based</td>
<td>SD7003, $\alpha = 4^\circ$, $Re = 22,000$</td>
</tr>
<tr>
<td></td>
<td>SD7003, $\alpha = 4^\circ$, $Re = 60,000$</td>
</tr>
<tr>
<td></td>
<td>SD7003, $\alpha = 8^\circ$, $Re = 60,000$</td>
</tr>
</tbody>
</table>
are compared against a classical empirical method. All three approaches were employed to develop a family of Index Quality error estimators: $IQ_{k-emp}$, $IQ_{k-ke}$, and $IQ_{k-tke}$ for LES. For both numerical test cases, the error estimators are applied to first predict the distribution of the numerical TKE then contours of Index Quality.

### 5.1.1 Periodic hill test case

**Introduction**

Our first test case is the periodic hill, whose geometry and grid are shown in figure 5.1, with periodic boundary conditions in both streamwise and spanwise directions, and no-
slip conditions are applied at the upper and lower boundaries. The Reynolds number based on the hill height and mean bulk velocity at the hill crest is \( Re = 10,600 \). A pressure forcing term [52] is added to the streamwise momentum and energy equations in order to drive the flow to maintain a constant Reynolds number during the simulation. The forcing term is initiated with \( f_{\rho U;init} = 0 \) at \( t = 0 \) and is corrected for each flow through period,

\[
f_{\rho U;new} = f_{\rho U;old} - \frac{m(\bar{U} - 1)}{U} f_{\rho U;old},
\]

(5.1)

where \( \bar{U} \) is the time-averaged streamwise velocity within the current flow through period and \( m = 1.7 \) is a constant estimated based on a friction factor analysis [52]. Similarly, the source term for the energy equation is as such, \( f_{\rho E} = U f_{\rho U} \). The flow is highly unsteady featuring separation from the continuous surface and the separation point oscillates over a large range on the wall. The mean flow is characterized by a separation bubble with an established separation and reattachment point. The form of the bubble depends on two factors: the position of the separation point and the turbulent intensity on the top of the bubble, which determines the level of energy exchange from the mean flow to the bubble region. The experimental data [9], an LES with wall function on a fine grid of 4.6M [98] and a very fine wall-resolved LES on 13.1M grid points [81] serve as the reference data.

Two levels of grids are available for the study. The coarse grid has \( 160 \times 160 \times 64 \) grid points, while the fine grid is refined from the coarse grid only in the spanwise direction with \( 160 \times 160 \times 128 \) grid points. The first layer of cells satisfies \( y^+ \approx 1 \), which ensures wall-resolved LES on both the upper and lower surfaces. The goal of the study is to apply the error estimators to the coarse grid based on the temporal and spanwise spatially averaged solution and refine only 5% of cells with the largest error.

**Flow solution**

The simulations were launched on coarse and fine grids for 100 flow through periods, and the flow field is averaged over 30 flow through periods in time and the spanwise direc-
Fig. 5.2 (a) shows the size of the separation bubble with the contour of the captured TKE. The coarse grid shows an early flow reattachment due to an over-estimation of the TKE level in the region above the separation bubble, the phenomenon is also reported in [98] for a coarse grid. A refinement in the spanwise direction allows for a lower TKE level and a better capture of the bubble length as shown in Fig. 5.2 (b).

Fig. 5.3 provides

<table>
<thead>
<tr>
<th>Grid</th>
<th>Size</th>
<th>((x/h)_{sep})</th>
<th>((x/h)_{reat})</th>
<th>(L_{bubble})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temmerman et al. [98]</td>
<td>4.6M</td>
<td>0.22</td>
<td>4.72</td>
<td>4.5</td>
</tr>
<tr>
<td>Breuer et al. [9]</td>
<td>13.1M</td>
<td>0.19</td>
<td>4.69</td>
<td>4.5</td>
</tr>
<tr>
<td>Coarse</td>
<td>1.6M</td>
<td>-0.93</td>
<td>4.06</td>
<td>4.99</td>
</tr>
<tr>
<td>Fine</td>
<td>3.3M</td>
<td>0.22</td>
<td>4.67</td>
<td>4.45</td>
</tr>
<tr>
<td>IQ(_\eta)-emp adapted</td>
<td>2.1M</td>
<td>0.14</td>
<td>3.95</td>
<td>3.81</td>
</tr>
<tr>
<td>IQ(_k)-emp adapted</td>
<td>2.1M</td>
<td>0.21</td>
<td>4.41</td>
<td>4.2</td>
</tr>
<tr>
<td>IQ(_k)-ke adapted</td>
<td>2.1M</td>
<td>-0.93</td>
<td>4.99</td>
<td>5.92</td>
</tr>
<tr>
<td>IQ(_k)-tke adapted</td>
<td>2.1M</td>
<td>0.22</td>
<td>4.55</td>
<td>4.35</td>
</tr>
</tbody>
</table>
further evidence that the coarse grid incorrectly captures a backflow layer on the top of the hill which is removed in the fine grid through spanwise refinement. Table 5.2 confirms that the coarse grid incorrectly predicts the separation point by estimating the separation prior to the top of the hill at a negative $X$ coordinate and predicts an early reattachment of the flow, while the fine grid shows good agreement with the reference LES data, even with comparatively smaller grid size.

**Evaluation of numerical TKE**

![Numerical dissipation](image)

**Figure 5.4:** Numerical dissipation, $\epsilon_n$, based on: (a) empirical approach; (b) KE-based approach; (c) TKE-based approach.

The numerical TKE $k_{\text{num}}$ is evaluated using all three approaches presented in Section 3.2. First, the time-averaged numerical dissipation, $\bar{\epsilon}_n$, is evaluated and the results are shown in Fig. 5.4. The results using the empirical formula, shown in the top-left-hand corner, only highlights the mixing layer above the separation bubble. The KE-based approach of Schranner et al. [89] highlights the intensively turbulent region near the separation point, while not targeting the mixing layer between $2 < X < 3.2$. The approach
Figure 5.5: Profile of contributions from different terms to KE numerical dissipation (Eq. 3.18, time-averaged) at: (a) $X = 0.5$; (b) $X = 4$.

Figure 5.6: Profile of contributions from different terms to TKE numerical dissipation (Eq. 3.37, time-averaged) at: (a) $X = 0.5$; (b) $X = 4$.

also shows high dissipation in a thin layer near the wall within the separation bubble $2 < X < 4$, and in a small near-wall region on the upstream side of the hilltop starting from $X \approx 8.5$, where flow separation starts to appear. Generally, the region between the
hills with $Y < 1$ shows positive numerical dissipation. Negative dissipation is shown in the region above the hill for $Y > 1$, where the convective flux dominates and the turbulence intensity is low, as discussed in Section 3.2.1. A similar trend was reported by Castiglioni and Domaradzki [12] who observed negative numerical dissipation in laminar regions far from the wall. In such regions a combination of low velocity gradients and an absence of a turbulent shear layer lead to a diminished role of the dissipation term, $\epsilon_n$, from Eq. 3.18. In addition, following Eq. 3.20 and as reported by [12] we observe a division of two small quantities ($\overline{\epsilon_n}$ and $S_{ij}\frac{du_i}{dx_j}$) which lead to unreasonable values of the numerical viscosity. Moreover the convective and pressure flux terms from Eq. 3.18 dominate over the turbulence dissipation and this eventually results in an estimation of negative numerical dissipation. Thus an application of Eq. 3.21 eliminates the impacted control volumes from adaptation. Lastly, we examine the developed TKE numerical dissipation from Fig. 5.4 (bottom). A quick survey of the contour and a comparison against the KE-based approach, reveals the removal of the negative numerical dissipation in the laminar region and an emphasis along the boundary layer and separated regions. As we traverse down towards the wall, the numerical dissipation begins to show higher value when approaching the mixing layer at the hill top level at $Y \approx 1$, where the production term, $P$, and the convective term, $F_k$, overwhelms the remaining contributions. As we approach the lower wall, the boundary layer is particularly highlighted, where the viscous and turbulent transport terms, $F_\nu$, as well as the dissipation terms, $\epsilon_\nu$ and $\epsilon_{\text{inter}}$, prevail due to high mean velocity gradients.

To provide a more thorough comparison between the KE-and TKE-based approaches, we plot and compare in Figs. 5.5 and 5.6 the contributions from all the terms in Eqs. 3.18 and 3.37 at two streamwise locations: at $X = 0.5$ shortly after the flow separation and $X = 4$ immediately before the flow reattachment. From Fig. 5.5 (a) at $X = 0.5$ as we trace from the lower to the upper wall, in the shear layer region of $Y \approx 1$ the KE numerical dissipation, $\epsilon_n$, reaches its maximum value, driven primarily by the convective term. As we move towards the upper wall the KE numerical dissipation is characterized by the
convective flux term as well as work due to pressure which results in a constant weak negative value. At $X = 4$, the KE numerical dissipation is dominated by the convective and pressure work terms which results in positive values in the lower turbulent region but negative in the upper largely laminar region. Fig. 5.6 shows the TKE numerical dissipation profile and the contributions from different items in Eq. 3.37 at the same positions of $X = 0.5$ and $X = 4$. It is observed in Fig. 5.6 (a) that at $X = 0.5$ the lower wall shows high TKE numerical dissipation contributed by the convection and production of TKE. The remaining terms play a minor role and all terms diminish as we move towards the upper wall. At the downstream location, $X = 4$, an equivalent observation is noted; however, the trends encompass a larger area. Comparing the two Figs. 5.5 and 5.6 the TKE based approach emphasizes the separated region. While the KE numerical dissipation is driven by the convection and pressure terms, the TKE approach is driven by the production and convection of TKE with a larger concentration on the boundary layer region.

![Figure 5.7: Numerical TKE, $k_{num}$, based on: (a) empirical approach; (b) KE-based approach; (c) TKE-based approach.](image)
Having established clear differences between the KE- and TKE-based approaches, we now center our discussion on the numerical TKE $k_{num}$ that is evaluated based on the empirical approach (Eq. 3.14), KE-based approach (Eq. 3.18), and TKE-based approach (Eq. 3.37) and we compare their contours in Fig. 5.7. As Eq. 3.14 demonstrates, the empirical approach is based on the modeled TKE and as such highlights the highly turbulent region, while diminishes as it approaches the wall. The empirical-based formula only shows elevated values in the mixing layer above the separation bubble with a peak value of 0.014, while the KE-based approach mainly targets the near-wall region in the separation bubble with a higher peak value of 0.044. The comparatively low numerical viscosity in the mixing layer leads to a low numerical TKE since the formula in Eq. 3.20 relates the numerical eddy viscosity, $\nu_{num}$, to the ratio between $\bar{\epsilon}_n$ and $S_{ij} \frac{\partial u_i}{\partial x_j}$. Although the mixing layer figures elevated values of numerical dissipation $\bar{\epsilon}_n; S_{ij} \frac{\partial u_i}{\partial x_j}$ also shows increased values in this turbulent region, resulting in largely low values of $k_{num}$. The TKE-based approach is able to target both the mixing layer and the boundary layer with a peak value of 0.013. The targeted boundary layer includes three domains, the separation point region, the reattachment point region, and a small near-wall region on the upstream side of the hill top region with $7.5 < X < 8.6$. The targeted regions are well aligned with the area with a high value of numerical dissipation, $\bar{\epsilon}_n$, as shown in Fig. 5.4.

**Error estimation**

In this subsection, we employ the three presented numerical TKE evaluation approaches within the Index Quality based error estimators: $IQ_\nu$, $IQ_\eta$, and $IQ_k$, leading to nine error estimators namely $IQ_{\nu,\eta,k-emp}$, $IQ_{\nu,\eta,k-ke}$ and $IQ_{\nu,\eta,k-tke}$. The error estimation based on the $IQ_\nu$ estimator are shown in Fig. 5.8. If we are to target the lowest quality region in the computational domain according to the error estimator, then the central region of the computational domain as well as a small region of the mixing layer near the separation point will require refinement. Three subfigures based on the three versions of $k_{num}$ lead to minimal differences in targeted regions. The $IQ_\nu$ estimator is a function of the ratio
Figure 5.8: Error estimation on coarse grid based on $IQ_\nu$ estimator using: (a) $IQ_\nu-\text{emp}$; (b) $IQ_\nu-\text{ke}$; (c) $IQ_\nu-\text{tke}$.

Figure 5.9: Error estimation on coarse grid based on $IQ_\eta$ estimator using: (a) $IQ_\eta-\text{emp}$; (b) $IQ_\eta-\text{ke}$; (c) $IQ_\eta-\text{tke}$.
between $\nu_{\text{eff}}$ and $\nu$ as shown in Eq. 3.1, thus only highly turbulent regions where $\nu_{\text{eff}}$ has large values will be identified. Without normalization against proper length and velocity scales, neither the turbulent shear layer near the separation point nor the boundary layer is targeted. It should be mentioned that the $IQ_{\nu-ke}$ estimator shows raised values in most of the computational domain outside the separation bubble region. These regions are mostly dominated by convection and the KE-based approach tends to estimate non-physical negative numerical dissipation, which is clipped by Eq. 3.21, leading to zero numerical TKE. As a consequence, following Eq. 3.2 and 3.3, $IQ_{\nu-ke}$ will have no contribution from $\nu_{\text{num}}$ in those regions and thus show steep values. Next, we present the $IQ_{\eta}$ error estimation in Fig. 5.9. The estimator targets domains similar to that of $IQ_{\nu}$; moreover, all versions of $k_{\text{num}}$ lead to very similar results.

![Figure 5.10:](image)

**Figure 5.10:** Error estimation on coarse grid based on $IQ_k$ estimator using: (a) $IQ_{k-emp}$; (b) $IQ_{k-ke}$; (c) $IQ_{k-tke}$.

Lastly, we present the $IQ_k$ error estimator in Fig. 5.10. The indicator $IQ_{k-emp}$ with the empirical formula of $k_{\text{num}}$ targets primarily the mixing layer above the separation bubble. The indicator $IQ_{k-ke}$ based on the evaluation of KE numerical dissipation provides
Figure 5.11: Automatically generated adapted grid based on: (a) $IQ_{\eta\text{-emp}}$; (b) $IQ_{k\text{-emp}}$; (c) $IQ_{k\text{-ke}}$; (d) $IQ_{k\text{-tke}}$.

an unexpected outcome, by exhibiting high values (over 90%) in most of the flow field and targets the near-wall region on the downstream side of the hill. Unlike $IQ_{k\text{-emp}}$, $IQ_{k\text{-ke}}$ does not target the mixing layer that is present above the separation bubble as a low-quality region, since the region is dominated by high strain rate and shows a low numerical eddy viscosity, $\nu_{\text{num}}$, and numerical TKE, $k_{\text{num}}$. The indicator $IQ_{k\text{-tke}}$ based on the TKE numerical dissipation targets both the mixing layer and the near-wall region, including the separation point and the reattachment point. Since the correct capture of TKE in those regions is essential for the correct prediction of the bubble length as shown in [98], the indicator $IQ_{k\text{-tke}}$ is expected to efficiently aid grid adaptation for LES.

Simulations on adapted grids

We have established that the three presented versions of $k_{\text{num}}$ does not lead to a clear difference in the regions targeted for grid adaptation for both $IQ_{\nu}$ and $IQ_{\eta}$, while $IQ_{k\text{-emp}}$
Figure 5.12: Separation bubble and TKE contour on: (a) $IQ_{\eta-emp}$ adapted grid; (b) $IQ_{k-emp}$ adapted grid; (c) $IQ_{k-ke}$ adapted grid; (d) $IQ_{k-tke}$ adapted grid.

$IQ_{k-ke}$ and $IQ_{k-tke}$ do target disparate regions. Hence, we decided to carry out a comparative study based on adapted grids generated by $IQ_{\eta-emp}$, $IQ_{k-emp}$, $IQ_{k-ke}$ and $IQ_{k-tke}$ as shown in Fig. 5.11, based on the largest 5% of the error levels of the original cells. The simulation was stabilized on the adapted grids for 90 flow through periods before making an average over the final 30 flow through periods to ensure a meaningful comparison.

Fig. 5.12 (a), (b), (c) and (d) show the TKE field and the separation bubble captured on the $IQ_{\eta-emp}$, $IQ_{k-emp}$, $IQ_{k-ke}$ and $IQ_{k-tke}$ adapted grids. It can be observed that the level of captured TKE on $IQ_{k-emp}$ and $IQ_{k-tke}$ adapted grids is significantly reduced compared to the value on the coarse grid shown in Fig. 5.2 (a), while the $IQ_{\eta-emp}$ and $IQ_{k-ke}$ adapted grid still captures a high level of TKE. As shown in Table 5.2, $IQ_{\eta-emp}$, $IQ_{k-emp}$ and $IQ_{k-tke}$ adapted grids improve the incorrect location of the separation point, while the $IQ_{k-ke}$ adapted grid still shows an incorrect separation location and provide for a larger separation bubble, whose reattachment point reaches 4.99. The $IQ_{\eta-emp}$ and $IQ_{k-emp}$ adapted grids underestimate the length of the separation bubble by predicting
Figure 5.13: Reynolds stress tensor components profiles at $X = 2$: (a) $u'u'$ profile; (b) $v'v'$ profile; (c) $u'v'$ profile; (d) TKE profile.

an early reattachment similar to that on the original coarse grid. The $IQ_{k-tke}$ adapted grid is able to predict the most accurate location of reattachment point at $X = 4.55$. This confirms again that the size of the separation depends on the turbulent intensity captured on the top of the bubble.
Figure 5.13 shows the profiles of the Reynolds stress tensor components and the TKE compared with the reference LES and the experimental data at the slice $X = 2$. The studied slice spans across the main flow and the bubble regions, and is characterized by a high TKE value in the mixing layer above the bubble. The coarse grid over-estimates all the components and wrongly captures the boundary layer while the fine grid shows great comparison against the reference data. It is observed that the $IQ_{q-\text{emp}}$ adapted grid does not provide a discernible improvement over the coarse grid; while, the $IQ_{k-\text{emp}}$ adapted grid shows an improvement of the captured TKE level in most of the computational domain, except for the lower wall region where an over-estimation of the TKE level is still observed.

Due to the fact that the empirical formula estimates the $k_{\text{num}}$ value based on $k_{\text{sgs}}$, which tends to zero as it approaches the wall, the value of $k_{\text{num}}$ is low in the near-wall region, leading to a high value of estimated $IQ_{k-\text{emp}}$. Therefore, even the separation and reattachment regions are not targeted for refinement, which could explain the over-estimation of the TKE near the reattachment point on the $IQ_{k-\text{emp}}$ adapted grid. $IQ_{k-ke}$ targets the high value of numerical TKE near the wall in the bubble region and leads to a refinement in the vicinity of the reattachment point, providing for an improvement in the captured TKE level near the wall, while showing an over-estimation of TKE in the mixing layer on the top region of the separation bubble. The $IQ_{k-tke}$ adapted grid outperforms the other estimators by targeting all the essential regions including the mixing layer and the boundary layer, and by capturing the correct length of the separation bubble as well as a better level of TKE profile in the whole computational domain.
5.1.2 SD7003 test case, $\alpha = 8^\circ, Re = 60,000$

![Figure 5.14: SD7003 case geometry and grid.](image)

Introduction

The SD7003 belongs to the SD family of low-Reynolds number airfoils [91] designed to minimize drag losses associated with the laminar separation bubble. The flow shows a laminar separation near the leading edge and transitions to turbulent flow before reattachment. The correct prediction of the separation bubble length relies on the correct prediction of the TKE level around the bubble. Our numerical test case is the SD7003 airfoil case with $Re = 60,000$ which has been widely studied in references [34, 102]. We mainly focus on the case at an angle of attack $\alpha = 8^\circ$, where the flow shows more turbulent features. The C-grid extends to approximately 25 chord lengths around the airfoil. The computational domain extends in the spanwise direction by $0.2c$ following Uranga et al. [102] who showed that a domain span of $0.2c$ was sufficient for capturing spanwise structures. An original coarse grid of 2.16M cells (shown in Fig. 5.14) and the correspondingly refined grid with 7.99M cells are studied for comparison. To ensure the flow reaches the statistically steady state, simulations are launched over nondimensionalized time $T = \frac{U}{c} = 120$, and the flow field is averaged in time over the final $T = 30$ and in the spanwise direction to evaluate the error estimators and perform requisite flow analysis. The proposed error estimators are then applied to the coarse grid in order to generate...
higher quality grids. Only a small percentage (5%) of the original grid cells are targeted and refined. The goal is to target critical regions where the grid refinement will lead to an improvement of the simulation quality, including the prediction of lift and drag coefficients and the structure of the separation bubble, with less additional computational cost compared to the fine grid.

Flow solution

Results on two levels of grids are available in Table 5.3, compared with the reference LES [34, 111] and experimental [90, 91] results. There are two key observations. First, the noted range for the aerodynamic coefficients in the experimental data is due to differences in the spanwise boundary setup [90]. Radespiel et al. [80] reported that the non-two-dimensional wake flow pattern results in a strong influence of the spanwise measurement position on the drag coefficient. Hence, due to the uncertainty in the measured

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Table 5.3: Feature-based grid adaptation: case summary for SD7003, \( Re = 60,000, \alpha = 4^\circ \).

<table>
<thead>
<tr>
<th>Simulation</th>
<th>DOF</th>
<th>Sep.</th>
<th>Reat.</th>
<th>Length</th>
<th>( C_i )</th>
<th>( C_d )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Garmann et al. [34]</td>
<td>54M</td>
<td>0.031</td>
<td>0.303</td>
<td>0.272</td>
<td>0.917</td>
<td>0.0447</td>
</tr>
<tr>
<td>Vermeire et al. [111]</td>
<td>2.3M</td>
<td>0.031</td>
<td>0.345</td>
<td>0.314</td>
<td>0.946</td>
<td>0.0529</td>
</tr>
<tr>
<td>Selig et al. [90, 91]</td>
<td>Exp</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.88 ( \sim ) 0.95</td>
<td>0.03 ( \sim ) 0.04</td>
</tr>
<tr>
<td>Coarse</td>
<td></td>
<td>2.16M</td>
<td>0.1368</td>
<td>0.4451</td>
<td>0.3083</td>
<td>0.9618</td>
</tr>
<tr>
<td>Fine</td>
<td>7.99M</td>
<td>0.0201</td>
<td>0.3349</td>
<td>0.3148</td>
<td>0.9433</td>
<td>0.05273</td>
</tr>
<tr>
<td>( IQ_{k-\text{emp}} ) adapted</td>
<td></td>
<td>2.76M</td>
<td>0.1062</td>
<td>0.3473</td>
<td>0.2411</td>
<td>0.9246</td>
</tr>
<tr>
<td>( IQ_{k-\text{ke}} ) adapted</td>
<td></td>
<td>2.76M</td>
<td>0.1214</td>
<td>0.4225</td>
<td>0.3011</td>
<td>0.9395</td>
</tr>
<tr>
<td>( IQ_{k-\text{tke}} ) adapted</td>
<td></td>
<td>2.76M</td>
<td>0.0430</td>
<td>0.3026</td>
<td>0.2596</td>
<td>0.9193</td>
</tr>
</tbody>
</table>

Table 5.4: Feature-based grid adaptation: grids information for SD7003 cases.

<table>
<thead>
<tr>
<th>Simulation</th>
<th>DOF</th>
<th>( \Delta s^+ )</th>
<th>( \Delta n^+ )</th>
<th>( \Delta z^+ )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Garmann et al. [34]</td>
<td>54M</td>
<td>( \approx 10 )</td>
<td>( \approx 0.2 )(^1)</td>
<td>( \approx 10 )</td>
</tr>
<tr>
<td>Uranga et al. [102]</td>
<td>1.8M</td>
<td>-</td>
<td>( \approx 2.0 )</td>
<td>( \approx 53 )</td>
</tr>
<tr>
<td>Vermeire et al. [111]</td>
<td>2.3M</td>
<td>( \approx 22 )</td>
<td>( \approx 0.6 )</td>
<td>( \approx 20 )</td>
</tr>
<tr>
<td>Coarse</td>
<td>2.16M</td>
<td>( \approx 24 )</td>
<td>( \approx 3 )</td>
<td>( \approx 40 )</td>
</tr>
<tr>
<td>Fine</td>
<td>7.99M</td>
<td>( \approx 17 )</td>
<td>( \approx 1 )</td>
<td>( \approx 20 )</td>
</tr>
<tr>
<td>adapted</td>
<td>2.76M</td>
<td>( \approx 12 )</td>
<td>( \approx 1.5 )</td>
<td>( \approx 20 )</td>
</tr>
</tbody>
</table>

---

\(^1\)Value from [34] is based on maximum \( \Delta n^+ \).
Figure 5.15: Separation bubble and TKE contour on: (a) coarse grid; (b) fine grid; (c) $I Q_{k-emp}$ adapted grid; (d) $I Q_{ke}$ adapted grid; (e) $I Q_{tke}$ adapted grid.

coefficients, two reliable LES results [34, 111] are used as benchmark values. Second, there is relatively good agreement between the two LES benchmark values [34, 111] in terms of the separation point but less so on the reattachment point, and lift and drag coefficients. We believe differences in the computational grid setup may have contributed to the observed differences. Garmann et al. [34] reported that the grid resolution in the vicinity of the separation was a strong influence on the proper capture of the flow field.
and provided values for the minimum non-dimensional normal distance at the streamwise location \( x/c = 0.1 \). We have tabulated the data in Table 5.4 and compared the values against other references as well as results achieved in this work. The normal distance of the first solution point off the surface of the airfoil is calculated as \( \Delta n^+ = u_r y / \nu \) where \( u_r = \sqrt{C_f / 2 U_\infty} \) and \( C_f \approx 0.01 \) at the streamwise location \( x/c = 0.1 \) [102]. The measure of the cell resolution for the streamwise \( (\Delta s^+) \) and spanwise \( (\Delta z^+) \) directions are calculated in the same way and given in Table 5.4. Garmann et al. [34] studied three levels of grids ranging from 6.7M to 12M and adopted a large computational domain extending to 100 chord lengths. As shown in Table 5.4 the boundary layer is extremely refined for the grid used in [34] with a \( \Delta n^+ \approx 0.2 \). However, Uranga et al. [102] showed that a much coarser grid was able to provide sufficient resolution for the test case through a grid study using implicit LES, where they employed a grid with a computational domain that extended to 6 chord lengths with 1.8M degrees of freedom (DOF) and a \( \Delta n^+ \approx 2 \) at \( x/c = 0.1 \). A validation of our in-house code for \( \alpha = 4^\circ \) resulted in \( C_l \) and \( C_d \) coefficients within 3% of difference from [102]. Following [102], Vermeire et al. [111] adopted the same computational domain with a finer grid resulting to a \( \Delta n^+ \approx 0.6 \) at \( x/c = 0.1 \). Based on the computational grids adopted in [34, 102, 111], we employed a computational domain that stretched to 25 chord lengths, 2.16M DOF, and a \( \Delta n^+ \approx 3 \) to serve as our coarse grid while the fine grid would be approximately 7.99M DOF and a \( \Delta n^+ \approx 1 \). As expected, our coarse grid estimates a delayed separation and reattachment of the flow, and also overestimates the lift coefficient \( C_l \) and underestimates the drag coefficient \( C_d \) compared to the fine grid and the reference LES results. The fine grid shows an overestimation of both \( C_l \) and \( C_d \) compared to [34], but show excellent agreement against [111]. The presented results highlight a strong correlation between the bubble length and the aerodynamic performance coefficients. Both the reported fine grid and [111] have equivalent bubble lengths and hence comparable \( C_l \) and \( C_d \) values. Fig. 5.15 (a) and (b) present the size of the separation bubble along with the contour of the captured TKE on the coarse and fine grids. Fig. 5.15 (c) to (e) present flow solutions on adapted grids. These results will be
discussed in a subsequent Section 5.1.2. The delay and overestimation of the length of
the separation bubble on the coarse grid are due to the incorrect delayed prediction of the
transition point and an underestimation of the turbulence level above the bubble region.
As a result, the boundary layer is incorrectly captured on the coarse grid which leads to
the observed errors in $C_l$ and $C_d$. The corresponding fine grid is able to better capture the
separation bubble with a correct length as shown in Fig. 5.15 (b) and Table 5.3.

**Evaluation of numerical TKE**

In order to provide for the Index Quality on the coarse grid, the numerical TKE is esti-
mated based on the three approaches presented in Section 3.2. It is observed in Fig. 5.16
that all three approaches only show positive values of the numerical TKE and highlight
similar regions that include the leading edge area and the shear layer on top of the sep-
aration bubble starting at $X \approx 0.2$ where flow transitions to be turbulent. The main
difference relies on the captured $k_{num}$ value level and the boundary layer. The KE-based
approach shows a comparatively higher value of numerical TKE compared to other ap-
proaches. The TKE-based approach is able to highlight the near-wall region on the upper
surface of the airfoil after the transition, especially targeting the boundary layer on the
upper surface for a high value of numerical TKE even though the modeled TKE is low
in the boundary layer; while both the empirical and KE-based approaches fail to flag the
boundary layer. Recalling that the KE-based approach estimates the numerical eddy vis-
cosity $\nu_{num}$ based on the ratio between $\bar{\epsilon}_n$ and $S_{ij} \frac{\partial u_i}{\partial x_j}$ as shown in Eq. 3.20, the high value
of $S_{ij} \frac{\partial u_i}{\partial x_j}$ in the boundary layer due to a large velocity gradient actually leads to a low
estimated value of numerical eddy viscosity $\nu_{num}$, resulting in a low value of estimated
$k_{num}$ following Eq. 3.3.

**Error estimation**

As shown in Fig. 5.17, all three error estimators target the stagnation point, as well as the
turbulent region in the shear layer above the separation bubble where high values of nu-
Figure 5.16: Numerical dissipation, $\epsilon_{nn}$, based on: (a) empirical approach; (b) KE-based approach; (c) TKE-based approach.

Numerical TKE is estimated. $IQ_{k-ke}$ targets an even larger region above the separation bubble compared to the other error estimators; where, some of the cells along block interfaces are featured due to irregular transitioning between block faces. In the case of $IQ_{k-tke}$, it targets the boundary layer on the upper surface due to elevated levels of numerical TKE as well as the entire separation bubble including the laminar separation point. It should
be mentioned that the family of Index Quality error estimators is grounded on the assumption that the flow is in a fully turbulent regime [17], while in the studied case, the region $X < 0.2$ is laminar where both captured and modeled TKE show low values, such that the performance of the estimators in such regions primarily depends on the estimation of numerical TKE. The adapted grids are generated based on a 5% refinement from the coarse grid and Fig. 5.18 gives an overview of the adapted grids based on three error
estimators. As we can see the wake region is targeted by all the error estimators due to its turbulent nature. Since we are more interested in the performance of the error estimators in the near-wall region, we present the zoom-in view of the adapted grids in Fig. 5.19 for the three error estimators.

![Figure 5.18: Far view of (a) $IQ_{k-emp}$ adapted grid; (c) $IQ_{k-ke}$ adapted grid; (d) $IQ_{k-tke}$ adapted grid.](image)

**Figure 5.18:** Far view of (a) $IQ_{k-emp}$ adapted grid; (c) $IQ_{k-ke}$ adapted grid; (d) $IQ_{k-tke}$ adapted grid.
Figure 5.19: Close view of (a) $IQ_{k-emp}$ adapted grid; (c) $IQ_{k-ke}$ adapted grid; (d) $IQ_{k-tke}$ adapted grid.

Figure 5.20: Profile lines normal to the airfoil surface located at $0.1c$ through $0.5c$. 

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Simulation on adapted grids

The simulation was carried out on the adapted grids and the results are presented in Table 5.3 and Fig. 5.15. It is observed that the location of the separation and reattachment points are improved on all adapted grids, which led to earlier separation and reattachment compared to the coarse grid. Fig. 5.15 shows that $IQ_{k-emp}$ and $IQ_{k-tke}$ perform better than $IQ_{k-ke}$ in terms of the prediction of the location, the length and the thickness of the separation bubble, as well as the location of the transition to turbulence, while the $IQ_{k-emp}$ adapted grid overestimates the level of TKE. The correct capture of the location and the size of the separation bubble highly depends on the correct estimation of the TKE level. The $C_l$ and $C_d$ values tended toward the fine grid results as expected; however, the $IQ_{k-tke}$ provided values that are in good agreement against [34] instead of the fine grid. This is primarily due to a separation length that is more in line with [34].

Profiles normal to the wall are studied in five different locations as shown in Fig. 5.20. The profiles are taken every $0.1c$ at $X = 0.1$ to 0.5 and provide an insight into the size of the separated region. The streamwise mean velocity $U$ and the squared fluctuations $u'u'$ are studied at the stated locations and compared against the reference values. Fig. 5.21 shows that the $IQ_{k-tke}$ adapted grid leads to the best prediction of the mean velocity at all five locations by providing results close to that on the fine grid and reference LES. Fig. 5.21 (c) shows that the flow is reattached at $X = 0.3$ for the $IQ_{k-tke}$ adapted grid similar to the reference LES, while other grids still show backflow in the boundary layer. The octree data structure in the code results in the refinement of the targeted cells by a factor of 8, such that the adapted grids are in fact finer than the fine grid in the targeted regions. The $u'u'$ profiles are shown in Fig. 5.22. We observe that at $X = 0.1$, only the $IQ_{k-tke}$ adapted grid is able to estimate the correct level of TKE. At a downstream location of $X = 0.2$, the coarse grid and the $IQ_{k-ke}$ adapted grid show very low level of captured $u'u'$ and fail to predict the start of transition. The $IQ_{k-tke}$ adapted grid also underestimates the level of TKE at this location. Further downstream at $X = 0.3$, which is near the flow reattachment, the $IQ_{k-tke}$ adapted grid captures $u'u'$ at the same level as reference LES [34].
while other grids show either an overestimation ($IQ_{k−ke}$ adapted grid and fine grid) or an underestimation ($IQ_{k−emp}$ adapted grid and coarse grid). At the downstream locations $X = 0.4$ and $X = 0.5$ the $IQ_{k−tke}$ adapted grid compares well against the reference LES and fine grid values, and outperforms $IQ_{k−emp}$ and $IQ_{k−ke}$ adapted grids.

The history of lift and drag coefficients during $T = 20$ is also studied on the coarse, fine and adapted grids and results are shown in Fig. 5.23 and 5.24. All simulations have reached statistically steady state. The coarse grid shows the highest peak $C_l$ and lowest peak $C_d$ among all five grids. All adapted grids lead to a reduced $C_l$ value and an increased $C_d$ value. $IQ_{k−emp}$ adapted grid shows a periodic $C_d$ spike due to the predicted vortex shedding. The prediction of the lift and drag are highly dependent on the correct capture of the flow structure within the bubble. The $IQ_{k−tke}$ adapted grid provides a stable prediction and improvement of both $C_l$ and $C_d$ by the refinement in the turbulent mixing layer and boundary layer for better capture of the separation bubble.
Figure 5.21: Streamwise mean velocity $U$ profiles at (a) $X = 0.1$; (b) $X = 0.2$; (c) $X = 0.3$; (d) $X = 0.4$; (e) $X = 0.5$. 
Figure 5.22: $u'u'$ profiles at (a) $X = 0.1$; (b) $X = 0.2$; (c) $X = 0.3$; (d) $X = 0.4$; (e) $X = 0.5$. 
Figure 5.23: Time-history of the lift coefficient on coarse, fine and adapted grids.

Figure 5.24: Time-history of the drag coefficient on coarse, fine and adapted grids.
5.2 Adjoint-based grid adaptation

In this section, the numerical validation on the SD 7003 airfoil case under various flow conditions are used to validate the proposed adjoint-based error estimator, which includes the entire grid adaptation pipeline and a grid convergence study. The geometry and basic grids are explained in detail in section 5.1.2 and shown in Fig. 5.14. Our numerical validation comprises of three flow conditions: first, at a Reynolds number of $Re = 22,000$ and angle of attack $\alpha = 4^\circ$; the second, at $Re = 60,000$ and $\alpha = 4^\circ$ and the third, at $Re = 60,000$ and $\alpha = 8^\circ$. It should be mentioned that instead of using a high order scheme and implicit LES as employed by authors [34,102,111], we adopted a second-order finite volume scheme with a WALE SGS model, and as such we performed our numerical investigation on a larger computational grid. The resolution of the boundary layer in our study is similar to that in reference [102]. To ensure the flow reaches statistically steady state, simulations are launched over nondimensionalized time $T = \frac{U}{c} = 120$, and the flow field is averaged in time over the final $T = 30$ and in the spanwise direction to evaluate the error estimators and perform requisite flow analysis. The proposed adjoint-based error estimators are then applied to the coarse grid in order to generate higher quality grids. We use the total drag on the airfoil as the objective function. The goal is to target critical regions where grid refinement will lead to an improvement of the solution quality, especially the objective function, with less additional computational cost.

Profiles normal to the wall are used to study the near-wall behaviors of the captured flow in different locations as shown in Fig. 5.25. The profiles are taken every $0.1c$ from $X = 0.1$ to $1.0$ and provide an insight into the size of the separated region. The streamwise mean velocity $U$
Table 5.5: Adjoint-based grid adaptation: case summary for SD7003, $Re = 22,000$, $\alpha = 4^\circ$.

<table>
<thead>
<tr>
<th>Simulation</th>
<th>DOF</th>
<th>Sep.</th>
<th>Reat.</th>
<th>Length</th>
<th>$C_l$</th>
<th>$C_d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uranga et al. [102]</td>
<td>1.85M</td>
<td>0.2239</td>
<td>0.9378</td>
<td>0.7139</td>
<td>0.6458</td>
<td>0.0429</td>
</tr>
<tr>
<td>Coarse</td>
<td>2.16M</td>
<td>0.1974</td>
<td>0.9040</td>
<td>0.7066</td>
<td>0.6264</td>
<td>0.0430</td>
</tr>
<tr>
<td>Fine</td>
<td>7.99M</td>
<td>0.2262</td>
<td>0.9493</td>
<td>0.7231</td>
<td>0.6568</td>
<td>0.0423</td>
</tr>
<tr>
<td>Adjoint-adapted (ap1)</td>
<td>2.76M</td>
<td>0.2510</td>
<td>0.9168</td>
<td>0.6658</td>
<td>0.6305</td>
<td>0.0421</td>
</tr>
<tr>
<td>Adjoint-adapted (ap2)</td>
<td>2.76M</td>
<td>0.2463</td>
<td>0.8937</td>
<td>0.6474</td>
<td>0.6143</td>
<td>0.0402</td>
</tr>
</tbody>
</table>

and the squared fluctuations $u'u'$ are studied at the stated locations and compared against the reference values.

5.2.1 SD7003 test case, $\alpha = 4^\circ$, $Re = 22,000$

Flow solution

Results on two levels of grids are available in Table 5.5, compared with the reference LES [102] result. As we can see, there is good agreement between our results on both coarse and fine grids and the LES benchmark values [102] in terms of the separation and reattachment point, as well as lift and drag coefficients. Under the current Reynolds number of 22,000 both coarse and fine grids have sufficient resolution with the first layer cell at a $\Delta n^+ < 1$ such that the boundary layer is well resolved. The fine grid shows slightly better agreement against the reference LES values [102] while the coarse grid estimates an early separation and reattachment of the flow, and also underestimates the lift coefficient $C_l$ and overestimates the drag coefficient $C_d$ compared to the fine grid and the reference LES results. Fig. 5.26 (a) and (b) present the size of the separation bubble along with the streamwise velocity contour on the coarse and fine grids and a zoom-in view of the comparison between the bubble shape on coarse and fine grids is shown in Fig. 5.27 (a) and (b). It can be observed that although the difference is minimal, a higher thickness of the separation bubble near the reattachment point is captured by the fine grid. Fig. 5.27 (c) and (d) as well as Fig. 5.26 (c) and (d) present flow solutions on adjoint-based adapted grids. These results will be discussed in a subsequent Section 5.2.1. The wall
normal streamwise velocity profiles are illustrated in Fig. 5.28, where despite a minimal difference at \( X = 0.2 \), the velocity profiles gradually diverge as we traverse from the leading edge while the general trend is consistent. Most notable is the larger separation observed at \( X = 0.8 \) for the fine grid.

![Streamwise velocity profiles](image)

**Figure 5.26**: Streamwise velocity \( U \) contour and separation bubble for \( Re = 22,000 \) and \( \alpha = 4^\circ \) on (a) coarse grid; (b) fine grid; (c) adjoint-based adapted grid based on approximation 1; (d) adjoint-based adapted grid based on approximation 2.
Figure 5.27: Zoom-in view of streamwise velocity $U$ contour and separation bubble for $Re = 22,000$ and $\alpha = 4^\circ$ on (a) coarse grid; (b) fine grid; (c) adjoint-based adapted grid based on approximation 1; (d) adjoint-based adapted grid based on approximation 2.

Unsteady adjoint evaluation

Applying the two unsteady adjoint approximations presented in Chapter 4, the adjoint $\psi_{h,n}^H$ contours for the components that correspond respectively to the $\rho$, $\rho U$, $\rho V$ and $\rho E$ are shown in Fig. 5.29 for approximation 1 and Fig. 5.30 for approximation 2. The adjoint solution provides the sensitivity of the objective function to local residuals. For example, Fig. 5.29 (b) highlights the presence of non-zero values for the $x$-momentum adjoint in
the vicinity of the leading and trailing edges as well as along the upper surface of the airfoil. These regions experience large changes in the $x$-component of the velocity gradient where both flow deceleration at the leading edge and acceleration over the upper surfaces have a considerable impact on the pressure distribution and hence the drag coefficient. As for Fig. 5.29 (c), apart from the leading and trailing edges, the $y$-momentum adjoint emphasizes the aft region on the upper surface in the proximate location of the separation bubble.

**Figure 5.28:** Streamwise velocity $U$ profile for $Re = 22,000$ and $\alpha = 4^\circ$ at (a) $X = 0.2$; (b) $X = 0.4$; (c) $X = 0.6$; (d) $X = 0.8$. 
Figure 5.29: Adjoint solution for (a) $\rho$, (b) $\rho U$, (c) $\rho V$, and (d) $\rho E$ for $Re = 22,000$ and $\alpha = 4^\circ$ using approximation 1.

Generally, the targeted regions by the two approaches are similar with a more pronounced concentration by approximation 1. Both approximations provide for a smooth adjoint solution throughout the computational domain. The $x$-momentum adjoint shows a slight difference between the two approximations, where approximation 1 highlights the entire near-wall region on the upper surface, while approximation 2 primarily targets the front half of the near-wall region and omits the boundary layer on the aft part of the air-
Figure 5.30: Adjoint solution for (a) $\rho$, (b) $\rho U$, (c) $\rho V$, and (d) $\rho E$ for $Re = 22,000$ and $\alpha = 4^\circ$ using approximation 2.

foil. As for the $y$-momentum adjoint, there is a larger emphasis on the aft upper surface by approximation 1.

Error estimation

The time-averaged residual on the fine grid of the projected solution $\overline{R}_h(u^H)$ used for both approximations is shown in Fig. 5.31. The derivation of the local error estimate as shown in subsection 4.1 through 4.3 was based on the assumption that the coarse grid
solution satisfies the unsteady residual at each time step, $R^*_H(u_H)$ exactly and hence for a statistically steady flow, we should expect the time-averaged residual on the coarse grid $\bar{R}_H(u_H)$ to be at machine precision; however, in practise this is not feasible. For the results presented in this work, $\bar{R}_H(u_H)$ is approximately three orders of magnitude smaller than $\bar{R}_h(u^H_h)$. This ensures that the dual-weighted time-averaged residual that provides for the local error estimate is sufficiently accurate to provide the proper trends for the purpose of grid adaptation.
Elevated levels of the residual typically start from the region of separation and continue into the turbulent wake for all four variables. The near-wall region close to the leading edge especially shows steep values for the $\rho E$ residual; where, flow deceleration and energy dissipation occur. The error estimation based on the computable correction are shown in Fig. 5.32 for approximation 1 and in Fig. 5.33 for approximation 2. The error estimation provides an indication of the highly sensitive regions where the grid refinement contributes to the accurate resolution of the objective function.

Figure 5.32: Adjoint-based error estimation and adapted grid for $Re = 22,000$ and $\alpha = 4^o$ using approximation 1.

Compared to the time-averaged residual value shown in Fig. 5.31, the error estimation based on the dual-weighted residual (Fig. 5.32 and Fig. 5.33) instead highlights the leading edge and trailing edge regions, along the boundary layer, as well as the turbulent mixing layer above the separation bubble. The boundary layer on most of the upper surface is targeted. Both approximations demonstrate very similar error estimation results, where approximation 2 stresses more of the wake region due to a lower adjoint solution value in the aforementioned region. The case figures a laminar separation bubble which transitions to turbulent flow after flow separation and reattaches on the upper surface of the airfoil. The correct capture of the size and position of the separation bubble, as well
as the capture of the boundary layer play an important role in the prediction of the drag coefficient.

**Simulation on adapted grids**

Two adapted grids are generated based on a 5% refinement according to both approximations as shown in Fig. 5.32 and 5.33. The simulation was stabilized on the adapted grids until statistically steady state and the time-averaged results are shown in Table 5.5. It is observed that the location of the separation point moves upstream on both adapted grids compared to the coarse grid, while the *approximation 1* adapted grid performs better than the *approximation 2* adapted grid in terms of the predicted location of the reattachment point. Both approximations lead to a lower predicted value of the drag coefficient compared to the coarse grid, but only *approximation 1* shows improvement on both $C_l$ and $C_d$ values which align well with our fine grid and the reference LES results. *Approximation 2* adapted grid leads to an underestimation of both $C_l$ and $C_d$, due to an underestimation of the separation bubble length. The error estimator aims to target critical regions which lead to a precise prediction of the objective function, the total drag, and the prediction
of the drag is highly dependent on the correct capture of the flow structure inside the bubble. The detail of the separation bubble near reattachment is shown in Fig 5.27. It is shown that approximation 1 is able to predict a later reattachment and a thicker bubble, which is close to the bubble captured on the fine grid, while the bubble length and thickness on approximation 2 is closer to the coarse grid. Fig. 5.28 shows the streamwise velocity profiles on the upper surface along the separation bubble at $X = 0.2, 0.4, 0.6$ and $0.8$. It is shown that both adapted grids lead to an obvious improvement of the captured velocity at $X = 0.2, 0.4$ and $0.6$ compared to the coarse grid. At position $X = 0.8$, the solution to the adapted grid based on approximation 2 remains as it was with the coarse grid, while the profile captured on approximation 1 agrees perfectly with our fine grid, which indicates a better prediction of the flow structure in the separation bubble near reattachment. Fig. 5.34 demonstrates the profile of Reynolds stress tensor components in the streamwise direction $u'u'$ at $X = 0.2, 0.4, 0.6$ and $0.8$ (location shown in Fig. 5.25). It is seen that the coarse grid overestimates $u'u'$ at all four locations. Both adapted grids are able to capture $u'u'$ at the correct level and the location of the peak value at all stations, especially at $X = 0.2$ and $0.4$ where, approximation 1 is more inline with the results of the fine grid.
Figure 5.34: $u'u'$ profile for $Re = 22,000$ and $\alpha = 4^\circ$ at (a) $X = 0.2$; (b) $X = 0.4$; (c) $X = 0.6$; (d) $X = 0.8$. 
Table 5.6: Adjoint-based grid adaptation: case summary for SD7003, Re = 60,000, α = 4°.

<table>
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<th>Simulation</th>
<th>Size</th>
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<th>Reat.</th>
<th>Length</th>
<th>$C_l$</th>
<th>$C_d$</th>
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<td>0.666</td>
<td>0.459</td>
<td>0.612</td>
<td>0.0241</td>
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<td>Vermeire et al. [111]</td>
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<td>0.480</td>
<td>0.608</td>
<td>0.0247</td>
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<td>Galbraith and Visbal [32]</td>
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<td>0.65</td>
<td>0.42</td>
<td>0.59</td>
<td>0.021</td>
</tr>
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<td>Skarolek and Miyaji [93]</td>
<td>2.0M</td>
<td>0.201</td>
<td>0.657</td>
<td>0.456</td>
<td>0.599</td>
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</tr>
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<td>0.5876</td>
<td>0.3876</td>
<td>0.5736</td>
<td>0.0226</td>
</tr>
<tr>
<td>Fine</td>
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<td>0.1969</td>
<td>0.6631</td>
<td>0.4662</td>
<td>0.6098</td>
<td>0.0227</td>
</tr>
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<td>2.76M</td>
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<td>0.5887</td>
<td>0.3999</td>
<td>0.5790</td>
<td>0.0233</td>
</tr>
<tr>
<td>Adjoint-adapted 7%</td>
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<td>0.5863</td>
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<td>0.5890</td>
<td>0.0227</td>
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<tr>
<td>Adjoint-adapted 12%</td>
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<td>0.5980</td>
<td>0.4200</td>
<td>0.6023</td>
<td>0.0227</td>
</tr>
</tbody>
</table>

5.2.2 SD7003 test case, α = 4°, Re = 60,000

Flow solution

We revisit the test case but now increase the Reynolds number to 60,000 while keeping the angle of attack at 4 degrees. The case attracts more interest, since it requires finer cells to resolve the boundary layer and the transitional behavior of the separation bubble. Table 5.6 shows the time-averaged flow solution on our coarse and fine grids, compared with the reference LES [32, 93, 102, 109] results. Compared to the lower Reynolds number case shown in Fig. 5.26, the higher Reynolds number case figures a smaller separation bubble, since transition occurs sooner, leading to an earlier flow reattachment. Generally the reference LES results in [102, 111] show good agreement in the flow separation, reattachment location, lift and drag coefficients. Our fine grid shows perfect agreement with the LES benchmark values where the predicted separation and reattachment point, as well as lift and drag coefficients are all in acceptable range. The coarse grid provides for a reasonable prediction of the drag coefficient, but underestimates the separation bubble length by predicting an early reattachment of the flow, and also underestimates the lift coefficient $C_l$. As expected, there is a larger difference between the coarse and fine grid results compared to that observed for the lower Reynolds number case. At Re = 60,000, the coarse grid is insufficient to accurately resolve the boundary layer with the first layer
Figure 5.35: Adjoint solution for (a) $\rho$, (b) $\rho U$, (c) $\rho V$, and (d) $\rho E$ for $Re = 60,000$ and $\alpha = 4^\circ$ using approximation 1.

cell at $\Delta n^+ \approx 3$, and Fig. 5.39 (a) and (b) present the size of the separation bubble along with the streamwise velocity contour on the coarse and fine grids.

Unsteady adjoint evaluation

Since both approximations provide similar error estimation for the test case with $Re = 22,000$ and $\alpha = 4^\circ$, and the approximation 1 adapted grid performed better than the approximation 2 adapted grid as shown in subsection 5.2.1, we decided to only focus on approximation 1 presented in section 4.2 for the current case. The contours of the adjoint solution
Figure 5.36: Absolute value of time-averaged residual of (a) $\rho$, (b) $\rho U$, (c) $\rho V$, and (d) $\rho E$ for $Re = 60,000$ and $\alpha = 4^\circ$.

$\psi_{h,n}^H$ are shown in Fig. 5.35. Compared to the adjoint solution at a lower Reynolds flow condition shown in Fig. 5.29, the current flow condition figures higher value of the adjoint solution. The highlighted areas are generally similar but all variables target smaller regions closer to the airfoil along with a decrease in the boundary layer thickness due to the increase of the Reynolds number.
Figure 5.37: Adjoint-based error estimation for $Re = 60,000$ and $\alpha = 4^\circ$ using approximation 1.

Error estimation

The time-averaged residual on the fine grid of the projected solution $\overline{R}_h(u_h^f)$ is shown in Fig. 5.36. Large values are found in the turbulent wake region for all four variables $\rho$, $\rho U$, $\rho V$, and $\rho E$ but the wake is narrower compared to the case with $Re = 22,000$ and $\alpha = 4^\circ$ shown in Fig. 5.31. The near-wall region close to the leading edge shows especially elevated values for the $\rho E$ residual, where flow deceleration and energy dissipation occur. The adjoint-based error estimation was carried out for approximation 1 and the result is shown in Fig. 5.37. Compared to the error estimation result for the case with $Re = 22,000$ and $\alpha = 4^\circ$ shown in Fig. 5.33, the error estimation highlights a narrow region especially focusing on both the upper and lower airfoil surface, as well as the turbulent mixing layer above the separation bubble. The boundary layer on most of the upper surface and part of the lower surface is targeted. The wake region with $X > 1.3$ is omitted due to the low value of the adjoint solution as shown in Fig. 5.37.
Simulation on adapted grids

In order to provide for a more detailed study of the error estimator. Four adapted grids are generated based on a 5%, 7%, 10% and 12% refinement according to the error estimation result and the generated grids are shown in Fig. 5.38. The simulations on the adapted grids were stabilized until statistically steady state and the resulting time-averaged flow separation bubble location, as well as the lift and drag coefficients, are shown in Table 5.6.
Figure 5.39: Streamwise velocity $U$ contour and separation bubble for $Re = 60,000$ and $\alpha = 4^\circ$ on (a) coarse grid; (b) fine grid; (c) adjoint-based adapted grid with 5\% refinement; (d) adjoint-based adapted grid with 7\% refinement; (e) adjoint-based adapted grid with 10\% refinement; (f) adjoint-based adapted grid with 12\% refinement.
and Fig. 5.39 (c) through (f). It is observed that the coarse grid already captures well
the drag coefficient and all adapted grids show similar values. The coarse grid shows
a clear underestimation of the lift coefficient. With an increased refinement percentage
from 5% to 12%, the captured lift coefficient increases gradually and converges to the
value captured by the fine grid and the reference LES result when the refinement per-
centage reaches 12%. The convergence trend of the lift and drag coefficient is further
illustrated in Fig. 5.40. It is shown in Table 5.6 that the coarse grid predicts an early flow
reattachment, thus a short separation bubble. The adapted grids with 5% to 10% refine-
ment do not show clear improvement in terms of the predicted flow reattachment location
as well as the length of the separation bubble, while the adapted grid with 12% refinement
demonstrates a delayed flow reattachment compared to the other adapted grids, but the
predicted bubble length is still shorter than the fine grid and the reference LES results.

Fig. 5.41 provides for more insight on the flow structure in the near-wall region, espe-
cially in the separation bubble, with the streamwise velocity profiles at $X = 0.2, 0.3, 0.4,$
$0.6, 0.8$ and $0.9$ (location shown in Fig. 5.25). At $X = 0.2$ the difference between the ve-
locity profile captured by the coarse and fine grids is minimal. Coarse grid shows a slight
underestimation of the streamwise mean velocity $U$ in the boundary layer. All adapted
grids show similar flow behavior compared to the fine grids. From $X = 0.3$ we can ob-
serve the flow separation and a more obvious underestimation of $U$ on the coarse grid, as
well as the improvement provided by the adapted grids. Similar flow behavior is shown
at $X = 0.4$ where the $U$ profile captured by all the four adapted grids align well with the
fine grid result. At $X = 0.6$ the fine grid shows a backflow in the near-wall region while
on the coarse grid the flow reattachment occurs before the location at $X = 0.6$, thus the
coarse grid always predicts a positive $U$ profile at the location $X = 0.6$. The adapted grids
show a velocity profile similar to the coarse grid, which confirms the incorrect prediction
of the early reattachment. At further downstream locations of $X = 0.8$ and $X = 0.9$,
the coarse grid provides for an underestimation of the streamwise mean velocity $U$ com-
Figure 5.40: Grid convergence study for (a) $C_l$ and (b) $C_d$ for adjoint-adapted grids, compared with fine grid benchmark.

Compared to the fine grid results, and all adapted grids are able to show an improvement and provide for comparable results against the fine grid.

The profile of the Reynolds stress component $u'u'$ is studied at the same chordwise locations and the comparison is shown in Fig. 5.42. At the start of flow separation $X = 0.2$, the coarse grid has an overestimation of turbulence by estimating a value of $u'u'$ one order
Figure 5.41: Streamwise velocity $U$ profile for $Re = 60,000$ and $\alpha = 4^\circ$ at (a) $X = 0.2$; (b) $X = 0.3$; (c) $X = 0.4$; (d) $X = 0.6$; (e) $X = 0.8$; (f) $X = 0.9$.

higher than the prediction on the fine grid. The 5%, 7%, and 10% refined grids are able to avoid the overestimation of $u' u'$ as shown in 5.42 (a), but their predictions are below
Figure 5.42: $u'v'$ profile for $Re = 60,000$ and $\alpha = 4^\circ$ at (a) $X = 0.2$; (b) $X = 0.3$; (c) $X = 0.4$; (d) $X = 0.6$; (e) $X = 0.8$; (f) $X = 0.9$.

the value captured by the fine grid. However, at the 12% refinement, the solution is in perfect alignment with the fine grid prediction. Similar behavior is observed at location
$X = 0.3$ and $X = 0.4$ before the flow reattachment. At locations $X = 0.6, 0.8$ and $0.9$ which are situated near or after the flow reattachment, an underestimation of the $u'u'$ value is observed on the coarse grid and the adapted grids are able to capture an increased level of $u'u'$ and provide for more comparable results to the fine grid.

### 5.2.3 SD7003 test case, $\alpha = 8^\circ, Re = 60,000$

In this subsection we maintain the Reynolds number at 60,000 but increase the angle of attack to 8 degrees. This flow condition has been employed for the numerical validation of our feature-based error estimator in subsection 5.1.2. Compared to the lower angle of attack flow condition studied in section 5.2.2, the higher angle of attack case figures an even shorter but thicker separation bubble, with even earlier transition and flow reattachment. The flow condition serves to demonstrate the advantage of fast convergence of integral quantities on adapted grids provided by the adjoint-based error estimator over feature-based and manually refined grids.

$IQ_{k-tke}$ is a feature-based error estimator for LES which evaluates the local grid quality by a cell-based Index Quality (IQ) [17]. The detailed derivation is presented in section 3.2. Briefly speaking, the TKE equation is employed to estimate the impact of the inherent numerical dissipation on the capture of the local TKE, which is then employed to evaluate the effective TKE to build a family of Index Quality-based error estimators. In summary, the $IQ_{k-tke}$ error estimator provides the percentage of resolved over total TKE with a proper consideration of the impact brought by numerical dissipation. The numerical validation in section 5.1 demonstrates its advantages over traditional feature-based error estimators for a better capture of pertinent flow features and estimation of local numerical and modeling errors. As discussed in subsection 5.1.2 and 5.2.2, the first layer cell on the manually generated coarse grid has a $\Delta n^+ \approx 3$, thus it is unable to sufficiently resolve the boundary layer. Therefore, we decided to also study a series of manually refined grids especially focusing on the near-wall region for comparison against the adjoint-based adapted grids.
Figure 5.43: Streamwise velocity $U$ contour and separation bubble for $Re = 60,000$ and $\alpha = 8^\circ$ on (a) coarse grid; (b) fine grid.

Flow solution

The flow solution on two levels of grids are available in Table 5.7, compared with the reference LES [34,111]. As mentioned in subsection 5.1.2, although experimental results are available in [90,91], the measured aerodynamic coefficients in the experimental data show great discrepancy due to differences in the spanwise boundary setup [90]. It is reported in [80] that the non two-dimensional wake flow pattern results in a strong influence of the spanwise measurement position on the drag coefficient and causes some uncertainty in the measured lift and drag coefficients. Hence we used two reliable LES results [34,111] as benchmark values. Our coarse grid estimates a delayed separation and reattachment of the flow, and also overestimates the lift coefficient $C_l$ and underestimates the drag coefficient $C_d$ compared to the fine grid and the reference LES results. The fine grid shows an overestimation of both $C_l$ and $C_d$ compared to [34], but shows excellent agreement against [111]. The presented results highlight a strong correlation between the bubble length and the aerodynamic performance coefficients. Both the reported fine grid and [111] have equivalent bubble lengths and hence comparable $C_l$ and $C_d$ values.
### Table 5.7: Adjoint-based grid adaptation: case summary for SD7003, $Re = 60,000, \alpha = 8^\circ$.

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</tr>
<tr>
<td>Manually adapted 7%</td>
<td>3M</td>
<td>0.0317</td>
<td>0.2837</td>
<td>0.2520</td>
<td>0.9012</td>
<td>0.0461</td>
</tr>
<tr>
<td>Manually adapted 10%</td>
<td>3.36M</td>
<td>0.0308</td>
<td>0.2709</td>
<td>0.2401</td>
<td>0.9353</td>
<td>0.0465</td>
</tr>
<tr>
<td>Manually adapted 12%</td>
<td>3.6M</td>
<td>0.0322</td>
<td>0.2579</td>
<td>0.2257</td>
<td>0.9463</td>
<td>0.0458</td>
</tr>
</tbody>
</table>

Fig. 5.43 presents the size of the separation bubble along with the contour of the captured TKE on the coarse and fine grids. The delay and overestimation of the length of the separation bubble on the coarse grid are due to the incorrect prediction of the transition point and an underestimation of the turbulence level above the bubble region. As a result, the boundary layer is incorrectly captured on the coarse grid which leads to the observed errors in $C_l$ and $C_d$. The corresponding fine grid is able to better capture the separation bubble with a correct length as shown in Fig. 5.43 (b) and Table 5.7.

**Unsteady adjoint evaluation**

The contours of the adjoint solution $\psi_{h,n}^H$ are shown in Fig. 5.44. when compared to the corresponding solution at a lower angle of attack shown in Fig. 5.35. The $x$-momentum adjoint is more pronounced on the aft part of the airfoil; while the $y$-momentum and energy-adjoints show similar results compared to the $\alpha = 4^\circ$ case (Fig. 5.35). Since the
Figure 5.44: Adjoint solution for (a) $\rho$, (b) $\rho U$, (c) $\rho V$ and (d) $\rho E$ for $Re = 60,000$ and $\alpha = 8^\circ$ using approximation 1.

flow condition figures a thicker but shorter separation bubble, the density-adjoint solution features a shorter but more prominent region, $0 < X < 0.4$ on the upper surface.

Error estimation

The time-averaged residual on the fine grid of the projected solution $\overline{R}_h(u_h^H)$ is shown in Fig. 5.45. As detailed in subsection 5.2.1, the time-averaged residual on the coarse grid $\overline{R}_H(u_H)$ is three orders of magnitude lower than $\overline{R}_h(u_h^H)$ and hence the local error estimate is adequate for the aim of mesh adaptation. Comparing the case with $Re =$
60,000 and $\alpha = 4^\circ$ shown in Fig. 5.36, the main difference is that the leading edge area exhibits very high values of residual for all four variables. At the larger angle of attack, the separation point is shifted closer to the leading edge and the transition is triggered sooner, leading to a wider turbulent mixing layer above the airfoil and a thicker wake region. The error estimation is shown in Fig. 5.46, where the largest errors are prevalent in the leading edge, the separation bubble and the mixing layer; predominantly in regions with abrupt changes in the pressure gradient.

![Figure 5.45](image)

**Figure 5.45:** Absolute value of time-averaged residual of (a) $\rho$, (b) $\rho U$, (c) $\rho V$ and (d) $\rho E$ for $Re = 60,000$ and $\alpha = 8^\circ$ using approximation 1.
Figure 5.46: Adjoint-based error estimation and adapted grid using approximation 1.

Grid convergence study

For the current case, a thorough grid study is carried out for three error estimators: Adjoint, $IQ_{k-tke}$ [53] and wall-distance based. The primary study is based on the proposed adjoint-based error estimator with six adapted grids generated with refinements from 1% to 15%, and the goal is to research the convergence trend of the flow features and the integral quantity including the lift and drag coefficients. All grid refinements are based on the adjoint-based error estimation shown in Fig. 5.46 and the generated grids are shown in Fig. 5.47. For comparison, six adapted grids generated using the $IQ_{k-tke}$ error estimator [53] with the same refinement percentages are carried out as shown in Fig. 5.48. We also present a series of manually refined grids based on wall-distance with refinement percentages from 5% to 12% as a baseline comparison for grid adaptation, as shown in Fig. 5.49, to demonstrate the efficiency of adjoint-based error estimator in targeting the critical regions to improve the accuracy of a chosen integrated function. This strategy was chosen instead of a complete uniform refinement to ensure the total grid size is still
Figure 5.47: Adjoint-based adapted grid for $Re = 60,000, \alpha = 8^\circ$ based on (a) 1%, (b) 5%, (c) 7%, (d) 10%, (e) 12% and (f) 15% refinement.
Figure 5.48: $IQ_{k-tke}$-based adapted grid for $Re = 60,000$, $\alpha = 8^\circ$ based on (a) 1%, (b) 5%, (c) 7%, (d) 10%, (e) 12% and (f) 15% refinement.
Figure 5.49: Adapted grids based on wall distance (a) 5% refinement, (b) 7% refinement, (c) 10% refinement, (d) 12% refinement.

manageable. As we can see, the adjoint-based error estimator primarily targets the region above the upper surface. The $IQ_{k-tke}$ based adapted grids tend to highly refine the wake of the airfoil, due to the turbulent nature of the region, which leads to high modeled and numerical TKE [53].

The simulations on all the adapted grids were stabilized until statistically steady state. The grid convergence of the separation bubble location as well as the lift and drag coefficients for all three series of grids are shown in Table 5.7. Fig. 5.50 further illustrates a comparison of the convergence trends of the adapted grid based on the three error estimators. It can be observed that the adjoint-based adapted grids show a more rapid convergence of the captured separation bubble for refinements above 7% comparing to the $IQ_{k-tke}$
Figure 5.50: Grid convergence study for (a) flow separation and (b) flow reattachment location on adjoint-, $IQ_{k-tke}$- and wall distance-adapted grids.

and wall-distance adapted grids; where, we observe that both the flow separation and reattachment points remain the same even with further grid refinement. Fig. 5.51 shows the time-averaged TKE contour on adjoint-based adapted grids and confirms the same convergence trend by showing the TKE level stabilized as the grid is refined based on the adjoint-based error estimator. In comparison, the $IQ_{k-tke}$ based adapted grids show a
Figure 5.51: Captured TKE and separation bubble on adjoint-based adapted grid based on (a) 1%, (b) 5%, (c) 7%, (d) 10%, (e) 12% and (f) 15% refinement.
Figure 5.52: Grid convergence study for (a) $C_l$ and (b) $C_d$ for adjoint-, $IQ_k$-tke- and wall distance-adapted grids.

trend of delayed flow reattachment as the grid is refined to 5%. As the grid is further refined, the size of the separation bubble converges to a length of 0.2965 at 15% refinement. The separation bubble based on the wall-distance adapted grids also show a convergence trend while with a lower convergence rate than that of the adjoint-based adapted grids.
Fig. 5.52 shows the $C_l$ and $C_d$ trends with respect to the grid refinement on three series of adapted grids. All three series of grids lead to a similar final value of $C_l$ and $C_d$ as the grid is refined; however, the adjoint-based adapted grids does converge to the final value at a higher rate and the same is true for the drag coefficient, $C_d$.

The near-wall flow behaviors on the adjoint-based adapted grids are further studied. Profiles at $X = 0.1$ to 0.5 (location shown in Fig. 5.25) are illustrated in Fig. 5.53 and 5.54. We will investigate the impact of the grid refinement based on three critical observations: first, the location and size of the separation; second, the velocity gradient in the vicinity of the wall; and third, the maximum velocity. At $X = 0.1$, the separation is well underway since the reference LES values [34, 111] place the point of separation at 0.031. A 5% grid refinement with 2.76M grid points provides for a solution that is comparable across the boundary layer to that achieved by the fine grid solution with approximately 8M points. The same is observed at the other chordwise locations and most notably at $X = 0.3$ and $X = 0.4$. Fig. 5.53 (c) provides a clear illustration of the impact of grid refinement. Here the coarse grid shows a thick layer of backflow with a negative $U$ value, whereas the 5% refined grid agrees exactly with the fine grid; while the 7% to 15% refined grids show very similar behavior and good agreement against the reference LES, indicating a convergence of the flow pattern. The octree data structure in the code results in the refinement of the targeted cells by a factor of 8, such that the adapted grids are in fact finer than the fine grid in the targeted regions. As the percentage of refined grids are increased further to 7%, the trend at all chordwise locations is towards the reference LES data [34]. As for the velocity gradient, a 1% refinement is insufficient to provide the proper capture of the boundary layer; however with at least 5% refinement the wall velocity gradient compares well against the benchmark except at $X = 0.3$ where 7% is required. Lastly, we investigate the maximum velocity achieved as that observed in Fig. 5.25). Similar to that seen for the velocity gradient, with at least a 7% refinement, the velocity distributions tend towards the LES benchmark values. The computational cost as a percentage of the flow solve for the adjoint-based and $IQ_{k-\text{tke}}$-based error estimation are compared in Tables 5.8 and 5.9.
Figure 5.53: Streamwise velocity $U$ profile for $Re = 60,000$ and $\alpha = 8^\circ$ at (a) $X = 0.1$; (b) $X = 0.2$; (c) $X = 0.3$; (d) $X = 0.4$; (e) $X = 0.5$. 
Table 5.8: Computational cost for adjoint-based grid adaptation process.

<table>
<thead>
<tr>
<th>Steps in grid adaptation process</th>
<th>Time Cost (% of one flow solve)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Evaluation of ( \frac{\partial R_h}{\partial u_h} \bigg</td>
<td>_{u^H_h} ) and ( \frac{\partial J_h}{\partial u_h} \bigg</td>
</tr>
<tr>
<td>Time averaging ( \frac{\partial R_h}{\partial u_h} \bigg</td>
<td>_{u^H_h} ) and ( \frac{\partial J_h}{\partial u_h} \bigg</td>
</tr>
<tr>
<td>Adjoint Linear Solve</td>
<td>3%</td>
</tr>
<tr>
<td>Evaluation of ( R_h(u^H_h) )</td>
<td>1%</td>
</tr>
<tr>
<td>Total Cost</td>
<td>12%</td>
</tr>
</tbody>
</table>

Table 5.9: Computational cost for \( I Q_{k-tke} \)-based grid adaptation process.

<table>
<thead>
<tr>
<th>Steps in grid adaptation process</th>
<th>Time Cost (% of one flow solve)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Evaluation of numerical dissipation ( \epsilon_n ) at each time step</td>
<td>3%</td>
</tr>
<tr>
<td>Evaluation of time-averaged flow solution ( \bar{u}_i )</td>
<td>1%</td>
</tr>
<tr>
<td>Evaluation of captured and modeled TKE, ( k_{res} ) and ( k_{mod} )</td>
<td>1%</td>
</tr>
<tr>
<td>Evaluation of numerical TKE, ( k_{num} )</td>
<td>1%</td>
</tr>
<tr>
<td>Total Cost</td>
<td>6%</td>
</tr>
</tbody>
</table>

For the presented cases, one flow solve amounts to 100 flow-through periods that were used to arrive at statistically steady state solutions. There are two main observations. First, although the adjoint-based grid adaptation shows an increased cost than that of the \( I Q_{k-tke} \)-based grid adaptation, both approaches still only represent a negligible cost compared to the LES flow solver. Second, most of the computational cost for the adjoint-based grid adaptation resides on the write-to-disk of the flow Jacobian and the sensitivity of the functional, which could be further improved by an in-memory computation pipeline.

To provide a more thorough impact of the grid refinement on the flow statistics, we compare the Reynolds stress tensor component, \( u'u' \) at the same chordwise locations in Fig. 5.54. At a location \( X = 0.2 \) the coarse grid underestimates the turbulence level while the 1% refined grid significantly increases the estimated turbulence as shown in Fig. 5.54 (b), while a higher refinement percentage leads to the convergence of the cap-
tured turbulence level. The fine grid result provides for the correct distribution and magnitude for the Reynolds stress over the coarse grid; however, the refined grids approach the LES benchmark values both in terms of the peak magnitude and location. This is evident in Fig. 5.54 (b) where with even with a 5% refinement the results are markedly better than that of the fine grid. This characteristic is repeated at all subsequent chordwise stations.
Figure 5.54: \( u'u' \) profile for \( Re = 60,000 \) and \( \alpha = 8^\circ \) at (a) \( X = 0.1 \); (b) \( X = 0.2 \); (c) \( X = 0.3 \); (d) \( X = 0.4 \); (e) \( X = 0.5 \).
Chapter 6

Conclusion and Future Work

This chapter presents the main conclusions which can be drawn from this research. It highlights the contributions and key aspects of the proposed error estimators for LES grid adaptation and lists several topics which remain open for future work.

6.1 Feature-Based Error Estimation for LES

In the first part of this work, we focus on proposing a feature-based error estimator for LES grid adaptation. Two new approaches are proposed to evaluate the numerical TKE and estimate the Index Quality for LES grid adaptation. The first approach relies on the numerical dissipation of the kinetic energy equation (KE-based approach) and demonstrated promising outcomes but its propensity to result in negative values in laminar regions reduced its effectiveness. The second approach relies on the numerical dissipation of the turbulent kinetic energy equation (TKE-based approach) for LES. The latter approach overcame the shortcomings of the KE-based technique by stressing high numerical dissipation within boundary layers and turbulent regions. The proposed methods were compared against a classical empirical method for evaluating the numerical TKE. All three approaches were employed to develop a family of Index Quality error estimators: $IQ_{k-emp}$, $IQ_{k-ke}$, and $IQ_{k-tke}$ for LES. Its capabilities were demonstrated for the
periodic hill and the SD7003 airfoil test cases, where we contrasted their differences by first studying the distribution of the numerical TKE then contours of Index Quality. All three IQ error estimators target the shear layer and turbulent mixing layer on the top of the separation bubble for the periodic hill and the separated region for the SD 7003 airfoil. However, the developed $IQ_{k-tke}$ added the boundary layer and reduced if not eliminated the tendency of the KE-based approach from producing negative numerical dissipation.

One complete grid adaptation cycle is performed for both test cases. Generally, the adapted grids based on all error estimators are able to improve the quality of the LES results. The $IQ_{k-emp}$ estimator was able to target the turbulent mixing layer and the adapted grid improved the size of the separation bubble; however, the estimator failed to target the boundary layer. Unlike the empirical approach, the $IQ_{k-ke}$ estimator was able to target the near-wall region however previously confirmed reports [12] of negative values were observed. As such the estimator failed to target the laminar separation bubble in the SD7003 case. We found that the $IQ_{k-tke}$ estimator was able to balance the refinement between the mixing layer above the bubble and the boundary layer for both cases, which led to the best performance in terms of capturing correctly the Reynolds stress tensor component values and the length of the separation bubble on the corresponding adapted grid.

6.2 Adjoint-Based Error Estimation for LES

In the second part of this work, a novel approach has been proposed for developing an adjoint-based error estimator for grid adaptation for LES. Two approximation methods are proposed, namely approximation 1 and approximation 2, to solve the adjoint problem for statistically steady LES flows, aiming to reduce the computational cost and ensure stability. The former approach builds a single-solve adjoint equation based on the time-averaged residual and the time-averaged objective function. The approach requires the storage of the time-averaged Jacobian and the sensitivity of the functional in a forward
time integration and avoids the need to solve an unsteady adjoint. The latter approach relies on converting the unsteady flow solution obtained by LES to a RANS-type steady flow solution, and perform the steady adjoint-based error estimation for the converted solution. Both approximations lead to a single-solve adjoint equation and improve largely the storage and computational cost. The involvement of the time-averaging process in a chaotic system ensures the convergence of the adjoint solver.

Numerical validation was carried out using the SD7003 case under two different flow conditions and one complete grid adaptation cycle was performed. It is observed under $Re = 22,000$ and $\alpha = 4^\circ$ that the approximation 1-generated grid outperforms the approximation 2-generated grid for better capture of the flow structure in the separation bubble as well as a better prediction of the integral quantity. Three error estimators, including the manual-, feature- and adjoint-based estimators, were applied to the flow condition $Re = 60,000$ to generate a series of grids with increasing refinement percentages. It is observed from a grid convergence study that the adjoint-based adapted grid provides for fast convergence of the integral quantity; specifically, the total lift and drag coefficients. The proposed adjoint-based error estimator is able to target the leading and trailing edge regions, the boundary layer near the separation and reattachment points as well as the transitional region, which helps the correct prediction of the length and reattachment of the separation bubble.

6.3 Future Work

This dissertation developed an automatic grid adaptation system based on feature- and adjoint-based error estimators. Their cost efficiency and performance, as well as their potential to be applied to industrial cases are demonstrated for various numerical test cases. At the same time, the current study possesses several limitations and the following future work could greatly advance grid adaptation for LES based on the proposed feature- and adjoint-based error estimators:
• In the current thesis, the numerical validations for both feature- and adjoint-based error estimators focus on moderate Reynolds number cases (with $Re$ ranging from $1 \times 10^4$ to $6 \times 10^4$) with homogeneous flow conditions in the spanwise direction. Further validation could employ more complex flow conditions, including three-dimensional flows with greater inhomogeneous spanwise variations or highly compressible flows with the presence of shocks.

• In the framework of the current dissertation, the flow solver is performed using the octree data structure, but the linear solver for the local numerical TKE (feature-based error estimation) and for the adjoint equation (adjoint-based error estimation) are based on structured grids, which limits the current validation to a single level refinement. Future work will extend all the current linear solvers to an octree data structure and perform multiple adaptation cycles and quantify and compare the results against the benchmark refined grids.

• We focused on quantifying the local error by a scalar value using isotropic error estimators and performed the grid adaptation using the octree data structure. Further extension will include developing anisotropic feature- and adjoint-based error estimators based on the current work and extend the current octree data structure to a binary tree data structure in order to include directional information.

• The current adjoint-based grid adaptation pipeline is based on storing a total number of $N$ flow Jacobians and sensitivities of the functional on disk. Future work will consider the use of checkpointing to avoid the need to store the entire flow history but strike a balance between minimizing the storage cost while increasing the computational time to evaluate the time-averaged Jacobian for the adjoint system.
Bibliography


