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# Effect of compressibility on strong shock and turbulence interactions

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## Abstract

The interactions between turbulent flows and shock waves are important in many natural processes as well as scientific and engineering applications. One of the fundamental building blocks in these complex processes and applications is the canonical problem of isotropic turbulence and a normal shock. Unfortunately, even this fundamental problem is not well understood. Recent direct numerical simulation (DNS) results of perfect gas flow showed some new trends in turbulent statistics as mean Mach number is increased. In this paper, we first conduct extensive DNS studies on canonical strong shock and turbulence interaction problem of perfect gas flow with mean Mach numbers ranging from 2 to 30, with the emphasis on investigating the effect of compressibility. The results show that maximum values of variance of streamwise vorticity fluctuations first increase and then decrease as shock strength is increased. The peak of streamwise vorticity fluctuations is observed for shock and turbulence interactions with Mach 2.8 shock. For stronger than Mach 2.8 shocks, there is a decrease in streamwise vorticity fluctuations. The amplification of Reynolds stress $R_{11}$ decreases as mean Mach number is increased till 8.8, which is consistent with findings of linear interaction analysis. This trend, however, reverses as shock strength is increased beyond Mach 8.8. For stronger than Mach 8.8 shocks, Reynolds stress $R_{11}$ is amplified as mean Mach number keeps increasing. Since gas temperature increases dramatically after strong shocks, we are also working on DNS of non-equilibrium flow, where non-equilibrium flow effects including internal energy excitations, translation-vibration energy relaxation, and chemical reactions among different species are considered based on the 5-species air chemistry and recently thermal property models. The code and corresponding thermo-chemical models have been tested on two cases of non-equilibrium flow over cylinders.

## 1. Introduction

The interactions between turbulent flows and shock waves are important in many natural processes as well as scientific and engineering applications, such as volcanic eruption, supernova explosion, detonation, medical application of shock wave lithotripsy to break up kidney stones, and energy application of the implosion of a cryogenic fuel capsule for inertial confinement fusion where very high rates of compression and expansion waves are generally observed. These phenomena are strongly nonlinear and proven to be very complex to understand with existing tools. One of the fundamental building blocks in these complex processes and applications is the canonical problem of the interaction of isotropic turbulence and a normal shock. The underlying physics in

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strong shock and turbulence interaction is essential for better understanding of such processes and applications. Unfortunately, even this fundamental problem is not well understood.

A schematic of canonical strong shock and turbulence interaction problem is shown in Fig. 1. In such flows, the coupling between shock wave and turbulent flow is very strong. Complex linear and nonlinear mechanisms are involved which alter the dynamics of the shock motion and can cause considerable changes in the structure of turbulence and its statistical properties. This fundamental shock and turbulence interaction problem has been a challenge for experimentalists, theorists and computational researchers for more than fifty years.

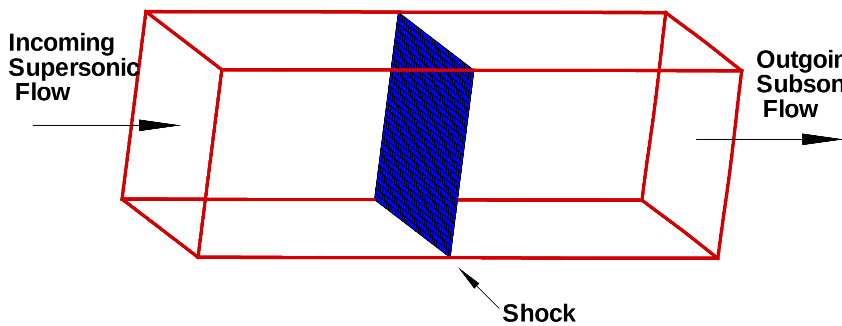



*Fig. 1. A schematic of canonical strong shock and turbulence interaction problem [1].*

## 1.1 Background

Theoretical studies in the field of shock and turbulence interaction have been attempted mostly through linear interaction analysis where small perturbations in flow are considered. Kovasznay [2] showed that for weak fluctuations of density, pressure, and entropy, turbulent fluctuations about mean uniform flow can be decomposed into vorticity, acoustic, and entropy modes. It was shown that at first-order approximation, each of these modes evolves independently in the inviscid limit. Modifications of random small fluctuations of pressure, entropy and vorticity after passing through shock or flame were studied by Moore [3] and Kerrebrock [4]. It was found that all modes of disturbances are generated in the downstream flow if any of the modes is presented in the upstream flow. More recent theoretical studies of shock and turbulence interaction were carried out by Goldstein [5], Lee et al. [6, 7], Mahesh et al. [8, 9] and Fabre et al. [10]. It was found in these studies that root mean square values of fluctuating pressure, temperature, and density as well as different components of turbulent kinetic energy are amplified across the shocks. Despite several assumptions, linear interaction analysis satisfactorily predicts essential characteristics of the interaction.

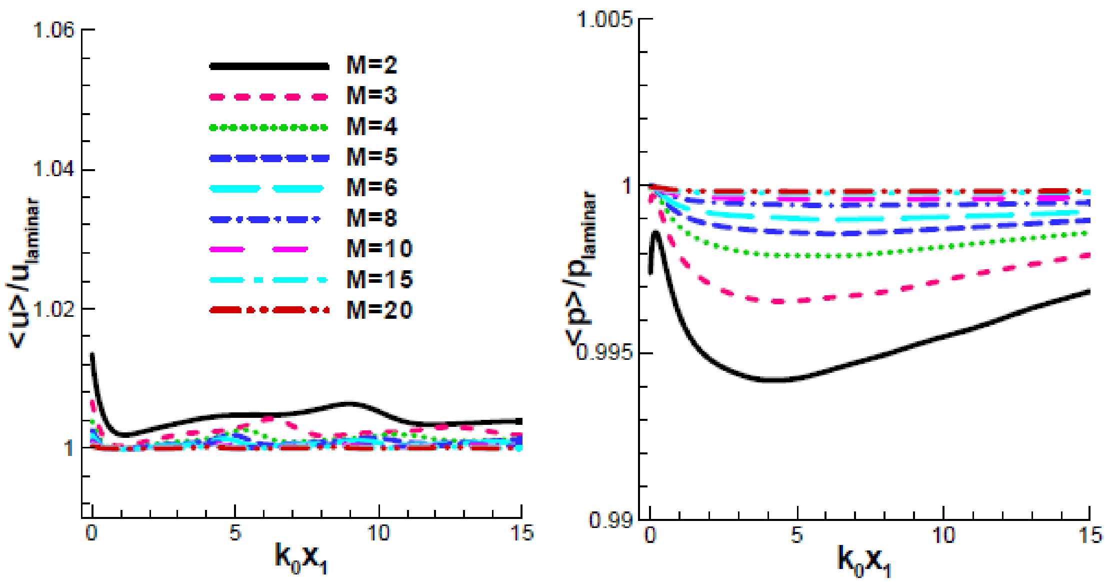
Since theoretical studies are valid only for very small perturbations, various attempts have been made towards DNS of shock and turbulence interactions since the early 80s. Initial efforts in this area were focused on the interaction of shock with simple disturbance waves. In 1981, Pao and Salas [11] fitted the shock at inflow boundary and solved Euler equation with finite difference discretization to study a shock/vortex interaction. Shock-fitting computations with pseudo-spectral (Zang et. al [12]) and spectral techniques (Hussaini et al [13, 14]) were later used to treat the problems in which a single vortex, a vortex sheet, an entropy spot or acoustic wave interacts with the shock.

The results obtained from these numerical efforts confirmed the linear theory for weak shocks. With the advent of essentially non-oscillatory (ENO) and related schemes, a number of shock-capturing schemes for compressible flows have been tested for interaction of shock with small disturbances. Although limited to low Mach numbers, these studies mostly confirm the linear interaction analysis results [14-16].

For studies of a fully turbulent field interacting with shocks, DNS methods and large eddy simulations (LES) have been used. However these different types of methods give different results when interaction with shock is considered [17]. Most of the recent DNS studies have been on various aspects of interaction of a normal shock with freestream turbulence for relatively weak shock at small Mach numbers. For example, Mahesh et al. [8, 9] did extensive DNS studies on the interaction of a normal shock with an isotropic turbulence. The mean shock Mach numbers were in the range of 1.29 to 1.8. They found that the upstream correlation between the vorticity and entropy fluctuations has strong influence on the evolution of the turbulence across the shock. Lee et al. [7] investigated the effect of Mach numbers on isotropic turbulence interacting with a shock wave. The range of Mach numbers was from 1.5 to 3.0. A shock-capturing scheme was developed to simulate the unsteady interaction of turbulence with shock waves. It was found that turbulence kinetic energy is amplified across the shock wave, and this amplification tends to saturate beyond Mach 3. Hannapel et al. [18] computed shock and turbulence interaction of a Mach 2 shock with a third-order shock-capturing scheme based on the essentially non-oscillatory (ENO) algorithm. Jamme et al. [19] carried out a DNS study of the interaction between normal shock waves of moderate strength (Mach 1.2 and Mach 1.5) and isotropic turbulence. Adams and Shariff [20, 21] proposed a class of upwind-biased finite-difference schemes with a compact stencil for shock and turbulence interaction simulation. They used the non-conservative upwind scheme in smooth region while a shock-capturing ENO scheme was turned on around discontinuities. This idea of hybrid formulation was improved by Pirozzoli [22] who used similar hybrid formulation for a compact weighted essentially non-oscillatory (WENO) scheme with conservative formulation for simulation of shock and turbulence interaction. Ducros et al. [23] conducted LES studies on shock and turbulence interaction by using a second-order finite volume scheme. The method was then used to simulate the interaction of a Mach 1.2 shock with homogeneous turbulence.

It is noticed that flows with stronger than Mach 3 shocks have not been considered in the past for shock and turbulence interaction problems. High-order shock-capturing schemes have been the methods of choice in most previous numerical simulation studies of shock and turbulence interaction [8, 9, 24, 25]. However, popular shock-capturing schemes are not very accurate in this regard as they inherently use numerical dissipation in the whole computational domain. Moreover, spurious numerical oscillations have also been observed when solving strong shock and turbulence interaction problems with shock-capturing schemes [26]. Moreover, in shock-capturing schemes, the shock spreads over a few grid points. With strong shocks, the thickness of the shock front decreases which requires more resolution for shock-capturing schemes. Thus, constraint due to choice of algorithms has been one of the main limitations in past studies. DNS results are currently available for $\mathrm{Re}_\lambda = 12 - 22$, where $\mathrm{Re}_\lambda$ is Reynolds number based Taylor microscale $\lambda$. However, the typical Reynolds number in real shock and turbulence interaction experiments are $\mathrm{Re}_\lambda = 200 - 750$ [27]. The highest Reynolds number of flow that can be resolved using DNS is bounded by the available computational resources. It was estimated that for DNS of shock and turbulence interaction with $Re_\lambda \approx 100$ around $19\times10^9$ grid points were needed [28]. Prohibitively large computational resources are needed for better understanding of realistic flow situations and inadequate computational resources have been another limitation in past studies.

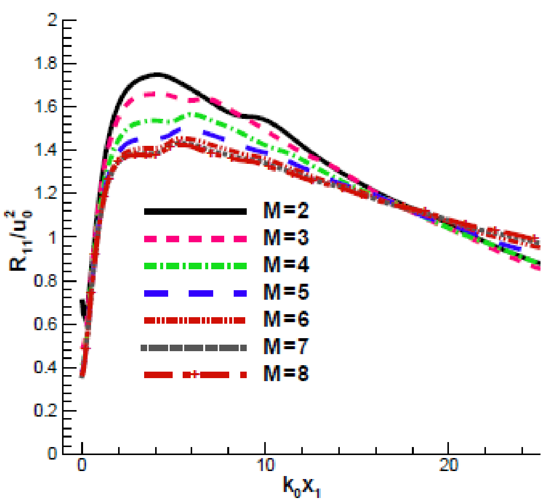
To avoid such problems in existing numerical simulation tools, Rawat and Zhong [1, 29] recently proposed a unique approach of using a high-order shock-fitting and shock-capturing method. The main shock is treated by the shock-fitting method as a sharp boundary of the computational domain. The weak or secondary shocks behind the main shock induced by interactions of the main shock and turbulence are captured by high-order shock-capturing methods. The shock dynamics is governed by a combination of shock jump conditions and a comparability relation from the flow behind main shock. In this way, the interaction of the main shock with freestream turbulence is computed accurately. Compared to shock-capturing methods, the main advantage of the shock-fitting method is uniform high-order accuracy for flow containing shock waves and no spurious oscillations [30]. On the contrary, most of the popular shock-capturing methods are only first-order accurate at the shock and may incur spurious numerical oscillations near the shock. Rawat and Zhong applied the shock-fitting method to DNS studies on strong shock and turbulence interactions of perfect gas flow. The range of shock Mach number is $M = 2-20$. Their results agreed well with those from linear theory and other numerical efforts for weaker than Mach 8 shocks. However, as they increased the shock strengths to the values beyond those considered in the past, new trends were observed. Specifically, it was found that, in post-shock turbulent flow, the mean value of streamwise velocity is larger than corresponding laminar values whereas the mean value of pressure is smaller than corresponding laminar values (Fig. 2). The difference between turbulent and laminar values decreases as shock strength is increased.




*(a) streamwise velocity* *(b) pressure*

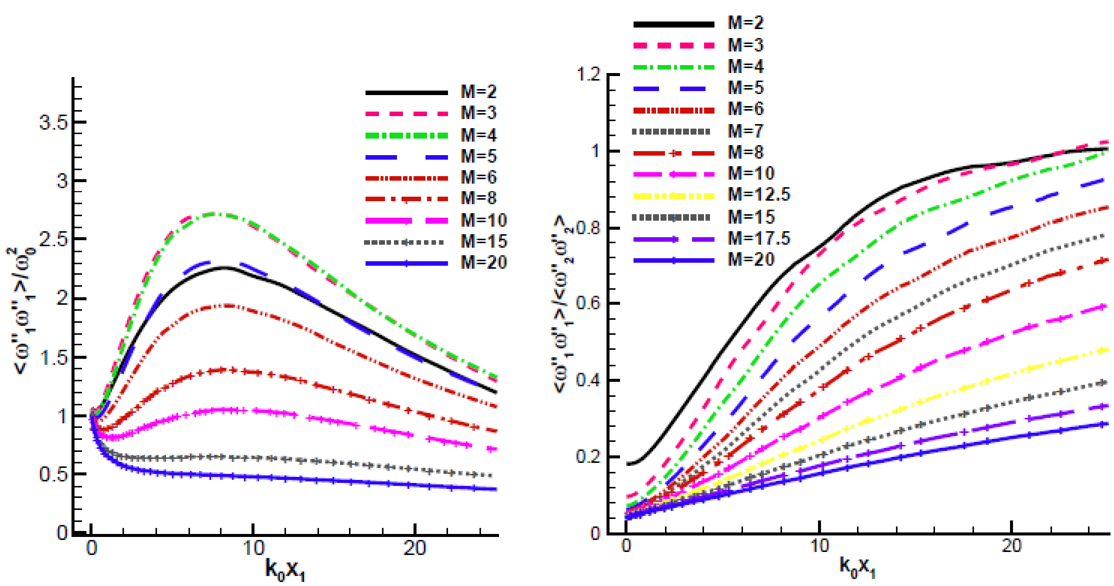
*Fig. 2. Comparison of mean values of flow variables in post-shock turbulent flow with the corresponding laminar values[29].*

Figure 3 shows the amplification in streamwise velocity fluctuations for cases with different shock Mach number. It was observed to decrease for weaker than Mach 8 shocks, which is in accordance with the linear theory results. This trend, however, reverses for stronger shocks. Same trends were observed for turbulent kinetic energy. Their calculations also showed that, contrary to the previous findings for weaker shocks, increasing shock strength does not simply increase the streamwise vorticity fluctuations. In fact, beyond a certain Mach number, amplification in streamwise vorticity fluctuations decreases and the flow's return to isotropy is delayed (Fig. 4).




*(a) M = 2-8* *(b) M = 8 - 20*

*Fig. 3. The amplification in streamwise velocity fluctuations at different shock Mach number [29]*




*(a) vorticity flucuation* *(b) variation of anisotropy*

*Fig. 4. Streamwise vorticity fluctuations values for inflow of* $Re_\lambda$ *= 29:2 and Mt = 0.124 [29]*

The above results are quite interesting and exciting. Basically, for very strong shock, new trends of turbulence statistics appear which is never observed in previous researches for weak shocks. But for turbulent flow interacting with very strong shocks, gas temperature increases dramatically after strong shocks. It is well known that thermal properties of air strongly depend on the temperature [31]. For example, at temperatures above 2000-2500 K, vibration energy mode is fully excited and $O_2$ starts dissociating. Around 4000 K, $O_2$ is completely dissociated and $N_2$ starts dissociating. Therefore, non-equilibrium flow effects including internal energy excitations, translation-vibration energy relaxation, and chemical reactions among different species need to be considered in DNS studies.

### 1.2 Objectives

A study of the literature in the field of shock and turbulence interactions shows that these complex configurations are part of a number of important applications but the current scientific understanding of strong shock and turbulence interactions in complex configurations and the ability to reliably predict these strongly nonlinear flows remain limited. We want to carry out DNS studies on large scale computations of strong shock and turbulence interactions, including non-equilibrium flow effects. The overall objective of this paper is to conduct extensive DNS studies on strong shock and turbulence interactions of perfect gas flow to obtain more quantitative results and to validate our new 3-D high-order shock-fitting code for DNS of non-equilibrium flow. DNS studies on canonical strong shock and turbulence interaction problem of perfect gas flow are extensively conducted with mean Mach numbers ranging from 2 to 30, with the emphasis on investigating the effect of compressibility.

In the past years, interest in various types of vehicles in hypersonic flow regime produced numerous structured grid based non-equilibrium flow solvers. Laura, DPLR, and US3D are the most frequently referenced and are intensively validated against each other [32]. These codes are efficient in solving non-equilibrium flows. However, they are generally second- and third-order solvers, which may not be good enough for accurate simulation of shock and turbulence interactions. We are also working on DNS studies on strong shock and turbulence interaction of non-equilibrium flow, where non-equilibrium flow effects including internal energy excitations, translation-vibration energy relaxation, and chemical reactions among different species are considered based on the 5-species air chemistry and recently thermal property models. The new shock-fitting code is implemented based on a two-temperature model. It is assumed that translational and rotational energy modes are in equilibrium at the translational temperature whereas vibration energy and electronic energy are in equilibrium at the vibration temperature. The flow solver uses the fifth-order shock-fitting method of Zhong [33] with local Lax-Friedrichs flux splitting. In this paper, a high-order shock-fitting non-equilibrium flow solver based on 5-species air chemistry and recently thermo-chemical models are implemented and tested on two cases of non-equilibrium flow over cylinders. DNS results on shock and turbulence interaction of perfect gas flow and non-equilibrium flow will be used to produce a set of highly resolved databases which will be used to develop turbulence models.

## 2. Governing equations and numerical methods

### 2.1 Governing equation

The governing equations for non-equilibrium flows based on 5-species air chemistry are Navier-Stokes equation with source terms (no radiation). Specifically, they consist of the following equations.

$$\frac{\partial \rho_s}{\partial t}+\frac{\partial}{\partial x_j}(\rho_s u_j)-\frac{\partial}{\partial x_j}(\rho D_s \frac{\partial y_s}{\partial x_j})=\omega_s \tag{1}$$

$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial x_j}(\rho u_i u_j + p\delta_{ij})-\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\mu\frac{\partial u_k}{\partial x_k}\delta_{ij}\right]=0 \tag{2}$$

$$\frac{\partial \rho E}{\partial t}+\frac{\partial}{\partial x_j}(\rho H u_j)-\frac{\partial}{\partial x_j}\left[u_i\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}u_i\mu\frac{\partial u_k}{\partial x_k}\delta_{ij}\right]$$
$$-\frac{\partial}{\partial x_j}\left(\rho\sum_{s=1}^{5}h_s D_s\frac{\partial y_s}{\partial x_j}\right)-\frac{\partial}{\partial x_j}\left(K\frac{\partial T}{\partial x_j}+K_V\frac{\partial T_V}{\partial x_j}\right)=0 \tag{3}$$

$$\frac{\partial \rho e_V}{\partial t}+\frac{\partial}{\partial x_j}(\rho e_V u_j)-\frac{\partial}{\partial x_j}(\rho\sum_{s=1}^{5}e_{V,s}D_s\frac{\partial y_s}{\partial x_j})-\frac{\partial}{\partial x_j}\left(K_V\frac{\partial T_V}{\partial x_j}\right)=\sum_{s=1}^{3}Q_{T-V,s}+\sum_{s=1}^{5}\omega_s e_{V,s} \tag{4}$$

where,

$$\rho=\sum_{s=1}^{5}\rho_s \qquad y_s=\frac{(c_s/M_s)}{\sum_{i=1}^{5}(c_i/M_i)}$$

$$p=\sum_{s=1}^{5}p_s \qquad p_s=\frac{\rho_s\bar{R}T}{M_s}$$

$$E=\frac{u_i u_i}{2}+\sum_{s=1}^{5}\frac{\rho_s e_s}{\rho} \qquad H=E+\frac{p}{\rho}$$

$\bar{R}$ is the universal gas constant. All the terms in the above governing equations are in non-dimensionalized form where important characteristics of the flow upstream of the shock are used for non-dimensionalization. Simulation of incoming isotropic turbulence is carried out as a temporal simulation in a periodic box. Initial conditions for periodic box are random fluctuations in flow variables with prescribed spectra (with $k_0$ as the most energetic wave number) and given velocity fluctuations. Root mean square (rms) values of these velocity fluctuations $u_0^*$, upstream fluid density $\rho_1^*$ and temperature $T_1^*$ are chosen to non-dimensionalize all the flow variables and functions. Length is non-dimenionalized by $k_0\lambda_0^*/2$ where $\lambda_0^*$ is the Taylor microscale. In DNS of perfect gas flow, the source terms and all terms relating to vibration energy ($K_V$ & $e_V$) are neglected. The viscosity coefficient μ is determined by the power law,

$$\mu=\mu_0(T/T_0)^{0.76} \tag{5}$$

where $\mu_0$ and $T_0$ are reference values. The thermal conductivity K is computed from the Prandtl number, which is assumed constant at 0.7. Detail models of thermal properties in DNS of non-equilibrium flow are discussed later,

The corresponding matrix form of governing equations is as follows,

$$\frac{\partial U}{\partial t}+\frac{\partial F_1}{\partial x}+\frac{\partial F_2}{\partial y}+\frac{\partial F_3}{\partial z}+\frac{\partial G_1}{\partial x}+\frac{\partial G_2}{\partial y}+\frac{\partial G_3}{\partial z}=S \tag{6}$$

Where F stands for inviscid flux,
G stands for viscous flux,
S stands for source terms.

$$U=\left(\rho_1,\rho_2,\ldots,\rho_{11},\rho u,\rho v,\rho w,\rho E,\rho e_V\right)^{\mathrm{T}}$$

The corresponding inviscid and viscous fluxes are

$$F_j=\begin{pmatrix}\rho_1 u_j\\ \rho_2 u_j\\ \vdots\\ \rho_5 u_j\\ \rho u u_j+p\delta_{1j}\\ \rho v u_j+p\delta_{2j}\\ \rho w u_j+p\delta_{3j}\\ \rho H u_j\\ \rho e_V u_j\end{pmatrix}\qquad G_j=\begin{pmatrix}\rho_1 v_{1j}\\ \rho_2 v_{2j}\\ \vdots\\ \rho_5 v_{5j}\\ -\tau_{1j}\\ -\tau_{2j}\\ -\tau_{3j}\\ -u_i\tau_{ij}+q_j+q_{Vj}+\sum_{s=1}^{5}\rho_s h_s v_{sj}\\ q_{Vj}+\sum_{s=1}^{5}\rho_s e_{V,s} v_{sj}\end{pmatrix}$$

Source term is as follows,

$$S=\begin{pmatrix}\omega_1\\ \omega_2\\ \vdots\\ \omega_5\\ 0\\ 0\\ 0\\ 0\\ \sum_{s=1}^{3}(Q_{T-V,s}+\omega_s e_{V,s})\end{pmatrix}$$

In above equations, $v_{sj}=u_{sj}-u_j$ is diffusion velocity of species s.

## 2.2 Coordinate transform

The flow solver uses structured grids, and the following grid transform is applied.

$$\begin{cases}x=x(\xi,\eta,\zeta,\tau)\\ y=y(\xi,\eta,\zeta,\tau)\\ z=z(\xi,\eta,\zeta,\tau)\\ t=\tau\end{cases}\Leftrightarrow\begin{cases}\xi=\xi(x,y,z,t)\\ \eta=\eta(x,y,z,t)\\ \zeta=\zeta(x,y,z,t)\\ \tau=t\end{cases} \tag{7}$$

Jacobian of the transform is,

$$J = \begin{vmatrix} x_\xi & y_\xi & z_\xi & 0 \\ x_\eta & y_\eta & z_\eta & 0 \\ x_\zeta & y_\zeta & z_\zeta & 0 \\ x_\tau & y_\tau & z_\tau & 1 \end{vmatrix} \tag{8}$$

With the transform relation, the governing equations in ($\xi, \eta, \zeta, \tau$) coordinate system are written as

$$\frac{\partial(JU)}{\partial\tau} + \frac{\partial\tilde{F}_1}{\partial\xi} + \frac{\partial\tilde{F}_2}{\partial\eta} + \frac{\partial\tilde{F}_3}{\partial\zeta} + \frac{\partial\tilde{G}_1}{\partial\xi} + \frac{\partial\tilde{G}_2}{\partial\eta} + \frac{\partial\tilde{G}_3}{\partial\zeta} = JS \tag{9}$$

Where

$$\tilde{F}_1 = J\xi_x F_1 + J\xi_y F_2 + J\xi_z F_3 + JU\xi_t$$
$$\tilde{F}_2 = J\eta_x F_1 + J\eta_y F_2 + J\eta_z F_3 + JU\eta_t$$
$$\tilde{F}_3 = J\zeta_x F_1 + J\zeta_y F_2 + J\zeta_z F_3 + JU\zeta_t$$
$$\tilde{G}_1 = J\xi_x G_1 + J\xi_y G_2 + J\xi_z G_3$$
$$\tilde{G}_2 = J\eta_x G_1 + J\eta_y G_2 + J\eta_z G_3$$
$$\tilde{G}_3 = J\zeta_x G_1 + J\zeta_y G_2 + J\zeta_z G_3$$

## 2.3 Numerical method

The governing equations are solved by the fifth-order shock-fitting method of Zhong [33]. For the thermally non-equilibrium and chemically reacting system (6) in the direction, $\mathrm{k} = (k_1, k_2, k_3)$, the corresponding inviscid flux term is

$$\mathrm{F} = \begin{pmatrix} \rho_1\,\mathrm{k\,u} \\ \rho_2\,\mathrm{k\,u} \\ \rho_3\,\mathrm{k\,u} \\ \rho_4\,\mathrm{k\,u} \\ \rho_5\,\mathrm{k\,u} \\ \rho u\,\mathrm{k\,u} + pk_1 \\ \rho v\,\mathrm{k\,u} + pk_2 \\ \rho w\,\mathrm{k\,u} + pk_3 \\ \rho H\,\mathrm{k\,u} \\ \rho e_V\,\mathrm{k\,u} \end{pmatrix} \tag{10}$$

Hence the Jacobian of flux is defined as,

$$\mathrm{A} = \frac{\partial\mathrm{F}}{\partial\mathrm{U}} = L\Lambda R \tag{11}$$

$$A = |\mathrm{k}| \begin{bmatrix} \tilde{U}(\delta_{sr} - c_s) & c_s n_x & c_s n_y & c_s n_z & 0 & 0 \\ \tilde{\gamma}_r n_x - \tilde{U}u & -\beta u n_x + u n_x + \tilde{U} & -\beta v n_x + u n_y & -\beta w n_x + u n_z & \beta n_x & \phi n_x \\ \tilde{\gamma}_r n_y - \tilde{U}v & -\beta u n_y + v n_x & -\beta v n_y + v n_y + \tilde{U} & -\beta w n_y + v n_z & \beta n_y & \phi n_y \\ \tilde{\gamma}_r n_z - \tilde{U}w & -\beta u n_z + w n_x & -\beta v n_z + w n_y & -\beta w n_z + w n_z + \tilde{U} & \beta n_z & \phi n_z \\ \tilde{\gamma}_r \tilde{U} - \tilde{U}H & -\beta u \tilde{U} + H n_x & -\beta v \tilde{U} + H n_y & -\beta w \tilde{U} + H n_z & \beta \tilde{U} + \tilde{U} & \phi \tilde{U} \\ -\tilde{U} e_V & e_V n_x & e_V n_y & e_V n_z & 0 & \tilde{U} \end{bmatrix}$$

$$R = \begin{bmatrix} a^2 \delta_{sr} - c_s \tilde{\gamma}_r & \beta u c_s & \beta v c_s & \beta w c_s & -\beta c_s & -\phi c_s \\ -\tilde{V} & l_x & l_y & l_z & 0 & 0 \\ -\tilde{W} & m_x & m_y & m_z & 0 & 0 \\ \tilde{\gamma}_r - \tilde{U}a & a n_x - \beta u & a n_y - \beta v & a n_z - \beta w & \beta & \phi \\ \tilde{\gamma}_r + \tilde{U}a & -a n_x - \beta u & -a n_y - \beta v & -a n_z - \beta w & \beta & \phi \\ -e_V \tilde{\gamma}_r & \beta u e_V & \beta v e_V & \beta w e_V & -\beta e_V & a^2 - \phi e_V \end{bmatrix}$$

$$L = \begin{bmatrix} \delta_{sr} / a^2 & 0 & 0 & c_s / 2a^2 & c_s / 2a^2 & 0 \\ u / a^2 & l_x & m_x & (u + a n_x) / 2a^2 & (u - a n_x) / 2a^2 & 0 \\ v / a^2 & l_y & m_y & (v + a n_y) / 2a^2 & (v - a n_y) / 2a^2 & 0 \\ w / a^2 & l_z & m_z & (w + a n_z) / 2a^2 & (w - a n_z) / 2a^2 & 0 \\ \left[ \beta (u^2 + v^2 + w^2) - \tilde{\gamma}_r \right] / \beta a^2 & \tilde{V} & \tilde{W} & (H + a\tilde{U}) / 2a^2 & (H - a\tilde{U}) / 2a^2 & -\phi / \beta a^2 \\ 0 & 0 & 0 & e_V / 2a^2 & e_V / 2a^2 & 1 / a^2 \end{bmatrix}$$

The eigenvalues of Jacobian matrix (11) are

$$\lambda_{1,2,5} = |\mathrm{k}| \tilde{U} \tag{12}$$

$$\lambda_3 = |\mathrm{k}| (\tilde{U} + a) \tag{13}$$

$$\lambda_4 = |\mathrm{k}| (\tilde{U} - a) \tag{14}$$

where subscript “s” refers to row s and species s, whereas subscript “r” refers to column r and species r. Both s and r vary from 1 to 5 in the present model. The unit vector $\mathrm{n}$ is defined from vector k as

$$\mathrm{n} = (n_x, n_y, n_z) = \frac{(k_1, k_2, k_3)}{|\mathrm{k}|}$$

$\mathrm{l} = \left( l_x, l_y, l_z \right)$ and $\mathrm{m} = \left( m_x, m_y, m_z \right)$ are two unit vectors such that $\mathrm{n}$, $\mathrm{l}$, and $\mathrm{m}$ are mutually orthogonal.

$$\tilde{U} = u n_x + v n_y + w n_z$$

$$\tilde{V} = u l_x + v l_y + w l_z$$

$$\tilde{W} = u m_x + v m_y + w m_z$$

The derivative of pressure respecting to conservative variables comes from

$$dp = \beta(d\rho E - ud\rho u - vd\rho v - wd\rho w) + \phi d\rho e_V + \tilde{\gamma}_s d\rho_s \tag{15}$$

where

$$\beta = \frac{\bar{R}}{\rho \sum_s c_s c_{v,tr}^s} \sum_{r=1}^{5} \frac{\rho_r}{M_r} \tag{16}$$

$$\phi = \frac{\bar{R}}{\rho C_{v,V}} \frac{\rho_e}{M_e} - \beta \tag{17}$$

$$\tilde{\gamma}_s = \frac{\bar{R} T_q}{M_s} + \beta \frac{u^2 + v^2 + w^2}{2} - \beta e_s - \phi e_{V,s} \tag{18}$$

$$a^2 = \sum_{s=1}^{5} c_s \tilde{\gamma}_s + \beta \left[ H - (u^2 + v^2 + w^2) \right] + \phi e_V = \left(1 + \beta\right) \frac{p}{\rho} \tag{19}$$

In equation (18), $T_q = T_V$ when s is an electron, otherwise, $T_q = T$ .

The main computational method we will use is a fifth-order shock fitting code [33]. The flow variables behind the shock are determined by Rankine-Hugoniot relations across the main shock and a characteristic compatibility relation from behind the shock. With the assumptions of "frozen" flow (no chemical reactions and energy relaxations when flow passes through the shock), the species mass fractions and vibration temperature keep constant on the two sides of the shock where translation temperature jumps across the shock. In this way, shock jumps conditions for total density, momentum and total energy are the same as those for perfect gas. In addition, the compatibility relation relating to the maximum eigenvalue in wall normal direction is used.

In shock-fitting method, the velocity and location of the shock are solved as part of the solutions. In the interior, compressible Navier-Stokes equations are solved in fully conservative form. An explicit finite difference scheme is used for spatial discretization of the governing equation, the inviscid flux terms are discretized by a fifth-order upwind scheme, and the viscous flux terms are discretized by a sixth-order central scheme. For the inviscid flux vectors, the flux Jacobians contain both positive and negative eigenvalues. A simple local Lax-Friedrichs scheme is used to split vectors into negative and positive wave fields. For example, the flux term F in Eq. (10) can be split into two terms of pure positive and negative eigenvalues as follows

$$F = F_+ + F_- \tag{20}$$

where $F_+ = \frac{1}{2}\left(F + \lambda U\right)$ and $F_- = \frac{1}{2}\left(F - \lambda U\right)$ and λ is chosen to be larger than the local maximum eigenvalue of F′.

$$\lambda = \frac{|\nabla \eta|}{J} \left( \sqrt{\left(\varepsilon c\right)^2 + u'^2} + c \right) \tag{21}$$

where

$$u' = \frac{\eta_x u + \eta_y v + \eta_z w + \eta_t}{|\nabla \eta|} \tag{22}$$

The parameter ε is a small positive constant added to adjust the smoothness of the splitting. The fluxes $F_+$ and $F_-$ contain only positive and negative eigenvalues respectively. Therefore, in the spatial discretization, the derivative of the flux F is split into two terms

$$\frac{\partial F}{\partial \eta} = \frac{\partial F_+}{\partial \eta} + \frac{\partial F_-}{\partial \eta} \tag{23}$$

where the first term on the right hand side is discretized by the upwind scheme and the second term by the downwind scheme.

The fifth-order explicit scheme utilizes a 7-point stencil and has an adjustable parameter α as follows

$$u_i' = \frac{1}{hb_i}\sum_{k=-3}^{3} a_{i+k}u_{i+k} - \frac{\alpha}{6!\,b_i}h^5\left(\frac{\partial^6 u}{\partial x^6}\right)_i + \dots \tag{24}$$

where $\alpha_{i\pm3} = \pm 1 + \frac{1}{12}\alpha,\ \alpha_{i\pm2} = \mp 9 - \frac{1}{2}\alpha,\ \alpha_{i\pm1} = \pm 45 + \frac{5}{4}\alpha,\ \alpha_i = -\frac{5}{3}\alpha$ and $b_i = 60$ . The scheme is upwind when $\alpha < 0$ and downwind when $\alpha > 0$. It becomes a 6-order central scheme when $\alpha = 0$ which is used for discretizing viscous terms. However, for shock and turbulence interaction problems, sufficiently high turbulence intensities might produce secondary shocks behind the main shock. To handle such cases, shock-capturing methods are used to solve the flow behind the main shock. All our methods are coded based on message passing interface (MPI) is used for communication in the parallel computations.

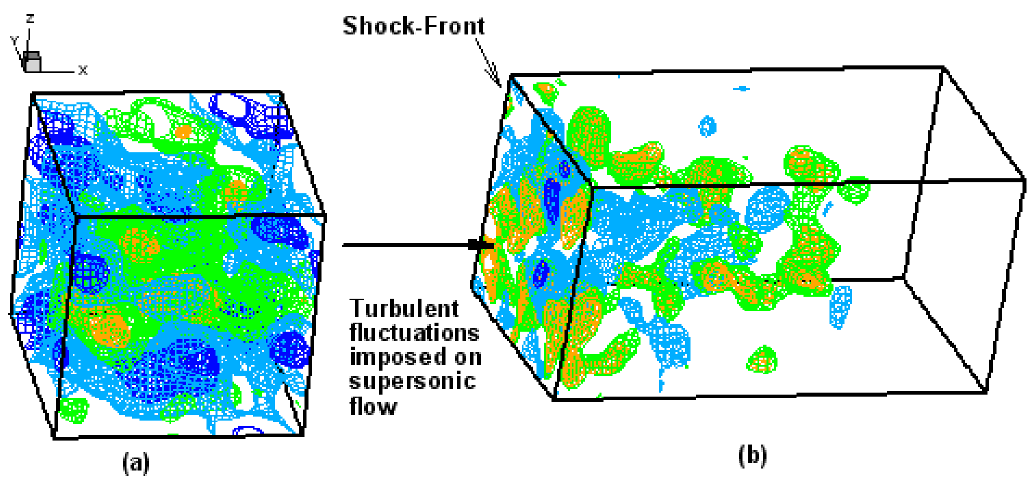



*Fig. 5. Schematic showing typical density contours and computational domains for simulation of shock-turbulence interaction using shock-fitting algorithm [1].*

With the shock-fitting algorithm for the problem shown in Fig. 1, there is no need to solve the supersonic flow upstream of the shock. Hence, computational domain for the shock-fitting method for shock and turbulence interaction consists of flow only downstream of the shock. The supersonic turbulent flow ahead of the shock can be computed in a separate simulation. A schematic of the shock-fitting implementation for the shock-turbulence interaction problem is shown in Fig. 5. The inflow turbulence is generated using a separate direct numerical simulation as shown in Fig. 5(a). We compute decaying isotropic turbulence in a periodic box to generate the realistic turbulent fluctuations that can be used as incoming turbulence for the shock-fitting algorithm. The computational domain for implementation of shock-fitting algorithm is shown in Fig. 5(b). The shock front forms the left boundary of the computational domain.

The turbulent fluctuations generated from Fig. 5(a) are imposed on supersonic flow and used as inflow condition at the shock following the Taylor's hypothesis that is valid for small turbulent intensities ($M_t < 0.5$ and $u'_{1rms} / \overline{u}_1 < 0.15$) [34]. For higher turbulent intensities, it is advisable to carry out simulation of spatially decaying turbulence which is more expensive. From the temporal simulations inside a periodic box, we obtain values of flow variables at fixed grid points of the box. Moreover, when the turbulent box is convected through the shock in the shock-fitting computations, the shock-points generally do not align with grid points of the turbulent box. Hence, values on the supersonic side of the shock are computed using interpolations. Since in our shock-fitting formulation the grids move in only one direction (X-direction in Fig. 5(b)), one dimensional Fourier interpolation is sufficient for this purpose. As a boundary condition, shock-fitting formulation needs the values of the time derivatives of conservative variables ahead of the shock according to the isotropic field which using Taylor's hypothesis are taken as appropriate spatial derivatives. Together with one characteristic coming to the shock from the high pressure side, these values determine the time derivatives at the downstream side. Thus, they are calculated from the corresponding upstream values, using the Rankine–Hugoniot conditions. Periodic boundary conditions are used in the transverse directions and non-reflecting characteristic boundary conditions are used at the subsonic exit of the computational domain.

## 3. Strong shock and turbulence interaction

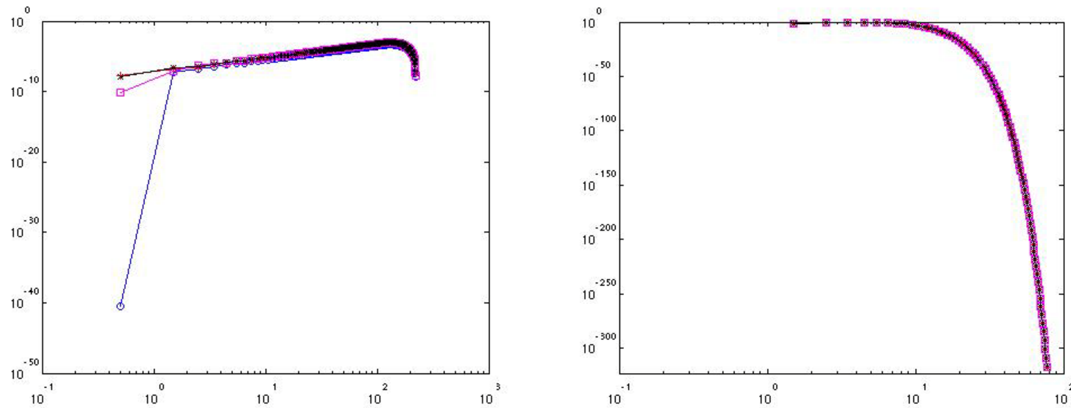
The extensive DNS studies on strong shock and turbulence interaction of perfect gas flow are similar to those of Rawat and Zhong [29]. The main objective is to obtain more quantitative results. Therefore, validation of the shock-fitting method and grid convergence of DNS results are neglected. In this paper, we conduct extensive DNS studies of canonical strong shock and turbulence interaction problem for perfect gas flow with mean Mach numbers ranging from 2 to 30, with the emphasis on investigating the effect of compressibility.

### 3.1 Decaying isotropic turbulence in the periodic box

Simulation of decaying isotropic turbulence in a periodic box is started with initial conditions generated using the algorithm given by Erlebacher et al [35]. The algorithm is based on generating random fields for fluctuations of flow variables and imposing a given spectrum. Following spectrum is imposed on the fluctuations of flow variables,

$$E(k) \propto k^4 \exp\left[-2\left(k / k_0\right)^2\right] \tag{25}$$

where $k = \sqrt{k_1^2 + k_2^2 + k_3^2}$ is the wave number of fluctuation and $k_0$ is the most energetic wave number. Figure 6 shows the energy spectra of fluctuations of flow variables before and after imposing the prescribed spectra. The fluctuation shown in Fig. 6(b) is used as initial conditions for the inflow simulation. This method offers flexibility to generate various turbulent regimes.




*(a) random fluctuations* *(b) scaled fluctuations*

*Fig. 6. Spectra of fluctuations of flow variables.*

The most important parameters that govern the physics of shock and turbulence interactions are turbulent Mach number $M_t$ and Reynolds number based on Taylor microscale $\lambda$. These quantities are defined as follows:

$$M_t = q/\overline{c} \tag{26}$$

$$\mathrm{Re}_\lambda = \overline{\rho} u_{rms} \lambda / \overline{\mu} \tag{27}$$

where,

$$q = \left(\widetilde{u_i^{"} u_i^{"}}\right)^{\frac{1}{2}} \tag{28}$$

For any given variable $f$, $\overline{f}$ denotes an ensemble average and $\tilde{f}$ is mass-weighted average i.e. $\tilde{f} = \overline{\rho f} / \overline{\rho}$. Deviation from ensemble average and mass-weighted average is denoted as $f^{'}$ and $f^{"}$ respectively. Subscript '1' has been used to denote the quantities upstream of the shock. Speed of sound is denoted as $c$, $u_{rms} = \left(\widetilde{u_1^{"2}}\right)^{1/2}$ and Taylor microscale is $\lambda = (\lambda_1 + \lambda_2 + \lambda_3)/3$ where

$$\lambda_\alpha = \left[ \overline{u'^2_\alpha} \Big/ \overline{\left( \frac{\partial u'_\alpha}{\partial x_\alpha} \right)^2} \right]^{1/2} \qquad (\alpha = 1, 2 \text{ or } 3) \tag{29}$$

With the non-dimensionalized governing equations following parameters are used as initial condition for generating initial random fluctuations: upstream mean density, $\rho_1 = 1$, temperature $T_1 = 1$, initial rms value of velocity fluctuations $u_{rms}^0 = 1$, $\mathrm{Pr} = 0.7$, $\gamma = 1.4$. Any values of initial turbulent Mach number, $M_{t0}$, and initial Reynolds number, $\mathrm{Re}_{\lambda 0}$ are can be chosen. Non-dimensionalized gas constant is given by $R = 3/\gamma M_{t0}^2$ and reference viscosity is given as $\mu_0 = \rho_1 u_{rms}^0 \lambda_0 / \mathrm{Re}_{\lambda,0}$ $\lambda_0 = 2/k_0$.

The initial conditions are assigned in a box of dimension $(2\pi)^3$ and compressible Navier-stokes equations are solved using periodic boundary conditions in all three directions until reasonably realistic turbulence is achieved. Skewness of velocity derivatives is a measure of inertial non-linearity of turbulence. Skewness of streamwise velocity derivatives is an important parameter to be monitored during the simulation of decaying isotropic turbulence, which is defined as follows,

$$S_1 = \overline{\left(\partial u_1' / \partial x_1\right)^3} \Big/ \overline{\left[\left(\partial u_1' / \partial x_1\right)^2\right]}^{3/2} \tag{30}$$

For the parameters considered here, a realistic turbulence should have $S_1$ in the range -0.4 to -0.6 [9, 24, 25]. In all of our calculations of inflow turbulence we found that $S_1$ reaches steady state in $t \sim \lambda_0 / u_{rms}^0$. Figures 7 and 8 show variations of various statistics obtained from simulations for flow with initial parameters $M_{t0} = 0.175$ and $\mathrm{Re}_{\lambda 0} = 135$, and $M_{t0} = 0.15$ and $\mathrm{Re}_{\lambda 0} = 50$, respectively. These computations were performed with $256^3$ grid points. Apart from $S_1$, we also plot turbulent Mach number, $M_t$, variance of velocity fluctuations, Reynolds number based on Taylor microscale, $\mathrm{Re}_\lambda$, and variance of dilatation fluctuations, $d = \partial u_i / \partial x_i$. It can be seen that velocity fluctuations are dissipated with the time, leading to decay in turbulent Mach number as well as Taylor microscale. Sudden increase in dilatation is due to completely solenoidal initial conditions and has been reported in previous studies as well [36, 37].

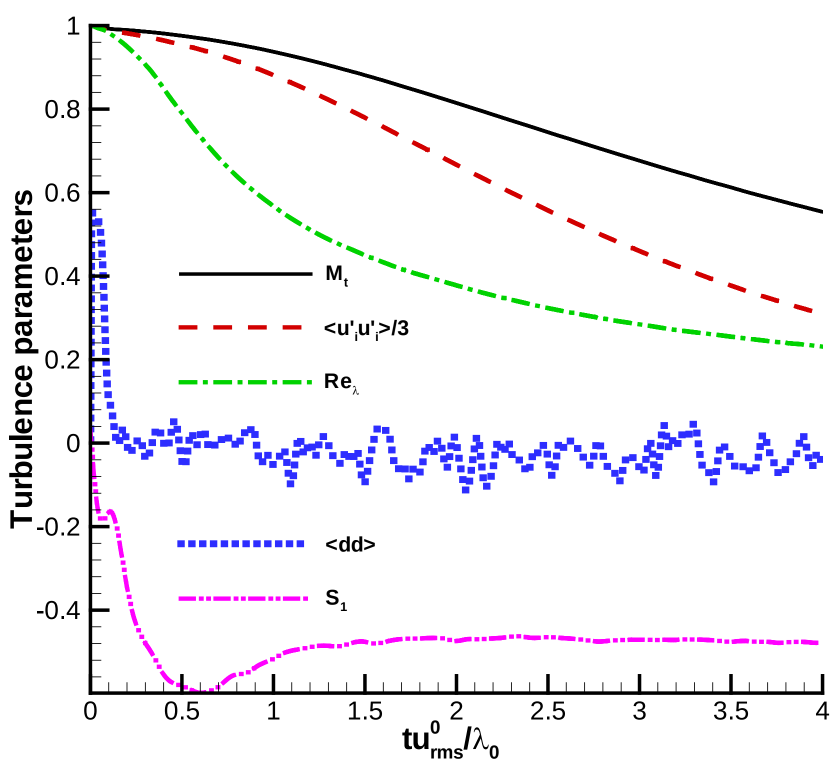



*Fig. 7. Variation of various turbulence statistics in simulation of decaying isotropic turbulence ($M_{t0} = 0.175, \mathrm{Re}_{\lambda 0} = 135$).*

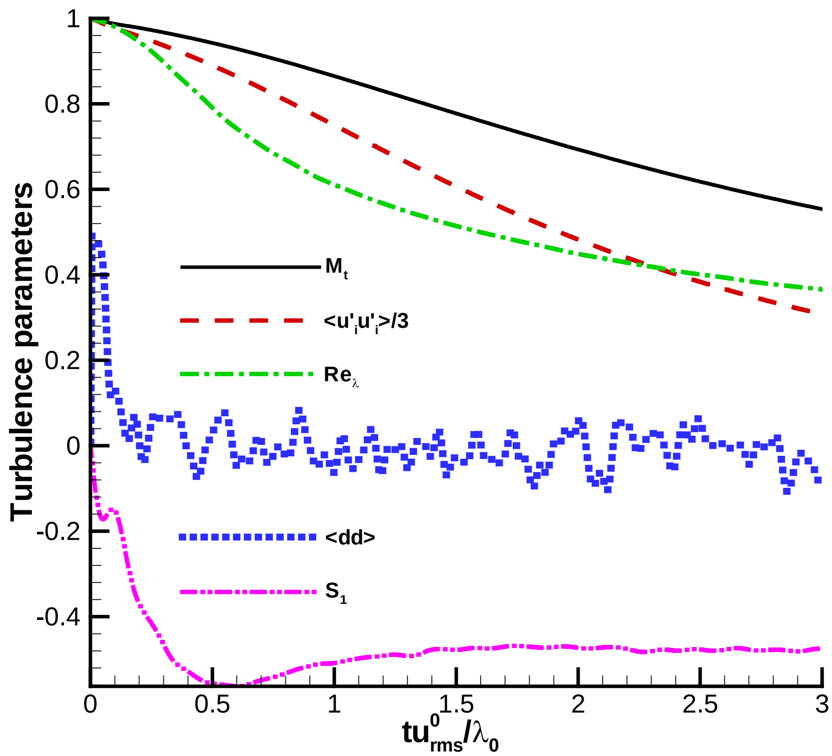



*Fig. 8. Variation of various turbulence statistics in simulation of decaying isotropic turbulence ($M_{t0} = 0.15$, $\mathrm{Re}_{\lambda 0} = 50$).*

After the skewness of velocity derivative, $S_1$, becomes steady to have value between -0.4 and -0.6, we choose a flow-field with desired values of $M_t$ and $\mathrm{Re}_\lambda$ as inflow condition for the shock-fitting computations. One can vary the flow conditions of decaying isotropic turbulence to obtain well developed realistic turbulence with desired statistical properties.

### 3.2 Shock and turbulence interaction

As discussed in previous sections, the shock-fitting method is best utilized for incoming turbulence of low turbulence intensities interacting with very strong shocks. In this paper, we present results from 4 different cases of inflow conditions which are listed in Table 1. Specifically, we compute 4 cases of DNS computations with varying incoming flow of turbulence intensities $M_t$ from 0.083 to 0.143, mean Mach number from 2 to 30, and Reynolds number, $\mathrm{Re}_\lambda$, from 18.9 to 52.4. Inflow conditions of Cases I & II are obtained from the decaying isotropic turbulence computation for flow with initial parameters $M_{t0} = 0.175$ and $\mathrm{Re}_{\lambda 0} = 135$ at $tu^0_{rms}/\lambda_0$ = 2.0 and 3.0 as shown in Fig. 7. Whereas inflow conditions of Cases III & IV are obtained from the decaying isotropic turbulence computation for flow with initial parameters $M_{t0} = 0.15$ and $\mathrm{Re}_{\lambda 0} = 50$ at

$tu_{rms}^{0}/\lambda_0$ = 2.0 and 3.0 as shown in Fig. 8. In this paper, the results from all the 4 cases of simulations are similar. Therefore, only the results of Cases I & III are discussed.

***Table 1: Cases of inflow conditions used in DNS of shock and turbulence interaction.***

| | $M_1$ | $M_t$ | $Re_\lambda$ | Grids |
|---|---|---|---|---|
| Case I | 2 - 30 | 0.143 | 52.4 | $256^2 \times 512$ |
| Case II | 10 - 30 | 0.118 | 39.4 | $256^2 \times 512$ |
| Case III | 2 - 30 | 0.104 | 23.1 | $256^2 \times 512$ |
| Case IV | 10 - 30 | 0.083 | 18.9 | $256^2 \times 512$ |

The computational domain for DNS of shock and turbulence interaction is shown in Fig. 5(b). The shock forms the left boundary of the computational domain. The turbulent fluctuations generated from Fig. 5(a) on a periodic box of dimensions $2\pi^3$ are imposed on supersonic flow and used as inflow condition at the shock. For shock-fitting computations, we use a domain of size $4\pi \times 2\pi^2$ and same non-dimensionalization is used as used for inflow computations. Uniform conditions corresponding to laminar Rankine-Hugoniot jump conditions are used as initial condition for simulation of post-shock flow. As the shock interacts with the incoming flow, transients are generated. Several flow-through of inflow box are needed before turbulence statistics in post-shock flow reach a steady state.

It is observed from previous shock-turbulence interaction simulations that turbulent fluctuations are generally much stronger just behind the shock. Hence, to appropriately resolve the flow it is advisable to cluster more grid points near the shock. The grid-spacing in transverse direction is determined by the need to resolve all the lengthscales in DNS of turbulent flow. For simulation of isotropic flows, it has been suggested that one should resolve a wavelength of $4.5\eta_s$ where $\eta_s$ is the Kolmogorov length scale for the flow in the computational domain [38]. With our high-order finite-difference scheme such resolution will require a grid spacing of $2.0\eta_s$ in transverse direction. On the upstream side of the shock, the Kolmogorov length scale is defined as $\eta_0 \approx 0.51\lambda/\sqrt{\mathrm{Re}_\lambda}$. Larsson and Lele [39] have recently presented the relation for change in Kolmogorov length scale across the shock which leads to $\eta_s \approx \eta_0 (\rho_s/\rho_u)^{-11/8} (p_s/p_u)^{3/8}$ [28]. Assuming $\lambda \approx 2/k_0$, more than $6.1 k_0 \sqrt{\mathrm{Re}_\lambda} (\rho_s/\rho_u)^{11/8} (p_s/p_u)^{-3/8}$ grids are needed in transverse directions. Based on these requirements, we chose to use 256 grid points in transverse direction.

For computations of statistics, we need averaging over transverse directions as well as in time as the turbulence behind the shock is stationary and homogeneous in spanwise directions. We found that storing and computing averages from 60 instantaneous flow-fields during time interval T is necessary for statistical convergence, where T represents the time needed for flow-through of one length of periodic box. Figure 9 shows the streamwise-streamwise Reynolds Stress, $R_{11} = \widetilde{u_1'' u_1''}$ (normalized by inflow Reynolds Stress), computed for one flow-through of inflow box at several different points in time.

These calculations are for inflow conditions of $M_1 = 30$, $M_t = 0.143$ and $\mathrm{Re}_\lambda = 52.4$. All of these cases used 60 snapshots for averaging the statistics.

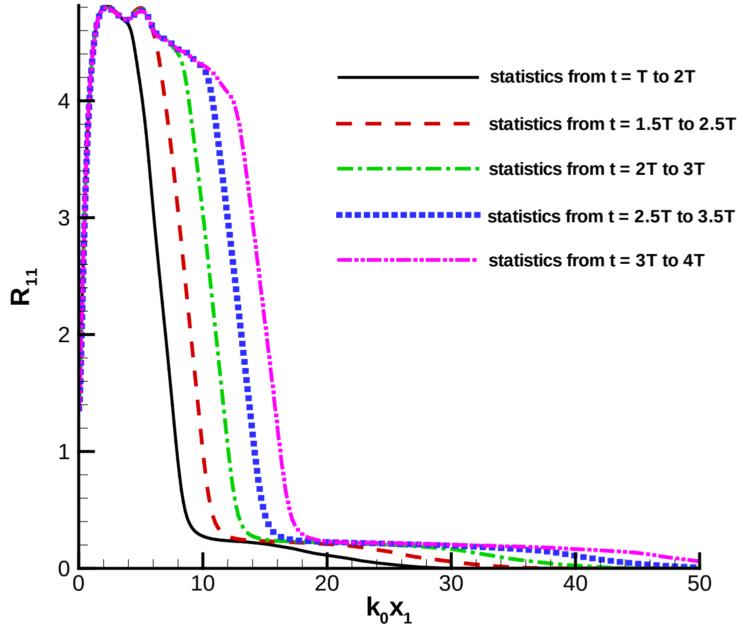



*Fig. 9. The streamwise-streamwise Reynolds stress computed using 60 snapshots of flow-fields at different points in time (case I, $M_1 = 30$).*

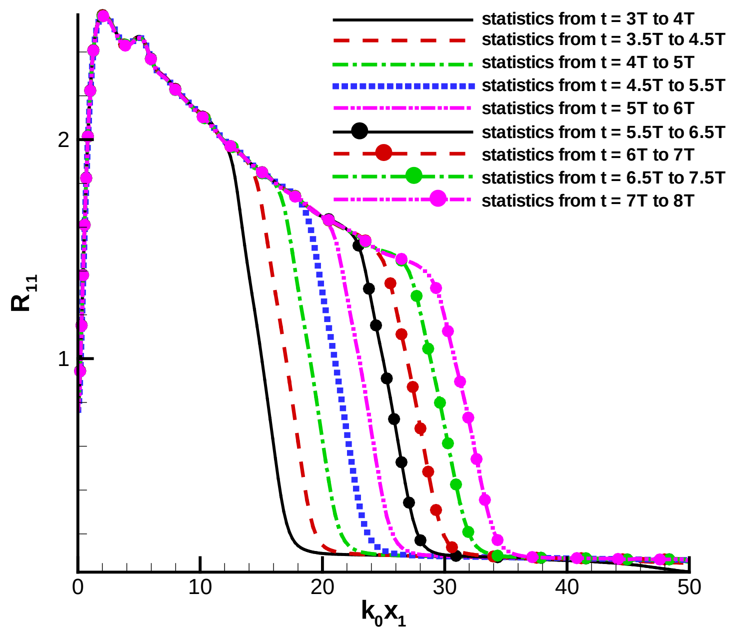


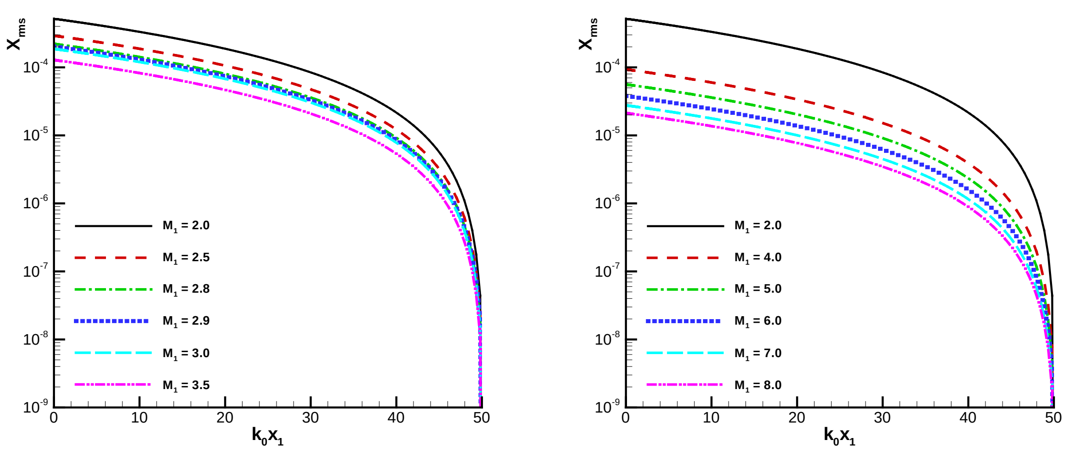

*Fig. 10. The streamwise-streamwise Reynolds stress computed using 60 snapshots of flow-fields at different points in time (case III, $M_1 = 30$).*

It can be seen that statistics reach steady state in longer region behind the shock wave as time progresses. It was observed that we obtain steady state in a region of length $14/k_0$ behind the shock after 4 flow-through lengths of the inflow. Similar statistics of the streamwise-streamwise Reynolds Stress for inflow conditions of $M_1 = 30$, $M_t = 0.104$ and $\mathrm{Re}_\lambda = 23.1$ are shown in Fig. 10. Again, it is observed that statistics reach steady state in longer region behind the shock wave as time progresses. We obtain steady state in a region of length $30/k_0$ behind the shock after 8 flow-through lengths of the inflow.

### 3.3 Effect of compressibility on shock fluctuation

In shock and turbulence interaction, the shock gets distorted. To estimate effect of compressibility on shock deformations, we plot RMS values of the fluctuations in streamwise coordinate, $x_{rms}$, in Fig. 11 for case I computations. Here, $k_0x_1 = 0$ represents the shock whereas $k_0x_1 \approx 50$ represents the exit boundary of the computational domain. It is the fluctuation of shock front that leads to the fluctuations of streamwise coordinate. At $k_0x_1 = 0$, fluctuation of streamwise coordinate is the shock fluctuation. After that, fluctuations of streamwise coordinate keep decreasing until they go to zero at $k_0x_1 = 0$. Figure 11 shows that increasing shock-strength reduces shock deformation. The result is quite reasonable. For fixed freestream isotropic turbulence, it is much difficult to distort a stronger shock.

To further examine the dependence of shock deformation on inflow parameters, we also compute results using linear interaction analysis of Mahesh [40]. Linear interaction analysis predicts shock fluctuation being almost linearly proportional to the turbulence intensity ($M_t/M_1$). The shock fluctuation predictions from linear interaction analysis assume perfectly incompressible fluctuations in inviscid fluid. Our computations, on the other hand, solve relatively viscous flows using developed turbulence. In general, for very strong shocks, it is seen that linear interaction analysis underpredicts the shock displacement fluctuations. Similar conclusion can be drawn in Fig. 12, where RMS values of the fluctuations in streamwise coordinate for case III computations are plotted.



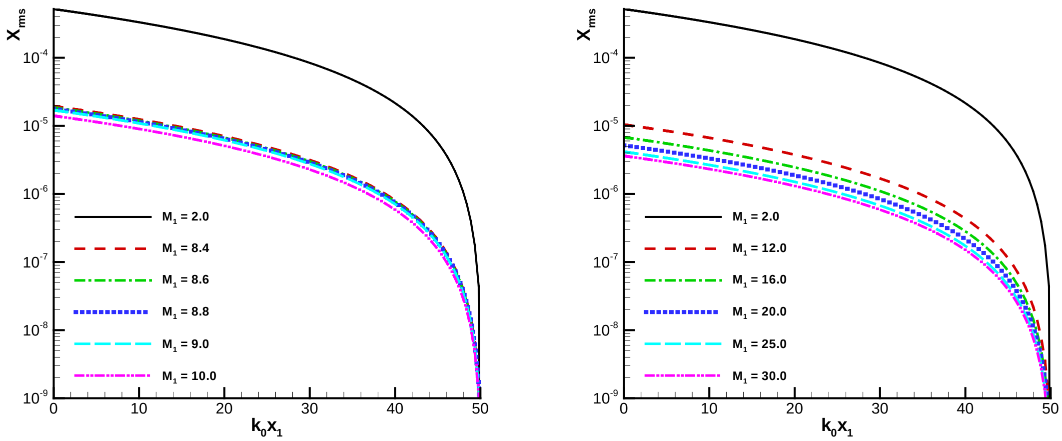



*Fig. 11. Root mean square values of fluctuations in streamwise coordinate (case I).*

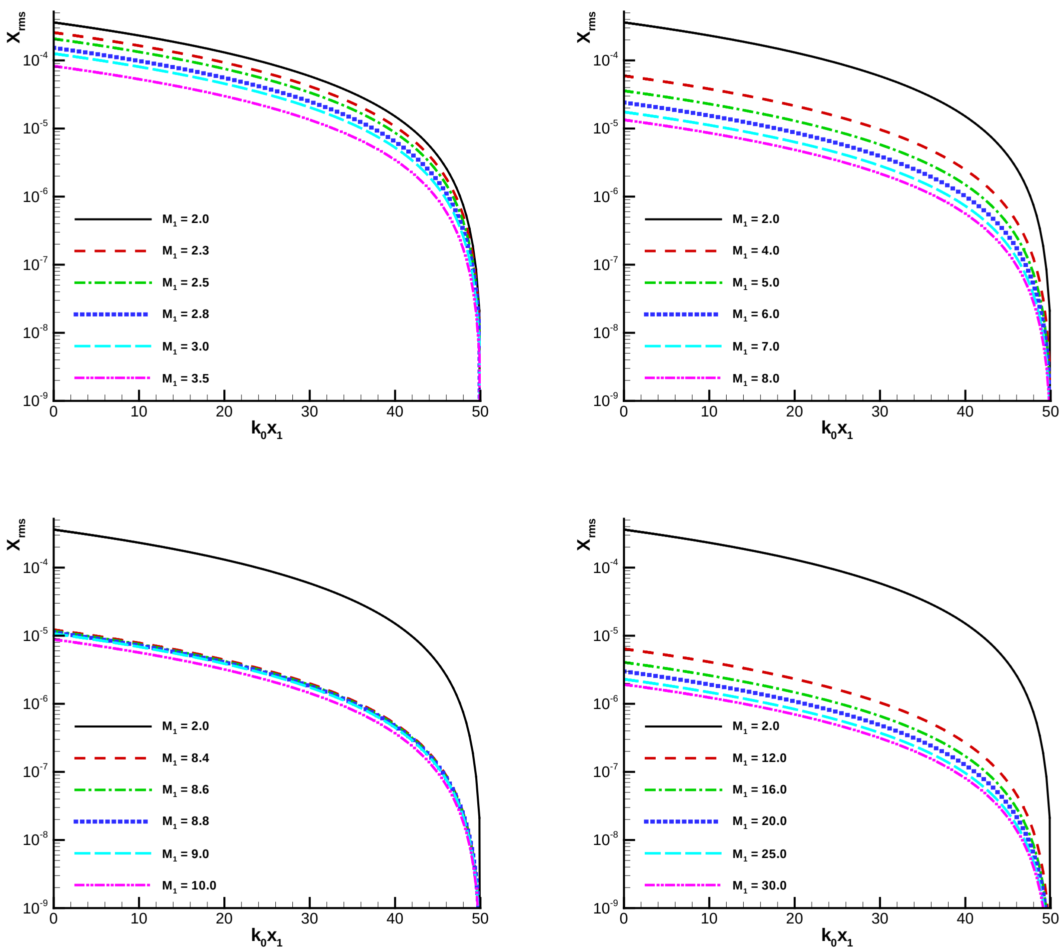



*Fig. 12. Root mean square values of fluctuations in streamwise coordinate (case III).*

### 3.4 Effect of compressibility on mean flow

For the post-shock flows in shock and turbulence interactions, the linear theory results assume fluctuations around the mean values given by Rankine-Hugoniot jump conditions. Lele [41] used results of rapid distortion theory to find shock-jump relations in turbulent flows. A drift velocity in normal shock moving through a turbulent flow was found to be necessary to sustain the laminar density ratio corresponding to the stationary shock. This corresponds to a smaller jump in mean density and pressure of turbulence flow across the shock than that predicted by jump conditions. In Figs. 13 and 14, we present the profiles of density and streamwise velocity behind the shock for inflow conditions of case I. Just downstream of the shock, mean values change rapidly. Mean velocity first decreases and then increases while mean density shows a compression of the flow followed by an expansion. It is observed that mean density behind the shock is lower than that in corresponding laminar flow, which is consistent with those reported in the literature [39]. We also observe in Figs. 13 and 14 that as mean Mach number value of incoming flow is increased at fixed values of turbulent Mach number and Reynolds number, the difference between laminar and turbulent post-shock mean values decreases.

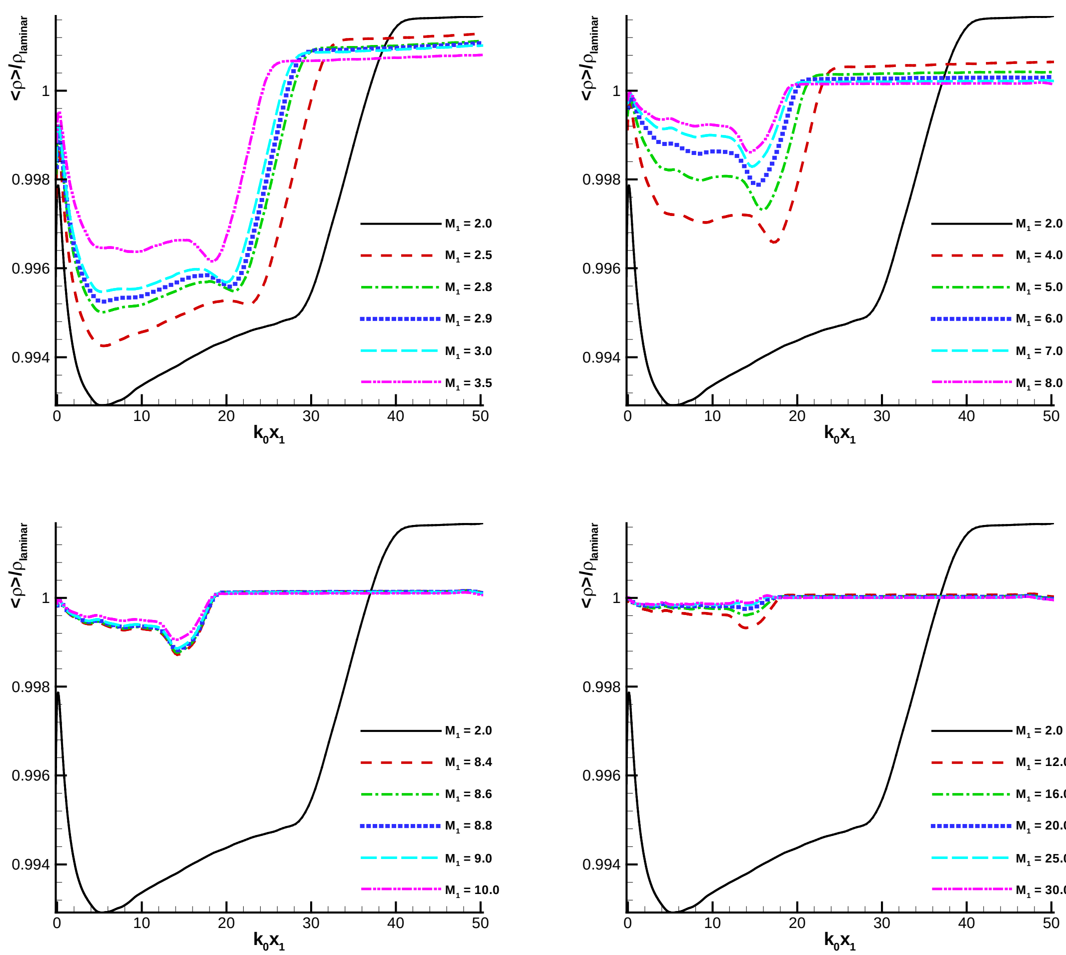



*Fig. 13. Mean values of density behind the shock for inflow conditions of case I.*

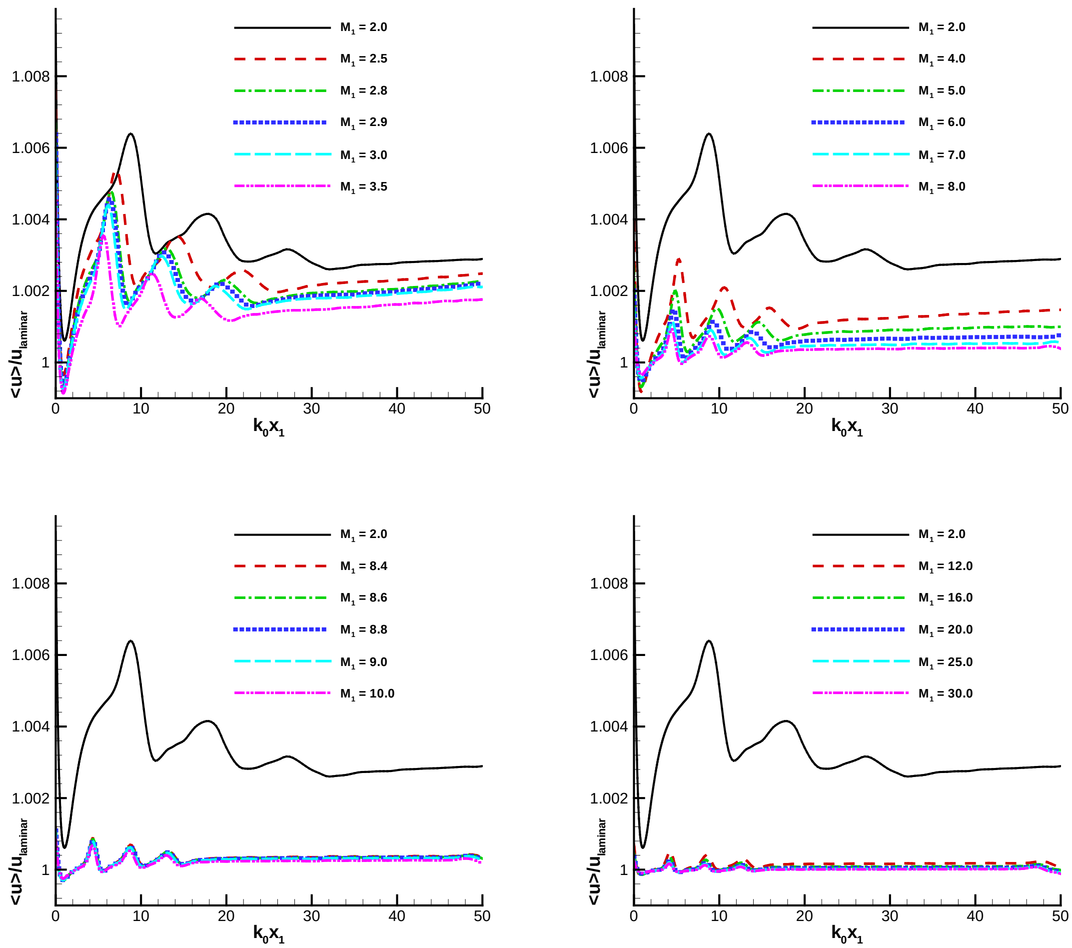
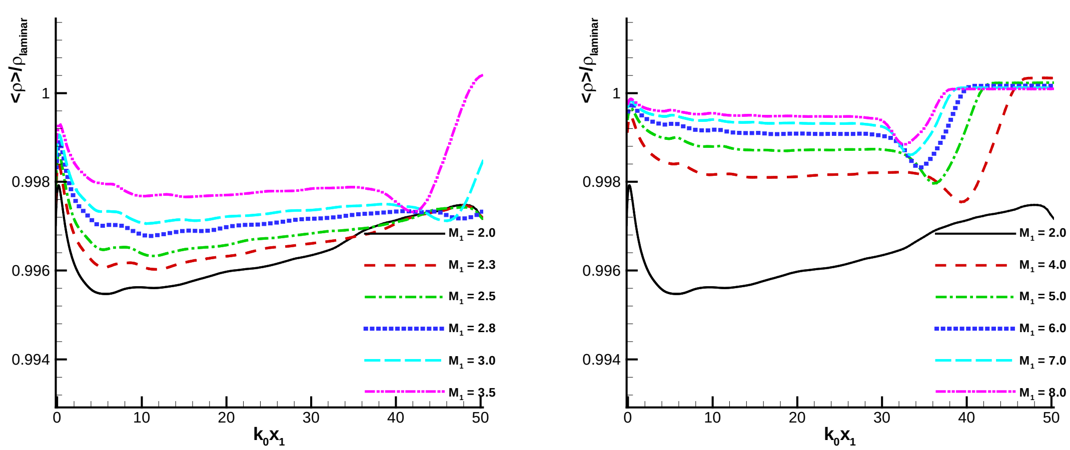



*Fig. 14. Mean values of streamwise velocity behind the shock for inflow conditions of case I.*

Again, similar conclusion can be drawn in Figs. 15 and 16, where mean values of density and streamwise velocity behind the shock for case III computations are plotted.



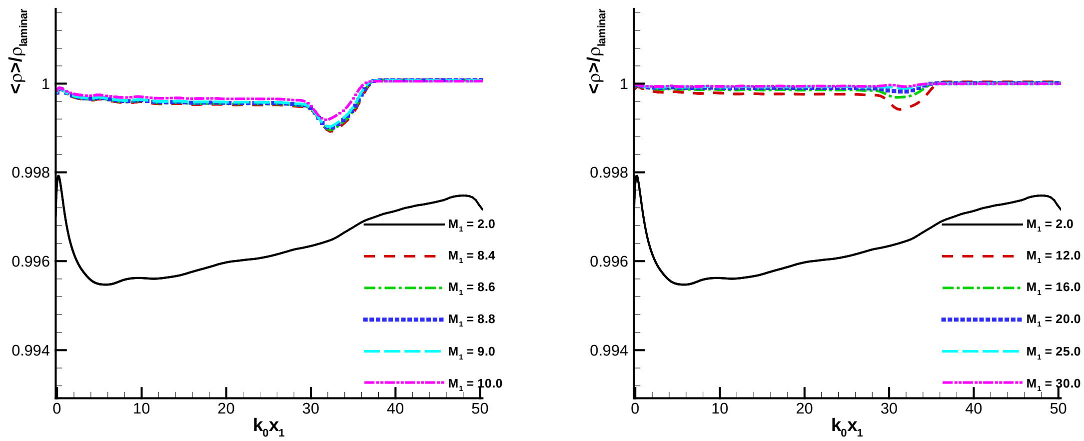



*Fig. 15. Mean values of density behind the shock for inflow conditions of case III.*

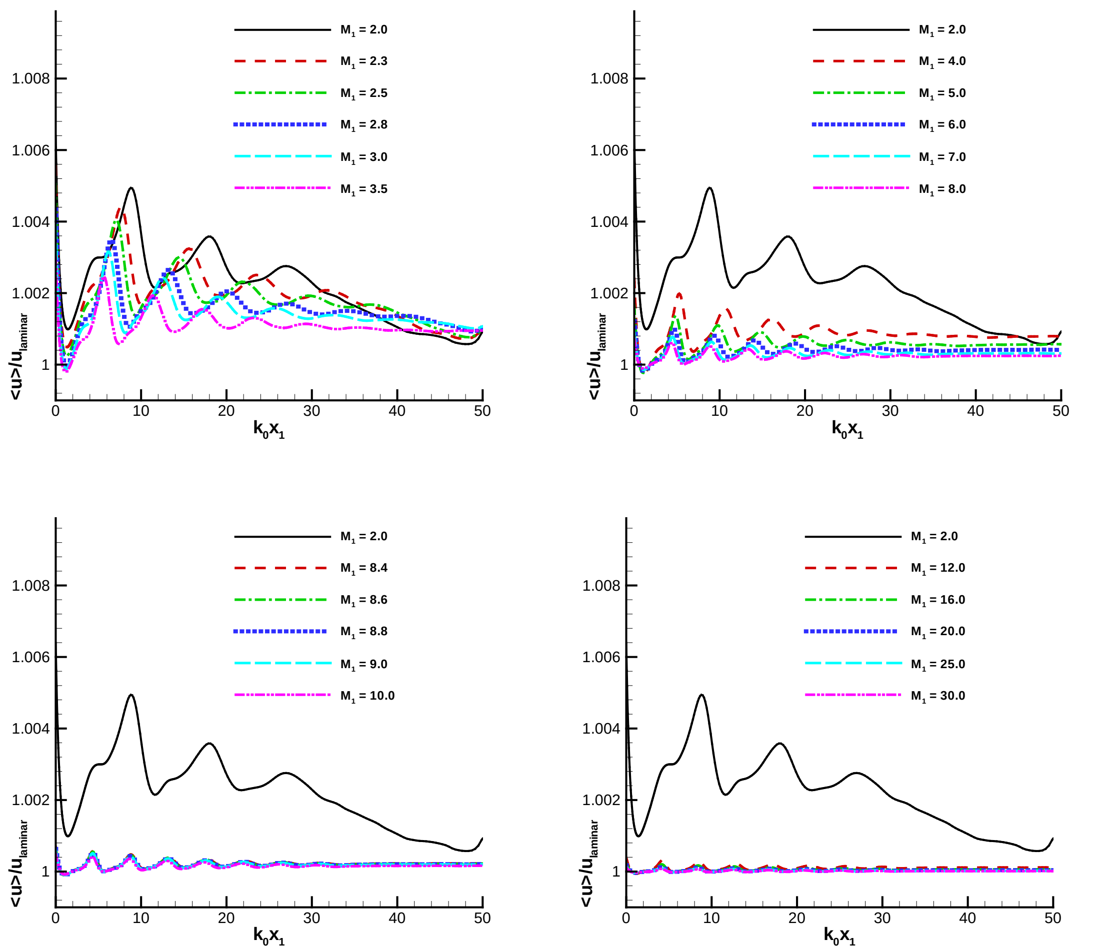



*Fig. 16. Mean values of streamwise velocity behind the shock for inflow conditions of case III.*

### 3.5 Effect of compressibility on vorticity variance

For the quasi-incompressible inflow turbulence, one of the most important contributions to the dissipation of turbulent kinetic energy is expected from the vorticity fluctuations. Linear interaction analysis predicts an increase in the transverse vorticity values which is expected to remain constant downstream of the shock. Amplitude of streamwise vorticity fluctuations is expected to remain unchanged throughout the computational domain. We observe these trends at the shock. However, downstream of the shock considerable non-linear effects are observed since both streamwise and transverse vorticity values change significantly moving away from the shock.

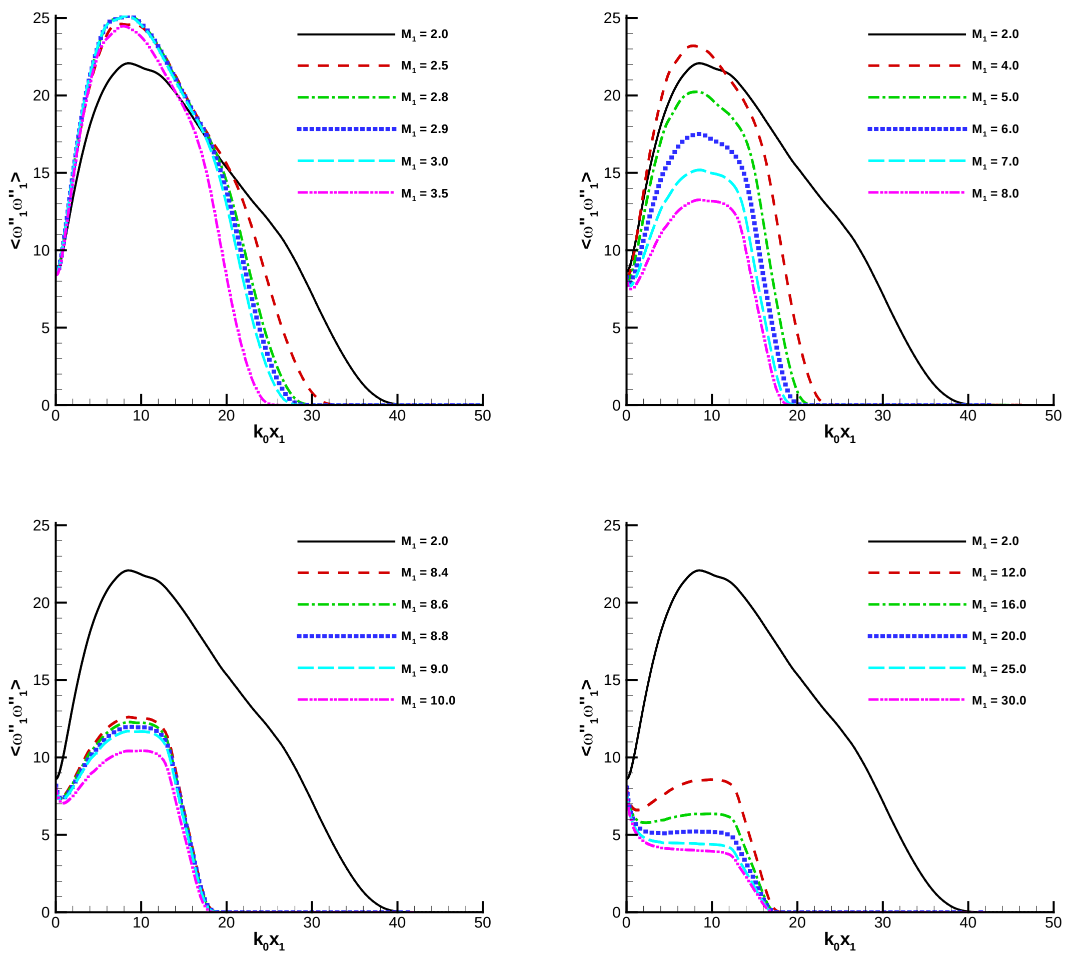



*Fig. 17. Effect of increasing mean Mach number on the variance of streamwise vorticity for inflow conditions of case I.*

Evolutions of variance in streamwise vorticity fluctuations, $\widetilde{\omega_1'' \omega_1''}$ , is presented in Figs. 17 and 18 with the varying shock strengths but using same inflow turbulence of case I and case III, respectively. Figure 17 shows that, for weaker than Mach 12 shocks in case I, streamwise vorticity increases behind the shock. In case III, Figure 18 shows that, for weaker than Mach 7 shocks, streamwise vorticity increases behind the shock. Such increase is attributed to the non-linear tilting and stretching of vorticity and has also been reported in the past studies [7, 39]. Both figures show that maximum values of variance of streamwise vorticity fluctuations first increase and then decrease as the shock strength is increased. Furthermore, the peak of streamwise vorticity fluctuations is observed for shock and turbulence interactions with Mach 2.8 shock. In past, researchers [7, 39] considered weaker than Mach 3 shocks for such comparisons and concluded that effect of increasing shock strength is to simply increase the amplification of streamwise vorticity fluctuations. Although our results agree to these trend for lower Mach numbers, we see that for stronger than Mach 2.8 flows there is a decrease in streamwise vorticity. It is observed that non-linear tilting and stretching is suppressed by the viscous dissipation and streamwise vorticity continuously decreases downstream of the shock for stronger than Mach 12 shocks in Case I and for stronger than Mach 7 shocks in Case III. Therefore, the suppression of vorticity tilting and stretching in post-shock flow strongly depends on the inflow conditions.

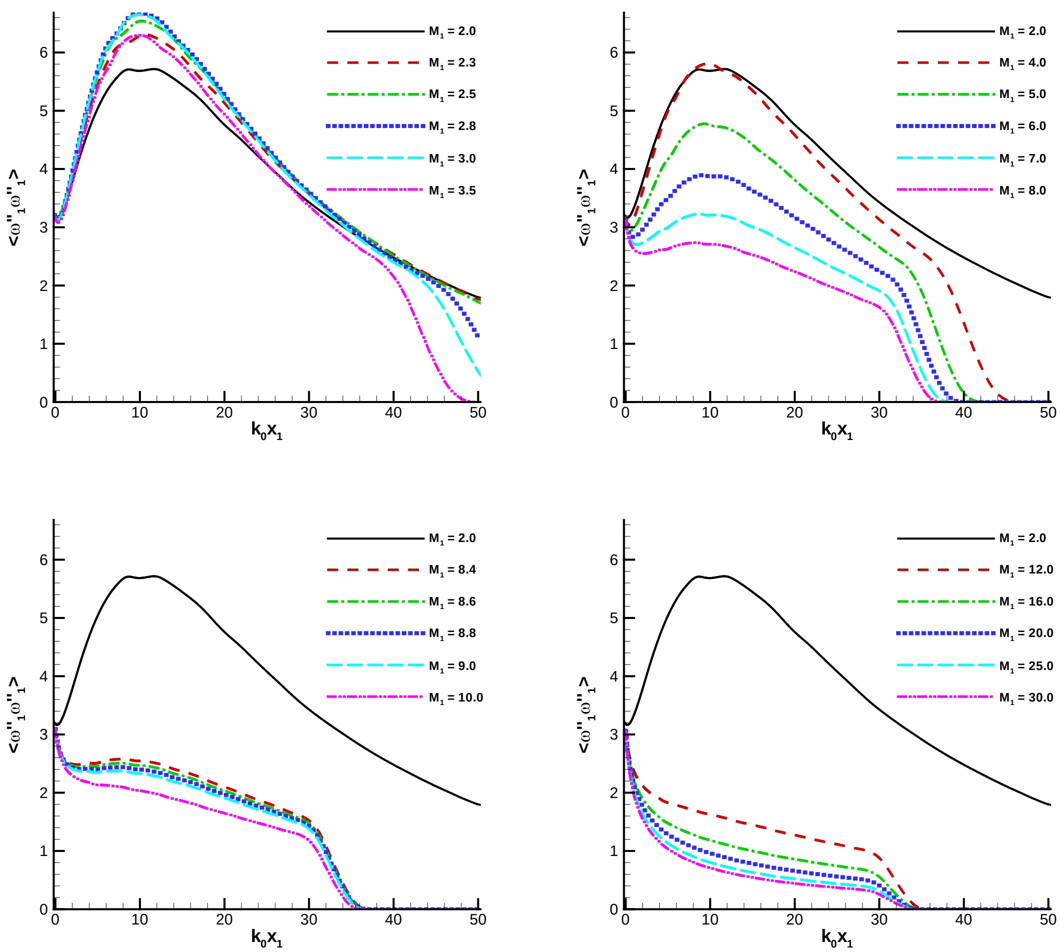



*Fig. 18. Effect of increasing mean Mach number on the variance of streamwise vorticity for inflow conditions of case III.*

### 3.6 Effect of compressibility on Reynolds stress $R_{11}$

Linear interaction analysis predicts that the amplification in turbulent kinetic energy saturates for stronger than Mach 3 shocks. Moreover, amplification of variance of streamwise-streamwise Reynolds stresses, $R_{11}$, is expected to decrease beyond Mach 3 shocks. We varied mean Mach number of the incoming flow from 2 to 30 for all cases of inflow conditions to see the effect of compressibility on shock turbulence interactions.

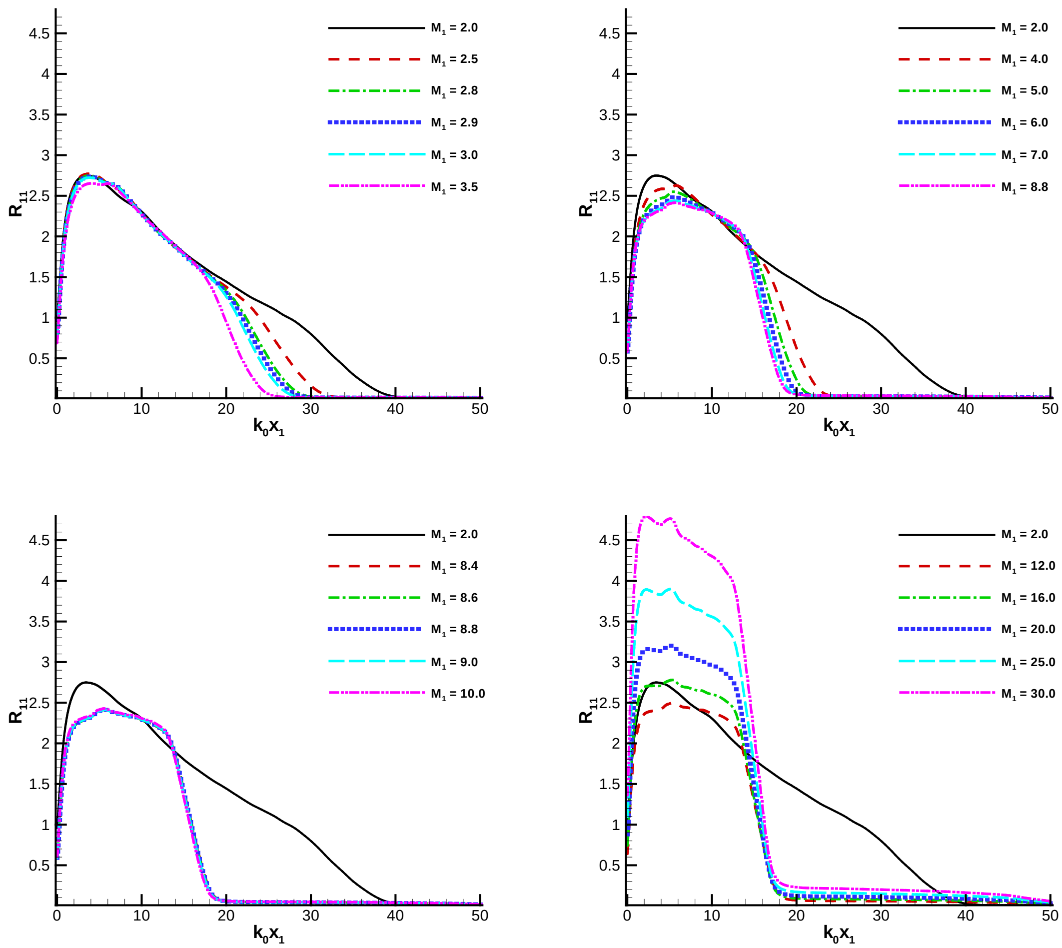



*Fig. 19. Evoluations in streamwise-streamwise Reynolds stresses for inflow conditions of case I.*

Streamwise variation of $R_{11}$ for various shock strengths is shown in Fig. 19 for inflow conditions of case I. Similar variations were observed in all the inflow cases considered in this paper. In general, the $R_{11}$ values evolve rapidly behind the shock for all the shock strengths considered and reach maximum value before $x_0 = 10/k_0$ . It is observed that maximum amplification of Reynolds stress $R_{11}$ decreases as the Mach number of the mean flow is increased till 8.8. The decrease in $R_{11}$ is consistent with findings of linear interaction analysis. This trend, however, reverses as shock strength is increased beyond Mach 8.8. For stronger than Mach 8.8 shocks, the Reynolds stress $R_{11}$

is amplified as mean Mach number is increased. Similar conclusion can be drawn in Fig. 20, where streamwise variation of $R_{11}$ for various shock strengths for inflow conditions of case III is shown.

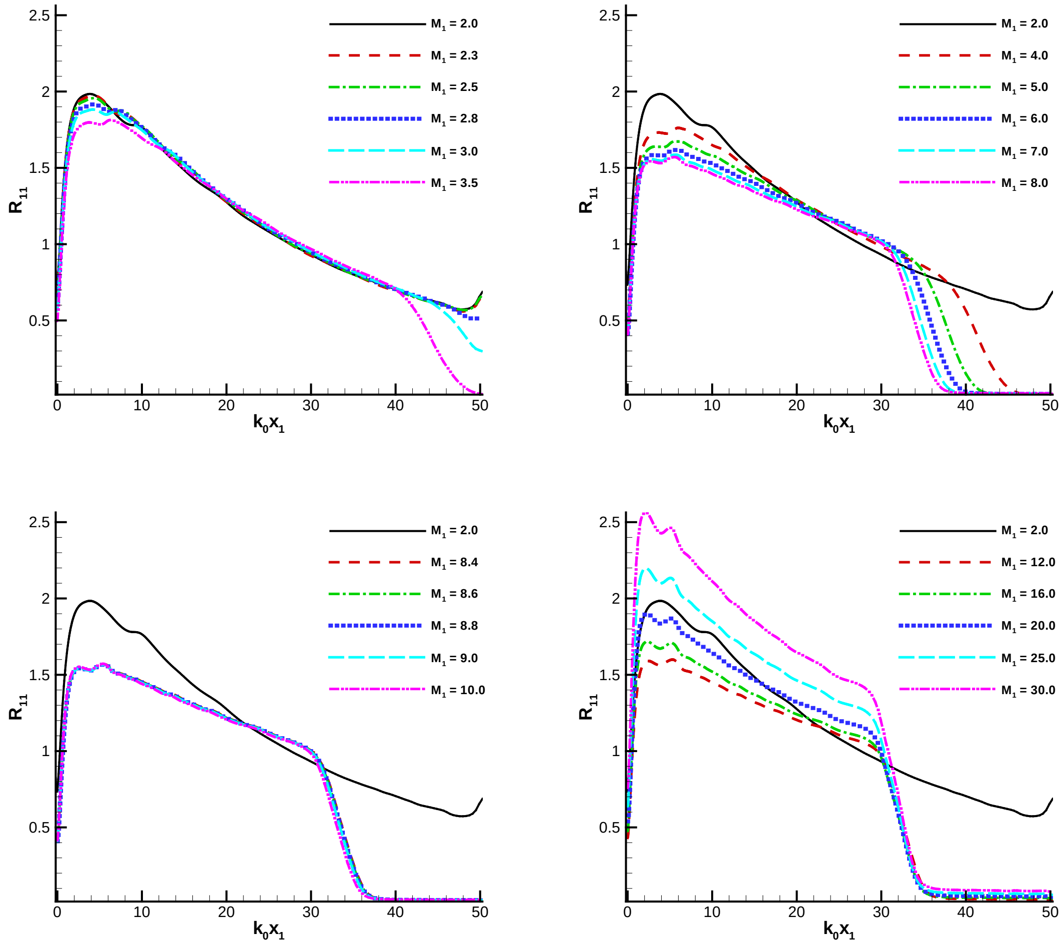



*Fig. 20. Evoluations in streamwise-streamwise Reynolds stresses for inflow conditions of case III.*

## 4. Non-equilibrium models

### 4.1 Model of vibration and electron energy

To consider the high temperature effects, the model of vibration and electron energy used in Hash et al.'s paper [32] are implemented in the code. Vibration energy and electron energy are considered separately with different formula. Specific total enthalpy of species and specific heat in constant pressure of species are defined as,

$$h_s = c_{vs}T + \frac{p_s}{\rho_s} + E_V + h_s^0 \tag{31}$$

$$c_p^s = c_v^s + \frac{\overline{R}}{M_s} + c_V^s \tag{32}$$

where $h_s^0$ is the generation enthalpy of species. The variables on the right hand side of equations (31) and (32) are calculated from the following formula,

$$E_V = (e_v + e_{els}) = \frac{\bar{R}}{M_s}\left( \sum_{s=1}^{3} \frac{\theta_{vs}}{e^{\theta_{vs}/T_V} - 1} + \sum_{s=1}^{5} \frac{\sum_{i=1}^{\infty} g_{i,s}\theta_{el,i,s} \exp(-\theta_{el,i,s}/T_V)}{\sum_{i=0}^{\infty} g_{i,s} \exp(-\theta_{el,i,s}/T_V)} \right)$$

$$c_v^s = c_{vtr,s} + c_{vrot,s} \quad c_{vtr,s} = \frac{3\bar{R}}{2M_s} \qquad c_{vrot,s} = \begin{cases} \frac{\bar{R}}{M_s} & (s = 1,3) \\ 0 & (otherwise) \end{cases}$$

$$c_V^s = \frac{\bar{R}}{M_s}\left\{ \frac{(\theta_{vs}/T_V)^2 e^{\theta_{vs}/T_V}}{\left(e^{\theta_{vs}/T_V} - 1\right)^2} + \frac{\left[\sum_{i=1}^{\infty} g_{i,s} \left(\theta_{el,i,s}/T_V\right)^2 \exp(-\theta_{el,i,s}/T_V)\right]}{\sum_{i=0}^{\infty} g_{i,s} \exp(-\theta_{el,i,s}/T_V)} \right.$$
$$\left. - \frac{\left[\sum_{i=1}^{\infty} g_{i,s}\theta_{el,i,s} \exp(-\theta_{el,i,s}/T_V)\right]\left[\sum_{i=0}^{\infty} g_{i,s} \left(\theta_{el,i,s}/T_V^2\right) \exp(-\theta_{el,i,s}/T_V)\right]}{\left(\sum_{i=0}^{\infty} g_{i,s} \exp(-\theta_{el,i,s}/T_V)\right)^2} \right\}$$

The related parameters are listed in Table 2 and Table 3.

Table 2. Electronic energy states for 5-species air

| Species | Θ (K) | g | Species | Θ (K) | g | Species | ΘO (K) | g |
|---|---|---|---|---|---|---|---|---|
| N2 | 0 | 1 | O2 | 1.13916e4 | 2 | NO | 8.88608e4 | 4 |
| N2 | 7.22316e4 | 3 | O2 | 1.89847e4 | 1 | NO | 8.98176e4 | 4 |
| N2 | 8.57786e4 | 6 | O2 | 4.75597e4 | 1 | NO | 8.98845e4 | 2 |
| N2 | 8.60503e4 | 6 | O2 | 4.99124e4 | 6 | NO | 9.04270e4 | 2 |
| N2 | 9.53512e4 | 3 | O2 | 5.09227e4 | 3 | NO | 9.06428e4 | 2 |
| N2 | 9.80564e4 | 1 | O2 | 7.18986e4 | 3 | NO | 9.11176e4 | 4 |
| N2 | 9.96827e4 | 2 | NO | 0 | 4 | N | 0 | 4 |
| N2 | 1.04898e5 | 2 | NO | 5.46735e4 | 8 | N | 2.76647e4 | 10 |
| N2 | 1.11649e5 | 5 | NO | 6.31714e4 | 2 | N | 4.14931e4 | 6 |
| N2 | 1.22584e5 | 1 | NO | 6.59945e4 | 4 | O | 0 | 5 |
| N2 | 1.24886e5 | 6 | NO | 6.90612e4 | 4 | O | 2.27708e2 | 3 |
| N2 | 1.28248e5 | 6 | NO | 7.0500e4 | 4 | O | 3.26569e2 | 1 |
| N2 | 1.33806e5 | 10 | NO | 7.49106e4 | 4 | O | 2.28303e4 | 5 |
| N2 | 1.40430e5 | 6 | NO | 7.62888e4 | 2 | O | 4.86199e4 | 1 |
| N2 | 1.50496e5 | 6 | NO | 8.67619e4 | 4 | | | |
| O2 | 0 | 3 | NO | 8.71443e4 | 2 | | | |

Table 3. Parameters used vibration energy model

| *Species* | $h_s^0$ (J/kg) | $M_s$ (g) | $\theta_{vs}$ (K) |
|---|---|---|---|
| N2 | 0 | 28 | 3395 |
| O2 | 0 | 32 | 2239 |
| NO | 2.996123e6 | 30 | 2817 |
| N | 3.362161e7 | 14 | - |
| O | 1.543119e7 | 16 | - |

### 4.2 Thermal properties

For the 5-species air, a more complex model of thermal properties is applied [42]. According to this model, thermal properties are calculated as follows,

$$\mu = \sum_s \frac{m_s \gamma_s}{\sum_r \gamma_r \Delta_{sr}^{(2)}(T)} \ \textbf{(g/cm-sec)} \tag{33}$$

$$K_T = \frac{15}{4} k \sum_s \frac{\gamma_s}{\sum_r a_{sr} \gamma_r \Delta_{sr}^{(2)}(T)} \ \textbf{(J/cm-sec-K)} \tag{34}$$

In above equation, $a_{sr} = 1 + \dfrac{\left[1-(m_s/m_r)\right]\left[0.45-2.54(m_s/m_r)\right]}{\left[1+(m_s/m_r)\right]^2}$

$$K_R = k \sum_{s=1,2,3} \frac{\gamma_s}{\sum_r \gamma_r \Delta_{sr}^{(1)}(T)} \ \textbf{(J/cm-sec-K)} \tag{35}$$

$$K_{V-E} = k \frac{C_{V,V}}{R} \sum_{s=1}^{5} \frac{\gamma_s}{\sum_r \gamma_r \Delta_{sr}^{(1)}(T)} \ \textbf{(J/cm-sec-K)} \tag{36}$$

To calculate viscosity and heat conductivity, from equation (33) to equation (36), the collision terms are as follows,

$$\Delta_{sr}^{(1)}(T) = \frac{8}{3}\left[\frac{2 m_s m_r}{\pi R T (m_s + m_r)}\right]^{1/2} 10^{-20} \pi \Omega_{sr}^{(1,1)}(T) \ \textbf{(cm-sec)}$$

$$\Delta_{sr}^{(2)}(T) = \frac{16}{3}\left[\frac{2 m_s m_r}{\pi R T (m_s + m_r)}\right]^{1/2} 10^{-20} \pi \Omega_{sr}^{(2,2)}(T) \ \textbf{(cm-sec)}$$

Collision integrals involving neutrals (Non-Coulombic collision integrals) are

$$\pi \Omega_{sr}^{(l,j)}(T) = D T^{\left[A(\ln T)^2 + B \ln T + C\right]} \ (\overset{0}{\mathrm{A}}{}^2) \tag{37}$$

Species diffusion coefficients are defined as,

$$D_s = \frac{(1-y_s)}{\sum_{r \neq s} (y_r / D_{sr})} \tag{38}$$

where $y_s$ is the molar fraction. For binary diffusion between heavy particles,

$$D_{sr} = \frac{kT}{p\Delta_{sr}^{(1)}(T)}$$

### 4.3 Chemical source terms

Five reactions are considered for the five species air, i.e.,

$$N_2 + M = 2N + M$$
$$O_2 + M = 2O + M$$
$$NO + M = N + O + M$$
$$N_2 + O = NO + N$$
$$NO + O = O_2 + N$$

Correspondingly, the reaction rates are calculated as follows,

$$R_1 = \sum_m \left[ -k_{f_1 m} \frac{\rho_{N_2}}{M_{N_2}} \frac{\rho_m}{M_m} + k_{b_1 m} \frac{\rho_N}{M_N} \frac{\rho_N}{M_N} \frac{\rho_m}{M_m} \right]$$
$$R_2 = \sum_m \left[ -k_{f_2 m} \frac{\rho_{O_2}}{M_{O_2}} \frac{\rho_m}{M_m} + k_{b_2 m} \frac{\rho_O}{M_O} \frac{\rho_O}{M_O} \frac{\rho_m}{M_m} \right]$$
$$R_3 = \sum_m \left[ -k_{f_3 m} \frac{\rho_{NO}}{M_{NO}} \frac{\rho_m}{M_m} + k_{b_3 m} \frac{\rho_N}{M_N} \frac{\rho_O}{M_O} \frac{\rho_m}{M_m} \right]$$
$$R_4 = -k_{f_4} \frac{\rho_{N_2}}{M_{N_2}} \frac{\rho_O}{M_O} + k_{b_4} \frac{\rho_{NO}}{M_{NO}} \frac{\rho_N}{M_N}$$
$$R_5 = -k_{f_5} \frac{\rho_{NO}}{M_{NO}} \frac{\rho_O}{M_O} + k_{b_5} \frac{\rho_{O_2}}{M_{O_2}} \frac{\rho_N}{M_N}$$

Finally, the source terms are as follows,

$$\begin{cases} \omega_{N_2} = M_{N_2}(R_1 + R_4) \\ \omega_{O_2} = M_{O_2}(R_2 - R_5) \\ \omega_{NO} = M_{NO}(R_3 - R_4 + R_5) \\ \omega_N = M_N(-2R_1 - R_3 - R_4 - R_5) \\ \omega_O = M_O(-2R_2 - R_3 + R_4 + R_5) \end{cases}$$

The forward and backward reaction rate coefficients have the form of

$$k_f\left(\bar{T}\right) = C_f \bar{T}^{\eta_f} \exp\left(-\theta_f / \bar{T}\right)$$
$$k_b\left(T\right) = \frac{k_f(T)}{k_{eq}(T)}$$

For dissociation reactions, $\bar{T} = \sqrt{TT_V}$ . For the other reactions, the control temperature is T. The equilibrium constant of chemical reaction is obtained using the curve fits of Park [43], i.e.,

$$k_{eq} = \exp(a_1 z^{-1} + a_2 + a_3 \ln z + a_4 z + a_5 z^2)$$

### 4.4 Energy relaxation

In two temperature model, energy relaxation only happens between translation energy and vibration & electron energy, which can be expressed as

$$Q_{T-v,s} = \rho_s \frac{e_{vs}^*(T) - e_{vs}}{\tau_{vs}} \tag{39}$$

where, $e_{vs}^*(T)$ is the vibration energy per unit mass of species s evaluated at the local translational temperature.

$$\tau_{vs} = \left\langle \tau_{s,L-T} \right\rangle + \tau_{cs} = \frac{\sum_r y_r}{\sum_r y_r / \tau_{sr,L-T}} + \frac{1}{a_s \sigma_v N_s} \qquad \left(a_s = \sqrt{\frac{8\bar{R}T}{\pi M_s}}\right)$$

$$\tau_{sr,L-T} = \frac{1}{p} \exp\left[ A_{sr} \left( T^{-1/3} - 0.015 \mu_{sr}^{1/4} \right) - 18.42 \right] \text{ (p in atm)}$$

$$A_r = 1.16 \times 10^{-3} \mu_{sr}^{1/2} \theta_{vs}^{4/3} \qquad \mu_{sr} = \frac{M_s M_r}{(M_s + M_r)}$$

$$S_s = 3.5 \exp\left( -\frac{\theta_s}{T_{shk}} \right) \qquad \sigma_v = 10^{-21} \left( \frac{50,000}{T} \right)^2$$

Here, $\theta_s$ is a defined characteristic temperature.

## 5. Test of shock-fitting method and nonequilibrium models

The two-temperature model of air has been implemented to the fifth-order shock-fitting method with recent models of thermochemical models. Here we focus our tests on shock-fitting method and thermo-chemical models.

### 5.1 Hornung's Nitrogen dissociation over 1 inch radius cylinder

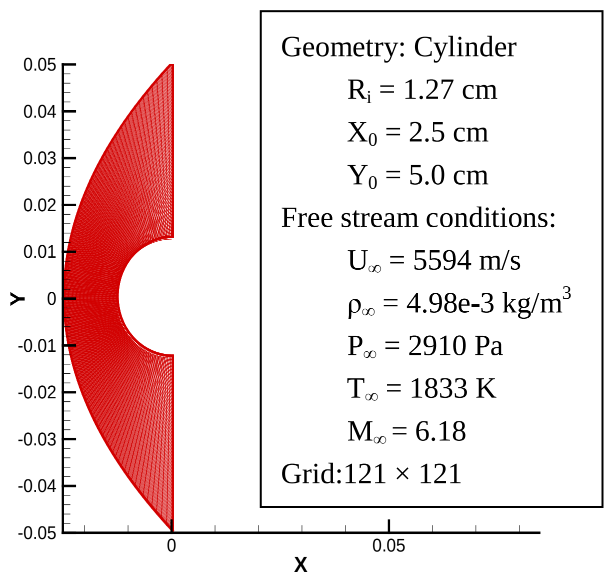


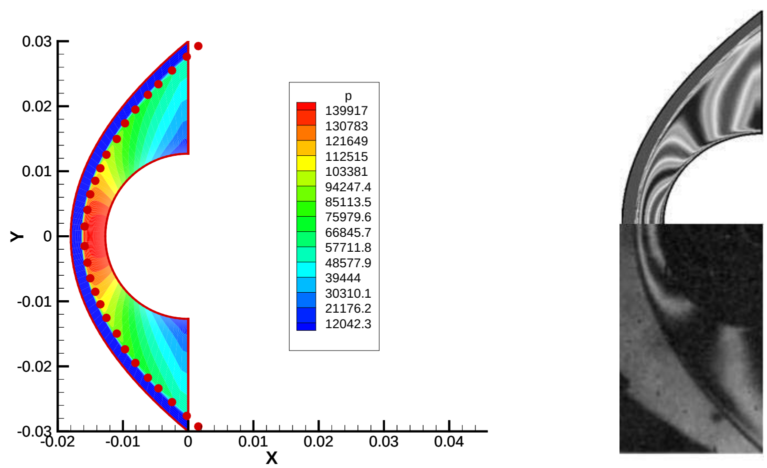

*Fig. 21. Geometry and free stream flow conditions*

The flow conditions of Hornung's experiment [44] are listed in Fig. 21, together with a schematic of the grid used in numerical simulations. This experimental study focused on the flow field relating to Nitrogen dissociation over 1 inch radius cylinder. The mass fractions of initial gas are as follows,

$$C_{N2} = 0.927,\ C_N = 0.073$$
$$C_{O2} = C_{NO} = C_O = 0$$

In this case, the five-species air model is used.

Our numerical simulation results are compared with the experimental measurement of Hornung obtained from his paper. As shown in Figs. 22 and 23, the shock standoff distance agrees well with experiment and the fringe pattern matches quite well with Hornung's experimental measurements. The test result on this case validated that the implementations of nonquilibrium and reactive flow solver to the high-order shock-fitting code is accurate.




(a) (b)

*Fig. 22. Comparisons with experimental measurements: (a) shock standoff distance (Dots stands for Hornung's experimental measurement); (b) fringe patterns (the lower half is Hornung's experimental measurement).*

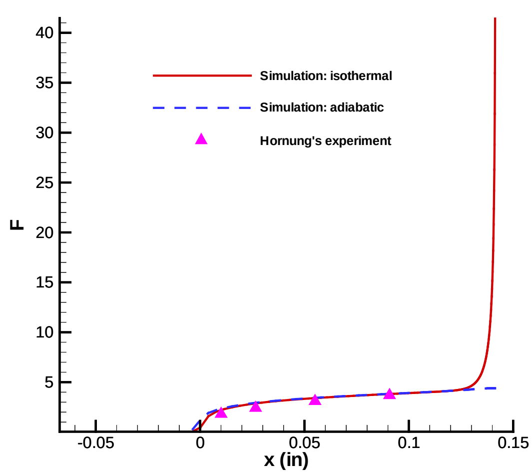



*Fig. 23. Quantitative comparison of fringe number along the stagnation line.*

## 5.2 Gnoffo's air dissociation over 1 meter radius cylinder

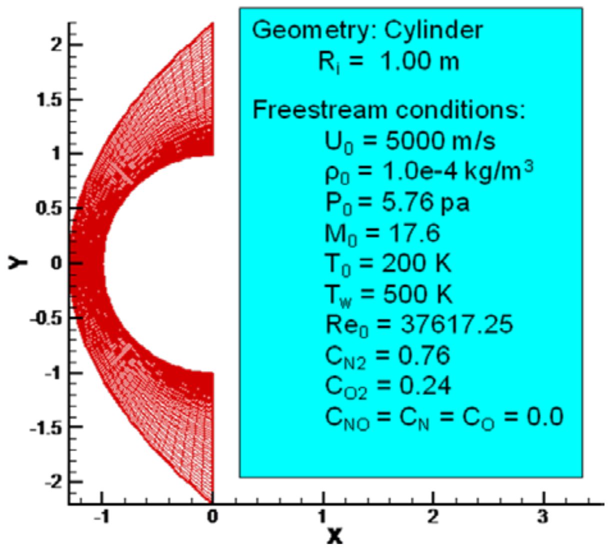


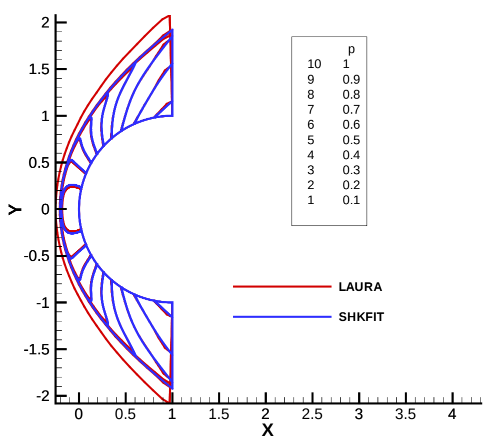

*Fig. 24. Mesh sturcture and flow conditions of the test case.*

Figure 24 shows the mesh and flow conditions of the test case: 5-species air over a 1-meter radius cylinder. The temperatures on the cylinder are equal to Tw (= 500 K). Catalytic boundary conditions are applied on the wall for species mass fraction. Total density is computed from pressure and translational temperature. Then species densities are calculated with total density and mass fraction. Total energy and vibration energy are calculated using species densities and two temperatures. The mass fractions of initial gas are as follows,

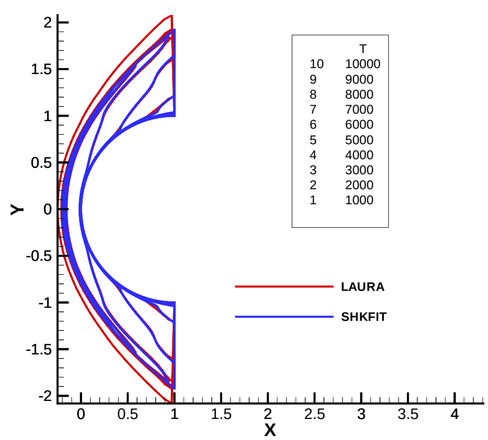
CN2 = 0.76, CO2 = 0.24

CNO = CN = CO = 0

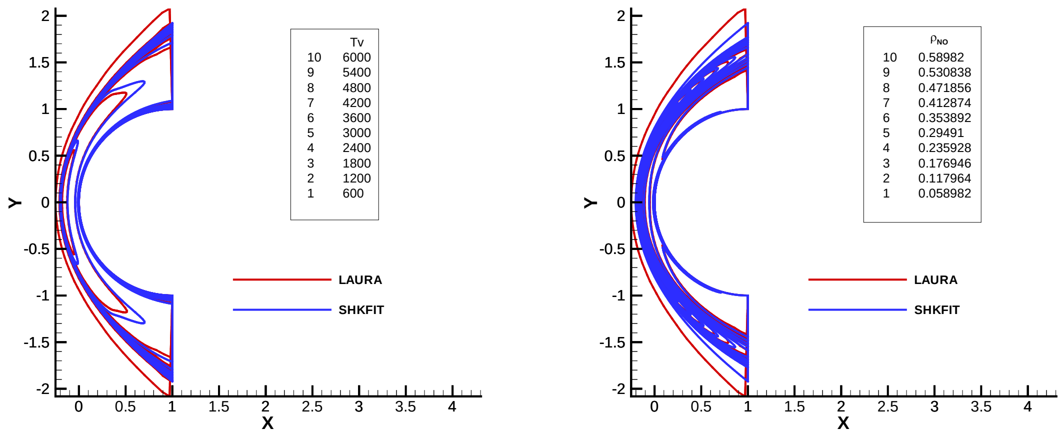
To make the results comparable, flow conditions are exactly the same as what Gnoffo used in his simulation. The simulation results are compared with Gnoffo's results obtained from Laura.




(a) Pressure



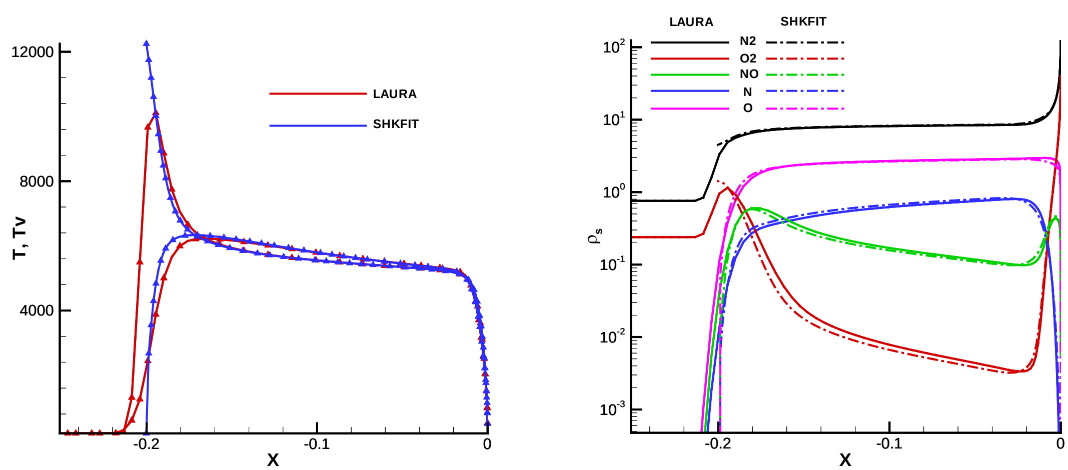

(b) Translation temperature




(c) Vibration temperature (d) Species density of NO

*Fig. 25. Comparisons of flow field contours obtained from shock-fitting code with those obtained from Laura simulation.*

Figure 25 compares flow field contours obtained from current shock-fitting code with those obtained from Laura code. From the contours of pressure, temperatures, and NO density, it is found that shock standoff distances of the two sets of simulations have a good agreement. In addition, the flow fields near the wall have a good agreement. Near the shock, there is small discrepancy between the two sets of solution, mainly due to the different treatment of shock wave. Unlike the shock-fitting code, shock-capturing TVD scheme is applied in Laura code. Figure 25(c) shows that the vibration temperature of shock-fitting solution is significant different from that of Laura in the shock layer, which is mainly caused by the different models of vibration and electronic energy. Laura code used curved fitted vibration and electronic energy [45], whereas we used separate models for vibration energy and electronic energy.




(a) Temperatures (b) Species densities

*Fig. 26. Comparisons of flow variables along the stagnation line obtained from shock-fitting code with those obtained from Laura simulation.*

Since we have detailed flow field information obtained from the Laura code, we can also compare the distributions of flow variables along the stagnation line or along the cylinder surface. For example, figure 26 compares flow variables along the stagnation line obtained from current shock-fitting code with those obtained from Laura code. These two figures also show that shock standoff distances of the two sets of simulations have a good agreement considering the different treatment of the bow shock. The distributions of temperatures and species densities along the stagnation line have a good agreement near the wall and have small discrepancy near the shock. Again, the discrepancy near the shock is due to the different treatment of shock wave. Overall, Figures 25 and 26 indicate that our shock-fitting non-equilibrium flow solver is reliable for the simulation of strong shock and turbulence interaction.

## 6. Summary and Future Plan

In current paper, we first conduct extensive DNS studies on the canonical strong shock and turbulence interaction problem of perfect gas flow with mean Mach numbers ranging from 2 to 30. The objectives of perfect gas flow simulations are to obtain more quantitative results and to investigate the effect of compressibility. DNS of perfect gas flow show that increasing shock-strength reduces the shock deformation. For very strong shocks, linear interaction analysis underpredicts the shock displacement fluctuations. Behind the shock, mean velocity first decreases and then increases while mean density shows a compression of the flow followed by an expansion. As mean Mach number value of incoming flow is increased, the difference between laminar and post-shock turbulent mean values decreases.

The results also show that maximum values of variance of streamwise vorticity fluctuations first increase and then decrease as the shock strength is increased. The peak of streamwise vorticity fluctuations is observed for shock and turbulence interactions with Mach 2.8 shock. For stronger than Mach 2.8 shocks, there is a decrease in streamwise vorticity fluctuations. In addition, the suppression of vorticity tilting and stretching in post-shock flow strongly depends on the inflow conditions. The amplification of Reynolds stress $R_{11}$ decreases as mean Mach number is increased till 8.8, which is consistent with findings of linear interaction analysis. This trend, however, reverses as shock strength is increased beyond Mach 8.8. For stronger than Mach 8.8 shocks, Reynolds stress $R_{11}$ is amplified as mean Mach number keeps increasing. More analyses on DNS results of perfect gas flow are ongoing.

Since gas temperature increases dramatically after strong shocks and thermal properties of air strongly depend on the temperature, non-equilibrium flow effects including internal energy excitations, translation-vibration energy relaxation, and chemical reactions among different species need to be considered in DNS studies. We will continue working on DNS of non-equilibrium flow, where non-equilibrium flow effects are considered based on the 5-species air chemistry and recently thermal property models. The code has been tested on two cases of non-equilibrium flow over cylinders. Although no numerical result is yet obtained for strong shock and turbulence problem at high shock Mach number with non-equilibrium effects.

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