NUMERICAL SIMULATIONS AND ANALYSES OF SHOCK WAVE-BOUNDARY LAYER INTERACTIONS

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ABSTRACT

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Shock-boundary layer interaction (SBLI) is becoming one of the benchmark problems in the high-speed flow modeling and simulation community. The interaction of shock wave with the boundary layer is a very complex phenomenon that requires high-fidelity numerical methods like direct numerical simulation (DNS) and large-eddy simulation (LES) to capture the flow physics. In this study, SBLI is examined for various flow conditions using DNS and LES.

In the first part of this study, DNSs are conducted for a Mach 2.75 turbulent boundary layer interacting with an impinging shock at three different shock incidence angles. Instantaneous flow visualizations show the effect of shock on turbulence structure in the shock-boundary layer interaction zone and also in the flow downstream of the interaction region. The separation bubbles exhibit highly unsteady and three-dimensional behavior and are larger for stronger shocks but the maximum probability of flow separation is found to be independent of the shock strength. A detailed examination of the terms in the turbulent kinetic equation shows a strong coupling exists between the mean and turbulent fields in the interaction region with energy being continuously exchanged from one field to another. However, the compressibility-related terms in the transport equations for turbulent kinetic energy and enstrophy are found to be small for the simulated flows.

In the second part of this study, data generated by DNS for a Mach 2.75 zero-pressure gradient turbulent boundary layer interacting with shocks of different intensities are used for *a priori* analysis of subgrid-scale (SGS) turbulence and various terms in the compressible filtered Navier-Stokes equations. The behavior of SGS stresses and their components, namely, Leonard, Cross and Reynolds components, is examined in various regions of the flow for different shock intensities and filter widths. The backscatter in various regions of the flow is found to be significant only instantaneously while the ensemble-averaged statistics indicate no significant backscatter. The budgets for the SGS kinetic energy equation are examined for a better understanding of shock-tubulence interactions at the subgrid level and also with the aim of providing useful information for one-equation LES models. A term-by-term analysis of the SGS terms in the filtered total energy equation indicate that while each term in this equation is significant by itself, the net contribution by all of them is relatively small. This observation is consistent with our *a posteriori* analysis.

In the third part of the study, assessments of several existing SGS LES models along with a new model are made for SBLI through systematic *a priori* and *a posteriori* analyses. In the problem chosen for this study, the incident shock is strong enough to generate a marginal separation of the boundary layer near the interaction region, hence providing the SGS models with a non-trivial challenge. The effect of SGS stress term on the resolved velocity field is found to be significant and shock-dependent. The subgrid-scale models tested include the mixed-time-scale model, the dynamic Smagorinsky model, the dynamic mixed model and a new dynamic model, termed the compressible serial decomposition model. A priori analysis indicate that the new dynamic model is more accurate than other SGS closures. A posteriori tests also indicate better predictions of DNS results by the LES employing the compressible serial decomposition model.

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TABLE OF CONTENTS

nock Wave/Boundary Layer In ical Simulation	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
SBLI	. 9 . 10 . 12 . 13 . 16 . 21 . 24
SBLI	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
· · · · · · · · · · · · · · · · · · ·	. 12 . 13 . 16 . 21 . 24
	. 13 . 16 . 21 . 24
	. 16 . 21 . 24
	. 21 . 24
	. 24
· · · · · · · · · · · · · · · · · · ·	
sure Comparisons	. 31
	. 34
•••••••••••••••••••••••••••••••••••••••	. 39
	. 51
	. 57
ale Turbulence for Shock Boun	dory
ale 101 bulence for Shock-Doun	uary 60
	. 00
	. 00
	. 02
um equation	. 00
	. 00
	. 10
rgies	. 00
rgies	. 98
rgies	. 100
rgies	. 100
	ergies

3.1	Introduction	.09
3.2	Governing Equations	.12
3.3	Subgrid-Scale Models	15
3.4	Numerical Method	.19
3.5	Results	.20
	3.5.1 Computational Setup and Parameters	.20
	3.5.2 A Priori Assessment $\ldots \ldots \ldots$	25
	3.5.3 A Posteriori Assessment	.39
3.6	3D effects of lateral walls on SBLI	48
3.7	Conclusions	53
BIBLI	OGRAPHY	55

LIST OF TABLES

Table 1.1	Simulation Parameters for DNS of SBLI.	12
Table 1.2	Boundary layer parameters for the incoming boundary layer	13
Table 1.3	Separation and Interaction lengths.	31
Table 1.4	Legend and colors for turbulent kinetic energy budget plots	42
Table 1.5	Legend and colors for enstrophy budget plots	52
Table 2.1	Color and legend for filtered total energy plots	79
Table 2.2	Color and legend for k_{sgs} and normal SGS stress budget plots	91
Table 3.1	Simulation Parameters for DNS of Mach 2 SBLI	120
Table 3.2	Simulation Parameters for LESof Mach 2 SBLI	121
Table 3.3	Separation region sizes	144

LIST OF FIGURES

Figure 1.1	Instantaneous density contours overlaid with modified Ducros shock sensor values. The critical regions identified by the shock sensor are shown in red. For interpretation of the references to color in this and all other figures, the reader is referred to the electronic version of this dissertation	8		
Figure 1.2	The wall pressure spectra at $x=23\delta_{ref}$ for the "auxiliary" DNS	11		
Figure 1.3	(a) Van Driest transformed mean streamwise velocity profile and(b) density-scaled Reynolds stresses of the incoming boundary layerSymbols represent DNS data of Pirozzoli and Bernardini [1]			
Figure 1.4	Instantaneous streamwise density gradient contours for Case III. Contour levels are evenly spaced between -1 and 1	17		
Figure 1.5	Instantaneous numerical schlieren visualizations at an $x-y$ symmetry plane. (a) Case I, (b) Case II, (c) Case III	18		
Figure 1.6	(a) Instantaneous velocity fluctuations and, (b) instantantaneous temperature fluctuations along the mean sonic plane for Case II. \ldots	20		
Figure 1.7	Differences between Reynolds- and Favre-averaged quantities at $X^* = -1.1$. (a) velocity, (b) temperature.	22		
Figure 1.8	Differences between Reynolds- and Favre-averaged quantities at $X^* = -0.5$. (a) velocity, (b) temperature.	23		
Figure 1.9	(a) Comparison of C_f computed using Reynolds- and Favre-averaged quantities. (b) Percentage difference in C_f computed by Reynolds- and Favre-averaged quantities. The results shown are for Case II	25		
Figure 1.10	Comparisons for $\langle \rho' u'_i u'_j \rangle$. (a) for different shock intensities. $X^* = -1.1$, (b) $X^* = 0.25$.	26		
Figure 1.11	Instantaneous streamwise skin-friction coefficient contours. The con- tour levels are evenly spaced between -6×10^{-3} and 0. (a) Case I, (b) Case II, (c) Case III	28		

Figure 1.12	Instantaneous spanwise skin-friction coefficient contours. The con- tour levels are evenly spaced between -5×10^{-3} and 5×10^{-3} . (a) Case I, (b) Case II, (c) Case III				
Figure 1.13	Comparisons for the probability of flow reversal for different shock intensities.				
Figure 1.14	Comparisons for mean skin-friction coefficient for different shock in- tensities				
Figure 1.15	Mean wall pressure distribution for different shock intensities plotted with different scalings.				
Figure 1.16	igure 1.16 (a) Instantaneous wall pressure fluctuations for Case II. (b) Stream wise evolution of r.m.s. of wall pressure fluctuations for different shock intensities.				
Figure 1.17	R.M.S. of thermodynamic fluctuations at different streamwise locations for Case II. (a) pressure, (b) temperature				
Figure 1.18	Contours of turbulent fluctuations of thermodynamic variables for Case II. (a) r.m.s. of pressure fluctuations, (b) r.m.s. of density fluctuations	38			
Figure 1.19	Turbulent and fluctuating Mach numbers at different streamwise lo- cations for Case II. (a) M_t , (b) $\langle M' \rangle$	40			
Figure 1.20	Turbulent kinetic energy budget for Case II at $X^* = -1.1.$	42			
Figure 1.21	Turbulent kinetic energy budgets at $X^* = -0.5$. (a) Case II, (b) Case III	44			
Figure 1.22	Turbulent kinetic energy budgets at $X^* = 0.25$. (a) Case II, (b) Case III	46			
Figure 1.23	Turbulent kinetic energy budgets at $X^* = 1.5$. (a) Case II, (b) Case III	47			
Figure 1.24	(a) Streamwise evolution of turbulent kinetic energy along the mean sonic line. (b) Streamwise evolution of turbulent kinetic energy budget along the sonic line	48			

Figure 1.25	Evolution of dissipation term and its components along the mean sonic line.	51
Figure 1.26	Enstrophy budget for Case II at $X^* = -1.1.$	53
Figure 1.27	Enstrophy budgets at $X^* = -0.5$. (a) Case II, (b) Case III	54
Figure 1.28	Enstrophy budgets at $X^* = 0.25$. (a) Case II, (b) Case III	55
Figure 1.29	Enstrophy budgets at $X^* = 1.5$. (a) Case II, (b) Case III	56
Figure 2.1	SGS stresses at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$. Black solid line for τ_{11} , black dashed line for τ_{22} , black dash-dot line for τ_{33} , black dots for τ_{12} , red solid line for ksgs.	69
Figure 2.2	SGS stresses at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = 0.25$, (b) $X^* = 1.5$. Black solid line for τ_{11} , black dashed line for τ_{22} , black dash-dot line for τ_{33} , black dots for τ_{12} , red solid line for ksgs	70
Figure 2.3	PDFs of τ_{12} SGS stresse as obtained from the instantaneous filtered DNS data for $\overline{\Delta} = 8\Delta_{DNS}$.	71
Figure 2.4	SGS stress decomposition at different streamwise locations as ob- tained from the filtered DNS data for $\theta = 7.75^{\circ}$ and $\overline{\Delta} = 4\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$. Black solid line for τ_{11} , black dashed line for L_{11} , black dash-dot line for C_{11} , black dots for R_{11}	73
Figure 2.5	SGS stress decomposition at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{\circ}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = 0.25$, (b) $X^* = 1.5$. Legend same as in Fig. 2.4	74
Figure 2.6	SGS stress decomposition at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 16\Delta_{DNS}$. (a) $X^* = -0.5$, (b) $X^* = 0.25$. Legend same as in Fig. 2.4	76
Figure 2.7	Various SGS terms in the filtered total energy equation at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$. See Table. 2.1 for legend.	80

Figure 2.8	Skin-friction coefficient predictions as obtained from <i>a posteriori</i> LES calculations for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. Solid black line for filtered DNS, red dashed line for LES1, blue dash-dot line for LES2.	82		
Figure 2.9	Turbulent Reynolds stress at different streamwise locations as ob- tained from <i>a posteriori</i> LES calculations for $\theta = 7.75^{\circ}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$. Solid black line for filtered DNS, red dashed line for LES1, blue dash-dot line for LES2	84		
Figure 2.10	Turbulent heat flux at different streamwise locations as obtained from a posteriori LES calculations for $\theta = 7.75^{\circ}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$. Legend same as in Fig. 2.9			
Figure 2.11	The ratio of SGS kinetic energy to the total kinetic energy $(k_{sgs}/(k_{sgs}+E_r))$ at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^o$ and $\overline{\Delta} = 4\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$	87		
Figure 2.12	$k_{sgs}/(k_{sgs} + E_r)$ at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^o$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$.	88		
Figure 2.13	$k_{sgs}/(k_{sgs}+E_r)$ at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^o$ and $\overline{\Delta} = 16\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$.	89		
Figure 2.14	$k_{sgs}/(k_{sgs} + E_r)$ as obtained from the filtered DNS data for different shock intensities with $\overline{\Delta} = 8\Delta_{DNS}$. (a) $\theta = 6^{\circ}$, (b) $\theta = 7.75^{\circ}$, (c) $\theta = 9.25^{\circ}$. The contours levels are uniformly spaced between 0 and 0.5. The figures are shown not to scale for clarity	90		
Figure 2.15	SGS kinetic energy (k_{sgs}) budget at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$. See Table. 2.2 for legend	93		
Figure 2.16	SGS kinetic energy (k_{sgs}) budget at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = 0.25$, (b) $X^* = 1.5$. See Table. 2.2 for legend	94		

Figure 2.17	Instantaneous contours of SGS production as obtained from the fil- tered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. Only the backscatter regions are shown. 50 uniformly spaced contour levels between 0.0 and 0.005. (a) $X^* = -1.1$, (b) $X^* = -0.5$, (c) $X^* = 0.25$, (d) $X^* = 1.5$	07
	$\Lambda = 1.5.\ldots$	91
Figure 2.18	Probability of backscatter in the $x - y$ symmetry plane as obtained from filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$.	98
Figure 2.19	Directionally filtered SGS stresses as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$ at $X^* = -1.1$. (a) τ_{11} , (b) τ_{22} . solid black line for <i>x</i> -only filter, dashed black line for <i>y</i> -only filter, red dash-dot line for <i>z</i> -only filter	101
Figure 2.20	Directionally filtered SGS stresses as obtained from the filtered DNS data for $\theta = 7.75^{\circ}$ and $\overline{\Delta} = 8\Delta_{DNS}$ at $X^* = -1.1$. (a) τ_{33} , (b) τ_{12} . solid black line for <i>x</i> -only filter, dashed black line for <i>y</i> -only filter, red dash-dot line for <i>z</i> -only filter	102
Figure 2.21	Directionally filtered SGS stresses as obtained from the filtered DNS data for $\theta = 7.75^{\circ}$ and $\overline{\Delta} = 8\Delta_{DNS}$ at $X^* = -0.5$. (a) τ_{11} , (b) τ_{22} . solid black line for <i>x</i> -only filter, dashed black line for <i>y</i> -only filter, red dash-dot line for <i>z</i> -only filter	103
Figure 2.22	Directionally filtered SGS stresses as obtained from the filtered DNS data for $\theta = 7.75^{\circ}$ and $\overline{\Delta} = 8\Delta_{DNS}$ at $X^* = -0.5$. (a) τ_{33} , (b) τ_{12} . solid black line for <i>x</i> -only filter, dashed black line for <i>y</i> -only filter, red dash-dot line for <i>z</i> -only filter	104
Figure 2.23	Directionally filtered SGS stresses as obtained from the filtered DNS data for $\theta = 7.75^{\circ}$ and $\overline{\Delta} = 8\Delta_{DNS}$ at $X^* = 0.25$. (a) τ_{11} , (b) τ_{22} . solid black line for <i>x</i> -only filter, dashed black line for <i>y</i> -only filter, red dash-dot line for <i>z</i> -only filter	105
Figure 2.24	Directionally filtered SGS stresses as obtained from the filtered DNS data for $\theta = 7.75^{\circ}$ and $\overline{\Delta} = 8\Delta_{DNS}$ at $X^* = 0.25$. (a) τ_{33} , (b) τ_{12} . solid black line for <i>x</i> -only filter, dashed black line for <i>y</i> -only filter, red dash-dot line for <i>z</i> -only filter	106
Figure 3.1	An $x - y$ slice of the sample DNS grid	122
Figure 3.2	A schematic of the computational procedure for DNS and LES of SBLI	.123

Figure 3.3	Flow structure in a typical shock/boundary layer interaction configu- ration. Vortex structures identified using λ_2 criterion [2] and colored based on the local values of instantaneous velocity magnitude			
Figure 3.4	Van Driest transformed mean streamwise velocity profile of the in- coming boundary layer in inner scaling calculated from DNS data at $x = 6$. Black dashed line represents $U_{VD}^+ = y^+$ and Eq. (1.14) is represented by black dash-dot line	125		
Figure 3.5	Density-scaled profiles of Reynolds stresses obtained by DNS at $x = 6$	5.126		
Figure 3.6	Leonard, Cross and Reynolds parts of the spanwise-averaged τ_{11} SGS stress component at $x = 6$ for $\overline{\Delta} = 4\Delta_{DNS}$. total stress - black solid line; L_{11} - dashed black line; C_{11} - dash-dot red line; R_{11} - blue dotted line.	128		
Figure 3.7	Leonard, Cross and Reynolds parts of the spanwise-averaged τ_{11} SGS stress component at $x = 6$ for $\overline{\Delta} = 8\Delta_{DNS}$. total stress - black solid line; L_{11} - dashed black line; C_{11} - dash-dot red line; R_{11} - blue dotted line.	129		
Figure 3.8	Spanwise-averaged values of the trace-free τ_{11} component of SGS stress tensor at (a) $x = 6$, (b) $x = 10$. Legend : open triangles = True stresses, dotted black line = Modeled-MTSM, dash-dot green line = Modeled-DSM, dashed blue line = Modeled-DMM, solid red line = Modeled-CSDM	131		
Figure 3.9	Spanwise-averaged isocontours of trace-free τ_{11} SGS stress component. (a) True stress, (b) Modeled-DSM, (c) Modeled-DMM, (d) Modeled-CSDM	132		
Figure 3.10	Spanwise-averaged values of the τ_{12} SGS stress component at (a) $x = 10$, (b) $x = 15$. See Fig. 3.8 for legend.	133		
Figure 3.11	Spanwise-averaged values of q_1 SGS heat flux component at (a) $x = 10$, (b) $x = 15$. See Fig. 3.8 for legend	135		
Figure 3.12	Correlation coefficients between the true and the modeled values of τ_{11} SGS stress for different values of density gradient parameter ψ . Legend : open circles = DSM, open triangles = DMM, open squares = CSDM.	137		

Figure 3.13	Correlation coefficients between the true and the modeled values of q_1 heat flux component for different values of density gradient parameter ψ . Legend : open circles = DSM, open triangles = DMM, open squares = CSDM	138		
Figure 3.14	Variations of backscatter with the density gradient parameter $\psi.~$	139		
Figure 3.15	Correlation coefficients for the SGS dissipation, ε_{sgs} , as a function of the density gradient parameter ψ as predicted by CSDM			
Figure 3.16	Turbulent kinetic energy profiles at $x = 6$. Legend : open circles = DNS, open triangles = Filtered DNS, crosses = LES-No-Model, dotted black line = LES-MTSM, dash-dot green line = LES-DSM, dashed blue line = LES-DMM, solid red line = LES-CSDM	141		
Figure 3.17	One-dimensional energy spectra in spanwise direction at $x = 6$ and $y \approx 0.07$	142		
Figure 3.18	Evolution of mean skin-friction coefficient, C_f . See Fig. 3.16 for legend	.143		
Figure 3.19	Evolution of mean wall-pressure, P_w . See Fig. 3.16 for legend	145		
Figure 3.20	Van-Driest transformed mean streamwise velocity profiles in inner scaling. (a) $x = 10$, (b) $x = 15$. Black dashed line represents law of the wall. See Fig. 3.16 for legend.	147		
Figure 3.21	Comparisons of R_{11} Reynolds stress component obtained by DNS and LES. (a) $x = 6$, (b) $x = 10$. See Fig. 3.16 for legend	149		
Figure 3.22	Comparisons of R_{22} Reynolds stress component obtained by DNS and LES. (a) $x = 10$, (b) $x = 15$. See Fig. 3.16 for legend 1			
Figure 3.23	Instantaneous slices of temperature contours at different streamwise locations for 3DSBLI.	152		

Chapter 1

Parametric Investigations of Shock Wave/Boundary Layer Interactions Using Direct Numerical Simulation

1.1 Introduction

Shock-turbulent boundary layer interaction (SBLI) is becoming one of the benchmark problems for high-speed flow modeling and simulations. This problem has mainly been studied in two flow configurations, a compression corner and a flat plate turbulent boundary layer with an incident shock. In the former, the shock is generated as a result of the geometry of the surface on which the boundary layer is developing. In the latter, the shock is generated from an external source and impinges on the boundary layer. In either case, turbulence is amplified across the shock and the boundary layer experiences a strong adverse pressure gradient which may lead to its separation. An important feature of the separated boundary layer is the low-frequency, large-scale unsteadiness of the shock that has been observed in experiments and numerical studies, but is yet to be fully understood. The characteristic frequency of the shock oscillation is generally an order or two magnitudes smaller than the characteristic frequency of the incoming boundary layer. The reflected SBLI problem has been receiving significant attention in recent years even though one of the earliest experimental studies was performed more than four decades ago [3]. In this experimental study, the shock deflection angle (θ) varied between 2^o and 10.5^o while the Mach number was kept constant at 2.5. Measurements were made using pitot probes and wall-pressure taps and flow visualizations were made using surface oil and optical techniques like schlieren and shadowgraph techniques. The experimental results indicated that the boundary layer remains attached for weaker incident shocks but separates for stronger incident shocks. The interaction region for the separated boundary layer was shown to exhibit a complex pattern with the primary reflected shock followed by an expansion wave and then a series of compression waves near the reattachment point.

Dupont et al.[4] studied the interaction of an impinging oblique shock with a flat-plate turbulent boundary layer at M = 2.3 using PIV technique. The primary focus was on the unsteadiness of the reflected shock. Measurements were made for different incidence shock angles θ which varied between 7° and 9.5°. By analyzing the wall-pressure signals in the interaction region, the authors found some low-frequency oscillations in the second part of the recirculation bubble. The characteristic frequency of these oscillations was found to be close to that of the reflected shock suggesting that the reflected shock unsteadiness could be related to the unsteadiness in the recirculation bubble. The effect of interaction strength on the unsteadiness of separation bubble was experimentally investigated by Souverein et al. [5]. From their experimental data, the authors inferred the following: when no separation occurs, unsteadiness of the shock motion is correlated with the incoming boundary layer; when mean flow separation occurs, the shock motion exhibits a strong correlation with the unsteadiness of the separation bubble; when incipient separation occurs, the shock unsteadiness appeared to be related to a superposition of both upstream and downstream flow conditions. Touber and Sandham^[6] studied the effect of shock strength on SBLI using large-eddy simulation (LES). They replicated three different experimental configurations and found a good agreement between LES and experiments. They showed that for low-to-moderate shock intensities, the length of SBLI region, when scaled by the upstream boundary layer thickness, is linearly proportional to the shock intensity scaled by the upstream wall shear stress. Using LES, Morgan et al. [7] carried out extensive parametric studies of SBLI for various wedge angles, Reynolds numbers, streamwise and spanwise domain sizes. They found that the Reynolds number did not have any significant effect on the separation bubble size. Increasing the wedge angle led to an increased size of the interaction region but did not necessarily cause a higher probability of reversed flow.

A state-of-the-art DNS calculations were performed by Pirozzoli and Bernardini [8] for a Mach 2.25 boundary layer interacting with an oblique shock. The numerical strategy relied on a hybrid scheme that used a high-order non-dissipative central scheme [9] in the shockfree regions and a fifth-order WENO scheme in the shock regions. A very long streamwise domain size was used to avoid possible adverse effects of the recycling-rescaling procedure and also to capture the recovery of boundary layer to an equilibrium state downstream of the interaction region. While the differences in Reynolds numbers prevented a definite one-toone comparison with experiments, the DNS was able to reproduce the overall flow structure of SBLI observed in experiments.

The main objectives of the present study are to examine SBLI under various flow conditions and to improve the basic understanding of SBLI by a detailed analysis of DNS data. The Mach number of the incoming boundary layer is kept fixed at 2.75 and the strength of the interacting shock is varied by varying the flow deflection angle, θ . Three different flow deflection angles, $\theta = 6^{\circ}$, 7.75° and 9.25°, are considered. The selected flow parameters lie on the higher end of DNS studies performed to date on SBLIs. The DNS calculations are performed using a hybrid numerical methodology that uses a minimally dissipative central scheme [9] in the shock-free regions of the flow and a very robust monotonicity preserving scheme [10, 11] in the shock regions. More details on the numerical method are described in Sec. 1.2. The effect of interacting shock strength on various flow quantities, mean and turbulent statistics is examined. The contributing terms to the turbulent kinetic energy and enstrophy variations are examined with the aim of explaining the effect of shock on turbulence, for providing useful information for high-order turbulence models and also for testing the accuracy of DNS calculations.

1.2 Computational Methodology

1.2.1 Governing equations

For the current DNS computations, we solve the compressible, three-dimensional Navier-Stokes equations in conservative form. The dimensionless equations read as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} \left(\rho u_j \right) = 0 \tag{1.1}$$

$$\frac{\partial}{\partial t}\left(\rho u_{i}\right) + \frac{\partial}{\partial x_{j}}\left(\rho u_{i}u_{j}\right) = -\frac{\partial p}{\partial x_{i}} + \frac{\partial \sigma_{ij}}{\partial x_{j}}$$
(1.2)

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j} \left(E + p \right) u_j = \frac{\partial}{\partial x_j} \left(\sigma_{ij} u_i \right) - \frac{\partial Q_j}{\partial x_j} , \qquad (1.3)$$

where the viscous stress and heat flux terms are obtained from the following Newtonian models:

$$\sigma_{ij} = \frac{2\mu}{Re} \left[\frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right]$$
(1.4)

$$Q_j = \frac{-\mu}{(\gamma - 1)RePrM_\infty^2} \frac{\partial T}{\partial x_j}$$
(1.5)

Here, the temperature dependence of μ is based on Sutherland's law, $\mu(T) = T^{1.5}(1 + C)/(T + C)$ with C = 0.82. In Eq. (3.3), E is the total energy defined as

$$E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho u_i u_i \tag{1.6}$$

Finally, the thermodynamic variables, ρ , p and T are linked by the ideal gas law,

$$p = \frac{\rho T}{\gamma M_{\infty}^2}.\tag{1.7}$$

1.2.2 Numerical scheme

DNS and LES of turbulent flows require low dissipation numerical schemes to avoid unphysical damping of "small" scales due to numerical dissipation. In the presence of shocks, it becomes necessary to use shock-fitting schemes to prevent spurious oscillations near the shock regions introduced due to the Gibbs phenomenon. While standard shock-capturing schemes like WENO or monotonicity preserving scheme (MP) [10, 11] successfully capture the shock without any spurious oscillations, they can be dissipative in the regions away from the shock and may reduce the accuracy of the solution. It should be noted that DNS computations of SBLI have been performed using WENO [12, 13, 14, 15] and MP [16] schemes with a good degree of accuracy. However, these schemes are not suitable for flows at higher Reynolds numbers or flows with strong shock/turbulence interactions. An ideal solver for numerical simulations of shock/turbulence interactions should have very low numerical dissipation in the regions away from the shock and should also successfully capture the shock without introducing any spurious oscillations. One way to achieve this goal is to use a hybrid scheme which incorporates a very low dissipation central-difference scheme in shock-free regions and a shock-capturing algorithm in regions near the shock. The switch between the two algorithms can be made by using a shock sensor. This hybrid methodology has been successfully used for various shock/turbulence interaction simulations [17, 8, 18].

In the present study, we use a similar hybrid methodology to discretize the convective terms in Eqs. (3.1), (3.2) and (3.3). In the shock regions, we employ a fifth-order MP scheme. (It should be noted that the order of accuracy degenerates to first-order near discontinuities). This scheme has proved to be very robust for a wide variety of problems and has lesser numerical dissipation and faster grid convergence when compared to a standard WENO scheme [11]. The details of MP scheme can be found in Ref. [11]. In smooth regions of the flow, the convective terms are cast in a split form [19, 9, 18]:

$$\frac{\partial\rho u_{j}\varphi}{\partial x_{j}} = \frac{1}{4} \frac{\partial\rho u_{j}\varphi}{\partial x_{j}} + \frac{1}{4} \left(u_{j} \frac{\partial\rho\varphi}{\partial x_{j}} + \rho \frac{\partial u_{j}\varphi}{\partial x_{j}} + \varphi \frac{\partial\rho u_{j}}{\partial x_{j}} \right) \\
+ \frac{1}{4} \left(\rho u_{j} \frac{\partial\varphi}{\partial x_{j}} + \rho \varphi \frac{\partial u_{k}}{\partial x_{j}} + u_{j} \varphi \frac{\partial\rho}{\partial x_{j}} \right)$$
(1.8)

where φ is unity for the continuity equation, velocity components (u_j) for the momentum equations and $H = \gamma/(\gamma - 1)p/\rho + u_k u_k/2$ for the total energy equation. The casting of convective terms in spilt form ensures global conservation of total kinetic energy in the limit of inviscid, incompressible flow and ensures strong numerical stability. Pirozzoli [9] has shown that the above split form for convective terms can be cast in a locally conservative form:

$$\frac{\partial \rho u_j \varphi}{\partial x_j} \Big|_{x=x_j} = \frac{1}{\Delta x} \left(\hat{f}_{j+1/2} - \hat{f}_{j-1/2} \right) , \qquad (1.9)$$

and be approximated using a central-difference operator of the form:

$$Df_{j} = \sum_{l=1}^{L} \frac{a_{l}}{\Delta x} \left(f_{j+l} - f_{j-l} \right) .$$
 (1.10)

This is achieved by defining the numerical flux as:

$$\hat{f}_{j+1/2} = 2\sum_{l=1}^{L} a_l \sum_{m=0}^{l-1} (\widetilde{\rho, u, \varphi})_{j-m,l}$$
(1.11)

where

$$(\widetilde{f,g,h})_{j,l} = \frac{1}{8}(f_l + f_{j+l})(g_l + g_{j+l})(h_l + h_{j+l}) .$$
(1.12)

Since the above formulation is based on central differencing, there is no additional numerical dissipation induced as in upwind schemes. Also, since the split form ensures strong numerical stability, there is no need for the use of spectral-type filters [20] which may also introduce artificial dissipation. In the present study, we use a sixth-order accurate central scheme (L = 3) for the formulation of convective terms in split form.

The switch between MP scheme and the central-difference scheme is made using a modified form of Ducros sensor [8]:

$$\Theta = \frac{(\nabla \cdot u)^2}{(\nabla \cdot u)^2 + |\nabla \times u|^2 + (u_\infty/\delta)^2} , \ 0 \leqslant \Theta \leqslant 1$$
(1.13)

In the present study, we use a threshold value of $\Theta = 0.075$ to distinguish between shock and shock-free regions, i.e., for regions where $\Theta \ge 0.075$, MP scheme is implemented and in all the other regions, the central-difference scheme is used. The hybridization is achieved by first computing the values of Θ in the computational domain and pre-marking the critical regions.



Figure 1.1: Instantaneous density contours overlaid with modified Ducros shock sensor values. The critical regions identified by the shock sensor are shown in red. For interpretation of the references to color in this and all other figures, the reader is referred to the electronic version of this dissertation.

Next, the fluxes are computed in the entire domain using the central-difference scheme. In critical regions, the fluxes are then selectively replaced by using the MP scheme. For the treatment of interfaces between the shock and shock-free regions, a padding of 3 points on either side of the interface point is used to prevent the incursion of non-dissipative central-difference scheme into the shock regions [8, 21]. In Fig. 1.1, we show the instantaneous density contours overlaid with the shock sensor values in an x - y symmetry plane for $\theta = 7.75^{\circ}$. The regions highlighted in red are identified as critical regions by the shock sensor and a switch is made to MP scheme for computing the convective fluxes in these regions.

The viscous and diffusion terms are cast in a "Laplacian" form [22] for proper representation of diffusion effects at the highest resolved wavenumbers and also for improved numerical stability. We found that when using a non-dissipative scheme for discretizing the convective terms, as done in the present study, it is necessary to use the non-conservative form for discretizing the viscous and diffusion terms which otherwise could lead to numerical oscillations in the solution, particularly near the wall. The viscous and diffusion terms are computed using a sixth-order central compact scheme [20] for both first and second derivatives. The time integration is performed using an explicit third-order Runge-Kutta scheme.

1.2.3 Inflow turbulence generation

The generation of a realistic inflow boundary condition for turbulent boundary layers is very important. Several methods are described in the literature, each with their own merits and demerits. In the present study, we adopt a two-step approach to prescribe the inflow turbulence for SBLI simulations. This is similar to the method used in Refs. [16, 15, 23]. First, we first perform an auxiliary DNS for a canonical zero-pressure gradient turbulent boundary layer. The domain size for the auxiliary simulation was $37.7\delta_{ref} \times 15\delta_{ref} \times 3.5\delta_{ref}$ in the streamwise (x), wall-normal (y) and spanwise (z) directions, respectively. Here, δ_{ref} is the boundary layer thickness at the inlet of the auxiliary DNS. The useful part of the domain in the streamwise direction was only until $x = 24\delta_{ref}$ after which is the sponge region [24] which is used to drive the flow to a uniform state towards the exit of the domain. The corresponding grid resolution for the auxiliary simulation was $1464 \times 202 \times 193$. The grid was uniform in the streamwise direction until $x = 24\delta_{ref}$ and stretched in the sponge region. The grid was also uniform in the spanwise direction. In the wall-normal direction, grid points were clustered near the wall using a hyperbolic sine transformation. In terms of wall units, the streamwise and spanwise grid spacings were $\Delta x^+ = \Delta z^+ \approx 4.5$ (the reference quantities are taken at $x = 23\delta_{ref}$). In the wall-normal direction, 100 points were located within $y/\delta_{ref} = 1$ and with the node next to the wall located at a distance of $\Delta y^+ \approx 0.6$. For prescribing the inflow boundary condition for the auxiliary DNS, we used the recyclingrescaling method similar to the one described in Ref. [25]. The recycling station was located at a distance of $23\delta_{ref}$ from the inlet of the domain. Once the flow reached a statistically steady state, a time-history of all the primitive variables were stored in a y - z plane located at a distance of $23\delta_{ref}$ from the inlet for a total length of approximately $360\delta_{ref}/U_{\infty}$. This "inflow box" was then used as the inflow boundary condition for SBLI simulations. The total length of the inflow box $(360\delta_{ref}/U_{\infty})$ was sufficient to carry out the SBLI simulations without having to recycle the inflow box. To establish that the recycling procedure used for auxiliary DNS does not introduce any spurious periodicity, we show the spectra of wall pressure at the recycling station in Fig. 1.2. Evidently, we do not see any phase locking due to the recycling procedure. As explained in Ref. [25], if a phase locking were to occur, a peak in the spectra would appear at $f_{rec} = U_c/x_{rec}$ where $U_c \approx 0.8U_{\infty}$ and $x_{rec} = 23\delta_{ref}$. This would correspond to $f_{rec} = 0.0348U_{\infty}/\delta_{ref}$ (indicated by a vertical line in Fig. 1.2).

At the outflow of auxiliary DNS, a supersonic exit condition was used. At the top boundary, a symmetry boundary condition was applied to all the primitive variables and a periodic boundary condition was used in the spanwise direction.

1.2.4 Computational setup for DNS of SBLI

The primary motivation for using the inflow box method in our DNS computations was to keep the incoming flow identical for all three selected flow deflection angles. Additionally, this inflow box can also be used for other DNS and LES computations. The computational parameters for the SBLI simulations conducted in this paper for various shock intensities are given in Table 1.1. In this table, P_2/P_1 is the pressure ratio across the incident shock.



Figure 1.2: The wall pressure spectra at $x = 23\delta_{ref}$ for the "auxiliary" DNS.

For all simulations, the grid is uniform in streamwise and spanwise directions. Similar to the auxiliary DNS, the useful part of the domain in the streamwise direction extends only up to $x = 23.5\delta_{ref}$ after which is the sponge region. In the wall-normal direction, the nodes are clustered near the wall using a hyperbolic sine function to resolve the boundary layer. It should be noted that the inflow box generated from the auxiliary DNS had 202 and 193 grid points in the wall-normal and spanwise directions, respectively. However, for the SBLI simulations, we increased the number points in both y and z to improve the resolution (See Table 1.1). Hence, the inflow box was interpolated to the SBLI DNS grid in y and z directions using a third-order polynomial. Since the time step for SBLI computations is controlled by the CFL condition, a third-order polynomial interpolation was used to obtain

Parameter	Case I	Case II	Case III
M_{∞}	2.75	2.75	2.75
heta	6^{o}	7.75^{o}	9.25^{o}
P_{2}/P_{1}	1.51	1.69	1.86
L_x	$23.5\delta_{ref}$	$23.5\delta_{ref}$	$23.5\delta_{ref}$
L_y	$15\delta_{ref}$	$13\delta_{ref}$	$13\delta_{ref}$
L_z	$3.48\delta_{ref}$	$3.48\delta_{ref}$	$3.48\delta_{ref}$
N_x	1440	1632	1632
N_{y}	252	302	302
N_z	234	234	234
Δx^+	4.1	3.45	3.45
Δy_w^+	0.6	0.6	0.6
Δz^+	3.45	3.45	3.45

Table 1.1: Simulation Parameters for DNS of SBLI.

the inflow values at an arbitrary time t. As in the case for the auxiliary DNS, a sponge layer is used at the outlet to damp out the fluctuations, thus enabling the use of a simple extrapolation for all variables. At the top boundary, a symmetry boundary condition is applied to all variables. The bottom boundary is an isothermal wall with wall temperature set equal to the adiabatic wall temperature of the undisturbed boundary layer. A no-slip condition is used for the three velocity components and the density at the wall is computed using the unsteady characteristic boundary condition [26, 27].

1.3 Results

The DNS results for three different shock intensities or deflection angles, $\theta = 6^{\circ}$, 7.75° and 9.25° are discussed in this section. For convenience, we refer to simulations with $\theta = 6^{\circ}$, 7.75° and 9.25° as Cases I, II and III, respectively. The ensemble-averaged statistics reported in this paper are obtained by averaging in time and the homogeneous spanwise direction.

δ_0	δ_1	δ_2	Re_{δ_2}	C_{f}
$1.484\delta_{ref}$	$0.4418\delta_{ref}$	$0.102\delta_{ref}$	2070	2.42×10^{-3}

Table 1.2: Boundary layer parameters for the incoming boundary layer.

The time integration was for at least one time period of the low-frequency oscillation of the reflected shock system. The time period of the shock system was estimated *a priori* using the data presented in Fig. 7 of Ref. [4] and assuming a characteristic frequency of $St_L = 0.03$, which is the typical value observed in most experimental and numerical studies. For calculating/presenting various statistics, we use either Reynolds decomposition $(\langle \phi \rangle = \phi - \phi')$ or Favre decomposition $(\{\phi\} = \phi - \phi'', \{\phi\} = \langle \rho\phi \rangle / \langle \rho \rangle)$ of the variables.

In the discussion of results for SBLIs, it is customary to use a non-dimensional streamwise coordinate defined as $X^* = (x - X_o)/L$. Here X_o is the nominal shock impingement location and L is the length of the interaction region, defined as the region between the nominal shock impingement location (X_o) and the apparent origin of the reflected shock. As done in other studies, the apparent origin of the reflected shock is obtained by extrapolating the mean reflected shock to the wall. In the present study, the nominal shock impingement location was kept fixed at $X_o = 15\delta_{ref}$ for all three DNS calculations. Using X^* as the streamwise coordinate, the interaction region is located between $-1 \leq X^* \leq 0$.

The flow parameters for the incoming (undisturbed) boundary layer are shown in Table 1.2. For evaluating these parameters, data at the reference station $x = 9\delta_{ref}$ was chosen. For the purpose of this study, the boundary layer thickness (δ_0) is defined as the location where the mean spanwise vorticity reaches 0.5% of its maximum value.

1.3.1 Accuracy of DNS

To assess the accuracy of our DNS calculations, we first compare the mean and turbulence quantities of the incoming boundary layer with the DNS results of Pirozzoli and Bernardini [1] which were at Mach 2. For this purpose $x = 9.0\delta_{ref}$, which is located just upstream of the interaction region for Case III, is chosen as the reference station. Figure 1.3(a) shows the Van-Driest transformed mean streamwise velocity profile of the incoming boundary layer. The universal linear relationship, $U^+ = y^+$, (shown using dash-dot line in the figure) is exhibited by the incoming boundary layer for $y^+ \leq 5$ and there is a logarithmic behavior between $30 \leq y^+ \leq 60$. The logarithmic behavior is in a very good agreement with the log-law profile (shown using dashed line in the figure) given by Eq. (1.14)

$$U_{VD}^{+} = \frac{1}{K}\ln(y^{+}) + C \tag{1.14}$$

where

$$K = 0.41, \quad C = 5.1$$

The differences in the wake region are due to the differences in Reynolds numbers computed using momentum thickness and wall properties $(Re_{\delta_{2w}})$. In the present DNS calculations, $Re_{\delta_{2w}} \approx 1000$ while in the DNS calculations of Pirozzoli and Bernardini [1], $Re_{\delta_{2w}} \approx 1300$. The density-scaled Reynolds stresses are shown in Fig. 1.3(b) in outer scaling. Once again, a very good agreement is obtained between our current DNS results and DNS results of Pirozzoli and Bernardini [1].

The accuracy of the incoming boundary layer statistics does not necessarily guarantee



(b)

Figure 1.3: (a) Van Driest transformed mean streamwise velocity profile and, (b) densityscaled Reynolds stresses of the incoming boundary layer. Symbols represent DNS data of Pirozzoli and Bernardini [1]

the accuracy of results in the interaction region and also downstream of the interaction region. Since there are no experimental data available in the range of current simulations, it is very important to establish the numerical accuracy of present DNS calculations in different ways. The numerical accuracy of current DNS calculations, both in the upstream and the downstream regions of the interaction, were assessed by checking the sum of all the terms in the turbulent kinetic energy equation, which in theory should be equal to zero for a converged solution. The net sum of all the terms in turbulent kinetic energy equation was found to be negligible compared to the leading order terms. These results, discussed in detail in a later section, and all the other results obtained for different grids indicate the numerical accuracy of our DNS data through out the simulated domain.

1.3.2 Flow Visualizations

The complex features of SBLI are shown through the streamwise density gradient contours for Case III in Fig. 1.4. The strong amplification of turbulence behind the reflected shock is apparent from the density gradient contours in this figure. Also notice that the flow appears more fine-grained downstream of the interaction region, indicating the effect of shock on different turbulent length scales. The formation of expansion fan (represented by negative values of the density gradient) is also evident behind the reflected shock. The expansion fan region is followed by a series of compression waves which arise due to the reattachment of boundary layer which mimics the effect of a compression corner.

The effect of shock strength on the shock-boundary layer interaction can be qualitatively examined by looking at the instantaneous numerical schlieren visualizations of the flow obtained from DNS data (Fig. 1.5). We use the density gradient parameter defined in Ref. [13] for flow visualizations in Fig. 1.5. The dark regions indicate regions of high



Figure 1.4: Instantaneous streamwise densitygradient contours for Case III. Contour levels are evenly spaced between -1 and 1.

density gradients. One can clearly observe that the origin of reflected shock shifts upstream with increasing shock intensity and the reflected shock is followed by a series of stronger compression waves. Also notice that the strength of the reflected shock increases with an increase in shock intensity.

The overall behavior of the boundary layer can be examined by looking at the flow in a plane parallel to the wall, i.e., in an x - z plane. It is recommended to examine the streamwise evolution of flow structures in a fixed y/δ plane [1]. However, the presence of shock makes the computation of boundary layer thickness (δ) in the interaction region difficult. Hence, we chose the mean sonic plane, i.e., the plane wall-normal location at which the mean Mach number is equal to 1, instead of a fixed y/δ plane. Additionally, the mean sonic plane approximately represents the beginning of the supersonic regime in the boundary layer.



Figure 1.5: Instantaneous numerical schlieren visualizations at an x - y symmetry plane. (a) Case I, (b) Case II, (c) Case III.

Figure 1.6 shows the instantaneous velocity and temperature fluctuations along the mean sonic plane. For the incoming boundary layer, the velocity and temperature fields exhibit a typical streaky structure with alternating low and high momentum regions observed in a canonical zero-pressure-gradient boundary layer. These structures can sometimes extend to lengths of around 40 δ and are referred to as superstructures. Some SBLI studies [28] have postulated that these superstructures may be responsible for the low-frequency oscillation of the shock system. In the region upstream of the interaction region, the velocity and temperature fields are negatively correlated, i.e., high-momentum regions correspond to low-temperature regions and vice-versa. In the separation region (indicated by the two vertical lines), the streaky flow structure is observed in the initial part of the region but it soon becomes "chaotic" and "isotropic" with a finer structure compared to the incoming flow. From a numerical perspective, this is very important because conventional shock capturing or upwind schemes cannot accurately capture the turbulence downstream of the interaction region due to their inherent numerical dissipation. The shock appears to enhance mixing in the boundary layer too. The anti-correlation between the velocity and temperature fields drops in the interaction region and also downstream of the interaction region. For the incoming boundary layer, the correlation between velocity and temperature field is approximately -0.85 along the mean sonic line but drops to -0.55 in the interaction region and regions downstream of the shock. This indicates the weakening of Reynolds analogy assumptions in the interaction region and regions downstream of the shock. We also examined the behavior of velocity and temperature fluctuations in the x-z plane along which the turbulent kinetic energy was maximum and found similar results.



Figure 1.6: (a) Instantaneous velocity fluctuations and, (b) instantantaneous temperature fluctuations along the mean sonic plane for Case II.

1.3.3 Reynolds- and Favre-Averaging

For a turbulent variable f, the Reynolds-averaged value $\langle f \rangle$ is related the Favre-averaged variable $\{f\}$ by the following equation:

$$\langle f \rangle - \{f\} = \langle f'' \rangle . \tag{1.15}$$

Both Reynolds- and Favre-averaged forms of the flow statistics may be used for analysis of compressible flows. Huang et al. [29] compared Reynolds- and Favre-averaged quantities for a supersonic channel flow at Mach numbers of 1.5 and 3.0 and observed small variations between them in regions close to the wall. Here we examine the two forms of averaging for different shock intensities before discussing the flow statistics for SBLI.

Figure 1.7 shows the difference between the two kinds of averaging for the mean streamwise velocity and temperature at $X^* = -1.1$, which corresponds to the incoming boundary layer not yet affected by the shock. For the streamwise velocity, the maximum difference is about -2.5% w.r.t. the Reynolds-averaged velocity and it is observed to be near the wall. For the static temperature, the maximum difference is about 1.5% w.r.t. the Reynolds-averaged temperature but the difference persists to a greater distance along the wall-normal direction. The difference between Reynolds- and Favre-averaged total temperature was found to be less than 0.4% w.r.t. the Reynolds-averaged quantity and can be considered negligible. In the interaction region ($X^* = -0.5$), the maximum difference between Reynolds-averaged and Favre-averaged velocity increases to 5% for all three shock intensities (Fig. 1.8(a)). For the temperature (Fig. 1.8(b)), there is only a marginal increase to 1.75%. In summary, differences between the two forms of averaging appear to be largely independent of the shock intensities and relatively small for the selected cases.



(a)



Figure 1.7: Differences between Reynolds- and Favre-averaged quantities at $X^* = -1.1$. (a) velocity, (b) temperature.




Figure 1.8: Differences between Reynolds- and Favre-averaged quantities at $X^* = -0.5$. (a) velocity, (b) temperature.

Since the differences in the two forms of averaging are more significant near the wall, it can influence the prediction of skin-friction coefficient (C_f) . In Fig. 1.9, the C_f values computed from Reynolds- and Favre-averaged velocities for Case II are compared. As evident from the figure, the differences mainly occur in the interaction region and downstream of the interaction region.

The relationship between the Reynolds- and Favre-averaged turbulent stresses is given by

$$\{u_i''u_j''\} = \langle u_i'u_j'\rangle - \langle u_i''\rangle\langle u_j''\rangle + \langle \rho'u_i'u_j'\rangle/\langle \rho\rangle$$
(1.16)

Consistent with supersonic channel flow DNS results [29], our results show that the term associated with the product of two mean Favre-averaged fluctuations, $\langle u_i'' \rangle \langle u_j'' \rangle$ is approximately 1% of the Favre-averaged stress value in all the regions of flow. On the other hand, the triple correlation term $\langle \rho' u_i' u_j' \rangle$ is not negligible, particularly in the outer regions of the boundary layer, as can be seen in Fig. 1.10. Although, it should be noted that the magnitude of stresses is small in the outer regions of the boundary layer. Similar results are observed for turbulent heat flux terms.

1.3.4 Flow Reversal Comparisons

Figure 1.11 shows instantaneous streamwise skin-friction coefficient (C_{fx}) contours for the three cases considered in this paper. The streamwise skin-friction coefficient is defined as

$$C_{fx} = \frac{2\sigma_{xy}}{\rho_{\infty}U_{\infty}^2} \tag{1.17}$$



Figure 1.9: (a) Comparison of C_f computed using Reynolds- and Favre-averaged quantities. (b) Percentage difference in C_f computed by Reynolds- and Favre-averaged quantities. The results shown are for Case II.





(b)

Figure 1.10: Comparisons for $\langle \rho' u'_i u'_j \rangle$. (a) for different shock intensities. $X^* = -1.1$, (b) $X^* = 0.25$.

where σ_{xy} is the x - y component of the shear stress at the wall. Only regions with $C_{fx} < 0$ are shown to illustrate the extent of boundary layer separation. The locations of mean separation and mean reattachment points in this figure are indicated by the dashed vertical lines. The effect of shock intensity on the extent of flow separation is evident from the larger separation regions created by shocks with higher intensities. The instantaneous data show much larger separation zones than the corresponding mean separation zones (denoted by dashed vertical lines). Additionally, the separation regions are not continuous and are distributed non-uniformly in the spanwise direction. This shows that the separation bubbles are highly unsteady and three-dimensional.

To further illustrate the 3D nature of flow in the interaction region, instantaneous spanwise skin-friction coefficient (C_{fz}) contours are shown in Fig. 1.12. C_{fz} is defined as

$$C_{fz} = \frac{2\sigma_{yz}}{\rho_{\infty}U_{\infty}^2} \tag{1.18}$$

The incoming boundary layer is statistically homogeneous in the spanwise direction and more-or-less "uniform" but we observe several patches of high C_{fz} values in the separation region as well as in the regions downstream of the reattachment point. This indicates that the flow is three-dimensional, at least instantaneously, not only in the separation region but also downstream of the reattachment point, where the boundary layer is recovering back to an equilibrium state.

For an additional characterization of the unsteady and intermittent nature of flow separation, we computed the statistical probability of flow reversal ($\overline{\gamma}$) at the wall. According to the classification by Simpson [30], incipient detachment (ID) occurs when the instantaneous flow reversal happens about 1% of the time, intermittent transitory detachment (ITD) oc-





(b)



(c)

Figure 1.11: Instantaneous streamwise skin-friction coefficient contours. The contour levels are evenly spaced between -6×10^{-3} and 0. (a) Case I, (b) Case II, (c) Case III.





(b)



(c)

Figure 1.12: Instantaneous spanwise skin-friction coefficient contours. The contour levels are evenly spaced between -5×10^{-3} and 5×10^{-3} . (a) Case I, (b) Case II, (c) Case III.



Figure 1.13: Comparisons for the probability of flow reversal for different shock intensities.

curs when the instantaneous backflow happens 20% of the time and transitory detachment (TD), which in practice coincides with the mean flow reversal, occurs when the flow reversal happens 50% of the time. The streamwise variation of $\overline{\gamma}$ for the three cases with different shock intensities is shown Fig. 1.13. All three cases show a maximum flow reversal probability between 65 – 70%. As evident from the figure, with an increase in shock strength, the probability of flow reversal extends to regions further downstream of the interaction region. However, by increasing the strength of the incident shock, the maximum probability of flow reversal does not change very much. This behavior was also observed by Morgan et al. [7] in their LES studies.

Henceforth, for convenience, the streamwise skin-friction coefficient (C_{fx}) will be referred

Parameter	Case I	Case II	Case III
$L_{sep} \\ L/\delta_0$	$\begin{array}{c} 0.915\delta_{ref} \\ 2.04 \end{array}$	$\frac{1.76\delta_{ref}}{2.49}$	$\frac{3.3\delta_{ref}}{3.44}$

Table 1.3: Separation and Interaction lengths.

to as just skin-friction coefficient and will be denoted by C_f . Figure 1.14 shows the streamwise distribution of mean skin-friction coefficient for the three cases simulated with different shock strengths. The abscissa of the plot has been modified to coincide the mean separation points for all three cases and all three cases exhibit appreciable mean separation bubbles. The separation lengths (L_{sep}) and the interaction lengths (L) for Cases I, II, and III are given in Table 3.3. Dupont et al. [4] proposed a linear relationship (for weak-to-moderate interactions) between the length of the interaction region (L) and the shock intensity. The interaction lengths computed in the present simulations agree well with the data presented in Fig.7 of Ref. [4]. Interestingly, Fig. 1.14 shows that the rate of decrease of C_f ahead of the mean separation point is similar for all three cases, even though the recovery rates vary.

1.3.5 Mean and Fluctuating Wall-Pressure Comparisons

The streamwise variations of mean wall-pressure for Cases I, II and III are shown in Fig. 1.15. In Fig. 1.15(a), the mean wall-pressure is again plotted against the streamwise coordinate whose origin has been shifted to the mean separation point. The mean wall pressure for all three cases begin to rise upstream of the mean separation point, i.e., before $x - x_{sep} = 0$. Also, similar to the trends shown for C_f , the rate of increase of wall-pressure is similar for all



Figure 1.14: Comparisons for mean skin-friction coefficient for different shock intensities.

three cases during the initial part of the interaction. When the non-dimensional mean wall pressure, $P^* = (P_w - p_1)/(p_2 - p_1)$ (p_1 and p_2 are the pressures upstream and downstream of the incident shock, respectively) is plotted against X^* (Fig. 1.15(b)), the profiles show a reasonable collapse across and downstream of the interaction region. However, the collapse becomes poor as the shock intensity increases [4] since the non-dimensionalization is valid only for the inviscid limit.

Figure 1.16(a) shows the instantaneous wall-pressure fluctuations for Case II. In the incompressible separated boundary layer DNS study by Na and Moin [31], the wall pressure fluctuations were found to be lower in the separated region compared to the region downstream of the reattachment point. However, in the present study, we find that the





Figure 1.15: Mean wall pressure distribution for different shock intensities plotted with different scalings.

wall-pressure fluctuations are high even in the separation region (between the dashed vertical lines in the figure). The streamwise evolution of r.m.s. of wall pressure fluctuations, normalized by the mean wall pressure and plotted against X^* , are shown in Fig. 1.16(b). The data show a reasonable collapse, particularly for Case II and Case III, in the regions downstream of the interaction region. Also note that the peak of the r.m.s. wall pressure fluctuation moves upstream with increasing shock strength when plotted in this scaling.

1.3.6 Thermodynamic Variables

Figure 1.17 shows the variation of r.m.s. values of thermodynamic variables along the wallnormal direction at different streamwise locations for Case II. At all the streawise stations, the pressure fluctuations (normalized by the mean pressure) are nearly constant in the nearwall regions, as shown in Fig. 1.17(a). For the incoming boundary layer $(X^* = -1.1)$, the maximum pressure fluctuations intensity is approximately 4% of the mean value. However, in the interaction region $(X^* = -0.5)$, the r.m.s. value of pressure increases to 12%. The spike in the r.m.s. pressure profile seen at this station is due to the shock, and as shown in the figure, there is a very sharp increase in pressure fluctuations across the shock. As we move to downstream stations, the intensity of pressure fluctuations decreases, although the peak values keep shifting to the outer part of the boundary layer. The variations in static temperature fluctuations (Fig. 1.17(b)) due to the shock are not as significant as those of the pressure. However, for the incoming boundary layer $(X^* = -1.1)$, the r.m.s. values of temperature fluctuations are quite significant with a peak value reaching to about 12% of the mean temperature. In the interaction region $(X^* = -0.5)$ there is a modest increase in the peak value of r.m.s. temperature fluctuations. Even the jump in the temperature plot across the shock (indicated by the spike) is not as strong as that in the pressure plot.





Figure 1.16: (a) Instantaneous wall pressure fluctuations for Case II. (b) Streamwise evolution of r.m.s. of wall pressure fluctuations for different shock intensities.

In the downstream stations, the r.m.s. temperature fluctuation values drop to the values comparable to those found in the incoming boundary layer. Also, similar to the r.m.s. of pressure fluctuations, the peak values of temperature r.m.s. keep shifting towards the outer part of the boundary layer as we move to downstream stations. The fluctuations in the total temperature (not shown) are not negligible, even for the incoming boundary layer. Interestingly, for the selected streamwise stations, the maximum value of total temperature fluctuations occur at $X^* = 0.25$, and not at $X^* = -0.5$, which is in the interaction region. And, unlike the fluctuations for pressure and static temperature, the fluctuations in total temperature are not so much affected by the shock, which is evident from the absence of spikes in the total temperature plots.

To get a better understanding of the global behavior of various thermodynamic variables and their turbulent fluctuations, we show the contours of their r.m.s. in Fig. 1.18 for Case II. Figures. 1.18(a) and 1.18(b) show contours of pressure and density, respectively. The highest fluctuations in the thermodynamic variables are observed in the interaction region. The oscillations in pressure and density are shown to propagate along the reflected shock and the strength of the fluctuations propagating along the reflected shock are shown to increase with increasing incident shock strengths. Although the intensity of pressure and density fluctuations decreases as we go further along the reflected shock towards the freestream, they could be partly because of the grid coarsening.

A convenient and important parameter for predicting the effects of compressibility in supersonic turbulent flows is the turbulent Mach number, M_t . It is defined as the ratio of twice the turbulent kinetic energy and the mean speed of sound,

$$M_t = \frac{\{u_i'' u_i''\}}{\langle c \rangle} . \tag{1.19}$$





Figure 1.17: R.M.S. of thermodynamic fluctuations at different streamwise locations for Case II. (a) pressure, (b) temperature.



Figure 1.18: Contours of turbulent fluctuations of thermodynamic variables for Case II. (a) r.m.s. of pressure fluctuations, (b) r.m.s. of density fluctuations.

Another useful quantity is the fluctuation Mach number $(\langle M' \rangle)$ which is the r.m.s. of the Mach number fluctuations. Compressibility effects in turbulence are predicted to become important when M_t exceeds 0.3. In Fig. 1.19, we show the profiles for M_t and $\langle M' \rangle$ at various streamwise locations for Case II. Both M_t and $\langle M' \rangle$ show similar trends with $\langle M' \rangle$ exhibiting slightly larger values. The incoming boundary layer shows a peak M_t value of approximately 0.3 and it increases to 0.55 at $X^* = -0.5$. As we go to regions downstream of the interaction region, the peak value of M_t reduces, but the location of peak moves towards the outer part

of the boundary layer, similar to pressure and temperature fluctuations. Unlike M_t , $\langle M' \rangle$ experiences a sharp jump across the shock, which can be seen in its profile at $X^* = -0.5$. Similar trends are observed for the other two cases with the difference being the magnitude of peak values which are higher for stronger shocks, as expected.

1.3.7 Turbulent Kinetic Energy Budget

Useful information for turbulence modeling can be obtained by looking at various terms in the turbulent kinetic energy (TKE) transport equation. The transport equation for turbulent kinetic energy $(k = 1/2\{u''_iu''_i\})$ is given by

$$\frac{\partial \langle \rho \rangle k}{\partial t} = C + P - \epsilon + T + V + \Pi + D \tag{1.20}$$

where $C, P, \epsilon, T, V, \Pi, D$ are the contributions from mean convection/advection, production, viscous dissipation, transport, viscous diffusion, pressure dilatation and mass diffusion terms, respectively. The expressions for these terms are given below.

$$C = -\frac{\partial \langle \rho \rangle \{u_j\}k}{\partial x_j}$$

$$P = -\langle \rho \rangle \{u_i'' u_j''\} \frac{\partial \{u_i\}}{\partial x_j}$$

$$\epsilon = \langle \sigma_{ij}' \frac{\partial u_i''}{\partial x_j} \rangle$$

$$T = T_t + T_p = -\frac{\partial}{\partial x_j} \left[\frac{1}{2} \{u_i'' u_i'' u_j''\} \right] - \frac{\partial}{\partial x_j} \left[\langle p' u_j' \rangle \right]$$

$$V = \frac{\partial \langle \sigma_{ij}' u_i'' \rangle}{\partial x_j}$$





Figure 1.19: Turbulent and fluctuating Mach numbers at different streamwise locations for Case II. (a) M_t , (b) $\langle M' \rangle$.

$$\Pi = \langle p' \frac{\partial u''_i}{\partial x_i} \rangle$$
$$D = \langle u''_i \rangle \left[\frac{\partial \langle \sigma_{ij} \rangle}{\partial x_j} - \frac{\partial \langle p \rangle}{\partial x_i} \right]$$

The production term (P) generates the turbulent kinetic energy through the mean velocity gradient. This term is responsible for the energy transfer between mean flow kinetic energy and the turbulent kinetic energy. The transport term consists of two parts, turbulent transport term (T_t) and pressure transport term (T_p) . The contributions from the pressure transport term (T_p) and the pressure dilatation term (II) together are known as the pressure work. The pressure dilatation term is responsible for the energy transfer between the turbulent kinetic energy and the mean internal energy and is significant only when the compressibility effects become important. The pressure transport term is responsible for the redistribution of energy to the inhomogeneous flow regions. As stated in Ref. [32], the mass diffusion term (D) is usually associated with variable inertia effects for flows with low turbulent Mach numbers. But at higher turbulent Mach numbers, this term can also include the effects of compressibility. Note that the mass diffusion term involves the Reynolds-averaged value of the Favre fluctuation of the velocity which, as we have shown earlier, is small and primarily confined to regions close to the wall.

Figure 1.20 shows the turbulent kinetic energy budget for the incoming boundary layer, i.e., at $X^* = -1.1$. Since the profiles are similar for all the three cases at this location, we show the results only for Case II. The legend for various terms in the turbulent kinetic energy equation is given in Table 1.4. The results at $X^* = -1.1$ are representative of a typical zero-pressure gradient boundary layer. Near the wall, viscous dissipation is balanced by the viscous diffusion term and away form the wall, the production term largely balances the



Figure 1.20: Turbulent kinetic energy budget for Case II at $X^* = -1.1$.

Term	Color	Line style
convection (C)	green	solid
production (P)	black	solid
dissipation (ϵ)	red	solid
turbulent transport (T_t)	blue	solid
pressure transport (T_p)	blue	dashed
viscous diffusion (V)	black	solid line with open circles
pressure dilatation (Π)	black	open squares

Table 1.4: Legend and colors for turbulent kinetic energy budget plots.

viscous dissipation term and the turbulent transport term. The advection term is negligible for the incoming boundary layer due to the absence of any significant mean strain rates in the flow direction. The sum of all the terms in Eq. 1.20 is shown by the dashed red line and it indicates excellent numerical accuracy of our DNS calculations.

The profiles at $X^* = -0.5$ are shown in Fig. 1.21. At this location, the pressure transport

term becomes important near the wall (indicating the redistribution of TKE to the inhomogeneous directions) and cancels the other two important terms, the viscous diffusion and the viscous dissipation terms. The dissipation near the wall increases with generally higher dissipation for higher shock intensities. Since dissipation is largely associated with small scales of the flow, larger dissipation indicates more small scales are formed due to the interaction of the boundary layer with the shock. As a result of the boundary layer interaction with the shock, the peak value of production term increases by almost four times which results in the amplification of turbulent kinetic energy at this location. Also, the peak of production term shifts away from the wall into the mixing layer region developing over the separation bubble. As shown earlier, the height of the separation bubble increases with an increase in shock intensity and this explains the shifting of the peak away from the wall with increasing shock intensity. Away from the wall, the convection term becomes significant, again due to the formation of mixing layer over the separation bubble, and helps in balancing out the production term in the outer part of the boundary layer. The turbulent transport term has both positive and negative contributions in the boundary layer. Near the wall, it has a positive contribution and compensates for the draining of the energy due to viscous dissipation. Near the regions where the production term attains its peak, the turbulent transport term is negative to counter the production term but once again its contribution becomes positive in the outermost region of the boundary layer to balance out the convective term. Once again note the excellent balance between all the contributing terms which is indicated by the dashed red line.

At $X^* = 0.25$ (Fig. 1.22), again the pressure transport term, the viscous diffusion term and the viscous dissipation term cancel each other near the wall. For Case I (not shown), the production term exhibits two peaks, one in the inner layer and the other in the outer





(b)

Figure 1.21: Turbulent kinetic energy budgets at $X^* = -0.5$. (a) Case II, (b) Case III.

layer, with the inner peak having a larger value. For Case II (Fig. 1.22(a)) and Case III (Fig. 1.22(b)), the inner peaks are just beginning to form. This indicates the varying rates of boundary layer recovery towards an equilibrium state for different shock intensities. The peaks of production in the outer part of the boundary layer are balanced by the turbulent transport and viscous dissipation terms. The convection term is positive in the inner part of the boundary layer to negate the effect of viscous dissipation but becomes negative in the outer part to balance the production and turbulent transport terms.

At $X^* = 1.5$ (Fig. 1.23), a recovery towards an equilibrium state is still in process with the peak of production term moving back towards the wall, although the peak in the outer layer still exists. The convection term becomes small again at $X^* = 1.5$ compared to the previous two stations and the pressure transport term continues to be important near the wall. The significance of the pressure transport term in the interaction region and also downstream of the interaction region indicates the effect of shock in redistributing the TKE in the inhomogeneous directions. In other words, the shock tends to make the flow more homogeneous near the wall. The compressibility related terms like Π and D are found to be negligible at all the four selected streamwise locations.

The behavior of TKE and various terms in the turbulent kinetic energy budget across the interaction region can be examined by looking at their evolution along the mean sonic line (Fig. 1.24). We show the results only for Case II since similar observations are made for the other two cases. Figure 1.24(a) shows the evolution of TKE along the mean sonic line. During the first half of the interaction region, TKE increases significantly, it then drops sharply before increasing again. This behavior can be explained by examining various terms in the TKE transport equation.

Along the mean sonic line, the production term in the incoming boundary layer is bal-





Figure 1.22: Turbulent kinetic energy budgets at $X^* = 0.25$. (a) Case II, (b) Case III.





Figure 1.23: Turbulent kinetic energy budgets at $X^* = 1.5$. (a) Case II, (b) Case III.



Figure 1.24: (a) Streamwise evolution of turbulent kinetic energy along the mean sonic line. (b) Streamwise evolution of turbulent kinetic energy budget along the sonic line.

anced by the turbulent transport and the viscous dissipation terms. Due to the interaction of the turbulence with the shock, the production term increases in the interaction region. The production term couples the mean flow kinetic energy and the turbulent kinetic energy. Hence, a positive increase in the production term means energy is transferred from the mean flow to the turbulent field (which explains the increase in TKE in Fig. 1.24(a)). The loss of energy from the mean flow is due to the bulk flow deceleration caused by the shock-generated adverse pressure gradient. The adverse pressure gradient also causes boundary layer separation and, hence the lift-up of vortical structures which leads to an increased contribution from the convection term. In the first half of the interaction region, the convection and viscous dissipation terms balance the contributions by the production and turbulent transport terms. At approximately $X^* = -0.4$, the production term becomes negative and the convection term becomes positive. This is due to the formation of the expansion region in the boundary layer that causes a local flow acceleration and the energy transfer from the turbulent field to the mean field (This explains the sharp drop in TKE in Fig. 1.24(a)). The pressure dilatation term is both negative and positive in the interaction region. The negative values of Π_d (which indicates a loss in turbulent kinetic energy and gain in mean internal energy in this region) occur near the foot of the incident shock while positive values occur around the expansion fan region (which indicates a loss of energy from the mean internal energy to the turbulent field). Hence, the compressibility effects are confined only to a small part of the interaction region. Similar to the pressure dilatation term, the pressure transport term is also significant in the expansion and compression regions of the interaction zone. As we go downstream of the interaction zone, production is once again balanced by turbulent transport and viscous dissipation.

The streamwise evolution of various terms in the TKE transport equation along the locus

of maximum TKE (which in the interaction region would approximately correspond to the centerline of the mixing layer) exhibit behavior similar to that along the mean sonic line except for the pressure-dilation term whose contribution was found to be negligible along the locus of maximum TKE.

The viscous dissipation term in the TKE equation can be decomposed into solenoidal (ϵ_s) , dilatation (ϵ_d) and inhomogeneous components (ϵ_I) .

$$\epsilon = \epsilon_s + \epsilon_d + \epsilon_I \tag{1.21}$$

where

$$\begin{aligned} \epsilon_s &= \langle \mu \rangle \langle \omega'_i \omega'_i \rangle \\ \epsilon_d &= \frac{4}{3} \langle \mu \rangle \langle \frac{\partial u'_k}{\partial x_k} \frac{\partial u'_l}{\partial x_l} \rangle \\ \epsilon_I &= 2 \langle \mu \rangle \left[\frac{\partial^2 \langle u'_i u'_j \rangle}{\partial x_i x_j} - 2 \frac{\partial}{\partial x_i} \langle u'_i \frac{\partial u'_j}{\partial x_j} \rangle \right] \end{aligned}$$

Figure 1.25 shows the streamwise variation of viscous dissipation and its components along the mean sonic line. As evident from the figure, the solenoidal part is the most significant component of the three. Similar to the pressure-dilatation term in the TKE equation, the dilatational dissipation is only noticeable in the interaction region. From Fig. 1.25, we also see that the solenoidal dissipation, and the total dissipation, increases across the interaction region which suggests the amplification of vorticity variance or enstrophy across the interaction region. The effect of shock on various terms in the enstrophy equation are discussed in the next section.



Figure 1.25: Evolution of dissipation term and its components along the mean sonic line.

1.3.8 Enstrophy budget

The transport equation for enstrophy $(\Omega = 1/2 \langle \omega'_i \omega'_i \rangle)$ is given below.

$$\underbrace{\langle u_{j} \rangle \frac{\partial \Omega}{\partial x_{j}}}_{I} = \underbrace{\langle \omega_{i}' \omega_{j}' \rangle \frac{\partial \langle u_{i} \rangle}{\partial x_{j}}}_{II} + \underbrace{\langle \omega_{i}' \omega_{j}' \frac{\partial u_{i}'}{\partial x_{j}} \rangle}_{III} - \underbrace{\Omega \frac{\partial \langle u_{k} \rangle}{\partial x_{k}}}_{IV} - \underbrace{\Omega \frac{\partial \langle u_{k} \rangle}{\partial x_{k}}}_{IV} - \underbrace{\langle \Omega \frac{\partial u_{k}'}{\partial x_{k}} \rangle}_{VI} + \underbrace{\varepsilon_{ijk} \langle \omega_{i}' \frac{\partial \rho}{\partial x_{j}} \frac{\partial \rho}{\partial x_{j}} \frac{\partial \rho}{\partial x_{j}}}_{VII} + \underbrace{\varepsilon_{ijk} \langle \omega_{i}' \frac{\partial \rho}{\partial x_{j}} \left[\frac{1}{\rho} \frac{\partial \sigma_{kq}}{\partial x_{q}} \right] \rangle}_{VII} - \underbrace{\langle \Omega u_{j}' \rangle}_{VI} - \underbrace{\langle \omega_{i}' u_{j}' \rangle \frac{\partial \langle \omega_{i} \rangle}{\partial x_{j}}}_{IX} + \underbrace{\langle \omega_{j} \rangle \langle \omega_{i}' \frac{\partial u_{i}'}{\partial x_{j}} \rangle}_{X} - \underbrace{\langle \omega_{i} \rangle \langle \omega_{i}' \frac{\partial u_{k}'}{\partial x_{k}} \rangle}_{XI}$$

$$(1.22)$$

In this equation, term I represents the convection term, term II is the production/destruction of enstrophy due to the mean velocity gradient, term III is the self-stretching due to the

Term	Color	Line style
I	black	dotted
II	black	dash-dot
III	black	solid
VII	black	dashed
X	black	solid with open triangles

Table 1.5: Legend and colors for enstrophy budget plots.

fluctuating vorticity field, term IV is the vorticity-mean dilatation, term V is the vorticityfluctuating dilatation, term VI represents the generation of vorticity due to baroclinic torques, term VII is the viscous diffusion term, term VIII is the turbulent transport term, term IX is the production of enstrophy due to mean vorticity field, term X is associated with the interaction of the fluctuating stretching term ($\omega'_i \nabla u'_i$) with the mean vorticity and term XI represents the interaction of the mean vorticity with the stretching term associated with the dilatation term.

Not all terms are important in the enstrophy transport equation before, within and after the interaction zone. In Fig. 1.26, we show the dominant terms in the enstrophy transport equation at $X^* = -1.1$. The legend for the enstrophy budget plots is given in Table 1.5. Near the wall, terms III and X have positive contributions to the enstrophy budget and they are balanced by terms II and VII. As we go away from the wall, the stretching term (X) becomes zero and the production term (II) becomes positive to compensate for the stretching term (X).

In the interaction region at $X^* = -0.5$ (Fig. 1.27), the two most dominant terms are the self-stretching term (III) and the viscous dissipation term (VII) and they balance each others effects. The increase of enstrophy (and viscous dissipation in the TKE equation)



Figure 1.26: Enstrophy budget for Case II at $X^* = -1.1$.

in the interaction region is primarily due to the stretching term (III). There is a small contribution from the convection term (I) and as the shock strength increases, the production term (II) becomes less significant. At $X^* = 0.25$ (Fig. 1.28), the stretching term (X) and the production term (II) again become significant near the wall with varying degrees of contributions for different shock intensities. The convection term (I) becomes negligible at this location. As we go further downstream to $X^* = 1.5$ (Fig. 1.29), where the boundary layer is in the process of reaching an equilibrium state once again, the dominant terms in the enstrophy transport equation show behavior similar to the one observed at $X^* = -1.1$. Again, terms III and X have positive contributions to the enstrophy evolution near the wall and are balanced by terms II and VII. The contribution of the baroclinic term (VI) was found to be negligible at all the selected streamwise locations. Similar to the pressure-dilatation term (II) in the transport equation for the turbulent kinetic energy, the baroclinic term (VI) is also associated with the effects of compressibility.



(b)

Figure 1.27: Enstrophy budgets at $X^* = -0.5$. (a) Case II, (b) Case III.



Figure 1.28: Enstrophy budgets at $X^* = 0.25$. (a) Case II, (b) Case III.



Figure 1.29: Enstrophy budgets at $X^* = 1.5$. (a) Case II, (b) Case III.

1.4 Summary and Conclusions

Direct numerical simulations are carried out for shock waves of different intensities interacting with a Mach 2.75 flat-plate turbulent boundary layer. The numerical method used for discretizing the Euler terms is based on a hybrid strategy that uses a sixth-order, non-dissipative central-differencing scheme in the shock-free regions and a robust fifth-order monotonicity preserving scheme in the regions around the shock. The accuracy of DNS calculations are verified by comparing the incoming boundary layer statistics with the published literature and also by checking the balance of all the terms in the turbulent kinetic energy transport equation.

Visualizations of instantaneous flow velocity and temperature in the planes parallel to the wall clearly indicate the significant and complex effects of shock on the turbulence structure. As expected, the flow downstream of the shock becomes more chaotic with a fine-grained structure and the mixing is also enhanced. The change of length scales downstream of the shock is very significant from a numerical perspective since it places additional constraints on the downstream grid and also the dissipative properties of the numerical scheme. The anti-correlation between velocity and temperature fields are found to be reduced across the interaction region indicating a breakdown of the strong Reynolds analogy. The differences between Reynolds- and Favre-averaged velocities are more significant than those for temperature but are only important near the wall and in the interaction region, as reflected in the skin-friction coefficient computations. The increase in shock intensity does not appear to increase the differences between Reynolds- and Favre-averaging.

As expected, the separation region grows with increasing shock intensity due to an increased adverse pressure gradient. Instantaneous flow reversal analysis indicate that the flow reversals are highly unsteady and three dimensional. The effect of shock strength on the boundary layer interaction is clearly visible in the flow reversal comparisons. However, the maximum probability of flow reversal does not increase with increasing shock intensity, an observation also made in the LES studies by Morgan et al. [7]. The length of interaction regions computed from the present DNS calculations show very good agreement with experimental results (Fig. 7 in Ref. [4]). The wall pressure fluctuations measured by the r.m.s. of pressure show a reasonable collapse downstream of the interaction region when normalized by mean wall-pressure and plotted against the non-dimensional streamwise coordinate, X^* . The fluctuations of thermodynamic properties are intensified in the interaction region with pressure showing the largest amplification in the interaction region.

The turbulent kinetic energy (TKE) budgets are examined for a better understanding of shock effects on turbulence. Various terms in the TKE equation showed similar behavior for different shock intensities when measured at the same non-dimensional streamwise locations, X^* . The streamwise evolution of TKE and terms contributing to its evolution are also examined along the mean sonic line. The increase in TKE in the interaction region is primarily due to an increase in the production term. The production term is found to be negative in the expansion fan region after the impinging shock, indicating a loss of energy from the turbulence to the mean flow. This effect is stronger for higher shock intensities. The pressure dilatation term and the dilatational dissipation are found to be significant only in the regions surrounding the shock. The pressure dilatation term is negative near the foot of the reflected shock which indicates an energy transfer from turbulence to the mean internal energy. In the expansion fan region, the pressure dilatation is positive and responsible for a net energy transfer from mean internal energy to the turbulence. All these indicate a strong and dynamic coupling exists between the turbulent and mean fields in
the interaction region with energy being continuously exchanged between the two fields. Despite the relatively high values of incoming Mach number and interacting shocks, the compressibility-related terms like the pressure dilatation term are found to be negligible in the TKE equation in most of the flow regions although the turbulent Mach number exceeded 0.3, a conventional threshold for the turbulent compressibility effects to become important. Examination of the enstrophy budgets also revealed that the baroclinic term, a term associated with compressibility effects, was negligible even for the highest shock intensity. The vortex stretching term in the enstrophy transport equation is found to be primarily responsible for the net increase in enstrophy in the shock-turbulence interaction region.

Chapter 2

A Priori Analysis of Subgrid-Scale Turbulence for Shock-Boundary Layer Interactions

2.1 Introduction

Large-eddy simulations (LES) are becoming increasingly popular for high speed flow computations due to the current restrictions on performing direct numerical simulations (DNS) and the short-comings of Reynolds-averaged Navier-Stokes simulations (RANS). In LES, only the large scales in the flow are explicitly computed and the small scales are modeled using a subgrid-scale (SGS) model. Unlike the turbulence models used in RANS, which are mostly of the two-equation type, the commonly used subgrid-scale (SGS) models for LES are the zero-equation eddy-viscosity type models. These models, despite their simplicity, may still perform well because they model only the small (or unresolved) scales which are generally more homogeneous than the large turbulent scales.

Shock-boundary layer interaction (SBLI) is becoming a benchmark problem in the highspeed flow modeling community due to its unique characteristics. Firstly, the setup for SBLI flow is simple enough for DNS and LES but it is of great practical significance. Secondly,

the interaction of shock with the boundary layer is very complex and requires high-fidelity numerical methods like DNS and LES to correctly capture the flow physics. With the obvious limitations of DNS, the focus is on LES to provide a reasonably accurate description of the flow. The development of models for LES of high speed (supersonic) flows, including SBLI, is a continuing research. There have been several LES computations of SBLIs. Garnier et al. [33] were the first to conduct LES of SBLI for a flow Mach number of 2.3 and a flow deflection angle of $\theta = 8^{\circ}$. Their LES results were in good agreement with the available experimental data. Using the mixed time scale SGS closure, Touber and Sandham [34] were able to reproduce the experimentally-observed characteristic frequency of the reflected shock system. In another separate LES study [6], they compared their LES results with those from three different experimental configurations. Pirozzoli et al. [35] examined the capabilities of LES and RANS models to predict unsteady flow characteristics of SBLI. Jammalamadaka et al. [16] evaluated the performances of several SGS models for the problem of SBLI by comparing DNS and LES results and found that dynamic similarity-type models gave good predictions. LES has also been used to study SBLI in compression corners. [36, 37]

In LES of incompressible flows, the only terms requiring models are the SGS stresses which appear in the filtered momentum equations. Several types of models are employed for the SGS stresses in incompressible flows, the most common being the zero-equation eddyviscosity type models. These models have also been used for modeling the SGS stresses in compressible flows with varying degrees of success. However, in LES of compressible flows, in addition to SGS terms in the filtered momentum equations, there are several terms in the filtered energy equation which also require modeling. The modeling of SGS terms in the energy equation has been a bit of a grey area for LES of compressible flows where some terms are modeled while the others are neglected. There have been some studies that examined the behavior of SGS terms in the filtered energy equation but these studies have been limited to relatively simple subsonic flows [38, 39]. In complex flows like SBLI that involve both shock and turbulence, the behavior of SGS terms in the LES equations is largely unexplored. The main objective of the present study is to examine the behavior of various SGS terms appearing in the compressible filtered Navier-Stokes equations for SBLIs. This is primarily done through *a priroi* analysis of DNS data for SBLI [40]. The description of the DNS database is described in the next section. The contribution of various components of SGS fluxes in various regions of the flow is examined. We also examine the budgets for SGS kinetic energy to study the effect of shock on subgrid-level turbulence and with the aim of providing useful information for one-equation SGS LES models. To the authors' knowledge, this is the first comprehensive attempt to examine the behavior of SGS correlations/terms in supersonic flows of the type seen in SBLIs.

2.2 DNS data

This study is based on *a priori* analysis of DNS data we have recently generated for SBLI [40]. The setup for the DNS of SBLI was a typical impinging oblique shock interacting with a zero-pressure gradient turbulent boundary layer developing on a flat plate. The DNS computations were performed for three different shock intensities to examine the effect of shock intensity on SBLI. The incoming freestream Mach number for the turbulent boundary layer was 2.75 and the flow deflection angles for impinging oblique shock were $\theta = 6^{\circ}$, 7.75° and 9.25°. For the selected flow deflection angles, all three cases exhibited mean flow separation. It was also shown in the DNS study [40] that the shock wave significantly affects the mean and turbulent quantities and these effects were amplified for higher shock intensities. With these results in view, we can expect the shock to have a similar effect on various SGS terms.

The computational algorithm used for generating the DNS data was based on a hybrid methodology. Hybrid numerical methodologies are popular for shock/turbulence simulations. In regions away from the shock, we used a minimally dissipative central scheme [9] to compute the Euler terms in the Navier-Stokes equations. For enhanced numerical stability and accuracy, the Euler terms were cast in a split-form [41, 9]. Interested readers are referred to Refs. [9, 41] for a detailed description of the method. In regions surrounding the shock, a fifth-order monotonicity-preserving (MP) scheme [10, 11] was used. Taking advantage of the hyperbolic nature of the Euler terms, and also for improved numerical stability, the fluxes were computed in the characteristic space and then transformed back to the physical space. The flux-splitting in characteristic space was done using Lax-Friedrich's method. Details on characteristic transformation can be found in Refs. [42, 43, 11]. The MP scheme has proven to be very robust for a wide variety of problems involving discontinuities like shocks and also has lesser numerical dissipation in comparison to the standard WENO scheme [44]. However, for the present DNS setup, MP scheme alone was not sufficient to resolve all scales in the flow. The switch between the central scheme and MP scheme was made using a dilatationbased shock sensor [8]. More details on the hybridization can be found in Refs. [21, 8]. The diffusive terms of the Navier-Stokes equations were computed using sixth-order compact central schemes [20]. The diffusive terms were cast in a non-conservative form [22] for enhanced numerical stability and also to ensure finite molecular dissipation at all wavelengths. In our experience, it is necessary to use the non-conservative form for the diffusive terms when the Euler terms are cast in a split form and computed using very low dissipation central schemes. Otherwise, unphysical oscillations appear in the solution, particularly in regions close to the wall.

While the details of the DNS can be found in Ref. [40], some computational details are given here for a better understanding of the results presented in this paper. The grid spacings in wall-units for DNS of SBLI were as follows: in the streamwise direction, $\Delta x^+ = 4.1$ for $\theta = 6^{\circ}$ and $\Delta x^+ = 3.45$ for $\theta = 7.75^{\circ}$ and 9.25° . In the homogeneous spanwise direction, $\Delta z^+ = 3.45$. The grid was clustered near the wall and the node immediately next to the wall was located at a distance of $\Delta y^+ \approx 0.6$. For the incoming boundary layer, Reynolds number based on the momentum thickness and freestream quantities was 2070. The accuracy of the incoming boundary layer statistics was verified by comparing them against results published in the literature [1]. However, the accuracy of incoming boundary layer characteristics does not necessarily guarantee the accuracy of solution in the interaction region and regions downstream. In the absence of any experimental data, the accuracy of DNS calculations in these regions was verified by grid-sensitivity assessment and by checking the sum of all terms in the turbulent kinetic energy (TKE) equation. An accurate and converged solution would result in a near zero sum of all the contributing terms in the TKE equation. For the DNS calculations, the sum was indeed found to be negligible compared to the leading order terms in the TKE equation in all the flow regions. In our opinion, this is a better way to ensure numerical accuracy for DNS of turbulent flows when compared to the standard practice of conducting grid refinement studies. Our studies showed that carrying grid refinement studies with MP scheme (which is based on an upwind scheme) alone gave converged results for various second-order statistics at $\Delta x^+ = \Delta z^+ = 4.1$, but the contributing terms in the turbulent kinetic energy equation were not found to be in full balance, even after further refinement of the grid, possibly because of the numerical dissipation of the scheme. Although increasing the grid resolution would theoretically increase our ability to capture smallest scales in the flow, the numerical dissipation of the scheme may prevent us from doing so. The hybrid method employed here [40] generated fully accurate data in all flow regions with the selected grids.

2.3 Results

The results presented in this section are obtained from either using a single realization of instantaneous filtered DNS data or an ensemble average of the data. For ensemble averaging, averages were taken in time and homogeneous spanwise direction. The duration for temporal averaging was $T \approx 15\delta/U_{\infty}$, with δ being the boundary layer thickness of the incoming boundary layer and U_{∞} the free stream velocity. The primary motivation to do ensemble averaging was to reduce the numerical noise in the results for a better interpretation. We stress that we were not looking to obtain fully converged statistics at low frequencies, which would need much longer integration.

One of the parameters studied in this paper is the filter width. Three different filter widths are considered: $\overline{\Delta} = 4\Delta_{DNS}$, $\overline{\Delta} = 8\Delta_{DNS}$ and $\overline{\Delta} = 16\Delta_{DNS}$, where $\overline{\Delta}$ is the characteristic size of the filter and Δ_{DNS} is the characteristic size of the DNS grid. In this study, filtering operations were performed mostly in the streamwise (x) and spanwise (z) directions where the grid was uniform. Filtering in the wall-normal (y) direction was avoided because of the complexities associated with filtering on non-uniform grids. It should be noted that this is a standard practice for wall-bounded flows. Filtering was performed in the physical space using a top-hat filter with the filtered variable, ϕ , obtained using the relation:

$$\overline{\phi} = \frac{1}{\overline{\Delta}} \int_{-\overline{\Delta}/2}^{\overline{\Delta}/2} \phi \mathrm{d}\xi \tag{2.1}$$

The integral was evaluated using the trapezoidal rule and the resulting 1-D discrete filter is given by: l=N/2

$$\overline{\phi}_i = \sum_{l=-N/2}^{l=N/2} a_l \phi_{i+l} \tag{2.2}$$

where the coefficients a_l are the corresponding coefficients of the trapezoidal rule and N = 4, 8 and 16 for $\overline{\Delta} = 4\Delta_{DNS}$, $8\Delta_{DNS}$ and $16\Delta_{DNS}$, respectively. Multi-dimensional filtering was performed by applying the above 1-D filter consecutively in each direction. For LES of compressible flows, it is customary to use a Favre-filtered variable, ϕ , which is given by $\tilde{\phi} = \overline{\rho \phi}/\overline{\rho}$.

Since the simulated SBLI has two inhomogeneous directions (x and y), various SGS terms are compared along the wall-normal direction at selected streamwise locations. The streamwise stations were located at $X^* = -1.1$, -0.5, 0.25 and 1.5. Here, X^* is the nondimensional streamwise coordinate defined as $X^* = (x - X_I)/L$, where X_I is the nominal shock impingement location and L is the length of the interaction region, defined as the distance between the nominal shock impingement location and the extrapolated wall-location of the reflected shock. The interaction region is then defined as the region between $-1 \leq X^* \leq 0$. Hence, $X^* = -1.1$ would correspond to the the incoming (pre-shock) boundary layer, $X^* = -0.5$ is located in the middle of the interaction region and $X^* = 0.25$ and 1.5 are located downstream of the interaction region.

2.3.1 SGS terms in the filtered momentum equation

There are no unclosed terms in the filtered continuity equation when Favre-filtering is used.

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_j} \left(\overline{\rho} \widetilde{u}_j \right) = 0 \tag{2.3}$$

However, unclosed terms appear in the filtered momentum equation which require modeling. The filtered momentum equation is obtained by applying the filtering operator to the compressible Navier-Stokes equations. The dimensionless form is given by:

$$\frac{\partial}{\partial t} \left(\overline{\rho} \widetilde{u}_{i} \right) + \frac{\partial}{\partial x_{j}} \left(\overline{\rho} \widetilde{u}_{i} \widetilde{u}_{j} \right) + \frac{\partial \overline{p}}{\partial x_{i}} = \frac{\partial \widetilde{\sigma}_{ij}}{\partial x_{j}} - \frac{\partial \tau_{ij}}{\partial x_{j}} + \frac{\partial}{\partial x_{j}} \left(\overline{\sigma}_{ij} - \widetilde{\sigma}_{ij} \right),$$

$$\tau_{ij} = \overline{\rho} \left(\widetilde{u}_{i} \widetilde{u}_{j} - \widetilde{u}_{i} \widetilde{u}_{j} \right) \\
\widetilde{\sigma}_{ij} = \frac{2\mu(\widetilde{T})}{\operatorname{Re}} \left[\frac{1}{2} \left(\frac{\partial \widetilde{u}_{i}}{\partial x_{j}} + \frac{\partial \widetilde{u}_{j}}{\partial x_{i}} \right) - \frac{1}{3} \frac{\partial \widetilde{u}_{k}}{\partial x_{k}} \delta_{ij} \right] \\
\overline{\sigma}_{ij} = \frac{2\mu(T)}{\operatorname{Re}} \left[\frac{1}{2} \left(\frac{\partial u_{i}}{\partial x_{j}} + \frac{\partial u_{j}}{\partial x_{i}} \right) - \frac{1}{3} \frac{\partial u_{k}}{\partial x_{k}} \delta_{ij} \right]$$

$$(2.4)$$

where μ is the dynamic viscosity of the fluid and Re is the reference Reynolds number. The tilde denotes Favre-filtered value, $\tilde{\phi} = \overline{\rho\phi}/\overline{\rho}$. The last term in Eq. (3.9) is due to the nonlinearities and differences in Favre and regular filtering operations. This term was found to be negligible by Vreman et al. [38] and also in the present study. Like in low-speed flows, the most important unclosed term in the momentum equation is the SGS stress, τ_{ij} . The profiles of τ_{ij} at various streamwise locations are shown in Fig. 2.1 and Fig. 2.2. The results are shown only for $\theta = 7.75^o$ and $\overline{\Delta} = 8\Delta_{DNS}$ since similar trends are observed for other shock intensities and filter widths. In all figures, the wall-normal coordinate (y) is normalized by the incoming boundary layer thickness (δ_0) . At $X^* = -1.1$, the profiles look very similar to the turbulent Reynolds stresses with τ_{11} being the dominant stress. Similar to the turbulent Reynolds stresses, peaks for various SGS stresses occur close to the wall and are unaffected by the shock at this streamwise location. In the interaction region at $X^* = -0.5$, however, the effect of shock is significant on the SGS stresses. All the SGS stress components are amplified and their peaks move away from the wall into the mixing layer developing over the separation bubble. This trend is once again similar to that seen for the turbulent Reynolds stresses. At $X^* = 0.25$, all the three normal SGS stress components exhibit very similar peak values. While the peak value for τ_{11} decreases in magnitude from $X^* = -0.5$ to $X^* = 0.25$, those for τ_{22} and τ_{33} are increased between these two locations. The shock appears to have made the subgrid-level turbulence more isotropic at this location. The reason for this behavior is discussed in a later section where the transport equations for normal SGS stress are examined. At $X^* = 1.5$, the peak value for τ_{11} shifts back to the near wall region, but those for τ_{22} and τ_{33} are still located away from the wall. Hence, we see a very complex behavior exhibited by various components of the SGS stress tensor.

The effect of shock strength on SGS stresses can be better understood by looking at the PDFs of different stress components. The PDFs were obtained using a single realization of the filtered DNS data in the regions between $5.0 \le x \le 20.0, 0.0 \le y \le 1.0$ and $0.0 \le z \le 3.5$. Figure 2.3 shows the PDFs for τ_{12} . It is clear that as the shock strength increases, the PDFs become wider, indicating the probability for large SGS stress values to occur in the flow is higher. Hence, for stronger shocks more energy is present at the subgrid level. This was also observed in the R.M.S. values of SGS stresses for different shock strengths. For the same filter width, the peak R.M.S. of SGS stresses were higher for stronger shocks in the interaction region and downstream of the shock.

The SGS stress, τ_{ij} , can be decomposed into generalized Leonard stress (L_{ij}) , Cross stress (C_{ij}) and Reynolds stress (R_{ij}) parts [45, 46].

$$\tau_{ij} = L_{ij} + C_{ij} + R_{ij} , \qquad (2.5)$$



Figure 2.1: SGS stresses at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$. Black solid line for τ_{11} , black dashed line for τ_{22} , black dash-dot line for τ_{33} , black dots for τ_{12} , red solid line for ksgs.



(b)

Figure 2.2: SGS stresses at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = 0.25$, (b) $X^* = 1.5$. Black solid line for τ_{11} , black dashed line for τ_{22} , black dash-dot line for τ_{33} , black dots for τ_{12} , red solid line for ksgs.



Figure 2.3: PDFs of τ_{12} SGS stresse as obtained from the instantaneous filtered DNS data for $\overline{\Delta} = 8\Delta_{DNS}$.

where

$$L_{ij} = \overline{\rho} \left(\widetilde{\widetilde{u}_i \widetilde{\widetilde{u}}_j} - \widetilde{\widetilde{u}}_i \widetilde{\widetilde{u}}_j \right)$$
$$C_{ij} = \overline{\rho} \left(\widetilde{u'_i \widetilde{u}_j} + \widetilde{\widetilde{u}_i u'_j} - \widetilde{u}'_i \widetilde{\widetilde{u}}_j - \widetilde{\widetilde{u}}_i \widetilde{u}'_j \right)$$
$$R_{ij} = \overline{\rho} \left(\widetilde{u'_i u'_j} - \widetilde{u}'_i \widetilde{u}'_j \right)$$

 L_{ij} is closed as it is represented by only the resolved variables. R_{ij} is only a function of unresolved components and C_{ij} is a function of both resolved and unresolved components. Hence, when it comes to modeling SGS stresses, the mixed-type models [46] are expected to perform better because they include the Leonard stress part in the model formulation.

The decomposition of τ_{11} stress for $\overline{\Delta} = 4\Delta_{DNS}$ are shown in Fig. 2.4. At all selected streamwise locations, L_{11} has the maximum contribution towards the total SGS stress. The contribution of R_{11} is the smallest at $X^* = -1.1$ but increases as we go to downstream stations. Since R_{11} is represented by only the unresolved scales, an increase in its value indicates generation of scales smaller than the characteristic filter width by the shock. However, the contribution of C_{11} remains largely unchanged through all the regions of the flow for filter width of the size $\overline{\Delta} = 4\Delta_{DNS}$. The shapes of all the individual components of the SGS stress are very similar to the total SGS stress. This suggests similar kind of models, say similarity-type model, can be used to model individual stress parts. The compressible serial decomposition model [16] is one such example. LES calculations with filter widths of the size $\overline{\Delta} = 4\Delta_{DNS}$ can be termed as "fine-scale" LES. The LES studies in Refs. [34, 6] are some examples of "fine-scale" LES.

The Leonard, Cross and Reynolds components of τ_{11} stress for $\overline{\Delta} = 8\Delta_{DNS}$ are shown in Fig. 2.5. Once again, at $X^* = -1.1$ and $X^* = -0.5$ (not shown), the Leonard stress component has the largest contribution. However, at $X^* = 0.25$, the Reynolds part of the total SGS stress has nearly the same contribution as the Leonard part. At $X^* = 1.5$, the contribution of R_{11} exceeds that of L_{11} . This once again highlights the effect shock has on the small scales in the flow and subsequently, the SGS stresses. For the filter width $\overline{\Delta} = 8\Delta_{DNS}$, accurate modeling of R_{ij} becomes important to correctly predict the behavior of SGS stresses, and consequently the flow. LES calculations conducted with filter widths of the size $\overline{\Delta} = 8\Delta_{DNS}$ can be termed as "coarse-scale" LES.

For very large filter widths of the size $\overline{\Delta} = 16\Delta_{DNS}$ (Fig. 2.6), a very significant part of turbulent scales are removed by the filtering operator. Hence, the unresolved scales



Figure 2.4: SGS stress decomposition at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 4\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$. Black solid line for τ_{11} , black dashed line for L_{11} , black dash-dot line for C_{11} , black dots for R_{11} .



Figure 2.5: SGS stress decomposition at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = 0.25$, (b) $X^* = 1.5$. Legend same as in Fig. 2.4.

represented by R_{ij} become very dominant in all the flow regions. At these filter widths, the LES can be termed as "very-large-scale" LES or VLES. No model currently exists to accurately capture the behavior of SGS stresses at such large filter widths. For even larger widths, we would be approaching the realm of RANS computations.

We have seen the effect of filter width on the behavior of individual parts of the SGS stress. It is evident that with change in filter width, different parts of the SGS stress become dominant in different regions of the flow. For example, for $\overline{\Delta} = 8\Delta_{DNS}$, the Leonard stress part is important mostly in the pre-shock region, while the Reynolds stress part is very important in the shock and post-shock regions. Clearly, choosing the SGS stress model for simulations of shock-turbulence interactions is not very straightforward and is dependent on the filter width and shock strength.

2.3.2 SGS terms in the filtered energy equation

The energy conservation for compressible flow simulations can be achieved by solving different forms of energy equations [47], e.g., the transport equation for internal energy, enthalpy or the total energy. However, for flows involving shocks, it is often better to use the conservative form of governing equations which makes the total energy equation an appropriate choice. The filtered equation for total energy is obtained by applying the filtering operator to the exact (DNS) total energy equation and subtracting the equation for SGS kinetic energy from it [38]. The dimensionless form of the filtered total energy equation is given by:

$$\frac{\partial \widetilde{E}}{\partial t} + \frac{\partial}{\partial x_j} \left(\widetilde{E} + \overline{p} \right) \widetilde{u}_j = \frac{\partial}{\partial x_j} \left(\widetilde{\sigma}_{ij} \widetilde{u}_i \right) - \frac{\partial \widetilde{Q}_j}{\partial x_j} - B_1 - B_2 - B_3 + B_4 + B_5 + B_6 - B_7, \quad (2.6)$$



Figure 2.6: SGS stress decomposition at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 16\Delta_{DNS}$. (a) $X^* = -0.5$, (b) $X^* = 0.25$. Legend same as in Fig. 2.4.

where

$$\widetilde{E} = \frac{\overline{p}}{\gamma - 1} + \frac{1}{2} \overline{\rho} \widetilde{u}_{i} \widetilde{u}_{i}$$

$$Q_{j} = \frac{-\mu}{(\gamma - 1) \text{RePr} M_{\infty}^{2}} \frac{\partial T}{\partial x_{j}}$$

$$B_{1} = \frac{1}{\gamma - 1} \frac{\partial}{\partial x_{j}} (\overline{pu_{j}} - \overline{p} \widetilde{u}_{j})$$

$$B_{2} = \overline{p} \frac{\partial u_{k}}{\partial x_{k}} - \overline{p} \frac{\partial \widetilde{u}_{k}}{\partial x_{k}}$$

$$B_{3} = \frac{\partial}{\partial x_{j}} (\tau_{kj} \widetilde{u}_{k})$$

$$B_{4} = \tau_{kj} \frac{\partial \widetilde{u}_{k}}{\partial x_{j}}$$

$$B_{5} = \overline{\sigma_{kj}} \frac{\partial u_{k}}{\partial x_{j}} - \widetilde{\sigma}_{kj} \frac{\partial \widetilde{u}_{k}}{\partial x_{j}}$$

$$B_{6} = \frac{\partial}{\partial x_{j}} (\overline{\sigma}_{ij} \widetilde{u}_{i} - \widetilde{\sigma}_{ij} \widetilde{u}_{i})$$

$$B_{7} = \frac{\partial}{\partial x_{j}} (\overline{Q}_{j} - \widetilde{Q}_{j})$$

The term B_1 in Eq. (3.10) is proportional to the divergence of SGS heat flux term (when pressure is replaced by density and temperature using the equation of state), B_2 is the pressure-dilatation term, B_3 is the SGS transport term, B_4 is the SGS production (or sometimes also referred to as the SGS dissipation) and B_5 is the SGS contribution to the molecular dissipation. Terms B_6 and B_7 arise due to the differences between Favre and regular filtering operations and were found to be negligible in the present study.

The modeling of B_1 can be based on a similarity-type closure,

$$B_1 = \frac{1}{\gamma(\gamma - 1)M_{\infty}^2} \frac{\partial}{\partial x_j} \left[\overline{\rho} \left(\widetilde{\widetilde{u}_j \widetilde{T}} - \widetilde{\widetilde{u}}_j \widetilde{\widetilde{T}} \right) \right]$$
(2.7)

or a gradient-diffusion type closure,

$$B_1 = -\frac{\partial}{\partial x_j} \left(\frac{\overline{\rho}\nu_t}{\gamma(\gamma - 1)Pr_t M_\infty^2} \frac{\partial \widetilde{T}}{\partial x_j} \right)$$
(2.8)

where γ is the ratio of specific heats, Pr_t is the SGS turbulent Prandtl number and ν_t is the SGS eddy-viscosity. The model for the pressure-dilatation term, B_2 , is often neglected in many practical LES computations. Vreman et al. [48] proposed a similarity model for this term as:

$$B_2 = C_{\pi} \left[\overline{\overline{p}_{ij}} \frac{\partial \widetilde{u}_i}{\partial x_j} - \overline{\overline{p}_{ij}} \frac{\partial \widetilde{\widetilde{u}}_i}{\partial x_j} \right]$$
(2.9)

The SGS terms B_3 and B_4 are computed directly using the model for τ_{ij} . For modeling the dissipation term, B_5 , Vreman et al. [48] proposed several different types of models:

$$B_5^{(1)} = C_1 \left[\overline{\widetilde{\sigma}_{ij} \frac{\partial \widetilde{u}_i}{\partial x_j}} - \overline{\widetilde{\sigma}}_{ij} \frac{\partial \widetilde{\widetilde{u}}_i}{\partial x_j} \right] , \qquad (2.10)$$

$$B_5^{(2)} = C_2 \overline{\rho} \frac{k^{3/2}}{\Delta} \quad , k = \left(\widetilde{\widetilde{u}_i \widetilde{u}_i} - \widetilde{\widetilde{u}_i} \widetilde{\widetilde{u}_i}\right)/2 \; , \tag{2.11}$$

$$B_5^{(3)} = C_3 \overline{\rho} \frac{k^{3/2}}{\Delta} \quad , k = \sqrt{3/4} \nu_t |\tilde{S}|$$
 (2.12)

where k is the modeled SGS kinetic energy. The first model is based on the similarity idea and the last two are based on the concept of balancing the production and dissipation of SGS kinetic energy.

The object of discussion here is not to make an appraisal of different SGS models but to give a quantitative estimate of each SGS term in Eq. 3.10 using the DNS data. In Fig. 2.7 we show various SGS terms in the filtered total energy equation at different streamwise locations for $\theta = 7.75^{\circ}$ and $\overline{\Delta} = 8\Delta_{DNS}$. The trends are similar for other shock intensities

Term	Color	Line style
$B_1 \\ B_2 \\ B_3 \\ B_4 \\ B_5$	black black black black blue	solid dashed dash-dot dotted solid

Table 2.1: Color and legend for filtered total energy plots.

and filter widths. The divergence of filtered molecular heat flux $(\partial \tilde{Q}_j / \partial x_j)$ is also plotted in Fig. 2.7 for showing the relative importance of each SGS term. The choice of $\partial \tilde{Q}_j / \partial x_j$ as the reference is arbitrary. The net contribution by all SGS terms in the filtered energy equation is shown by the dotted red line. This would signify the importance of modeling the terms in the filtered total energy equation.

At $X^* = -1.1$, the two dominant terms are B_1 and B_3 which have opposite signs. The net contribution by B_1 , B_2 , B_3 , B_4 , and B_5 is very small compared to $\partial \tilde{Q}_j / \partial x_j$. This suggested that for the incoming boundary layer which is a supersonic canonical turbulent boundary layer, the modeling of B_1 , B_2 , B_3 , B_4 , and B_5 terms in the total energy equation can be ignored. This is confirmed in our *a posteriori* tests which will be discussed later.

At $X^* = -0.5$, which is located in the middle of the interaction region, the peak values of most terms are comparable to that of $\partial \tilde{Q}_j / \partial x_j$. The values of SGS molecular dissipation (B_5) and the SGS production terms (B_4) increase in the interaction region, which is an effect of shock interacting with the subgrid-level turbulence. The overall contribution of all the SGS terms has some significance in the inner and outer part of the boundary layer. The net contribution follows the trend of B_5 near the wall and in the outer layer, its peak is



(a)



Figure 2.7: Various SGS terms in the filtered total energy equation at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$. See Table. 2.1 for legend.

comparable to B_1 . At $X^* = 0.25$ and $X^* = 1.5$ (not shown), the net contribution of SGS terms, B_1 , B_2 , B_3 , B_4 , and B_5 , is negligible in the outer part of the boundary layer and is only significant near the wall. Hence, the shock affects each SGS term differently in different flow regions, which is shown by the relative importance of the net contribution of B_1 , B_2 , B_3 , B_4 , and B_5 in different flow regions.

To assess the importance of modeling SGS terms in the total energy equation in practical LES calculations, we carried out two different *a posteriori* tests: one in which no models for SGS terms in the filtered total energy equation were used (LES1) and in the other, models for B_1 , B_3 , B_4 and B_5 were implemented in the LES calculations (LES2). In LES2, the similarity model for the pressure-dilatation term (B_2) given by Eq. (2.9) caused numerical instability and, therefore, was not used. For the term B_1 , the gradient-diffusion model (Eq. (3.24)) is used and B_5 was modeled using Eq. (2.11). To model the SGS stresses in momentum equations, the mixed-time scale model [34] was used. This model has yielded acceptable results for LES of SBLI and is also relatively inexpensive when compared to the dynamic Smagorinsky model or the dynamic mixed model. A posteriori tests were performed for two different shock intensities, $\theta = 7.75^{\circ}$ and $\theta = 9.25^{\circ}$. The LES grid was four times coarser than the DNS grid in the x and z directions. To avoid filtering in the wall-normal direction, the grid in this direction was kept the same as the DNS grid. The setup for LES calculations were similar to the one described in Ref. [16] where the inflow boundary condition for both LES and DNS were kept consistent.

In Fig. 2.8, we show the skin-friction predictions by the two LES calculations for $\theta = 7.75^{\circ}$. The result from filtered DNS is also shown for comparison. As evident from the figure, there is no significant effect of modeling the terms B_1 , B_3 , B_4 and B_5 in the energy equation except for small differences in the interaction region. It should be mentioned here that by



Figure 2.8: Skin-friction coefficient predictions as obtained from *a posteriori* LES calculations for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. Solid black line for filtered DNS, red dashed line for LES1, blue dash-dot line for LES2.

ignoring the model for B_5 , we observed some differences in C_f predictions between LES1 and LES2 downstream of the interaction region. Similar results were observed for $\theta = 9.25^{\circ}$.

Figure 2.9 shows the $\langle u'u' \rangle$ Reynolds stress profiles for $\theta = 7.75^{\circ}$ at $X^* = -1.1$ and -0.5. The modeling of (or the lack of) SGS terms in the total energy equation apparently has no significant effect on the Reynolds stress profiles at $X^* = -1.1$, as also observed in our *a priori* analysis. However, there are some differences between the LES calculations conducted with and without SGS models (LES1 and LES2) in the interaction region and downstream of the interaction region. In fact, modeling the SGS terms in the total filtered energy equation slightly deteriorates the results in these regions. This could be because the

model for the pressure-dilatation term (B_2) was ignored, and our *a priori* results indicated that this term is not negligible. The same behavior is also observed for the turbulent heat flux term, $\langle u'T' \rangle$, shown in Fig. 2.10. Evidently, LES calculations conducted with no models for B_1 , B_3 , B_4 and B_5 in the filtered total energy equation give better results than those conducted with some of these terms modeled.

The modeling of isotropic part of the SGS stress (τ_{kk}) is often neglected in LES of compressible flows. To assess the importance of this term, we also carried out LES simulations with and without models for τ_{kk} . In one simulation, τ_{kk} was assumed to be proportional to L_{kk} (similarity-type model) and in another simulation, it was neglected. The results obtained with the similarity model were similar to those obtained with no model for τ_{kk} .

2.3.3 Resolved and residual kinetic energies

The filtered kinetic energy can be decomposed into resolved kinetic energy (E_r) and residual or SGS kinetic energy (k_{sgs}) .

$$\frac{1}{2}\widetilde{u_i u_i} = \underbrace{\frac{1}{2}}_{E_r} \underbrace{\widetilde{u_i u_i}}_{k_{sqs}} + \underbrace{\frac{1}{2}}_{k_{sqs}} \underbrace{(\widetilde{u_i u_i} - \widetilde{u_i \widetilde{u_i}})}_{k_{sqs}}$$
(2.13)

The ratio $k_{sgs}/(k_{sgs} + E_r)$ provides us with the information on how much SGS energy is present in the flow in comparison to the total filtered kinetic energy. We have computed the ratio of $k_{sgs}/(k_{sgs} + E_r)$ from SBLI DNS data for $\theta = 7.75^o$ and different filter widths. The results for $\overline{\Delta} = 4\Delta_{DNS}$ at different streamwise locations are shown in Fig. 2.11. The cross symbol on the plots indicates the location of peak values of k_{sgs} . At $X^* = -1.1$, the contribution of k_{sgs} is only 2.5% near the wall and just 1% at the location of peak k_{sgs} . This



(a)



(b)

Figure 2.9: Turbulent Reynolds stress at different streamwise locations as obtained from *a* posteriori LES calculations for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$. Solid black line for filtered DNS, red dashed line for LES1, blue dash-dot line for LES2.



(a)



(b)

Figure 2.10: Turbulent heat flux at different streamwise locations as obtained from *a posteriori* LES calculations for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$. Legend same as in Fig. 2.9.

indicates that at pre-shock locations, the flow is over-resolved by LES with $\overline{\Delta} = 4\Delta_{DNS}$. At $X^* = -0.5$, the ratio increases to 15% near the wall and 5% near the maximum k_{sgs} location which are acceptable values for LES. In further downstream locations, the ratio drops again but is still higher than that of the incoming boundary layer values. With larger filter widths, the contribution of k_{sgs} to the total filtered kinetic energy increases as expected. For example, with $\overline{\Delta} = 8\Delta_{DNS}$ (Fig. 2.12), the ratio $k_{sgs}/(k_{sgs} + E_r)$ at the location of peak k_{sgs} increases from 2.5% to 12% as we go from $X^* = -1.1$ to -0.5. For $\overline{\Delta} = 16\Delta_{DNS}$ (Fig. 2.13), the contribution of k_{sgs} to the total filtered kinetic energy in the interaction region is as high as 60% near the wall. The results in Figs. 2.11, 2.12 and 2.13 elucidate the significant effect of shock on the distribution of SGS energy in different regions of the flow. Also note that these results were obtained using ensemble-averaged filtered DNS data. Instantaneous filtered DNS data can give even higher ratios. With such significant changes occurring in the distribution of SGS kinetic energy in the flow, it is important for an LES model to accurately predict the behavior of k_{sgs} .

The effect of shock strength on SGS kinetic energy is evident in the contours of $k_{sgs}/(k_{sgs}+E_r)$ in Fig. 2.14. The results are shown for $\overline{\Delta} = 8\Delta_{DNS}$. Note that the *y*-axis is in logarithmic scale for a better illustration of the near-wall results. As observed in Fig. 2.14, the maximum value for the ratio is approximately 0.4 in the interaction region for all three shock strengths (The slightly higher values predicted for $\theta = 6^{\circ}$ compared to $\theta = 7.75^{\circ}$ and $\theta = 9.25^{\circ}$ is possibly due to different grids used for cases with different shock angles). Hence, the filter width is a more important parameter than the shock strength for the SGS kinetic energy.

To better understand the behavior of SGS kinetic energy, we examine the transport equation k_{sgs} below. This would also provide useful information for the one-equation SGS



Figure 2.11: The ratio of SGS kinetic energy to the total kinetic energy $(k_{sgs}/(k_{sgs} + E_r))$ at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 4\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$.



Figure 2.12: $k_{sgs}/(k_{sgs} + E_r)$ at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^o$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$.



Figure 2.13: $k_{sgs}/(k_{sgs} + E_r)$ at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^o$ and $\overline{\Delta} = 16\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$.



Figure 2.14: $k_{sgs}/(k_{sgs} + E_r)$ as obtained from the filtered DNS data for different shock intensities with $\overline{\Delta} = 8\Delta_{DNS}$. (a) $\theta = 6^{\circ}$, (b) $\theta = 7.75^{\circ}$, (c) $\theta = 9.25^{\circ}$. The contours levels are uniformly spaced between 0 and 0.5. The figures are shown not to scale for clarity.

models which make use of k_{sgs} transport equation. The transport equation for the SGS kinetic energy is given by:

Term	Color	Line style
convection (I) turbulent transport (II) pressure-dilatation (III) pressure-transport (IV) viscous diffusion (V) viscous dissipation (VI) production (VII) SGS diffusion (VIII)	black red green blue black black blue green	solid solid transport dashed dash-dot dashed dashed

Table 2.2: Color and legend for k_{sgs} and normal SGS stress budget plots.

$$\frac{\partial \overline{\rho}k_{sgs}}{\partial t} + \underbrace{\frac{\partial}{\partial x_k} \overline{\rho} \widetilde{u}_k k_{sgs}}_{I} + \underbrace{\frac{1}{2} \frac{\partial}{\partial x_k} \left(\overline{\rho} \widetilde{u}_i \widetilde{u}_i \widetilde{u}_k - \overline{\rho} \widetilde{u}_i \widetilde{u}_i \widetilde{u}_k \right)}_{II} = \underbrace{\left(\underbrace{p \frac{\partial u_k}{\partial x_k} - \overline{p} \frac{\partial \widetilde{u}_k}{\partial x_k} \right)}_{III} - \underbrace{\frac{\partial}{\partial x_k} \left(\overline{p} \overline{u}_k - \overline{p} \widetilde{u}_k \right)}_{V} + \underbrace{\frac{\partial}{\partial x_k} \left(\overline{\sigma} \widetilde{u} \overline{k} \overline{u}_i - \widetilde{\sigma} \widetilde{u}_i \widetilde{u}_i \right)}_{V} - \underbrace{\left(\underbrace{\sigma} \widetilde{u} \widetilde{k} \frac{\partial u_i}{\partial x_k} - \widetilde{\sigma} \widetilde{u} \widetilde{k} \frac{\partial \widetilde{u}_i}{\partial x_k} \right)}_{VI} - \underbrace{\frac{\partial}{\nabla u_k} \widetilde{u} \widetilde{u} \widetilde{u} \widetilde{u}_k}_{VII} + \underbrace{\frac{\partial}{\partial x_k} \widetilde{u} \widetilde{u} \widetilde{u} \widetilde{u}_i}_{VIII} + \underbrace{\frac{\partial}{\partial x_k} \widetilde{u} \widetilde{u} \widetilde{u} \widetilde{u}_i}_{VIII} + \underbrace{\frac{\partial}{\partial x_k} \widetilde{u} \widetilde{u} \widetilde{u} \widetilde{u}_i}_{VIII} + \underbrace{\frac{\partial}{\partial x_k} \widetilde{u} \widetilde{u} \widetilde{u} \widetilde{u} \widetilde{u}_i}_{VIII} + \underbrace{\frac{\partial}{\partial x_k} \widetilde{u} \widetilde{u} \widetilde{u} \widetilde{u} \widetilde{u}}_{VIII} + \underbrace{\frac{\partial}{\partial x_k} \widetilde{u} \widetilde{u} \widetilde{u} \widetilde{u}}_{VIII} + \underbrace{\frac{\partial}{\partial x_k} \widetilde{u} \widetilde{u} \widetilde{u} \widetilde{u} \widetilde{u}}_{VIII} + \underbrace{\frac{\partial}{\partial x_k} \widetilde{u} \widetilde{u} \widetilde{u} \widetilde{u}}_{VIII} + \underbrace{\frac{\partial}{\partial x_k} \widetilde{u} \widetilde{u} \widetilde{u} \widetilde{u} \widetilde{u}}_{VIII} + \underbrace{\frac{\partial}{\partial x_k} \widetilde{u} \widetilde{u}}_{VIII} + \underbrace{\frac{\partial}{\partial x_k} \widetilde{u} \widetilde{u}}_{VIII} + \underbrace{\frac{\partial}{\partial x_k} \widetilde{u}}_{VII} + \underbrace{\frac{\partial}{\partial x_k} \widetilde{u}}_{VI} + \underbrace{\frac{\partial}{\partial x_k} \widetilde{u}}_{$$

In this equation, term I is the convection term, term II is the SGS turbulent transport/diffusion, term III is the pressure-dilatation, term IV is the pressure-velocity transport, term V is the viscous diffusion, term VI is the viscous dissipation, term VII is the SGS production (sometimes also referred to as SGS dissipation) and term VIII is the SGS diffusion. Notice that terms III, IV, VI, VII and VIII also appear in the filtered total energy equation (Eq. 3.10) simply because the transport equation for k_{sgs} is used to derive the filtered total energy equation. We once again use the filtered DNS results for $\theta = 7.75^{\circ}$ and $\overline{\Delta} = 8\Delta_{DNS}$ to study the behavior of each term in Eq. (2.14) at selected streamwise locations. The budget for k_{sgs} transport equation at various streamwise locations are shown in Fig. 2.15 and Fig. 2.16.

At $X^* = -1.1$, the two most dominant terms are the turbulent transport (II) and the SGS diffusion (VIII) terms and and as shown in Fig. 2.15 they cancel out each others contributions to the SGS kinetic energy. Knight et al. [49] proposed the following model for computing the turbulent transport term (II):

$$\frac{1}{2}\overline{\rho}\big(\widetilde{u_i u_i u_k} - \widetilde{u_i u_i}\widetilde{u_k}\big) \approx \widetilde{u}_i \tau_{ik} \tag{2.15}$$

which is exactly the same as the SGS diffusion term (VIII). Hence, in the fully developed supersonic boundary layers, terms II and VIII can be neglected together in the modeling of transport equation for k_{sgs} . The pressure-dilatation (III) is not negligible and has similar contribution as the pressure-velocity term (IV) but with an opposite sign. Hence these two terms also cancel out each others contributions for the incoming boundary layer. Near the wall, the viscous diffusion term (V) balances the contribution from the viscous dissipation (VI) term (similar to turbulent kinetic energy). The production (VII) term is responsible for the generation of k_{sgs} . A positive contribution from the production term implies energy transfer from the resolved kinetic energy (E_r) or resolved field to the SGS kinetic energy (k_{sgs}) or residual field (analogous to the energy transfer from mean and turbulent kinetic energy fields in RANS) which is known as forward-scatter. It is, however, possible for the energy to be transferred from the SGS/residual field to the resolved field, referred to as backscatter. Under such circumstances, there would be a net negative contribution from the production term (VII) to the k_{sgs} transport equation.



Figure 2.15: SGS kinetic energy (k_{sgs}) budget at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = -1.1$, (b) $X^* = -0.5$. See Table. 2.2 for legend.



(a)



Figure 2.16: SGS kinetic energy (k_{sgs}) budget at different streamwise locations as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. (a) $X^* = 0.25$, (b) $X^* = 1.5$. See Table. 2.2 for legend.
At $X^* = -0.5$ in the interaction region, all the contributing terms to the k_{sgs} are amplified in their magnitudes. The production term (VII) is the most dominant term in the interaction region which explains the increase in k_{sgs} in this region (Fig. ??). Once again, the turbulent transport (II) and the SGS diffusion (VIII) terms balance each other and hence can be ignored together in the modeling of k_{sgs} equation. The pressure-dilatation term (III) is significant near the wall, and unlike the incoming boundary layer at $X^* = -1.1$, where it is balanced by the pressure transport term (IV), the modeling of this term cannot be ignored in the interaction region. The viscous dissipation term is also significant near the wall, where it balances the contributions from pressure-dilatation (III) and the viscous-diffusion (VI), and also away from the wall where it balances the production (VII) term. Hence accurate modeling of this term is also important.

At $X^* = 0.25$, similar to $X^* = -0.5$, the terms which need modeling are the pressuredilatation (III), pressure-velocity (IV), viscous diffusion (V), viscous dissipation (VI) and the production (VII) term. The contribution from the pressure-dilatation term is comparable to the production term near the wall. At $X^* = 1.5$, the profiles of these two terms look similar to the profiles at $X^* = -1.1$. At all the selected streamwise locations, the turbulent transport (II) term and the SGS diffusion (VIII) term cancel each others contributions and hence have a net zero effect on k_{sgs} equation and can be ignored together.

Earlier we had shown the behavior of various SGS stress components in different regions of the flow. It was observed that τ_{22} and τ_{33} SGS increase in magnitude from $X^* = -0.5$ to $X^* = 0.25$ while the τ_{11} component showed a decrease between these two locations. The reason for this behavior can be examined by looking at the transport equation for the normal SGS stresses (τ_{ii}). On examination of the transport equation for the normal SGS stresses, it was observed that at $X^* = -1.1$ the production terms for τ_{22} and τ_{33} are negligible and the entire production of k_{sgs} comes from τ_{11} . At $X^* = 0.25$, the production term for τ_{22} and τ_{33} becomes significant and this explains their behavior at $X^* = 0.25$.

2.3.4 Backscatter

As discussed earlier, a positive contribution from the SGS production term to the SGS kinetic energy equation indicates an energy transfer from the resolved field to the residual field. It is, however, also possible for the energy to be transferred back from the residual field to the resolved field (backscatter). The ensemble-averaged values of the SGS production term indicated no significant backscatter, i.e., the SGS production term always had a positive contribution to the SGS kinetic energy equation. However, instantaneous flow realizations show that backscatter does indeed occur in various regions of flow. This can be observed in Fig. 3.14 where the instantaneous contours of the SGS production term in a y - z plane at four different streamwise locations are shown. The results in this figure are from the instantaneous filtered DNS data for $\theta = 7.75^{\circ}$ and $\overline{\Delta} = 8\Delta_{DNS}$. Only regions indicating backscatter are shown. Figure 3.14 shows that significant backscatter does indeed occur instantaneously. For example, at $X^* = -1.1$, backscatter occurs in 11% of the selected y - zplane and at $X^* = -0.5$, it occurs in 16% of that flow region. However, no backscatter is observed in the ensemble-averaged data. This might explain why constant-coefficient SGS eddy-viscosity models, which cannot account for the energy backscatter, yield acceptable results for many steady flow calculations. However, we would like to emphasize here that shocks do have a very significant effect on the energy transfer between resolved and SGS scales and generally increase the backscatter, mainly because they increase "small-scale" turbulence.

To better understand the effect of shock on energy transfer and backscatter, we computed



Figure 2.17: Instantaneous contours of SGS production as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$. Only the backscatter regions are shown. 50 uniformly spaced contour levels between 0.0 and 0.005. (a) $X^* = -1.1$, (b) $X^* = -0.5$, (c) $X^* = 0.25$, (d) $X^* = 1.5$.

the probability of backscatter in the simulated flow. Figure 2.18 shows the contours for the probability of backscatter for $\theta = 7.75^{\circ}$ and $\overline{\Delta} = 8\Delta_{DNS}$. Analogous to the definitions used by Simpson [30] for identifying flow reversal, a probability greater than 50% would mean backscatter occurs in the mean flow. As shown in Fig. 2.18 the maximum probability in



Figure 2.18: Probability of backscatter in the x - y symmetry plane as obtained from filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$.

majority of flow regions does not exceed the 40% value and only in the regions close to the shock, particularly in the expansion fan region, the probability reaches close to 50%. This is similar to the production term in turbulent kinetic energy equation where the the production term had negative contribution in the expansion fan region [40]. Figure 2.18 also shows that the shock increases the probability of backscatter in the interaction region $(-1 \le X^* \le 0)$ and in the regions downstream of the interaction. Hence the shock affects the dynamics of energy transfer between the resolved and residual fields.

2.3.5 Directional filtering

In all the results discussed until now, filtering was performed only in x and z directions, which is a common practice for wall-bounded flows. To examine the effect of shock on SGS fluctuations in each spatial direction, it would be useful to examine the amount of SGS energy present in each spatial direction. To study this, filtering operations were performed in only one spatial direction, i.e., x-only and z-only directions. Additionally, filtering was also performed in y- only direction using the 1-D filter function given by Eq. (2.2). The filter coefficients were evaluated using the trapezoidal rule for non-uniform grids. It should be noted that the 1-D filter (Eq. (2.2)) is a symmetric filter and is ill-defined at the wall. Hence, near the wall, the grid points dictated by the filter width were ignored while computing the filtered value. Nevertheless, the results discussed here are very useful and help us to better understand the effects of directional filtering on LES quantities. The results are presented for $\theta = 7.75^{\circ}$ and $\overline{\Delta} = 8\Delta_{DNS}$ and at $X^* = -1.1$, -0.5 and 0.25.

Figures 2.19 and 2.20 show the spatial variations of τ_{11} , τ_{22} , τ_{33} and τ_{12} SGS stresses along the wall-normal direction at $X^* = -1.1$. For τ_{11} , the maximum SGS energy occurs near the wall in y and z directions, as indicated by the y-only and z-only filtered values. Very little energy is present in the streamwise direction which is evident in the x-only filtered results. This indicates a slow growth of SGS turbulence in the streamwise direction. It also explains why the grids are relatively coarse in the x direction compared to z and y directions in LES of boundary layers (eg. Ref. [50]). While the overall τ_{22} stress values are small relative to those for τ_{11} , important contributions are observed for the x-only and z-only filters. The contribution from the y-only filter is negligible which indicates that the SGS turbulence does not change significantly in the wall-normal direction for τ_{22} . For τ_{33} , while the stress values are small relative to τ_{11} , they are still significant in all three spatial directions. This suggests that τ_{33} is more homogenous than τ_{11} and τ_{22} . The peak for τ_{33} with z-only filtering occurs near the wall, while the peak is away from the wall for the x-only filtered τ_{33} . The net effect of a combined x - z filter results in the peak being shifted away from the wall, as seen in Fig. 2.1(a). We should also mention here that the τ_{12} SGS stress is almost entirely due to the SGS fluctuations in the spanwise direction.

In Figs. 2.21 and 2.22, we show the results for τ_{11} , τ_{22} , τ_{33} and τ_{12} SGS stresses in the interaction region at $X^* = -0.5$. While the z-only filtered τ_{11} stress is still the most dominant one, the contribution from the x-only filtered τ_{11} stress increases in the interaction region, indicating that the SGS fluctuations for the streamwise velocity component increase in the streamwise direction due to the shock. The near wall peak for y-only filtered τ_{11} stress disappears at this location because of the separation bubble. The trends for τ_{22} and τ_{12} are similar to those at $X^* = -1.1$. For τ_{33} , the x-only and z-only filtered stresses are of nearly same magnitude, indicating that the z component of SGS stress is more homogeneous. At $X^* = 0.25$ (Figs. 2.23 and 2.24), the trends for τ_{11} are same as at $X^* = -0.5$ except that the near-wall peak for y-only filtered τ_{11} reappears and there is also a second peak away from the wall. For τ_{33} , the x-only filtered stress values exceed the z-only filtered values, suggesting that the streamwise SGS fluctuations are more important. In general, the shock seems to homogenize the normal components of SGS stresses by increasing the SGS fluctuations in the streamwise direction.

2.4 Conclusions

A detailed analysis of various subgrid-scale terms in the filtered equations for large-eddy simulation (LES) of compressible flows is made using accurate DNS database for shockboundary layer interaction (SBLI) that resolves the flow both upstream and downstream of the interaction region. The SGS stresses were examined in different flow regions and their behavior were found to be generally similar to those of turbulent Reynolds stresses. The Leonard, Cross and Reynolds parts of the SGS stresses were also examined in different





Figure 2.19: Directionally filtered SGS stresses as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$ at $X^* = -1.1$. (a) τ_{11} , (b) τ_{22} . solid black line for *x*-only filter, dashed black line for *y*-only filter, red dash-dot line for *z*-only filter





Figure 2.20: Directionally filtered SGS stresses as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$ at $X^* = -1.1$. (a) τ_{33} , (b) τ_{12} . solid black line for *x*-only filter, dashed black line for *y*-only filter, red dash-dot line for *z*-only filter





Figure 2.21: Directionally filtered SGS stresses as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$ at $X^* = -0.5$. (a) τ_{11} , (b) τ_{22} . solid black line for *x*-only filter, dashed black line for *y*-only filter, red dash-dot line for *z*-only filter







Figure 2.22: Directionally filtered SGS stresses as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$ at $X^* = -0.5$. (a) τ_{33} , (b) τ_{12} . solid black line for *x*-only filter, dashed black line for *y*-only filter, red dash-dot line for *z*-only filter







Figure 2.23: Directionally filtered SGS stresses as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$ at $X^* = 0.25$. (a) τ_{11} , (b) τ_{22} . solid black line for *x*-only filter, dashed black line for *y*-only filter, red dash-dot line for *z*-only filter







Figure 2.24: Directionally filtered SGS stresses as obtained from the filtered DNS data for $\theta = 7.75^{o}$ and $\overline{\Delta} = 8\Delta_{DNS}$ at $X^* = 0.25$. (a) τ_{33} , (b) τ_{12} . solid black line for *x*-only filter, dashed black line for *y*-only filter, red dash-dot line for *z*-only filter

regions of the flow for three different filter widths, $\overline{\Delta} = 4\Delta_{DNS}$, $8\Delta_{DNS}$ and $16\Delta_{DNS}$ and shock intensities. For the smallest filter width, the contribution of the Leonard stress component was found to be the most dominant in all the flow regions, suggesting that the mixed-type models could be appropriate for LES with such filter widths. For intermediate filter width ($\overline{\Delta} = 8\Delta_{DNS}$), the Leonard stress component was dominant for the incoming boundary layer while the Reynolds stress component's contribution became very significant in the regions downstream of the shock. These suggest that accurate modeling of the Reynolds stress part of the SGS stress is important close to the shock. For very large filter widths ($\overline{\Delta} = 16\Delta_{DNS}$), the Reynolds stress part of the SGS stress dwarfs the contributions from the other two parts.

To further study the shock effect on compressible boundary layer flow, the SGS terms in the filtered total energy equation were examined in various regions of the flow using the ensemble-averaged DNS data. It was observed that while the individual unclosed SGS terms in the filtered energy equation had sizable contributions by themselves, the combined contribution from all the terms was relatively small when compared to the divergence of filtered molecular heat flux term. To confirm this, two different *a posteriori* LES calculations were performed in which SGS terms in the total energy equation were either neglected or modeled via suggested models in the literature. The skin-friction coefficient predictions between the two LES calculations showed no significant differences. Interestingly, comparison of the turbulent stress and heat flux profiles show that the modeling of SGS terms in the total energy equation slightly deteriorate the LES predictions in comparison to DNS. This could be partly because the model for the pressure-dilatation term was ignored as it was found to cause numerical instability to the LES calculations. Based on these observations, one could argue that it is probably better to ignore the SGS terms in the total energy equation altogether instead of modeling just a few terms. These results are, however, for the total energy equation only and might not be valid for the internal energy or enthalpy equations.

The transport equation for SGS kinetic energy was examined using ensemble-averaged values with the aim providing useful information to aid in the development of one-equation LES models. The turbulent transport and the SGS diffusion term were found to balance each others contributions in all the regions of the flow suggesting that modeling of these two terms can be safely ignored for boundary layers and SBLIs. The contribution from the pressure-dilatation term was not negligible and became more significant in the interaction region and downstream of the interaction region. Hence, the modeling of this term cannot be ignored, which is commonly is done. The ensemble-averaged production term was found to have a positive contribution at all the selected streamwise locations and also in the majority of flow region. This suggested there were no backscatter regions in the flow, where energy is transferred back from the residual field to the resolved field. However, examination of instantaneous flow samples indicated that backscatter does indeed occur in the flow. To quantify the occurrence of backscatter, its probability was computed and was found to be less than 50% in all of the flow regions with higher values in the expansion fan region. Making an analogy to Simpson's flow reversal definitions [30], less than 50% probability indeed confirms that backscatter does not occur in the mean flow in the majority of flow regions. The high probability of negative energy transfer from residual field to the resolved filed in the expansion fan region is reminiscent of the behavior of production term in the turbulent kinetic energy equation, which also has a negative contribution in the expansion fan region.

Chapter 3

SGS Models and their Applications to LES of Shock-Boundary Layer

Interactions

3.1 Introduction

Shock boundary layer interactions (SBLI) are important to a wide range of applications [51]. The shock wave can significantly alter the structure of supersonic boundary layers and depending on the strength of shock, the boundary layer may even separate in the vicinity of shock impingement location. There is an amplification of turbulence across the shock and in the case of boundary layer separation, the shock oscillates at a frequency lower than the characteristic frequency of the incoming flow [4, 14, 12, 34, 13]. To understand and predict the complex SBLI phenomena, high-fidelity simulations, i.e., direct numerical simulation (DNS) and large-eddy simulation (LES), are needed. DNS is limited to simple geometries and low-to-moderate Reynolds number flows. LES can be conducted at higher Reynolds numbers and for flows in complex geometries but only computes the large scales and has some limitations in wall-bounded flows [52]. Although the filtered equations for LES are derived from Navier-Stokes equations with no major assumptions, there are several unclosed terms appearing in the filtered momentum and energy equations. These terms are often represented in terms of resolved quantities through subgrid-scale (SGS) closures. The use of models to include the effects of small scales introduces an uncertainty into the computations. Also, many of the SGS models were originally developed for incompressible flows. Their application to high speed flows, particularly the shock-turbulence interaction locations where turbulence and shock effects are both important, has not been fully tested or justified.

The most common type of SGS models used for LES are zero-equation models developed based on the eddy-viscosity and isotropic SGS interaction assumptions which are not necessarily valid in SBLI. Scale-similarity models [46, 53] and dynamic models [46, 54] are developed to replace or improve the original eddy-viscosity models. However, it is still not clear how these eddy-viscosity, similarity or mixed models behave in shock-turbulence regions.

The problem of shock wave interacting with a boundary layer has primarily been studied in two configurations, incident shock interacting with an already fully developed flat-plate supersonic turbulent boundary layer [8, 55, 5, 4, 33] and shock-boundary layer interaction in a compression corner [23, 13, 15]. The focus of the present study is on the incident SBLI. An important characteristic of SBLI is the low-frequency oscillation of the shock system. Although a few DNS studies [15, 14, 13, 12, 23] of low-frequency shock oscillations have been reported, the computational cost associated with such simulations is still very significant at reasonably high Reynolds numbers, Mach numbers and shock intensities.

LES method has also been used, particularly in recent years, for studying the main characteristics of SBLI. Garnier et al. [33] were the first to conduct LES of SBLI for a flow Mach number of 2.3 and a flow deflection angle of $\theta = 8$ deg. They compared their LES results with the available experimental data for similar flow conditions and found a good agreement between the numerical and experimental results. More recently, Touber and Sandham [34] studied the low-frequency oscillations in SBLI problem using LES with a new inflow generation technique based on digital filters [56] and the mixed-time-scale closure for SGS stresses. They also examined the effect of spanwise domain size on the separation bubble and recommended that the spanwise width be at least the same as the separation bubble size. Their results were in good agreement with the experiment. Morgan et al. [57] studied the low-frequency behavior of shock motion using an improved rescaling/recycling method [58]. However, they used no SGS model in their LES studies, arguing that the artificial viscosity they used for shock capturing mimicked the behavior of an SGS model. Morgan et al. [7] also carried out extensive parametric studies of SBLI for various wedge angles, Reynolds numbers, streamwise and spanwise domain sizes. They found that the Reynolds number did not have any significant effect on the separation bubble size. Increasing the wedge angle led to an increased size of the interaction region but did not necessarily guarantee higher probability of reversed flow. Pirozzoli et al. [35] used LES and RANS models to study SBLI under the conditions of incipient separation. By comparing with experimental results, they found that both LES and RANS were able to qualitatively predict some basic features of the interaction.

Given the importance and complexity of shock-turbulence interactions at small scales, the SGS models are expected to play an important role in the flow development and quantitative predictions of SBLI under various flow conditions. Our main objectives in this study are to systematically assess the performance of several widely used SGS models along with a new dynamic model for SBLI simulations and to evaluate the effects of shock and compressibility on the models. Comparisons are made, both *a priori* and *a posteriori*, with the DNS data for an incident 34° oblique shock interacting with a flat-plate turbulent boundary layer at Mach 2. For these selected flow conditions, the boundary layer exhibits a marginal mean

flow separation.

The organization of the paper is as follows. In Sections 3.2 and 3.3, the governing equations and SGS models are presented. In Section 3.4 we describe the numerical method. The computational setup and parameters and simulation results are given in Section 3.5 followed by concluding remarks in Section 3.7.

3.2 Governing Equations

Written in conservative form, the non-dimesionalized form of governing equations solved in DNS read as

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

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j}$$
(3.2)

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j} \left(E + p \right) u_j = \frac{\partial}{\partial x_j} \left(\sigma_{ij} u_i \right) - \frac{\partial Q_j}{\partial x_j} , \qquad (3.3)$$

where the viscous stress and heat flux terms are obtained from the following models:

$$\sigma_{ij} = \frac{2\mu}{Re} \left[\frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right]$$
(3.4)

$$Q_j = \frac{-\mu}{(\gamma - 1)RePrM_{\infty}^2} \frac{\partial T}{\partial x_j}$$
(3.5)

Here, the temperature dependence of μ is based on Sutherland's law, $\mu(T) = T^{1.5}(1 + C)/(T + C)$ with C = 0.65. In Eq. (3.3), E is the total energy defined as

$$E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho u_i u_i \tag{3.6}$$

Finally, the thermodynamic variables, ρ , p and T are linked by the ideal gas law,

$$p = \frac{\rho T}{\gamma M_{\infty}^2}.$$
(3.7)

The filtered equations for LES are obtained by applying the standard filtering and Favre filtering operators to Eqs. (3.1), (3.2), (3.3) and (3.7). The final dimensionless form of the filtered continuity, momentum and energy equations are

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_j} \left(\overline{\rho} \widetilde{u}_j \right) = 0 \tag{3.8}$$

$$\frac{\partial}{\partial t}\left(\overline{\rho}\widetilde{u}_{i}\right) + \frac{\partial}{\partial x_{j}}\left(\overline{\rho}\widetilde{u}_{i}\widetilde{u}_{j}\right) = -\frac{\partial\overline{p}}{\partial x_{i}} + \frac{\partial\overline{\sigma}_{ij}}{\partial x_{j}} - \frac{\partial\tau_{ij}}{\partial x_{j}} + \frac{\partial}{\partial x_{j}}\left(\overline{\sigma}_{ij} - \overline{\sigma}_{ij}\right), \qquad (3.9)$$

$$\frac{\partial \widetilde{E}}{\partial t} + \frac{\partial}{\partial x_j} \left(\widetilde{E} + \overline{p} \right) \widetilde{u}_j = \frac{\partial}{\partial x_j} \left(\widetilde{\sigma}_{ij} \widetilde{u}_i \right) - \frac{\partial \widetilde{Q}_j}{\partial x_j} - B_1 - B_2 - B_3 + B_4 + B_5 + B_6 - B_7, \quad (3.10)$$

where the SGS stress term τ_{ij} and the filtered viscous stresses $\tilde{\sigma}_{ij} \ \overline{\sigma}_{ij}$ and are given by

$$\tau_{ij} = \overline{\rho}(\widetilde{u_i u_j} - \widetilde{u}_i \widetilde{u}_j) \tag{3.11}$$

$$\widetilde{\sigma}_{ij} = \frac{2\mu(\widetilde{T})}{Re} \left[\frac{1}{2} \left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial \widetilde{u}_k}{\partial x_k} \delta_{ij} \right]$$
(3.12)

$$\overline{\sigma}_{ij} = \frac{\overline{2\mu(T)}}{Re} \left[\frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right]$$
(3.13)

$$\widetilde{Q}_j = \frac{-\mu(\widetilde{T})}{(\gamma - 1)RePrM_\infty^2} \frac{\partial \widetilde{T}}{\partial x_j}$$
(3.14)

The last term on the RHS of Eq. (3.9) appears as a result of non-linearities in the viscous flux terms due to filtering. Vreman et al. [38] found this term to be negligible for compressible mixing layer. The same is assumed to be valid in the present study. The choice of total energy equation for energy conservation, although is not unique, is appropriate for formulating the Navier-Stokes equations in conservative form which is necessary for flows with discontinuities.

In Eq. (3.10), \tilde{E} is the Favre-filtered value of the modified total energy and the subgrid scale terms B_1 , B_2 , B_3 , B_4 , B_5 , B_6 , and B_7 are defined as

$$B_{1} = \frac{1}{\gamma - 1} \frac{\partial}{\partial x_{j}} (\overline{pu_{j}} - \overline{p}\widetilde{u}_{j})$$

$$B_{2} = \overline{p} \frac{\partial u_{k}}{\partial x_{k}} - \overline{p} \frac{\partial \widetilde{u}_{k}}{\partial x_{k}}$$

$$B_{3} = \frac{\partial}{\partial x_{j}} (\tau_{kj}\widetilde{u}_{k})$$

$$B_{4} = \tau_{kj} \frac{\partial \widetilde{u}_{k}}{\partial x_{j}}$$

$$B_{5} = \overline{\sigma_{kj}} \frac{\partial u_{k}}{\partial x_{j}} - \widetilde{\sigma}_{kj} \frac{\partial \widetilde{u}_{k}}{\partial x_{j}}$$

$$B_{6} = \frac{\partial}{\partial x_{j}} (\overline{\sigma}_{ij}\widetilde{u}_{i} - \widetilde{\sigma}_{ij}\widetilde{u}_{i})$$

$$B_{7} = \frac{\partial}{\partial x_{j}} (\overline{Q}_{j} - \widetilde{Q}_{j})$$

Equations (3.8), (3.9), (3.10) are completed by the filtered state equation.

$$\overline{p} = \frac{\overline{\rho} \ \widetilde{T}}{\gamma M_{\infty}^2} \tag{3.15}$$

The terms which need modeling are τ_{ij} , B_1 , B_2 , B_3 , B_4 , B_5 , B_6 , and B_7 . The modeling of these terms is described in the next section.

3.3 Subgrid-Scale Models

The filtered equations presented in previous section require closures for the unclosed SGS terms. Several models have been proposed including the eddy-viscosity type ones in which the deviatoric part of the SGS stress is modeled as

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = -2\overline{\rho}\nu_t \left[\frac{1}{2}\left(\frac{\partial\widetilde{u}_i}{\partial x_j} + \frac{\partial\widetilde{u}_j}{\partial x_i}\right) - \frac{1}{3}\frac{\partial\widetilde{u}_k}{\partial x_k}\delta_{ij}\right]$$
(3.16)

To compute the isotropic part of the SGS stress, τ_{kk} , Yoshizawa [59] proposed the following model,

$$\tau_{kk} = 2C_I \overline{\rho} \overline{\Delta}^2 |\tilde{S}|^2, \qquad (3.17)$$

where $|\tilde{S}| = \sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$, $\overline{\Delta}$ is the characteristic filter width and C_I is the model constant which is typically chosen as 0.006 for isotropic turbulence or computed dynamically [54, 60]. However, Eq. (3.17) correlates poorly with the DNS data for compressible isotropic turbulence [61].

In this study, four different SGS stress models, namely, the mixed-time-scale model (MTSM), the dynamic Smagorinsky model (DSM), the dynamic mixed model (DMM) and a new dynamic model, termed the compressible serial decomposition model (CSDM) are examined. A brief description of each model is given below.

 Mixed-Time-Scale Model (MTSM): The mixed time scale model has been used by Touber and Sandham [34] for LES study of low-frequency unsteadiness in SBLI. Although this model gives an incorrect asymptotic behavior of eddy-viscosity near the wall, it has been found to yield acceptable results for SBLI. The model details are given in the following set of equations.

$$\nu_t = C_{MTS} k_{es} T_S \tag{3.18}$$

$$k_{es} = \left[\widetilde{u}_i - \widetilde{\widetilde{u}}_i\right] \left[\widetilde{u}_i - \widetilde{\widetilde{u}}_i\right]$$
$$T_S^{-1} = \left(\frac{\overline{\Delta}}{\sqrt{k_{es}}}\right)^{-1} + \left(\frac{C_T}{|\widetilde{S}|}\right)^{-1}$$
$$\widetilde{\widetilde{u}}_i = \frac{\overline{\rho}\widetilde{u}_i}{\overline{\rho}}$$
$$C_{MTS} = 0.03, C_T = 10$$

 Dynamic Smagorinsky Model (DSM): In the dynamic Smagorinky model, the Smagorinsky coefficient, C_s, is computed dynamically [62]. The compressible form of the model is given by,

$$\nu_t = C_s \overline{\Delta}^2 |\widetilde{S}| \tag{3.19}$$

$$C_s = -\frac{\langle (G_{ij} - \frac{1}{3}G_{kk}\delta_{ij})M_{ij}\rangle}{\langle 2\overline{\Delta}^2 M_{ij}M_{ij}\rangle}$$
(3.20)

In Eq. (3.20), $\langle \rangle$ denotes the averaging in homogeneous direction and the tensors G_{ij} and M_{ij} are computed by the following relations.

$$G_{ij} = \widehat{\overline{\rho}\widetilde{u}_i\widetilde{u}_j} - \frac{\widehat{\overline{\rho}\widetilde{u}_i\overline{\rho}\widetilde{u}_j}}{\widehat{\overline{\rho}}}$$
$$M_{ij} = \left(\frac{\widehat{\Delta}}{\overline{\Delta}}\right)^2 \widehat{\overline{\rho}}|\widehat{\widetilde{S}}| \left(\widehat{\widetilde{S}}_{ij} - \frac{1}{3}\widehat{\widetilde{S}}_{kk}\delta_{ij}\right) - \overline{\overline{\rho}}|\widetilde{S}| \left(\widetilde{\widetilde{S}}_{ij} - \frac{1}{3}\widetilde{S}_{kk}\delta_{ij}\right)$$

The characteristic width of the test filter, $\widehat{\Delta}$, is chosen to be twice of the grid filter width, $\overline{\Delta}$.

3. Dynamic Mixed Model (DMM): One of the known drawbacks of eddy-viscosity models is the inherent assumption that SGS stress and resolved strain rate tensors are 'aligned'. This assumption is generally not correct, particularly in wall-bounded flows where there is significant anisotropy. The model predictions also correlates poorly with the DNS data. The dynamic mixed model (DMM) addresses these issues by including the Leonard part of stress tensor in the model. This results in 'lesser' modeling since Leonard stress is respresented only by the resolved quantities and a better representation of energy back-scatter to the resolved scales. Salvetti and Banerjee [46] and Vreman [53] used the DMM model in their *a priori* analysis and *a posteriori* simulations of compressible (but subsonic) homogeneous turbulence and planar mixing layer. The model is described in the following equations.

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = \left(L_{ij} - \frac{1}{3}L_{kk}\delta_{ij}\right) - 2\overline{\rho}\nu_t \left[\frac{1}{2}\left(\frac{\partial\widetilde{u}_i}{\partial x_j} + \frac{\partial\widetilde{u}_j}{\partial x_i}\right) - \frac{1}{3}\frac{\partial\widetilde{u}_k}{\partial x_k}\delta_{ij}\right]$$
(3.21)

$$L_{ij} = \overline{\rho} \left(\widetilde{\widetilde{u}_i \widetilde{\widetilde{u}}_j} - \widetilde{\widetilde{u}_i} \widetilde{\widetilde{\widetilde{u}}_j} \right)$$
$$\nu_t = C_m \overline{\Delta}^2 |\widetilde{S}|$$
$$C_m = -\frac{\left\langle \left[\left(G_{ij} - \frac{1}{3} G_{kk} \delta_{ij} \right) - \left(H_{ij} - \frac{1}{3} H_{kk} \delta_{ij} \right) \right] M_{ij} \right\rangle}{\langle 2 \overline{\Delta}^2 M_{ij} M_{ij} \rangle}$$
$$H_{ij} = \widehat{\overline{\rho} \widetilde{\widetilde{u}_i} \widetilde{\widetilde{u}_j}} - \frac{\widehat{\overline{\rho} \widetilde{\widetilde{u}_i} \widetilde{\overline{\rho} \widetilde{\widetilde{u}_j}}}}{\widehat{\overline{\rho}}}$$

4. Compressible Serial Decomposition Model (CSDM): The SGS stress tensor τ_{ij} can be decomposed into modified Leonard stress, modified Cross stress and modified Reynolds stress components (Eq. 3.25). In the dynamic mixed model, the Cross term and the Reynolds term are modeled together using an eddy-viscosity type model [46]. In the compressible serial decomposition model, they are modeled using a similarity type model following the same dynamic procedure used for DSM or DMM. For the sake of brevity, we refrain from describing the details of the model in this paper. Further details about this model can be found in Ref. [63, 64]. The basic formulation for CSDM is given below.

$$\tau_{ij} = L_{ij} + C_{\alpha} F_{ij} \tag{3.22}$$

$$F_{ij} = \overline{\rho} \left(\widetilde{\widetilde{v}_i \widetilde{v}_j} - \widetilde{\widetilde{v}}_i \widetilde{\widetilde{v}}_j \right)$$
$$C_\alpha = \frac{\langle \left[G_{ij} - H_{ij} \right] N_{ij} \rangle}{\langle N_{ij} N_{ij} \rangle}$$
$$N_{ij} = \overline{\rho} \widehat{\widetilde{v}_i} \widehat{\widetilde{v}_j} - \frac{\overline{\rho} \widehat{\widetilde{v}_i} \overline{\rho} \widehat{\widetilde{v}_j}}{\overline{\rho}}$$
$$\widetilde{v}_i = \widetilde{u}_i - \widetilde{\widetilde{u}}_i$$

In the filtered total energy equation, the term B_1 is modeled as

$$B_1 = -\frac{\partial}{\partial x_j} \left(\frac{\overline{\rho}\nu_t}{\gamma(\gamma - 1)Pr_t M_\infty^2} \frac{\partial \widetilde{T}}{\partial x_j} \right)$$
(3.23)

for the eddy-viscosity type models. For the mixed type models which includes the dynamic mixed model and the new compressible serial decomposition model, B_1 is modeled as

$$B_{1} = -\frac{\partial}{\partial x_{j}} \left(\frac{\overline{\rho}\nu_{t}}{\gamma(\gamma-1)Pr_{t}M_{\infty}^{2}} \frac{\partial \widetilde{T}}{\partial x_{j}} \right) + \frac{1}{\gamma(\gamma-1)M_{\infty}^{2}} \frac{\partial q_{j}^{L}}{\partial x_{j}}$$

$$q_{j}^{L} = \overline{\rho} \left(\widetilde{\widetilde{u_{j}}\widetilde{T}} - \widetilde{\widetilde{u}_{j}}\widetilde{\widetilde{T}} \right)$$

$$(3.24)$$

For CSDM, we use MTSM to compute the eddy-viscosity used in modeling B_1 . The turbulent Prandtl number, Pr_t , is assumed to have a constant value of 0.89 for the simulated boundary layer. Once τ_{ij} is known, B_3 and B_4 are computed from their definitions. The other unclosed terms, B_2 , B_5 , B_6 , and B_7 were neglected by Garnier et al. [33] in their LES of SBLI and the same is done here.

3.4 Numerical Method

Numerical simulation of shock-turbulence interactions require high-order numerical schemes for accurate computations of both the shock wave and turbulence. Since it is very difficult to resolve the shock structure, the use of a shock-fitting scheme that treats the shock as a discontinuity becomes necessary. In this study, we use a recently developed seventh-order Monotonicity-Preserving (MP) [11, 10] scheme to discretize the Euler fluxes. The MP scheme has proved to be less dissipative and more accurate than the standard WENO scheme [11] for shock and turbulence calculations. To discretize the viscous fluxes, we use a sixth-order compact scheme [20] with a fourth-order boundary formulation. The viscous terms are discretized in conservative form. However, for the sake of comparison, we also performed LES computations with the viscous terms discretized in Laplacian form [22] and found no significant differences between the two forms of discretization. The governing equations are integrated in time by a third-order low-storage Runge-Kutta scheme. The details of numerical method are presented in Ref. [11] and also in Appendix A.

3.5 Results

3.5.1 Computational Setup and Parameters

The computational parameters for DNS and LES are listed in tables 3.1 and 3.2, respectively.

Parameter	Value	Comment
M_{∞} Pr $Re_{\delta_{ref}}$ Re_{δ_2} T	2.0 0.72 13500 1475 1.717T	at $x = 6$
$ \begin{array}{c} L_w \\ L_x \\ L_y \\ L_z \\ N_x \\ N_w \end{array} $	$ \begin{array}{c} 1.7171_{\infty} \\ 20\delta_{ref} \\ 13\delta_{ref} \\ 3\delta_{ref} \\ 1333 \\ 252 \end{array} $	
$ \begin{array}{c} N_{z} \\ \Delta x^{+} \\ \Delta y_{w}^{+} \\ \Delta z^{+} \\ \beta \end{array} $	$201 \\ 3.89 \\ 0.65 \\ 3.89 \\ 34^{o}$	at $x = 6$ at $x = 6$ at $x = 6$
$ \begin{array}{c} \theta \\ X_I \\ C_f \end{array} $	4.67^{o} $10\delta_{ref}$ 0.0031	at $x = 6$

Table 3.1: Simulation Parameters for DNS of Mach 2 SBLI

In these tables, $Re_{\delta_{ref}}$ is the Reynolds number based on the reference boundary layer thickness, δ_{ref} (computed from DNS data as described below), and the freestream velocity, density and viscosity. Re_{δ_2} is the Reynolds number based on momentum thickness (δ_2) and the freestream quantities. Also in tables 3.1 and 3.2, x, y and z denote the streamwise, wall-normal and spanwise directions, respectively. The grid is uniform in x and z directions.

Parameter	Value	Comment
M_{∞}	2.0	
Pr	0.72	
$Re_{\delta_{ref}}$	13500	
T_w	$1.717T_{\infty}$	
L_x	$20\delta_{ref}$	
L_y	$13\delta_{ref}$	
L_z	$3\delta_{ref}$	
N_x	333	$1/4^{th}$ of DNS
N_y	252	
N_z	51	$1/4^{th}$ of DNS
β	34^{o}	
heta	4.67^{o}	
X_I	$10\delta_{ref}$	

Table 3.2: Simulation Parameters for LESof Mach 2 SBLI

In the wall-normal direction, a hyperbolic sine function was used upto $y \approx 5\delta_{ref}$ and then the grid was smoothly varied to a uniform spacing up to the top boundary. In this work, the wall-normal grid resolution is identical for both DNS and LES since filtering is performed only in x and z directions. A sample x - y slice of the DNS grid is shown in Fig. 3.1. For clarity, we only show every other 20^{th} grid point in the x direction and every other 4^{th} grid point in the y direction. The grid in the blue region after x = 20 is coarse and indicates sponge region.

When comparing LES results with DNS results, particularly when making model assessments as being done in the present study, it is important to minimize the effects of inlet boundary condition on simulations. In order to keep the inflow boundary condition consistent for both DNS and LES, we first carried out an "auxiliary" DNS of a canonical turbulent boundary layer with a rescaling-recycling inflow condition similar to that used by Pirrozzoli et al. [25]. Once the flow reached a statistically steady condition, a time-history of primitive



Figure 3.1: An x - y slice of the sample DNS grid.

variables was collected at a y - z plane located at a distance of 23 boundary layer thicknesses from the inlet (this was also the location of recycling plane). A total of 5000 samples were collected for a period of $T = 75\delta_{ref}/U_{\infty}$ which corresponded to approximately 3 flowthrough times and were periodically used as the inflow boundary condition for both DNS and LES of SBLI. The inflow turbulence generation method employed in this work is similar to that previously used in other SBLI simulations [23, 65, 36]. For LES, the inflow DNS quantities were filtered in x and z directions using a box filter in physical space and then down-sampled onto the LES grid. It should be noted here that the streamwise flow varibles at the inflow boundary are obtained from a time-dependent periodic box data. Thus, for filtering in x-direction, Taylor's hypothesis was used to convert the temporal coordinate into a spatial coordinate using a convection velocity of U_{∞} . A schematic of the computational procedure is shown in Fig. 3.2.

At the outlet, a sponge layer [24] is used and supersonic exit condition is applied to all variables. At the wall, no-slip isothermal wall with wall temperature (T_w) close to the adiabatic wall temperature is used. The wall pressure is computed by assuming that the



Figure 3.2: A schematic of the computational procedure for DNS and LES of SBLI.

pressure remains constant across the boundary layer, i.e., $\partial p/\partial y = 0$. Symmetry boundary condition is applied to all variables at the freestream and at the spanwise boundaries periodic boundary condition is used. The shock is introduced at the inlet boundary by imposing discontinuous conditions according to the Rankine-Hugoniot relations.

In order to evaluate the performance of SGS models for SBLI simulations, the flow statistics at three different streamwise locations, (i) x = 6, upstream of the mean separation point, (ii) x = 10, downstream but very close to the mean reattachment point and (iii) x = 15, further downstream of the mean reattachment point, are compared. Here, all the spatial coordinates are non-dimensionalized by the reference boundary layer thickness δ_{ref} unless otherwise stated.

Figure 3.3 illustrates a typical impinging shock-turbulent boundary layer interaction. The shock is identified using the modified Ducros shock sensor [8] and the vortex structures are identified using λ_2 criterion [2]. The vortex structures are shown through isosurfaces of $\lambda_2 = -3$ and colored based on the local velocity magnitude. The effect of shock on turbulence is clearly very significant.



Figure 3.3: Flow structure in a typical shock/boundary layer interaction configuration. Vortex structures identified using λ_2 criterion [2] and colored based on the local values of instantaneous velocity magnitude.

To demonstrate the validity of our DNS results, Van Driest transformed mean streamwise velocity profile of the incoming boundary layer is compared in Fig. 3.4 with zero-pressure gradient Mach 2 DNS results of Pirozzoli and Bernardini [1] for two different Reynolds numbers. The mean DNS velocity profile shows a linear relationship, $U_{VD}^+ = y^+$, until $y^+ \approx 6$ and a logarithmic behavior (Eq. (1.14)) between $y^+ \approx 30$ and $y^+ \approx 100$. The density-scaled profiles of Reynolds stresses are shown in Fig. 3.5 in wall units. Evidently, there is a good comparison between the density-scaled profiles of the current DNS with those of Pirozzoli and Bernardini. [1]. To further establish the numerical accuracy of current DNS



Figure 3.4: Van Driest transformed mean streamwise velocity profile of the incoming boundary layer in inner scaling calculated from DNS data at x = 6. Black dashed line represents $U_{VD}^+ = y^+$ and Eq. (1.14) is represented by black dash-dot line.

data, we computed various terms in the turbulent kinetic energy equation at different regions of the flow and found them to be in balance.

3.5.2 A Priori Assessment

The four models described in Sec. 3.3 are tested *a priori* for the SBLI problem using a single realization of instantaneous DNS data. Although *a priori* testing of SGS models provides only a partial assessment of LES, it is still a good direct method of evaluating the models.



Figure 3.5: Density-scaled profiles of Reynolds stresses obtained by DNS at x = 6.

To make useful conclusions, filtered values from the DNS data are down-sampled onto an LES grid four times coarser than the DNS grid in the streamwise and spanwise directions. The modeled SGS fluxes are then computed on the LES grid and compared with the true SGS fluxes. The filter function used for filtering the DNS data is a box filter in physical space and filtering is performed only in x and z directions.

Following Germano's [45] redefinition of stresses, the SGS stress tensor can be decom-

posed into modified Leonard's stress, Cross stress and Reynolds stress components.

$$\tau_{ij} = L_{ij} + C_{ij} + R_{ij} \tag{3.25}$$

where

$$L_{ij} = \overline{\rho} \left(\widetilde{\widetilde{u}_i \widetilde{u}_j} - \widetilde{\widetilde{u}}_i \widetilde{\widetilde{u}}_j \right)$$
$$C_{ij} = \overline{\rho} \left(\widetilde{u'_i \widetilde{u}_j} + \widetilde{\widetilde{u}_i u'_j} - \widetilde{u}'_i \widetilde{\widetilde{u}}_j - \widetilde{\widetilde{u}}_i \widetilde{u}'_j \right)$$
$$R_{ij} = \overline{\rho} \left(\widetilde{u'_i u'_j} - \widetilde{u}'_i \widetilde{u}'_j \right)$$

Figures 3.6 and 3.7 show the three parts of SGS stress tensor τ_{11} for two different filter widths, $\overline{\Delta} = 4\Delta_{DNS}$ (Fig. 3.6) and $\overline{\Delta} = 8\Delta_{DNS}$ (Fig. 3.7), where Δ_{DNS} is the characteristic size of DNS grid. Note that since the LES grid is four times coarser than the DNS grid in x and zdirections, $\Delta_{LES} = 4\Delta_{DNS}$. Hence, $\overline{\Delta} = 4\Delta_{DNS}$ would imply that the characteristic filter width and the characteristic LES grid size are the same, i.e., $\overline{\Delta} = \Delta_{LES}$. As expected, the magnitude of subgrid-scale tensor τ_{11} increases with filter width. The modified Leonard's stress component (L_{ij}) and the modified Reynolds stress component (R_{ij}) have the largest and the smallest contributions, respectively, when $\overline{\Delta} = 4\Delta_{DNS}$. However, the contribution of R_{ij} increases significantly and becomes comparable to L_{ij} near the wall and to C_{ij} away from the wall when the filter width is doubled, i.e., $\overline{\Delta} = 8\Delta_{DNS}$. This is expected since the Reynolds part of the total stress represents the unresolved scales and as the filter width is increased, the contribution of unresolved scales also increases. Henceforth, in the results and discussions of a priori assessment of SGS models we use $\overline{\Delta} = 8\Delta_{DNS}$ since it presents a greater challenge for SGS models to correctly capture the behavior of SGS stresses and



Figure 3.6: Leonard, Cross and Reynolds parts of the spanwise-averaged τ_{11} SGS stress component at x = 6 for $\overline{\Delta} = 4\Delta_{DNS}$. total stress - black solid line; L_{11} - dashed black line; C_{11} - dash-dot red line; R_{11} - blue dotted line.

fluxes.

Figure 3.8 shows the comparison between the true and the modeled values of spanwiseaveraged trace-free τ_{11} SGS stress tensor. The reported τ_{11} values are normalized by the local mean wall shear stress and are plotted against the wall-normal distance normalized by viscous length scale. Since the eddy-viscosity models assume an alignment between the stress and the strain-rate tensors and do not take into account the Leonard stress component, they compare very poorly with the true stress. On the other hand, the DMM and CSDM account



Figure 3.7: Leonard, Cross and Reynolds parts of the spanwise-averaged τ_{11} SGS stress component at x = 6 for $\overline{\Delta} = 8\Delta_{DNS}$. total stress - black solid line; L_{11} - dashed black line; C_{11} - dash-dot red line; R_{11} - blue dotted line.

for the Leonard's term and, understandably, show a better agreement with the true stress values. In fact, CSDM predicts the trend of true stress better than the DMM. These trends are reiterated in Fig. 3.9 where we compare the spanwise-averaged contours of τ_{11} . For the sake of brevity, we only compare DSM, DMM and CSDM predictions with the exact values in this figure. It is evident that the shape and levels of isocontours predicted by DMM and CSDM are similar to those considered to be exact while the DSM's predictions seem to be very poor. Between DMM and CSDM, the contours of CSDM show a greater similarity to the contours of true τ_{11} stress.

Figure 3.10 shows the spanwise-averaged plots of τ_{12} SGS stress tensor. The DSM gives a marginally improved prediction for τ_{12} as compared to τ_{11} predictions. The eddy-viscosity models assume the stress components to be proportional to the strain-rate components. Near the wall, the gradients are generally very high in the wall-normal direction as compared to the gradients parallel to the wall. This makes the x - y component of strain-rate tensor more significant and hence, a better prediction of τ_{12} . The predictions of MTSM are the poorest since the turbulent viscosity computed by the model is small compared to the turbulent viscosity computed by DSM. The DMM and CSDM again show better agreement with the true stress in comparison to other models. Again, the predictions by CSDM are qualitatively better than those of DMM.

A priori analysis of SGS models indicate that DSM and DMM correctly predict the Smagorinsky coefficient, C_s , to be zero at the wall. However, at other locations C_s values predicted by the DMM are found to be smaller and fluctuate less than those of DSM. This is consistent with the results previously reported in the literature [46]. The dynamic coefficient of CSDM is not of the same order as the dynamic coefficients of DSM or DMM. Its value is generally an order of magnitude greater than DMM or DSM. However, the fluctuations in CSDM's coefficient are smaller than those of DMM.

Figure 3.11 shows the spatial variations of the streamwise component of SGS heat flux $q_k = \overline{\rho} \left(\widetilde{u_k T} - \widetilde{u}_k \widetilde{T} \right)$ along the wall-normal direction. For eddy-viscosity type models, q_k is modeled as

$$q_k = -\frac{\overline{\rho}\nu_t}{Pr_t}\frac{\partial \widetilde{T}}{\partial x_k} \tag{3.26}$$


Figure 3.8: Spanwise-averaged values of the trace-free τ_{11} component of SGS stress tensor at (a) x = 6, (b) x = 10. Legend : open triangles = True stresses, dotted black line = Modeled-MTSM, dash-dot green line = Modeled-DSM, dashed blue line = Modeled-DMM, solid red line = Modeled-CSDM.



Figure 3.9: Spanwise-averaged isocontours of trace-free τ_{11} SGS stress component. (a) True stress, (b) Modeled-DSM, (c) Modeled-DMM, (d) Modeled-CSDM.



Figure 3.10: Spanwise-averaged values of the τ_{12} SGS stress component at (a) x = 10, (b) x = 15. See Fig. 3.8 for legend.

For the dynamic mixed model, it is modeled as,

$$q_k = -\frac{\overline{\rho}\nu_t}{Pr_t}\frac{\partial \widetilde{T}}{\partial x_k} + q_k^L \tag{3.27}$$

where \boldsymbol{q}_k^L is the Leonard part of the heat flux vector computed as,

$$q_k^L = \overline{\rho} \left(\widetilde{\widetilde{u}_k \widetilde{T}} - \widetilde{\widetilde{u}}_k \widetilde{\widetilde{T}} \right)$$

For the CSDM, the SGS heat flux is modeled as,

$$q_k = q_k^L + C_\beta q_k^F \tag{3.28}$$

$$\begin{split} q_k^F &= \overline{\rho} \left(\widetilde{\widetilde{v}_k} \widetilde{\theta} - \widetilde{\widetilde{v}_k} \widetilde{\widetilde{\theta}} \right) \\ C_\beta &= \frac{\langle [G_k - H_k] \, N_k \rangle}{\langle N_k N_k \rangle} \\ G_k &= \overline{\rho} \widetilde{\widetilde{u}_k} \widetilde{T} - \frac{\overline{\rho} \widetilde{\widetilde{u}_k} \overline{\rho} \widetilde{T}}{\overline{\rho}} \\ H_k &= \overline{\rho} \widetilde{\widetilde{\tilde{u}}_k} \widetilde{\widetilde{T}} - \frac{\overline{\rho} \widetilde{\widetilde{u}}_k \overline{\rho} \widetilde{\widetilde{T}}}{\overline{\rho}} \\ N_k &= \overline{\rho} \widetilde{\widetilde{v}_k} \widetilde{\widetilde{\theta}} - \frac{\overline{\rho} \widetilde{\widetilde{v}_k} \overline{\rho} \widetilde{\widetilde{\rho}}}{\overline{\rho}} \\ v_k &= \widetilde{u}_k - \widetilde{\widetilde{u}}_k \\ \theta &= \widetilde{T} - \widetilde{\widetilde{T}} \end{split}$$

Similar to τ_{11} and τ_{12} results shown in Figs. 3.8 and 3.10, the best predictions are given by CSDM. Similar trends are observed for other components of SGS stresses and heat fluxes.



Figure 3.11: Spanwise-averaged values of q_1 SGS heat flux component at (a) x = 10, (b) x = 15. See Fig. 3.8 for legend.

To better illustrate the performance of models, we have plotted in Fig. 3.12 and Fig. 3.13 the correlation coefficients between the true and modeled SGS stress and heat flux components. The correlations are plotted against a non-dimensional parameter termed ψ which is a measure of the filtered density gradient. The parameter ψ is similar to the parameter NS used by Wu and Martin [13] in their numerical schlieren visualizations and is defined as

$$\psi = 1.0 - \exp\left[-10.0\left(\phi - \phi_{\min}\right) / \left(\phi_{\max} - \phi_{\min}\right)\right] , \qquad (3.29)$$

where $\phi = |\nabla \overline{\rho}|$ is the magnitude of the filtered density gradient. This transformation amplifies the small density gradients in the flow. Here, we chose the data in the domain between [5.0, 0.0, 0.0] and [20.0, 1.0, 3.0] for computing the correlation coefficients. The maximum and the minimum values of ψ are then found within this domain and the interval between the minimum and maximum values is divided into 10 equal sub-intervals. The correlation coefficients for τ_{11} and q_1 corresponding to each sub-interval are shown for DSM, DMM and CSDM in Fig 3.12 and Fig 3.13. Evidently, the correlation coefficients are higher for DMM and CSDM, which is consistent with other *a priori* results we have shown in this paper. Between DMM and CSDM, the CSDM gives higher correlations, which is again consistent with other a priori results shown earlier. Interestingly, for all models the general trend is that the correlation coefficient for SGS heat fluxes, and to a lesser extent for the SGS stresses. increases with an increase in the density gradient magnitude. A possible but not definite explanation for this trend is provided in Fig. 3.14 where the amount of backscatter or reverse energy transfer from subgrid field to the resolved resolved field for various levels of ψ are shown. The backscatter occurs in the the regions where the SGS dissipation, $\varepsilon_{sgs} \equiv \tau_{ij}S_{ij}$ is positive, i.e., $\tau_{ij}\tilde{S}_{ij} > 0$. Figure 3.14 shows that the amount of backscatter generally



Figure 3.12: Correlation coefficients between the true and the modeled values of τ_{11} SGS stress for different values of density gradient parameter ψ . Legend : open circles = DSM, open triangles = DMM, open squares = CSDM.

decreases with an increase in density gradient. The SGS models tested here are expected to perform better when the transfer of energy from the unresolved to resolved scales is minimal. This is corroborated in Fig. 3.15 where it is shown that the correlation coefficient between the true and modeled SGS dissipation decreases appreciably for CSDM in the backscatter regions. The same trend is also observed for DSM and DMM, although the correlation coefficient for CSDM in the backscatter regions is still higher than other models.

Analogous to the SGS kinetic energy dissipation, ε_{sgs} , we have the SGS scalar 'dissipation', $\varepsilon_{\phi_{sgs}}$, which appears in the SGS or residual scalar variance equation. For temperature,



Figure 3.13: Correlation coefficients between the true and the modeled values of q_1 heat flux component for different values of density gradient parameter ψ . Legend : open circles = DSM, open triangles = DMM, open squares = CSDM.

the SGS scalar dissipation is defined as,

$$\varepsilon_{\phi_{sgs}} = q_k \frac{\partial \widetilde{T}}{\partial x_k} \tag{3.30}$$

The 'backscatter' for temperature occurs when the temperature variance values transfer from the unresolved to resolved fields (i.e., $\varepsilon_{\phi sgs} > 0$). Similar to that for ε_{sgs} , the backscatter for $\varepsilon_{\phi sgs}$ shown in Fig. 3.14 decreases with increasing density gradient parameter ψ , although the decrease in $\varepsilon_{\phi sgs}$ with ψ is much more pronounced than that for ε_{sgs} . This again might explain why the correlation coefficients for the SGS heat fluxes increase with increasing ψ .



Figure 3.14: Variations of backscatter with the density gradient parameter ψ .

3.5.3 A Posteriori Assessment

In the *a posteriori* assessment of SGS models, the Reynolds-averaged statistics (represented by $\langle \rangle$) are obtained by averaging in time over a period of $60\delta_{ref}/U_{\infty}$ and in the homogeneous spanwise direction. The time period used for statistical averaging was found to be sufficient for the convergence of second-order statistics. The LES statistics are compared with those obtained from the filtered DNS (FDNS) data. The FDNS data was obtained by filtering and averaging DNS data on the fly. The characteristic width of the filter function employed for LES computations and for filtering the DNS data was chosen to be twice the characteristic size of the LES grid, with filtering being performed only in x and z directions, i.e., $\overline{\Delta} = 2\sqrt{\Delta x \Delta z}$. In LES of compressible flows, the isotropic part of SGS stress (τ_{kk}) cannot be neglected. Here, to model τ_{kk} in MTSM, DSM and DMM, we use the trace of modified Leonard stress, i.e., $\tau_{kk} \approx L_{kk}$.

Figure 3.16 shows the turbulent kinetic energy profiles at x = 6. In addition to FDNS and LES results with different SGS models, we also show the profiles of DNS and LES without SGS model (No-Model). The effect of SGS model is quite clear in the turbulent kinetic energy profiles. Since in all LES calculations we use the same filtered inflow velocity, the



Figure 3.15: Correlation coefficients for the SGS dissipation, ε_{sgs} , as a function of the density gradient parameter ψ as predicted by CSDM.



Figure 3.16: Turbulent kinetic energy profiles at x = 6. Legend : open circles = DNS, open triangles = Filtered DNS, crosses = LES-No-Model, dotted black line = LES-MTSM, dash-dot green line = LES-DSM, dashed blue line = LES-DMM, solid red line = LES-CSDM.

profiles for turbulent kinetic energy are the same at inlet. However at x = 6, as shown in Fig. 3.16, the LES predictions with different SGS models significantly differ from each other. The prediction by LES with No-Model is comparable to DNS but not FDNS. In fact, LES with No-Model even slightly over-predicts the peak DNS value. On coarser grids like the ones used in our LES, without an SGS model there is an energy build-up at smaller scales which cannot be dissipated properly and leads to an over-prediction of turbulent kinetic energy and perhaps even a failure of the simulations at higher Reynolds numbers. This clearly demonstrates the necessity of SGS models. In Fig. 3.17, the 1D-energy spectra obtained by LES with No-Model, MTSM and CSDM is compared with that of FDNS. The spectra for LES with No-Model and MTSM show an over-prediction at all wavenumbers, which is consistent with the over-prediction of turbulent kinetic energy in Fig. 3.16. At higher wavenumbers, the MTSM provides a slightly better comparison than No-Model. The CSDM, on the other hand, shows a very good agreement with the FDNS spectra, particularly at higher wavenumbers where it correctly predicts the decay of energy. Comparing the spectra for FDNS and LES with No-model suggests that our numerical scheme is not excessively dissipative.



Figure 3.17: One-dimensional energy spectra in spanwise direction at x = 6 and $y \approx 0.07$.



Figure 3.18: Evolution of mean skin-friction coefficient, C_f . See Fig. 3.16 for legend.

Figure 3.18 shows the skin-friction coefficient, C_f obtained from FDNS and LES data. The skin-friction coefficient is defined as

$$C_f = \frac{1}{2} \frac{\rho_w}{\rho_\infty} \left(\frac{u_\tau}{U_\infty}\right)^2 \tag{3.31}$$

Figure 3.18 shows that the shock is strong enough for creating a small recirculation region in the flow. The predictions by various models can be compared in three different flow regions: upstream of the separation point, in the interaction region and downstream of the reattachment point. The C_f predictions by the new model (CSDM) are very good upstream of the separation point. For example, at x = 6 the difference between FDNS and CSDM results is only +1.5% (positive sign indicates over-prediction by the model). All other SGS models under-predict C_f with DSM giving the poorest prediction. At x = 6, the errors of No-Model, MTSM, DSM and DMM are -8%, -10%, -17% and -7%, respectively. It should be noted that the C_f values of FDNS and LES are identical at the inflow boundary. The inset in Fig. 3.18 shows the evolution of C_f downstream of the inflow boundary. The under-prediction of C_f by MTSM, DSM and DMM downstream of inflow boundary indicates the inability of these models to accurately model the SGS stresses. On the other hand, the new model properly accounts for the SGS effects as LES results with CSDM are very close to those of FDNS.

Table 3.3: Separation region sizes

	FDNS	No-Model	MTSM	DSM	DMM	CSDM
L_{sep}	$0.54\delta_{ref}$	$0.58\delta_{ref}$	$0.6\delta_{ref}$	$0.94\delta_{ref}$	$0.62\delta_{ref}$	$0.36\delta_{ref}$

In the interaction region, none of the SGS models are accurate and can completely capture the FDNS results. Table 3.3 shows the lengths of separation bubble obtained from FDNS and LES data. While LES with No-Model, MTSM, DSM and DMM over-predict the size of separation region with varying degrees, the FDNS results are under-predicted by CSDM. LES with No-Model, MTSM and DMM predict the onset of separation well but compared to FDNS, the mean separation point occurs earlier when DSM is employed or delayed when CSDM is used. Downstream of the reattachment point, the predictions by MTSM and CSDM are in good agreement with FDNS, although it should be noted that MTSM under-predicted C_f upstream of the mean separation point. Similar to results shown upstream of separation, LES with No-Model, DSM or DMM under-predict C_f .

Figure 3.19 shows the downstream variations of mean wall pressure normalized by the



Figure 3.19: Evolution of mean wall-pressure, P_w . See Fig. 3.16 for legend.

upstream wall pressure. It can be observed in this figure that the wall pressure begins to rise at x = 7.2 even though the nominal impingement location is at x = 10 which is due to the upstream propagation of the disturbances through the subsonic region of the boundary layer. In general, all models predict the FDNS data satisfactorily. The CSDM predicts the pressure rise at a slightly later location in comparison to other models and also in comparison to FDNS.

Figure 3.20 compares the Van Driest transformed mean streamwise velocity profiles in inner scaling at different streamwise locations. At x = 6 (not shown), the FDNS profile exhibits a log-law profile (Eq. 1.14) between $30 < y^+ < 100$. At this location, the boundary

layer is unaffected by the shock and exhibits the profile of a canonical turbulent boundary layer. Also, at this location LES results obtained by CSDM are in excellent agreement with those of FDNS. However, the results obtained by LES with No-Model, MTSM and DMM are different than those of FDNS. DSM seems to be the least accurate model. Since the velocity profiles are normalized by friction velocity, u_{τ} , the variations in the slope of logarithmic function for various models is directly related to the C_f predictions. At x = 10(Fig. 3.20(a)), just downstream of the mean reattachment point, the velocity profiles do not exhibit any logarithmic behavior although the universal near-wall $U^+ = y^+$ behavior is still obeyed. Once again, CSDM shows the best agreement with FDNS profile in comparison to other models. At x = 15 (Fig. 3.20(b)), the boundary layer starts to relax back to a canonical boundary layer profile although it has not fully recovered from the effect of adverse pressure gradient induced by the shock. At this location, the profile exhibits a logarithmic-like behavior albeit with different constants and a stronger wake region. This is very similar to a separated incompressible boundary layer [31]. All models show reasonably good agreement with FDNS at this location. Overall, the predictions by CSDM are more accurate than other tested models for mean streamwise velocity at all three streamwise locations.

Figure 3.21 compares the R_{11} Reynolds stress component obtained by DNS and LES at different locations. At x = 6 (Fig. 3.21(a)), LES with any model or with No-Model over-predicts R_{11} with No-Model giving the largest values. However, the best agreement with FDNS profile is obtained by the CSDM. At x = 10 (Fig. 3.21(b)), the peak value of R_{11} increases due to the shock and this trend is well captured by LES. Again, the best agreement with FDNS profile is obtained by CSDM. Interestingly, the LES results obtained by No-Model and those with eddy-viscosity models are very similar at this location. Similar



Figure 3.20: Van-Driest transformed mean streamwise velocity profiles in inner scaling. (a) x = 10, (b) x = 15. Black dashed line represents law of the wall. See Fig. 3.16 for legend.

trends are observed at x = 15 (not shown), although the predicted LES trends do not quite match with those of FDNS.

For the R_{22} component of Reynolds stress, Fig. 3.22 again shows a general trend of overpredicting the FDNS stresses by LES employing No-model, MTSM, DMM or even CSDM at all selected locations, even though the best prediction is by CSDM. At x = 15, the predictions by MTSM and No-Model are similar. Similar behaviors are observed for the R_{33} and R_{12} component of Reynolds stress (not shown) with the best predictions given by CSDM at all three selected locations.

3.6 3D effects of lateral walls on SBLI

Up until now, majority of the SBLI simulations have been carried out with an assumption of homogeneity in the spanwise directions. Several experimental results indicate that the lateral walls of wind tunnel influence the physics of SBLI. A recent numerical study by Garnier [66] has shown that the corner separation generated due to the presence of lateral walls reduces the effective span of the wind tunnel, strengthens the interaction and the strongest fluctuations are found at the corners. This problem has been gaining a steady interest because of its practical relevance, for example, at the inlet of a scramjet.

To examine the effect of lateral walls on SBLI, some preliminary calculations have been performed. A unique approach was adopted to overcome the specific challenges to this problem. The first challenge was to generate a realistic turbulent state at the interaction region. The presence of lateral walls meant standard inflow turbulence generation methods for boundary layers could not be used. To generate a realistic turbulent state in the interaction region, an auxiliary LES simulation was first carried out. In the auxiliary LES, a laminar



Figure 3.21: Comparisons of R_{11} Reynolds stress component obtained by DNS and LES. (a) x = 6, (b) x = 10. See Fig. 3.16 for legend.



Figure 3.22: Comparisons of R_{22} Reynolds stress component obtained by DNS and LES. (a) x = 10, (b) x = 15. See Fig. 3.16 for legend.

boundary layer profile was specified at the inflow and the boundary layer was perturbed by a blowing-suction forcing at the wall [67]. This is achieved by computing the wall-normal velocity component at the wall in a region between $a \le x \le b$ using the following relation:

$$v(x, z, t) = U_{\infty} A f(x) g(z) h(t)$$
(3.32)

where

$$f(x) = 4\sin\theta(1 - \cos\theta)/\sqrt{27}$$
$$g(z) = \sum_{l=0}^{10} Z_l \sin(2\pi l(z/L_z + \phi_l))$$
$$\sum_{l=0}^{10} Z_l = 1, \ Z_l = 1.25Z_{l+1}$$
$$h(t) = \sum_{m=0}^{5} T_m \sin(2\pi m(\beta t + \phi_m))$$
$$\sum_{l=0}^{10} T_m = 1, \ T_m = 1.25T_{m+1}$$

The amplitude for the perturbations was chosen equal to A = 0.1 and the forcing frequency, $\beta = 0.1$. The domain size for the auxiliary LES was, x = 4.5in, y = 1.3in and z = 0.5in. The blowing and suction strip was placed between $0.5in \leq x \leq 1in$. The freestream Mach number was 2.75. The Smagorinsky SGS model was used for the computations. Once the flow reached a realistic turbulent state downstream, a time history of primitive variables was stored from a selected downstream plane. This 'inflow box' was then used periodically for the main SBLI simulation. The second challenge was the generation of an impinging shock. A compression ramp with an inviscid/slip wall boundary condition at the freestream was used to generate the impinging shock. The wedge angle was equal to 6° . In Fig. 3.23 we show the y-z slices for instantaneous temperature contours. The nominal shock impingement location was at x = 3 and as can be seen in the figure, the mixing is enhanced in the interaction region and also downstream of the interaction region and there is a very significant influence of the boundary layers developing on the lateral walls. It should be noted that the spanwise width for these computations was only 0.5in which is very narrow and hence, 3D effects are expected to be very strong for narrow spanwise domain widths. A further detailed analysis is required to make a direct comparison between the cases with and without lateral walls.



Figure 3.23: Instantaneous slices of temperature contours at different streamwise locations for 3DSBLI.

3.7 Conclusions

A priori and a posteriori assessments of SGS models are made for the problem of 34^o incident shock wave interacting with a Mach 2 turbulent boundary layer via direct numerical simulation (DNS) and large-eddy simulation (LES) data. In both DNS and LES, the Euler terms of the governing equations are solved by a new seventh-order monotonicity preserving scheme while the diffusion terms are solved by a sixth-order compact finite difference scheme. The SGS stress and scalar flux models tested are the mixed time scale model (MTSM), the dynamic Smagorinsky model (DSM), the dynamic mixed model (DSM) and the new compressible serial decomposition model (CSDM).

A priori testing of the models indicate the superiority of similarity-type models like DMM and CSDM over eddy-viscosity type closures like DSM. Between DMM and CSDM, the predictions by CSDM are more accurate. The decomposition of SGS fluxes into Leonard, Cross and Reynolds components shows the importance of taking into account the Leonard component since it is a major contributor toward the total SGS stress or heat flux. For larger filter widths, the contribution of Reynolds component also becomes important since it represents the direct effect of unresolved scales. Hence, a proper modeling of this term is also necessary for accurate LES computations. The compressible serial decomposition model uses a similarity concept to model this term and it is more accurate than the eddy-viscosity type model employed by the dynamic mixed model. This is clearly reflected in the correlation coefficients computed between the true and modeled SGS stresses and heat fluxes. The correlation coefficients computed for the three dynamic models are found to increase with increasing the density gradient magnitude. A possible but by no means definite explanation for this trend can be the amount of backscatter which is shown to decrease with increasing density gradient magnitudes.

A posteriori comparisons made for mean velocity profiles and filtered Reynolds stresses indicate the significance of SGS model effect and are generally consistent with our *a priori* testing of SGS models. For a posteriori assessment of the models, special attention was made to keep the inflow boundary condition consistent in DNS and LES. Also, the characteristic filter width for a posteriori assessment was chosen to be $\overline{\Delta} = 2\Delta_{LES}$ since, (a) it presents a greater challenge for the SGS models to correctly capture SGS terms behavior, and (b) it gives a better indication of model performance for higher Reynolds number flows where the grid requirements are more demanding. The skin-friction coefficient is shown to be best predicted by CSDM in comparison to other SGS models for the incoming boundary layer. In the interaction region, however, the predictions by CSDM is not very accurate, which might be due to CSDM not being sufficiently dissipative. The performance of other models is also not adequate. Overall, the LES results obtained by CSDM are found to be comparable with the FDNS values, despite the fact that the SGS terms B_2 , B_5 , B_6 , and B_7 are neglected in our LES calculations as is done in most LES studies of compressible flows. These terms represent the interactions between the resolved and unresolved fields and non-linear effects in the filtered energy equation. It is possible that these terms could be significant in shockturbulence interactions at higher shock intensities and/or flow Mach numbers, something that has to be tested in future studies. In general, the LES results obtained by CSDM appear to be very promising. However, certain features of the model need to be improved. Also, its predictions for other compressible turbulent flows needs to be further examined.

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