ABSTRACT

METTU, BALACHANDRA REDDY. Wall Modeled LES of Compressible Flows in Non-Equilibrium Conditions. (Under the direction of Pramod Subbareddy.)

A turbulent boundary layer is composed of a wide range of length scales and time scales. To resolve all these scales of motion, as with a DNS or traditional wall resolved LES, the grid sizes required scale roughly as the square/cube of the Reynolds number (Re). These requirements make high Re flows computationally very expensive. By modeling the effect of the motions close to the wall, as is proposed in wall modeled LES (WMLES) methods, the computation of high Re flows can be made significantly cheaper. To date, WMLES has been relatively less studied in application with strong compressibility effects.

In this study, we implement state-of-the-art wall models for these flows and examine the different challenges which are common to high-speed flow applications: isothermal cold wall conditions, the transition to turbulence, and shock boundary layer interactions (SBLI). It is observed that for cold-wall flows, a more empirical “mixed” scaling for the length scale appearing in the eddy viscosity formulation outperforms the classical semi-local scaling for obtaining predictions of heat-flux and skin-friction. For transitional flows, we develop a modified transition sensor that gave robust predictions for the high Mach number cases we examined. We find that the more computationally expensive non-equilibrium model with an eddy viscosity formulation based on the pressure gradient outperformed the standard equilibrium model for skin-friction predictions in SBLIs. A sensor for detecting regions of non-equilibrium flow was developed based on the resolved Reynolds stress. By using this sensor and switching to an exchange location closer to the wall in the non-equilibrium region for the equilibrium model gave skin-friction and heat flux results close to or even better than the non-equilibrium model at a far cheaper cost. WMLES was performed for SBLI at moderate to high Re with different wall temperature conditions. It was observed that WMLES was able to capture the expansion and shrinking of the separation bubble size when the wall was heated and cooled. Also observed was that using WMLES the low-frequency characteristics of SBLI at high Re was now possible. As a whole, it was seen that WMLES can become a promising tool for exploring the complex physics involved in turbulent high-speed flows at a significantly lower cost than wall resolved LES/DNS and with much higher fidelity compared to pure RANS simulations.

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Wall Modeled LES of Compressible Flows in Non-Equilibrium Conditions

by
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CHAPTER 1

Introduction

1.1 Motivation

The rapid growth in computational power and development of accurate numerical discretization methods in the last few decades has made computational fluid dynamics (CFD) a vital tool for research and industrial design. The current industry standards for turbulence modeling in CFD are still dictated by RANS (Reynolds Averaged Navier-Stokes) methods which suffer from low fidelity when faced with predicting complex turbulent flows that include phenomena such as crossflow, transition, separation, and shock boundary layer interactions (SBLI). Large eddy simulation (LES) has gained prominence in recent years to accurately simulate turbulent flow. Its use, however, has been largely limited to academic research at low Reynolds numbers (Re). For high Re flows commonly seen in industrial applications, LES becomes computationally infeasible due to the strict grid resolution requirements in the near-wall region. It was predicted by Spalart [74] that a wall resolved LES (WRLES) of a full aircraft at flight conditions might require more than 10^{11} grid points and 10^7 time steps. This high computational cost is mainly due to the need to resolve small-scale energy-carrying motions near the wall: a large fraction of the cells in the computational domain are used to resolve the near-wall region of the boundary layer. Figure 1.1 shows an instantaneous snapshot of temperature contours taken from a direct numerical simulation (DNS) of a turbulent boundary layer. The scales of motion near the wall become smaller and a more refined grid is needed to resolve these motions. At high Re, close to 90% of the grid cells are used to model this inner layer region (defined as $y^+ < 100$ or as $y/\delta < 0.15$, approximately) which spans a small fraction of the boundary layer. Note that the wall-normal distance y normalized by wall units is

Figure 1.1 Density contours from a slice extracted from the DNS of a turbulent boundary layer by Pirozzoli et al. [62]. To fully resolve all the motions in a DNS the grid scales as a Re^3 . The grid for resolving just the outer motions in the boundary layer scales linearly with Re whereas to resolve the thinner and streaky inner motions the grid scales as Re^2 . The inner scales are also more universal thus can be more easily for different flow scenarios.

defined as $y^+ = yu_\tau/\nu_w$, where $u_\tau = \sqrt{\tau_w/\rho_w}$, the friction velocity, is computed from the shear stress τ_w , kinematic viscosity ν_w and density ρ_w computed at the wall.

Figure 1.2 reproduces results from a grid requirement study by Choi & Moin [17] who show that the number of cells needed to resolve the inner layer scales as $Re^{13/7}$: a nearly quadratic dependence on the Re . The cost of direct numerical simulation (DNS), which is the most accurate tool available for simulating turbulent flow is even more prohibitive as the grid size scales as $Re^{37/14}$. As mentioned above, the Re^2 scaling of the grid size is imposed by the small dynamically important eddies close to the wall. One approach to circumventing this quadratic dependence of the grid size on Re for LES is to model the inner layer flow physics using a wall model and resolve just the outer layer motions which have a linear dependence with Re . The outer layer structures are presumed to be resolvable with grid spacings that are a (fixed) fraction of the outer length scale (boundary layer thickness, δ). The resulting grid sizes will then scale linearly with Re which makes these simulations much more feasible in practice.

Wall-Modeled LES (WMLES) has been applied extensively to canonical cases such as channels and adiabatic boundary layers. However, its utility in simulating flows in the compressible regime where significant heat transfer effects are present, for example in isothermal, cold wall cases or high Mach number ($M > 5.0$) SBLIs, is less well understood. RANS methods are known to produce poor predictions when it comes to high-speed separation and transition without extensive and case-specific tuning. For example, the various lines in the heat flux plot shown in figure 1.3 correspond to a blind comparison

Figure 1.2 The number of grid points (N) needed to resolve a turbulent boundary layer using LES as a function of Re is shown above. The above plot shows the significant cost reduction at high Re when resolving just the outer layer motions in a LES.

between experiments done at CUBRC and RANS simulations by various groups using different codes and models. This particular comparison is a Mach 6 flow on a cone-flare geometry, and the heat flux comparison near the shock interaction region is highlighted. The RANS results show a lot of uncertainty in terms of the separation length and the peak heat transfer. Another important aspect of these flows is the presence of cold walls (by which we mean that the ratio of the wall temperature to the adiabatic recovery temperature, (T_w/T_r) is small). The velocity scaling laws for boundary layers developing over cold walls are relatively less well understood and the temperature profile in such cases is non-canonical. By contrast, for adiabatic boundary layers, well-known transformations (van Driest) collapse the velocity profiles onto their incompressible counterparts. A preliminary calculation estimates that wall-resolved simulations at such conditions would require grids on the order of a billion cells. With wall modeling such high Reynolds number cases are more easily accessible. The broad question the current study would like to address is whether we can use WMLES to bridge the gap between CFD and experiments at conditions such as these.

Figure 1.3 The above plot corresponds to a blind comparison between experiments and CFD for a cone-flare geometry close to the SBLI region. Symbols denote experimental data obtained from experiments done by the CUBRC group. Lines denote RANS simulations performed by various CFD groups.

1.2 Overview of WMLES

1.2.1 Classifying Wall Models

Most wall models borrow ideas from the RANS theory to represent the inner layer motions. Paraphrasing Piomelli & Balaras [59] when the near-wall is grid coarse enough that it contains a large number of eddies, their average effect must be represented by the wall model. When the number of near-wall eddies in a grid cell is large enough and also the time step is much larger than the time-scale characteristic of these eddies, the inner layer can be assumed to be governed by the RANS equations, rather than the filtered Navier-Stokes equations solved in LES in the outer layer. This idea of a different set of equations being valid in different regions of the flow forms the basis of wall modeling methods.

The different wall modeling approaches which try to model the inner layer can be classified broadly into hybrid RANS-LES and WMLES methods. A broad schematic of various methods is shown in figure 1.4. The classic hybrid RANS-LES methods use a RANS model in the attached boundary layer region (or in severely under-resolved regions), and away from it, or in detached shear layers, they switch to LES. Seamless models like

Figure 1.4 A schematic illustrating the hierarchy of different methods of modeling the near-wall region.

DES [73] and its extensions (DDES [75], IDDES [69]) do this dynamically, where some combination of local grid size, distance to the wall, and the solution itself are used to construct switches between these two modes. With zonal DES approaches, the RANS and LES portions are fixed in the domain [21, 55]. The grids used for these methods are resolved in the wall-normal directions, with the requirement that the first cell spacing, $y_1^+ \approx 1$ is used as a guide to constructing the grid. The streamwise and spanwise grid spacings are set to resolve the outer length scale (like the boundary layer thickness; e.g. $\Delta x \approx 0.1\delta$, where x is the streamwise direction, δ is the local boundary layer thickness).

WMLES approaches are different in that the LES domain is defined conventionally up to the wall and the wall model is essentially used to supply boundary conditions to the LES. With wall-stress modeling methods, these boundary conditions are the shear stress and heat flux at the wall. The important distinction here is that the outer LES grid is not (inner-scaling) resolved in the wall-normal direction and the grid spacings in all three directions are scaled on outer length scales. An important practical aspect to be noted is that high aspect ratio cells typically used near the wall in wall-resolved approaches restrict the stable explicit time step due to the Courant–Friedrichs–Lewy (CFL) condition: consequently, implicit time-stepping schemes that can overcome the CFL

limit are often needed. These methods can be quite diffusive and are therefore not ideal for use in LES simulations where it is important to preserve the small-scale structure. Therefore, a wall-modeling approach that can stably employ reasonably large, stable, explicit time steps can be greatly advantageous.

1.2.2 Wall-Stress Modeling Methods

The most commonly used WMLES approaches, the wall-stress modeling methods, compute the wall shear stress, τ_w , and heat flux, q_w , by either numerically solving the full Reynolds averaged Navier-Stokes (RANS) equations near the wall, or a reduced set of boundary layer equations without the “non-equilibrium” terms (these are the unsteady, pressure gradient and convective terms) [43, 85, 18, 8, 4]. Since WMLES grids are coarse near the wall, LES by itself is not able to capture the sharp near-wall gradients that are common to turbulent flows. To overcome this, the wall model provides a viscous flux boundary condition for the LES in the form of τ_w and q_w by using instantaneous or time-filtered data at some location(s) from the LES field. In the present study, we use two variants of wall stress modeling: the *equilibrium model* solves a set of simplified ODEs, and the *non-equilibrium model* solves the full RANS equations in the near-wall region on a separate wall-adjacent grid. The non-equilibrium model is much more computationally expensive. The merits and deficiencies of both these models are discussed in the current study and a methodology is proposed to dynamically blend the LES and wall model stress in the equilibrium model context to obtain accurate results at a fraction of the cost of the full non-equilibrium model.

The ‘equilibrium’ assumption in the Navier-Stokes equations is reasonable in canonical cases such as channel flows and with attached zero pressure gradient boundary layers. However, if unsteady terms and pressure gradient effects dominate, as is the case with separated flows, shock boundary layer interactions, etc., the equilibrium assumption leads to poor predictions of skin friction and heat flux by this simplified wall model. Bodart & Larsson [9] were among the first to implement WMLES in an unstructured framework using the equilibrium model. Their simulation of a high Re flow on an airfoil showed that WMLES is a promising tool for use on complex geometries. Kawai & Larsson [44] have had some success in simulating SBLI using WMLES; this involved solving the full RANS partial differential equations for the wall model on a separate, auxiliary grid that covers the near-wall region. Park & Moin [57] have demonstrated that accurate skin-friction prediction is possible, both for transitional and separated flows using their non-equilibrium wall model which also solves the full RANS equations on an auxiliary mesh. Such non-

equilibrium wall models, however, don't have the simplicity of the equilibrium wall model which solves simpler ordinary differential equations (ODEs) locally. These methods also need the generation of an additional grid that wraps around the wall surfaces to support the wall model calculation. For complex flow geometries, this can be tough to implement.

Wang & Moin [83] showed that when a RANS-type eddy viscosity is used in wall-layer equations that contain nonlinear convective terms, its value must be adjusted such that it only accounts for only the unresolved part of the Reynolds stress. The Reynolds stress carried by the nonlinear terms in the boundary-layer equations is significant. Non-equilibrium wall models that do not need PDE solvers for the full RANS equations would be advantageous as they would not need to deal with accounting for the resolved Reynolds stresses and would not need additional grid generation. There are a few other wall models, like the integral wall model by Yang et al. [85] and its compressible extension (Catchirayer et al. [15]) which try to account for some of the non-equilibrium terms using a set of parameterized velocity and temperature profiles. The wall model by Komives et al. [45] tries to incorporate some of the non-equilibrium effects by adding source terms from the LES in combination with the SA-RANS turbulence model. Gonzalez et al. [33] derive a modified law of the wall to account for the convective and pressure gradient effects in their wall model. Models such as the dynamic slip model [13, 3], which do not use the equilibrium assumption also offer a good alternative. Chung & Pullin [18] have developed an ODE that governs the wall shear-stress based on the assumptions of wall-parallel filtering and wall-normal averaging. Using this ODE which in theory retains some of the non-equilibrium effects they develop a near-wall subgrid-scale model which has shown good results in separated flows [16]. Models such as these do not require the use of an additional grid and have shown promise for use in separated flow calculations but their application has been limited to incompressible flows.

Typically, wall-modeling approaches sample the flow field from the LES solution at some point near the wall. This is fed in as a boundary condition to the RANS model (either equilibrium or otherwise), which computes the wall shear stress and heat fluxes. These are then used as boundary conditions for the LES solution. An issue with this approach is that the near-wall LES solution is often contaminated by numerical and subgrid modeling errors. The highly anisotropic near-wall structures are poorly resolved, unless some special treatment is used to represent these structures statistically, as in done by Chung & Pullin [18]. It has been suggested [43] that this is the cause for the so-called log-layer mismatch (LLM) present in some WMLES solutions. The LLM is a shift in the normalized mean velocity profile due to an over or under-prediction of the wall stresses. Taking the LES input for the wall model from locations that are a few

cells away from the wall has been shown to reduce the LLM. Recently it was shown that temporal filtering of the LES input at the first wall point can also help reduce the strength of LLM [88]. A rationale for temporal filtering is that there is a certain time delay for the fluctuations in the velocity to be felt in the wall stress. The time filtering essentially decorrelates the unphysically high correlation between the LES velocity and the wall stresses when the LES input is taken at the first grid point. If we think about temporal filtering in a Lagrangian sense, we could interpret it as using the velocity of some particle at some shifted position downstream of the first wall cell location. The existence of inclined structures in the logarithmic region which are responsible for the fluctuations in velocity and the wall stress could explain the reason why temporal filtering leads to a reduction in LLM. Rajagopalan & Antonia [64] have shown that the correlation between wall shear and velocity is a maximum along directions aligned with these inclined structures. In their earlier work, Piomelli et al. [60] made use of this fact in their wall model by using the velocity at some distance downstream of the position where the wall stress is required.

1.2.3 Application in Compressible Flows

There have been a few studies using WMLES for compressible flow. Kawai & Larsson [44] have had success in performing simulations for SB LI ($M \approx 1.7$) using a non-equilibrium WMLES approach. Bermejo-Moreno et al. [6] demonstrate good agreement with experimental measurements for their oblique shock boundary layer interaction studies ($M \approx 2.0$) when using the equilibrium wall model. WMLES of compressible channel flow has been performed previously by Bocquet et al. [8] and Iyer & Malik [39] using the equilibrium wall model with some corrections for compressibility effects. Recently, Yang et al. [86] and Fu et al. [29] have shown that WMLES can accurately predict heat transfer rates in transitional hypersonic flow. Iyer & Malik [38] [37] have demonstrated a good match with experiments for the case of transonic flow over a wall-mounted hump and axis-symmetric compression ramp SB LI ($M \approx 2.9$) studied by them using an equilibrium and non-equilibrium model. WMLES can resolve the key unsteady features seen in the high Re transonic flow over an airfoil was shown by Fukushima & Kawai [30]. It was seen in the studies of Bermejo-Moreno et al. [6] and Zebiri et al. [90] that WMLES can capture the low-frequency unsteadiness seen in shock-induced separated flows. Supersonic compression ramp flows were studied in detail by Dawson et al. [23] in the context of WMLES. In the current study, we set up several supersonic and hypersonic flow cases that illustrate the different challenges at these conditions such as transition prediction,

cold wall boundary layers, and shock boundary layer interactions. Both the equilibrium and non-equilibrium wall models are tested on these cases and improvements in their formulations are proposed.

1.3 Governing Equations

We solve the Favre-filtered compressible Navier-Stokes equations that express conservation of mass, momentum and energy:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = 0 \quad (1.1)$$

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_i \tilde{u}_j - \tilde{\tau}_{ij} + \bar{p} \delta_{ij}) = \frac{\partial}{\partial x_j} (\mathcal{T}_{ij}) \quad (1.2)$$

$$\frac{\partial \bar{\rho} \tilde{E}}{\partial t} + \frac{\partial}{\partial x_j} ((\bar{\rho} \tilde{E} + \bar{p}) \tilde{u}_j - \tilde{\tau}_{ij} \tilde{u}_j - \tilde{q}_j) = \frac{\partial}{\partial x_j} (Q_j + \mathcal{J}_j) \quad (1.3)$$

$$\bar{p} = \bar{\rho} R \tilde{T}, \quad \tilde{E} = C_v \tilde{T} + \frac{1}{2} \tilde{u}_i \tilde{u}_i \quad (1.4)$$

In the equations above, ρ is density and u_j is the velocity along the x_j cartesian direction. τ_{ij} is the shear stress tensor and q_j is the molecular heat flux given by the Fourier's heat conduction law,

$$\tilde{\tau}_{ij} = \tilde{\mu} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \tilde{\mu} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij}, \quad \tilde{q}_j = \frac{\tilde{\mu} C_p}{Pr} \frac{\partial \tilde{T}}{\partial x_j} \quad (1.5)$$

We assume the gas is calorically perfect: the specific heats C_v and C_p are constant and the internal energy $e = C_v T$ is directly proportional to temperature. The specific heats follow the relation $C_p = C_v + R$ where R is the universal gas constant. A constant Prandtl number of $Pr = 0.72$ is used for all test cases. The viscosity is computed using the Sutherland's law for the compressible flows as

$$\mu = A_0 \frac{T^{3/2}}{T + B_0},$$

where A_0 and B_0 are constants. For some test cases, we alternatively use a power law viscosity,

$$\mu = \mu_r \left(\frac{T}{T_r} \right)^\omega,$$

where μ_r and T_r are reference values. We typically use $\omega = 2/3$.

The variables with a bar ($\bar{\phi}$) are grid-filtered quantities and the ones with the tilde ($\tilde{\phi} = \overline{\rho\phi}/\bar{\rho}$) denote Favre-filtered quantities. Note that no explicit filtering is used: the filtering is assumed to be implicit in the sense that the coarse grid resolution serves as the LES low pass filter. The application of the filtering process to the Navier-Stokes equations gives rise to unclosed subgrid terms which need to be modeled. Many of the subgrid terms which arise due to the variation of density and viscosity are negligible: the text by Garnier et al. [32] has a detailed discussion of these. The most significant subgrid scale terms which will be computed using an LES model are the SGS stress tensor ($\mathcal{T}_{ij}$), SGS heat flux (Q_j), and SGS turbulent diffusion ($\mathcal{J}_j$), given below,

$$\mathcal{T}_{ij} = -\bar{\rho}(\widetilde{u_i u_j} - \widetilde{u_i} \widetilde{u_j}) \quad (1.6)$$

$$Q_j = -C_p \bar{\rho}(\widetilde{T u_j} - \widetilde{T} \widetilde{u_j}) \quad (1.7)$$

$$\mathcal{J}_j = -\frac{\bar{\rho}}{2}(\widetilde{u_j u_i u_i} - \widetilde{u_j} \widetilde{u_i} \widetilde{u_i}) \quad (1.8)$$

1.4 Numerical Method

1.4.1 Finite Volume Approach

Consider the Navier-Stokes equations written in divergence form,

$$\frac{\partial U}{\partial t} + \frac{\partial(F_j + F_j^v)}{\partial x_j} = 0. \quad (1.9)$$

Here, U is the vector of conserved variables, F_j is the inviscid flux vector and F_j^v is the viscous flux vector

$$U = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{pmatrix}, \quad F_j = \begin{pmatrix} \rho u_j \\ \rho u u_j + \delta_{1j} p \\ \rho v u_j + \delta_{2j} p \\ \rho w u_j + \delta_{3j} p \\ \rho(E + p)u_j \end{pmatrix} \text{ and } F_j^v = \begin{pmatrix} 0 \\ \tau_{1j} \\ \tau_{2j} \\ \tau_{3j} \\ u_i \tau_{ij} + q_j \end{pmatrix}$$

By integrating the above equation over a control volume defined by the grid and using the Gauss' theorem we get the discretized form as,

$$\frac{\Delta U_i}{\Delta t_i} + \frac{1}{V_i} \sum_f \partial(\vec{F}_f + \vec{F}_f^v) \cdot \hat{n}_f S_f = 0. \quad (1.10)$$

Where U_i represents the volume average of U at the cell i and V_i the volume of the cell. The fluxes are computed at the face centers f of the control volume and summed up over all the faces after the dot product with the unit face normals $\hat{n}_f$ and face area S_f .

In this work, we split the inviscid flux F into two parts,

$$F = F_{\text{central}} + \alpha F_{\text{dissipative}}.$$

The centered (non-dissipative) inviscid fluxes are calculated using a fourth-order kinetic energy conserving scheme [78]. The dissipative part of the inviscid flux is extracted from the modified Steger-Warming scheme [48] and is damped by a shock-sensing multiplicative factor α . A very effective shock sensor is due to Ducros [25],

$$\alpha_D = \frac{\theta^2}{\theta^2 + \omega^2 + \epsilon}, \quad (1.11)$$

where θ is the dilation and ω is the vorticity magnitude. We use a modification suggested by Pirozzoli [61] in which he suggests using $\epsilon = (u_\infty/\delta)^2$, where δ is some estimate of the boundary layer thickness.

For very high Mach number flows, for stability reasons, we often also use the density-based switch (α_ρ) adapted from Ren, Zhang, et al. [65]. The density switch at a face $i + 1/2$ is computed as

$$\alpha_{\rho,i} = 1 - \frac{2\Delta_{i-1/2}\Delta_{i+1/2}}{\Delta_{i-1/2}^2 + \Delta_{i+1/2}^2 + \epsilon_\rho}$$

The blend of the Ducros and density switches at a face $i + 1/2$ is computed as,

$$\begin{aligned} \text{if } \alpha_{\rho,i+1/2} > 0.9, \quad & \alpha_{i+1/2} = \max(\alpha_{D,i+1/2}, \alpha_{\rho,i+1/2}), \\ \text{if } \alpha_{\rho,i+1/2} < 0.1, \quad & \alpha_{i+1/2} = \alpha_{D,i+1/2} \end{aligned}$$

$$\alpha_{D,i+1/2} = \max(\alpha_{D,i}, \alpha_{D,i+1}), \quad \alpha_{\rho,i+1/2} = \max(\alpha_{\rho,i}, \alpha_{\rho,i+1})$$

The highly diffusive density switch is activated only we encounter a large density gradient; otherwise, the Ducros switch is used.

The viscous fluxes F_j^v are discretized using a standard second-order accurate central scheme. For time integration, we use an explicit 3-stage total variation diminishing (TVD) Runge-Kutta method [34].

1.4.2 Sub-Grid Scale (SGS) Model

The sub-grid stresses and subgrid kinetic energy are modeled using the Smagorinsky model [71] and the model by Yoshizawa [89] respectively. The sub-grid scale (SGS) terms, namely the SGS stress tensor ($\mathcal{T}_{ij}$), SGS heat flux (Q_j), and the SGS turbulent diffusion ($\mathcal{J}_j$), given below, are the terms which we need to model. Here, we use the following (standard) closure,

$$\mathcal{T}_{ij} - \frac{\delta_{ij}}{3} \mathcal{T}_{kk} = -2C_s \Delta^2 \bar{\rho} |\tilde{S}| \tilde{S}_{ij}^* = \mu_t^{SGS} \tilde{S}_{ij}^* \quad (1.12)$$

$$\mathcal{T}_{kk} = -2C_I \Delta^2 \bar{\rho} |\tilde{S}|^2 \quad (1.13)$$

$$Q_j = -C_p \bar{\rho} \frac{C_s \Delta^2 |\tilde{S}|}{Pr_t^{SGS}} \frac{\partial \tilde{T}}{\partial x_j} = \lambda_t^{SGS} \frac{\partial \tilde{T}}{\partial x_j} \quad (1.14)$$

$$\mathcal{J}_j = -\tilde{u}_i \mathcal{T}_{ij}, \quad (1.15)$$

where μ_t^{SGS} and λ_t^{SGS} are the SGS eddy viscosity and SGS thermal conductivity. Note that the strain-rate tensor S_{ij} is defined as

$$S_{ij} = \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad S_{ij}^* = S_{ij} - \frac{\delta_{ij} S_{kk}}{3}$$

and the strain-rate magnitude is

$$|S| = \sqrt{2S_{ij}S_{ij}}.$$

As an alternative to using fixed values of the Smagorinsky constant C_s , C_I and the SGS turbulent Prandtl number Pr_t^{SGS} we compute them using the compressible form of the dynamic Smagorinsky model (DSM) by Moin et al. [53]. Typically the test-filtering and averaging (for C_s , C_I and Pr_t^{SGS}) needed for the dynamic model is performed in homogeneous directions, for example, in channel flows this would translate to averaging in spanwise planes. Since a homogeneous direction may not always exist for complex flows, the filtering/averaging in the current study is done locally for each grid cell based on linear interpolation from the face-centered values of the control volume. We use a simple filtering/averaging appropriate for unstructured meshes:

$$\hat{\phi} = \frac{1}{N_f} \sum_{N_f} \phi_f, \quad \phi_f = \phi_{c1} + \phi_{c2}$$

where N_f is the number of faces bounding a cell and ϕ_{c1} , ϕ_{c2} are the two cell-centered values adjacent to the face. To alleviate robustness issues due to (rare) extreme values of

Figure 1.5 The coefficients obtained from the dynamic Smagorinsky procedure are shown here. Red, C_s ; Blue, C_I ; Green, Pr_t^{SGS} ;

C_s and C_I , we ‘clip’ these values.

A note about boundary conditions is appropriate here. For WRLES, “natural” no-slip boundary conditions work well. However, for WMLES the dynamic procedure for the SGS viscosity is error-prone in the first few cells of the WMLES where the wall-normal grid spacing is extremely coarse. This is due to the application of the no-slip boundary condition at the wall which is not fully justified at such coarse resolution. This leads to an abnormally high peak in u' , the streamwise velocity RMS (root mean square), near the wall. This was also seen in the study of Bae et al. [2] who observed this effect when using a no-slip boundary condition for coarse grid LES. Applying a slip velocity boundary condition at the wall for the filtering/averaging in the dynamic model greatly improves the near-wall SGS model behavior and gives improved RMS predictions in the first few cells.

1.4.3 SGS Model Validation: Mach 3 Channel Flow

As an example validation study for the LES model, we present results from a compressible turbulent channel flow simulation with a bulk Mach number M_b set to 3 and a Karman number, $Re_\tau = 480$. DNS by Ulerich [81] is used as a reference for comparison. M_b is

based on the bulk velocity and the specified isothermal wall temperature T_w ,

$$M_b = \frac{u_b}{\sqrt{\gamma R T_w}}$$

As is standard, periodic boundary conditions are applied in streamwise and spanwise directions. Grid spacings that comply with typical wall resolved LES resolution requirements are used (shown in table 1.1). The streamwise velocity is initialized using a laminar profile with a bulk velocity of u_b , whereas the bulk velocity in the spanwise and wall-normal direction is initialized to zero. The velocity components in all directions are perturbed with random noise (with amplitude 0.2 times the bulk velocity u_b) at the onset. The temperature is initialized to T_w and the density is initialized to the bulk density ρ_b everywhere inside the channel. Note that no fluctuations are imposed on the density and temperature profiles.

Table 1.1 LES of compressible channel flow - grid details

$L_x \times L_y \times L_z$	$\Delta x^+ \times \Delta y_1^+ \times \Delta z^+$	$n_x \times n_y \times n_z$
$12.5\delta \times 2\delta \times 5\delta$	$40 \times 0.7 \times 24$	$150 \times 100 \times 100$

The source term driving the channel flow is computed by using the average wall shear stress combined with an unsteady relaxation term. The goal here is to conserve the mass flux. The source term, f_b , is added to the x-momentum equation and is given by

$$f_b = \frac{\langle \tau_w \rangle}{h} - 0.3 \frac{\langle q^n \rangle - \langle q^0 \rangle}{dt^n}. \quad (1.16)$$

Here q^n is the volume-averaged mass flux at the current iteration n , q^0 is the mass flux specified at the initial condition corresponding to a bulk Reynolds number of $Re_b = \rho_b u_b h / \mu_w = 5000$ and dt is the current time step value. $\langle \cdot \rangle$ denotes an average taken over the entire volume and h is the channel half-width. The source term added to the total energy equation, f_e , is computed locally at each cell center as $f_e = f_b \tilde{u}$. The factor of 0.3 is empirical and serves to stabilize the simulation.

The coefficients obtained from DSM, shown in figure 1.5, are reasonably close to values typically used for the Smagorinsky model in literature for compressible channel flows [50]. An excellent match for both the Favre-averaged velocity and temperature profiles for the LES and the DNS is seen in figures 1.6.a and 1.6.b. The resolved Reynolds stresses and temperature fluctuations are also well predicted as seen in figures 1.7.a and 1.7.b.

1.5 Chapter Summaries

- CHAPTER 2 details the wall modeling methods used in the current study: the equilibrium and the non-equilibrium models. Their implementation and the form of the RANS models used within them are discussed.
- CHAPTER 3 applies WMLES to flows at high Mach number and with cold wall conditions. The classical scaling laws derived for incompressible flows fail as the wall becomes colder. In combination with the lack of grid resolution near the wall for WMLES approaches this leads to erroneous temperature profiles. Analyzing the budget of the internal energy equation gives insight into where this error might be arising.
- CHAPTER 4 discusses how WMLES methods deal with transition via the use of a sensor that detects the transition to turbulence. A modified sensor based on the ratio of resolved turbulent kinetic energy and shear stress is formulated. This is tested on transitional hypersonic flows at different Reynolds numbers.
- CHAPTER 5 deals with a formulation that blends the LES and wall-model shear stresses (to address separated flows). A sensor for detecting regions of non-equilibrium flow is formulated. This blended stress formulation is applied in flows with strong non-equilibrium effects in the form of shock-induced separation at moderate to high Reynolds numbers.

(a)

(b)

Figure 1.6 (a) The Favre-averaged velocity $\bar{u}^+$ and (b) the mean temperature $(\bar{T}^+)$ computed from the LES (red) are compared with DNS [81] (black).

(a)

(b)

Figure 1.7 (a) Density weighted Reynolds stresses $\overline{u'u'}$ (red), $\overline{w'w'}$ (green), $\overline{v'v'}$ (blue) and $\overline{u'v'}$ (grey). (b) temperature fluctuations $\overline{T'T'}$ (red), the resolved turbulent heat flux $\overline{v'T'}$ (blue). LES (symbols); DNS (lines).

CHAPTER 2

Wall Modeling

2.1 Introduction

The wall modeling approach based on the equilibrium and non-equilibrium model is detailed in this chapter. Due to the assumptions on the state of the boundary layer in the equilibrium model, this reduces to solving a coupled ODE system to obtain the wall stress boundary condition for the outer LES. In contrast, the more computationally expensive non-equilibrium model needs the solution of coupled PDEs (the RANS equations) which adds complexity in terms of the numerics (advanced hyperbolic discretization methods) and implementation (MPI exchanges). The different eddy viscosity formulations, the grid resolution requirements for the outer LES, and the location of coupling between the LES and wall model are discussed in the following sections. Finally, both the models are validated for the most benign case of an incompressible channel flow.

2.2 Grid Resolution in WMLES

The classic hybrid RANS-LES methods [73, 21, 5] achieve cost reductions compared to wall resolved LES by using RANS in the boundary layer region, and away from the wall, or in detached shear layers, they switch to LES. RANS grids, in theory, do not have limits on the wall-parallel spacing whereas typical wall resolved LES require near-wall streamwise, spanwise, and wall-normal spacings of $\Delta x^+ \approx 40-80$, $\Delta z^+ \approx 20-50$ and $\Delta y^+ \approx 1-40$ respectively. With hybrid RANS-LES, these stringent wall-parallel grid size requirements are relaxed; we instead attempt to resolve the larger, outer scales of motion (on the order of δ , the boundary layer thickness). This leads to spacings of $\Delta x \approx 0.05-0.1\delta$ and

Figure 2.1 A typical grid used for hybrid RANS-LES simulations which are usually refined in the wall-normal direction as shown above. The green gridlines denote regions where the RANS model is used and the blue regions are where the LES model is active.

$\Delta z \approx 0.025\text{--}0.05\delta$. This significantly drops the cost of hybrid RANS-LES simulations for high Re flows. The wall-normal grid spacing still uses the $y_1^+ \approx 1$ criterion but uses rapid stretching away from the wall as is typically done with RANS grids. A schematic hybrid RANS-LES grid in which the RANS and LES portions of the grid are fixed (zonal hybrid RANS-LES) is portrayed in figure 2.1. The grids for WMLES methods follow similar specifications – with the major difference that the wall-normal spacing also is set as a fraction of the outer length scale, δ . This not only reduces the grid size but also allows the use of larger explicit time-steps.

2.3 The Equilibrium Model

The equilibrium wall model [43] is derived using standard boundary layer approximations, and the assumption that the unsteady and convective terms are approximately in balance with the pressure gradient. Assuming a quasi-2D flow, where, without loss of generality, y is assumed to be the wall-normal direction ($y = 0$ is the wall) and x , the wall-parallel direction in the direction of the outer flow, the RANS momentum and total energy equations become

$$\frac{d}{dy} \left((\mu + \mu_t) \frac{du}{dy} \right) = \underbrace{\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u u + p)}{\partial x} + \frac{\partial(\rho u v)}{\partial y}}_{S_m} \quad (2.1)$$

$$\frac{\partial p}{\partial y} = 0 \quad (2.2)$$

Figure 2.2 A flow chart depicting the different steps in the WMLES code (for both equilibrium and non-equilibrium models) is shown above. The Red boxes denote where the subroutines from the LES are called and the blue boxes denote when the wall model (WM) subroutines are active.

$$\frac{d}{dy} \left((\mu + \mu_t) u \frac{du}{dy} + C_p \left(\frac{\mu}{Pr} + \frac{\mu_t}{Pr_t^{wm}} \right) \frac{dT}{dy} \right) = \underbrace{\frac{\partial(\rho E)}{\partial t} + \frac{\partial(\rho H u)}{\partial x} + \frac{\partial(\rho H v)}{\partial y}}_{S_E} \quad (2.3)$$

The terms which are not seen in the above equations include the viscous terms which have derivatives of the form $\partial()/\partial x$, as well as the convective and viscous terms for the wall-normal momentum equation (2.2). These terms are omitted based on scaling arguments similar to the classical thin boundary layer approximations [72]. The right-hand side denotes the non-equilibrium terms for the momentum (S_m) and total energy equation (S_E) whose sum is typically small in attached zero pressure gradient flows. The resulting set of simplified equations used to model the near-wall layer are

$$\frac{d}{dy} \left((\mu + \mu_t) \frac{du}{dy} \right) = 0 \quad (2.4)$$

$$\frac{d}{dy} \left((\mu + \mu_t) u \frac{du}{dy} + C_p \left(\frac{\mu}{Pr} + \frac{\mu_t}{Pr_t^{wm}} \right) \frac{dT}{dy} \right) = 0 \quad (2.5)$$

A simple mixing-length model,

$$\mu_t = \kappa \sqrt{\rho |\tau_w|} y D_1(y), \quad D_1(y) = (1 - \exp(-y^*/A_1^+))^2 \quad (2.6)$$

is used to compute the eddy viscosity. $D_1(y)$ is the van Driest damping factor; the notation y^* is defined later. A constant turbulent Prandtl number ($Pr_t^{wm} = 0.9$) is used to model the turbulent eddy conductivity. The values of the constants used are $\kappa = 0.41$, $A_1^+ = 17$ and $Pr = 0.72$. These two coupled ODEs are solved on a one-dimensional stretched wall-normal grid at every wall face center, as illustrated in figure (2.3), with a domain that ranges between $y = 0$ and h_e (height of exchange location). This gives us the wall parallel velocity (u) and temperature (T) profiles in the near wall region. The pressure is assumed not to vary in y and is obtained from the LES solution at the exchange location, while density is computed using the pressure and temperature via the equation of state. Discretizing the ODEs using a second-order finite-volume method gives a tridiagonal system of equations which is efficiently solved using the Thomas algorithm. We solve the momentum and energy equations iteratively until the wall model velocity and temperature profiles have converged. At this point, τ_w and q_w computed from these profiles are given to the LES solver as wall flux boundary conditions.

Classically the scaled distance from the wall (y^*) that appears in the van Driest damping factor D_1 was equated to $y^+ = y u_\tau \rho_w / \mu_w$, based on its definition for incompressible flow. For compressible flow, this classical definition can lead to large errors in skin-friction

Figure 2.3 The ODEs for the equilibrium model are solved on a 1-D grid (green) refined in the wall normal direction which is embedded on each wall face of the LES grid (blue), such as one shown above.

[88]. Hence a more suitable definition for compressible flows given by $y^s = y \sqrt{\rho |\tau_w|} / \mu$ [58, 80], called the semi-local scaling (y^s), became popular. Recently, Iyer & Malik [39] proposed an empirical “mixed” scaling for the normalized wall distance that outperforms the semi-local scaling in terms of accurately predicting skin-friction when using WMLES. The mixed scaling (y^m) [39] is given as,

$$y^{m1} = \frac{y^s + y \rho_w u_\tau / \mu_w}{2}, \quad y^{m2} = \frac{y^s + y \rho u_\tau / \mu}{2}$$

$$y^m = \min[y^{m1}, y^{m2}]$$

Note that $u_\tau = \sqrt{|\tau_w| / \rho_w}$.

In terms of implementation, the wall model solver is run once before the start of the Runge-Kutta (RK) sub-iterations, and the profiles obtained are stored for their subsequent use to reduce the cost of solving the wall model at each RK sub-iteration. Numerical experimentation showed that solving the wall model at every RK sub-iteration did not lead to better accuracy in the predicted statistics (for the simple test cases used). A flow chart depicting the different steps in the WMLES code is shown in figure 2.2.

2.3.1 Solution Method

2.3.1.1 Wall Model Grid

A one-dimensional stretched grid from the wall face center to its corresponding exchange location in the LES is created for solving the wall model equations. First a mapping

between the wall face and the corresponding LES cell center is established. The nodes $(y_{f,j})$ and centers $(y_{c,j})$ for this 1D grid are

$$y_{f,j} = h_e \left(1 - \frac{\tanh(\alpha_s j/n)}{\tanh(\alpha_s)} \right)$$

$$y_{c,j} = 0.5 * (y_{f,j} + y_{f,j+1}),$$

where y is the distance from the wall, α_s is a stretching factor and n is the number of (finite-volume) cells in the wall model layer. Parameters α_s and n are chosen such that $y_{c,1}^+ < 1$ is approximately maintained in the attached regions of the WMLES. The wall corresponds to $y_{f,0} = 0$ and $y_{c,n+1} = h_e$ is the distance from the wall of the LES cell center (which also corresponds to the top ghost cell center in the wall model layer).

At the outset, the wall model solution is initialized with linear profiles for velocity and temperature,

$$\phi_j = \phi_e \frac{y_j}{h_e} + \phi_w \left(1 - \frac{y_j}{h_e} \right),$$

where ϕ_e and ϕ_w are values at the exchange location and wall respectively. The (constant) pressure in the wall model layer is $P_y = P_e$, the LES exchange location value. The density is obtained using the ideal gas equation, $\rho_j = P_e/(RT_j)$.

2.3.1.2 Momentum Equation

The discretization of the momentum equation 2.4 using a 1-D finite volume method for a cell center ‘ j ’ reads,

$$\mu' \frac{du}{dy} \Big|_{f,j+1/2} - \mu' \frac{du}{dy} \Big|_{f,j-1/2} = 0, \quad j = 1, \dots, n$$

$$\mu' = \mu + \mu_t.$$

The gradients of velocity or temperature are computed using standard finite differencing,

$$\frac{du}{dy} \Big|_{f,j+1/2} = \frac{u_{j+1} - u_j}{y_{j+1} - y_j}.$$

This gives rise to a tridiagonal system of equations for u_j ,

$$\left(\frac{\mu'}{dy} \Big|_{f,j+1/2} \right) u_{j+1} - \left(\frac{\mu'}{dy} \Big|_{f,j+1/2} + \frac{\mu'}{dy} \Big|_{f,j-1/2} \right) u_j + \left(\frac{\mu'}{dy} \Big|_{f,j-1/2} \right) u_{j-1} = 0$$

which is solved using the Thomas algorithm which is a simplified form of Gaussian elimination that can be used to solve tridiagonal systems efficiently.

2.3.1.3 Total Energy Equation

The discretization of the total energy equation is similar to that of the momentum equation.

$$\lambda' = \lambda + \lambda_t$$

$$\lambda' \frac{dT}{dy} \Big|_{f,j+1/2} - \mu' \frac{dT}{dy} \Big|_{f,j-1/2} = - \left(u\mu' \frac{du}{dy} \Big|_{f,j+1/2} - u\mu' \frac{du}{dy} \Big|_{f,j-1/2} \right)$$

The velocity terms are fixed and only the temperature is updated when solving the energy equation. $\lambda' = C_p(\mu/Pr + \mu_t/Pr_t)$ is the molecular plus turbulent thermal conductivity. The resulting tridiagonal system reads:

$$\left(\frac{\lambda'}{dy} \Big|_{f,j+1/2} \right) T_{j+1} - \left(\frac{\lambda'}{dy} \Big|_{f,j+1/2} + \frac{\lambda'}{dy} \Big|_{f,j-1/2} \right) T_j + \left(\frac{\lambda'}{dy} \Big|_{f,j-1/2} \right) T_{j-1} =$$

$$- \left(u\mu' \frac{du}{dy} \Big|_{f,j+1/2} - u\mu' \frac{du}{dy} \Big|_{f,j-1/2} \right).$$

The momentum and energy equations are solved in an uncoupled manner iteratively until the velocity and temperature profiles converge. Convergence is measured by taking the difference between velocity and temperature profiles for successive iterations and checking if the RMS of the difference is less than a prescribed tolerance (typically on the order of 10^{-6}). The u_{rms} and T_{rms} is given as,

$$u_{rms} = \sqrt{\sum_{j=1}^n \frac{(u_j^k - u_j^{k-1})^2}{n}}$$

$$T_{rms} = \sqrt{\sum_{j=1}^n \frac{(T_j^k - T_j^{k-1})^2}{n}}$$

Here $k, k - 1$ is the current and previous iteration for the wall model. Typically both the velocity and temperature converge within approximately 5-15 iterations for the cases in the current study.

2.3.2 Resolving Log-Layer Mismatch (LLM)

The wall model takes its input from the LES at some exchange location above the wall boundary: the choice of this point is of great importance since this directly affects the

quality of the overall solution. Since the LES is essentially under-resolved near the wall, the near-wall solution will be polluted by modeling and numerical errors [43]. Hence, the input for the wall model is from a point where these errors become less significant while making sure this exchange location lies within a region governed by the law of the wall. The recommended location is typically $\sim 0.1\delta$, where δ is the turbulent boundary layer thickness [43].

In terms of practical implementation, this method needs information from cells at some height above the wall: these cells may not ‘live’ on the same processor when running a code in parallel (depending on how the mesh is partitioned). This, in turn, adds additional complexity to the wall model in terms of grid partitioning and information exchange between processors which will not be ideal for simulations using unstructured grids or with complex geometries. An approach which was suggested by Yang et al. [88] was to use the first grid point of the wall with temporal filtering of the velocity (temperature and pressure also) as the input for the wall model. Temporal filtering is performed as follows,

$$\langle U \rangle_e^n = (1 - \epsilon)\langle U \rangle_e^{n-1} + \epsilon U_e^n \quad (2.7)$$

where ϵ is defined as $\epsilon = \Delta t/T_f$. The filtering time scale (T_f) is usually set to the wall diffusion time scale which is calculated as $T_f = h_e/\kappa u_\tau$. This operation denotes an exponential moving average using the weight $W(t) = \exp(-t/T)$ with a finite memory of time scale T . Time-filtering the Dirichlet boundary condition [88] helped in reducing the log-layer mismatch for their study but the usage of time-filtering in generals, such as in separated flows is not justified fully since the unsteady aspects of the flows also need to be preserved. In the current study, we ensure the exchange location obeys the requirements set by Kawai & Larsson [43] by taking $h_e = 0.07\text{--}0.1\delta$ for most cases and use the instantaneous values of primitives as the input to the wall model.

2.3.3 Validation: Incompressible Channel Flow

As a validation study for the wall model we conduct a channel flow simulation in the incompressible regime at $Re_\tau = 2000$. DNS of incompressible channel flow by Lee & Moser [47] is used as a reference for comparison. The Mach number chosen is $M = 0.3$, based on the bulk velocity and the specified isothermal wall temperature, and is reasonably close to the incompressible condition. Periodic boundary conditions are applied in both streamwise and spanwise directions. Uniform grid spacings are employed in all directions complying with typical WMLES resolution in outer units, as seen in table 2.1. The initialization procedure is similar to the WRLES case described previously in Chapter 1. The source

(a)

(b)

Figure 2.4 (a) The van Driest transformed mean velocity is compared with the DNS [47]. Black line, DNS; Red line, outer LES; Blue line, wall model solution; Circles, WMLES - 3rd grid point; Squares, WMLES - 1st point. (b) The resolved Reynolds stresses from top to bottom: $\overline{u'u'^+}$ (red), $\overline{w'w'^+}$ (blue), $\overline{v'v'^+}$ (green) and $\overline{u'v'^+}$ (black). Circles, WMLES - Exchange location at third point; Squares, WMLES - Exchange location at first point; Dotted lines, DNS.

term for driving the channel flow is computed by using the domain average of the wall shear stress predicted by the wall model combined with an unsteady term which makes sure the mass flux in the channel is conserved as done in equation (1.16).

Table 2.1 Quasi-incompressible channel flow - grid details

$L_x \times L_y \times L_z$	$\Delta x^+ \times \Delta y^+ \times \Delta z^+$	$\Delta x \times \Delta y \times \Delta z$	$n_x \times n_y \times n_z$
$6\delta \times 2\delta \times 3\delta$	$200 \times 120 \times 100$	$0.1\delta \times 0.06\delta \times 0.05\delta$	$60 \times 32 \times 60$
$25\delta \times 2\delta \times 10\delta$	$200 \times 60 \times 100$	$0.1\delta \times 0.03\delta \times 0.05\delta$	$250 \times 64 \times 200$

We observe in figure (2.4a) that the mean velocity profile beyond the exchange location agrees well with the DNS data when using the 3rd point from the wall as the exchange location. An error is induced in the velocity profile when we use the first point data: this results in an overprediction of the wall shear stress which makes the velocity profile dip in the outer region. This error in the mean profile when taking the first point is an example of the so-called Log-Layer Mismatch (LLM). In the present study, the exchange location which corresponds to the third grid point is at $y = 0.15\delta$ (here, δ is the channel half-width) which is in the log-layer region. The points below the exchange location in the WMLES solution have a large deviation from DNS both in the mean and the RMS (root mean square) due to the severely under-resolved cells close to the wall. Placing the exchange location further in the log-layer has been proven to improve the accuracy of the mean WMLES solution. Except for the $\overline{u'v'}$ component which seems to agree very well, the other components of the resolved Reynolds stress are underpredicted (especially the $\overline{u'u'}$ component): this is expected owing to the much coarser resolution in the outer region compared to the DNS. Overall the results are qualitatively very similar to previous WMLES of channel flows [9, 57, 8]. Note that we use the classic semi-local scaling for the eddy viscosity in the wall model, which is sufficient to get decent predictions in the low Mach number regime. A case with different streamwise/spanwise lengths ($L_x = 25\delta$, $L_z = 10\delta$) and finer wall-normal spacing was also performed (keeping the exchange location fixed) for the sake of verification. The results obtained for the mean statistics were very similar for both grids (not shown below). Thus we ensure grid convergence is achieved.

Figure 2.5 An additional 3-D grid refined in the wall-normal direction such as one shown above in green is needed to solve the RANS equations.

2.4 Non-Equilibrium Model

Non-equilibrium wall models that solve the fully coupled RANS equations in a layer close to the wall require an auxiliary wall-layer grid to be supplied, which needs to communicate with the overlying LES grid. Figure 2.5 shows a sketch illustrating the coupling between the LES and the RANS layers in such a setup.

Note that a local, one-dimensional mesh for equilibrium models is implicitly defined for any given LES grid, even for relatively complex geometries. This local mesh is typically generated by drawing normal lines starting from the wall face-centers, as shown in figure 2.6. In this study, we developed a “meshless” scheme to solve the RANS equations in the near-wall region which makes use of this implicitly defined mesh. The solution is updated on a mesh which is considered to be the union of the locally one-dimensional grid lines that would typically be used in an equilibrium wall model.

The full set of RANS equations are solved on this set of points using an upwind finite difference meshless scheme based on the work of Sridar & Balakrishnan [76]. Meshless schemes are different from the classical discretization methods like finite volume as they do not require a rigid set of points that define an area or volume with some form of connectivity binding them. They work on a cloud of points on which PDEs can be discretized. Various meshless schemes have been applied to compressible viscous flows with a great deal of accuracy, and have compared well with the results obtained from finite-volume schemes [42, 49, 76, 35, 41]. A description of the meshless method used in our non-equilibrium model, which we call the Meshless Line Solver (MLS), is given in the

Figure 2.6 An implicit grid defined by normal lines for the meshless non-equilibrium model and the cloud of points which form a representative stencil is shown above. Blue lines are part of the outer LES mesh and the green cloud of points forms the wall model mesh.

following section.

2.4.1 Meshless Line Solver (MLS): Solution Method

2.4.1.1 Wall Model Grid

The same 1D grid previously used for the equilibrium model is now extended to all 3 Cartesian coordinates x^i where $i = 1, 2, 3$,

$$x_{f,j}^i = x_w^i + (x_e^i - x_w^i) \left(1 - \frac{\tanh(\alpha_s j/n)}{\tanh(\alpha_s)} \right)$$

$$x_{c,j}^i = 0.5 * (x_{f,j}^i + x_{f,j+1}^i)$$

Here x_w^i and x_e^i are the coordinates for the wall face and exchange location cell center. Additional connectivity in the form of wall-to-wall face mapping needs to be generated in a pre-processing step which generates the cloud of neighboring points needed for solving the non-equilibrium model.

2.4.1.2 Discretization: Meshless Scheme

We solve the Reynolds-averaged Navier-Stokes equations, compactly written as,

$$\frac{\partial U}{\partial t} + \frac{\partial F^k}{\partial x^k} = 0, \quad k = 1, 2, 3 \quad (2.8)$$

Figure 2.7 For each point on the wall model grid a cloud of points nearby is created, which is used for the derivative computation in the non-equilibrium model.

where U represents the vector of conserved variables and F^k is the flux along the k -th cartesian direction. Meshless methods are similar to the finite difference family of schemes in terms of how they approximate the flux derivatives. The goal is to compute the upwinded flux derivative $\partial F^k / \partial x^k$ at point i given a set of neighboring points around it. The sketch in figure 2.7 shows a cloud of six points j_1 to j_6 surrounding point i . This cloud of points forms the three-dimensional stencil for our derivative computation.

The gradient of a generic scalar ϕ is computed at location i using weighted least-squares. The least-squares method for computing gradients is based on the Taylor series approximation of a function to its neighboring points. Given m neighbors, using Taylor series expansions, the gradient at a point i based on the weighted least-squares method can be computed by inverting the matrix system given in equation (2.10).

$$A_{kl} = \sum_{n=1}^m w_n \Delta x^k \Delta x^l, \quad b_k = \sum_{n=1}^m w_n \Delta \phi_n \Delta x^k \quad (2.9)$$

$$[A_{kl}] \left(\frac{\partial \phi}{\partial x_l} \right) = b_k \quad (2.10)$$

Here, $\sum^m$ denotes the sum over each i - j pair. The weighting functions, w_n , are the squares of the inverse distances between point i and any neighbor. The use of these weights leads to improved accuracy and conditioning of the least-squares procedure [51, 42]. Solving the matrix system in equation (2.10), we can evaluate the gradient of ϕ_i at

point i as a function of a geometric quantity a_{ij}^k and the respective difference of the scalar for each neighbor. The coefficients a_{ij}^k are the least-squares coefficients obtained for each i - j pair after inverting the matrix system. These least-square coefficients depend purely on the relative position of the point cloud with respect to point i . Thus, they can be precomputed and stored at each point before the simulation begins. Compactly, we can say

$$\frac{\partial \phi_i}{\partial x^k} = \sum_{j=1}^m a_{ij}^k \Delta \phi_{ij}, \quad \Delta \phi_{ij} = \phi_j - \phi_i. \quad (2.11)$$

To obtain the upwinded flux gradients [76] using the least-squares method we compute the upwind flux at each fictitious interface $(ij/2)$ between i and its neighbor j . In the current implementation, we assume this interface is midway between a i - j pair. The flux at interface $ij/2$ can be computed using any existing upwinded flux formulation. In the current study, the modified Steger-Warming scheme is used to compute the inviscid upwind flux $(F_{ij/2}^{inv,k})$, and a second-order accurate, centered approximation is used for the viscous flux $(F_{ij/2}^{vis,k})$.

The final discretized form reads,

$$\frac{U_i^{n+1} - U_i^n}{\Delta t^n} + \left[\sum_{k=1}^3 \sum_{j=1}^m 2a_{ij}^k (F_{ij/2}^k - F_i^k) \right]^{n+1} = 0 \quad (2.12)$$

The factor of 2 in the equation (2.12) is an artifact of assuming the interface for the flux computation is at the halfway point between each pair i - j . This essentially scales the previously obtained least-squares coefficients (a_{ij}^k) , in equation (2.11), by a factor of 2.

To remove the CFL time-step limitation in the wall model we use an implicit time-stepping method. A line relaxation method with first-order backward Euler time integration is used in the present study. 4-6 sub-iterations are sufficient (for the current study) for the implicit scheme to converge per wall model time-step. Note that the time-step for the wall model calculation is set by the LES solution and grid. Typical CFL values for the wall model in the present study are in the range ~ 20 -50. As with the equilibrium model, this system is solved once before the start of the RK sub-iterations to achieve a significant cost reduction. The added cost of the non-equilibrium model is about 150% which means the total cost of the simulation more than doubles. In comparison, the added cost of the equilibrium model is about 15% and that of the dynamic Smagorinsky LES model is about 30%. The high additional cost and complexity of solving the non-equilibrium model are its main drawbacks.

Figure 2.8 The solid red line is the value of corrected kappa κ_c obtained from the dynamic eddy viscosity correction procedure; Dashed black line, $\kappa = 0.41$.

2.4.2 Dynamic Eddy Viscosity Correction

A persistent problem in non-equilibrium wall models that solve the full RANS equations is traceable to the fact that the solution is necessarily unsteady (due to the time-varying boundary conditions from the unsteady LES solution imposed on the outer edge of the wall model solution). This gives rise to non-zero *resolved* Reynolds stress [83]. For the eddy viscosity used in the wall model to account only for the unresolved portion of the Reynolds stress, a “correction” procedure is needed. Wang & Moin [83] tried to match the RANS eddy viscosity with the SGS viscosity to dynamically calculate a “corrected” value of κ (which appears in the eddy-viscosity formulation), termed κ_c , at the exchange location which can account for this resolved stress in the wall model layer. A constant value of κ_c was used throughout the wall-normal direction and this resulted in better skin-friction predictions for their cases. This type of κ_c model using the SGS viscosity gave erroneous results in high Re boundary layers which was shown by Kawai & Larsson [44]. They proposed a linear variation of κ_c with the wall-normal distance combined with a user-defined slope α_c which gave significantly better results. But later it is shown by Park & Moin [57], that the optimal value of parameter α_c varies quite widely for different flow scenarios and hence proposed a new dynamic procedure without any ad-hoc user-defined parameters or assumptions on the shape of κ_c . The current study uses the dynamic correction proposed by Park & Moin [57]. It has to be noted that the use of this dynamic correction procedure does add significant computational cost to the non-equilibrium

model.

Consider the baseline mixing-length eddy-viscosity formulation in the non-equilibrium model given as,

$$\mu_t^a = \rho(\kappa y)^2 |S| D_{vd}(y), \quad D_{vd}(y) = (1 - \exp(-y^+/A_2^+))^2, \quad (2.13)$$

where D_{vd} is the van Driest damping function and the standard value of $A_2^+ = 26$ and $\kappa = 0.41$ is used in this wall model. ρ is the local density, $|S|$ is the strain rate magnitude and y is wall normal distance in the wall model domain. The corrected eddy viscosity μ_t^{wm} used in the wall model is given by

$$\mu_t^{wm} = \mu_t^a + \frac{\bar{\rho} \bar{R}_{ij} \bar{S}_{ij}^*}{\bar{S}_{mn}^* \bar{S}_{mn}^*}$$

where $\bar{R}_{ij} = -\overline{u_i' u_j'}$ is the resolved Reynolds stress computed inside the wall model using an exponential moving average with a time scale $T_f = L_x/U_\infty$ where L_x is the streamwise length of the domain and U_∞ is the free stream velocity.

$$\lambda_t^{wm} = \lambda_t^a + \frac{\bar{\rho} \bar{Q}_j^t \bar{Q}_j}{\bar{Q}_m \bar{Q}_n}$$

A similar correction procedure is used to account for the resolved turbulent heat flux $Q_j^t = \overline{u_j' T'}$ in the turbulent thermal conductivity λ_t using the averaged temperature gradient $Q_j = \partial T / \partial x_j$.

Note that values of the corrected κ_c which are negative or larger than 0.41 are clipped to zero and 0.41 respectively. The above dynamic procedure accounts for the resolved Reynolds stresses and turbulent heat flux without any ad-hoc parameters but is still limited by the simple mixing length model which in theory applies only to equilibrium flow scenarios. Another drawback of this method is it is computationally expensive in terms of storage and also the time needed for the Reynolds stresses to converge is of the order of several flow-through times. Using an averaging time, T_f , which is in the order of wall diffusion time scale ($h/(\kappa u_\tau)$) was also been tried but the κ_c obtained with such a small time scale (compared to L_x/U_∞) did not lead to good predictions for the mean flow profile.

2.4.3 Validation: Incompressible Channel Flow

The non-equilibrium model is validated for the basic test case of incompressible channel flow at $Re_\tau = 2000$. The grid, initialization, and source term computation details have been

Figure 2.9 (a) The van Driest transformed mean velocity is compared with the DNS [47]. Black line, DNS; Red line, outer LES; Blue line, wall model solution; Circles, WMLES - with eddy viscosity correction; Squares, WMLES - no correction in resolved stress.

described previously. Figure 2.8 shows the wall-normal distribution of the dynamically corrected κ in the non-equilibrium model. Note that the lowest value of κ is close to the exchange location which is where most of the resolved stress is generated. As we got close to the wall the κ value starts recovering to its normal value of 0.41. As shown in figure (2.9), not accounting for the resolved stress leads to the wall model profile at the exchange location tending to a slope of zero which in turn leads to an erroneous mean velocity profile in the outer LES.

3.1 Introduction

While the user base for WMLES is rapidly growing, so far, most of the reported WMLES studies have focused on incompressible or weakly compressible flows. For these cases, scaling laws (with Re , Mach number, etc.) for the mean and RMS velocity and temperature are well understood: this is in the sense that the mean density variation accounts for most differences when similar statistics from incompressible flow are compared. In terms of WMLES prediction accuracy, as we observed in Chapter 2, as long as the exchange location requirements are met and the boundary layer is in or near a state of equilibrium, WMLES can give accurate results in these cases.

Most hypersonic boundary layers have a cold wall – namely the surface temperature of the hypersonic vehicle is significantly less than the adiabatic wall temperature T_r . This occurs because of transient heating of the vehicle, active cooling or ablation of the surface, and/or re-radiative cooling of the surface. The mean temperature and density profiles in cold-wall boundary layers are not monotonic, unlike in cases with no heat transfer. The temperature peaks very close to the wall (figure 3.1.b), giving rise to a rapid change in density, temperature, and viscosity in the near-wall region. Also, the heat flux in the direction normal to the wall changes sign at the peak temperature location. There are structural changes as well – near-wall vortices in cold wall flows tend to be “fatter” and more elongated compared to their adiabatic wall counterparts.

Many of the incompressible velocity transformation and scaling laws when applied to such hypersonic cold wall cases (e.g., the van Driest transformation, Walz’s correlation) give systematic errors. Shown in figure 3.1.a is the van Driest transformed mean velocity

(a)

(b)

Figure 3.1 (a) The van Driest transformed velocity profile (black solid lines) and (b) temperature profile (black solid lines) for a Mach 6 cold wall boundary layer taken from the DNS of Subbareddy & Candler [77] is shown above. The different solid black lines in both figures are taken at different streamwise locations in the boundary layer. The grey line in figure 3.1.a is the log-law with the intercept $C = 6.4$. The classical log-law with $C = 5.2$ and the linear viscous sub-layer profiles $u^+ = y^+$ is given with the black dashed line. The grey line in figure 3.1.b is a scaled velocity profile and the symbols denote the prediction of temperature profiles from Walz's correlation.

profile from DNS of a Mach 6 turbulent boundary layer with a significantly cold wall ($T_w/T_r = 0.16$). A shift in the log-law intercept C from its classical value of 5.2 to 6.4 and a drop in slope for the viscous sub-layer is seen. At these conditions, the velocity and temperature are strongly coupled and the assumptions of minor variations in density and viscosity typically used for classical velocity scalings (Morkovin’s hypothesis) start to deteriorate. The mean temperature profile for cold wall boundary layers, as shown in figure 3.1.b, is also non-canonical and the sharp inner peak in the temperature profile would not be captured by the typical grids used in WMLES. There have been some recent attempts (e.g. Trettel & Larsson [80] and Volpiani et al. [82]) to develop universal scaling laws for velocity profiles at non-adiabatic wall conditions, however, a conclusive solution is not at hand. Most RANS models (including SA and SST) are calibrated using low-speed flow data and have not been thoroughly extended to capture significant compressibility and heat transfer effects.

In terms of WMLES investigations at these conditions, Yang & Lv [87] observed that using the classical van Driest type damping function in the eddy-viscosity definition can give errors of nearly 100% when used in WMLES. They observed, however, that the use of semi-local scaling to define the length scale [80] can greatly improve the accuracy in modeling the wall-stress. Recently, an empirical mixed scaling proposed by Iyer & Malik [39] has shown improved results compared with both the classical van Driest damping as well as damping based on the semi-local scaling. The current study evaluates the effect of these different damping functions in the context of WMLES for high Mach number flows with cold walls. Section 2.3 contains the details and definitions of these length scales.

3.2 Compressible Channel Flow

We start by closely examining supersonic cold wall channel flow where there is a much stronger coupling between the velocity and temperature profiles than the previously simulated incompressible channel flow. Note that some authors employ an additional source term for internal energy which forces the bulk temperature to match the DNS value [8, 39]: this approach is not used here. Broadly speaking, the mean temperature profile inside the channel develops as a balance between the production of heat due to viscous dissipation and the loss of heat through the walls. The production of internal energy below the buffer layer is absent or severely diminished in WMLES since the grid does not resolve the gradients of velocity near the wall which are responsible for this viscous heating. The current study investigates the effect of the absence of this viscous heating in WMLES. The exchange location is taken to be fixed at a height $h_e = 0.25\delta$

(a)

(b)

Figure 3.2 (a) The Favre-averaged velocity $\bar{u}^+$ and (b) the mean temperature ($\bar{T}^+$) computed from the WMLES are compared with the DNS (black). The dashed lines correspond to the wall model prediction. The above figure is comparing the different eddy viscosity damping functions for the Mach 3 case with $N_y = 32$.

(a)

(b)

Figure 3.3 (a) The Favre-averaged velocity $\bar{u}^+$ and (b) the mean temperature ($\bar{T}^+$) computed from the WMLLES are compared with the DNS (black). The dashed lines correspond to the wall model prediction. Grids with different wall-normal spacings (Red, $N_y = 32$; Blue, $N_y = 48$; Green, $N_y = 64$;) for the Mach 3 case are compared here, all of which use the mixed scaling.

(this is well in the log-layer at these Reynolds numbers). As seen in figure (3.2.a), when using the semi-local scaling for a channel flow with cold walls we see an error in the mean velocity prediction: the wall shear stress is over-predicted, causing a downward shift in the scaled profile. With the mixed scaling law [39] which was presented in recent literature (described in section 2.3), we obtain better predictions. However, this good match for the mean velocity does not translate to the temperature profile prediction, as can be seen in figure 3.2.b. Both the mixed and semi-local scaling fail to predict the bulk temperature in the channel for WMLES.

Table 3.1 WMLES of compressible channel flow - grid details

M	Re_τ	B_q	$L_x \times L_y \times L_z$	$n_x \times n_y \times n_z$
1.5	220	-0.05	$12.5\delta \times 2\delta \times 5\delta$	$150 \times 32/48/64 \times 100$
3.0	480	-0.14	$12.5\delta \times 2\delta \times 5\delta$	$150 \times 32/48/64 \times 100$
4.5	420	-0.27	$12.5\delta \times 2\delta \times 5\delta$	$150 \times 32/48/64 \times 100$

To investigate this further, a grid refinement study was done (details in table 3.1). Note that in all cases, the spacings in the streamwise and spanwise direction in wall units are $\Delta x^+ < 50$ and $\Delta y^+ < 25$, which correspond to typical wall resolved LES spacings. Since the streamwise/spanwise directions are well resolved, the source of error in WMLES is presumably due to the unresolved grid in the wall-normal direction. The grid is refined in the wall-normal direction by maintaining uniform spacing and keeping the exchange location height to be approximately the same.

As seen in figure 3.3.a, the velocity prediction does not change much: this is not surprising since this depends predominantly on the exchange location height and the eddy viscosity scaling used in the wall model. Also observed are good predictions in the outer region for the resolved Reynolds stress and turbulent heat flux in figure 3.5, for all the grids tested. However, the temperature profiles (in figure 3.3.b) do not show any improvement. Simulations with other Mach numbers ($M = 1.5, 4.5$) were also done (details in table 3.1). Note that with increasing Mach number, the non-dimensional heat transfer parameter,

$$B_q = \frac{q_w}{\rho_w C_p u_\tau T_w}$$

becomes more negative i.e. the wall gets relatively colder. The mean temperature profiles in figure 3.4 show that as the wall gets colder, the error in the bulk temperatures becomes systematically larger for WMLES (from 3-9%).

Figure 3.4 The mean temperature (normalized by the DNS center-line temperature T_c^{DNS}) from the WMLES (dashed lines) are compared with the DNS (solid lines). Mach 1.5, red; Mach 3.0, blue; Mach 4.5, green. Different Mach numbers for the WMLES grid with $N_y = 32$ using the mixed-scaling for the eddy viscosity are compared in the figure above.

To examine this further, the viscous dissipation term from the WMLES is plotted in figure 3.7 and the wall model plus the outer LES temperature profile are shown in figure 3.6. Notice that the shape of the temperature profile obtained from the wall model matches well with the near-wall DNS profile in figure 3.6. This shape of the near-wall temperature implies a certain heat-flux being applied to the outer LES. Consider a wall resolved LES/DNS, this outflow of heat is essentially coming from the near-wall region. However, in WMLES this near-wall viscous dissipation is absent, as seen in figure 3.7. The viscous dissipation is given by $\tilde{\phi} = \tilde{\tau}_{ij} \partial \tilde{u}_i / \partial x_j$, which is a function of the near-wall velocity gradients resolved in the outer LES. With grid refinement, we do observe an improvement in $\tilde{\phi}$ but that is nowhere close to what is predicted in a resolved simulation where the wall-normal resolution much finer (close to $\Delta y^+ < 1$). Since we are imposing the wall model q_w onto the channel, the net effect of this is to reduce the internal energy everywhere and thus resulting in lower bulk temperatures in the WMLES results.

3.3 Mach 6 Cold Wall Boundary Layer

Next, we assess WMLES predictions of cold wall turbulent boundary layers. Unlike the case with channel flows, the temperature profile in cold wall boundary layers is not monotonic:

(a)

(b)

Figure 3.5 (a) The resolved Reynolds stress $\overline{v'T'}^+$ and (b) the resolved turbulent heat flux $\overline{v'T'}^+$ computed from the WMLLES are compared with the DNS (black). The dashed lines correspond to the wall model prediction. Grids with different wall normal spacings (Red, $N_y = 32$; Blue, $N_y = 48$; Green, $N_y = 64$;) for the Mach 3 case are compared here, all of which use the mixed scaling.

Figure 3.6 The mean temperature ($\bar{T}^+$) computed from the WMLES is compared with the DNS of the Mach 3 channel flow. Blue, wall model solution; Red, outer LES solution; Black, DNS solution [81].

Figure 3.7 The viscous dissipation compared from WMLES and the resolved simulation is shown above for the Mach 3 channel flow (Red, $N_y = 32$; Blue, $N_y = 48$; Green, $N_y = 64$; Black, DNS).

Figure 3.8 Skin friction coefficient (C_f - red) and Stanton number (St - blue) comparison between the DNS and the WMLES. Lines with circles, WMLES with mixed scaling; Lines with squares, WMLES with semi-local scaling; Solid lines, DNS. Note that the inflow plane for the WMLES calculation is at $x/\delta = 0$.

Table 3.2 Mach 6 boundary layer - flow conditions and grid details

M_∞	Re_1	Re_{x_o}	$Re_{\delta_o^*}$	T_∞	T_w	T_w/T_r
6.0	$2.2 \times 10^7 \text{ m}^{-1}$	8.3×10^5	5000	254 K	300 K	0.16

$L_x \times L_y \times L_z \text{ (m)}$	$\Delta x^+ \times \Delta y_1^+ \times \Delta z^+$	$\Delta x \times \Delta y_1 \times \Delta z$	$n_x \times n_y \times n_z$
$0.5 \times 0.05 \times 0.025$	$110 \times 22 \times 56$	$0.067\delta \times 0.013\delta \times 0.033\delta$	$1404 \times 98 \times 200$

there is a peak in the profile that occurs very close to the wall (in the buffer layer). This peak is not resolvable when using grids with typical wall modeled LES spacings. The main goal for this part of the study was to find out if we can get reasonable predictions when simulating high Mach number flows with cold wall conditions.

The flow conditions for this case (shown in table 3.2) match those used by Subbareddy & Candler [77] in their DNS study. The boundary layer in the DNS transitions from a laminar to a turbulent state close to the inflow location. In later section 4.4, we present results from a fully matched spatial simulation of this flow. Here, since we are trying to isolate the effects of the cold wall condition, the inflow plane is placed at a streamwise location that is in the fully turbulent region of the DNS.

The adiabatic temperature ratio (T_w/T_r) in this case is around 0.16 which suggests strong non-adiabatic effects dominate the near-wall region which may not be fully resolved

by the grid used in the current WMLES. Uniform spacings conforming to typical WMLES resolutions in outer units are used in streamwise and spanwise directions. Close to the outflow, we use a buffer zone with grid stretching to mitigate adverse outflow boundary condition effects. In the wall-normal direction, uniformly distributed points were used up to the boundary layer thickness (δ) after which the grid was stretched gradually up to the upper boundary. Periodic boundary conditions are used in the spanwise direction. At the inflow, mean flow profiles from the DNS are imposed, and superimposed with synthetic turbulence: the turbulent inflow generation technique of Toubert & Sandham [79] is used for generating these turbulent fluctuations. Note that the reference thickness, δ , in what follows is the inflow boundary layer thickness.

The skin-friction curve plotted in figure 3.8, shows that there is a ‘development length’ of about 20δ downstream of the inflow plane (this is fairly typical of turbulence generation techniques), after which the C_f and Stanton number S_t curves from the WMLES start to closely track the DNS curves. The Stanton number S_t and skin-friction coefficient C_f is computed as,

$$S_t = \frac{q_w}{C_p \rho_\infty U_\infty (T_w - T_r)}, \quad C_f = \frac{2\tau_w}{\rho_\infty U_\infty^2}$$

Some mean flow statistics are plotted for this case in the figures 3.9 and 3.10. The slight log-layer mismatch in the mean velocity profile implies a minor over-prediction of the wall shear stress. There is a slight under-prediction of temperature in the outer region of the boundary layer but the inner layer profile (note that this is the wall-model prediction) consisting of the temperature peak shows good agreement. The normal component ($\overline{v'v'}$) of the resolved Reynolds stresses seems to be the most underpredicted compared to the other components. This is something that was not seen for the low Mach number cases. Overall the mean and RMS quantities are predicted to a reasonable degree of accuracy, with a maximum deviation of around 3% for the skin friction or heat transfer in the fully turbulent regime when using the mixed scaling. The error is around 9% when using the semi-local scaling. Thus, WMLES does seem to show promise even when posed with strong non-adiabatic conditions. The use of mixed scaling in such flows did lead to significantly better predictions for C_f and S_t .

3.4 Discussion

WMLES was applied to high-speed channel flows and boundary layers with significantly colder walls. For the channel flow improved prediction in the velocity profile was seen when using the mixed scaling. Lower bulk temperatures were observed in the WMLES

(a)

(b)

Figure 3.9 (a) The mean velocity and (b) the temperature profile computed from the WMLES are compared with the DNS. Black line, DNS; red line, outer LES; blue line, mean wall model solution; black dash-dotted line, exchange location in the WMLES. The profiles are taken at $x/\delta = 50$.

Figure 3.10 The density scaled resolved Reynolds stresses from the top to bottom: corresponding to $\overline{u'u'}$ (red), $\overline{w'w'}$ (blue), $\overline{v'v'}$ (green) and $\overline{u'v'}$ (yellow). Solid lines, DNS; Circles, WMLES. The profiles are taken at $x/\delta = 50$.

results for channel flow which was related to the lack of viscous dissipation in the outer LES. This discrepancy seen in channel flow did not seem to affect the boundary layer results in a dramatic way, where we observed that the wall model was able to capture the cold wall temperature peak accurately. It was observed that overall the mixed scaling provided better skin-friction and heat-flux predictions when compared to the semi-local scaling for cold wall boundary layers. WMLES is further applied to hypersonic flows with different challenges in the coming sections, but the results until now for cold wall conditions show promise.

4.1 Introduction

Transition prediction is a difficult task for any model: this is certainly the case for WMLES as well. Wall models use a turbulent eddy viscosity and the resulting turbulent profiles do not match those in the laminar/transitional regimes.

Prior WMLES studies on transitional flows proposed the use of a ‘transition sensor’ that attempts to detect the turbulent zone (essentially delineating laminar and turbulent regions). In locations where ‘laminar’ flow is detected, the wall model reverts to using a linear approximation for velocity and temperature gradients to predict wall shear stress and heat flux; the linear approximation typically uses the solution from the first off-all grid point [10]. Computing the shear-stress from the outer grid first point is often a reasonable approximation for the wall velocity gradient since near-wall velocity profiles are nearly linear in laminar regions. However, the temperature profiles, especially in cold wall flows, are non-linear with sharp gradients in the near-wall region: this suggests that using a wall model to predict the heat flux would be beneficial. The non-linearity of near-wall temperature profiles even in laminar flows is seen in figure 4.1.b. By comparison, a linear approximation for the near-wall velocity profile is much more accurate, as can be seen in figure 4.1.a.

In this study, we develop a modified transition sensor to detect laminar/turbulent flow regions. In regions detected as laminar, we solve the wall model with the turbulent eddy viscosity set to zero. The exchange location for the equilibrium wall model in such regions is taken to be the first off-wall cell: this gives reasonable predictions for the velocity and temperature gradient.

Figure 4.1 (a) Streamwise velocity and (b) temperature profiles taken from a laminar Mach 6 hypersonic cold wall boundary layer.

One limitation of WMLES to keep in mind for transitional flow cases is that the grid spacing in the wall-normal direction needs to be finer than needed by conventional fully turbulent simulations: typical wall-normal grid spacings for WMLES are scaled based on the turbulent boundary layer thickness and might be too coarse to resolve the thin pre-transitional laminar boundary layer. Previous studies using WMLES in transitional cases have used much finer grid spacings ($\Delta y_1^+ < 20$) to capture transition accurately [57, 10]. When using such a fine wall-normal spacing near the wall it may not always be possible to have the LES input taken at a distance even close to the value of 0.1δ . In the following sections, we describe the transition sensor and validate it for two cases at Mach 6 cold wall conditions at low and high Reynolds numbers.

4.2 Transition Sensor

A transition sensor (S_{tl}^k) was developed by Bodart & Larsson [10] [46] using the turbulent kinetic energy (k) normalized by the friction velocity (u_τ). They suggest using

$$S_{tl}^k = \frac{\widehat{\rho_w k}}{\widehat{\tau_w}}, \quad (4.1)$$

where the quantities with the hats are temporally filtered using an exponential moving average (similar to Meneveau et al. [52]). The Favre-averaging procedure is used to obtain the resolved turbulent kinetic energy ($\widehat{k}$) for the sensor:

$$\widehat{k} = \frac{\widehat{\rho u_i u_i}}{\widehat{\rho}} - \frac{\widehat{\rho u_i} \widehat{\rho u_i}}{\widehat{\rho}^2} \quad (4.2)$$

Note that time filtering for any quantity ϕ at a time step $n + 1$ is defined as

$$\hat{\phi}^{n+1} = \hat{\phi}^n + \left(\frac{dt^n}{T} \right) (\phi^n - \hat{\phi}^n), \quad (4.3)$$

where the time scale $T = 1/\sqrt{S_{ij}S_{ij}} = 1/|S|$ is computed from LES data at the exchange location $y = h_e$, and dt^n is the time step for the current iteration. This sensor has been successfully tested on transitional low Mach number flows [10, 57]. A potential issue with the computation of this sensor is that it depends on an estimate of τ_w which is itself an output of the wall model. This may not be ideal since τ_w can vary quite a lot between laminar and turbulent regions. Additionally, flow separation, τ_w goes close to zero which results in a large value of S_{ij}^k . There seems to be a recursive relation where the value of the sensor is dependent on the output of the wall model and the action of the wall model is dependent on whether the sensor is above some threshold. We suggest a modified transition sensor which is computed as

$$S_{tl}^m = 0.15 \frac{\hat{\rho}\hat{k}}{\hat{\mu}|\hat{S}|}, \quad (4.4)$$

where the time filtered quantities $\hat{k}$, $\hat{\rho}$, $\hat{\mu}$ and $|\hat{S}|$ are all computed using LES data at $y = h_{el}$ using the time scale shown before. This sensor was inspired by an empirical relation between turbulent kinetic energy and eddy viscosity proposed by Bradshaw et al. [14],

$$\nu_t \left| \frac{du}{dy} \right| = \sqrt{C_\mu} k,$$

where $C_\mu = 0.09$ and the constant 0.15 is equal to $\sqrt{C_\mu}/2$. The main modification is replacing u_τ with the norm of the strain-rate tensor. This modified sensor can be calculated entirely from the outer LES without requiring any input from the wall model and should remain relatively robust close to separated regions in the flow. The threshold value S_{tl}^0 is set by the user and usually varies from 0.1-0.25. If the value of the sensor at the LES exchange location goes below this then the eddy viscosity in the wall model is set to zero for the corresponding wall face. In the case of the equilibrium model, the closest cell to the wall is taken as the exchange location.

4.3 Mach 6 Transitional SBLI, Low Re

WMLES using the equilibrium wall model is tested against the DNS [66] of a Mach 6 transitional boundary layer interacting with an incident shockwave. Yang et al. [86] have

Figure 4.2 A schematic diagram of the oblique shock impinging on a laminar boundary layer is shown above. Downstream of the shock interaction the boundary layer transitions to turbulence.

Figure 4.3 Instantaneous snapshot of density gradient magnitude for the WMLES taken at $z/\delta_0^* = 20$. Seen is the boundary layer transitioning right after the interaction with the shock.

performed WMLES for this case previously using the equilibrium wall model. This current test case aims to compare the two transition sensors discussed in the previous section. This test case is a good measure of how well the transition sensor and the wall model can unravel the flow features close to the wall which are not resolved by the grid. A schematic of the flow is given in figure 4.2. Here we observe that the adverse pressure gradient caused by the impinging oblique shock produces a separation bubble. The inflow acoustic disturbances combined with the interaction of the shock cause the boundary layer to rapidly transition downstream of the separation bubble.

Information regarding the grid used in this case and the flow conditions are given in table 4.1. Here Re_1 refers to the unit Reynolds number, Re_{x_0} the inflow Reynolds number based on the distance from the leading edge of the flat plate, and $Re_{\delta_0^*}$ is based on the inflow displacement thickness (δ_0^*). We used 20 uniformly distributed points from the wall till a distance of $\delta = 5.1\delta_0^*$ (δ here is the boundary layer thickness at the outlet), giving us a first wall spacing of 0.05δ which seems to be slightly coarser than what was used by Yang et al. [86]. This places the exchange location height at 0.125δ which corresponds to the third cell from the wall. The grid is stretched to the upper boundary beyond a wall-normal distance of δ . Uniform streamwise spacing of 0.23δ is maintained till $300\delta_0^*$ after which the grid is stretched till the outflow boundary; this constitutes a buffer zone. Since this is a comparatively low Reynolds number flow the grid spacings normalized in wall units might seem finer than usual but when normalized with δ it obeys the typical WMLES resolution.

Table 4.1 Transitional SBLI - flow conditions and grid details.

M_∞	Re_1	Re_{x_0}	$Re_{\delta_0^*}$	T_∞	T_w/T_∞
6.0	$6.0 \times 10^6 \text{ m}^{-1}$	0.3×10^6	6830	65 K	4.5

$L_x \times L_y \times L_z$	$\Delta x^+ \times \Delta y_1^+ \times \Delta z^+$	$\Delta x \times \Delta y_1 \times \Delta z$	$n_x \times n_y \times n_z$
$350\delta_0^* \times 25\delta_0^* \times 45\delta_0^*$	$40 \times 8.7 \times 20$	$0.23\delta \times 0.05\delta \times 0.12\delta$	$300 \times 64 \times 72$

Periodic boundary conditions are imposed in spanwise directions. Rankine–Hugoniot shock jump conditions are applied at the upper boundary downstream of the shock to generate an oblique impinging shock with a 4° deflection angle. A similarity solution for the compressible laminar boundary layer [1] is imposed at the inlet combined with acoustic disturbances which are added to the inflow density profile, as done in the DNS [66]. The perturbations added to free stream density are computed as

$$\rho' = \rho_\infty A W(y) \sum_{j=0}^J \cos(2\pi jz/L_z + \phi_j) \sum_{k=1}^K \sin(2\pi f_k t + \psi_k) \quad (4.5)$$

where the cutoff wave numbers are $J = 16$ and $K = 20$. ϕ_j and ψ_k are random phases which are fixed for all the cases in this paper. The disturbance amplitude within the boundary layer is diminished using a damping function given below.

$$W(y) = 1 - \exp(-(y/\delta_0^*)^3)$$

The amplitude of the disturbances is $A = 10^{-3}$ for the WMLES whereas for the DNS it is $A = 5 \times 10^{-4}$. Since the WMLES grid is much coarser compared to the DNS it is not able to capture the growth of the disturbances in transitional regions. Hence we need to provide a higher amplitude to reach similar turbulence levels to that of the DNS [86].

In figure 4.3 we can distinctly see the main flow features, corresponding to the impinging oblique shock with the separation bubble, the reflected shock waves, and the transitioning boundary layer. The instantaneous Stanton number computed based on the heat flux predicted by the wall model in figure 4.5 shows a clear increase at the onset of transition. In figure 4.4.b we plot the spanwise time-averaged Heaviside function $H(x)$ value of the variable $x = S_{tl} - S_{tl}^0$. The threshold $S_{tl}^0 = 0.25$ is chosen for this case. If the sensor goes above the set threshold value the Heaviside function gives a value of 1 else it gives 0. The spanwise time average of the described function gives us an idea of how often the sensor detects turbulence in the domain. If this function value is 1 then it tells us that the eddy viscosity is activated in the wall model throughout the domain at every time instance conversely a value of 0 means there is no turbulence in that region and the eddy viscosity is set to zero. We observe that the modified transition sensor is much less noisy in the laminar region while being active more than 90% of the time in the turbulent region whereas the original sensor detects turbulence even before the shock interaction region which will result in higher skin friction and heat flux prediction in the laminar region. The many overshoots for the original sensor in the laminar region and separated region might be due to the low value of τ_w computed in those regions by the wall model. Also observed in figure 4.4.a is that the Stanton number (S_t) prediction to be slightly better for the modified sensor in the transitional region. At the end of the transitional region, we observe the Stanton number plot for the WMLES merges with the fully turbulent region of the DNS. Overall the modified sensor seems to show a much better behavior in the laminar and transitional region for this case compared to the original sensor.

(a)

(b)

Figure 4.4 (a) Comparison of the Stanton numbers with the heat flux computed from the wall model two sensors with the DNS (Black) (b) Comparison of regions with turbulence as detected by the two sensors. Blue, the original sensor; Red, the modified sensor.

Figure 4.5 Instantaneous isocontours of Stanton number computed from the wall model using the modified transition sensor are shown in the transitional region.

4.4 Mach 6 Transitional Boundary Layer, High Re

The transitional boundary layer in the case by Sandham et al. [66] was a low Re case for demonstrating the ability of the modified transition sensor. Now we try to capture the transition involved in the high Re case of Subbareddy & Candler [78] using WMLES. A similarity solution for the laminar compressible boundary layer [1] with perturbations is used at the inflow plane. A pair of counter-rotating vortices at the inflow plane, similar to the DNS, is used in the WMLES to cause transition making the boundary layer to become fully turbulent quite rapidly. The inflow disturbance is made up of dual pairs of counter-rotating streamwise vortices that create a sequence of “downwash” and “upwash” events in the boundary layer and cause it to transition. The perturbation velocities are computed from the stream function as,

$$\Psi = AU_{\infty}\bar{x}\bar{y}^3\bar{z}\exp\left(-\bar{x}^2 - \bar{y}^2 - \bar{z}^2\right), \quad u' = 0, \quad v' = \frac{\partial\Psi}{\partial z}, w' = \frac{\partial\Psi}{\partial y}$$

where $(\bar{x}, \bar{y}, \bar{z}) = (x/l_x, y/l_y, z/l_z)$ are the co-ordinates scaled by the characteristic lengths of the vortex perturbation and A is the strength of the disturbance as a fraction of the freestream velocity. In order to break the symmetry of the vortex spots and to introduce randomness to the inflow, the length scales of the disturbances (l_i) and the angle (θ_x) they make with the streamwise direction to vary in a random manner: they are sampled from sequences of random numbers in the range $\bar{l}_i \pm \delta l_i$ and $\bar{\theta}_x \pm \delta\theta_x$. The characteristic lengths which are normalized by the displacement thickness of the inflow laminar boundary layer (δ_0^*) $(l_x/\delta_0^*, l_y/\delta_0^*, l_z/\delta_0^*) = (4.5 \pm 1.5, 1 \pm 0.2, 4.5 \pm 1.5)$ and the

Figure 4.6 Iso-surfaces of “Q” colored by the streamwise velocity is shown above for the Mach 6 transitional boundary layer.

Figure 4.7 Instantaneous slice of density contour for the WMLES taken at $z = 0.0125$. The image is stretched in the wall normal direction by a factor of 2 for clarity.

Figure 4.8 Skin friction coefficient (C_f , red) and Stanton number (St , blue) comparison between the DNS and the WMLES. Colored circles, WMLES with mixed scaling; Colored squares, WMLES with semi-local scaling; Colored solid lines, DNS. The black dashed line denotes the scaled transition sensor ($S_{tl}^m/5$) employed in this case.

amplitude of perturbation $A = 0.5$ are matched with the DNS. The spot angles are allowed to vary from $\theta_x = [-2^\circ, 2^\circ]$, consistent with the DNS.

Table 4.2 Boundary layer - grid details.

$L_x \times L_y \times L_z$ (m)	$\Delta x^+ \times \Delta y_1^+ \times \Delta z^+$	$\Delta x \times \Delta y_1 \times \Delta z$	$n_x \times n_y \times n_z$
$0.5 \times 0.05 \times 0.025$	$200 \times 20 \times 100$	$0.1\delta \times 0.02\delta \times 0.05\delta$	$1404 \times 98 \times 200$

The grid (details in table 4.2) used in this case is similar to the one used in the previous chapter but is extended in the upstream streamwise direction to capture the full range from laminar to transitional to fully turbulent flow. Instantaneous flow visualizations are presented in figures 4.6 and 4.7. Hairpin-like vortices do seem to be captured by the WMLES, which can be seen in the iso-contours of Q-criterion. We can see the formation of inclined turbulent structures in the outer regions and acoustic waves propagating from the boundary layer in the instantaneous density contour. Thus even with a much coarser grid compared to the DNS we can capture some key flow features of the turbulent boundary layer. From the skin-friction plot in figure 4.8, it can be discerned that the transition location for the WMLES closely follows the DNS but the peak in skin-friction

and heat-flux at transition is underpredicted by the WMLES. In the fully turbulent region, a maximum deviation of around 5% for the skin friction or heat transfer is observed.

4.5 Discussion

WMLES of high Mach number flows undergoing the transition to turbulence was investigated. The modified transition sensor detailed in the text shows promise in such cases to differentiate between transitional and turbulent regions of the flow. It was observed that the transitional location was well predicted by the modified sensor but the peak in skin friction and heat flux at transition was not captured using WMLES. Transition prediction is still dependent on a user-set threshold and the WMLES for transitional flows is still not fully predictive. An issue with using WMLES for transitional cases is that there are not any clear standards by which the wall-normal grid spacing can be chosen. For transitional flows, thin boundary layers dictate that fine wall-normal spacings are needed to get the transition right. This is in contrast to well-validated WMLES grid resolution requirements which scale with the boundary layer thickness. Overall, reasonable heat-flux and skin-friction predictions were obtained for WMLES at both low and high Re considering the relatively coarse resolution which was employed.

Shock Boundary Layer Interactions

5.1 Introduction

Shock boundary layer interactions (SBLI) are common in high-speed flow applications and pose difficult challenges to turbulence modeling. The adverse pressure gradient caused due to a shock in such flows can lead to boundary layer separation. Flow separation causes intense, large-scale flow unsteadiness which can cause high-pressure loads on the air-frame and severe heating, which are very undesirable from an engineering perspective. Purely RANS-based approaches have difficulty in modeling this complex phenomenon. Considering that while using WMLES, the bulk of the boundary layer is resolved by the LES, our reliance on the accuracy of the RANS model is restricted to a small region close to the wall. With this reasoning, in theory, even with a simplistic mixing-length-based RANS model (used in the wall model), much higher accuracy can be obtained with WMLES when compared to hybrid RANS-LES or pure RANS-based methods.

The equilibrium (denoted by EQ) model is cheap, easy to implement across complex geometries, and does well in attached flows. The numerical and implementation complexity of the non-equilibrium model (NEQ) makes it less appealing for industrial applications. Considering its simplicity and low cost, there is an incentive to make improvements to the accuracy of the equilibrium model for use in complex flows. The main goal of this chapter is to examine how we can use information from the LES to improve the prediction for the equilibrium model under complex (“non-equilibrium”) conditions. The non-equilibrium model (and the eddy viscosity formulation within it) is also examined in detail, but the main focus is to improve the equilibrium model prediction. A robust sensor to detect the non-equilibrium regions is devised and applied to three different SBLIs at moderate to

Figure 5.1 A schematic diagram of the oblique shock impinging on a turbulent boundary layer with variable wall temperature is shown above.

high Re . Also investigated is the capability of WMLES to capture large-scale features of SBLI at different wall temperature conditions from hot to cold wall flows and the ability of it to capture the low-frequency characteristics of a ramp-type SBLI at high Re .

5.2 Mach 2.3 Oblique SBLI, Moderate Re

A comparison of the WMLES results to the DNS data of Bernardini et al. [7], who study the effects of wall heat transfer on the characteristics of the shock-induced separation bubble, is performed in this section. A schematic diagram of the shock boundary layer interaction with the step wall temperature change is shown in the figure 5.1. The adverse pressure gradient caused by the impinging oblique shock opposes the incoming fluid momentum and if the pressure gradient is high enough it causes the flow to reverse forming a separation bubble. The main effect of wall cooling as seen in the DNS was to reduce the separation region and a heated wall causes the opposite effect where the separated region expands. We wanted to see if WMLES can capture this behavior, especially when you are not resolving that inner layer dynamics. A moderate friction Reynolds number of $Re_\tau = 450$ is obtained downstream of the shock interaction in this case. Similar to the DNS the at some point, upstream of the shock interaction the temperature at the wall is smoothly changed to either a heated or cold wall.

The digital filtering technique of Toubert & Sandham [79] is used to produce synthetic

Figure 5.2 Instantaneous temperature contours near the shock interaction region for the quasi-adiabatic wall case is shown above.

turbulence at the inflow plane. Re_{δ_i} is the Reynolds number based on the inflow boundary layer thickness (δ_i). A sponge layer of length $30\delta_i$ is provided in the grid after a streamwise location of $x = 96\delta_i$ to remove spurious oscillations at the outflow. Uniform spacing in the streamwise (up to $x = 96\delta_i$) and spanwise directions is used. In the wall-normal direction, uniform spacing of Δy_1 is maintained until $3\delta_i$ after which the grid is smoothly stretched in y until the outflow. The oblique shock is introduced in the simulation by imposing the inviscid Rankine-Hugoniot jump conditions at the top boundary corresponding to the free-stream Mach number (M_∞) and the deflection angle (θ). Periodic boundary conditions are used in the span and an isothermal wall boundary condition with $T_w = s T_r$ is used, where T_r is the recovery temperature. In the current study, we have performed WMLES for wall temperature ratios of $s = 0.5, 1.0$, and 1.9 . Note that the total number of cells used for the WMLES is approximately 100 times smaller than the DNS which shows the cost savings achieved. The grid resolution seen in table 5.1 might seem finer than typical WMLES spacings in wall units but that's mainly due to the moderate Reynolds number of this case. The grid spacings in terms of the inflow boundary layer thickness agree well with the usual WMLES grid requirements.

Table 5.1 Mach 2.3 OSBLI - flow conditions and grid details.

M_∞	T_∞	θ	$\text{Re}_{\delta_{in}}$
2.28	145.5 K	8°	16750

$L_x \times L_y \times L_z (\times \delta_{in})$	$\Delta x \times \Delta y_1 \times \Delta z (\times \delta_{in})$	$n_x \times n_y \times n_z$
$126 \times 20 \times 5.5$	$0.1 \times 0.05 \times 0.05$	$1035 \times 98 \times 110$

Figure 5.3 Instantaneous velocity contours from wall-normal location $y = 0.1\delta_i$ near the shock interaction region for the quasi-adiabatic wall case is shown above.

Figure 5.4 (a) The van Driest transformed mean velocity is compared with the DNS for the adiabatic case. Black, DNS; Red, outer LES; Blue, EQ/NEQA wall model solution. (b) The density scaled resolved Reynolds stresses from the top to bottom: corresponding to $\overline{u'u'}$ (red), $\overline{w'w'}$ (green), $\overline{v'v'}$ (blue) and $\overline{u'v'}$ (grey). Symbols, WMLES; Lines, DNS.

Instantaneous snapshots of temperature and velocity contours in the shock interaction region are given in figures 5.2-5.3. The main flow characteristics like the inviscid oblique shock, the reflected shock emanating from the separation bubble, and the thickening of the boundary layer in the post-shock region can be observed in the temperature contours in figure 5.2. The upstream attached boundary layer region is observed in the figure 5.3, which consists of small-scale streaky structures. When these thin streaky structures come across the separation they are amplified and become much larger. After reattachment, they try to regain their streaky structure in the downstream region.

5.2.1 Baseline Results

A comparison between the WMLES and DNS for the incoming boundary layer at a location upstream of the shock-interaction region at $x_0 = 50\delta_i$ is done in figure 5.4 for the adiabatic case ($s = 1$). δ_0 is the boundary layer thickness at x_0 and $x^* = x - x_{imp}/\delta_0$

Figure 5.5 (a) Streamwise velocity and (b) temperature profiles from outer LES at $x^* = -5, -2, -1, 0, 5$ from left to right respectively are compared to the DNS for the nominally adiabatic case using the NEQA formulation.

is the coordinate system centered around the shock impingement point $x_{imp} = 69.5\delta_i$. A good match in both the mean and second-order statistics with DNS is obtained at this location. It is seen that the inner peak in streamwise RMS $(\overline{u'u'})$ is unresolved as expected in a wall modeled LES which resolves only the outer motions and a good agreement in the outer layer fluctuations is achieved. Qualitatively a good comparison in the outer region of the SBLI is obtained with the DNS as seen in the velocity and temperature profiles in figure 5.5 using the baseline NEQA formulation. This suggests that the major flow features near the shock are still dictated by the outer LES.

The skin-friction C_f and wall-pressure P_w obtained from WMLES are compared to the DNS for the nominally adiabatic wall case in figure 5.6 for the equilibrium model (EQ) and the non-equilibrium model with the baseline eddy viscosity formulation (NEQA). Both the models can get accurate skin-friction results upstream of the SBLI region. The small-scale features like the prominent "W" shaped C_f curve which is seen in the separated region for the DNS are absent in the WMLES results. The equilibrium model fails to predict the negative C_f in the separation bubble, unlike the non-equilibrium model. The assumption that the wall shear stress is aligned to the velocity vector at the exchange location means that the C_f prediction in the equilibrium wall model is strongly dependent on the grid resolution in the outer LES. If the time-averaged velocity at the exchange location is positive then the C_f obtained from the equilibrium model will also have the same sign. The non-equilibrium model differs in this aspect as it incorporates the adverse pressure-gradient effects in the inner layer and hence can predict a negative C_f in the separated region, although in this case, we see a large negative dip. Also observed is that

(a)

(b)

Figure 5.6 (a) C_f and (b) P_w comparison for the quasi-adiabatic case is shown above. Black, DNS; Blue, EQ model; Green, NEQA model.

the pressure rise seen in figure 5.6.b is better predicted by the NEQA model than the equilibrium model.

The eddy viscosity formulation which uses the classic van Driest damping (NEQA) predicts a high negative peak in C_f as seen for the NEQA model in figure 5.6.a. This is an effect of its dependence on u_τ which depletes the Reynolds stress in regions close to the separation. Also to be noted is that the dynamic eddy viscosity correction [57] which uses the inverse of the damping factor in computing the corrected κ value will further lower the value of eddy viscosity in separated regions. Writing the streamwise momentum equation in the following crude way:

$$\frac{d}{dy} \left((\mu + \mu_t) \frac{du}{dy} \right) = S_{neq} ,$$

where S_{neq} denotes the momentum being carried by the non-equilibrium terms which are typically imposed from the outer LES. This term is significant in the separated regions and if the Reynolds stress is depleted in such regions then this leads to an increase in du/dy to compensate for the momentum deficit. Thus, we get an unphysically large dip in C_f in regions where the DNS [7] which predicts a peak in Reynolds stresses has much smaller skin friction. In the following section, we look at modifications to the eddy viscosity in the non-equilibrium model to account for this increase in Reynolds stresses.

5.2.2 Eddy Viscosity Modifications

5.2.2.1 Formulation

The baseline mixing length model used for the eddy viscosity viscosity in the non-equilibrium model assumes the form

$$\mu_t^a = \rho(\kappa y)^2 |S| D_2(y), \quad D_2(y) = (1 - \exp(-y^+/A_2^+))^2, \quad (5.1)$$

where the standard value of $A_2^+ = 26$ is used in this case. Note that in regions of the flow near separation, the value of u_τ , which is typically computed locally at each wall face assumes values close to zero. As a consequence, the van Driest damping function takes on very small values and this results in the eddy viscosity being highly damped in these regions. Wall functions that use the pressure-gradient (or some non-dimensional representation of it) have been previously explored in the context of incompressible flows by (for e.g.) Skote & Wallin [70]. Eddy viscosity formulations that use a pressure-gradient parameter such as the one given by Duprat et al. [26] and Nituch et al. [56] have shown

promising results in adverse pressure-gradient, separated flows. The velocity scale in these formulations is given, on dimensional grounds, by $u_p = ((\mu/\rho^2)|dP_w/dx|)^{1/3}$. In this study, we explore the use of such pressure-gradient-based eddy viscosity formulations for shock-induced separated flows. A modified version of the eddy viscosity formulation by Duprat et al. [26] used in the present study is given by:

$$\alpha = u_\tau^2/(u_p^2 + u_\tau^2), \quad \alpha_* = \max[\alpha, (\tanh[10(\alpha - 0.5)] + 1)/2] \quad (5.2)$$

$$u_{\tau p}^2 = u_\tau^2 + (1 - \alpha_*)u_p^2, \quad y_p = y u_{\tau p}/\nu \quad (5.3)$$

$$D_p(y) = (1 - \exp(-y_p/A_3^+))^2, \quad A_3^+ = 1 + \alpha_*^3(A_2^+ - 1) \quad (5.4)$$

$$\mu_t^b = \rho(\kappa y)^2 |S| D_p(y) \alpha_*^{-0.5} (\alpha_* + y_p(1 - \alpha_*)^{1.5})^{0.5} \quad (5.5)$$

The eddy viscosity above is constructed such that in regions where pressure-gradient effects are negligible ($\alpha_* = 1$), it switches back to the standard mixing length model given in equation (5.1). The modification to α giving α_* is done so that the eddy viscosity does not react to small pressure-gradient fluctuations in attached boundary layer regions and is active only when it encounters a strong pressure gradient. Another type of eddy viscosity model, given in equation (5.6) below, uses just the damping function, $D_p(y)$:

$$\mu_t^c = \rho(\kappa y)^2 |S| D_p(y) \quad (5.6)$$

The eddy viscosity formulations from equations (5.1), (5.5) and (5.6) above are tested for the SBLI cases in the present study. The cases which use the non-equilibrium model with the above-mentioned eddy viscosity formulations are named NEQA, NEQB, and NEQC respectively.

5.2.2.2 Results

In figure 5.7, it is observed that the eddy viscosity formulation namely NEQB and NEQC can compensate for this eddy viscosity depletion in some form and thus can recover the skin friction in the separated region. But another drawback of such pressure-gradient-based formulations is that they might be triggered by small oscillations in pressure that need to be suppressed. In the present case, we observe that the upstream region of the shock interaction is affected due to the sensor α_* getting activated. This is also the reason C_f dips earlier for the NEQB and NEQC cases than the NEQA model. The early dip in C_f follows the early rise in P_w for NEQB and NEQC cases in figure 5.7.b. The NEQB formulation performs the best in trying to recover the skin friction in separation but also

(a)

(b)

Figure 5.7 (a) C_f and (b) P_w comparison for the quasi-adiabatic case is shown above. Black, DNS; Green, NEQA model; Blue, NEQC model; Red, NEQB model.

leads to the earliest dip in C_f . The small over-prediction in separation bubble length by the different eddy-viscosity formulations in the WMLES results is consistent with the study by Morgan et al. [54], where they observed that RANS models had a bias towards over-predicting separated regions at low Re conditions.

Seen in the figure 5.8 are the temperature contours on a spanwise and wall-normal plane. Here there is an almost adiabatic boundary layer coming in and at some point, upstream the wall temperature is changed to a heated or cold wall, which can be seen in the temperature contours. The effect of heating is to expand the interaction region and cooling shrinks the region. The expansion and shrinkage of the separation bubble due to the hot and cold wall temperatures can be seen from the skin-friction and wall-pressure plots using the NEQB model in figure 5.9. The reattachment skin-friction and wall-pressure are captured accurately by the NEQB model. Although we do observe that the separation length is slightly over-predicted across all cases.

5.2.3 Wall-Stress Blending

Both the equilibrium and non-equilibrium models are limited by their use of a RANS-based eddy viscosity which loses its robustness in separated flows. LES, in theory, is better equipped to handle separated flow regimes where the scales of motion are larger and slower moving compared to the attached regions. For separated flow regions, the WMLES cell closest to the wall might hold more accurate information than a cell away from the wall in such non-equilibrium regions – using the first cell as the exchange location may be beneficial. It has been observed in previous WMLES studies [26, 11], that reverting to a standard no-slip LES has given more accurate skin-friction results in separated regions when compared with the use of a wall model. Bose & Park [12] suggest that lowering the exchange location when the flow is subject to strong pressure-gradients can make the equilibrium assumption stronger since the contribution of the non-equilibrium terms to the wall-stress is lower (in an integral sense). Having a variable exchange location in the presence of non-equilibrium effects was also talked about by Kahraman & Larsson [40], who try to determine the most optimum wall model thickness using an apriori solution. When taking the exchange location away from the wall, you can produce shear in the wrong direction, especially in separated flows. This manifests in the equilibrium model not able to capture the negative C_f in separated regions even when there are pockets of negative flow in the mean velocity solution. Now the question arises how do we detect such regions dominated by non-equilibrium effects and suitably switch: either between the wall model and LES-defined wall-stress or the second option would be to reduce the

Figure 5.8 Instantaneous temperature contours at plane $y = 0.05\delta_0$ and $z = 0.5\delta_0$ are shown above for the WMLES cases of SBLI at cold, isothermal and heated wall conditions.

Figure 5.9 C_f and P_w comparisons are shown above for cold (blue), isothermal (black) and hot (red) wall cases. Symbols, DNS; Solid lines, NEQB model.

exchange location height (for the equilibrium model) to be closer to the wall to decrease the effect of the non-equilibrium terms.

5.2.3.1 Non-equilibrium Sensor

First, we formulate the sensor to detect regions of non-equilibrium flow. There are a few options, the classical definition of separation is defined by regions where the wall-stress changes sign $\tau_w < 0$. But this criteria is not very useful when looking at instantaneous turbulent flow. The second option was to look at the magnitude of the non-equilibrium terms averaged over a time scale. The non-equilibrium terms for the momentum equation are given as,

$$S_{neq} = \frac{dU_{||}}{dt} + u_i \frac{dU_{||}}{dx_i} + \frac{1}{\rho} \frac{dP}{dx_{||}}$$

These terms are typically negligible in equilibrium attached flows. But it is hard to determine what a sensible threshold or normalization we could use to differentiate separated regions. Some of the options which were investigated to devise a robust non-equilibrium sensor are detailed as follows.

An option based on the pressure gradient which we explored previously for the eddy viscosity in the non-equilibrium model is a valid candidate. In regions of flow separation, the value of $u_\tau = \sqrt{|\tau_w|/\rho_w}$, the velocity scale based on the wall shear stress assumes values close to zero. In such regions, another velocity scale based on the pressure-gradient (or some non-dimensional representation of it) has been previously explored in the context of incompressible flows. Eddy viscosity formulations that use a pressure-gradient parameter such as the one given by Duprat et al. [26] have shown promising results in adverse pressure-gradient, separated flows. The velocity scale in these formulations is given, on dimensional grounds, by $u_p = ((\mu_w/\rho_w^2)|dP_w/dx|)^{1/3}$. Note that since pressure doesn't vary in the wall model layer the pressure-gradient dP_w/dx is taken from the LES exchange location.

The blend of these two velocity scales gives us a sensor α' which can be used to differentiate regions of separation as u_τ decreases in magnitude and u_p becomes significant.

$$\alpha' = u_\tau^2/(u_p^2 + u_\tau^2), \quad \alpha_p = \max[\alpha', (\tanh[10(\alpha' - 0.5)] + 1)/2] \quad (5.7)$$

The modification to α' is done to get α_p so that it doesn't react to small pressure-gradient fluctuations in attached boundary layer regions and the switch to LES is only done when it encounters a strong enough pressure gradient. It was observed in our previous results with the NEQ model that the activation of this sensor in the upstream region of the shock

gave rise to larger separation lengths. Hence we try to explore other methods to detect separation which doesn't include the pressure gradient.

An idea that has been used in hybrid RANS-LES methods was to try to dynamically detect regions where the grid was too coarse for LES hence the solver would switch to a RANS model in such regions. Many popular hybrid approaches use this mechanism (e.g. the IDDES model by [69], Xiao et al. [84]) of detecting unresolved regions of the domain. Since in separated flow regimes the scales of motion are larger than attached regions than this would mean that the near-wall grid would be more resolved in separated regions. As to how resolved a grid is could be a good metric to differentiate attached and separated region. A classic criterion to check how resolved a grid is at a point was developed by Pope [63], which was the ratio of the resolved turbulent kinetic energy (k_{res}) and the resolved plus modeled turbulent kinetic energy ($k_{res} + k_{SGS}$) given as,

$$\alpha_{po} = \frac{k_{res}}{k_{res} + k_{SGS}} > 0.8$$

This criterion suggests that if the grid resolves more than 80% of the total turbulent kinetic energy (k) then the LES can be considered to be well resolved. It was shown by Davidson [20] and later by Xiao et al. [84] that this criterion was not robust enough due to the heavy dependence on the modeling of k_{SGS} . Also taking into account the near-wall SGS modeling errors typically seen in the cells close to the wall in WMLES a different criterion was needed.

A criterion for LES resolution was given by Xiao et al. [84], based on the total (resolved plus modeled) turbulent kinetic energy and the total dissipation rate (ε) as,

$$\alpha_{xi} = \frac{k^{3/2} \Delta}{\varepsilon}$$

where Δ was defined based on the cell volume V as $\Delta = V^{1/3}$ or $\Delta = \max[\Delta x, \Delta y, \Delta z]$.

Another criterion for quantifying the LES resolution, was developed by Davidson [20] based on the SGS dissipation rate, this was computed as,

$$\alpha_{da} = \frac{\varepsilon'_{SGS}}{\varepsilon_{SGS}}$$

$$\varepsilon'_{SGS} = \varepsilon_{SGS} - \langle \nu_t^{SGS} \rangle \frac{\partial \langle u_i \rangle}{\partial x_j} \frac{\partial \langle u_i \rangle}{\partial x_j}, \quad \varepsilon_{SGS} = \langle \nu_t^{SGS} \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} \rangle$$

Both α_{xi} and α_{da} sensors were relatively robust when applying different SGS models but lacked a sensible threshold value by which we could identify attached regions of the flow.

In the numerical experiments performed in this study using WMLES, for flows at different Reynolds numbers, both α_{xi} and α_{da} gave a wide range of values in the attached regions. Hence we formulate a more robust sensor based on the resolved Reynolds stress in the next section.

5.2.3.2 Sensor Based on Reynolds Stress

The non-equilibrium sensor based on the resolved Reynolds stress at the exchange location is discussed in this section. The formulation of the sensor begins with the equilibrium model equation which equates the wall-stress to the total stress at the exchange location which is the sum of the viscous and the modeled Reynolds stress in the wall model layer.

$$\langle \tau_w \rangle = \langle (\mu + \mu_t) \frac{du}{dy} \rangle^R = \tau^{vis} + \tau^{rey} \quad (5.8)$$

The same equation in terms of the LES variables would be equivalent to viscous, subgrid, and resolved Reynolds stress. The angular brackets denote an averaging over some time scale.

$$\langle \tau_w \rangle = \langle (\mu + \mu_t) \frac{du}{dy} \rangle^L - \langle \rho u' v' \rangle^L = \tau^{vis} + \tau^{sgs} + \tau^{res} \quad (5.9)$$

Since the time-averaged subgrid and viscous stresses are strictly positive in attached regions thus by comparing equations (5.8) and (5.9) would give us the following inequality for regions of equilibrium flow

$$\langle (\mu + \mu_t) du/dy \rangle_h^R = \langle \tau_w \rangle_h^R > -\langle \rho u' v' \rangle^L \quad (5.10)$$

The above inequality suggests that the resolved stress in the LES is lesser than the total stress which is equal to the wall-stress predicted by the equilibrium model. In separated regions where the equilibrium assumption is violated the inequality will not hold as the Reynolds stresses are known to peak in separated regions whereas the wall-stress would tend towards zero. Hence this inequality can be used to detect separated regions and blend the LES and wall model stresses in the form given below.

The above-formed inequality is used as a non-equilibrium sensor written as,

$$\alpha_r^1 = \begin{cases} 0, & \text{if } \langle u' v' \rangle / \langle 1.5 u_\tau^2 \rangle > 1 \\ 1, & \text{otherwise} \end{cases} \quad (5.11)$$

Note the factor of 1.5 multiplied to u_τ^2 so that small deviations from equilibrium in the

attached region do not lead to the sensor being activated and only when the shear stress drops significantly compared to the resolved stress, the switch is done. The current version of this sensor gives only binary values of 1 or 0. But this can easily be extended to give a smooth variation using a Tanh function. Using the Tanh function to get a smooth variation of the sensor did not significantly affect the results in the current study.

The time-filtering operation $\langle \phi \rangle^n$ for a variable ϕ at time step n is defined as

$$\langle \phi \rangle^n = (1 - \epsilon) \langle \phi \rangle^{n-1} + \epsilon \phi^n \quad (5.12)$$

where ϵ is defined as $\epsilon = \Delta t / T_f$. This operation denotes an exponential moving average using the weight $W(t) = \exp(-t/T_f)$ with a finite memory of time-scale T_f . The filtering time-scale (T_f) is taken as the wall diffusion time scale which is calculated as $T_f = h_e / \kappa u_\tau$. Since u_τ drops to low values in the separated regions, this would lead to large filtering time scales in such regions. An equivalent time-scale which is computed as $T_f = 1/(\kappa^2 |S|)$ from the LES exchange location is more robust in separated regions. Numerical experiments with both these time-scales were performed and in the current study, we did not observe a large difference in the final results when using either of the time scales.

For complex flows where a dominant flow direction cannot be determined the sensor is formulated by determining the wall-parallel direction as follows,

$$\begin{aligned} \vec{u} &= \vec{U} - v\vec{n}, \quad v = \vec{U} \cdot \vec{n} \\ \langle \rho u'_i v' \rangle &= \langle \rho u_i v \rangle / \langle \rho \rangle - \langle \rho u_i \rangle \langle \rho v \rangle / \langle \rho \rangle^2 \\ \alpha_r^1 &= \begin{cases} 0, & \text{if } |\langle u'_i v' \rangle| / \langle 1.5 u_\tau^2 \rangle > 1 \\ 1, & \text{otherwise} \end{cases} \end{aligned} \quad (5.13)$$

Here $\vec{u}$ is the wall-parallel velocity vector, v is the wall-normal velocity, and $\vec{U}$ is the velocity vector in Cartesian coordinates at the exchange location. Additional criteria defined to augment the sensor in equation 5.13 is based on the direction of the velocity vector in the exchange location cell and the first cell off the wall. If their dot product is negative i.e. their directions are opposite to each other the region is tagged as a non-equilibrium region.

$$\alpha_r^2 = \begin{cases} 0, & \text{if } \langle \vec{u}_e \rangle \cdot \langle \vec{u}_1 \rangle < 0 \\ 1, & \text{otherwise} \end{cases} \quad (5.14)$$

Where u_e and u_1 are the wall parallel velocity vectors at the exchange location and first cell off the wall in the LES. The equations 5.13-5.14 combined define the criterion for

Figure 5.10 Comparison of the skin-friction obtained from using the τ_{vis} (red) and τ_{dsm} (blue) formulations with the DNS [7] or experiments [68] (black) for SBLI at (a) moderate Re and (b) high Re.

non-equilibrium flow in the sensor. The final sensor is given by

$$\alpha_r = \min[\alpha_r^1, \alpha_r^2]$$

5.2.3.3 Choice of Blending

The blending between LES and wall model stress is defined as follows,

$$\tau_w = (1 - \alpha) \tau_w^L + \alpha \tau_w^R$$

Where τ_w^R is the wall-stress computed from the wall model at an exchange location $y = h_e$ away from the wall and τ_w^L is computed from the LES assuming a standard no-slip boundary condition. The value of 1 for blending factor α would translate to a region where the non-equilibrium effects are negligible and the equilibrium model can be used to model the wall-stress and heat-flux. Conversely when α tends to zero the WMLES would revert to a no-slip BC. In our current formulation, the wall heat-flux also uses the same blending factor α as the wall-stress as,

$$q_w = (1 - \alpha) q_w^L + \alpha q_w^R$$

Now we come to the question, as to how do we define the LES-stress τ_w^L . The first option is to just supply the wall-stress using the standard no-slip boundary condition

given as,

$$\tau_w^L = \mu_w \left. \frac{du}{dy} \right|_w$$

Which would mean taking a standard linear approximation of the velocity profile from the first cell to the wall. This assumes the fact that the subgrid-scale viscosity is zero at the wall. But this assumption is true only for wall resolved cases where the filtering length scale becomes smaller as you go close to the wall. Since in WMLES, the near-wall grid is much coarser this assumption is not valid [3]. We also explore the use of the first cell LES subgrid-scale viscosity when defining the LES-stress as,

$$\tau_w^L = \left(\mu_w + \mu_t^{SGS} \right) \left. \frac{du}{dy} \right|_w$$

The third option is where the τ_w^L and q_w^L are computed from the wall modeled solution by taking the exchange location to be the first cell off the wall at $y = h_1$.

It was observed that the first two approaches which involved using the first-cell linear approximation of the gradient were heavily dependent on the outer LES resolution in regions close to separation. Though using the LES-stress gave good results for moderate Re flows, we observed the solution deteriorated when going to high Re flows. This phenomenon of the deteriorating LES wall-stress at high Re is illustrated in figure 5.10. The wall-stress computed from the linear approximation of the velocity gradient from the first cell of the wall is shown in figure 5.10 for the oblique SBLI at moderate Re [7] and the ramp SBLI at high Re [68]. The WMLES study for the high Re SBLI by Settles et al. [68] will be detailed in the next section, here it is shown as a demonstration of the deteriorating LES-stress at high Re. The two stress formulations which are tested are, $\tau_{vis} = \mu_w (du/dy)|_w$ termed τ_{vis} and $\tau_{sgs} = (\mu_w + \mu_t^{SGS}) (du/dy)|_w$, where the μ_t^{SGS} is computed using the dynamic Smagorinsky model [53]. The τ_{vis} formulation is a bad approximation as we go to higher Re because the grid is much more unresolved when scaled in wall units. Whereas those based on μ_t^{SGS} are prone to near-wall SGS modeling errors, e.g. the huge peak in C_f obtained in the τ_{sgs} formulation at separation due to the large increase in μ_t^{SGS} at the shock. Also observed that τ_{sgs} varies quite largely between different SGS models, and hence the formulation would need to be tweaked for different SGS models. To avoid the errors in these two formulations, the primitives in the first cell are passed through the wall model to obtain a more robust computation of the wall-stress and heat-flux in non-equilibrium regions. Using the wall model by switching to the first cell off the wall as the exchange location gave robust predictions for all flow conditions tested in this study.

In the next few sections, we explore the non-equilibrium sensor (α_r) for shock separated

Figure 5.11 Instantaneous contours of the pressure-gradient sensor (α_p), Reynolds stress sensor (α_r) and wall-stress (τ_w) from the WMLES plotted near the SBLI region.

flows using this dynamic-switching of the exchange location. The equilibrium model with a fixed exchange location is termed the EQ model and the equilibrium model which switches the exchange location based on the value of α_r is termed the EQS model.

The switching between the two exchange locations is done as follows,

$$\tau_w, q_w = \begin{cases} \tau_1, q_1, & \text{if } \alpha_r = 0 \\ \tau_e, q_e, & \text{if } \alpha_r = 1 \end{cases} \quad (5.15)$$

Here τ_1, q_1 are the equilibrium wall model prediction of wall-stress and heat-flux using the first cell off the wall as the exchange location, and τ_e, q_e is an exchange location taken at a distance away from the wall which adheres to the recommendation by Kawai & Larsson [43].

In terms of implementation, this is trivial as the first cell off the wall would always be on the same processor thus we would not need any extra MPI exchanges. The wall model grid (y_{wm}) for the equilibrium model which was initially created during the preprocessing step for an exchange location of $y = h_e$ would just be scaled as

$$y_{wm} = \frac{h_1}{h_e} y_{wm}$$

when the first cell exchange location is used.

5.2.3.4 Results: Wall-Stress Blending

In figure 5.12, the two sensors based on the pressure-gradient (α_p) and resolved-stress (α_r) are plotted with the DNS wall-stress. It is observed that α_p does not dip completely towards zero in the separated region and recovers far too quickly. This is mainly due

Figure 5.12 A comparison of the two sensors α_p (blue) and α_r (red) (averaged in time) is shown above with $\tau_w/40$ from the DNS (black) for the quasi-adiabatic case.

to u_τ being computed from the absolute value of τ_w and hence on a time average, it's unlikely that this sensor would go towards zero completely. In the upstream region, the α_r sensor gives you a value of 1 where it detects equilibrium attached flow and in separation, it dips to 0. As the flow reattaches, the sensor slowly recovers back to a value of 1. α_r gives the variation we would want in the separated region and also the reattachment region following it where the boundary layer is attached but still can't be fully categorized as an equilibrium region as it is growing under an adverse pressure gradient. Even in the instantaneous contours in figure 5.11, you can see that the regions where the sensor detects non-equilibrium flow, these are the grey regions, are correlated to the low-speed events (in blue) in separation seen in the skin friction contour. In the following sections, we use α_r as the non-equilibrium sensor.

It is seen in figures 5.13.a-f, switching to the exchange location closer to the wall as done in the EQS model gives better skin-friction prediction compared to using a standard fixed exchange location as done in the EQ model. The improvement in the C_f for the EQS model over the EQ model is seen across all cases from cold to hot wall. The P_w prediction though is relatively unchanged across all cases. Thus we observe that by using the non-equilibrium sensor combined with the dynamic switching of the exchange location, we can get results close to or even better than the more expensive non-equilibrium model using the equilibrium model.

Figure 5.13 C_f and (b) P_w comparison cold (a-b), isothermal (c-d) and hot (e-f) wall cases. Black, DNS; Blue, Equilibrium model; Green, NEQB model; Red, EQS model.

Figure 5.14 A schematic diagram of the shock formed on the ramp impinging on a turbulent boundary layer is shown above. The separated region formed as a result of this interaction gives rise to an oscillatory separation shock (dotted lines).

5.3 Mach 2.9 Compression Ramp, High Re

The flow conditions for the compression ramp case have been chosen to replicate the experiment by Settles et al. [68]. This is a high Reynolds number case and unlike the previous SBLI study, this is not accessible to wall resolved LES/DNS. This case was also studied by Dawson et al. [23] and [27] in the context of WMLES and hybrid RANS-LES respectively. A schematic picture of ramp-type SBLIs and the time-averaged streamwise velocity contour of the flow close to the compression corner is shown in figure 5.14-5.15. Seen here is that the shock-boundary layer interaction results in the formation of a separation bubble upstream of the corner and this leads to the boundary layer going over the separated region to reattach at some region downstream on the ramp. This, in turn, results in the formation of a separation shock over this region. The separation shock is typically much weaker than the inviscid (incident) shock in this case but it does show a highly oscillatory nature whose unsteadiness is of great importance.

The wall boundary condition is taken to be adiabatic and standard periodic boundary conditions are applied on the spanwise boundaries. The digital filtering technique of Toubert & Sandham [79] is used to produce synthetic turbulence at the inflow plane. The digital filtering technique has been successfully applied to many different SBLIs and has known to not interfere with the low-frequency oscillations of the separation bubble

Figure 5.15 Time averaged contour of streamwise velocity u is shown in above near the shock interaction region. The dashed black line encloses the small region at the compression corner filled with negative u .

Figure 5.16 The grid used for the Mach 2.9 compression ramp case is shown above. Every fifth point is plotted in the mesh above for the sake of clarity.

Table 5.2 Mach 2.9 compression ramp - flow conditions and grid details.

M_∞	$Re_1 \text{ (m}^{-1}\text{)}$	Re_δ	Re_θ	Re_τ	θ
2.85	7.3×10^7	1.7×10^6	1.1×10^5	1.1×10^4	24°
<hr/>					
$L_x \times L_y \times L_z$	$\Delta x \times \Delta y_1 \times \Delta z$		$n_x \times n_y \times n_z$		
$50\delta \times 14\delta \times 4\delta$	$0.05\delta \times 0.03\delta \times 0.025\delta$		$937 \times 102 \times 160$

Figure 5.17 Instantaneous slices of temperature and skin-friction is plotted above for Mach 2.9 compression ramp case over the entire domain.

which is of interest for this case. The flow conditions and grid resolution details are provided in table 5.2. Uniform spacing in the spanwise and streamwise directions is used until $z = 44\delta_0$ after which a sponge layer is introduced where the streamwise spacing is stretched gently till the outflow domain. Uniform wall-normal spacing is maintained till about $3\delta_0$ from the wall after which the grid was stretched until the top outflow domain. A schematic of the grid used for this study and an instantaneous snapshot of the SBLI with the skin-friction contours is shown in figures 5.16-5.17. The coordinate system is centered around the compression corner, the streamwise location of which is x_{cor} . $x^* = (x - x_{cor})/\delta_0$ is the transformed coordinate where δ_0 is the incoming boundary layer thickness taken at $x^* = -9$. The experimental unit Reynolds number and Reynolds number based on the $0.99\delta_0$ boundary layer thickness is matched by the WMLES at $x^* = -9$. The friction-based Reynolds number Re_τ ranges from 9000-12000 for this case making this a significantly high Re flow compared to the previously studied cases.

5.3.1 Mean Flow Comparison

Seen in figure 5.18 is a comparison of experimental streamwise velocity profiles with the outer LES profiles at different streamwise locations near the compression corner. Excellent agreement is seen for the upstream boundary layer profiles. But as we enter the separated

Figure 5.18 The streamwise velocity profiles computed from the WMLES compared with experiments near the SBLI region. Red line, WMLES; Black circles, experiments. The profiles correspond to the streamwise locations at $x^* = -3, -1.5, -0.5, 0, 0.5, 1.5$, and 3 from left to right respectively.

Figure 5.19 (a) The wall-pressure and (b) the skin-friction computed from the WMLES are compared with the experiments. Red lines, WMLES with blended stress; Blue lines, standard equilibrium model; Black circles, experiments [68]; Black triangles, experiments [67] (corrected).

region profiles deteriorate in the near-wall region but the agreement is still good in the outer region for $y > 0.1\delta_0$. Note that the exchange location, in this case, is taken as the third cell off the wall at $y = 0.08\delta_0$ which is well in the log-layer region. As the flow reattaches downstream on the ramp the overall prediction gets better.

The wall-pressure and skin-friction comparison between WMLES results and the experimental data near the SBLI is given in figure 5.19. It is observed that switching to the first exchange location in the separation bubble can capture more of the negative C_f in the separation bubble and also separation length given by the two points where the C_f becomes negative is captured accurately with the use of the non-equilibrium sensor. The separation length L_{sep} comes out to be approximately $2\delta_0$ for this case. Also observed is the error in the C_f in the reattachment region in both the standard EQ model and EQS model. The EQS model does slightly better in the reattachment region than the EQ model here when comparing with the corrected C_f results [67]. But overall we see that C_f prediction lies well within the uncertainty of the experimental measurements. The wall-pressure shows excellent predictions compared to the experiments for both models.

5.3.2 Low-Frequency Unsteadiness

The low-frequency oscillations (LFO) of the shock seen in SBLIs is known to be an important phenomenon for designing aircraft structures. The unsteady loading caused by the pressure oscillations resonating with the aircraft panels can cause severe fatigue to the airframe [19]. Wall resolved LES has been known to accurately capture the low-frequency unsteadiness seen in many different SBLI [22, 79], but has been limited to low to moderate Re because of the high computational cost and flow-through times needed to capture the low-frequencies. As pointed out by Bose & Park [12], WMLES has the potential to capture these low-frequencies as this would require resolving the large-scale coherent structures [31, 24] and also do it at more realistic high Reynolds numbers.

To characterize the low-frequency unsteadiness in this study, we perform a Fourier transform of the time-series data obtained from the wall-pressure signal at each streamwise location on a line spanning over the SBLI region. The wall-pressure signal was segmented using Welch’s method with 50% overlaps and Hanning windows [79]. 15 segments were used to distribute data for the Welch’s method, this would correspond to a segment length in time of $300\delta_0/U_\infty$. The (physical) time the data was collected corresponds to approximately $2500\delta_0/U_\infty$ which came out to be around 2×10^5 computational time steps. To obtain a smoother PSD, the individual PSDs of three equidistant streamwise lines corresponding to $z/\delta_0 = 1, 2$, and 3 were averaged over the shock-interaction region.

Figure 5.20 (a) The weighted power spectral density (WPSD) map of pressure fluctuations near the SBLI region is plotted above

Figure 5.21 The Strouhal number in logarithmic scale is plotted versus the WPSD at an upstream location which is $x^* = -4$, close to the shock impingement location at $x^* = -2.25$ and at $x^* = -4$ which is a region downstream of the reattachment point.

Figure 5.22 The hollow cylinder-flare model being simulated in the current WMLES study is shown above.

The contour plot showing the weighted pre-multiplied power spectral density (WPSD) map over space and frequency domain is given in figure 5.20. The WPSD is obtained by multiplying the PSD with the non-dimensional frequency (given by the Strouhal number, which is defined as $S_r = f\delta_0/U_\infty$) and normalizing it with the integrated PSD over the frequency range. Slices of WPSD data at a location upstream of the shock impingement at $x^* = -4$, close to the shock impingement where the peak in low-frequency is observed at $x^* = -2.25$ and one far downstream after reattachment at $x^* = 3$ are plotted in figure 5.21. The peak in the WPSD upstream of the shock interaction lies around the frequencies $S_r \sim O(1)$ which is typical for turbulent boundary layers. A distinct low-frequency peak in WPSD is seen lying around S_r of 0.02-0.025. If we define the Strouhal number based on the separation length L_{sep} which is around $2\delta_0$ for this case, we would obtain a low-frequency peak at around S_r of 0.04-0.05. It is observed that the peak in WPSD shifts to lower frequencies $S_r \sim O(1)-O(10^{-1})$ after the reattachment at $x^* = 3$ when compared to the upstream boundary layer. This is related to the thickening of the boundary layer in the post-shock region which would lead to larger energetic scales of motion thus shifting the peak to lower frequencies. The overall trend seen in the pressure spectra follows the experimental study on low-frequency unsteadiness on ramp-type SBLIs by Erengil & Dolling [28]. The current study shows the capability of WMLES to capture the mean flow and low-frequency characteristics of SBLIs at high Re.

5.4 Mach 5.0 Compression Ramp, High Re

Figure 5.23 Instantaneous slice of the Mach number contour for the WMLES taken at $z = 0.05$ m combined with the instantaneous wall-stress plotted over the entire domain is shown above.

The wall model is now tested for hypersonic flow over a compression ramp. This case aims to test this sensor-based approach to the prediction of heat transfer in a strongly non-adiabatic and separated flow. The flow conditions are chosen to match the experiments done by Holden et al. [36] on their hollow cylinder-flare geometry (corresponding to “Run 17” from the CUBRC database). The experimental geometry is shown in figure 5.22, where approximately $1/10^{th}$ of the full geometry in the azimuthal direction is simulated. Note that we assume that axisymmetric effects are negligible and simulate a flat-plate version of this geometry.

Seen in figure 5.23, is that the full region from transition to the shock interaction is included in the simulation which is almost 3 m in length. A wall resolved LES grid would have a grid in the order of billion cells for this case. Whereas with WMLES this can be simulated at a much cheaper cost. In terms of computational cost, this is 2 orders of magnitude cheaper and if one includes the fact that a WMLES grid could take larger explicit timesteps, then this becomes almost 3 orders of magnitude.

This case exhibits strong non-equilibrium effects in the region where the oblique shock formed on the ramp interacts with the turbulent boundary layer. The flow-field for this

Figure 5.24 Instantaneous slice of density gradient magnitude contour for the WMLES taken at $z = 0.05 \text{ m}$, zoomed in at the SBLI region. The experimental schlieren image is given for comparison on the top left corner.

case is very similar to the one in section 5.3, the major difference being the onset of strong compressibility and heat-transfer effects due to the higher Mach number and cold wall conditions. Some of the important instantaneous flow features from the WMLES of this configuration can be observed in figures 5.23 and 5.24. The shock structure formed in the WMLES shows qualitative similarity to the one obtained in the experiments as seen in figure 5.24. Figure 5.23 illustrates the different challenges encountered in this case, as you need to resolve the thin laminar boundary layers close to the leading edge and also getting the right transition location. Downstream there are cold wall boundary layers which one needs to account for. And finally, there is separation and reattachment at the compression corner where RANS simulations fail to get the right peak heat-transfer and separation bubble size [36].

Table 5.3 Mach 5.0 compression ramp - flow conditions and grid details.

M_∞	T_∞	T_w	T_w/T_o	θ_{Ramp}
4.95	213.9 K	315.5 K	0.25	36°

$L_x \times L_y \times L_z \text{ (m)}$	$\Delta x \times \Delta y_1 \times \Delta z$	$n_x \times n_y \times n_z$
$3.22 \times 1 \times 0.125$	$0.06\delta \times 0.01\delta \times 0.03\delta$	$1915 \times 180 \times 168$

The flow conditions and grid details are summarized in table 5.3. Uniform grid spacings in the spanwise directions are used. A sponge layer is used after $x = 2.8 \text{ m}$ and $y = 0.5\delta$

Figure 5.25 The heat transfer computed from WMLES compared with experiments in the entire domain. Blue line, WMLES with standard EQ model; Black circles, experiments [36]; Grey dashed line, streamwise location of the compression corner.

for the streamwise and wall-normal directions respectively wherein the grid is stretched rapidly. δ , in this case, is taken to be the boundary layer thickness (99 %) of the incoming boundary layer taken at $x = 2$ m. The near-wall region contains 50 cells with a uniform wall-normal spacing which corresponds to Δy_1 , after which mild stretching is applied up to the beginning of the sponge layer. The wall-normal spacing might be sufficient in the turbulent regime but could still prove to be inadequate in the transitional region especially close to the leading edge where the boundary layer is only a few cells thick.

For capturing transition in this case we have used the modified transition sensor described in Chapter 4 with a threshold $S_{tl}^0 = 0.1$. Acoustic perturbations [66] have been imposed at the inlet with an amplitude of $A = 10^{-3}$ (similar to Section 4.3). The damping function $W(y)$ is taken to be 1.0 since the inflow plane is taken at the leading edge where the boundary just starts to develop.

In figure 5.25, the heat-flux over the entire domain is mapped from the leading edge to the reattachment. Good agreement with the experiment is obtained in the attached region upstream of the shock interaction. Figure 5.26 is a zoomed-in comparison of the heat-flux and wall-pressure from the WMLES using the EQ and EQS model. Firstly from the pressure plot for WMLES using the EQ model it is observed that the separation bubble size is slightly larger. Also, both the peak pressure and heat-flux at reattachment are underpredicted. Whereas the dynamic switching of the exchange location in the EQS

Figure 5.26 (a) The wall-pressure and (b) the heat-flux computed from the WMLES are compared with the experiments. Red lines, WMLES with EQS model; Blue lines, WMLES with EQ model; Black circles, experiments [36]

model within the non-equilibrium region can capture the heat-flux rise at separation and also the heat-flux rise while the flow reattaches on the ramp more accurately. We also observe that the pressure rise at the onset of separation to be more accurate for the EQS model. Both models though fail to capture the significant peak pressure at reattachment.

This underprediction in pressure at reattachment seen in WMLES results seems to be related to the high Mach number associated with this flow as the pressure rise on a similar geometry at Mach 3 (seen in section 5.3) was captured accurately with the equilibrium model. At high Mach numbers, the assumption of $dp/dy = 0$ breaks down and the wall-normal velocity fluctuations play a significant role [72]. The wall-normal momentum equation at such conditions takes the form,

$$\frac{\partial}{\partial y} (\bar{p} + \bar{\rho} \widetilde{v'v'}) = 0 \implies \bar{p}_w = \bar{p}_e + \bar{\rho} \widetilde{v'v'}|_e$$

where $-$ and $\sim$ denote Reynolds and Favre-averaging respectively. This means that the predicted wall-pressure p_w is a function of the exchange location pressure p_e and the (resolved plus modeled) wall-normal RMS ($\bar{\rho} \widetilde{v'v'}$). The boundary layer is impinging on the ramp surface at reattachment and due to this, the wall-normal stress is typically large in these regions. Since the equilibrium model does not model the wall-normal stress or account for wall-normal pressure variations this could be the reason for the poor wall-pressure prediction in the reattachment region. The isolated effect of not modeling the wall-normal stress is something that has not been looked at in prior studies and could play a significant role in high Mach number flows. Overall, we observe that even when using the simpler equilibrium model by switching the exchange location appropriately,

more accurate heat-flux results can be obtained in the non-equilibrium flow regions.

5.5 Discussion

WMLES was performed for SBLIs at different wall temperatures and Reynolds numbers. It was observed the WMLES was capable of capturing the large-scale expansion and shrinkage of separation at different wall temperatures. The non-equilibrium model using the pressure-based eddy viscosity gave better predictions than the standard EQ model at such conditions. It was shown that by dynamically shifting the exchange location using the non-equilibrium sensor the equilibrium model prediction can be improved for skin-friction and heat-transfer predictions in SBLIs. Also seen was that the low-frequency oscillations in SBLIs at high Re can be captured with WMLES. On the high Mach number ramp SBLI, we observed a good prediction for heat-transfer at reattachment but were under-predicting the wall pressure. The assumption of negligible wall-normal stress could be the culprit in this case. The effect of not modeling the wall-normal stress (in equilibrium models) is something that needs to be investigated in future studies. As a whole, it was observed that by using the equilibrium model with a few corrections for non-equilibrium flows, WMLES can capture many of the complex features of SBLI.

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APPENDIX

APPENDIX A

Validation for MLS

A.1 Fluxes

In this section, we have performed a few validation cases for the Meshless Line Solver (MLS) code which solves the 3D Navier-Stokes equations. MLS is used to solve the RANS equations which form the non-equilibrium model. It has to be noted that the fluxes in the MLS code are more diffusive compared to the outer LES solver. The RANS equations solved in the non-equilibrium model can be solved with a much more diffusive scheme with a lower order of accuracy in space and time as it doesn't need to capture the small-scale features of the flow like the outer LES solver. The final output of the MLS solver is to just return the wall-stress and heat-flux at the corresponding face connected to the outer LES exchange location. Note that in these validation cases the MLS code is run as a stand-alone CFD solver.

Attached is the common validation test case in figure A.1 for viscous fluxes (in the MLS solver) which is the Taylor-Green vortex problem that describes the decay of kinetic energy with time. For validating the inviscid fluxes which are computed using the modified Steger-Warming method [48] (in the MLS solver), the SOD shock-tube problem is simulated and compared with the theoretical values at time $t = 0.2$ s, as shown in figure A.2. A second-order MUSCL extrapolation of the conservative variables with the minmod limiter is used for the inviscid fluxes. Both the test problems were solved with a 100 point grid. Overall the inviscid and viscous fluxes seem to show an acceptable level of fidelity for these two validation problems.

Figure A.1 The decay of kinetic energy computed by the MLS code (symbols) is compared with the analytical curves (lines) at 4 different Reynolds numbers.

Figure A.2 A snapshot of density, pressure and velocity at $t = 0.2$ s is shown above the SOD shock-tube problem. The symbols denote the computation using the MLS code and the lines are given by the exact inviscid solution.

A.2 Laminar Boundary Layer

As a validation exercise for the non-equilibrium wall model (MLS), we perform a laminar hypersonic boundary layer simulation at isothermal cold-wall conditions. The free-stream conditions are similar to the ones used in the transitional SBLI by Sandham et al. [66]. The flow parameters and grid sizing are given in the table.A.1. Note that Re_1 refers to the unit Reynolds number and $Re_{\delta_0^*}$ is based on the inflow displacement thickness (δ_0^*) which is present in the laminar region of the transitional case. The objective here is to observe the effects of using a wall model under conditions when the grid is severely under-resolved. This can be important for cases such as the nose region of a hypersonic vehicle or the leading edge of an airfoil where the boundary layer is extremely thin and it is critical to model the correct boundary layer growth in such regions for predicting transition. The growth of the laminar boundary layer, in this case, is observed right from the leading edge of the flat plate.

This case is also important as it is a laminar flow and thus eliminates any errors being introduced through the inaccuracies in the subgrid/eddy viscosity modeling. Therefore any errors in our solution can be purely traced back to the errors being induced due to the coupling between the wall model and the outer CFD solver on a coarse mesh. Note that in this case the MLS solver and the outer CFD solver are coupled at the exchange location and wall as would be done in WMLES. In both solvers (MLS wall model and outer CFD solver), the subgrid/eddy viscosity is switched off and the spatial/temporal discretization for the fluxes is kept approximately the same.

Table A.1 Laminar boundary layer - flow conditions and grid details

M_∞	Re_1	$Re_{\delta_0^*}$	T_∞	T_w/T_∞
6.0	$6.0 \times 10^6 \text{ m}^{-1}$	6830	65 K	4.5

$L_x \times L_y (\delta_0^*)$	$\Delta x \times \Delta y_1 (\delta_0^*)$	$n_x \times n_y$
200×20	0.8×0.18	250×80

We observe in figure A.3 that the boundary layer resides completely inside the wall model layer until $x/\delta_0^* \approx 10$ after that there is a settling length of about $20\text{-}30\delta_0^*$ beyond which the boundary layer inside the wall model has adjusted with boundary layer growth in the outer region. The imprint of this behavior is felt on the wall shear stress and heat flux as seen in the skin-friction and Stanton number curves are shown in figures A.4 and

Figure A.3 The growth of the laminar boundary layer close to the leading edge seen in the non-equilibrium wall model layer (colored lines) and the outer layer (colored flood contour). The exchange location height is denoted by the horizontal black line at $y/\delta_0^* \approx 0.42$. The grid lines in grey represent the outer layer grid.

Figure A.4 Skin-friction coefficient (C_f) got from the wall model compared with a resolved grid solution. Black, resolved grid; Red, non-equilibrium model; Grey, equilibrium model; Grey dashed lines, mark the different regimes the boundary layer goes through.

Figure A.5 (a) Streamwise velocity profiles taken at $x/\delta_0^* = 10, 30, 50, 70, 90$ from left to right respectively. Lines, resolved grid solution; Circles, non-equilibrium model; Squares, Outer grid solution. Grey squares denote points in the outer grid below the exchange location. (b) Skin-friction coefficient (C_f) and Stanton number (S_t) got from the wall model compared with a resolved grid solution. Lines, resolved grid solution; Colored symbols, non-equilibrium model; Grey symbols, equilibrium model; Grey dashed lines, mark the different regimes the boundary layer goes through.

A.5.b. The three distinct regions in this case are marked for the C_f curve in figure A.4. The first region is the one where the boundary layer edge resides within the wall model layer ($x/\delta_0^* < 10$), the second region is the settling region where we observe the inflection point in the C_f curve ($10 < x/\delta_0^* < 40$) and the third region is where the boundary layer edge is well past the exchange location for the wall model ($x/\delta_0^* > 40$) after which skin-friction curve starts to tend to its normal behavior. Also seen in the contour plot in figure A.3 is beyond this third region where the C_f curve has settled, the wall model solution has fully merged with the outer grid solution which is denoted by the merging of contour lines.

Wall models typically operate with the assumption that the exchange location is well within the boundary layer edge. In the region $x/\delta_0^* < 40$, where the boundary layer growth in the non-equilibrium wall model and the outer layer is much different the solution is prone to errors as shown in the C_f curve. The equilibrium model which just relies on the exchange location solution for computing the wall shear stress shows a flat skin-friction curve until this point as it just sees free-stream values of velocity and temperature. This results in inaccurate boundary layer growth and a much larger streamwise length for the skin-friction curve to settle to its correct behavior. The non-equilibrium model which solves the full transport equations should, in theory, give us the correct skin-friction at $x/\delta_0^* < 40$. But it is limited by the errors creeping in through the Dirichlet boundary

Figure A.6 (a) Wall normal velocity and (b) temperature profiles taken at $x/\delta_0^* = 10, 30, 50, 70, 90$ from left to right respectively. Lines, resolved grid solution; Circles, non-equilibrium model; Squares, Outer grid solution. Grey squares denote points in the outer grid below the exchange location.

condition from the under-resolved cells of the outer layer. How to treat thin-laminar boundary layers accurately remains a challenge for current wall models. On the whole, however, it has been observed that the non-equilibrium model can model the boundary layer growth in a much better fashion compared to the equilibrium model even for a simple laminar boundary layer.

From the velocity and temperature profiles which are given in figure A.5 and A.6, we can observe that as we go further downstream, the profiles are better matched with their resolved counterparts. At the outflow, there are about 16 points in the boundary layer in the outer grid and as we go towards the leading edge it gets progressively more under-resolved. The blue and red profiles which are the closest to the leading edge show the most error. The profiles downstream which have about 10 points inside the boundary layer in the outer grid match well with the resolved grid solution. As a whole from this exercise, we can observe that when using the MLS as a wall model it can reproduce the compressible laminar boundary layer profile when coupled to an outer CFD solver.

A.3 Viscous Fluxes in MLS

A comprehensive description of the computation of the viscous fluxes F_v^{ij} in the MLS code at an interface ij which is halfway between the point i and its neighbor j is provided below. The notation used is the same as what was introduced in Chapters 1 and 2.

$$\left(\frac{du_m}{dx_n}\right)^{ij} = \sum_j a_n^{ij}(u_m^j - u_m^i)$$

$$\left(\frac{dT}{dx_m}\right)^{ij} = Q_m^{ij} = \sum_j a_m^{ij}(T^j - T^i)$$

$$S_{mn}^{ij} = \left(\frac{du_m}{dx_n} + \frac{du_n}{dx_m} - \frac{2}{3} \frac{du_k}{dx_k} \delta_{mn}\right)^{ij}$$

$$\mu' = \mu + \mu_t, \quad \lambda' = \lambda + \lambda_t$$

$$\sum_j F_v^i = \begin{pmatrix} 0 \\ \mu'^i \{\sum_j a_m^{ij}\} S_{1m}^{ij} \\ \mu'^i \{\sum_j a_m^{ij}\} S_{2m}^{ij} \\ \mu'^i \{\sum_j a_m^{ij}\} S_{3m}^{ij} \\ \lambda'^i \{\sum_j a_m^{ij}\} Q_m^{ij} + \mu'^i \{\sum_j a_m^{ij}\} S_{nm}^{ij} u_n^i \end{pmatrix}$$

$$e_m^{ij} = \frac{(x_m^j - x_m^i)}{||x^j - x^i||^2}$$

$$\left(\frac{du_m}{dx_n}\right)^{ij,f} = e_n^{ij}(u_m^j - u_m^i)$$

$$\left(\frac{dT}{dx_m}\right)^{ij,f} = Q_m^{ij,f} = e_m^{ij}(T^j - T^i)$$

$$S_{mn}^{ij,f} = \left(\frac{du_m}{dx_n} + \frac{du_n}{dx_m}\right)^{ij,f}, \quad D^{ij,f} = \frac{2}{3} \left(\frac{du_k}{dx_k}\right)^{ij,f}$$

$$u^{ij,f} = \frac{(u^i + u^j)}{2}, \quad T^{ij,f} = \frac{(T^i + T^j)}{2}$$

$$\mu'^{ij,f} = \mu[T^{ij,f}] + \frac{(\mu_t^i + \mu_t^j)}{2}, \quad \lambda'^{ij,f} = \lambda[T^{ij,f}] + \frac{(\lambda_t^i + \lambda_t^j)}{2}$$

$$F_v^{ij} = \begin{pmatrix} 0 \\ \mu'^{ij,f} \{a_m^{ij} S_{1m}^{ij,f}\} - \mu^{ij,f} \{a_1^{ij} D^{ij,f}\} \\ \mu'^{ij,f} \{a_m^{ij} S_{2m}^{ij,f}\} - \mu^{ij,f} \{a_2^{ij} D^{ij,f}\} \\ \mu'^{ij,f} \{a_m^{ij} S_{3m}^{ij,f}\} - \mu^{ij,f} \{a_3^{ij} D^{ij,f}\} \\ \lambda'^{ij,f} \{a_m^{ij} Q_m^{ij,f}\} + \mu'^{ij,f} \{a_m^{ij} S_{nm}^{ij,f} u_n^{ij,f}\} - \mu^{ij,f} D^{ij,f} \{a_m^{ij} u_m^{ij,f}\} \end{pmatrix}$$